# Full wwPDB EM Validation Report (i)

Feb 1, 2025 – 06:50 PM EST

| | | |
|---|---|---|
| PDB ID | : | 9CPC |
| EMDB ID | : | EMD-45802 |
| Title | : | Atomic model of porcine brain ventricles cilia doublet microtubule (48-nm periodicity) |
| Authors | : | Zeng, J.; Sun, C.; Zhang, R. |
| Deposited on | : | 2024-07-18 |
| Resolution | : | 3.65 Å(reported) |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

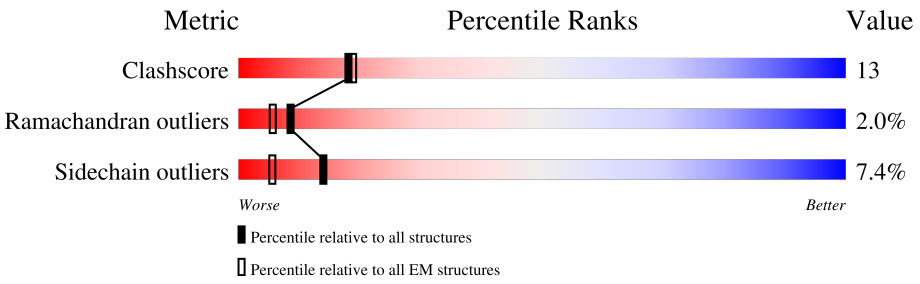
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.40 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1A | 1048 | 54% 55% 44% |
| 1 | 1B | 1048 | 14% 14% 86% |
| 2 | 1C | 685 | 23% 30% • 69% |
| 2 | 1D | 685 | 19% 30% • 69% |
| 3 | 1F | 262 | 65% 64% • 35% |
| 3 | 1G | 262 | 65% 32% 30% • 35% |
| 4 | 1H | 711 | 19% 26% • 73% |
| 4 | 1I | 711 | 12% 12% • 88% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | 1J | 711 | 12% 16% 84% |
| 5 | 1L | 620 | 20% 22% • • 75% |
| 5 | 1M | 620 | 27% 38% • 60% |
| 5 | 1N | 620 | 14% 15% • 83% |
| 6 | 1P | 1456 | 6% 6% 94% |
| 6 | 1Q | 1456 | 6% 5% 94% |
| 7 | 1S | 620 | 21% 86% 12% • • |
| 7 | 1T | 620 | 16% 47% 35% 15% • • |
| 7 | 1U | 620 | 18% 73% 25% • • |
| 8 | 1W | 549 | 41% 45% 12% 42% |
| 8 | 1X | 549 | 37% 30% 14% 5% • 50% |
| 8 | 1Y | 549 | 19% 25% 5% 70% |
| 8 | 1Z | 549 | 27% 30% 5% 64% |
| 9 | 2B | 552 | 39% 52% 14% • 32% |
| 9 | 2C | 552 | 6% 12% • 86% |
| 10 | 2E | 170 | 23% 52% 15% 32% |
| 10 | 2F | 170 | 28% 51% 16% • 32% |
| 10 | 2G | 170 | 25% 54% 12% • 32% |
| 11 | 2I | 256 | 41% 64% 20% 12% • • |
| 11 | 2J | 256 | 45% 79% 15% • • • |
| 11 | 2K | 256 | 43% 65% 20% 7% 7% |
| 12 | 2M | 257 | 35% 71% 14% 15% |
| 12 | 2N | 257 | 23% 71% 14% 15% |
| 12 | 2O | 257 | 25% 62% 21% • 15% |
| 12 | 2P | 257 | 18% 71% 14% 15% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 12 | 2Q | 257 | 20% 73% 12% 15% |
| 12 | 2R | 257 | 76% 66% 19% 15% |
| 13 | 2T | 193 | 18% 38% 37% 19% • • |
| 13 | 2U | 193 | 18% 40% 36% 18% • • |
| 13 | 2V | 193 | 15% 39% 36% 17% • • |
| 13 | 2W | 193 | 16% 39% 39% 15% • • |
| 13 | 2X | 193 | 17% 32% 41% 21% • • |
| 14 | 3A | 177 | 11% 51% 15% • 33% |
| 14 | 3B | 177 | 11% 51% 15% • 33% |
| 14 | 3C | 177 | 9% 54% 12% • 33% |
| 15 | 3E | 418 | 18% 83% 10% • 6% |
| 15 | 3F | 418 | 19% 78% 17% • 5% |
| 15 | 3G | 418 | 10% 27% 6% 67% |
| 15 | 3H | 418 | 17% 60% 11% 29% |
| 16 | 3J | 430 | 19% 74% 17% • 8% |
| 16 | 3K | 430 | 21% 61% 13% 27% |
| 16 | 3L | 430 | 18% 73% 18% • 8% |
| 16 | 3M | 430 | 11% 22% 5% 73% |
| 17 | 3O | 490 | 57% 62% 15% • 20% |
| 17 | 3P | 490 | 51% 41% 28% 10% • 20% |
| 17 | 3Q | 490 | 19% 14% 7% • • 73% |
| 17 | 3R | 490 | 41% 15% 26% 11% • 46% |
| 18 | 3T | 447 | 63% 72% 16% • 11% |
| 18 | 3U | 447 | 62% 72% 16% • 11% |
| 18 | 3V | 447 | 34% 32% 6% 62% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 18 | 3W | 447 | 49% 48% 10% 42% |
| 19 | 3Y | 377 | 26% 82% 12% 6% |
| 19 | 3Z | 377 | 94% |
| 20 | 4A | 379 | 41% 20% 18% 8% 52% |
| 20 | 4B | 379 | 24% 14% 9% 5% 70% |
| 21 | 4D | 640 | 26% 49% 16% 6% 27% |
| 21 | 4E | 640 | 25% 50% 17% 6% 27% |
| 21 | 4F | 640 | 28% 48% 18% 5% 27% |
| 22 | 4H | 748 | 22% 36% 11% 53% |
| 22 | 4I | 748 | 41% 59% 19% 18% |
| 22 | 4J | 748 | 39% 57% 20% 5% 18% |
| 22 | 4K | 748 | 31% 17% 9% 5% 68% |
| 23 | 4M | 272 | 35% 20% 25% 15% 38% |
| 23 | 4N | 272 | 32% 21% 23% 15% 38% |
| 23 | 4P | 272 | 28% 7% 12% 8% 68% |
| 23 | 4Q | 272 | 44% 15% 19% 13% 50% |
| 23 | 4R | 272 | 44% 14% 29% 17% 39% |
| 24 | 4O | 252 | 27% 10% 14% 9% 65% |
| 25 | 4T | 469 | 18% 25% 9% 65% |
| 26 | 4V | 377 | 40% 72% 26% |
| 26 | 4W | 377 | 64% 68% 29% |
| 27 | 4Y | 314 | 28% 67% 18% 15% |
| 27 | 4Z | 314 | 25% 64% 20% 14% |
| 28 | 5B | 230 | 44% 67% 17% 13% |
| 29 | 5D | 136 | 21% 51% 10% 38% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | 5E | 136 | 17% 20% 76% |
| 30 | 5G | 121 | 76% 57% 19% 23% |
| 31 | 5I | 879 | 24% 39% 10% 50% |
| 31 | 5J | 879 | 10% 9% 87% |
| 32 | 5L | 101 | 39% 75% 16% 9% |
| 33 | 5N | 495 | 51% 57% 10% 33% |
| 33 | 5O | 495 | 17% 26% 5% 69% |
| 34 | 5Q | 514 | 28% 42% 8% 49% |
| 34 | 5R | 514 | 19% 15% 13% 9% 61% |
| 35 | 5T | 196 | 68% 51% 17% 31% |
| 35 | 5U | 196 | 14% 13% 86% |
| 36 | 5W | 282 | 43% 60% 21% 18% |
| 36 | 5X | 282 | 48% 60% 19% 18% |
| 36 | 5Y | 282 | 39% 47% 17% 34% |
| 36 | 5Z | 282 | 12% 18% 79% |
| 37 | 6A | 135 | 47% 63% 22% 14% |
| 38 | 6C | 310 | 36% 46% 19% 32% |
| 38 | 6D | 310 | 6% 16% 5% 79% |
| 39 | 6F | 223 | 70% 57% 11% 30% |
| 39 | 6G | 223 | 70% 60% 10% 30% |
| 39 | 6H | 223 | 63% 50% 13% 37% |
| 39 | 6I | 223 | 69% 57% 14% 30% |
| 39 | 6J | 223 | 70% 60% 11% 30% |
| 39 | 6K | 223 | 69% 58% 13% 30% |
| 39 | 6L | 223 | 61% 46% 12% 39% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | AA | 447 | 16% 74% 24% |
| 40 | AE | 447 | 16% 79% 19% |
| 40 | AF | 447 | 14% 79% 19% |
| 40 | AG | 447 | 13% 73% 25% |
| 40 | AH | 447 | 15% 81% 17% |
| 40 | BA | 447 | 18% 75% 23% |
| 40 | BE | 447 | 15% 41% 38% 16% |
| 40 | BF | 447 | 15% 69% 28% |
| 40 | BG | 447 | 15% 72% 24% |
| 40 | BH | 447 | 12% 45% 38% 14% |
| 40 | BI | 447 | 24% 31% 36% 14% 17% |
| 40 | CA | 447 | 20% 35% 44% 17% |
| 40 | CE | 447 | 28% 70% 28% |
| 40 | CF | 447 | 23% 74% 23% |
| 40 | CG | 447 | 21% 74% 23% |
| 40 | CH | 447 | 18% 37% 42% 15% 5% |
| 40 | CI | 447 | 41% 72% 26% |
| 40 | DA | 447 | 22% 25% 47% 22% |
| 40 | DE | 447 | 29% 30% 43% 20% |
| 40 | DF | 447 | 24% 32% 42% 19% |
| 40 | DG | 447 | 29% 72% 25% |
| 40 | DH | 447 | 24% 33% 44% 17% |
| 40 | DI | 447 | 39% 28% 43% 22% |
| 40 | EA | 447 | 25% 70% 27% |
| 40 | EE | 447 | 35% 70% 26% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | EF | 447 | 24% 70% 27% |
| 40 | EG | 447 | 21% 70% 25% |
| 40 | EH | 447 | 16% 38% 38% 16% |
| 40 | EI | 447 | 32% 33% 37% 22% 5% |
| 40 | FA | 447 | 19% 38% 35% 22% |
| 40 | FE | 447 | 40% 73% 24% |
| 40 | FF | 447 | 22% 75% 22% |
| 40 | FG | 447 | 23% 74% 22% |
| 40 | FH | 447 | 23% 74% 23% |
| 40 | FI | 447 | 34% 72% 24% |
| 40 | GA | 447 | 19% 70% 26% |
| 40 | GE | 447 | 32% 32% 43% 20% |
| 40 | GF | 447 | 20% 73% 23% |
| 40 | GG | 447 | 18% 71% 23% |
| 40 | GH | 447 | 13% 38% 40% 16% |
| 40 | GI | 447 | 21% 37% 39% 17% |
| 40 | HA | 447 | 17% 72% 24% |
| 40 | HE | 447 | 32% 35% 37% 21% |
| 40 | HF | 447 | 17% 73% 24% |
| 40 | HG | 447 | 15% 77% 19% |
| 40 | HH | 447 | 18% 72% 24% |
| 40 | HI | 447 | 21% 69% 28% |
| 40 | IA | 447 | 19% 73% 24% |
| 40 | IE | 447 | 41% 72% 22% 6% |
| 40 | IF | 447 | 21% 72% 24% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | IG | 447 | 18% 71% 25% |
| 40 | IH | 447 | 16% 70% 26% |
| 40 | II | 447 | 20% 67% 30% |
| 40 | JA | 447 | 20% 73% 24% |
| 40 | JD | 447 | 27% 69% 28% |
| 40 | JE | 447 | 23% 71% 26% |
| 40 | JF | 447 | 21% 74% 21% |
| 40 | JG | 447 | 19% 77% 21% |
| 40 | JH | 447 | 21% 72% 25% |
| 40 | KA | 447 | 15% 74% 22% |
| 40 | KD | 447 | 15% 73% 23% |
| 40 | KE | 447 | 13% 71% 26% |
| 40 | KF | 447 | 16% 77% 19% |
| 40 | KG | 447 | 15% 73% 26% |
| 40 | KH | 447 | 15% 71% 27% |
| 40 | LA | 447 | 14% 74% 24% |
| 40 | LD | 447 | 11% 74% 22% |
| 40 | LE | 447 | 13% 78% 18% |
| 40 | LF | 447 | 5% 49% 33% 13% |
| 40 | LG | 447 | 44% 38% 13% |
| 40 | LH | 447 | 13% 75% 22% |
| 40 | MA | 447 | 6% 51% 35% 10% |
| 40 | MD | 447 | 14% 79% 18% |
| 40 | ME | 447 | 12% 77% 19% |
| 40 | MF | 447 | 5% 47% 36% 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | MG | 447 | 5% 46% 38% 12% |
| 40 | MH | 447 | 7% 50% 32% 15% |
| 40 | NA | 447 | 26% 70% 26% |
| 40 | ND | 447 | 24% 39% 39% 15% |
| 40 | NE | 447 | 29% 71% 25% |
| 40 | NF | 447 | 26% 72% 24% |
| 40 | NG | 447 | 27% 71% 25% |
| 40 | NH | 447 | 30% 71% 26% |
| 40 | OA | 447 | 24% 72% 25% |
| 40 | OD | 447 | 46% 67% 27% |
| 40 | OE | 447 | 28% 71% 25% |
| 40 | OF | 447 | 32% 69% 29% |
| 40 | OG | 447 | 28% 69% 28% |
| 40 | OH | 447 | 27% 30% 43% 20% |
| 40 | PA | 447 | 36% 68% 28% |
| 40 | PD | 447 | 63% 65% 26% 9% |
| 40 | PE | 447 | 39% 71% 26% |
| 40 | PF | 447 | 39% 69% 28% |
| 40 | PG | 447 | 39% 70% 26% |
| 40 | PH | 447 | 41% 68% 28% |
| 40 | QA | 447 | 45% 68% 28% |
| 40 | QE | 447 | 52% 62% 34% |
| 40 | QF | 447 | 39% 71% 25% |
| 40 | QG | 447 | 43% 69% 26% |
| 40 | QH | 447 | 49% 74% 23% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | RA | 447 | 42% 69% 27% |
| 40 | RE | 447 | 51% 67% 29% |
| 40 | RF | 447 | 42% 69% 26% |
| 40 | RG | 447 | 41% 66% 30% |
| 40 | RH | 447 | 47% 71% 25% |
| 40 | RI | 447 | 70% 62% 21% 16% |
| 40 | SA | 447 | 36% 65% 28% |
| 40 | SE | 447 | 47% 66% 31% |
| 40 | SF | 447 | 41% 66% 30% |
| 40 | SG | 447 | 36% 67% 29% |
| 40 | SH | 447 | 39% 65% 31% |
| 40 | SI | 447 | 70% 74% 22% |
| 40 | TA | 447 | 32% 72% 25% |
| 40 | TE | 447 | 48% 72% 24% |
| 40 | TF | 447 | 36% 71% 25% |
| 40 | TG | 447 | 36% 72% 25% |
| 40 | TH | 447 | 28% 70% 26% |
| 40 | TI | 447 | 52% 70% 26% |
| 40 | UA | 447 | 32% 73% 23% |
| 40 | UE | 447 | 42% 68% 28% |
| 40 | UF | 447 | 26% 34% 41% 19% |
| 40 | UG | 447 | 34% 70% 26% |
| 40 | UH | 447 | 27% 72% 25% |
| 40 | UI | 447 | 31% 29% 45% 21% |
| 40 | VA | 447 | 25% 72% 25% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | VF | 447 | 28% 71% 27% |
| 40 | VG | 447 | 17% 73% 23% |
| 40 | VH | 447 | 20% 78% 19% |
| 40 | VI | 447 | 24% 75% 23% |
| 40 | VJ | 447 | 23% 68% 28% |
| 40 | WA | 447 | 23% 74% 24% |
| 40 | WE | 447 | 24% 74% 24% |
| 40 | WF | 447 | 16% 71% 26% |
| 40 | WG | 447 | 17% 65% 31% |
| 40 | WH | 447 | 19% 73% 26% |
| 40 | WI | 447 | 19% 74% 23% |
| 41 | AB | 449 | 18% 71% 24% 5% |
| 41 | AL | 449 | 12% 74% 21% 5% |
| 41 | AM | 449 | 14% 73% 22% 5% |
| 41 | AN | 449 | 14% 72% 22% 5% |
| 41 | AO | 449 | 8% 47% 38% 9% 5% |
| 41 | AP | 449 | 17% 75% 20% 5% |
| 41 | BB | 449 | 15% 44% 35% 15% 5% |
| 41 | BL | 449 | 23% 71% 24% 5% |
| 41 | BM | 449 | 14% 39% 39% 15% 5% |
| 41 | BN | 449 | 20% 70% 24% 5% |
| 41 | BO | 449 | 15% 45% 34% 13% 5% |
| 41 | BP | 449 | 13% 40% 39% 14% 5% |
| 41 | CB | 449 | 23% 65% 30% 5% |
| 41 | CL | 449 | 26% 33% 40% 18% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | CM | 449 | 18% 41% 38% 13% • 5% |
| 41 | CN | 449 | 15% 34% 40% 18% • 5% |
| 41 | CO | 449 | 18% 34% 44% 16% • 5% |
| 41 | CP | 449 | 17% 35% 39% 18% • 5% |
| 41 | DB | 449 | 22% 30% 44% 18% • 5% |
| 41 | DL | 449 | 53% 27% 41% 22% 5% 5% |
| 41 | DM | 449 | 22% 29% 41% 21% • 5% |
| 41 | DN | 449 | 20% 25% 44% 21% 6% 5% |
| 41 | DO | 449 | 28% 69% 26% • 5% |
| 41 | DP | 449 | 22% 35% 38% 19% • 5% |
| 41 | EB | 449 | 20% 69% 25% • 5% |
| 41 | EL | 449 | 59% 61% 20% 19% |
| 41 | EM | 449 | 18% 30% 43% 20% • 5% |
| 41 | EN | 449 | 21% 70% 25% 5% |
| 41 | EO | 449 | 18% 74% 21% 5% |
| 41 | EP | 449 | 18% 36% 41% 15% • 5% |
| 41 | FB | 449 | 20% 73% 21% • 5% |
| 41 | FM | 449 | 24% 68% 27% 5% |
| 41 | FN | 449 | 21% 71% 24% 5% |
| 41 | FO | 449 | 19% 67% 28% 5% |
| 41 | FP | 449 | 25% 68% 26% • 5% |
| 41 | GB | 449 | 17% 73% 22% • 5% |
| 41 | GM | 449 | 21% 67% 28% • 5% |
| 41 | GN | 449 | 13% 36% 42% 15% • 5% |
| 41 | GO | 449 | 15% 70% 25% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | GP | 449 | 21% 67% 27% 5% |
| 41 | HB | 449 | 15% 73% 22% 5% |
| 41 | HM | 449 | 18% 68% 27% 5% |
| 41 | HN | 449 | 11% 39% 39% 14% 5% |
| 41 | HO | 449 | 14% 68% 26% 5% |
| 41 | HP | 449 | 17% 76% 19% 5% |
| 41 | HQ | 449 | 37% 70% 24% 5% |
| 41 | IB | 449 | 15% 72% 23% 5% |
| 41 | IM | 449 | 21% 69% 26% 5% |
| 41 | IN | 449 | 19% 69% 26% 5% |
| 41 | IO | 449 | 15% 72% 22% 5% |
| 41 | IP | 449 | 15% 67% 28% 5% |
| 41 | IQ | 449 | 22% 69% 25% 5% |
| 41 | JB | 449 | 14% 67% 28% 5% |
| 41 | JL | 449 | 20% 69% 25% 5% |
| 41 | JM | 449 | 11% 33% 42% 18% 5% |
| 41 | JN | 449 | 19% 69% 26% 5% |
| 41 | JO | 449 | 17% 75% 20% 5% |
| 41 | KB | 449 | 13% 71% 23% 5% |
| 41 | KL | 449 | 8% 41% 39% 14% 5% |
| 41 | KM | 449 | 14% 75% 19% 5% |
| 41 | KN | 449 | 15% 73% 22% 5% |
| 41 | KO | 449 | 14% 69% 26% 5% |
| 41 | KP | 449 | 26% 65% 21% 14% |
| 41 | LB | 449 | 8% 72% 23% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | LL | 449 | 10% 73% 22% 5% |
| 41 | LM | 449 | 11% 75% 20% 5% |
| 41 | LN | 449 | 11% 73% 22% 5% |
| 41 | LO | 449 | 10% 71% 23% 5% |
| 41 | LP | 449 | 12% 78% 18% 5% |
| 41 | MB | 449 | 12% 71% 24% 5% |
| 41 | ML | 449 | 9% 73% 22% 5% |
| 41 | MM | 449 | 11% 76% 19% 5% |
| 41 | MN | 449 | 11% 69% 25% 5% |
| 41 | MO | 449 | 5% 47% 36% 10% 5% |
| 41 | MP | 449 | 11% 71% 23% 5% |
| 41 | NB | 449 | 24% 69% 25% 5% |
| 41 | NL | 449 | 31% 68% 26% 5% |
| 41 | NM | 449 | 27% 73% 22% 5% |
| 41 | NN | 449 | 29% 67% 28% 5% |
| 41 | NO | 449 | 28% 72% 23% 5% |
| 41 | NP | 449 | 41% 64% 28% 7% |
| 41 | OB | 449 | 24% 66% 29% 5% |
| 41 | OL | 449 | 32% 67% 27% 5% |
| 41 | OM | 449 | 26% 67% 27% 5% |
| 41 | ON | 449 | 27% 65% 30% 5% |
| 41 | OO | 449 | 30% 64% 31% 5% |
| 41 | OP | 449 | 42% 68% 26% 5% |
| 41 | PB | 449 | 39% 63% 31% 5% |
| 41 | PL | 449 | 44% 66% 29% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | PM | 449 | 40% 67% 27% 5% |
| 41 | PN | 449 | 37% 71% 24% 5% |
| 41 | PO | 449 | 42% 70% 24% 5% |
| 41 | PP | 449 | 47% 67% 27% 5% |
| 41 | QB | 449 | 34% 23% 43% 24% 5% 5% |
| 41 | QL | 449 | 54% 69% 25% 5% |
| 41 | QM | 449 | 45% 66% 28% 5% |
| 41 | QN | 449 | 45% 67% 27% 5% |
| 41 | QO | 449 | 48% 72% 22% 5% |
| 41 | QP | 449 | 46% 23% 40% 27% 5% 5% |
| 41 | RB | 449 | 42% 69% 25% 5% |
| 41 | RL | 449 | 64% 71% 23% 5% |
| 41 | RM | 449 | 44% 66% 28% 5% |
| 41 | RN | 449 | 42% 68% 27% 5% |
| 41 | RO | 449 | 42% 65% 29% 5% |
| 41 | RP | 449 | 51% 67% 27% 5% |
| 41 | SB | 449 | 37% 66% 26% 5% |
| 41 | SL | 449 | 57% 58% 27% 15% |
| 41 | SM | 449 | 39% 70% 25% 5% |
| 41 | SN | 449 | 34% 71% 23% 5% |
| 41 | SO | 449 | 24% 28% 46% 17% 5% 5% |
| 41 | SP | 449 | 42% 67% 27% 5% |
| 41 | TB | 449 | 30% 71% 23% 5% |
| 41 | TL | 449 | 63% 66% 20% 14% |
| 41 | TM | 449 | 33% 65% 30% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 41 | TN | 449 | 27% 71% 23% 5% |
| 41 | TO | 449 | 26% 66% 28% 5% |
| 41 | TP | 449 | 32% 65% 29% 5% |
| 41 | UB | 449 | 29% 68% 26% 5% |
| 41 | UM | 449 | 32% 69% 26% 5% |
| 41 | UN | 449 | 29% 64% 30% 5% |
| 41 | UO | 449 | 23% 68% 26% 5% |
| 41 | UP | 449 | 19% 32% 41% 20% 5% |
| 41 | VB | 449 | 18% 69% 26% 5% |
| 41 | VN | 449 | 19% 71% 23% 5% |
| 41 | VO | 449 | 19% 68% 27% 5% |
| 41 | VP | 449 | 23% 68% 27% 5% |
| 41 | VQ | 449 | 21% 73% 22% 5% |
| 41 | WB | 449 | 18% 67% 28% 5% |
| 41 | WM | 449 | 12% 39% 37% 16% 5% |
| 41 | WN | 449 | 11% 37% 39% 16% 5% |
| 41 | WO | 449 | 22% 69% 26% 5% |
| 41 | WP | 449 | 17% 73% 22% 5% |
| 41 | WQ | 449 | 29% 73% 21% 6% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 42 | GTP | MB | 502 | - | - | X | - |
| 42 | GTP | MN | 501 | - | - | X | - |

# 2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 1114625 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Armadillo repeat-containing protein 4 isoform 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 1A | 587 | 4498 | 2806 | 817 | 843 | 32 | 0 | 0 |
| 1 | 1B | 149 | 1135 | 698 | 212 | 217 | 8 | 0 | 0 |

- Molecule 2 is a protein called Outer dynein arm-docking complex subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 1C | 211 | 1699 | 1076 | 297 | 317 | 9 | 0 | 0 |
| 2 | 1D | 211 | 1699 | 1076 | 297 | 317 | 9 | 0 | 0 |

- Molecule 3 is a protein called EF-hand calcium binding domain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | 1F | 171 | 1375 | 887 | 219 | 255 | 14 | 0 | 0 |
| 3 | 1G | 171 | 1375 | 887 | 219 | 255 | 14 | 0 | 0 |

- Molecule 4 is a protein called Coiled-coil domain-containing protein 114 isoform X2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | 1H | 195 | 1633 | 1001 | 326 | 299 | 7 | 0 | 0 |
| 4 | 1I | 88 | 727 | 439 | 150 | 134 | 4 | 0 | 0 |
| 4 | 1J | 115 | 973 | 601 | 189 | 180 | 3 | 0 | 0 |

- Molecule 5 is a protein called Outer dynein arm docking complex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | 1L | 155 | 1306 | 801 | 247 | 253 | 5 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 5 | 1M | 248 | 2086 | 1287 | 392 | 402 | 5 | 0 | 0 |
| | | | Total | C | N | O | | | |
| 5 | 1N | 103 | 865 | 539 | 164 | 162 | | 0 | 0 |

There are 72 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 1L | 478 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1L | 479 | ASP | - | insertion | UNP A0A5G2RIE6 |
| 1L | 480 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1L | 481 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1L | 482 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1L | 483 | GLU | - | insertion | UNP A0A5G2RIE6 |
| 1L | 484 | GLU | - | insertion | UNP A0A5G2RIE6 |
| 1L | 485 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1L | 486 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1L | 487 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1L | 488 | ARG | - | insertion | UNP A0A5G2RIE6 |
| 1L | 489 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1L | 490 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1L | 491 | GLN | - | insertion | UNP A0A5G2RIE6 |
| 1L | 492 | ASP | - | insertion | UNP A0A5G2RIE6 |
| 1L | 493 | VAL | - | insertion | UNP A0A5G2RIE6 |
| 1L | 494 | ARG | - | insertion | UNP A0A5G2RIE6 |
| 1L | 495 | GLY | - | insertion | UNP A0A5G2RIE6 |
| 1L | 496 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1L | 497 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1L | 498 | THR | - | insertion | UNP A0A5G2RIE6 |
| 1L | 499 | ILE | - | insertion | UNP A0A5G2RIE6 |
| 1L | 500 | THR | - | insertion | UNP A0A5G2RIE6 |
| 1L | 501 | GLN | - | insertion | UNP A0A5G2RIE6 |
| 1M | 478 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1M | 479 | ASP | - | insertion | UNP A0A5G2RIE6 |
| 1M | 480 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1M | 481 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1M | 482 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1M | 483 | GLU | - | insertion | UNP A0A5G2RIE6 |
| 1M | 484 | GLU | - | insertion | UNP A0A5G2RIE6 |
| 1M | 485 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1M | 486 | PRO | - | insertion | UNP A0A5G2RIE6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 1M | 487 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1M | 488 | ARG | - | insertion | UNP A0A5G2RIE6 |
| 1M | 489 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1M | 490 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1M | 491 | GLN | - | insertion | UNP A0A5G2RIE6 |
| 1M | 492 | ASP | - | insertion | UNP A0A5G2RIE6 |
| 1M | 493 | VAL | - | insertion | UNP A0A5G2RIE6 |
| 1M | 494 | ARG | - | insertion | UNP A0A5G2RIE6 |
| 1M | 495 | GLY | - | insertion | UNP A0A5G2RIE6 |
| 1M | 496 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1M | 497 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1M | 498 | THR | - | insertion | UNP A0A5G2RIE6 |
| 1M | 499 | ILE | - | insertion | UNP A0A5G2RIE6 |
| 1M | 500 | THR | - | insertion | UNP A0A5G2RIE6 |
| 1M | 501 | GLN | - | insertion | UNP A0A5G2RIE6 |
| 1N | 478 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1N | 479 | ASP | - | insertion | UNP A0A5G2RIE6 |
| 1N | 480 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1N | 481 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1N | 482 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1N | 483 | GLU | - | insertion | UNP A0A5G2RIE6 |
| 1N | 484 | GLU | - | insertion | UNP A0A5G2RIE6 |
| 1N | 485 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1N | 486 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1N | 487 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1N | 488 | ARG | - | insertion | UNP A0A5G2RIE6 |
| 1N | 489 | ALA | - | insertion | UNP A0A5G2RIE6 |
| 1N | 490 | PRO | - | insertion | UNP A0A5G2RIE6 |
| 1N | 491 | GLN | - | insertion | UNP A0A5G2RIE6 |
| 1N | 492 | ASP | - | insertion | UNP A0A5G2RIE6 |
| 1N | 493 | VAL | - | insertion | UNP A0A5G2RIE6 |
| 1N | 494 | ARG | - | insertion | UNP A0A5G2RIE6 |
| 1N | 495 | GLY | - | insertion | UNP A0A5G2RIE6 |
| 1N | 496 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1N | 497 | SER | - | insertion | UNP A0A5G2RIE6 |
| 1N | 498 | THR | - | insertion | UNP A0A5G2RIE6 |
| 1N | 499 | ILE | - | insertion | UNP A0A5G2RIE6 |
| 1N | 500 | THR | - | insertion | UNP A0A5G2RIE6 |
| 1N | 501 | GLN | - | insertion | UNP A0A5G2RIE6 |

- Molecule 6 is a protein called EFCAB6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | 1P | 84 | 704 | 456 | 126 | 119 | 3 | 0 | 0 |
| 6 | 1Q | 81 | 675 | 436 | 122 | 114 | 3 | 0 | 0 |

- Molecule 7 is a protein called Cilia- and flagella-associated protein 52.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | 1S | 611 | 4712 | 2983 | 817 | 883 | 29 | 0 | 0 |
| 7 | 1T | 611 | 4712 | 2983 | 817 | 883 | 29 | 0 | 0 |
| 7 | 1U | 611 | 4712 | 2983 | 817 | 883 | 29 | 0 | 0 |

- Molecule 8 is a protein called Cilia- and flagella-associated protein 45.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | 1W | 316 | 2722 | 1643 | 539 | 528 | 12 | 0 | 0 |
| 8 | 1X | 275 | 2293 | 1398 | 427 | 452 | 16 | 0 | 0 |
| 8 | 1Y | 162 | 1331 | 819 | 242 | 260 | 10 | 0 | 0 |
| 8 | 1Z | 196 | 1680 | 1016 | 338 | 323 | 3 | 0 | 0 |

- Molecule 9 is a protein called Cilia and flagella associated protein 210.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | 2B | 373 | 3205 | 1994 | 606 | 596 | 9 | 0 | 0 |
| 9 | 2C | 80 | 665 | 413 | 122 | 127 | 3 | 0 | 0 |

- Molecule 10 is a protein called Cilia and flagella associated protein 276.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | 2E | 115 | 930 | 577 | 173 | 177 | 3 | 0 | 0 |
| 10 | 2F | 115 | 930 | 577 | 173 | 177 | 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | 2G | 115 | 930 | 577 | 173 | 177 | 3 | 0 | 0 |

- Molecule 11 is a protein called Enkurin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | 2I | 247 | 2024 | 1294 | 350 | 373 | 7 | 0 | 0 |
| 11 | 2J | 247 | 2027 | 1296 | 350 | 373 | 8 | 0 | 0 |
| 11 | 2K | 237 | 1947 | 1244 | 336 | 359 | 8 | 0 | 0 |

- Molecule 12 is a protein called Parkin coregulated.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | 2M | 219 | 1767 | 1144 | 297 | 316 | 10 | 0 | 0 |
| 12 | 2N | 219 | 1767 | 1144 | 297 | 316 | 10 | 0 | 0 |
| 12 | 2O | 219 | 1767 | 1144 | 297 | 316 | 10 | 0 | 0 |
| 12 | 2P | 219 | 1767 | 1144 | 297 | 316 | 10 | 0 | 0 |
| 12 | 2Q | 219 | 1767 | 1144 | 297 | 316 | 10 | 0 | 0 |
| 12 | 2R | 219 | 1767 | 1144 | 297 | 316 | 10 | 0 | 0 |

- Molecule 13 is a protein called Cilia- and flagella-associated protein 20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | 2T | 185 | 1540 | 990 | 269 | 274 | 7 | 0 | 0 |
| 13 | 2U | 185 | 1540 | 990 | 269 | 274 | 7 | 0 | 0 |
| 13 | 2V | 185 | 1540 | 990 | 269 | 274 | 7 | 0 | 0 |
| 13 | 2W | 185 | 1540 | 990 | 269 | 274 | 7 | 0 | 0 |
| 13 | 2X | 185 | 1540 | 990 | 269 | 274 | 7 | 0 | 0 |

- Molecule 14 is a protein called Protein Flattop.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | 3A | 118 | 924 | 586 | 170 | 166 | 2 | 0 | 0 |
| 14 | 3B | 118 | 924 | 586 | 170 | 166 | 2 | 0 | 0 |
| 14 | 3C | 118 | 924 | 586 | 170 | 166 | 2 | 0 | 0 |

- Molecule 15 is a protein called Tektin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | 3E | 394 | 3216 | 1989 | 591 | 627 | 9 | 0 | 0 |
| 15 | 3F | 397 | 3241 | 2006 | 595 | 631 | 9 | 0 | 0 |
| 15 | 3G | 136 | 1096 | 675 | 207 | 211 | 3 | 0 | 0 |
| 15 | 3H | 298 | 2451 | 1517 | 447 | 481 | 6 | 0 | 0 |

- Molecule 16 is a protein called Tektin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | 3J | 397 | 3234 | 1990 | 599 | 629 | 16 | 0 | 0 |
| 16 | 3K | 316 | 2559 | 1578 | 463 | 503 | 15 | 0 | 0 |
| 16 | 3L | 397 | 3234 | 1990 | 599 | 629 | 16 | 0 | 0 |
| 16 | 3M | 114 | 939 | 572 | 184 | 181 | 2 | 0 | 0 |

- Molecule 17 is a protein called Tektin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | 3O | 391 | 3180 | 1957 | 581 | 627 | 15 | 0 | 0 |
| 17 | 3P | 391 | 3180 | 1957 | 581 | 627 | 15 | 0 | 0 |
| 17 | 3Q | 131 | 1058 | 654 | 192 | 207 | 5 | 0 | 0 |
| 17 | 3R | 264 | 2149 | 1319 | 393 | 428 | 9 | 0 | 0 |

- Molecule 18 is a protein called Tektin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | 3T | 398 | 3284 | 2024 | 605 | 637 | 18 | 0 | 0 |
| 18 | 3U | 399 | 3289 | 2027 | 606 | 638 | 18 | 0 | 0 |
| 18 | 3V | 170 | 1405 | 863 | 255 | 280 | 7 | 0 | 0 |
| 18 | 3W | 259 | 2121 | 1310 | 398 | 402 | 11 | 0 | 0 |

- Molecule 19 is a protein called RIB43A domain with coiled-coils 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | 3Y | 356 | 2977 | 1815 | 580 | 571 | 11 | 0 | 0 |
| 19 | 3Z | 22 | 194 | 121 | 33 | 39 | 1 | 0 | 0 |

- Molecule 20 is a protein called RIB43A-like with coiled-coils protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | 4A | 181 | 1485 | 891 | 294 | 286 | 14 | 0 | 0 |
| 20 | 4B | 115 | 943 | 561 | 185 | 193 | 4 | 0 | 0 |

- Molecule 21 is a protein called EF-hand domain containing 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | 4D | 468 | 3844 | 2478 | 648 | 702 | 16 | 0 | 0 |
| 21 | 4E | 468 | 3844 | 2478 | 648 | 702 | 16 | 0 | 0 |
| 21 | 4F | 468 | 3844 | 2478 | 648 | 702 | 16 | 0 | 0 |

- Molecule 22 is a protein called EF-hand domain-containing family member C2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | 4H | 354 | 2895 | 1866 | 483 | 532 | 14 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | 4I | 612 | 5027 | 3227 | 847 | 926 | 27 | 0 | 0 |
| 22 | 4J | 615 | 5055 | 3247 | 851 | 930 | 27 | 0 | 0 |
| 22 | 4K | 242 | 1983 | 1268 | 340 | 363 | 12 | 0 | 0 |

- Molecule 23 is a protein called Ciliary microtubule inner protein 2B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | 4M | 170 | 1330 | 859 | 229 | 235 | 7 | 0 | 0 |
| 23 | 4N | 170 | 1320 | 853 | 228 | 234 | 5 | 0 | 0 |
| 23 | 4P | 87 | 705 | 457 | 121 | 124 | 3 | 0 | 0 |
| 23 | 4Q | 136 | 1070 | 687 | 186 | 193 | 4 | 0 | 0 |
| 23 | 4R | 167 | 1319 | 851 | 229 | 232 | 7 | 0 | 0 |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 4M | 271 | ALA | - | insertion | UNP A0A8D1CRM3 |
| 4M | ? | - | SER | deletion | UNP A0A8D1CRM3 |
| 4N | 271 | ALA | - | insertion | UNP A0A8D1CRM3 |
| 4N | ? | - | SER | deletion | UNP A0A8D1CRM3 |
| 4P | 271 | ALA | - | insertion | UNP A0A8D1CRM3 |
| 4P | ? | - | SER | deletion | UNP A0A8D1CRM3 |
| 4Q | 271 | ALA | - | insertion | UNP A0A8D1CRM3 |
| 4Q | ? | - | SER | deletion | UNP A0A8D1CRM3 |
| 4R | 271 | ALA | - | insertion | UNP A0A8D1CRM3 |
| 4R | ? | - | SER | deletion | UNP A0A8D1CRM3 |

- Molecule 24 is a protein called Ciliary microtubule inner protein 2B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | 4O | 87 | 702 | 455 | 121 | 124 | 2 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 4O | 271 | ALA | - | insertion | UNP A0A8D1QC18 |

- Molecule 25 is a protein called Sperm-associated antigen 8 isoform 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | 4T | 162 | 1320 | 825 | 245 | 243 | 7 | 0 | 0 |

- Molecule 26 is a protein called Nucleoside diphosphate kinase homolog 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | 4V | 373 | 2946 | 1876 | 500 | 548 | 22 | 0 | 0 |
| 26 | 4W | 373 | 2946 | 1876 | 500 | 548 | 22 | 0 | 0 |

- Molecule 27 is a protein called Cilia and flagella associated protein 161.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 27 | 4Y | 267 | 2145 | 1359 | 378 | 395 | 13 | 0 | 0 |
| 27 | 4Z | 270 | 2160 | 1369 | 380 | 398 | 13 | 0 | 0 |

- Molecule 28 is a protein called Chromosome 1 C9orf135 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | 5B | 200 | 1625 | 1030 | 278 | 311 | 6 | 0 | 0 |

- Molecule 29 is a protein called Piercer of microtubule wall 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | 5D | 84 | 697 | 442 | 125 | 127 | 3 | 0 | 0 |
| 29 | 5E | 33 | 280 | 180 | 47 | 52 | 1 | 0 | 0 |

- Molecule 30 is a protein called Chromosome 1 C15orf65 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | 5G | 93 | 708 | 445 | 123 | 136 | 4 | 0 | 0 |

- Molecule 31 is a protein called EF-hand domain family member B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | 5I | 443 | 3576 | 2284 | 630 | 653 | 9 | 0 | 0 |
| 31 | 5J | 112 | 898 | 563 | 161 | 172 | 2 | 0 | 0 |

- Molecule 32 is a protein called Cilia and flagella associated protein 141.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | 5L | 92 | 736 | 460 | 140 | 130 | 6 | 0 | 0 |

- Molecule 33 is a protein called Meiosis-specific nuclear structural protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | 5N | 334 | 2883 | 1791 | 520 | 556 | 16 | 0 | 0 |
| 33 | 5O | 151 | 1277 | 783 | 242 | 245 | 7 | 0 | 0 |

- Molecule 34 is a protein called Cilia- and flagella-associated protein 53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | 5Q | 262 | 2216 | 1361 | 412 | 433 | 10 | 0 | 0 |
| 34 | 5R | 198 | 1671 | 1019 | 319 | 326 | 7 | 0 | 0 |

- Molecule 35 is a protein called CFAP107/C1orf158.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | 5T | 135 | 1118 | 732 | 196 | 188 | 2 | 0 | 0 |
| 35 | 5U | 28 | 223 | 141 | 41 | 41 | | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 5T | 40F | UNK | THR | conflict | UNP A0A8D1WB49 |
| 5U | 46 | UNK | THR | conflict | UNP A0A8D1WB49 |

- Molecule 36 is a protein called Cilia and flagella associated protein 77.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | 5W | 231 | 1868 | 1186 | 349 | 325 | 8 | 0 | 0 |
| 36 | 5X | 231 | 1868 | 1186 | 349 | 325 | 8 | 0 | 0 |
| 36 | 5Y | 185 | 1487 | 942 | 277 | 262 | 6 | 0 | 0 |
| 36 | 5Z | 59 | 488 | 310 | 93 | 83 | 2 | 0 | 0 |

- Molecule 37 is a protein called Cilia and flagella associated protein 144.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | 6A | 116 | 992 | 626 | 184 | 180 | 2 | 0 | 0 |

- Molecule 38 is a protein called Cilia-and flagella-associated protein 96.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 38 | 6C | 212 | 1698 | 1086 | 290 | 315 | 7 | 0 | 0 |
| 38 | 6D | 65 | 495 | 318 | 87 | 87 | 3 | 0 | 0 |

- Molecule 39 is a protein called Sperm acrosome associated 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | 6F | 157 | 1264 | 789 | 229 | 236 | 10 | 0 | 0 |
| 39 | 6G | 157 | 1264 | 789 | 229 | 236 | 10 | 0 | 0 |
| 39 | 6H | 141 | 1134 | 710 | 202 | 213 | 9 | 0 | 0 |
| 39 | 6I | 157 | 1264 | 789 | 229 | 236 | 10 | 0 | 0 |
| 39 | 6J | 157 | 1264 | 789 | 229 | 236 | 10 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | 6K | 157 | 1264 | 789 | 229 | 236 | 10 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 39 | 6L | 137 | 1095 | 694 | 190 | 204 | 7 | 0 | 0 |

- Molecule 40 is a protein called Tubulin alpha chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | AA | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | AE | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | AF | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | AG | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | AH | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | BA | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | BE | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | BF | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | BG | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | BH | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | BI | 373 | 2932 | 1855 | 501 | 555 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | CA | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | CE | 440 | 3438 | 2174 | 584 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | CF | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | CG | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | CH | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | CI | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | DA | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | DE | 435 | 3410 | 2157 | 579 | 652 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | DF | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | DG | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | DH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | DI | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | EA | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | EE | 435 | 3415 | 2161 | 580 | 652 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | EF | 435 | 3415 | 2161 | 580 | 652 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | EG | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | EH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | EI | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | FA | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | FE | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | FF | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | FG | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | FH | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | FI | 434 | 3402 | 2152 | 577 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | GA | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | GE | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | GF | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | GG | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | GH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | GI | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | HA | 435 | 3410 | 2157 | 579 | 652 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | HE | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | HF | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | HG | 434 | 3402 | 2153 | 578 | 649 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | HH | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | HI | 435 | 3415 | 2161 | 580 | 652 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | IA | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | IE | 420 | 3286 | 2074 | 557 | 633 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | IF | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | IG | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | IH | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | II | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | JA | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | JD | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | JE | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | JF | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | JG | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | JH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | KA | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | KD | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | KE | 434 | 3402 | 2153 | 578 | 649 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | KF | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | KG | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | KH | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | LA | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | LD | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | LE | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | LF | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | LG | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | LH | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | MA | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | MD | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | ME | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | MF | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | MG | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | MH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | NA | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | ND | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | NE | 434 | 3402 | 2153 | 578 | 649 | 22 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | NF | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | NG | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | NH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | OA | 436 | 3422 | 2165 | 581 | 654 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | OD | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | OE | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | OF | 436 | 3419 | 2163 | 581 | 653 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | OG | 436 | 3415 | 2160 | 580 | 653 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | OH | 436 | 3419 | 2163 | 581 | 653 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | PA | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | PD | 408 | 3196 | 2023 | 543 | 610 | 20 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | PE | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | PF | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | PG | 431 | 3384 | 2144 | 575 | 643 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | PH | 431 | 3384 | 2144 | 575 | 643 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | QA | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | QE | 431 | 3384 | 2144 | 575 | 643 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | QF | 431 | 3384 | 2144 | 575 | 643 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | QG | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | QH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | RA | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | RE | 431 | 3384 | 2144 | 575 | 643 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | RF | 431 | 3384 | 2144 | 575 | 643 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | RG | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | RH | 431 | 3384 | 2144 | 575 | 643 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | RI | 376 | 2962 | 1875 | 505 | 562 | 20 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | SA | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | SE | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | SF | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | SG | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | SH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | SI | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | TA | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | TE | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | TF | 432 | 3392 | 2148 | 576 | 646 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | TG | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | TH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | TI | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | UA | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | UE | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | UF | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 40 | UG | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | UH | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| 40 | UI | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| 40 | VA | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| 40 | VF | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| 40 | VG | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| 40 | VH | 434 | 3406 | 2155 | 578 | 651 | 22 | 0 | 0 |
| 40 | VI | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| 40 | VJ | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| 40 | WA | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| 40 | WE | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| 40 | WF | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |
| 40 | WG | 432 | 3390 | 2147 | 576 | 645 | 22 | 0 | 0 |
| 40 | WH | 440 | 3442 | 2177 | 585 | 658 | 22 | 0 | 0 |
| 40 | WI | 433 | 3398 | 2151 | 577 | 648 | 22 | 0 | 0 |

- Molecule 41 is a protein called Tubulin beta chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | AB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | AL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | AM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | AN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | AO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | AP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | BB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | BL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | BM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | BN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | BO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | BP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | CB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | CL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | CM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | CN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | CO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | CP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | DB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | DL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | DM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | DN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | DO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | DP | 428 | 3337 | 2096 | 577 | 637 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | EB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | EL | 364 | 2826 | 1775 | 489 | 538 | 24 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | EM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | EN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | EO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | EP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | FB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | FM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | FN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | FO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | FP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | GB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | GM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | GN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | GO | 428 | 3335 | 2095 | 574 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | GP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | HB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | HM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | HN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | HO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | HP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | HQ | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | IB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | IM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | IN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | IO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | IP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | IQ | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | JB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | JL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | JM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | JN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | JO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | KB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | KL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | KM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | KN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | KO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | KP | 386 | 3007 | 1892 | 519 | 573 | 23 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | LB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | LL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | LM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | LN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | LO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | LP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | MB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | ML | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | MM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | MN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | MO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | MP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | NB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | NL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | NM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | NN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | NO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | NP | 418 | 3264 | 2052 | 565 | 621 | 26 | 0 | 0 |
| 41 | OB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | OL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | OM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | ON | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | OO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | OP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | PB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| 41 | PL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | PM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | PN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | PO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | PP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | QB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | QL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | QM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | QN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | QO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | QP | 428 | 3327 | 2090 | 575 | 636 | 26 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | RB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | RL | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | RM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | RN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | RO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | RP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | SB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | SL | 381 | 2964 | 1861 | 512 | 567 | 24 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | SM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | SN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | SO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | SP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | TB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | TL | 387 | 3019 | 1899 | 521 | 576 | 23 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | TM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | TN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | TO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | TP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | UB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | UM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | UN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | UO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | UP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | VB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | VN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | VO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | VP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | VQ | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | WB | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | WM | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | WN | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | WO | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |

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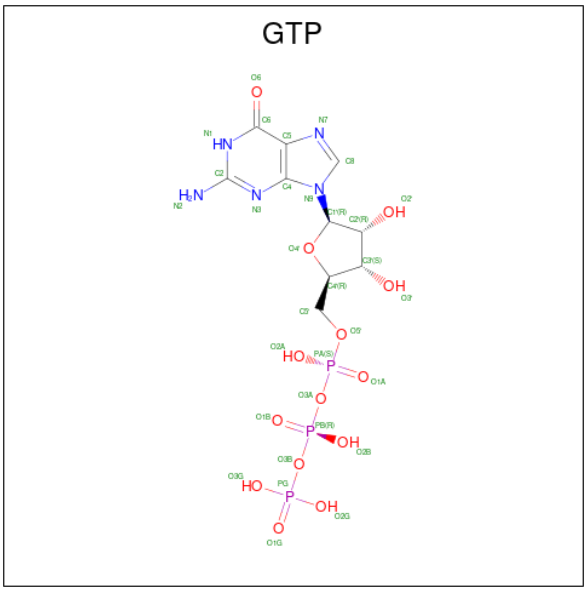
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | WP | 428 | 3341 | 2098 | 577 | 639 | 27 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 41 | WQ | 421 | 3285 | 2065 | 569 | 625 | 26 | 0 | 0 |

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 42 | AA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | AE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | AF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | AG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | AH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | BA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | BF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | BG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | BH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 42 | BI | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | BL | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | CA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | CE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | CF | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | CG | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | CH | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | CI | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | DA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | DE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | DF | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | DG | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | DH | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | DI | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | EA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | EF | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | EG | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | EH | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | EI | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | EL | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 42 | FB | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 42 | FE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | FI | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | FM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | FN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | FO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | GA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | GB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | GE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | GF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | GH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | GP | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | HA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | HB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | HE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | HH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | HM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | HP | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | IA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | IE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | IF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | IG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 42 | IH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | II | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | JA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | JB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | JD | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | JE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | JF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | JO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | KB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | KD | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | KE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | KM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | KN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | KO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | LA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | LB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | LD | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | LL | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | LM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | LO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | MB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 42 | MD | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | MH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | ML | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | MM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | MN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | ND | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | NE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | NG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | NM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | NN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | NO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | OB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | OD | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | OL | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | OM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | ON | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | OO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | PB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | PD | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | PE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 42 | PM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 42 | PN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | PO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | QF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | QG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | QL | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | QN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | QO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | RE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | RF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | RG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | RN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | RO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | RP | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | SG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | SH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | SL | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | SM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | SN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | SP | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | TF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | TG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 42 | TH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | TI | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | TL | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | TN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | UA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | UB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | UE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | UI | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | UM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | UO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | VA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | VB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | VF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | VN | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | VP | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | VQ | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | WA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | WE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | WF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | WG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 42 | WI | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

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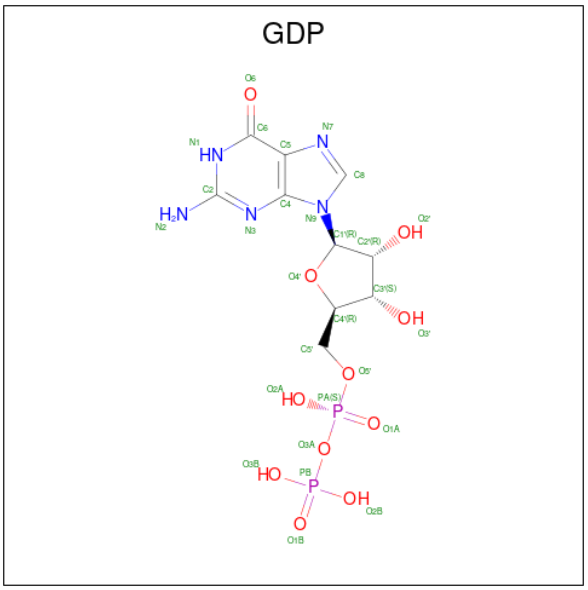
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 42 | WO | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

- Molecule 43 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 43 | AB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | AL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | AM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | AN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | AO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | AP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | BB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | BL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | BM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | BN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 43 | BO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | BP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | CB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | CL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | CM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | CN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | CO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | CP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | DB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | DL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | DM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | DN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | DO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | DP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | EB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | EL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | EM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | EN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | EO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | EP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | FB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 43 | FM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | FN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | FO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | FP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | GB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | GM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | GN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | GO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | GP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | HB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | HM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | HN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | HO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | HP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | HQ | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | IB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | IM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | IN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | IO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | IP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | IQ | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 43 | JB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | JL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | JM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | JN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | JO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | KB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | KL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | KM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | KN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | KO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | KP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | LB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | LL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | LM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | LN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | LO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | LP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | MB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | ML | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | MM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | MN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 43 | MO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | MP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | NB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | NL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | NM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | NN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | NO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | NP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | OB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | OL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | OM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | ON | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | OO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | OP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | PB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | PL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | PM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | PN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | PO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | PP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| | | | Total | C | N | O | P | |
| 43 | QB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 43 | QL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | QM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | QN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | QO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | QP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | RB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | RL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | RM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | RN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | RO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | RP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | SB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | SL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | SM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | SN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | SO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | SP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | TB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | TL | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | TM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | TN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

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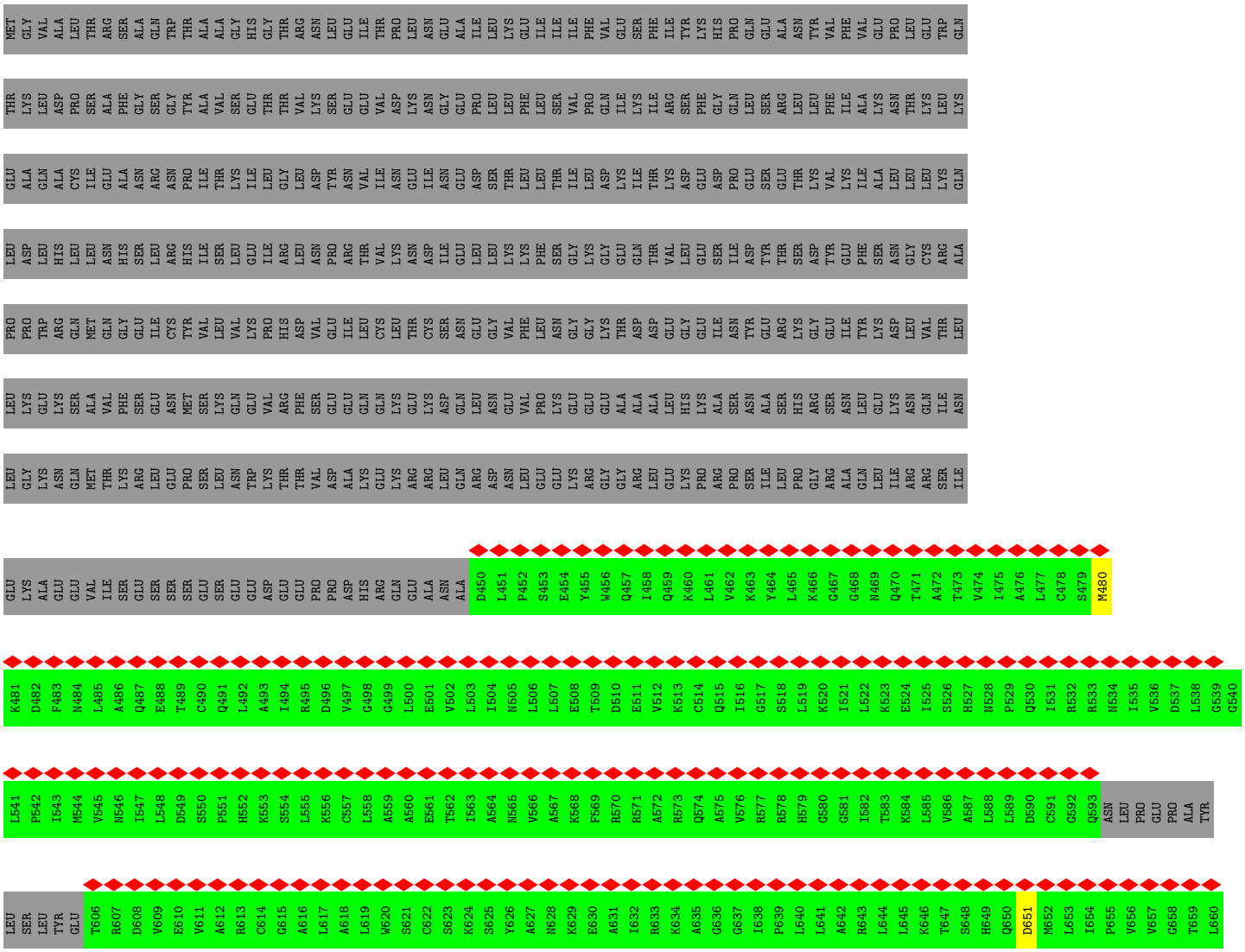
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 43 | TO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | TP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | UB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | UM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | UN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | UO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | UP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | VB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | VN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | VO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | VP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | VQ | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | WB | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | WM | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | WN | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | WO | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | WP | 1 | 28 | 10 | 5 | 11 | 2 | 0 |
| 43 | WQ | 1 | 28 | 10 | 5 | 11 | 2 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Armadillo repeat-containing protein 4 isoform 1

Chain 1A:



Q661 E662 C663 A664 S665 E666 E667 N668 Y669 R670 A671 A672 I673 K674 A675 E676 R677 I678 I679 E680 N681 L682 V683 K684 N685 L686 N687 S688 E689 N690 E691 Q692 L693 Q694 E695 H696 C697 A698 M699 A700 I701 Y702 Q703 C704 A705 E706 D707 E708 E709 T710 R711 D712 L713 V714 R715 L716 H717 G718 G719 L720

K721 P722 L723 A724 S725 L726 L727 N728 N729 T730 D731 N732 K733 E734 R735 L736 A737 A738 V739 T740 G741 A742 I743 W744 K745 C746 S747 I748 S749 K750 E751 N752 V753 I754 K755 F756 R757 E758 Y759 K760 A761 I762 E763 T764 L765 V766 G767 L768 L769 T770 D771 Q772 P773 E774 E775 V776 L777 V778 N779 V780

V781 G782 A783 L784 G785 E786 C787 C788 Q789 E790 H791 E792 N793 R794 V795 I796 V797 R798 R799 C800 G801 G802 I803 Q804 P805 L806 V807 N808 L809 L810 V811 G812 I813 N814 Q815 A816 L817 L818 N820 V821 T822 K823 A824 V825 G826 A827 C828 A829 V830 E831 P832 E833 S834 M835 M836 I837 I838 D839 R840

L841 D842 G843 V844 R845 L846 L847 W848 S849 L850 L851 K852 N853 P854 H855 A856 D857 V858 K859 A860 S861 A862 A863 W864 A865 L866 C867 P868 C869 I870 Q871 N872 A873 K874 D875 A876 G877 E878 M879 V880 R881 S882 F883 V884 G885 G886 L887 E888 L889 V890 V891 N892 L893 L894 K895 S896 D897 N898 K899 E900

V901 L902 A903 S904 V905 C906 A907 A908 I909 T910 N911 I912 A913 K914 D915 E916 E917 N918 L919 A920 V921 I922 T923 D924 H925 G926 V927 V928 P929 L930 L931 S932 K933 L934 A935 N936 T937 N938 N939 D940 K941 L942 R943 R944 H945 L946 A947 E948 A949 I950 S951 R952 C953 C954 M955 W956 G957 R958 N959 R960

V961 A962 F963 G964 E965 H966 K967 A968 V969 A970 P971 L972 V973 R974 Y975 L976 K977 S978 S979 D980 T981 N982 V983 H984 R985 A986 T987 A988 Q989 A990 L991 Y992 Q993 L994 S995 E996 N997 A998 D999 N1000 C1001 I1002 T1003 M1004 H1005 E1006 N1007 G1008 A1009 V1010 K1011 L1012 L1013 L1014 D1015 M1016 V1017 G1018 S1019 P1020

D1021 Q1022 D1023 L1024 Q1025 E1026 A1027 A1028 A1029 G1030 C1031 I1032 S1033 N1034 I1035 R1036 R1037 L1038 A1039 L1040 A1041 T1042 E1043 K1044 A1045 R1046 Y1047 T1048

- Molecule 1: Armadillo repeat-containing protein 4 isoform 1

Chain 1B:

MET GLY VAL ALA LEU THR ARG SER ALA GLN TRP THR ALA ALA GLY HIS GLY THR ARG ASN LEU GLU ILE THR PRO LEU ASN GLU ALA ILE LEU LYS GLU ILE ILE ILE PHE VAL GLU SER PHE ILE TYR LYS HIS PRO GLN GLU ALA ASN TYR VAL PHE VAL GLU PRO LEU GLU TRP GLN

THR LYS LEU ASP PRO SER ALA PHE GLY SER GLY TYR ALA ALA VAL SER GLU THR THR VAL LYS SER GLU GLU VAL ASP LYS ASN GLY GLU PRO LEU LEU PHE LEU SER VAL PRO GLN ILE LYS ILE ARG SER PHE GLY GLN LEU SER ARG LEU LEU PHE ILE ALA LYS ASN THR LYS LEU LYS

GLU ALA GLN ALA CYS ILE GLU ALA ASN ARG ASN PRO ILE THR LYS ILE LEU GLY LEU ASP ASN PRO ASN VAL ILE ASN GLU ILE ASN GLU ASP SER THR LEU LEU THR ILE LEU ASP LYS ILE THR LYS ASP GLU ASP PRO GLU SER GLU THR LYS VAL LYS ILE ALA LEU LEU LEU LYS GLN

LEU ASP LEU HIS LEU LEU ASN HIS SER LEU ARG HIS ILE SER LEU GLU ILE ARG LEU ASN PRO ARG THR VAL LYS ASN ASP ILE GLU LEU LEU LYS LYS PHE SER GLY LYS GLY GLU GLN THR VAL LEU GLU SER ILE ASP TYR THR SER ASP TYR GLU PHE SER ASN GLY CYS ALA

PRO PRO TRP ARG GLN MET GLN GLY GLU ILE CYS TYR VAL LEU VAL LYS PRO HIS ASP VAL GLU ILE LEU CYS LEU THR CYS SER ASN GLU GLY VAL PHE LEU ASN GLY LYS GLU GLU GLY GLY THR ASP ASP GLU GLY GLU ILE ASN TYR GLU ARG LYS GLY GLU ILE TYR LYS ASP LEU VAL THR LEU

LEU LYS GLU LYS SER ALA VAL PHE SER GLU ASN MET SER LYS GLN GLU VAL ARG PHE SER GLU GLU GLN GLN LYS GLU ASP GLN LEU ASN GLU VAL PRO LYS GLU GLU GLU ALA ALA ALA LEU HIS LYS ALA SER ASN ALA SER HIS ARG SER ASN LEU GLU ILE LYS ASN LEU ASN

LEU GLY LYS ASN GLN MET THR LYS ARG LEU GLU PRO SER LEU ASN TRP LYS THR THR VAL ASP ALA LYS GLU GLN ARG ASP ASN LEU ASN LEU GLU LYS ARG LYS ARG ARG LEU GLN ARG ASP ASN LEU GLU GLU LYS GLY GLY ARG GLU LYS PRO ARG PRO SER ILE LEU PRO GLY ARG ALA THR VAL ILE LEU LYS ARG ARG SER ILE

GLU LYS ALA GLU GLU VAL ILE SER GLU SER SER SER GLU SER GLU GLU ASP GLU PRO PRO ASP HIS ARG GLN GLU ALA ASN ALA ASP LEU PRO SER GLU TYR TRP GLN ILE GLN LYS LEU VAL LYS TYR LEU LYS GLY GLY ASN GLN THR ALA THR VAL ILE ALA LEU CYS SER MET

LYS ASP PHE ASN LEU ALA GLN GLU THR CYS GLN LEU ALA ILE ARG ASP VAL GLY GLY LEU GLU VAL LEU ILE ASN LEU LEU GLU THR ASP GLU VAL LYS CYS GLN ILE GLY SER LEU LYS ILE LEU LYS GLU ILE SER HIS ASN PRO GLN ILE ARG ARG ASN ILE VAL ASP LEU GLY GLY

LEU PRO ILE MET VAL ASN ILE LEU ASP SER PRO HIS LYS SER LEU LYS CYS LEU ALA ALA GLU THR ILE ALA ASN VAL ALA LYS PHE ARG ARG ARG ALA ARG GLN ALA VAL ARG ARG HIS GLY GLY ILE THR LYS LEU VAL ALA LEU LEU ASP CYS GLY GLN ASN LEU PRO GLU PRO ALA TYR

LEU SER LEU TYR GLU THR ARG ASP VAL GLU VAL ALA ARG CYS GLY ALA LEU ALA LEU TRP SER CYS SER LYS SER TYR ALA ASN LYS GLU ALA ILE ARG LYS ALA GLY GLY ILE PRO LEU LEU ALA ARG LEU LEU ASP MET GLN ILE PRO VAL VAL GLY THR LEU

GLN GLU CYS ALA SER GLU GLU ASN TYR ARG ALA ALA ILE LYS ALA GLU ARG ILE ILE GLU ASN LEU VAL LYS ASN LEU ASN SER GLU ASN GLU GLN LEU GLN GLU GLN HIS CYS ALA MET ALA ILE TYR GLN CYS ALA GLU ASP GLU GLU THR ARG ASP LEU VAL ARG LEU HIS GLY GLY LEU

LYS PRO LEU ALA SER LEU LEU ASN ASN THR ASP ASN LYS GLU ARG LEU ALA ALA VAL THR GLY ALA ILE TRP LYS CYS SER ILE SER LYS GLU ASN VAL ILE LYS PHE ARG GLU TYR LYS ALA ILE GLU THR LEU VAL GLY LEU LEU THR ASP GLN PRO GLU VAL LEU VAL ASN VAL

VAL GLY ALA LEU GLY GLU CYS CYS GLN GLU HIS GLU ASN ARG VAL ILE VAL ARG ARG CYS GLY GLY ILE GLN PRO LEU VAL ASN LEU LEU VAL GLY ILE ASN GLN ALA LEU LEU VAL ASN VAL THR LYS ALA VAL GLY GLU PRO GLU SER MET MET ILE ILE ASP ARG

LEU ASP GLY VAL ARG LEU LEU TRP SER LEU LEU LYS ASN PRO HIS ALA ASP VAL LYS ALA SER ALA ALA TRP ALA LEU CYS PRO CYS ILE GLN ASN ALA LYS ASP ALA GLY GLU MET VAL ARG SER PHE VAL GLY GLY LEU GLU LEU VAL VAL ASN LEU LEU LYS SER ASP ASN LYS E900

V901 L902 A903 S904 V905 C906 A907 A908 I909 T910 N911 I912 A913 K914 D915 E916 E917 N918 L919 A920 V921 I922 T923 D924 H925 G926 V927 V928 P929 L930 L931 S932 K933 L934 A935 N936 T937 N938 N939 D940 K941 L942 R943 R944 H945 L946 A947 E948 A949 I950 S951 R952 C953 C954 M955 W956 G957 R958 N959 R960

V961 A962 F963 G964 E965 H966 K967 A968 V969 A970 P971 L972 V973 R974 Y975 L976 K977 S978 S979 D980 T981 N982 V983 H984 R985 A986 T987 A988 Q989 A990 L991 Y992 Q993 L994 S995 E996 N997 A998 D999 N1000 C1001 I1002 T1003 M1004 H1005 E1006 N1007 G1008 A1009 V1010 K1011 L1012 L1013 L1014 D1015 M1016 V1017 G1018 S1019 P1020

D1021 Q1022 D1023 L1024 Q1025 E1026 A1027 A1028 A1029 G1030 C1031 I1032 S1033 N1034 I1035 R1036 R1037 L1038 A1039 L1040 A1041 T1042 E1043 K1044 A1045 R1046 Y1047 T1048

- Molecule 2: Outer dynein arm-docking complex subunit 4

Chain 1C:

MET ALA GLU GLN GLU ALA ASN G8 L9 R10 S11 T12 F13 P14 M17 A18 E19 G20 E21 R22 L25 C26 G27 E28 F29 A30 K31 A32 A33 H34 S35 F36 S37 L40 H41 L42 Q43 N44 G45 D46 K47 L50 V51 A52 R53 S54 K55 C56 F57 L58 K59 M60 G61 E62 L63 E64

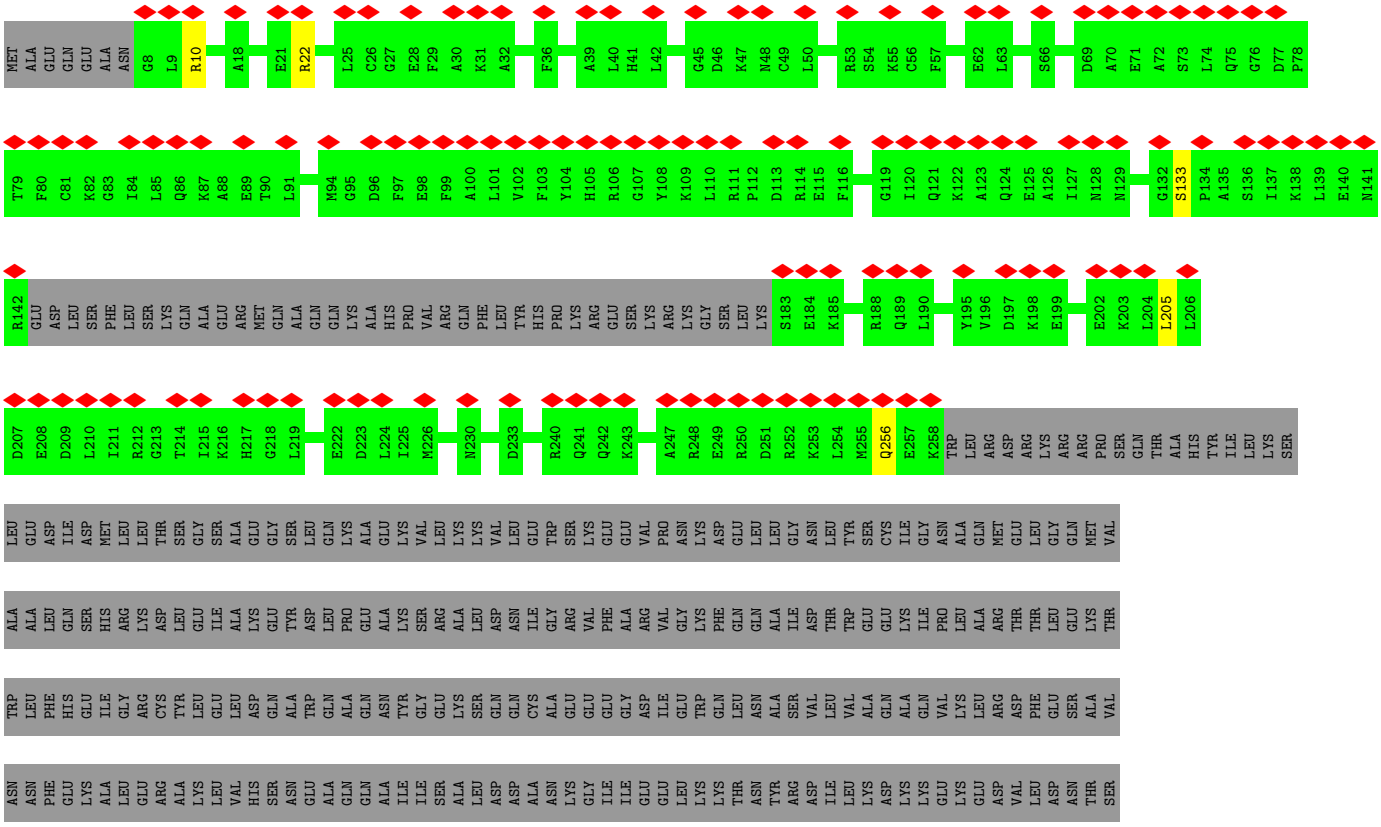
K65 A68 D69 A70 E71 A72 S73 L74 Q75 G76 D77 P78 T79 F80 C81 I84 L85 Q86 K87 A88 E89 T90 L91 M94 G95 D96 F97 E98 F99 A100 L101 V102 F103 Y104 H105 R106 G107 Y108 K109 L110 R111 P112 D113 R114 E115 F116 K117 V118 G119 I120 Q121 K122 A123 Q124 E125 A126 I127

N128 N129 S130 V131 G132 S133 S136 I137 K138 L139 E140 N141 R142 GLU ASP LEU SER PHE LEU SER LYS GLN ALA GLU ARG MET GLN ALA GLN GLN LYS ALA HIS PRO VAL ARG GLN PHE LEU TYR HIS PRO LYS ARG GLU SER LYS ARG LYS GLY SER LEU LYS S183 E184 K185 I186 V187 R188

Q189 E193 L194 E199 E202 K203 L204 L205 L206 D207 E208 D209 L210 I211 R212 G213 T214 I215 K216 H217 G218 L219 E222 D223 M226 T227 G228 I229 N230 Y231 L232 D233 T234 R235 F238 W239 R240 Q241 Q242 K243 P244 I245 Y246 A247 R248 E249 R250 D251 R252 K253 L254 M255 Q256 E257

• Molecule 2: Outer dynein arm-docking complex subunit 4

Chain 1D:



ALA LYS GLU LYS GLU ALA THR ARG ARG VAL ARG ASP GLU PRO GLU LYS VAL MET LYS ARG TRP GLU HIS GLU GLN MET GLU ASN GLU LYS GLU MET GLU GLY ASP LEU SER LYS ASP THR LEU GLY THR ALA ALA SER GLY GLN GLU GLY HIS GLU GLN ARG GLY ALA ILE GLU LYS ALA

SER PRO LEU ARG ARG THR GLU GLN ALA ALA MET GLY ARG ASP PRO GLY GLU ALA ALA LYS GLU HIS LEU GLY GLU ALA GLY ARG THR LEU SER GLU LEU LYS ARG GLY GLU THR ARG GLU ILE TYR ARG ARG PRO SER ASP LEU ASP GLN ASN LEU SER GLU GLU LEU SER THR ARG GLU

PRO GLU VAL LEU GLU LYS LYS LEU SER GLU THR GLY ARG GLY GLU SER GLU ARG LEU GLU LYS THR GLU SER GLU GLU ILE GLY GLU THR GLU ASN THR GLU GLU MET ARG LYS ASP GLU LYS GLU ASP GLU LEU ALA LEU GLU

- Molecule 3: EF-hand calcium binding domain 1

Chain 1F: 65% 64% • 35%

MET ASN SER VAL CYS LEU GLY LYS ASP THR ALA LEU THR LEU GLY ARG SER GLN GLN LEU SER VAL ALA LEU MET GLY VAL ASN LEU THR MET ASP ALA CYS ARG ARG PRO GLY ALA ALA VAL CYS LYS LEU THR CYS ALA GLU LEU LYS LEU GLY I53 K54 D55 G56 L57 N58 A59 C60

C61 Y62 I63 C64 I65 F66 S67 F68 T69 V70 N71 K72 F73 E74 V75 K76 C77 L78 I79 S80 L81 F82 Y83 N84 L85 V86 G87 ASP VAL THR GLU ARG GLN GLY VAL VAL VAL G98 L99 D100 R101 N102 A103 F104 R105 N106 I107 L108 H109 V110 T111 F112 G113 M114 T115 D116 D117 M118 I119 M120

D121 R122 V123 F124 R125 G126 F127 D128 K129 D130 N131 D132 G133 C134 V135 S136 V137 S138 E139 W140 V141 Y142 G143 L144 S145 V146 F147 L148 R149 G150 T151 L152 E153 E154 K155 M156 K157 Y158 C159 F160 E161 V162 F163 D164 L165 N166 G167 D168 G169 F170 I171 S172 K173 E174 E175 M176 V177 H178 M179 L180

K181 N182 S183 L184 L185 K186 Q187 PRO SER GLU GLU ASP PRO ASP GLU GLY ILE LYS ASP LEU VAL GLU ILE T204 L205 K206 K207 M208 D209 HIS ASP HIS ASP GLY LYS L216 S217 F218 P219 D220 Y221 E222 A223 A224 V225 R226 E227 E228 A229 L230 L231 L232 E233 A234 F235 G236 P237 C238 L239 P240

D241 P242 K243 S244 Q245 K246 E247 F248 E249 A250 Q251 V252 F253 K254 D255 PRO ASN GLU PHE GLY GLU VAL

- Molecule 3: EF-hand calcium binding domain 1

Chain 1G: 65% 32% 30% • 35%

MET ASN SER VAL CYS LEU GLY LYS ASP THR ALA LEU THR LEU GLY ARG SER GLN GLN LEU SER VAL ALA LEU MET GLY VAL ASN LEU THR MET ASP ALA CYS ARG ARG PRO GLY ALA ALA VAL CYS LYS LEU THR CYS ALA GLU LEU LYS LEU GLY I53 K54 D55 G56 L57 N58 A59 C60

C61 Y62 I63 C64 I65 F66 S67 F68 T69 V70 N71 K72 F73 E74 V75 K76 C77 L78 I79 S80 L81 F82 Y83 N84 L85 V86 G87 ASP VAL THR GLU ARG GLN GLY VAL VAL VAL G98 L99 D100 R101 N102 A103 F104 R105 N106 I107 L108 H109 V110 T111 F112 G113 M114 T115 D116 D117 M118 I119 M120

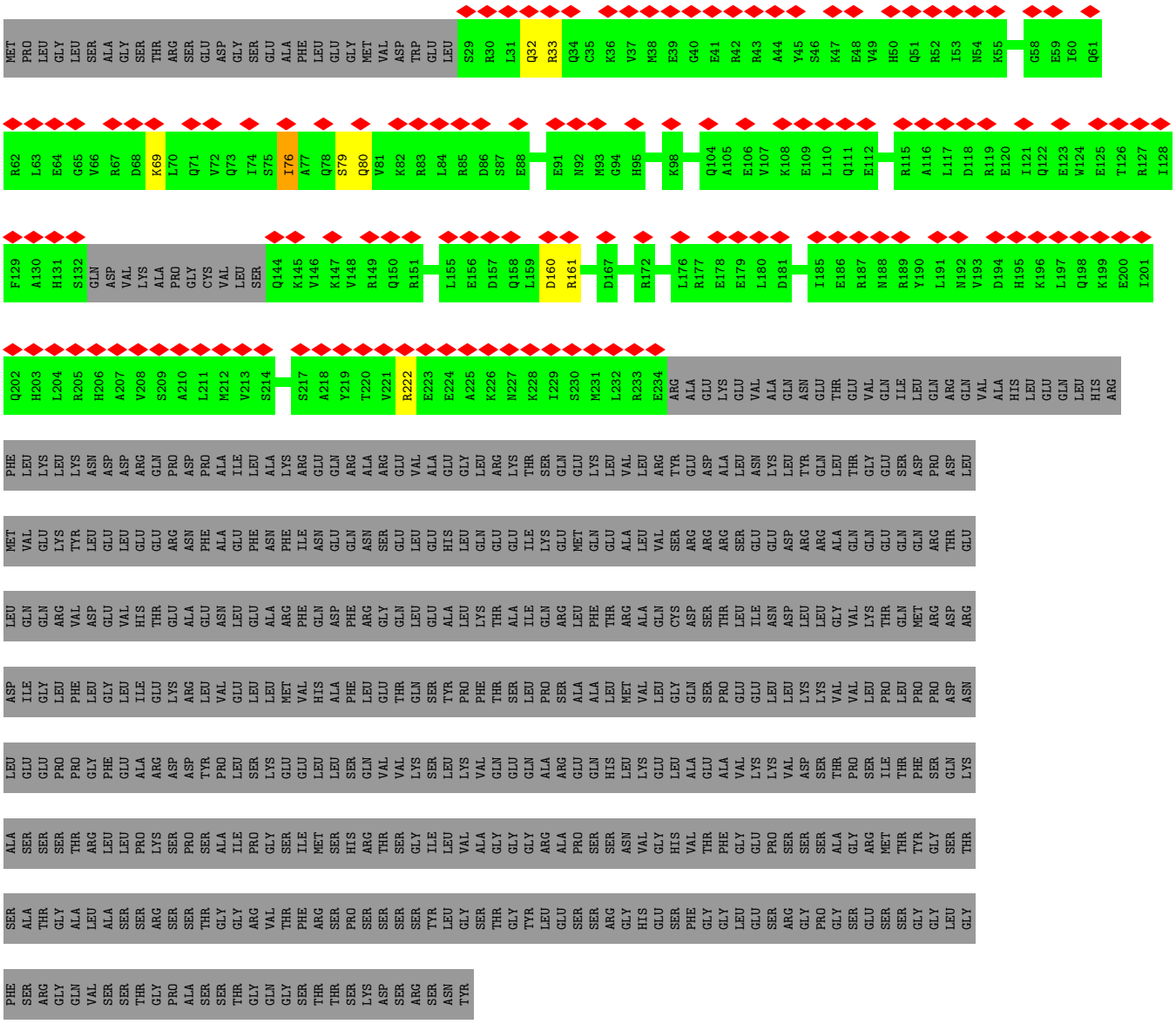
D121 R122 V123 F124 R125 G126 F127 D128 K129 D130 N131 D132 G133 C134 V135 S136 V137 S138 E139 W140 V141 Y142 G143 L144 S145 V146 F147 L148 R149 G150 T151 L152 E153 E154 K155 M156 K157 Y158 C159 F160 E161 V162 F163 D164 L165 N166 G167 D168 G169 F170 I171 S172 K173 E174 E175 M176 V177 H178 M179 L180

K181 N182 S183 L184 L185 K186 Q187 PRO SER GLU GLU ASP PRO ASP GLU GLY ILE LYS ASP LEU VAL GLU ILE T204 L205 K206 K207 M208 D209 HIS ASP HIS ASP GLY LYS L216 S217 F218 P219 D220 Y221 E222 A223 A224 V225 R226 E227 E228 A229 L230 L231 L232 E233 A234 F235 G236 P237 C238 L239 P240

D241 P242 K243 S244 Q245 K246 E247 F248 E249 A250 Q251 V252 F253 K254 D255 PRO ASN GLU PHE GLY GLU VAL

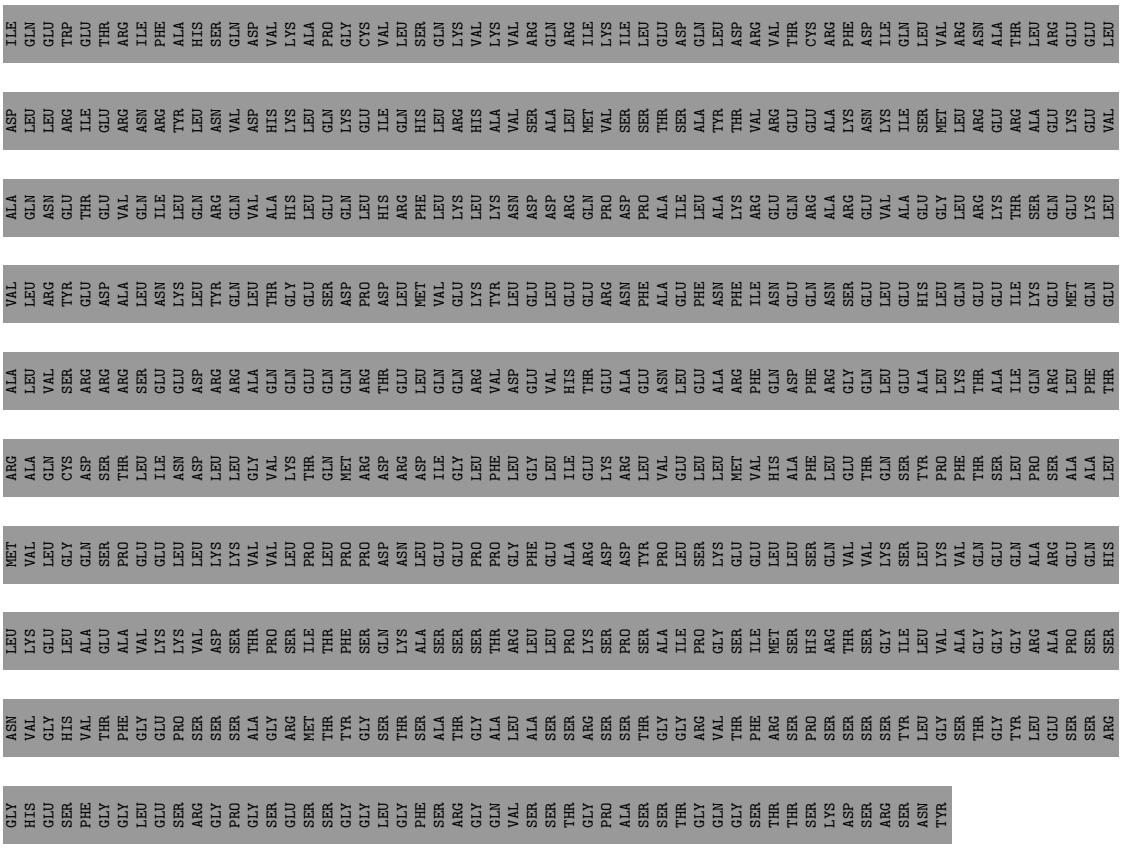
- Molecule 4: Coiled-coil domain-containing protein 114 isoform X2

Chain 1H:



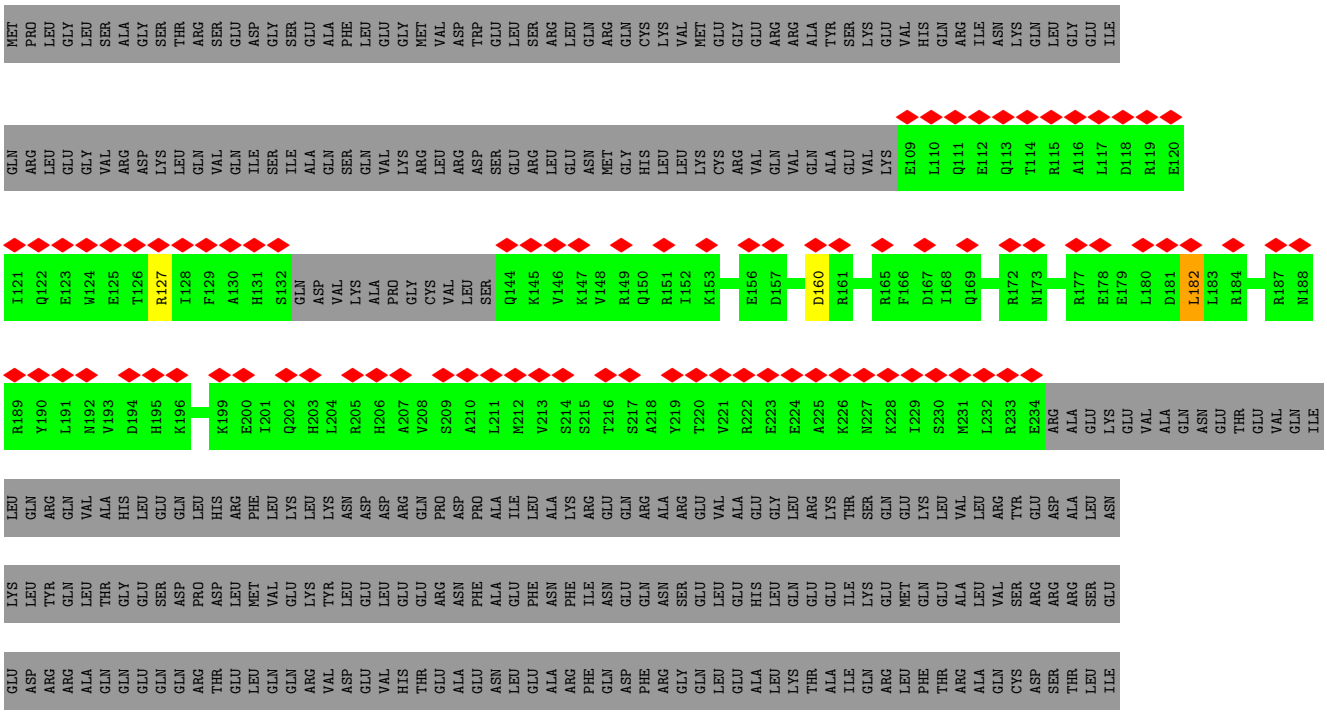

- Molecule 4: Coiled-coil domain-containing protein 114 isoform X2

Chain 1I:



- Molecule 4: Coiled-coil domain-containing protein 114 isoform X2

Chain 1J:



ASN ASP LEU LEU GLY VAL LYS THR GLN MET ARG ASP ARG ASP ILE GLY LEU PHE LEU GLY LEU ILE GLU LYS ARG LEU VAL GLU LEU LEU MET VAL HIS ALA PHE LEU GLU THR GLN SER TYR PRO PHE THR SER LEU PRO SER ALA ALA LEU MET VAL LEU GLY GLN SER PRO GLU GLU

LEU LEU LYS LYS VAL VAL LEU PRO LEU PRO PRO ASP ASN LEU GLU GLU PRO PRO GLY PHE GLU ALA ARG ASP ASP TYR PRO LEU SER LYS GLU GLU LEU LEU SER GLN VAL VAL LYS SER LEU LYS VAL GLN GLU GLN ALA ARG GLU GLN HIS LEU LYS GLU LEU ALA GLU ALA VAL LYS

LYS VAL ASP SER THR PRO SER ILE THR PHE SER GLN LYS ALA SER SER SER THR ARG LEU LEU PRO LYS SER PRO SER ALA ILE PRO GLY SER ILE MET SER HIS ARG THR SER GLY ILE LEU VAL ALA GLY GLY GLY ARG ALA PRO SER SER ASN VAL GLY HIS VAL THR PHE GLY GLU

PRO SER SER SER ALA GLY ARG MET THR TYR GLY SER THR SER ALA THR GLY ALA LEU ALA SER SER SER SER THR GLY GLY ARG VAL THR PHE ARG SER PRO SER SER SER SER TYR LEU GLY SER THR GLY TYR LEU GLU SER SER SER ARG GLY HIS GLU SER PHE GLY GLY LEU GLU

SER ARG GLY PRO GLY SER GLU SER SER GLY GLY LEU GLY PHE SER ARG GLY GLN VAL SER SER THR GLY PRO ALA SER SER THR GLY GLN GLY SER THR THR SER LYS ASP SER ARG SER ASN TYR

- Molecule 5: Outer dynein arm docking complex subunit 3

Chain 1L: 20% 22% 75%

MET THR SER PRO LEU CYS TRP ALA ALA SER ALA ASN ALA MET PRO SER GLN ASP GLN VAL SER ALA SER SER LYS GLY ARG GLY ASN GLN ALA GLN ALA LYS GLY HIS PRO GLN GLY LYS GLY SER VAL GLN ALA TRP GLN SER LEU HIS SER LYS ALA GLY PRO PHE HIS ALA SER GLU

GLY LYS SER THR VAL HIS THR GLN VAL ALA GLU LEU GLN ARG LYS ILE GLN LEU LEU GLU GLY ASP ARG LYS ALA PHE TYR GLU SER THR GLN TRP ASN ILE ARG LYS ASN GLN GLU THR ILE ASN GLN LEU ARG GLU GLU THR ARG VAL LEU GLN LEU LEU ALA ASP LEU LEU GLN

GLY ASP GLU LYS VAL VAL GLN ALA VAL ILE ARG GLU TRP LYS SER GLU LYS PRO TYR LEU LYS ASN ARG THR GLY GLN GLN ALA LEU GLU HIS LEU ASP HIS GLN LEU SER GLU LYS VAL K161 Q162 L163 N164 A165 L166 R167 H168 Q169 L170 G171 L172 R173 Q174 K175 W176 L177 E178 E179 L180

Q181 L182 Q183 H184 S185 L186 R187 E188 L189 E190 M191 A192 E193 A194 Q195 D196 R197 N198 T199 E200 K203 R206 N207 L208 E209 N210 R211 L212 E213 K214 A215 K218 A219 E220 E221 A222 E223 H224 Q231 L232 K233 E238 E239 S240 L241 E244 N245 R246 L247 D248 F249 M250 E251 A252

E253 R256 T257 K258 H259 E260 L261 E262 E263 L264 N265 V266 V267 N268 Q269 E270 A271 L272 N273 A274 R275 D276 I277 A278 K279 N280 Q281 L282 Q283 D284 L285 E286 E287 T288 V289 L290 R291 E292 R293 K294 K295 R296 D297 R298 Y299 L300 T301 E302 C303 K304 K305 R306 A307 E308 E309 R310 K311 L312 Q313

N314 E315 ARG MET GLU ARG LYS THR GLN ARG GLU ASP VAL LEU LEU HIS SER ASP ASP THR LEU GLN ASP SER GLN ARG SER LYS GLU GLU GLU LEU ARG ARG ARG ARG TRP SER MET TYR GLN MET GLU VAL LEU PHE GLY LYS VAL LYS ASP ALA THR GLY VAL ALA GLU THR HIS ALA VAL

VAL ARG ARG PHE LEU ALA GLN GLY GLU THR PHE THR GLN LEU GLU THR LEU LYS ILE GLU ASN GLU GLN MET LEU LEU ARG LEU LYS GLN GLU GLU LYS GLN ARG LEU GLN LYS LYS GLU LEU GLU ALA GLY LYS GLU ALA MET LEU LYS LYS TYR SER GLY GLU ALA MET LEU MET SER GLU GLN LYS LEU GLN LEU

GLN GLU ARG ILE LYS ALA GLU GLU GLN ARG ARG ALA ASP VAL GLN ASP ARG LEU GLU ARG THR MET ARG ALA MET HIS MET THR LYS GLU ALA LEU GLU HIS LEU ALA SER LYS LEU ASP HIS ILE THR VAL ALA ASP SER ALA PRO GLU PRO ARG ALA PRO GLU GLU ALA PRO PRO ARG HIS ILE ALA ASP ARG GLU

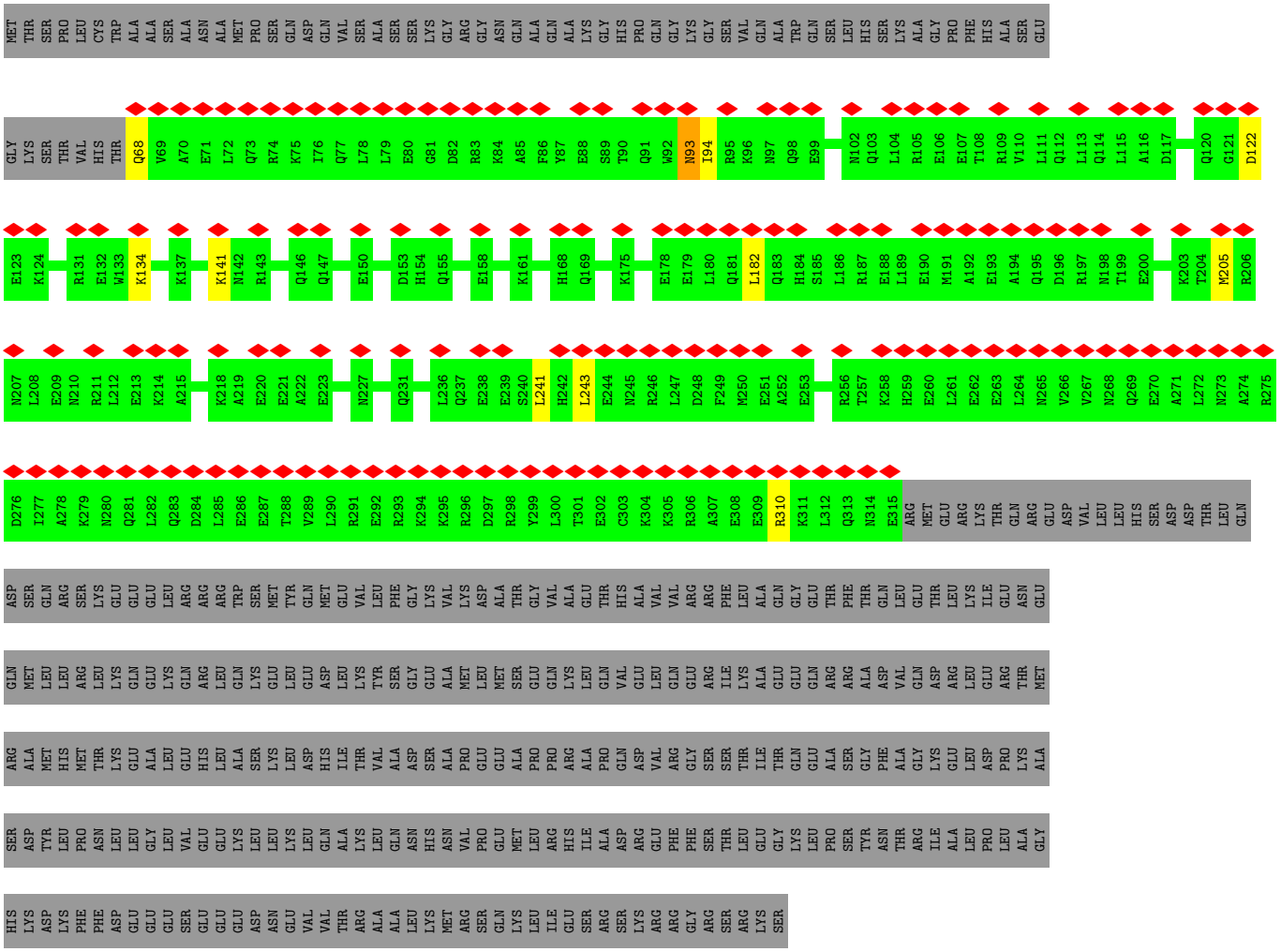
ARG GLY SER SER THR ILE THR GLN GLU ALA SER GLY PHE ALA GLY LYS GLU LEU ASP PRO LYS ALA SER ASP TYR LEU PRO ASN LEU LEU GLY LEU VAL GLU GLU LYS LEU LEU LYS LEU GLN ALA LYS LEU GLN LYS MET GLU GLU GLN LYS LYS LEU ALA ASP ARG GLU

PHE PHE SER THR LEU GLU GLY LYS LEU PRO SER TYR ASN THR ARG ILE ALA LEU PRO LEU ALA GLY HIS LYS ASP LYS PHE PHE ASP GLU GLU GLU SER GLU GLU GLU ASP ASN GLU VAL VAL THR ARG ALA ALA LEU LYS MET ARG SER GLN LYS LEU ILE GLU SER ARG SER LYS ARG

ARG GLY ARG SER ARG LYS SER

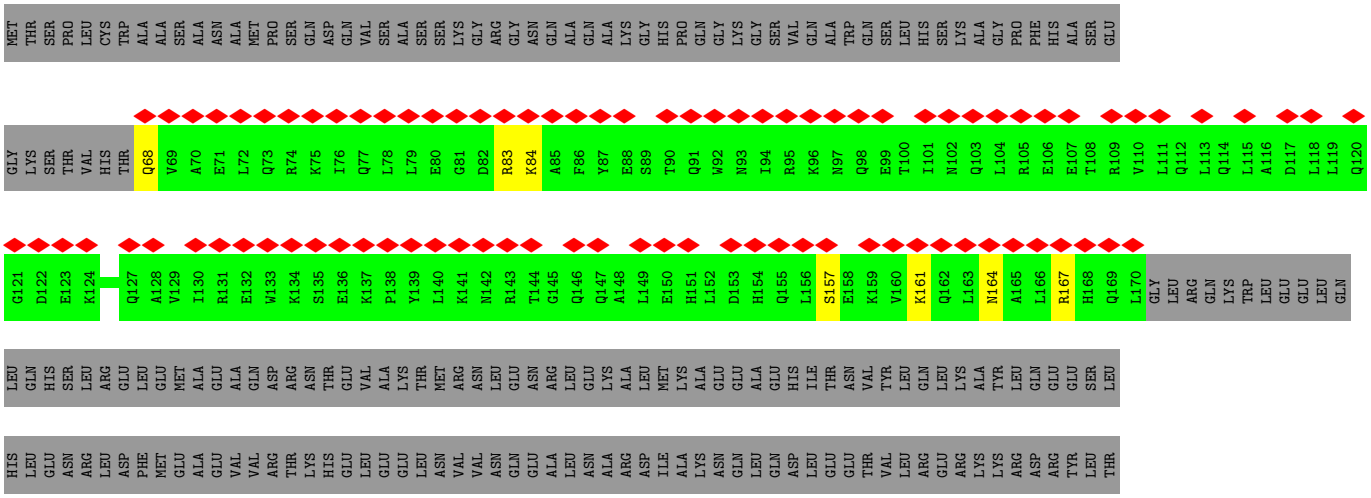
- Molecule 5: Outer dynein arm docking complex subunit 3

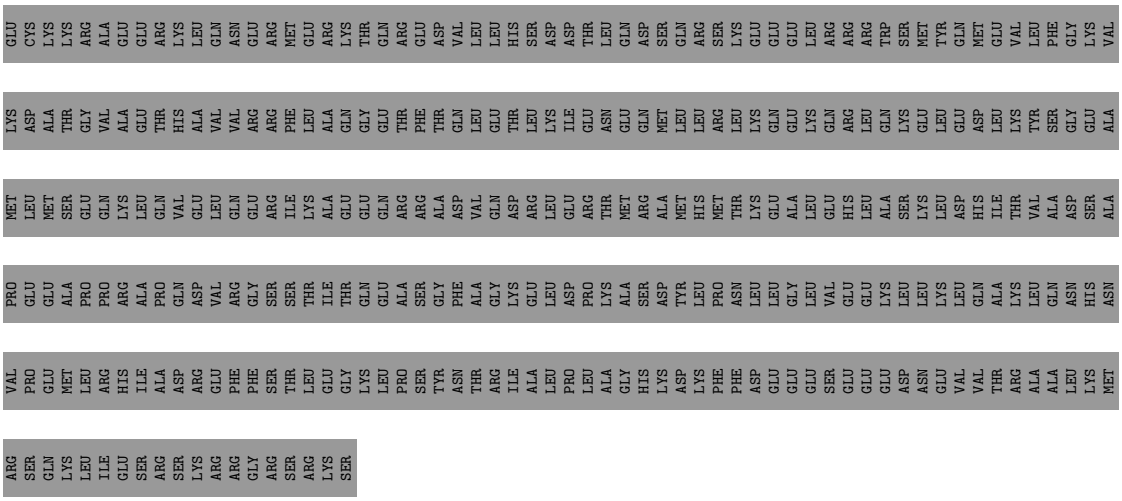
Chain 1M:




- Molecule 5: Outer dynein arm docking complex subunit 3

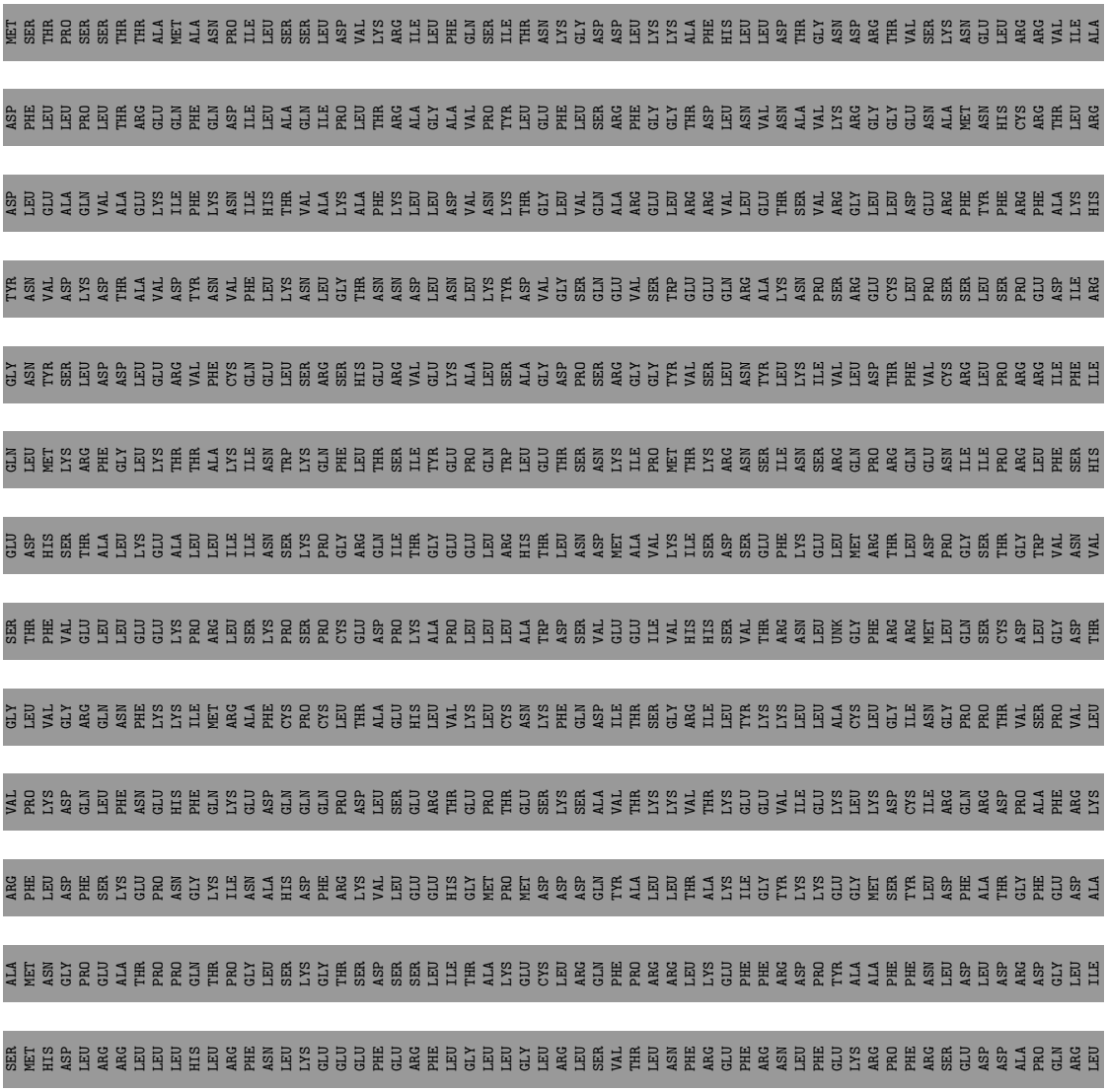
Chain 1N:

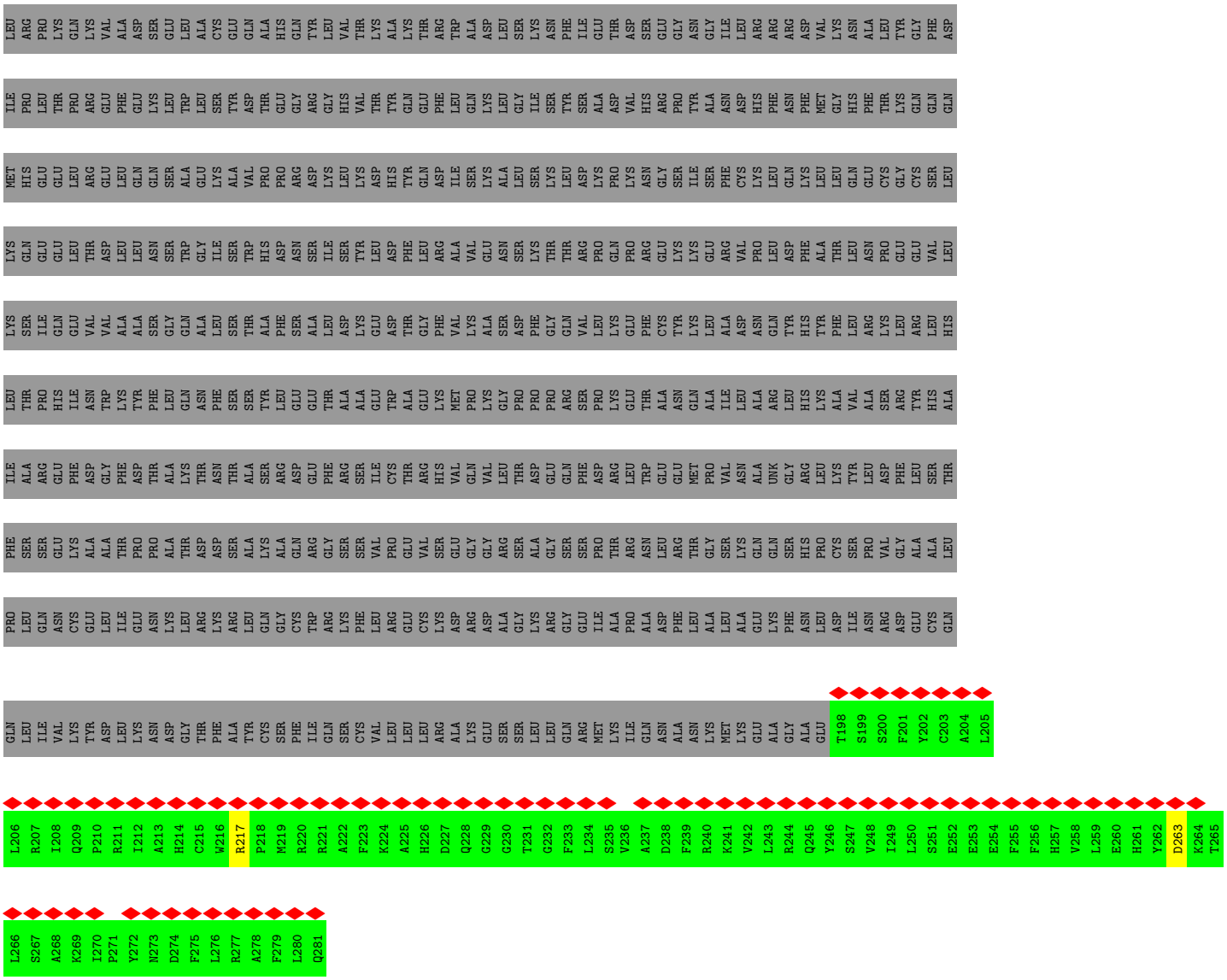





- Molecule 6: EFCAB6

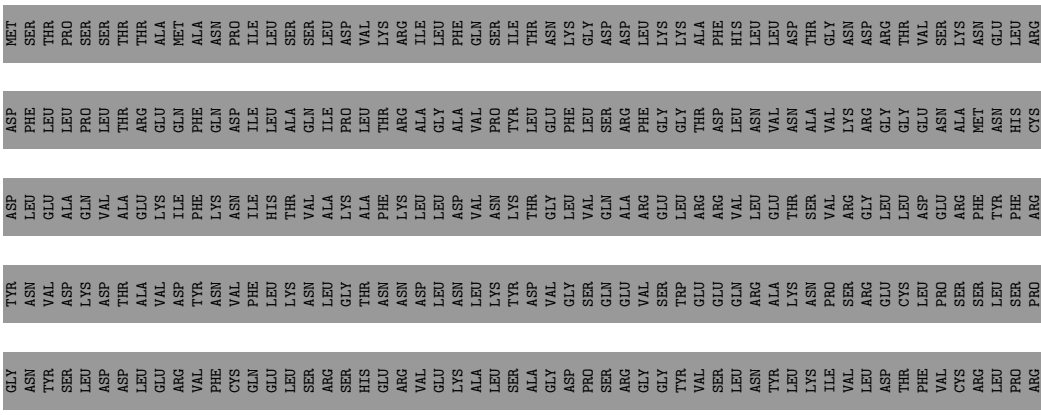
Chain 1P: 6% 6% 94%






- Molecule 6: EFCAB6

Chain 1Q: 6% 5% 94%



GLN LEU MET LYS ARG PHE GLY LEU LYS THR THR ALA LYS ILE ASN TRP LYS GLN PHE LEU THR SER ILE TYR GLU PRO GLN TRP LEU GLU THR SER ASN LYS ILE PRO MET THR LYS ARG ASN SER ILE ASN SER ARG GLN PRO ARG GLN GLU ASN ILE ILE PRO ARG LEU PHE SER HIS

GLU ASP HIS SER THR ALA LEU LYS GLU ALA LEU LEU ILE ILE ASN SER LYS PRO GLY ARG GLN ILE THR GLY GLU GLU LEU ARG HIS THR LEU ASN ASP MET ALA VAL LYS ILE SER ASP SER GLU PHE LYS GLU LEU MET ARG THR LEU ASP PRO GLY SER THR GLY TRP VAL ASN VAL

SER THR PHE VAL GLU LEU LEU GLU GLU LYS PRO ARG LEU SER LYS PRO SER PRO CYS GLU ASP PRO LYS ALA PRO LEU LEU LEU ALA TRP ASP SER VAL GLU GLU ILE VAL HIS HIS SER VAL THR ARG ASN LEU UNK GLY PHE ARG ARG MET LEU GLN SER CYS ASP LEU GLY ASP THR

GLY LEU VAL GLY ARG GLN ASN PHE LYS LYS ILE MET ARG ALA PHE CYS PRO CYS LEU THR ALA GLU HIS LEU VAL LYS LEU CYS ASN LYS PHE GLN ASP ILE THR SER GLY ARG ILE LEU TYR LYS LYS LEU LEU ALA CYS LEU GLY ILE ASN GLY PRO PRO THR VAL SER PRO VAL LEU

VAL PRO LYS ASP GLN LEU PHE ASN GLU HIS PHE GLN LYS GLU ASP GLN GLN PRO ASP LEU SER GLU ARG THR GLU PRO THR GLU SER LYS SER ALA VAL THR LYS LYS VAL THR LYS GLU GLU VAL ILE GLU LYS LEU LYS ASP CYS ILE ARG GLN ARG ASP PRO ALA PHE ARG LYS

ARG PHE LEU ASP PHE SER LYS GLU PRO ASN GLY LYS ILE ASN ALA HIS ASP PHE ARG LYS VAL LEU GLU GLU HIS GLY MET PRO MET ASP ASP GLN TYR ALA LEU LEU THR ALA LYS ILE GLY TYR LYS LYS GLU GLY MET SER TYR LEU ASP PHE ALA THR GLY PHE GLU ASP ALA

ALA MET ASN GLY PRO GLU ALA THR PRO PRO GLN THR PRO GLY LEU SER LYS GLY THR SER ASP SER SER LEU ILE THR ALA LYS GLU CYS LEU ARG GLN PHE PRO ARG ARG LEU LYS GLU PHE PHE ARG ASP PRO TYR ALA ALA PHE PHE ASN LEU ASP LEU ASP ARG ASP GLY LEU ILE

SER MET HIS ASP LEU ARG ARG LEU LEU LEU HIS LEU ARG PHE ASN LEU LYS GLU GLU GLU PHE GLU ARG PHE LEU GLY LEU LEU GLY LEU ARG LEU SER VAL THR LEU ASN PHE ARG GLU PHE ARG ASN LEU PHE GLU LYS ARG PRO PHE ARG SER GLU ASP ALA PRO GLN ARG LEU

LEU ARG PRO LYS GLN LYS VAL ALA ASP SER GLU LEU ALA CYS GLU GLN ALA HIS GLN TYR LEU VAL THR LYS ALA LYS THR ARG TRP ALA ASP LEU SER LYS ASN PHE ILE GLU THR ASP SER GLU GLY ASN GLY ILE LEU ARG ARG ARG ASP VAL LYS ASN ALA LEU TYR GLY PHE ASP

ILE PRO LEU THR PRO ARG GLU PHE GLU LYS LEU TRP LEU SER TYR ASP THR GLU GLY ARG GLY HIS VAL THR TYR GLN GLU PHE LEU GLN LYS LEU GLY ILE SER TYR SER ALA ASP VAL HIS ARG PRO TYR ALA ASN ASP HIS PHE ASN PHE MET GLY HIS PHE THR LYS GLN GLN

MET HIS GLU GLU LEU ARG GLU LEU GLN GLN SER ALA GLU LYS ALA VAL PRO PRO ARG ASP LYS LEU LYS ASP HIS TYR GLN ASP ILE SER LYS ALA LEU SER LYS LEU ASP LYS PRO LYS ASN GLY SER ILE SER PHE CYS LYS LEU GLN LYS LEU LEU GLN GLU CYS GLY CYS SER LEU

LYS GLN GLU GLU LEU THR ASP LEU LEU ASN SER SER TRP GLY ILE SER TRP HIS ASP ASN SER ILE SER TYR LEU ASP PHE LEU ARG ALA VAL GLU ASN SER LYS THR THR ARG PRO GLN PRO ARG GLU LYS LYS GLU ARG VAL PRO LEU ASP PHE ALA THR LEU ASN PRO GLU GLU VAL LEU

LYS SER ILE GLN GLU VAL VAL ALA ALA SER GLY GLN ALA LEU SER THR ALA PHE SER ALA LEU ASP LYS GLU ASP THR GLY PHE VAL LYS ALA SER ASP PHE GLY GLN VAL LEU LYS GLU PHE CYS TYR LYS LEU ALA ASP ASN GLN TYR HIS TYR PHE LEU ARG LYS LEU ARG LEU HIS

LEU THR PRO HIS ILE ASN TRP LYS TYR PHE LEU GLN ASN PHE SER SER TYR LEU GLU GLU THR ALA ALA GLU TRP ALA GLU LYS MET PRO LYS GLY PRO PRO PRO ARG SER PRO LYS GLU THR ALA ASN GLN ALA ILE LEU ALA ARG LEU HIS LYS ALA VAL ALA SER ARG TYR HIS ALA

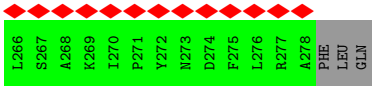
ILE ALA ARG GLU PHE ASP GLY PHE ASP THR ALA LYS THR ASN THR ALA SER ARG ASP GLU PHE ARG SER ILE CYS THR ARG HIS VAL GLN VAL LEU THR ASP GLU GLN PHE ASP ARG LEU TRP GLU GLU MET PRO VAL ASN ALA UNK GLY ARG LEU LYS TYR LEU ASP PHE LEU SER THR

PHE SER SER GLU LYS ALA ALA THR PRO PRO ALA THR ASP SER ALA LYS ALA GLN ARG GLY SER SER VAL PRO GLU VAL SER GLU GLY GLY ARG SER ALA GLY SER SER PRO THR ARG ASN LEU ARG THR GLY SER LYS GLN GLN SER HIS PRO CYS SER PRO VAL GLY ALA ALA LEU

PRO LEU GLN ASN CYS GLU LEU ILE GLU ASN LYS LEU ARG LYS ARG LEU GLN GLY CYS TRP ARG LYS PHE LEU ARG GLU CYS LYS ASP ARG ASP ALA GLY LYS ARG GLY GLU ILE ALA PRO ALA ASP PHE LEU ALA LEU ALA GLU LYS PHE ASN LEU ASP ILE ASN ARG ASP GLU CYS GLN

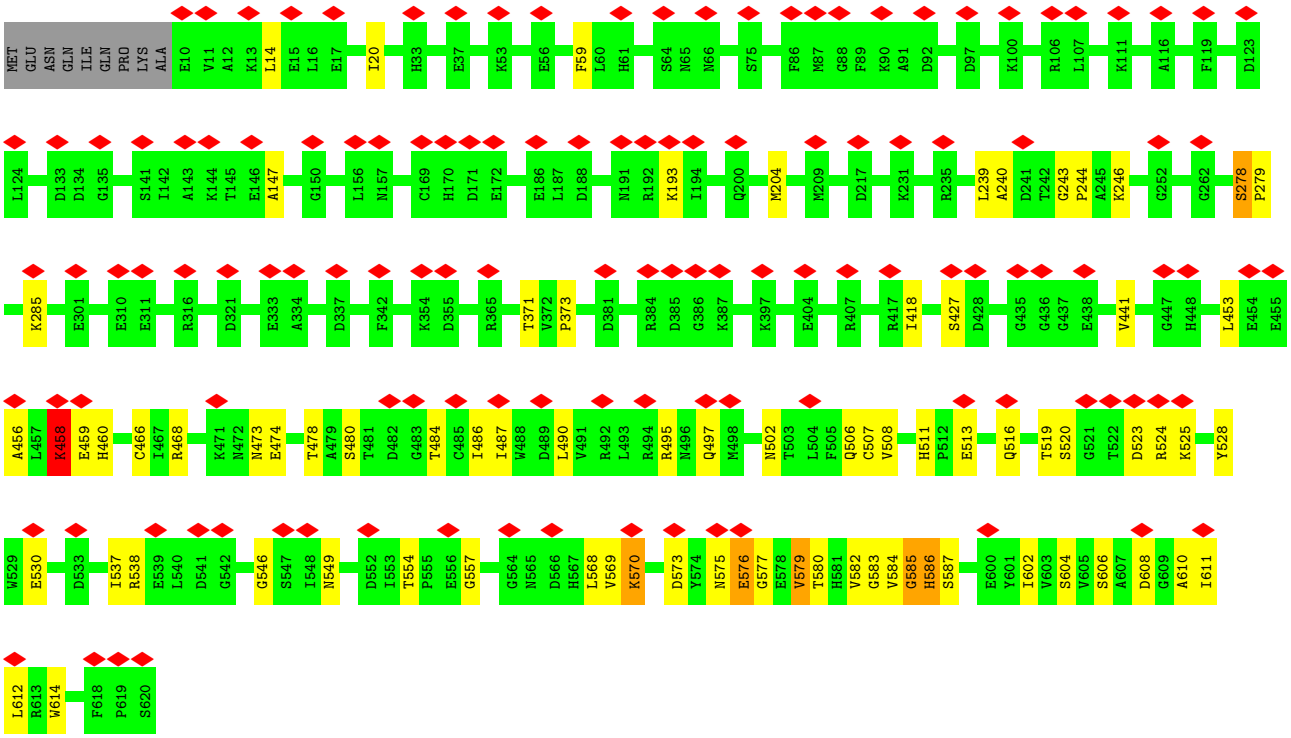
GLN LEU ILE VAL LYS TYR ASP LEU LYS ASN ASP GLY THR PHE ALA TYR CYS SER PHE ILE GLN SER CYS VAL LEU LEU LEU ARG ALA LYS GLU SER SER LEU LEU GLN ARG MET LYS ILE GLN ASN ALA ASN LYS MET LYS GLU ALA GLY ALA GLU T198 S199 S200 F201 Y202 C203 A204 L205

L206 R207 I208 Q209 P210 R211 I212 A213 H214 C215 W216 R217 P218 M219 R220 R221 A222 F223 K224 A225 H226 D227 Q228 G229 G230 T231 G232 F233 L234 S235 V236 A237 D238 F239 R240 K241 V242 L243 R244 Q245 Y246 S247 V248 I249 L250 S251 E252 E253 E254 F255 F256 H257 V258 L259 E260 H261 Y262 D263 K264 T265



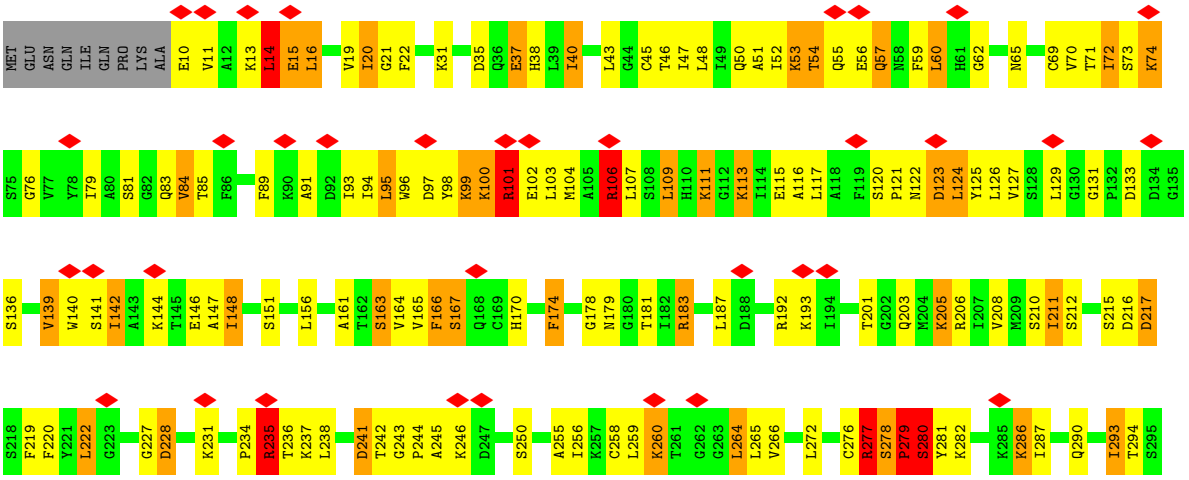

• Molecule 7: Cilia- and flagella-associated protein 52

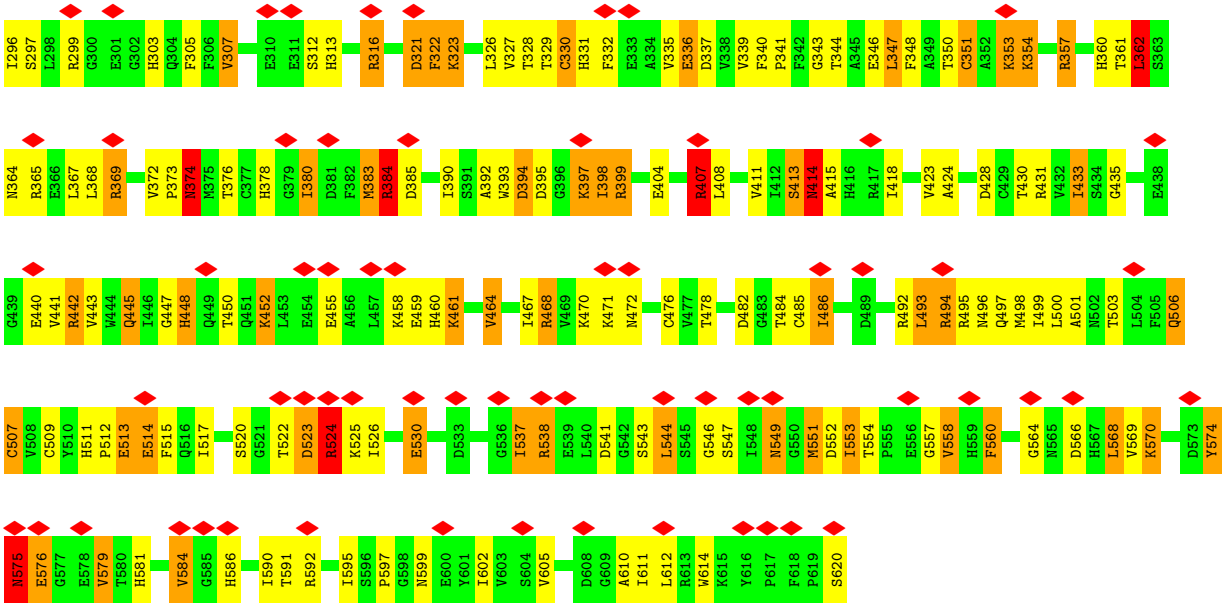
Chain 1S:




• Molecule 7: Cilia- and flagella-associated protein 52

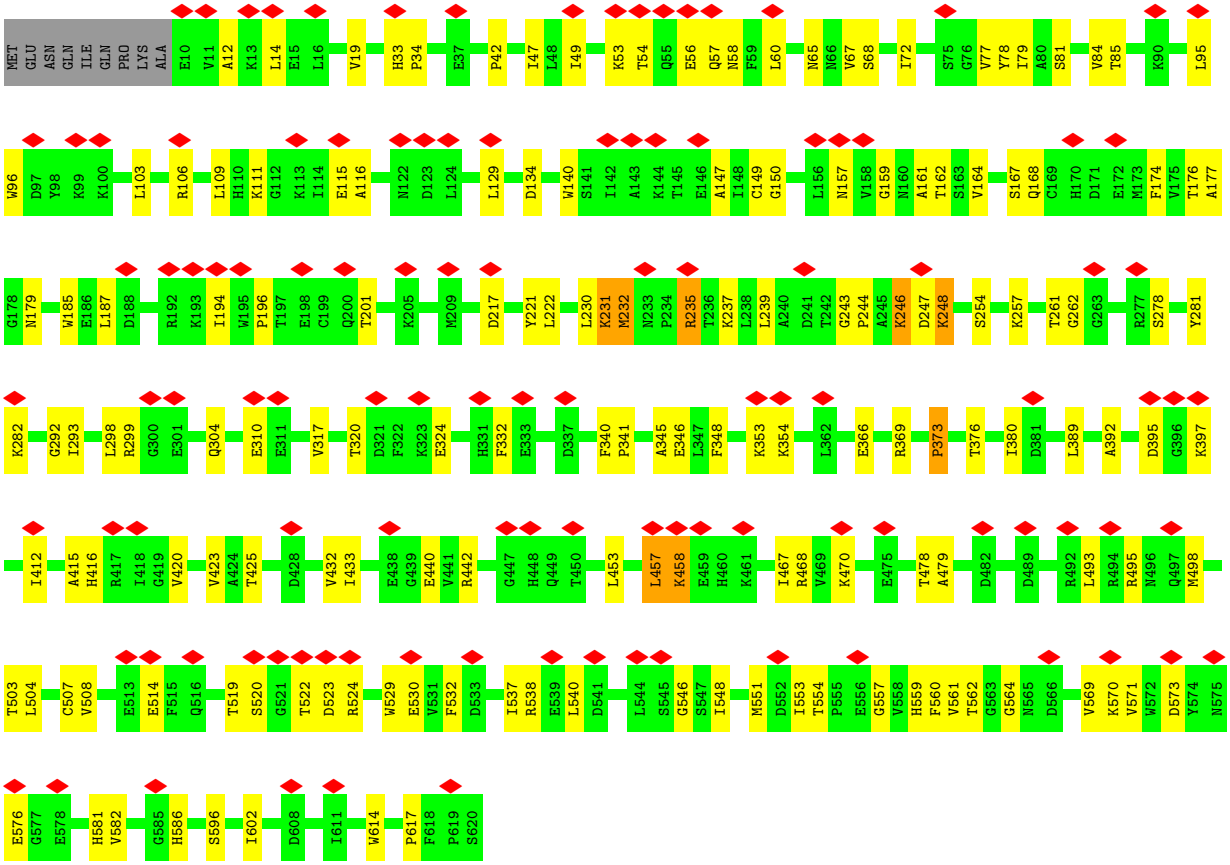
Chain 1T:





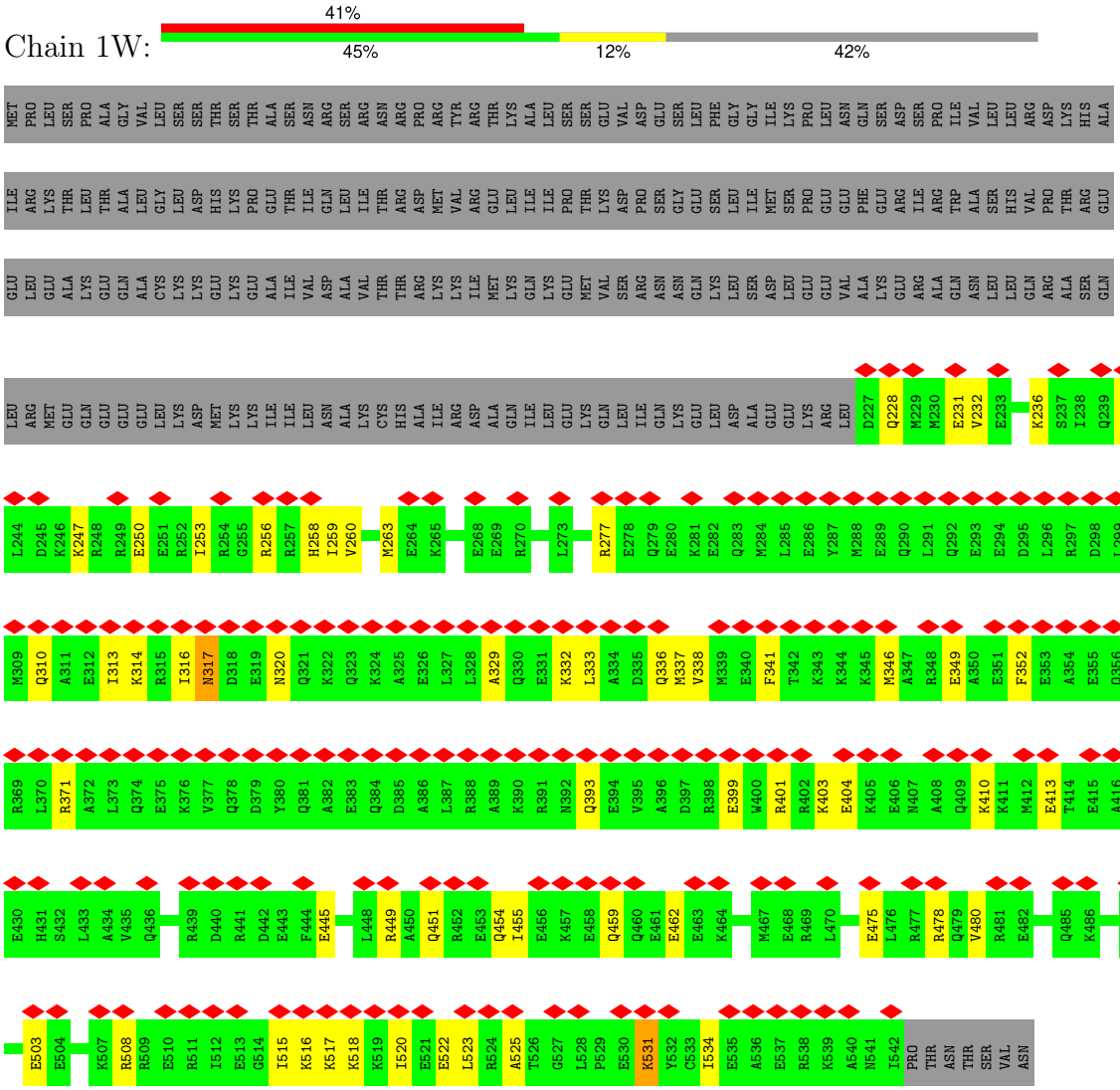

- Molecule 7: Cilia- and flagella-associated protein 52

Chain 1U:



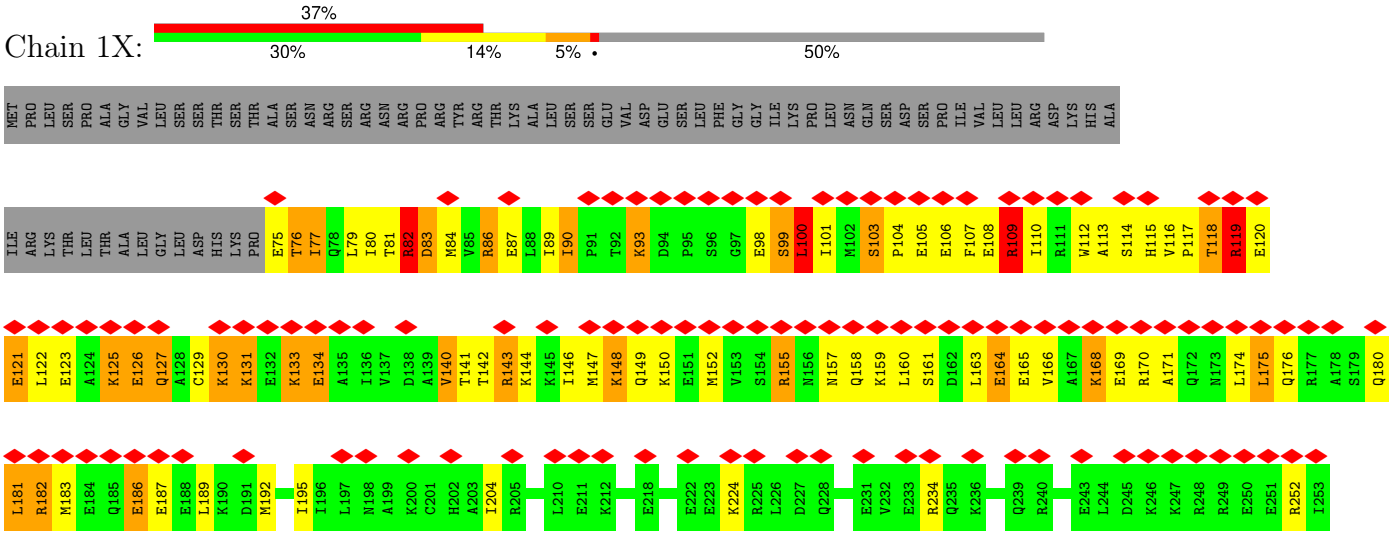

- Molecule 8: Cilia- and flagella-associated protein 45

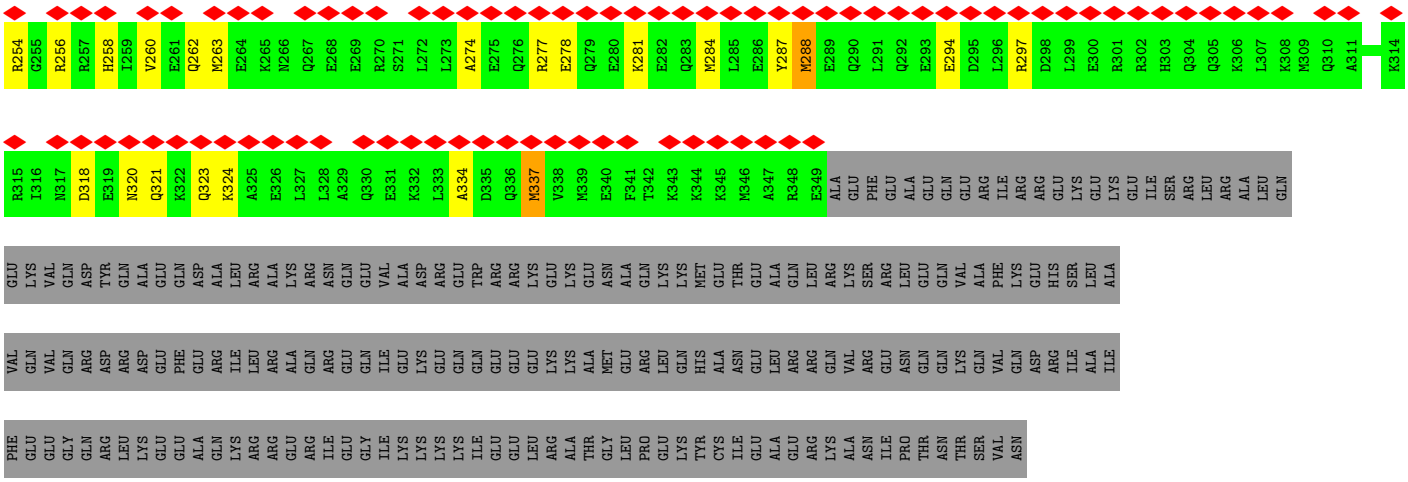
Chain 1W:




• Molecule 8: Cilia- and flagella-associated protein 45

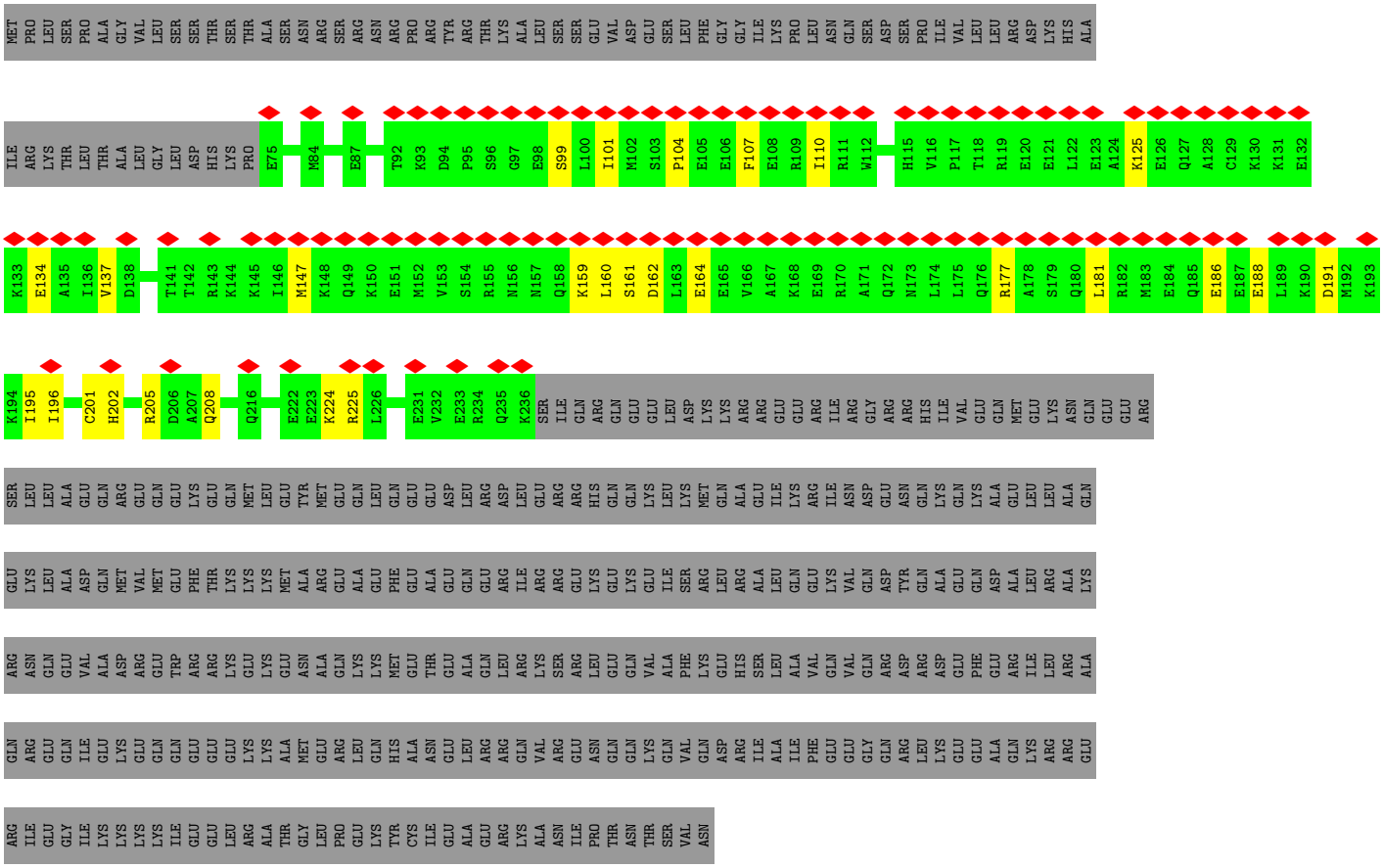
Chain 1X:






- Molecule 8: Cilia- and flagella-associated protein 45

Chain 1Y:




- Molecule 8: Cilia- and flagella-associated protein 45

Chain 1Z:

ILE ARG LYS THR LEU THR ALA LEU GLY LEU ASP HIS LYS PRO GLU THR ILE GLN LEU ILE THR ARG ASP MET VAL ARG GLU LEU ILE ILE PRO THR LYS ASP PRO SER GLY GLU SER LEU ILE MET SER PRO GLU GLU PHE GLU ARG ILE ARG TRP ALA SER HIS VAL PRO THR ARG GLU

GLU LEU GLU ALA LYS GLU GLN ALA CYS LYS LYS GLU LYS GLU ALA ILE VAL ASP ALA VAL THR THR ARG ASP LYS LYS ILE MET LYS GLN LYS GLU MET VAL SER ARG ASN ASN GLN LYS LEU SER ASP LEU GLU GLU VAL ALA LYS GLU ARG ALA GLN ASN LEU LEU GLN ARG ALA SER GLN

LEU ARG MET GLU GLN GLU GLU GLU LEU LYS LYS ASP MET LYS LYS ILE ILE LEU ASN ALA LYS CYS HIS ALA ILE ARG ASP ALA GLN ILE LEU GLU LYS GLN LYS GLU LEU ASP ALA GLU GLU LYS ARG LEU ASP GLN MET MET GLU VAL GLN GLN LYS SER ILE GLN ARG

GLN GLU GLU LEU ASP LYS LYS ARG ARG GLU GLU ARG ILE ARG GLY ARG ARG HIS ILE VAL GLU GLN MET GLU LYS ASN GLN GLU GLU ARG SER LEU LEU ALA GLU GLN ARG GLU GLN GLU LYS GLU GLN MET LEU GLU TYR MET GLU GLN LEU GLU GLU ARG GLN GLU

ARG ARG HIS GLN GLN LYS LEU LYS MET GLN ALA GLU ILE LYS ARG ILE ASN ASP GLU ASN GLN LYS GLN LYS ALA GLU LEU LEU ALA GLN GLU LYS LEU ALA ASP GLN MET VAL MET GLU PHE THR LYS LYS LYS MET A347 R348 E349 A350 E351 F352 E353 A354 E355 Q356 E357 R358 I359 R360

R361 E362 K363 E364 K365 E366 I367 S368 R369 L370 R371 A372 L373 Q374 E375 K376 V377 Q378 D379 Y380 Q381 A382 E383 Q384 D385 A386 L387 R388 A389 K390 R391 N392 Q393 E394 V395 A396 D397 R398 E399 W400 R401 R402 K403 E404 K405 E406 N407 A408 Q409 K410 K411 M412 E413 T414 E415 A416 Q417 L418 R419 K420

S421 R422 L423 E424 F428 H431 A434 V435 Q436 V437 Q438 R439 D440 R441 D442 E443 R446 I447 L448 R449 A450 Q451 R452 E453 Q454 I455 E456 K457 E458 Q459 Q460 E461 E462 E463 K464 E468 Q471 H472 A473 N474 E475 L476 R477 R478 Q479 V480 R481 E482 N483 Q484 Q485 K486 Q487

D490 R491 I492 A493 I494 F495 E496 E497 G498 Q499 R500 L501 K502 E503 E504 A505 Q506 K507 R508 R509 E510 R511 I512 E513 G514 I515 K516 K517 K518 K519 I520 E521 E522 L523 R524 A525 T526 G527 L528 P529 E530 K531 Y532 C533 I534 E535 A536 E537 R538 K539 A540 N541 I542 PRO THR ASN THR SER VAL ASN

- Molecule 9: Cilia and flagella associated protein 210

Chain 2B:

MET GLY THR SER GLU VAL VAL VAL ARG PHE GLY ARG ARG CYS GLY ARG ALA LYS GLU ILE THR GLU ILE LYS ASN TYR GLU GLU ASP GLN VAL LEU TYR PRO PRO LEU LEU PRO ASP LYS VAL ASP L43 R44 Q45 V46 T47 I48 I49 P50 H51 N52 E53 W54 E55 R56 I57 R58 D59 S60

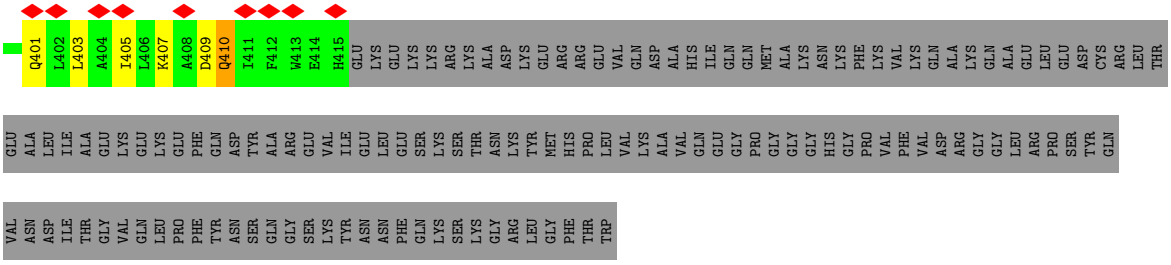
L61 D62 S63 L64 T65 R66 E67 A68 A69 H70 L71 R72 A73 K74 R75 K76 A77 K78 K79 E80 F83 R84 E87 V88 V89 K90 H91 W92 T93 N94 T95 Y96 M99 R100 K101 Q102 K103 L104 E105 A106 K107 K108 K109 R110 D111 E112 E113 I114 E115 A116 E117 R118 Q119 I120 L121 E124

E125 A126 I127 Y128 K129 Q130 G131 E132 R133 K134 K135 A136 I137 E138 Y139 Q142 Y143 E149 F154 H155 L160 S161 R162 V163 M164 K165 E166 R167 D168 A169 Q170 I171 Q174 K175 S176 K177 I178 K179 S180 D181 K182 K183 W184 E185 E186 Q187 L188 K189 L190 E193 K194 G195 F196 K197

E201 K202 A203 E204 K205 Q206 R207 R208 D209 R210 L213 A214 K215 D216 H217 L218 K219 Q220 I221 K222 E223 E228 V229 R230 R231 R232 E235 E236 K237 E241 I242 K243 Q244 Q245 N246 L247 L248 Y249 E250 I251 E252 M253 K254 K255 K256 L257 G258 M259 K260 K261 E262 K263 I264 N265 E266

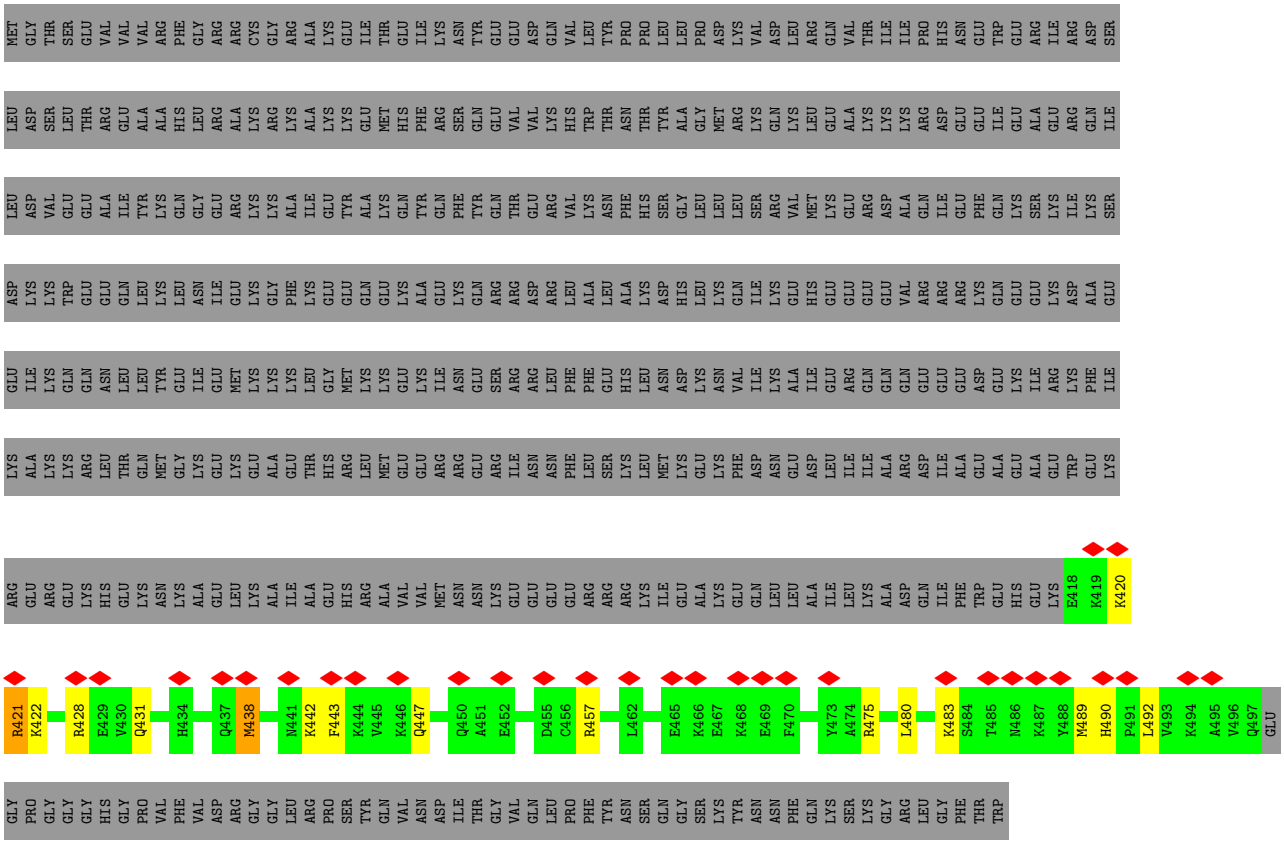
S267 R268 R269 L270 F271 F272 E273 H274 L275 N276 D277 K278 K282 A283 I284 E285 R286 Q287 Q288 Q289 E290 E291 E292 D293 E294 K295 I296 R297 K298 F299 I300 K301 A302 K303 K304 R305 Q308 K311 E312 K313 E314 A315 E316 T317 H318 R319 L320 M321 E322 E323 R324 R325 E326 R327 I328 N329 N330

F331 L332 S333 K334 L335 M336 K337 E338 K339 F340 D341 N342 E343 D344 L345 I346 I347 A348 R349 D350 E353 A354 E355 A356 E357 W358 E359 K360 R361 E362 R363 E364 K365 H366 E367 E372 L373 K374 A375 I376 A377 E378 H379 R380 N386 K387 E388 E389 E390 E391 R392 R393 R394 K395 I396 E397 A398



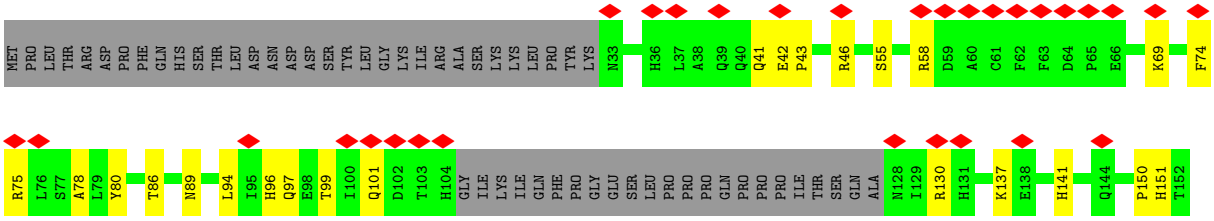

• Molecule 9: Cilia and flagella associated protein 210

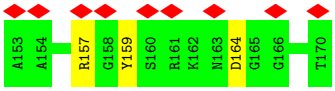
Chain 2C:




• Molecule 10: Cilia and flagella associated protein 276

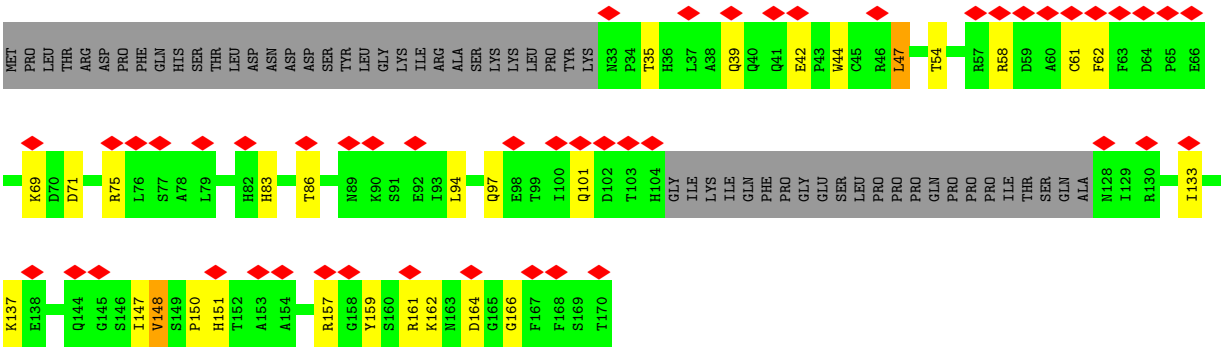
Chain 2E:





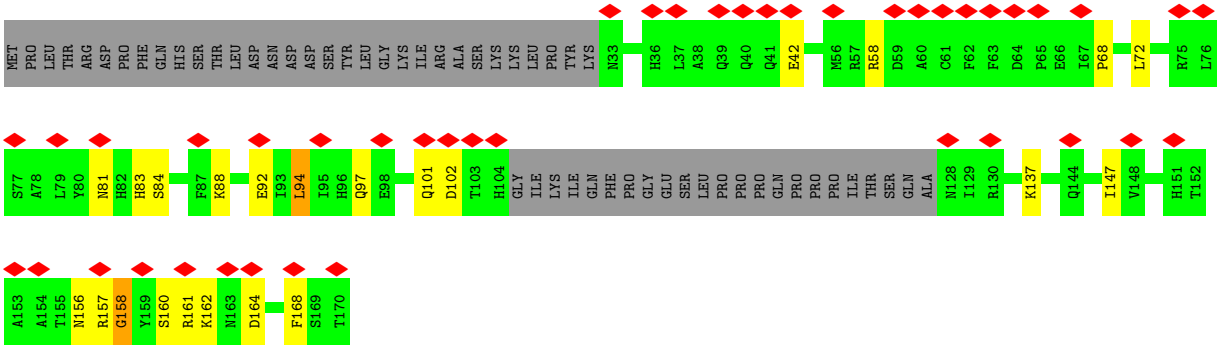

- Molecule 10: Cilia and flagella associated protein 276

Chain 2F:



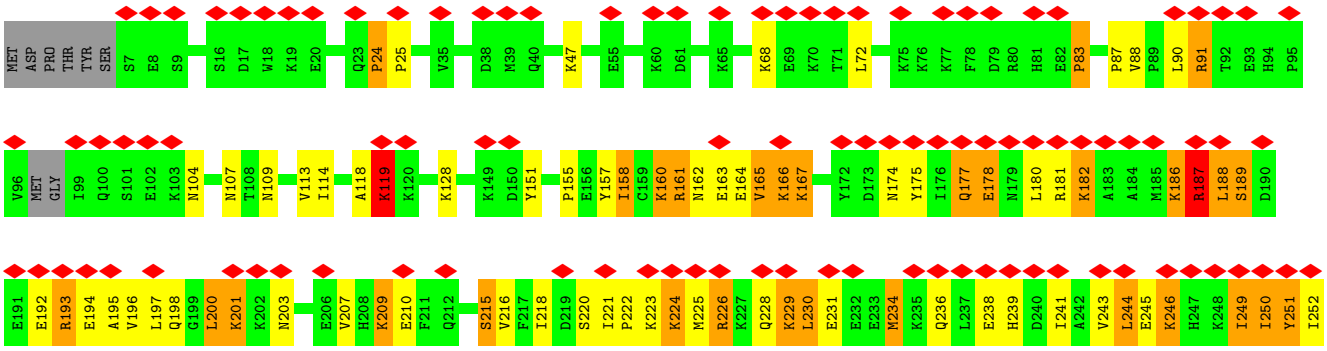

- Molecule 10: Cilia and flagella associated protein 276

Chain 2G:



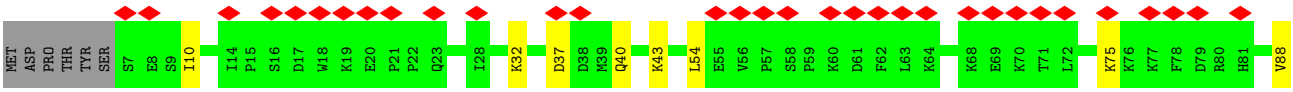

- Molecule 11: Enkurin

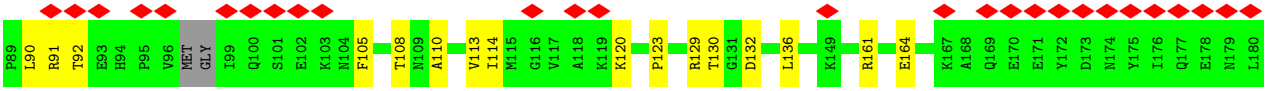
Chain 2I:

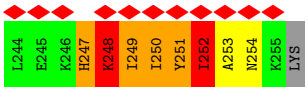


- Molecule 11: Enkurin

Chain 2J:

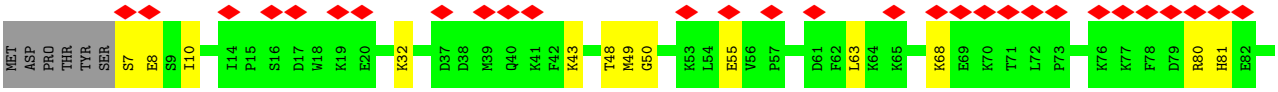


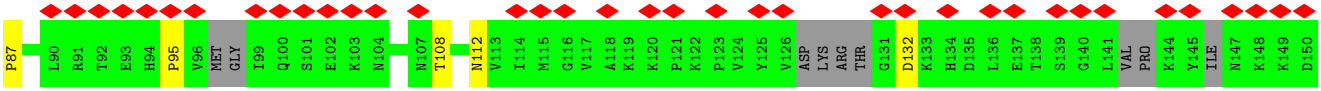



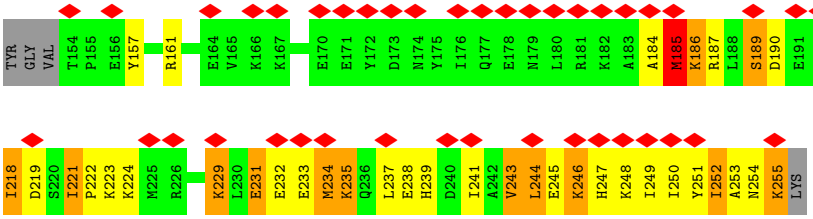



- Molecule 11: Enkurin

Chain 2K:



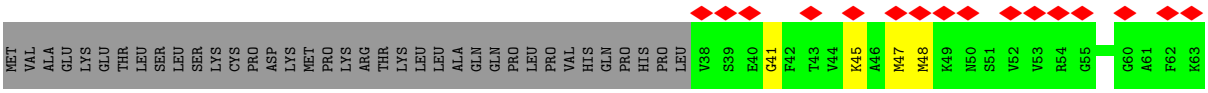



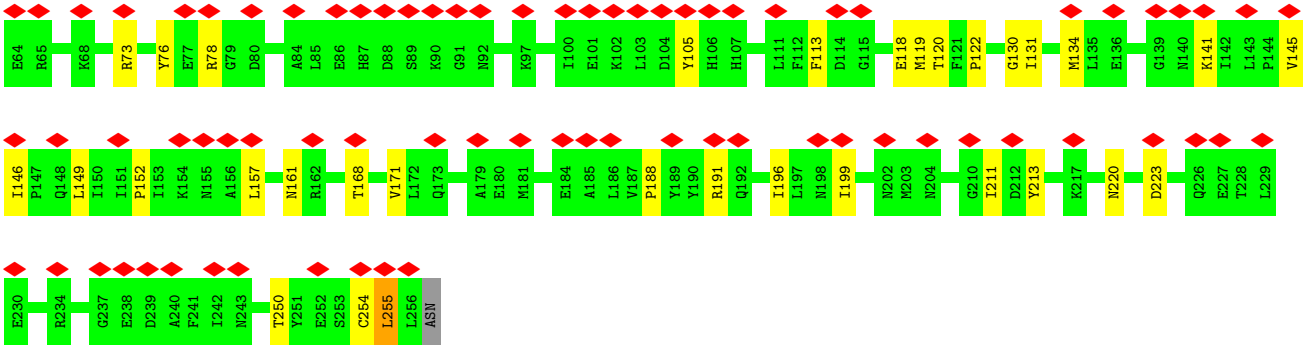




- Molecule 12: Parkin coregulated

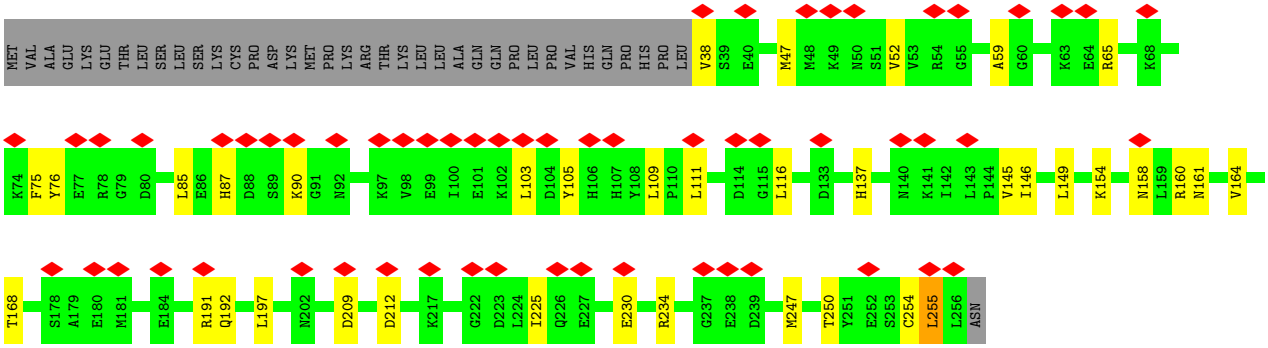
Chain 2M:





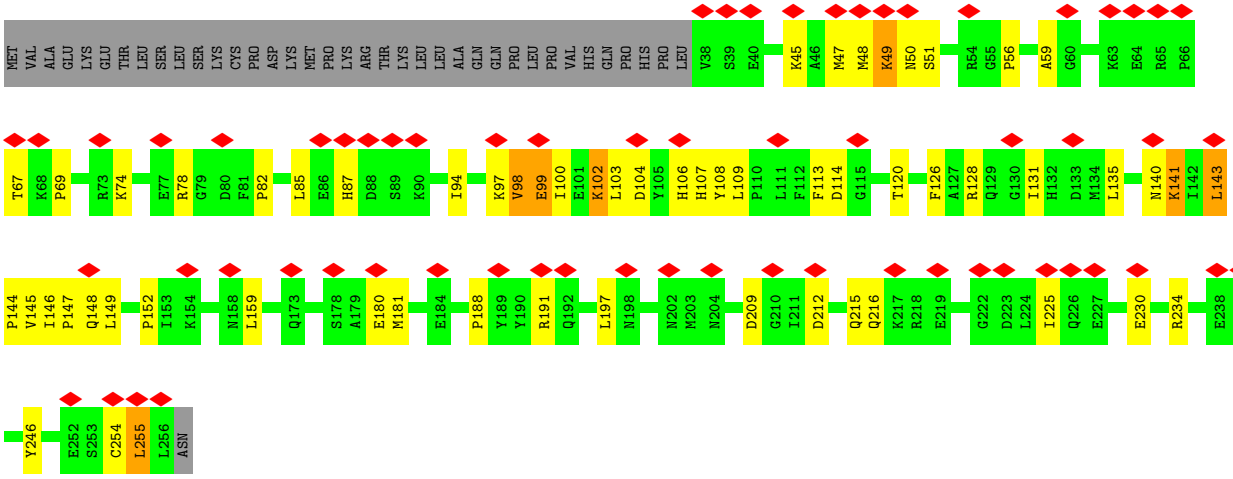

- Molecule 12: Parkin coregulated

Chain 2N:



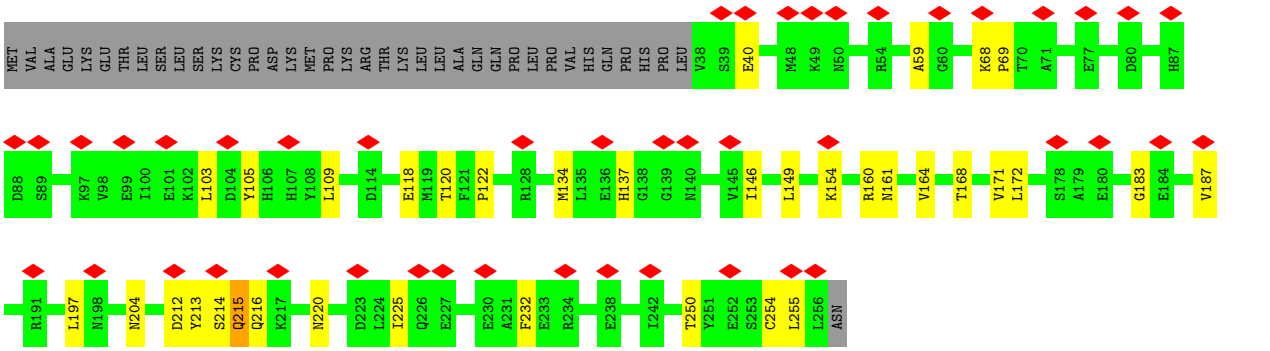

- Molecule 12: Parkin coregulated

Chain 2O:



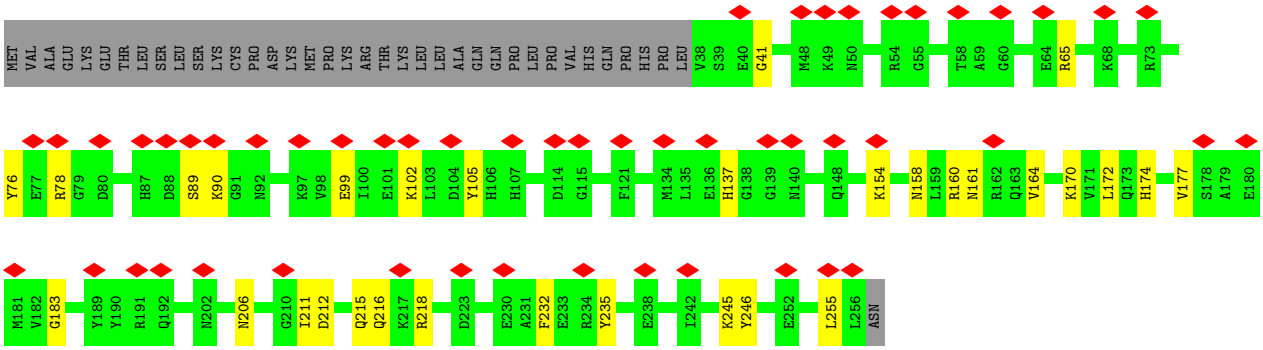

- Molecule 12: Parkin coregulated

Chain 2P:




• Molecule 12: Parkin coregulated

Chain 2Q:

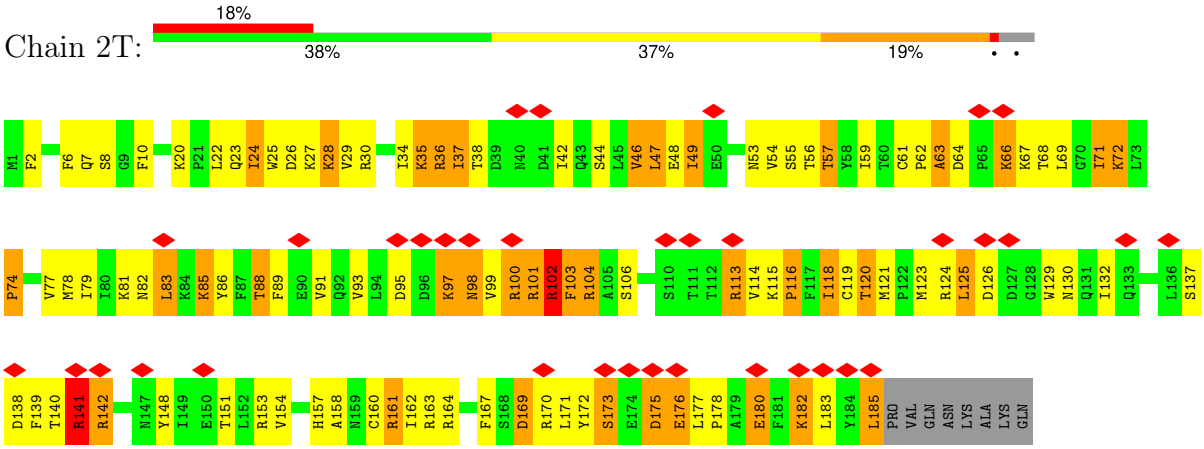



• Molecule 12: Parkin coregulated

Chain 2R:

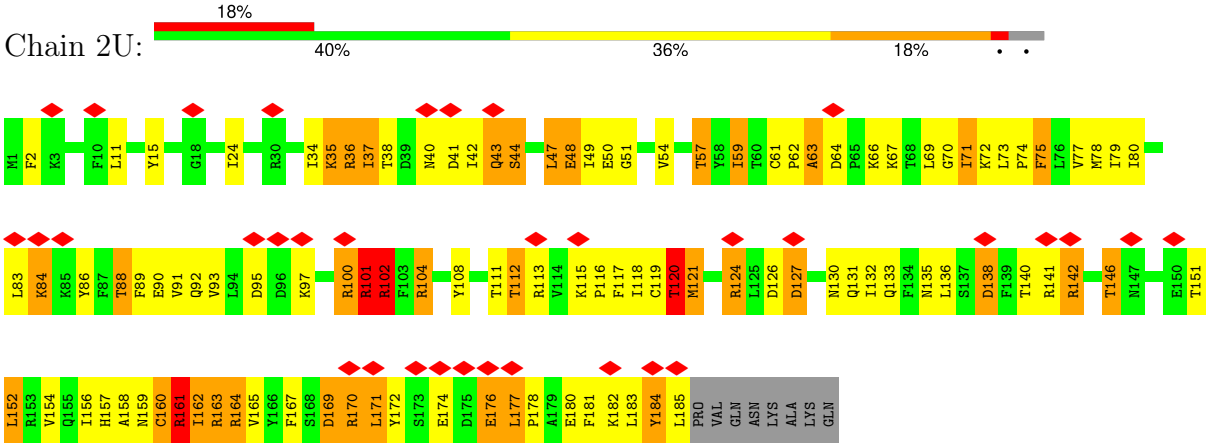
• Molecule 13: Cilia- and flagella-associated protein 20

Chain 2T:



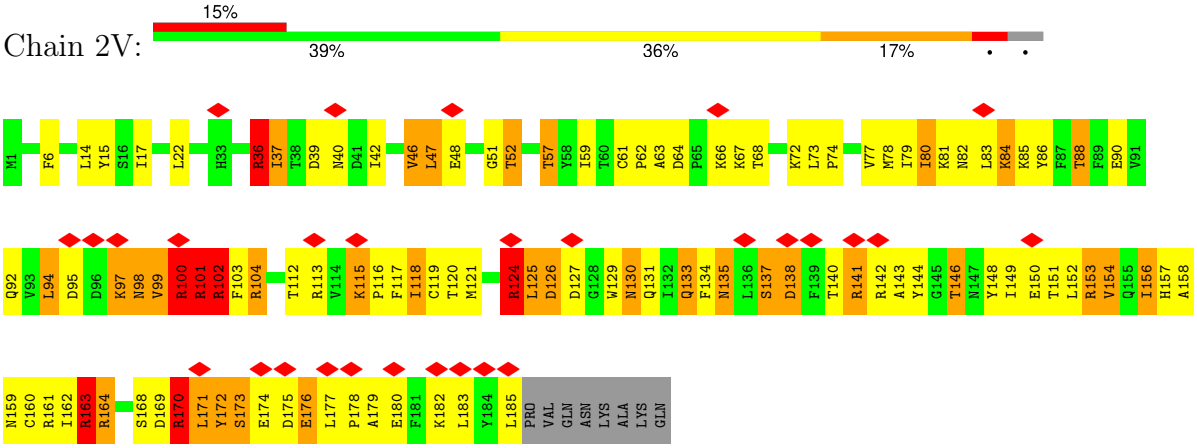

• Molecule 13: Cilia- and flagella-associated protein 20

Chain 2U:



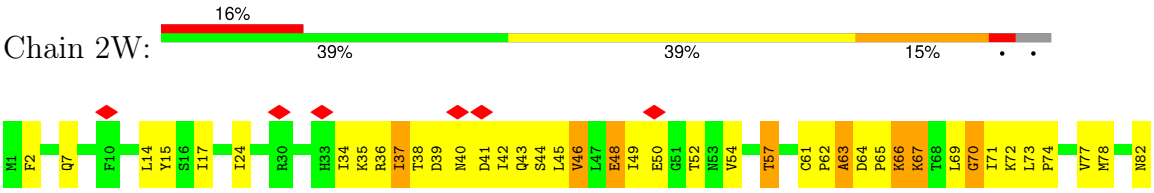

• Molecule 13: Cilia- and flagella-associated protein 20

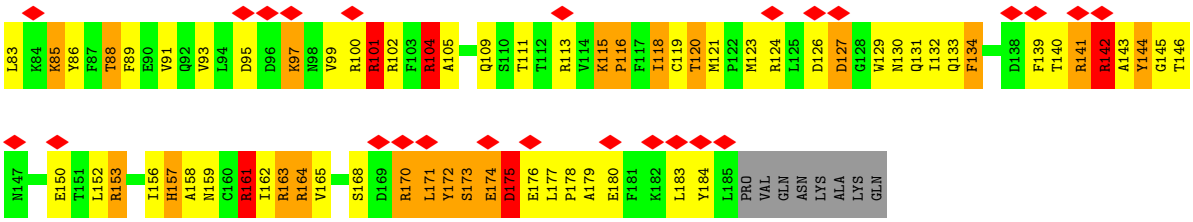
Chain 2V:




• Molecule 13: Cilia- and flagella-associated protein 20

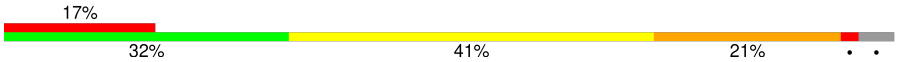
Chain 2W:

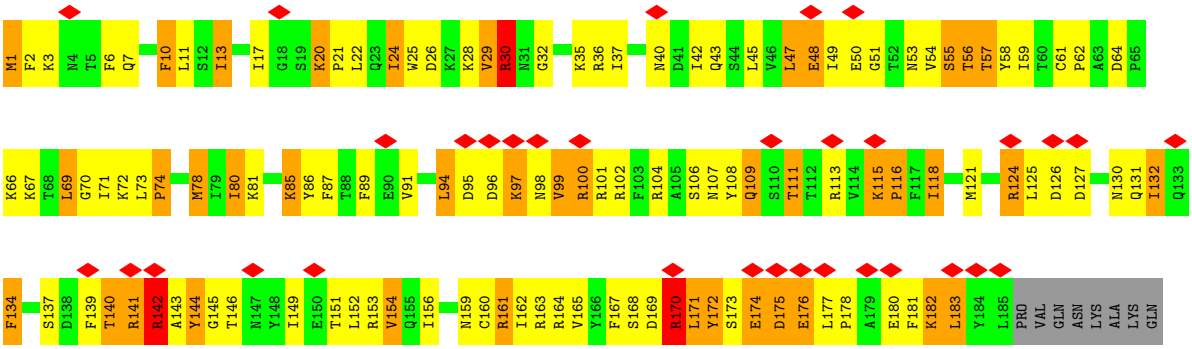





- Molecule 13: Cilia- and flagella-associated protein 20

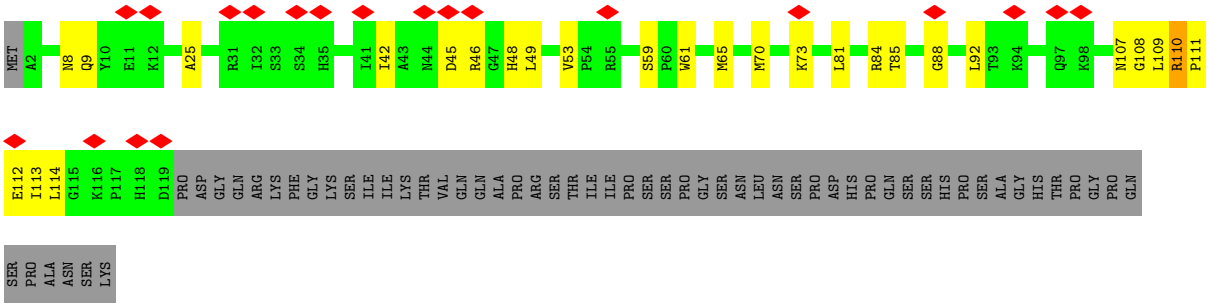
Chain 2X:



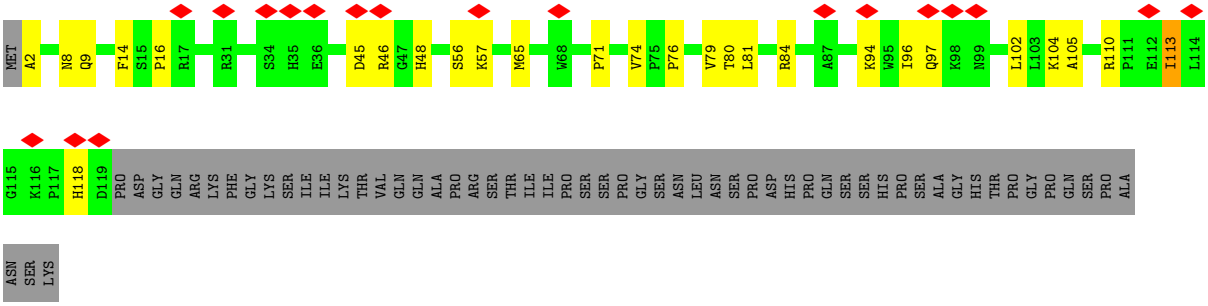

- Molecule 14: Protein Flattop

Chain 3A:



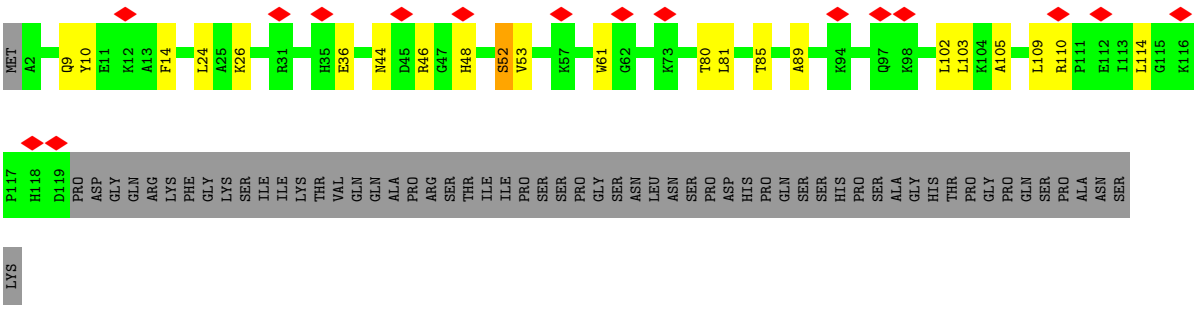

- Molecule 14: Protein Flattop

Chain 3B:



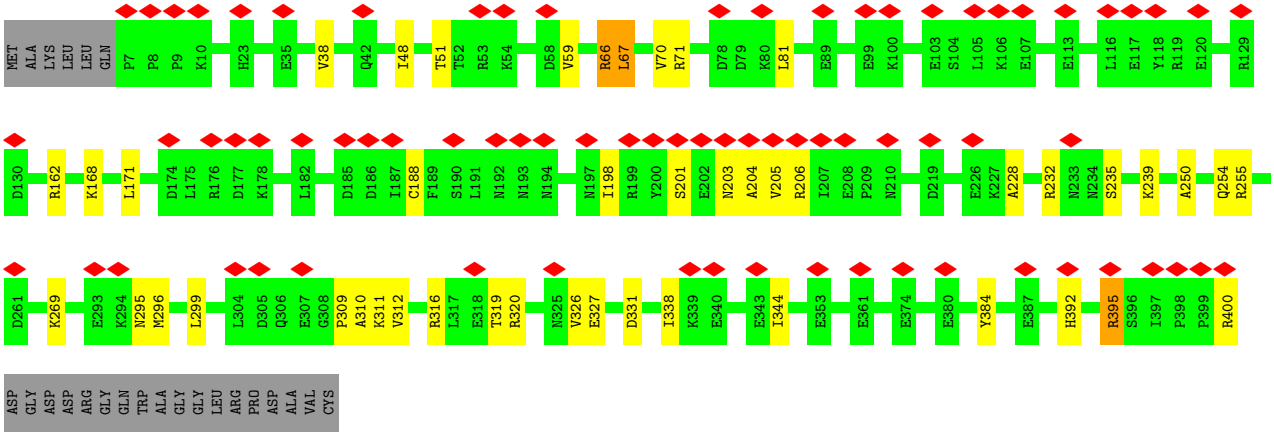

- Molecule 14: Protein Flattop

Chain 3C:



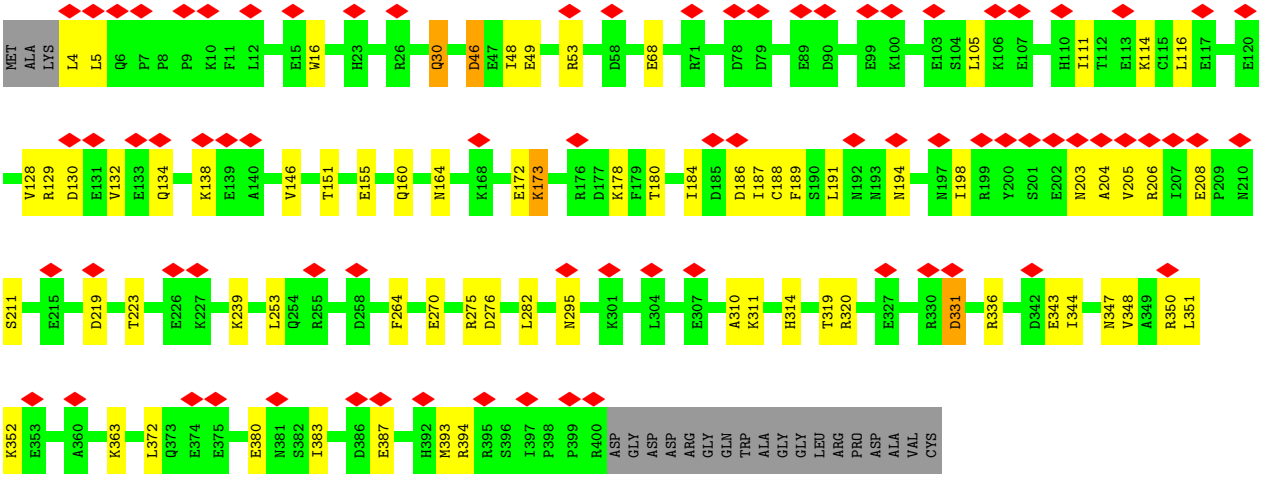

- Molecule 15: Tektin

Chain 3E:



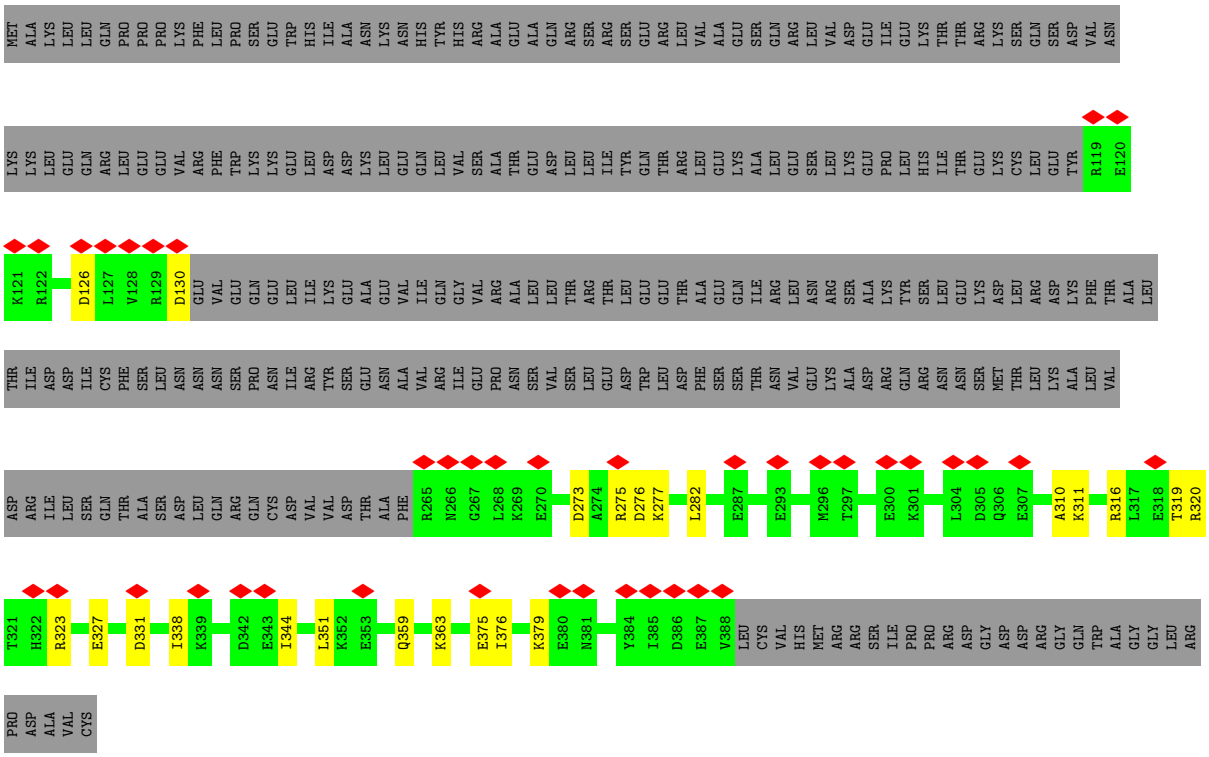

- Molecule 15: Tektin

Chain 3F:



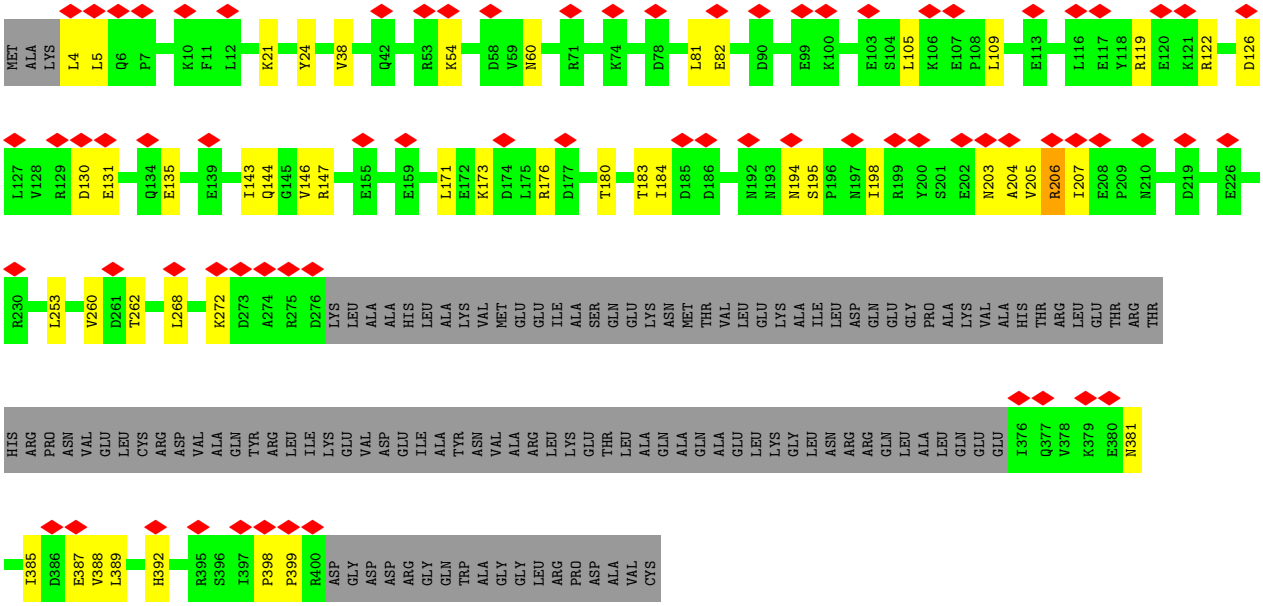

- Molecule 15: Tektin

Chain 3G:



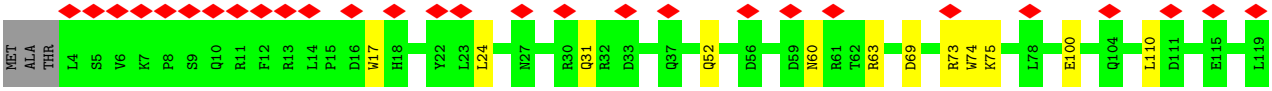

- Molecule 15: Tektin

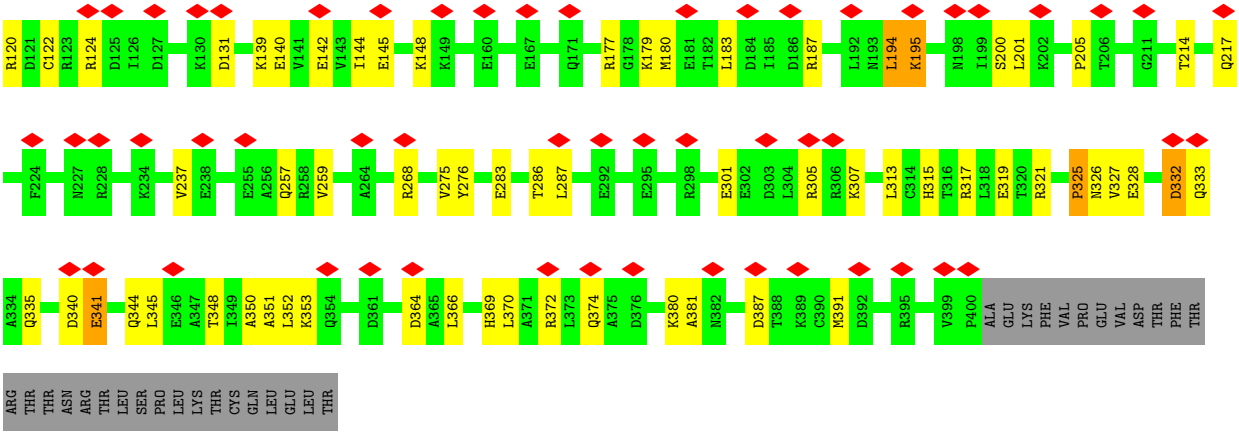
Chain 3H:




- Molecule 16: Tektin

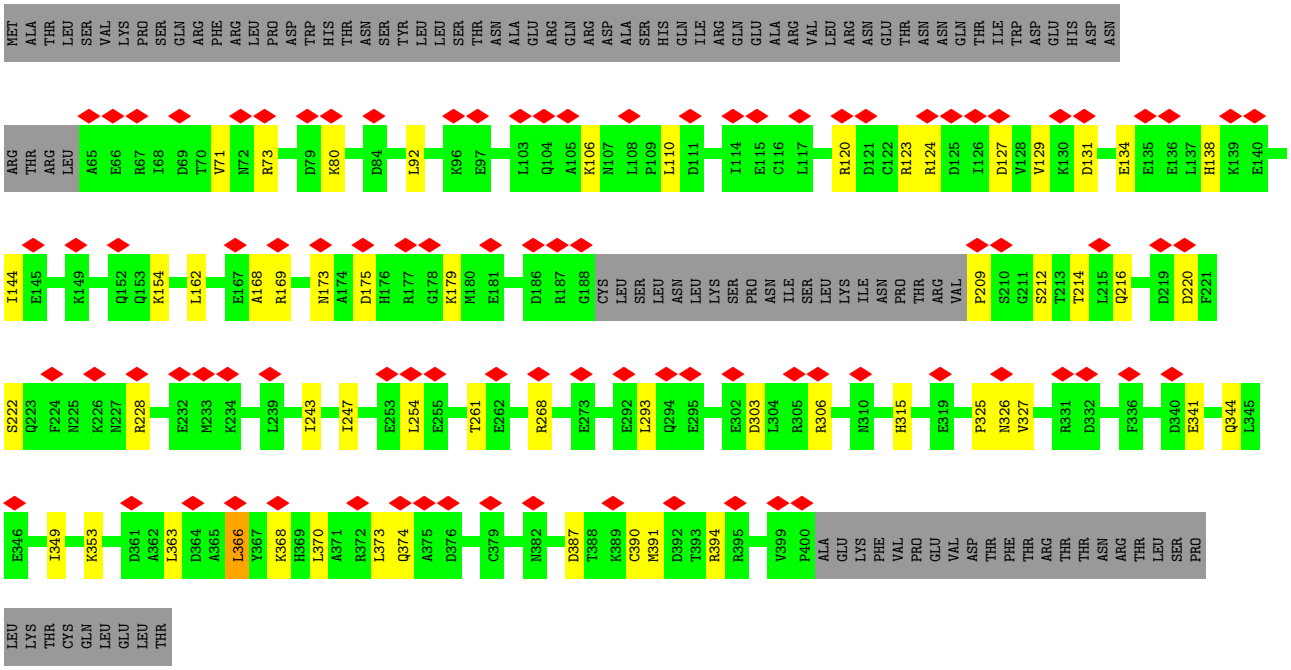
Chain 3J:





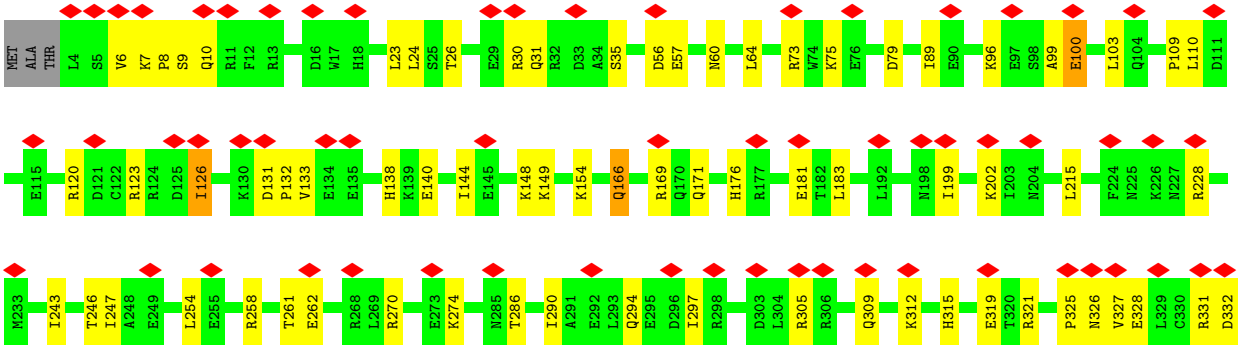

- Molecule 16: Tektin

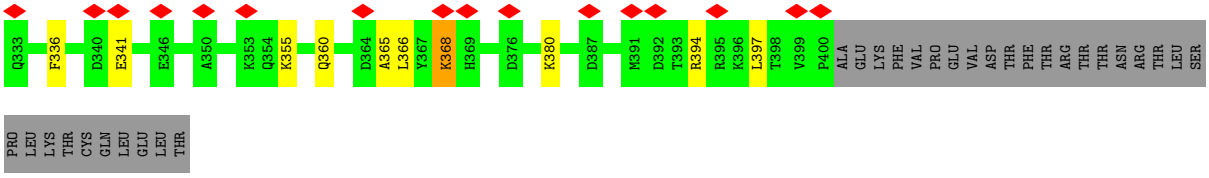
Chain 3K:




- Molecule 16: Tektin

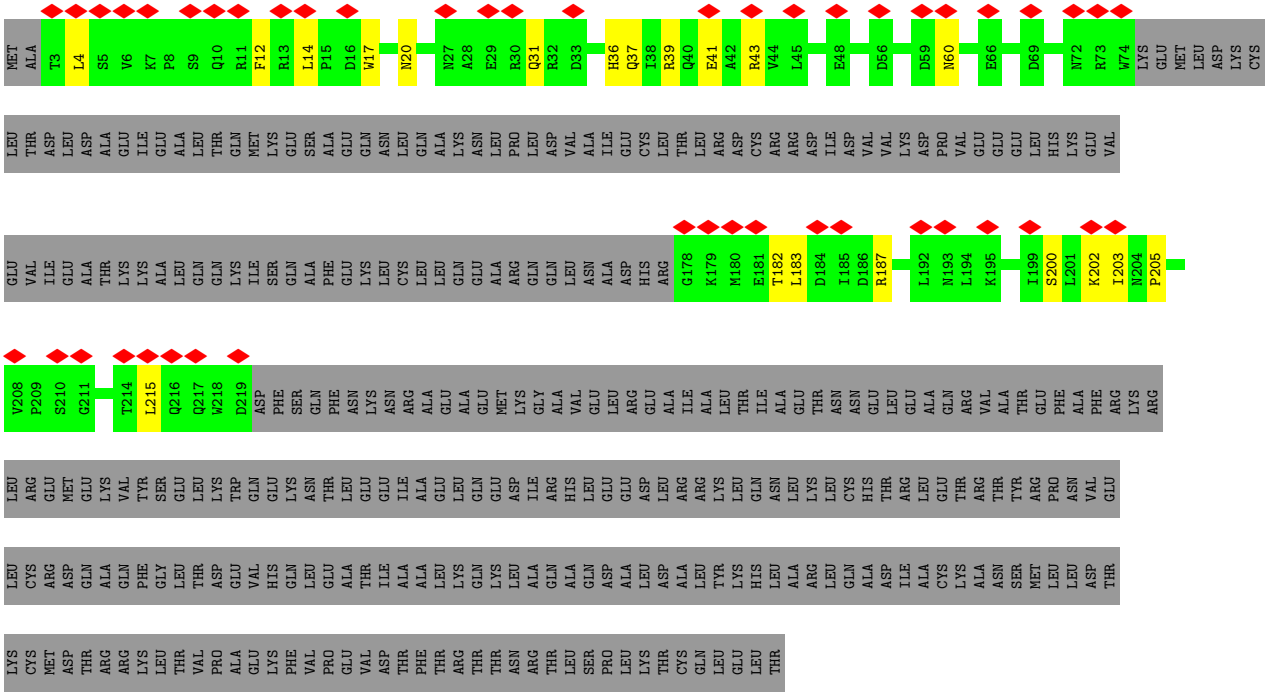
Chain 3L:





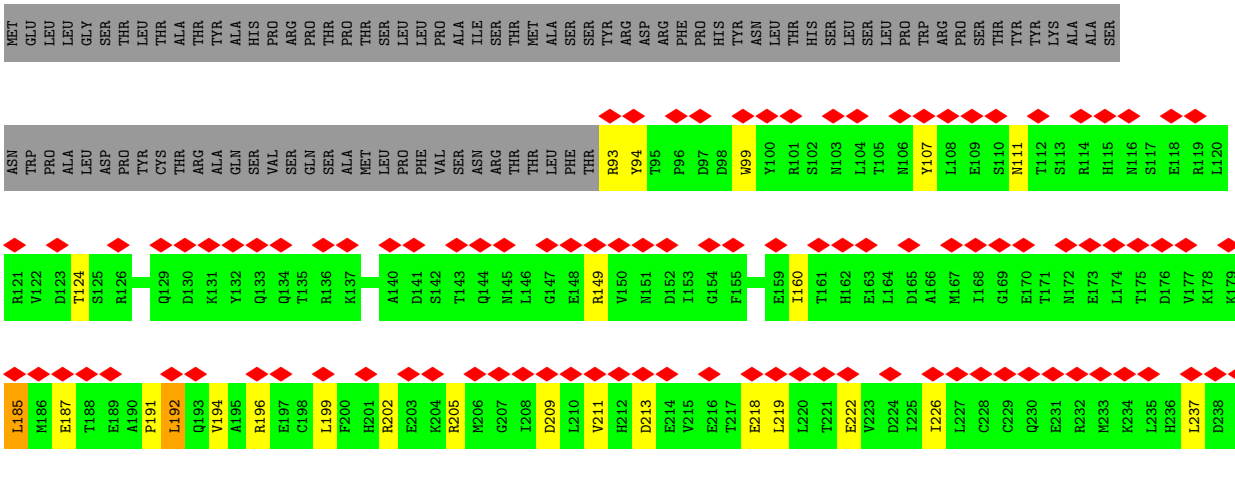

- Molecule 16: Tektin

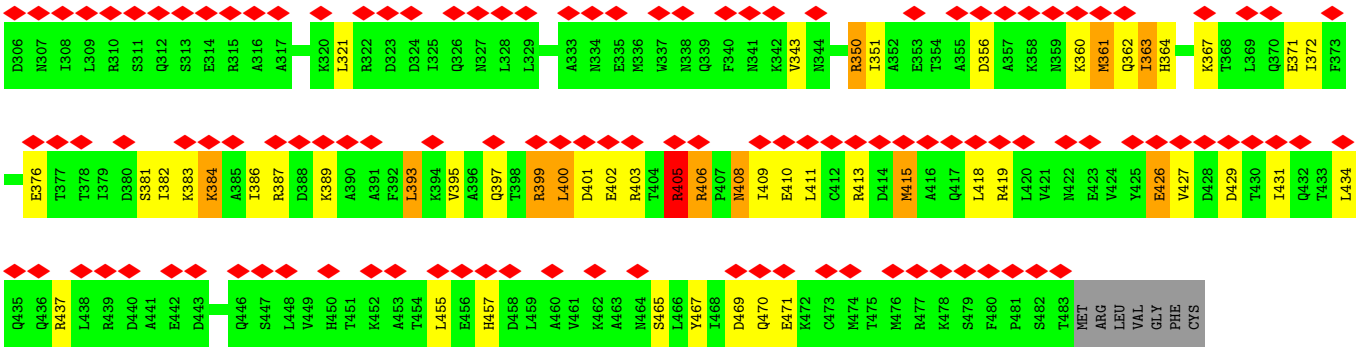
Chain 3M:




- Molecule 17: Tektin

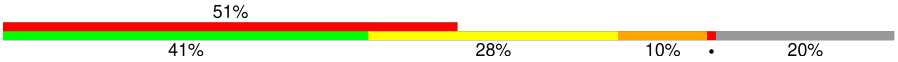
Chain 3O:

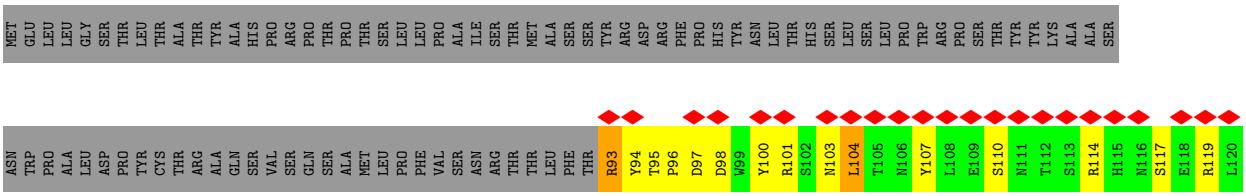





- Molecule 17: Tektin

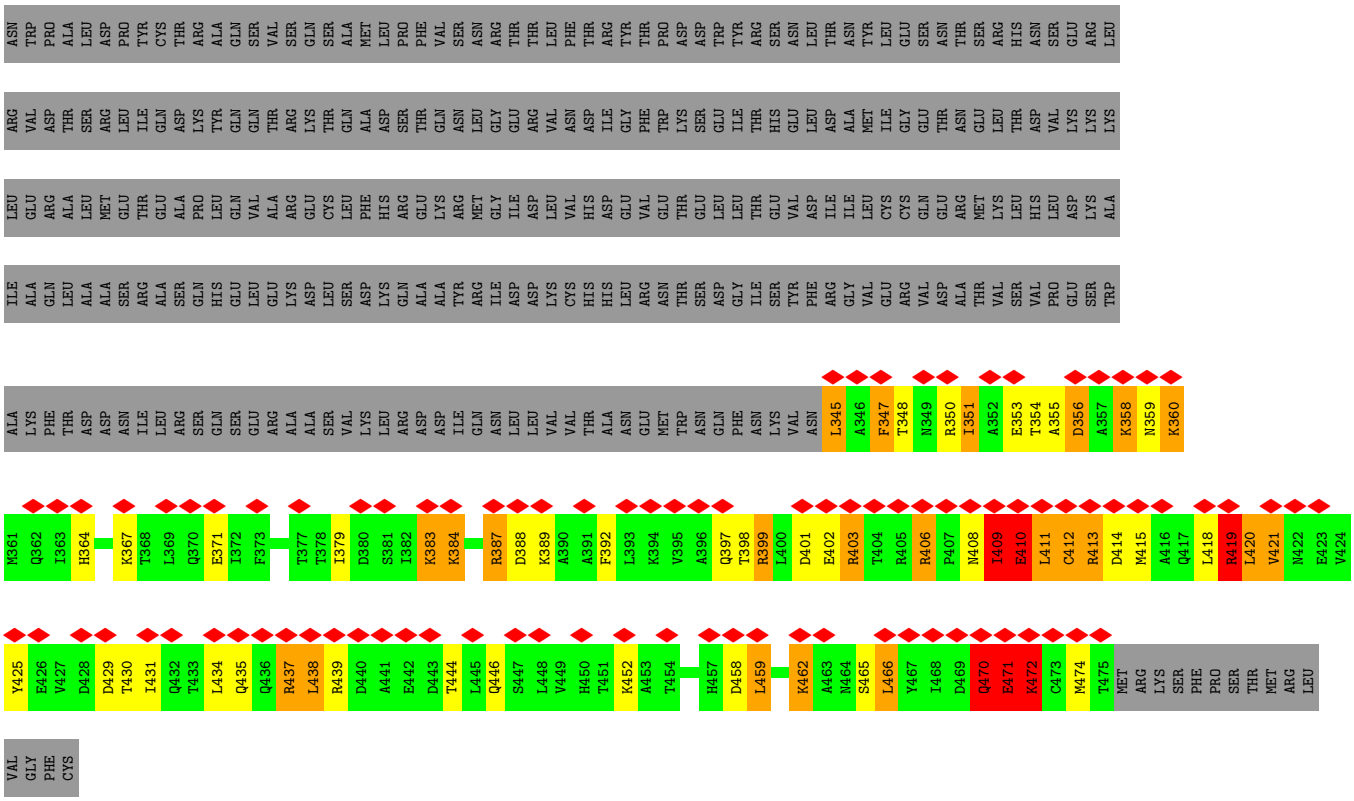
Chain 3P:



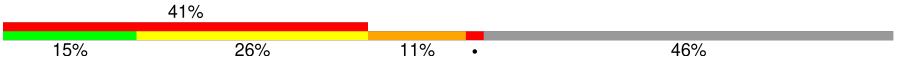

- Molecule 17: Tektin

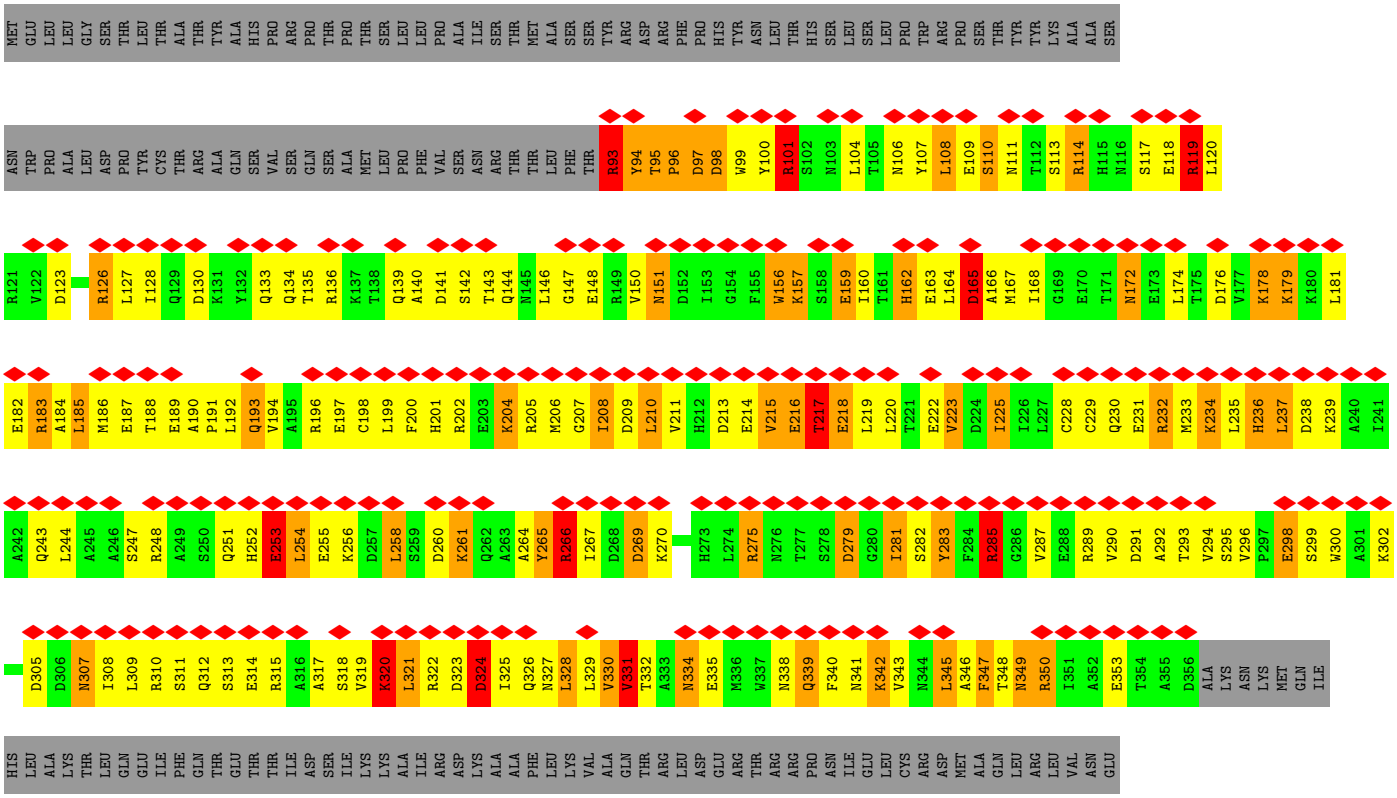
Chain 3Q:

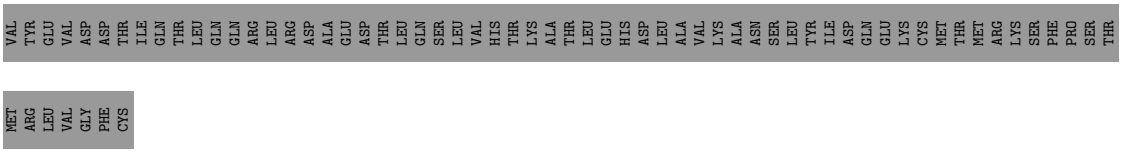


- Molecule 17: Tektin

Chain 3R:

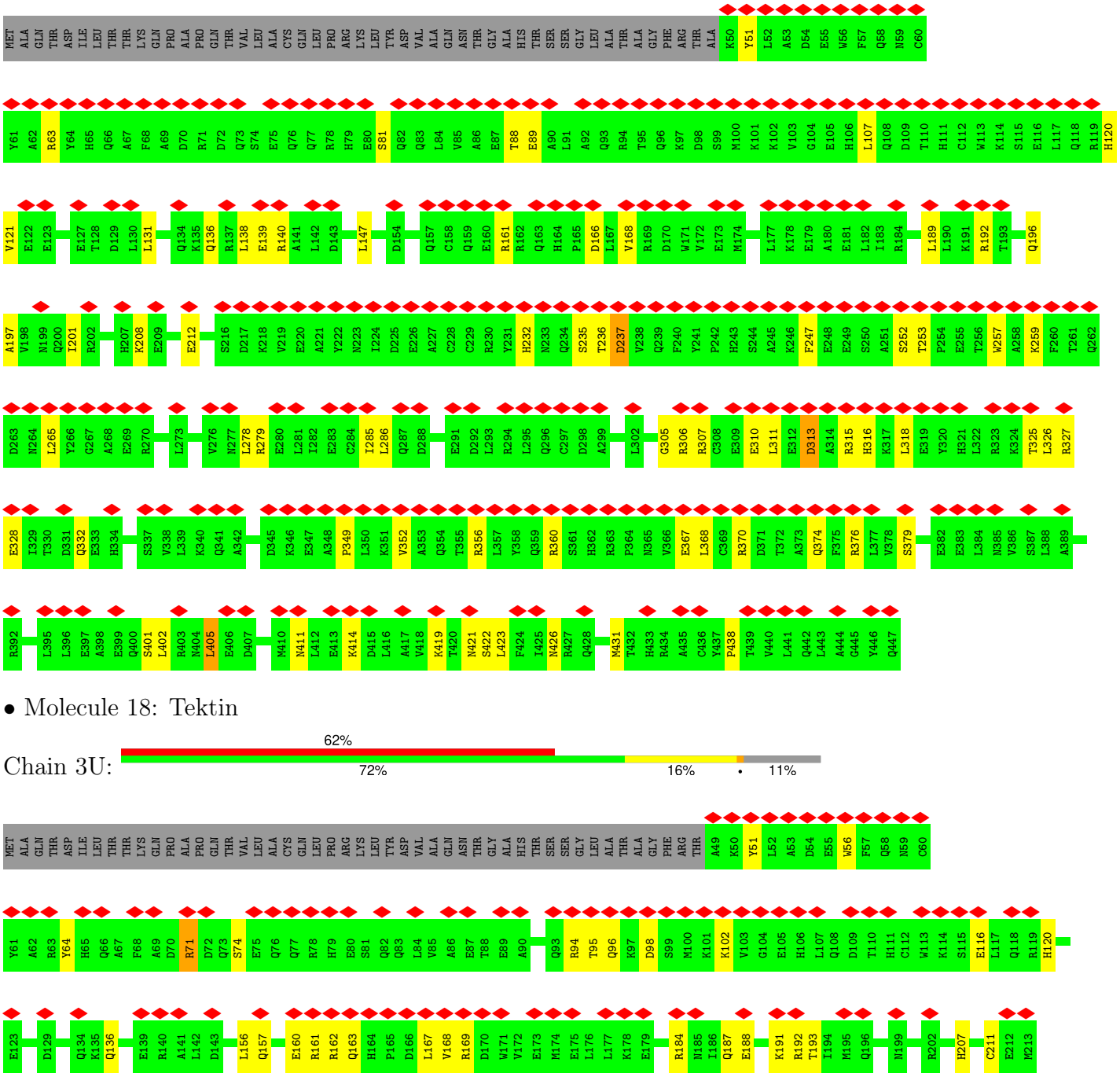





- Molecule 18: Tektin

Chain 3T:




- Molecule 18: Tektin

Chain 3U:

G214 W215 S216 D217 K218 V219 E220 A221 Y222 N223 I224 D225 E226 A227 C228 C229 R230 Y231 H232 N233 Q234 S235 T236 D237 V238 Q239 F240 Y241 P242 H243 S244 A245 K246 F247 E248 E249 S250 A251 S252 T253 P254 E255 T256 W257 A258 K259 F260 T261 Q262 D263 N264 L265 Y266 G267 A268 E269 R270 E271 R272 L273

V276 W277 L278 R279 E280 L281 I282 E283 C284 I285 I286 Q287 D288 T289 A290 E291 D292 L293 R294 L295 Q296 C297 D298 N301 L302 A303 F304 G305 R306 R307 C308 E309 E310 L311 E312 D313 A314 R315 H316 K317 I318 E319 Y320 H321 L322 R323 K324 T325 L326 R327 E328 I329 T330 D331 Q332 E333 H334 N335

V336 S337 V338 L339 K340 Q341 A342 V343 K344 D345 K346 E347 A348 P349 L350 K351 V352 A353 Q354 T355 R356 L357 Y358 Q359 R360 S361 H362 R363 P364 N365 V366 E367 L368 C369 R370 D371 T372 A373 Q374 F375 R376 L377 V378 S379 E380 V381 E382 E383 L384 N385 V386 S387 L388 A389 T390 L391 R392 E393 K394 L395

L396 E397 A398 E399 Q400 S401 L402 R403 N404 L405 E406 D407 M410 N411 L412 E413 K414 D415 L416 A417 V418 K419 T420 N421 S422 L423 R427 Q428 K429 C430 M431 T432 C436 Q442 L443 Y446 Q447

- Molecule 18: Tektin

Chain 3V:

MET ALA GLN THR ASP ILE LEU THR THR LYS GLN PRO ALA PRO GLN THR VAL LEU ALA CYS GLN LEU PRO ARG LYS LEU TYR ASP VAL ALA GLN ASN THR GLY ALA HIS THR SER SER GLY LEU ALA THR ALA GLY PHE ARG T48 A49 K50 Y51 L52 A53 D54 E55 W56 F57 Q58 N59 C60

Y61 A62 R63 Y64 H65 Q66 A67 F68 A69 D70 R71 D72 Q73 S74 E75 Q76 Q77 R78 H79 E80 S81 Q82 Q83 L84 V85 A86 E87 T88 E89 A90 L91 A92 Q93 R94 T95 Q96 K97 D98 S99 M100 K101 K102 V103 G104 E105 H106 L107 Q108 D109 T110 H111 C112 W113 K114 S115 E116 L117 Q118 R119 H120

V121 E122 E123 A126 E127 T128 D129 L130 L131 L132 A133 GLN LYS GLN ARG LEU GLU ARG ALA LEU ASP ALA THR ALA LEU PRO PHE SER ILE ALA THR ASP ASN LEU GLN CYS GLN GLU ARG ARG GLN HIS PRO ASP LEU VAL ARG ASP TRP VAL GLU MET GLU LEU LEU LYS GLU ALA GLU

LEU ILE ARG ASN ILE GLN GLU LEU LEU LYS ARG THR ILE MET Q196 A197 V198 N199 Q200 I201 R202 L203 E206 H207 K208 E209 T210 C211 E212 M213 D217 K218 V219 E220 A221 Y222 N223 I224 D225 E226 A227 C228 C229 R230 Y231 H232 N233 Q234 S235 T236 D237 V238 Q239 F240 Y241 P242 H243 S244

A245 K246 F247 E248 E249 S250 A251 S252 T253 P254 E255 T256 W257 A258 K259 F260 T261 Q262 D263 N264 L265 Y266 G267 A268 E269 R270 E271 R272 L273 A274 N277 L278 R279 GLU LEU ILE GLU CYS ILE LEU GLN ASP THR ALA GLU ASP LEU ARG LEU GLN CYS ASP ALA VAL ASN LEU ALA PHE GLY

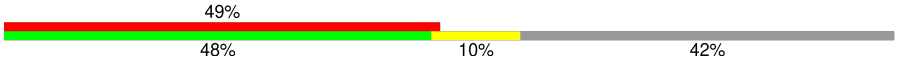
ARG ARG CYS GLU GLU LEU GLU ASP ALA ARG HIS LYS LEU GLU TYR HIS LEU ARG LYS THR LEU ARG GLU ILE THR ASP GLN GLU HIS ASN VAL SER VAL LEU LYS GLN ALA VAL LYS ASP LYS GLU ALA PRO LEU LYS VAL ALA GLN THR ARG LEU TYR GLN ARG SER HIS ARG PRO ASN

VAL GLU LEU CYS ARG ASP THR ALA GLN PHE ARG LEU VAL SER GLU VAL GLU GLU GLU LEU ASN VAL SER LEU ALA THR LEU ARG GLU LYS LEU LEU GLU ALA GLU GLN SER LEU ARG ASN LEU GLU ASP THR ARG MET ASN LEU GLU LYS ASP LEU ALA VAL LYS THR ASN SER LEU PHE ILE

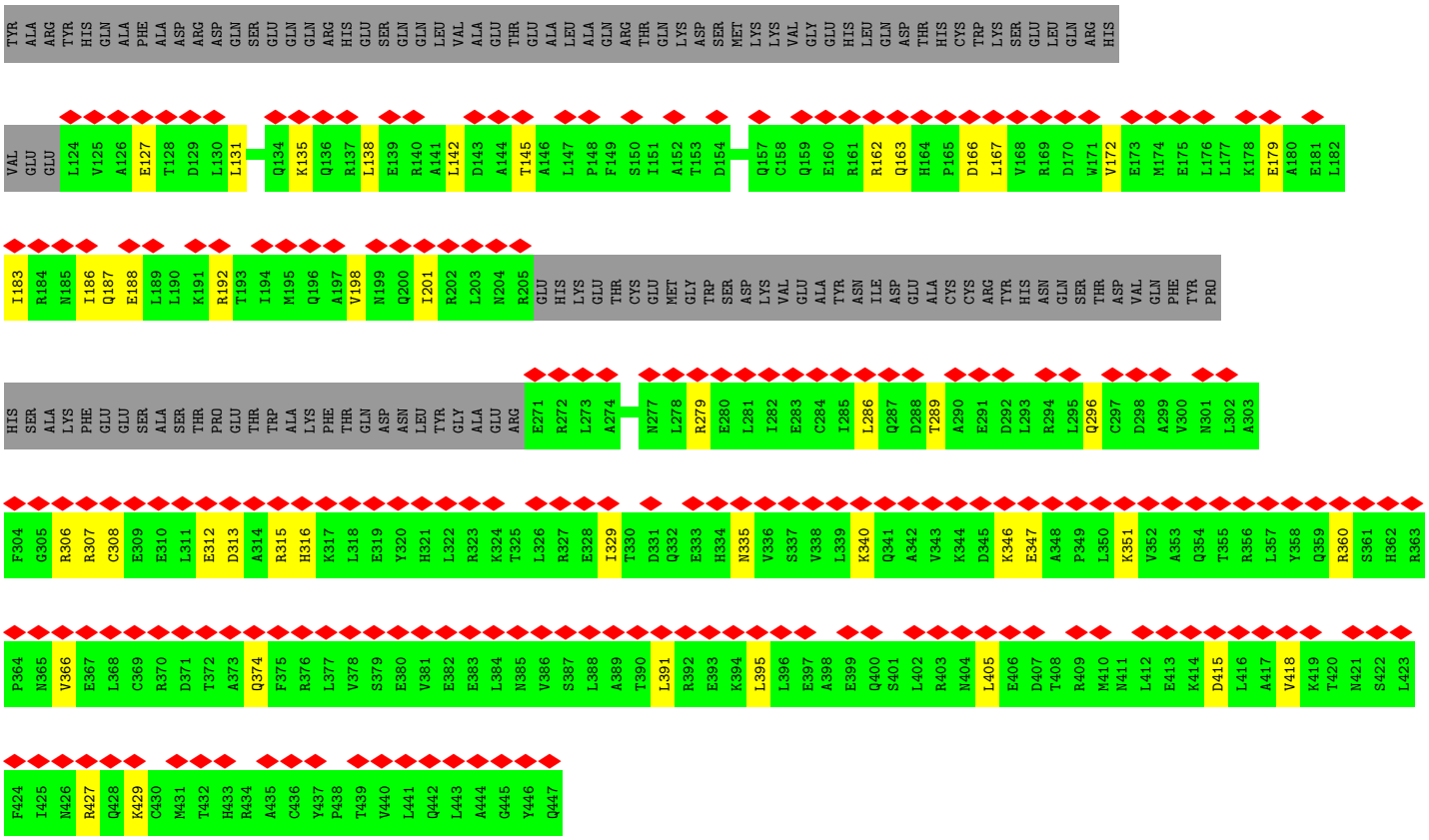
ASN ARG GLN LYS CYS MET THR HIS ARG ALA CYS TYR PRO THR VAL LEU GLN LEU ALA GLY TYR GLN

- Molecule 18: Tektin

Chain 3W:

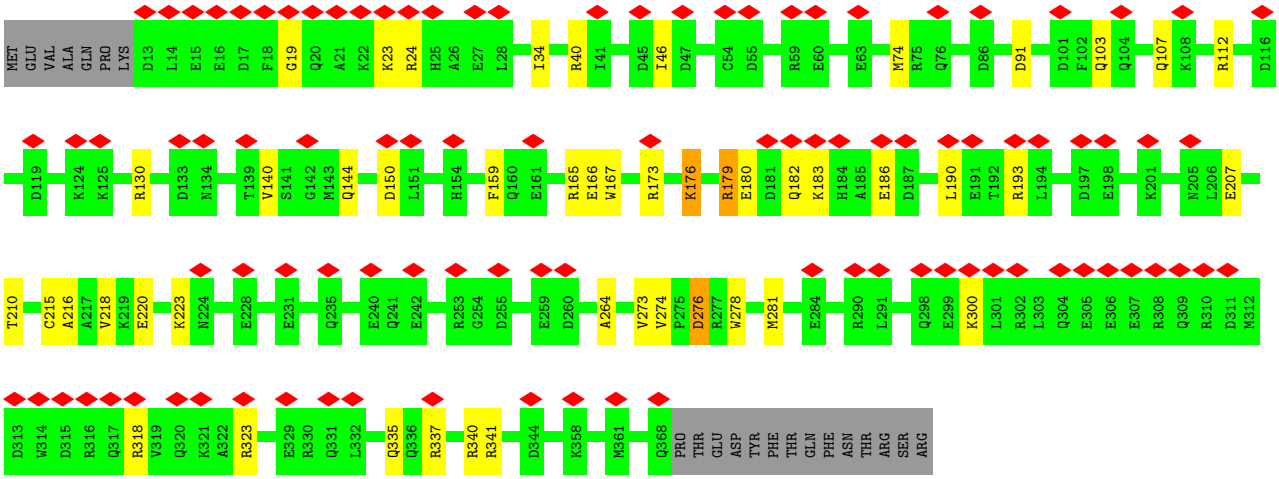



MET ALA GLN THR ASP ILE LEU THR THR LYS GLN PRO ALA PRO GLN THR VAL LEU ALA CYS GLN LEU PRO ARG LYS LEU TYR ASP VAL ALA GLN ASN THR GLY ALA HIS THR SER SER GLY LEU ALA THR ALA GLY PHE ARG THR ALA LYS TYR LEU ALA ASP GLU TRP PHE GLN ASN CYS



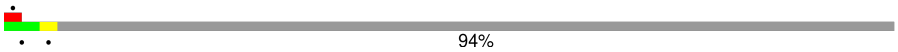
• Molecule 19: RIB43A domain with coiled-coils 2

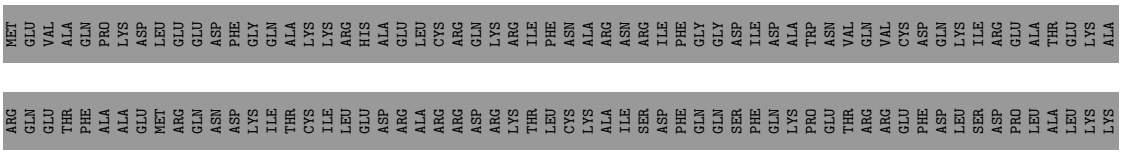
Chain 3Y:



• Molecule 19: RIB43A domain with coiled-coils 2

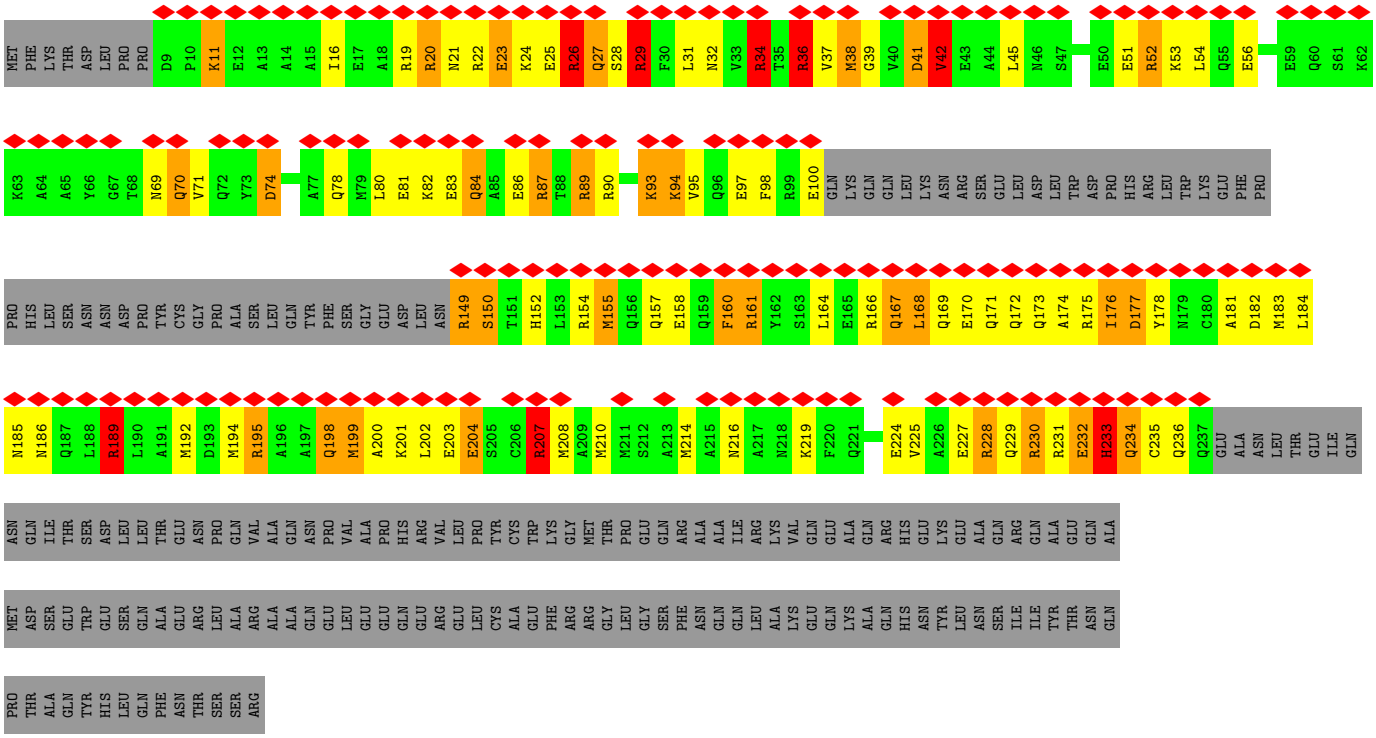
Chain 3Z:



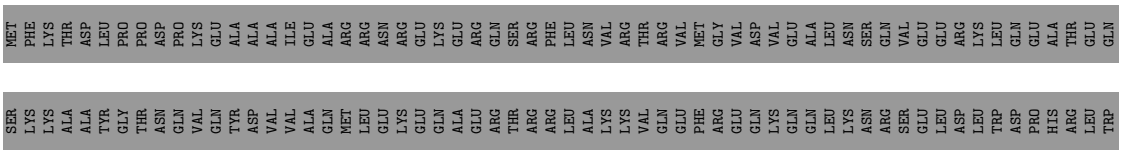
• Molecule 20: RIB43A-like with coiled-coils protein 1

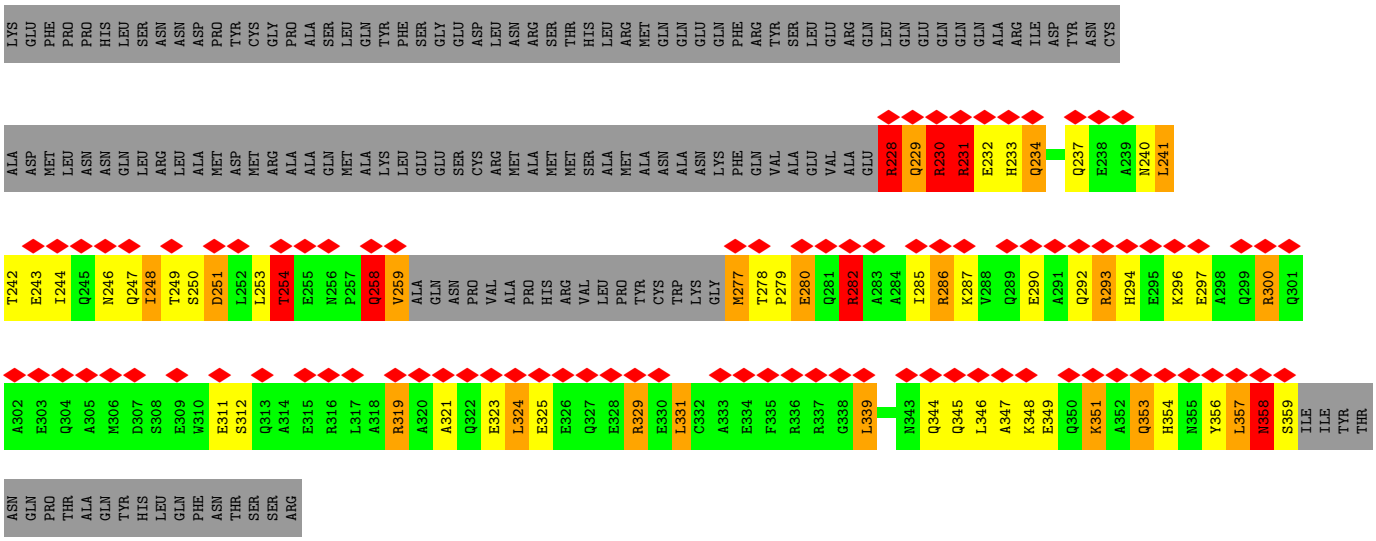
Chain 4A:



• Molecule 20: RIB43A-like with coiled-coils protein 1

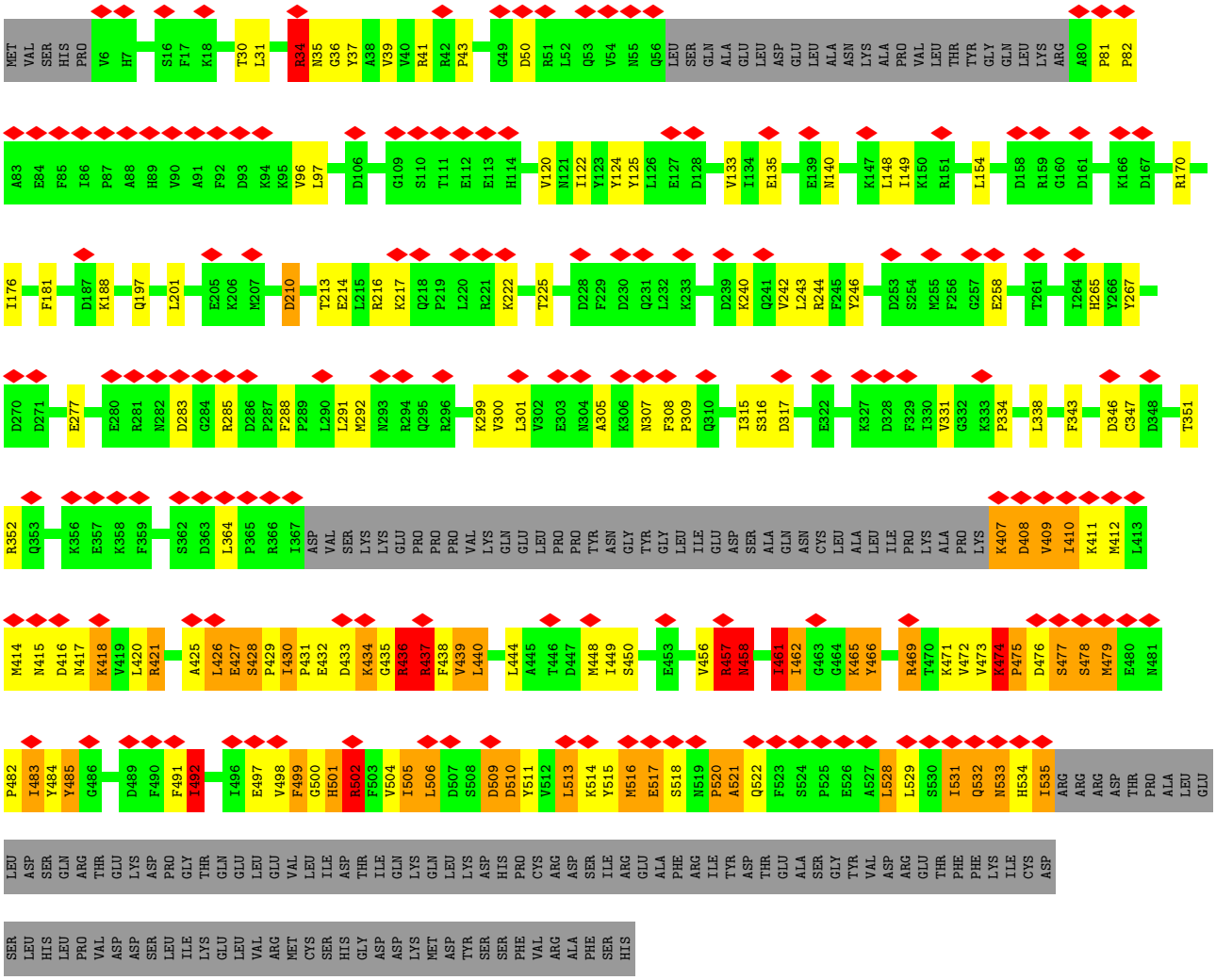
Chain 4B:





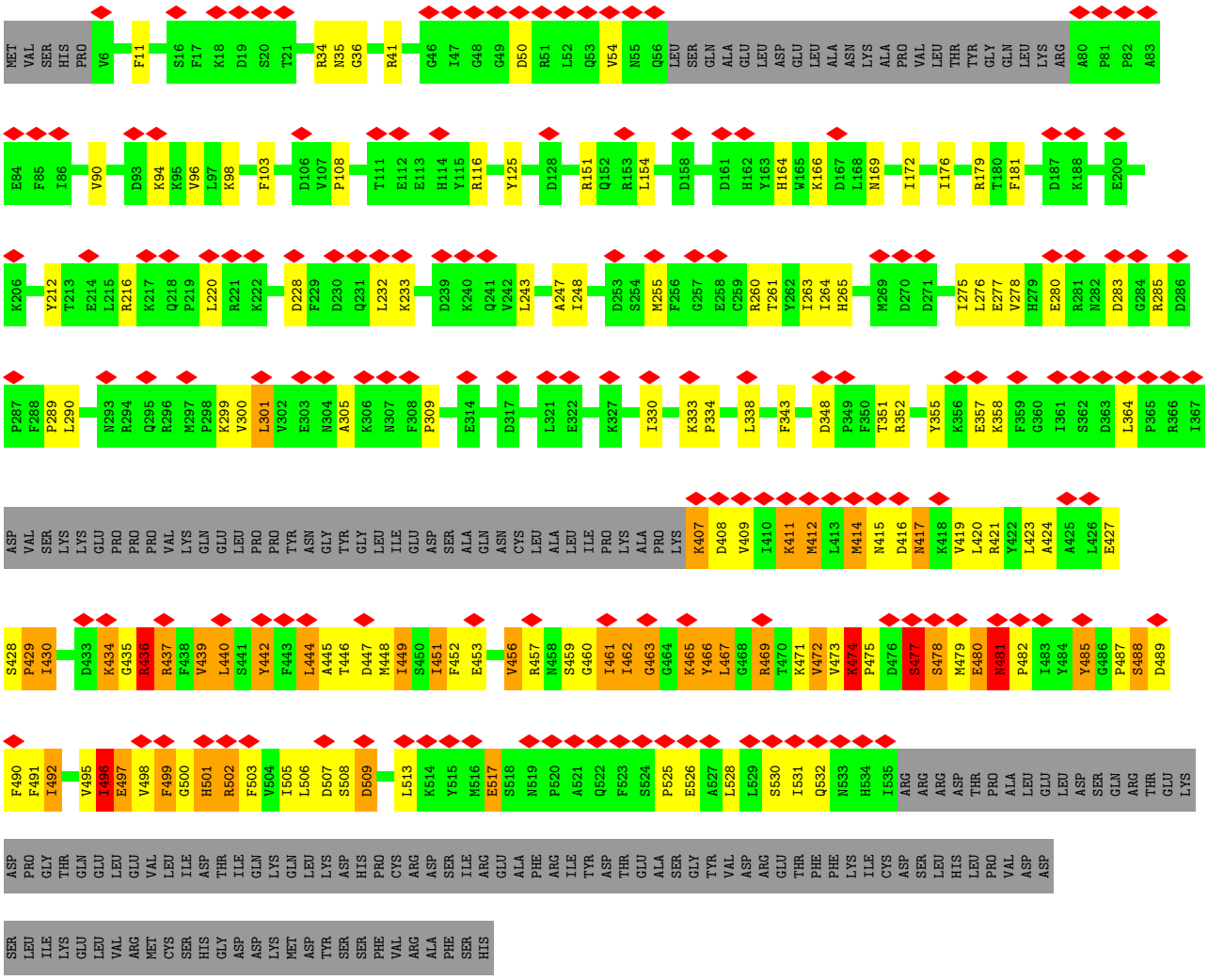
- Molecule 21: EF-hand domain containing 1

Chain 4D:



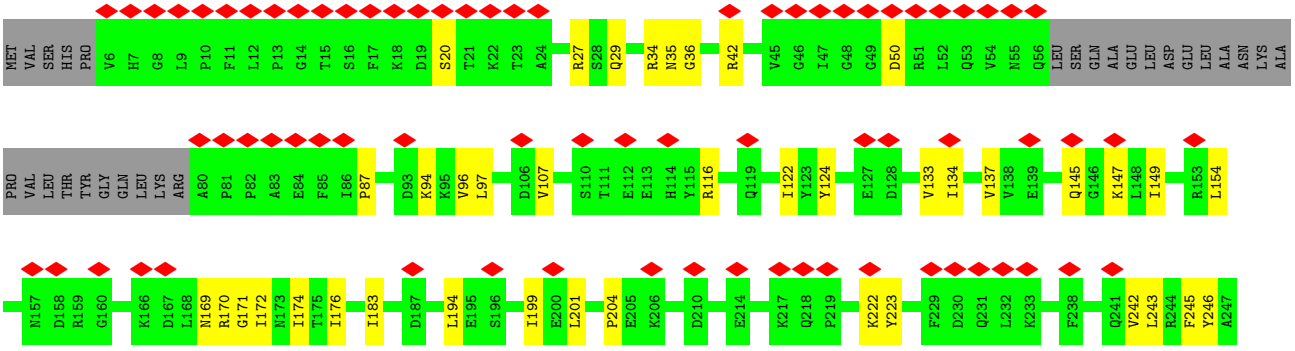
• Molecule 21: EF-hand domain containing 1

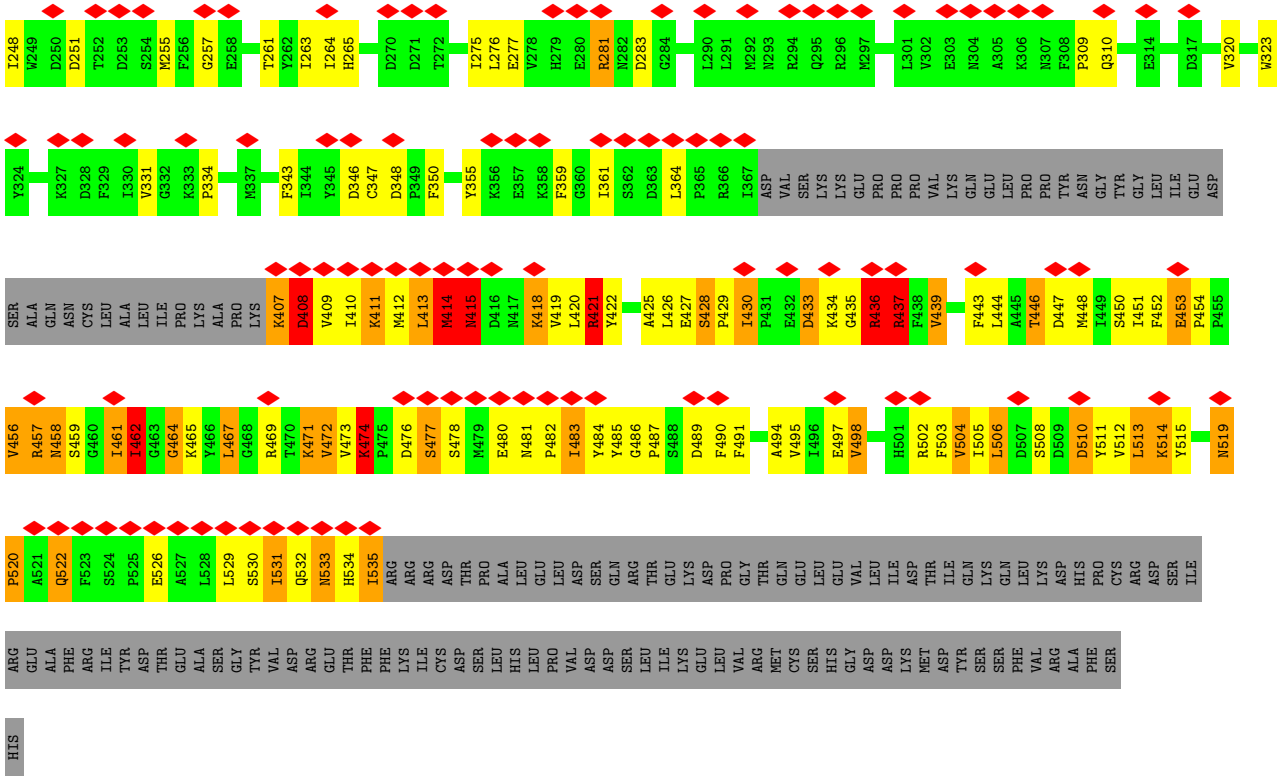
Chain 4E:




• Molecule 21: EF-hand domain containing 1

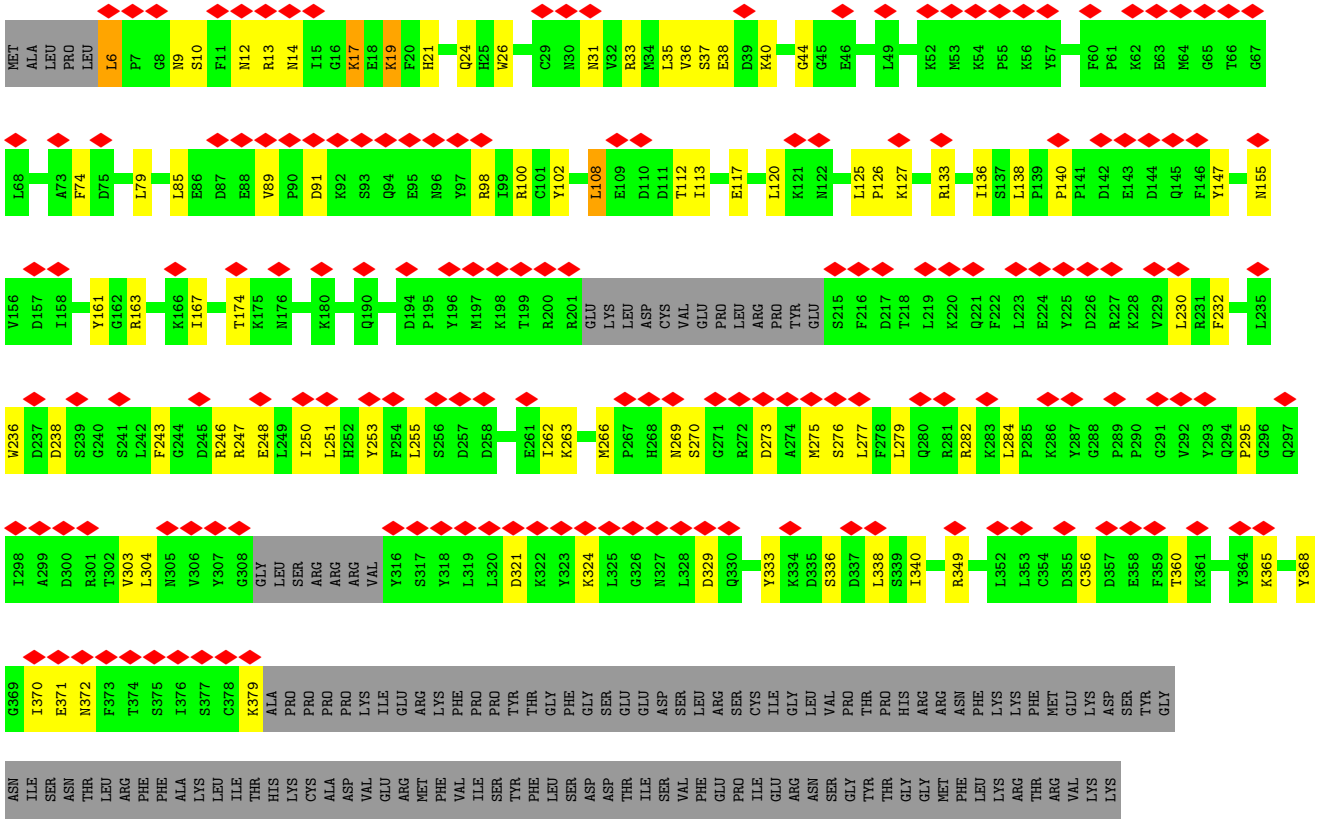
Chain 4F:

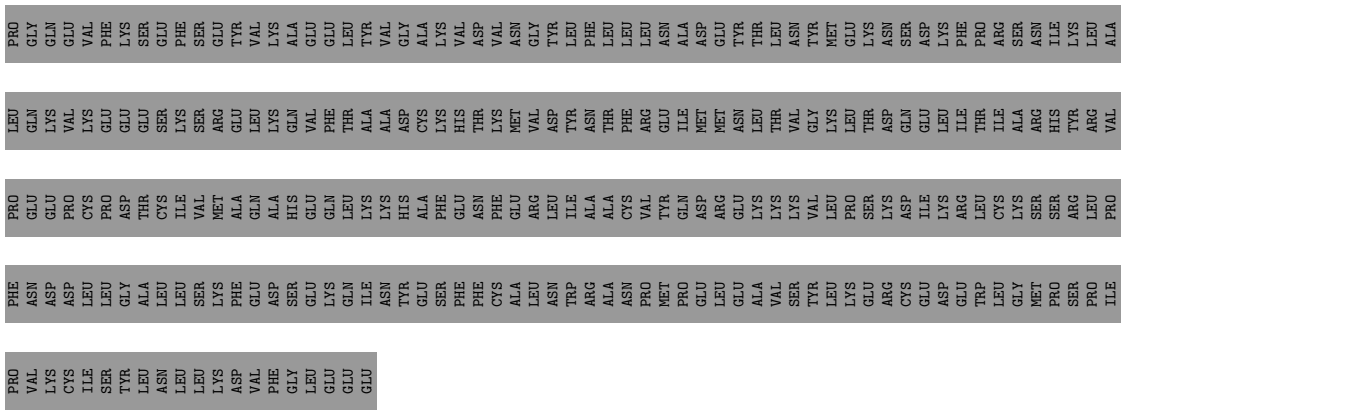




• Molecule 22: EF-hand domain-containing family member C2

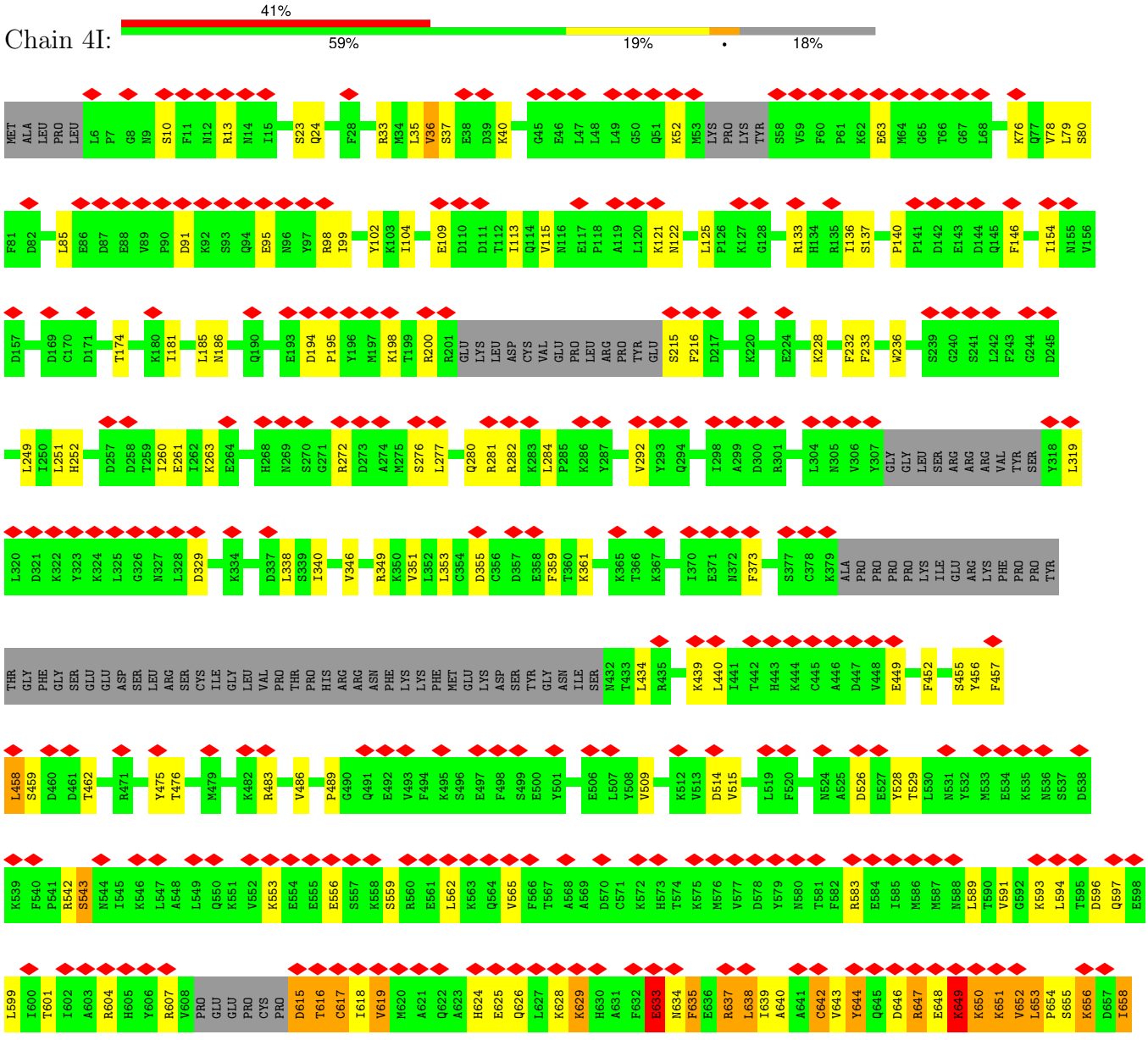
Chain 4H:

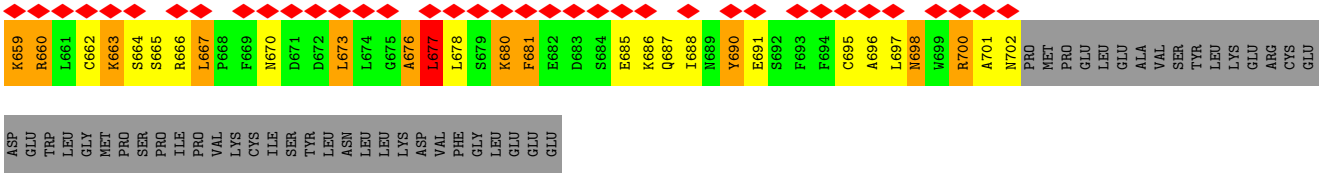




- Molecule 22: EF-hand domain-containing family member C2

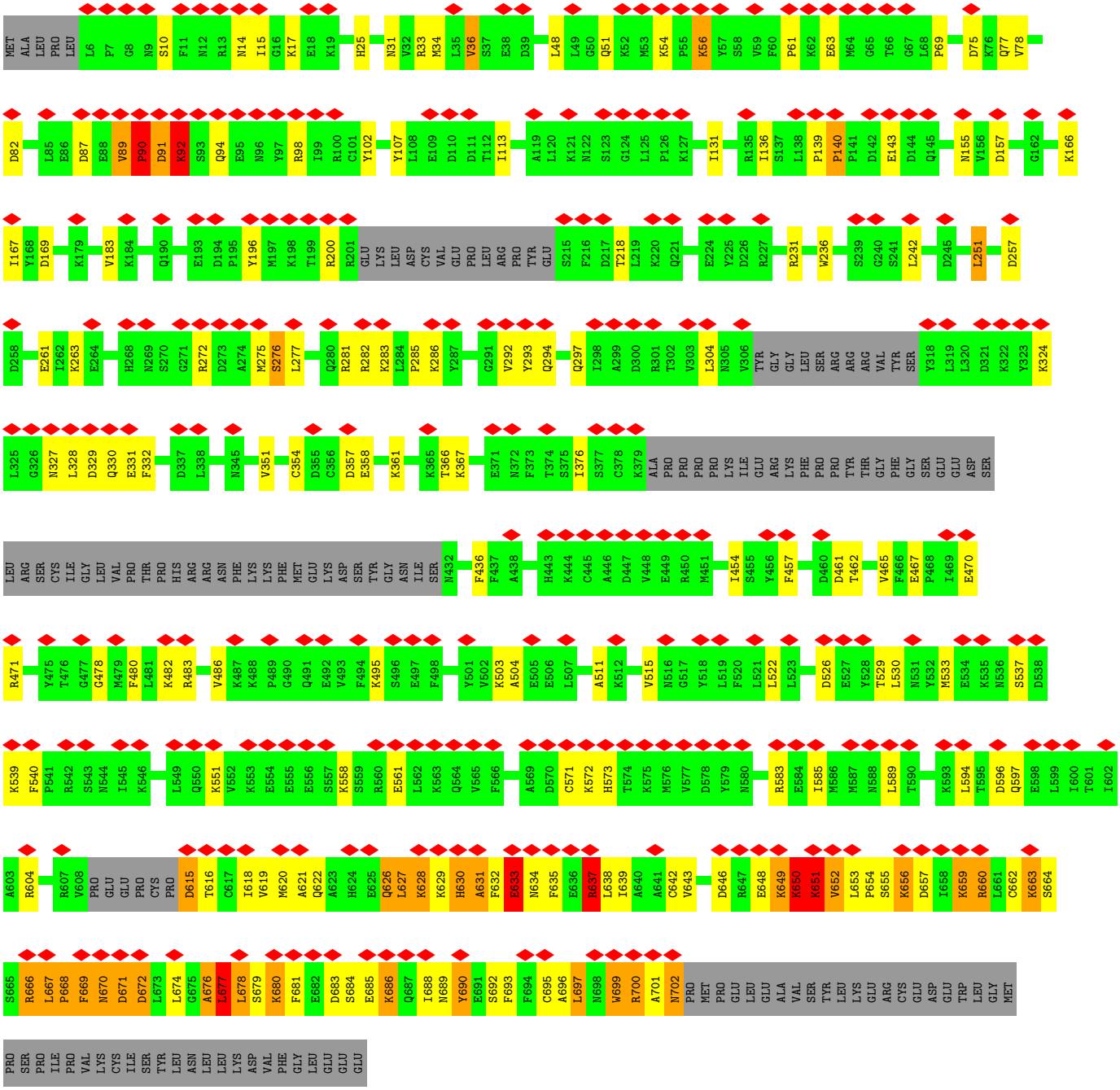
Chain 4I:





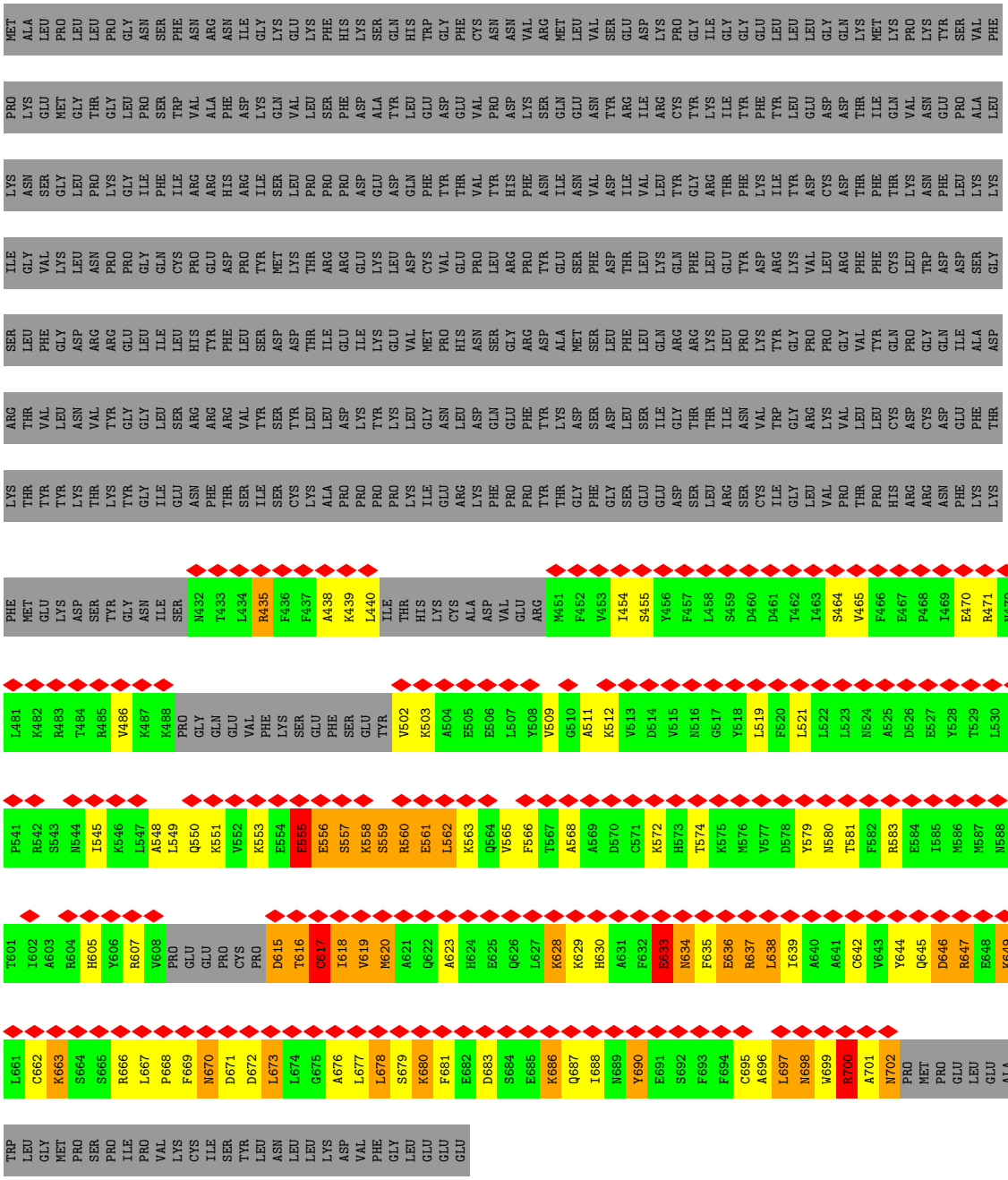

• Molecule 22: EF-hand domain-containing family member C2

Chain 4J:



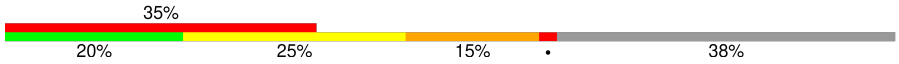

• Molecule 22: EF-hand domain-containing family member C2

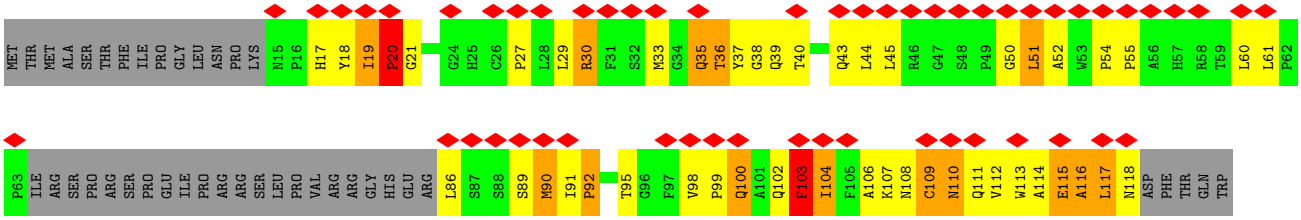
Chain 4K:

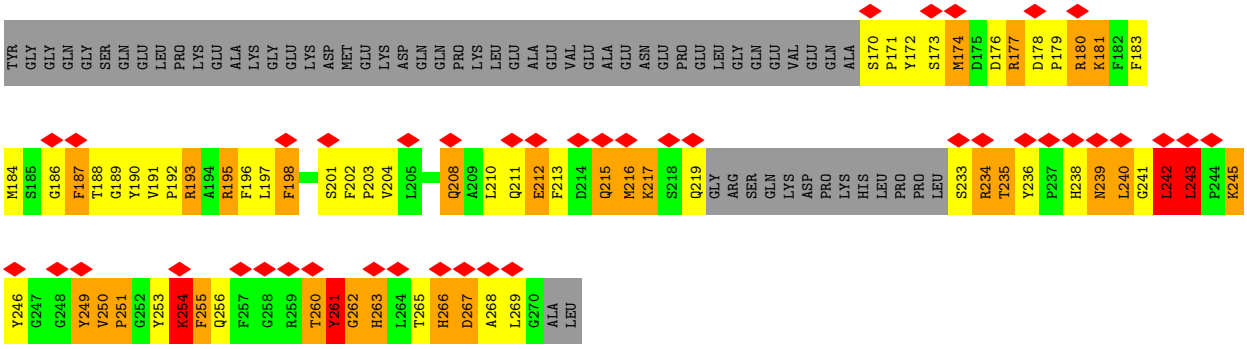


• Molecule 23: Ciliary microtubule inner protein 2B

Chain 4M:

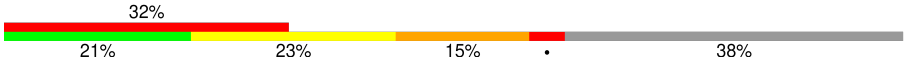


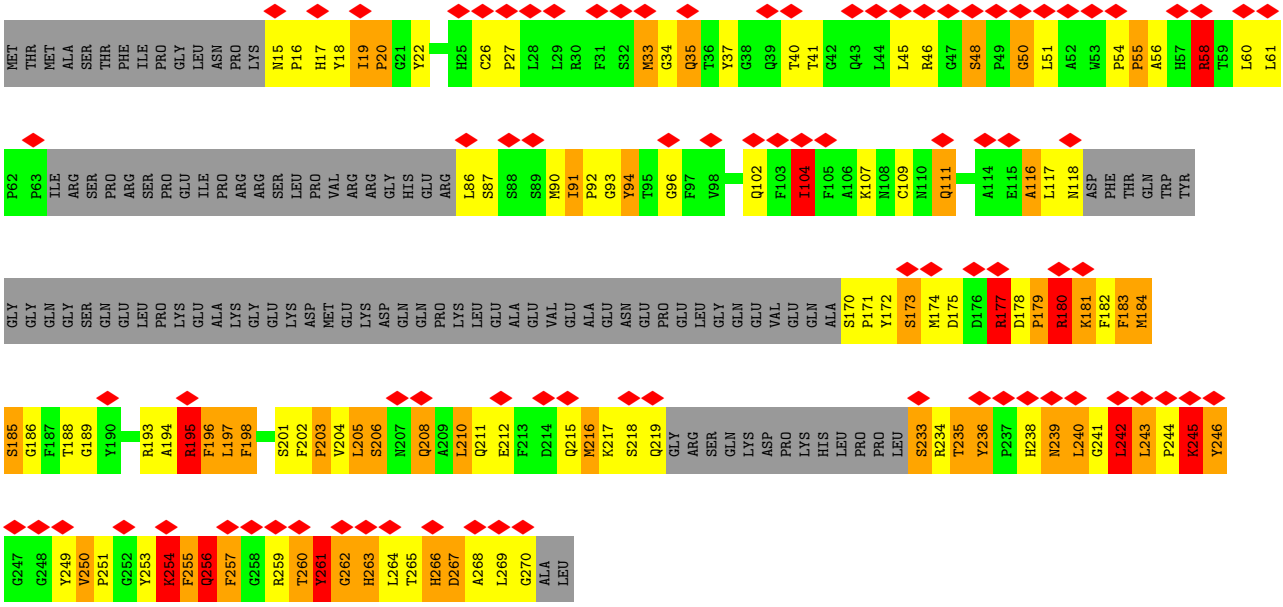






• Molecule 23: Ciliary microtubule inner protein 2B

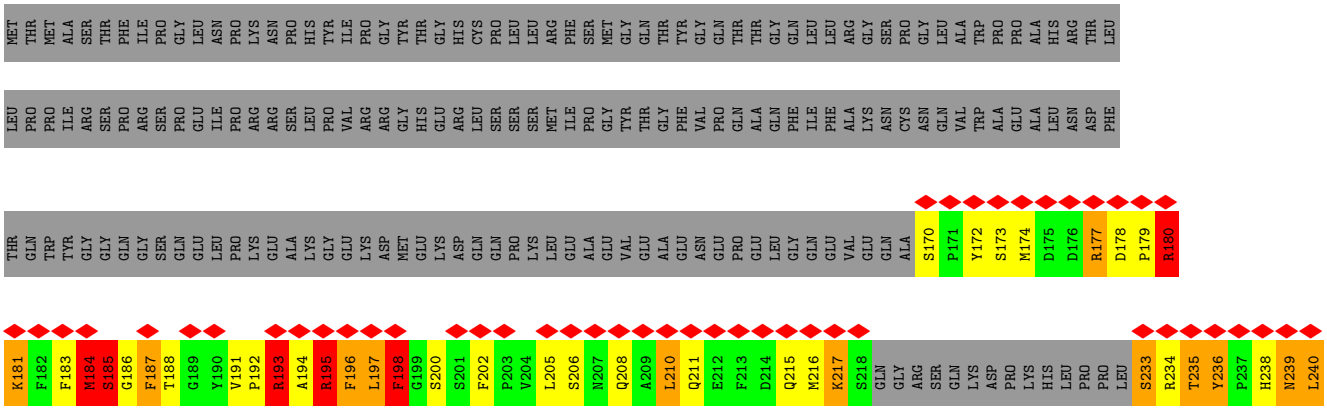
Chain 4N:

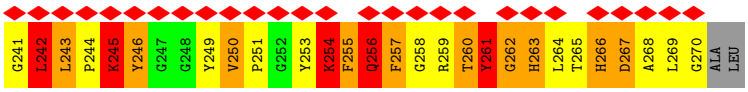



• Molecule 23: Ciliary microtubule inner protein 2B

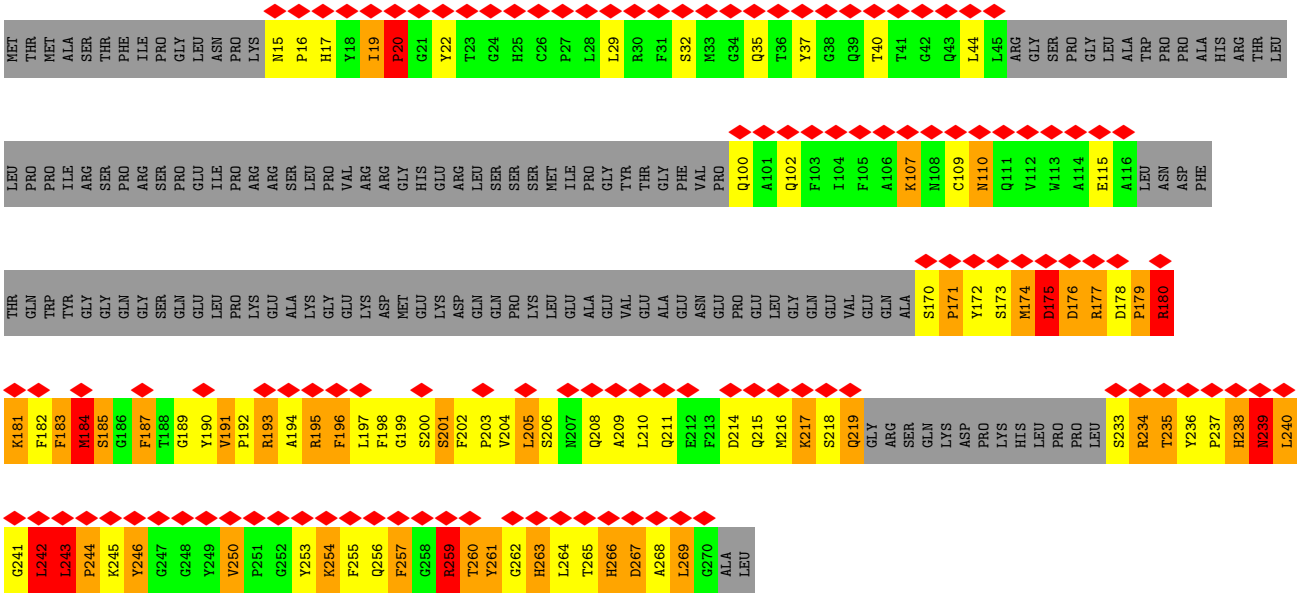
Chain 4P:





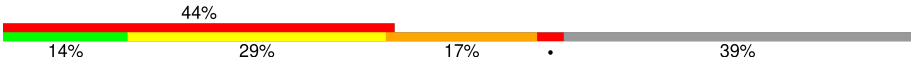

• Molecule 23: Ciliary microtubule inner protein 2B

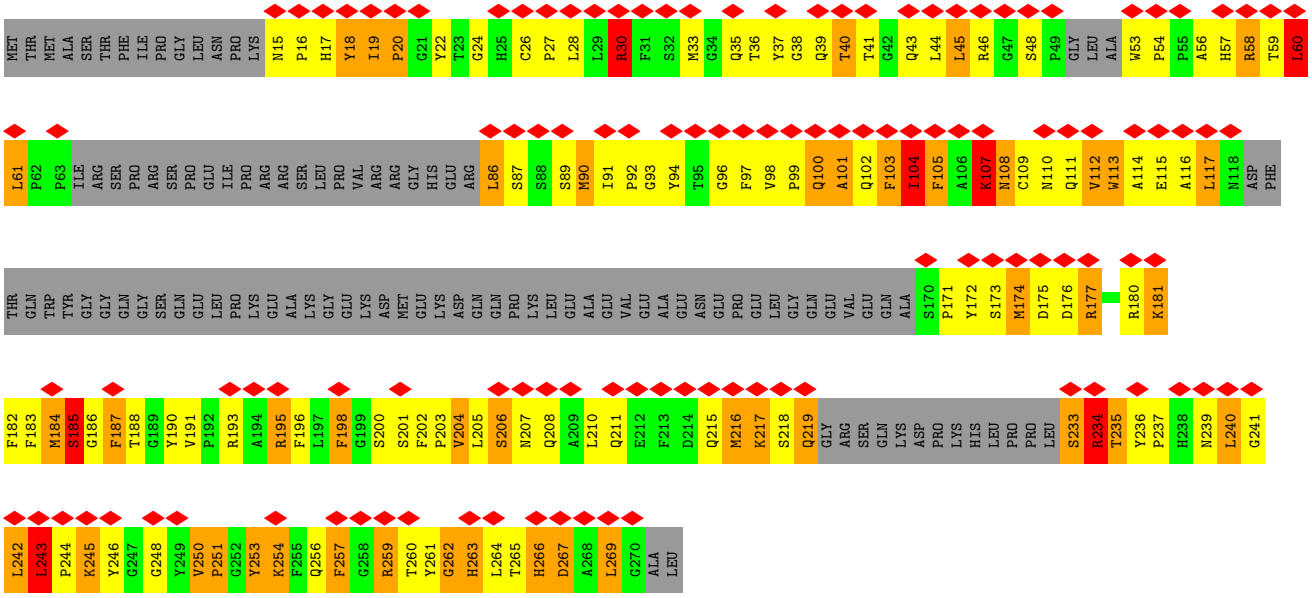
Chain 4Q:




• Molecule 23: Ciliary microtubule inner protein 2B

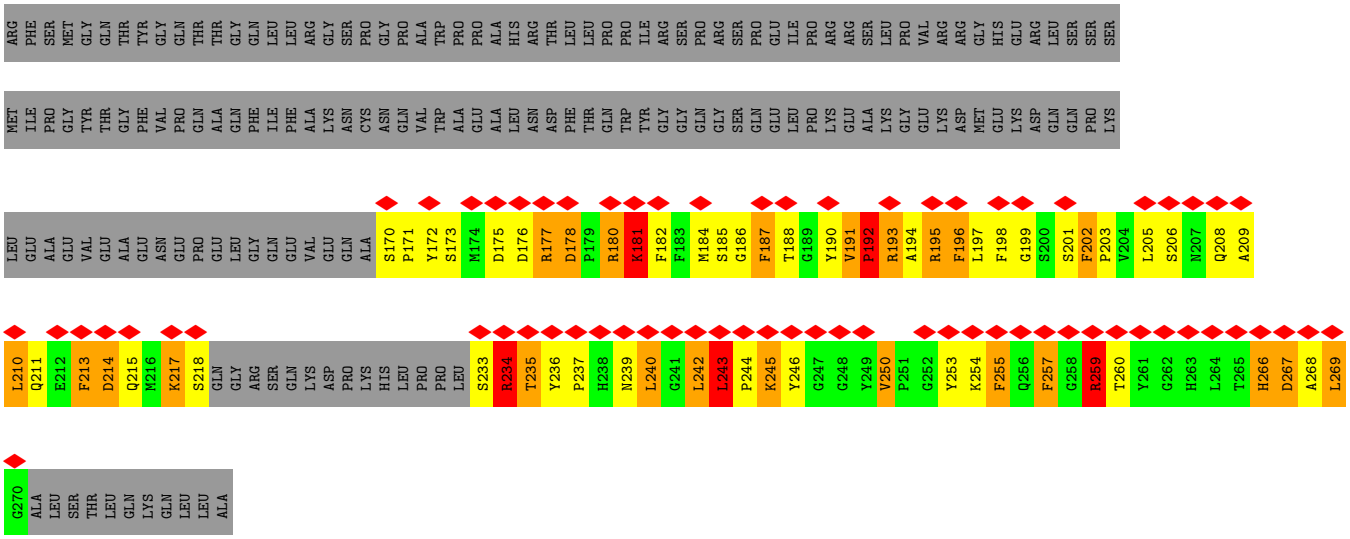
Chain 4R:



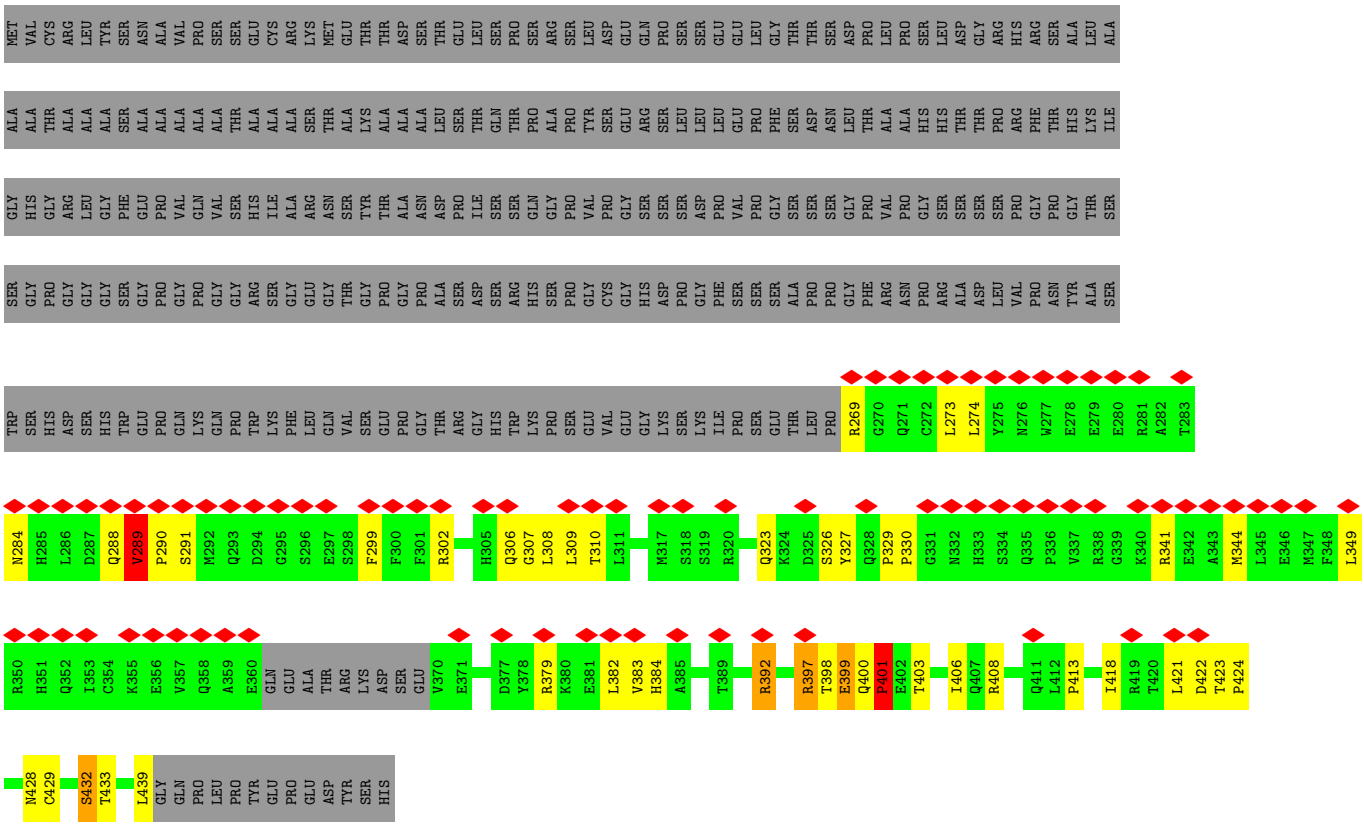

• Molecule 24: Ciliary microtubule inner protein 2B

Chain 4O:



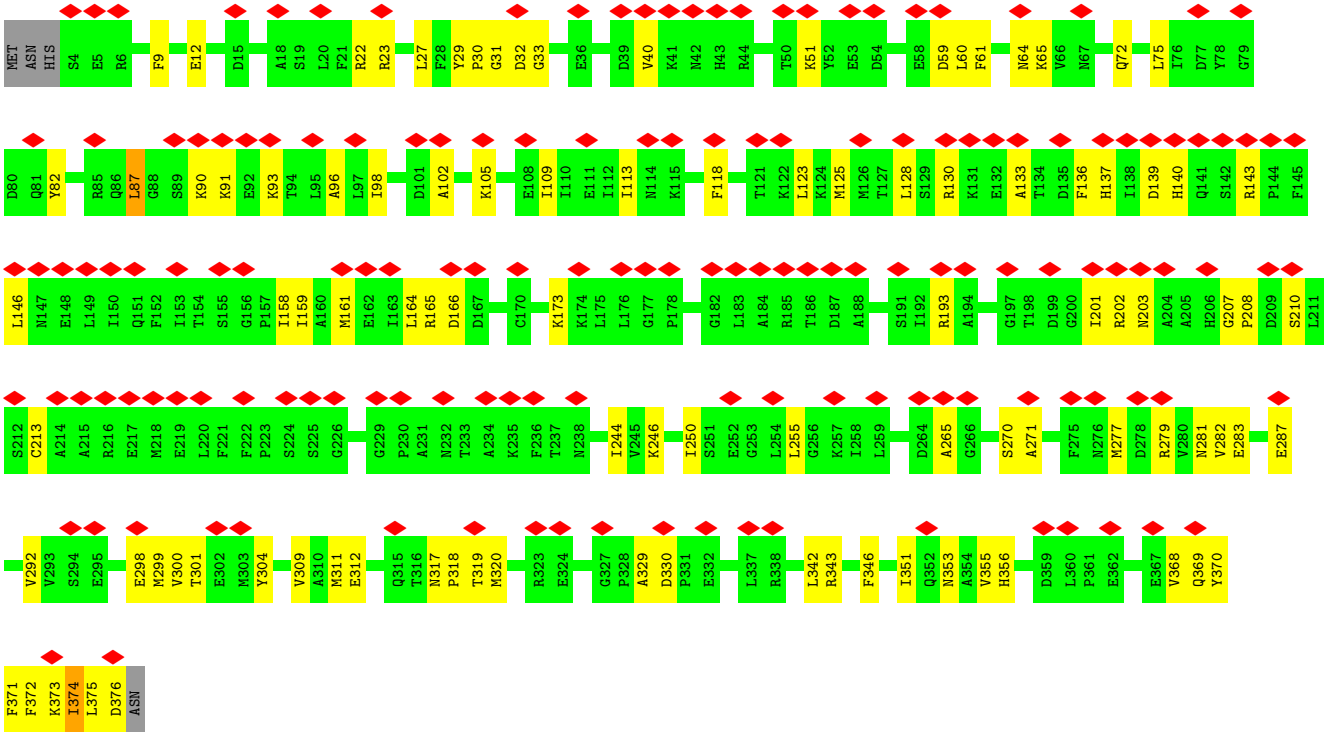

- Molecule 25: Sperm-associated antigen 8 isoform 1

Chain 4T:



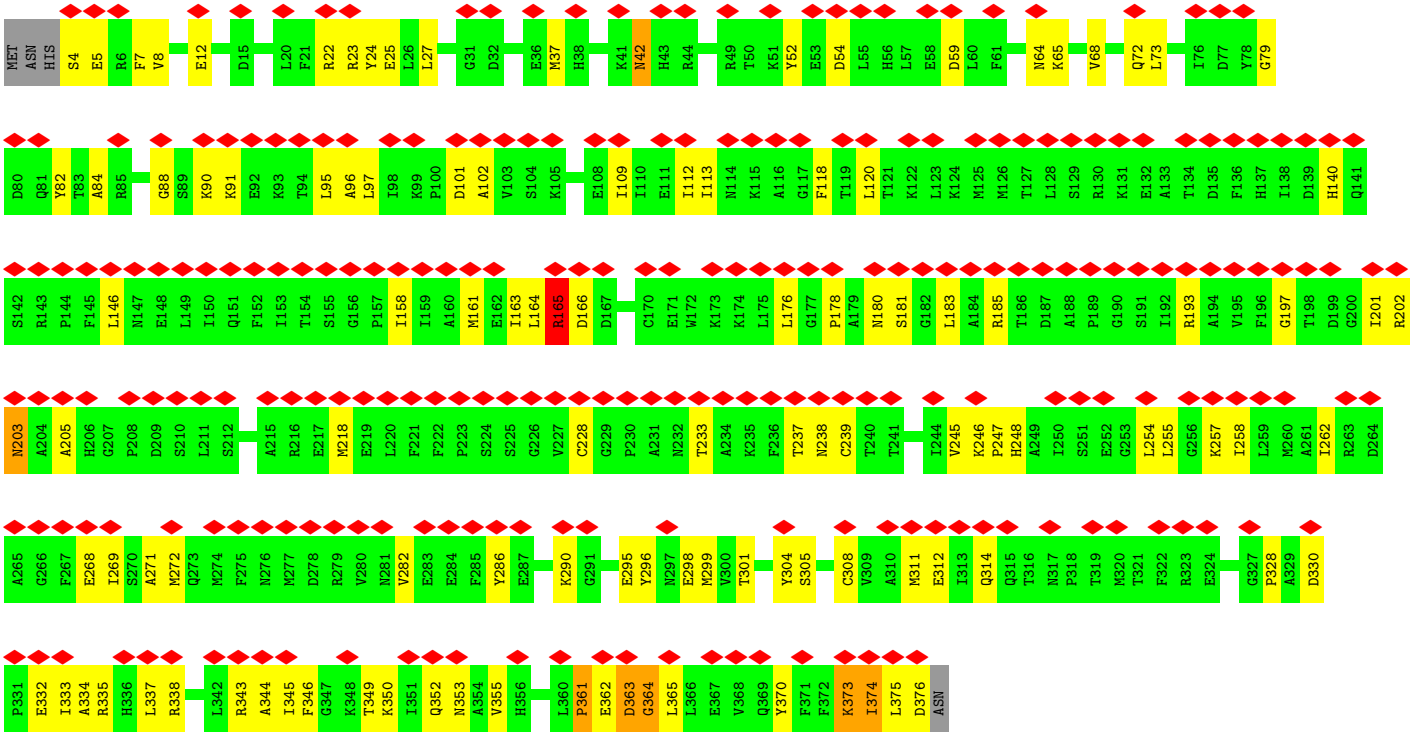

- Molecule 26: Nucleoside diphosphate kinase homolog 7

Chain 4V:



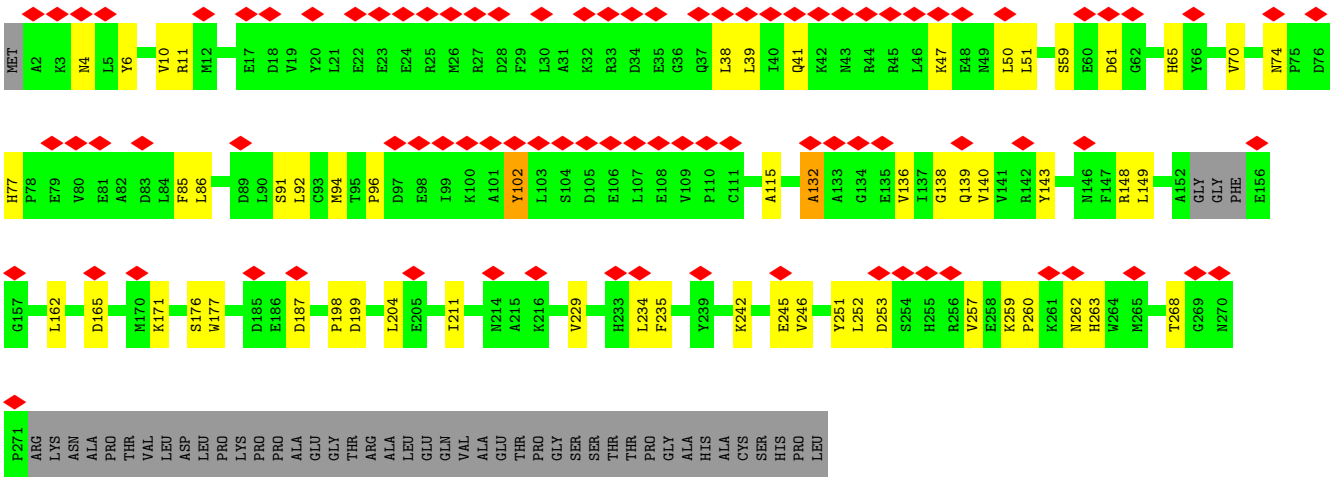

- Molecule 26: Nucleoside diphosphate kinase homolog 7

Chain 4W:



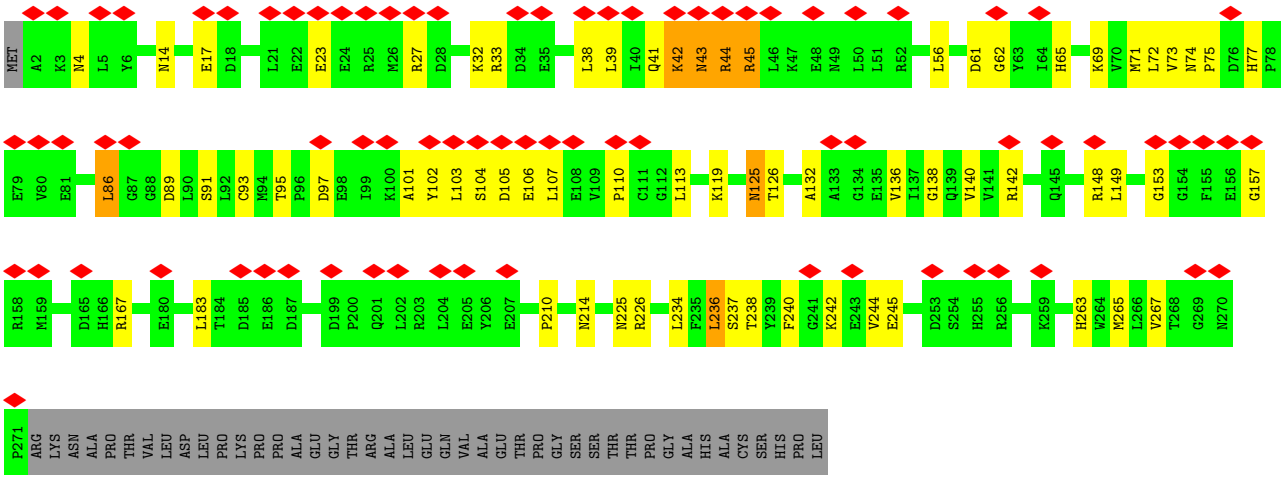

- Molecule 27: Cilia and flagella associated protein 161

Chain 4Y:



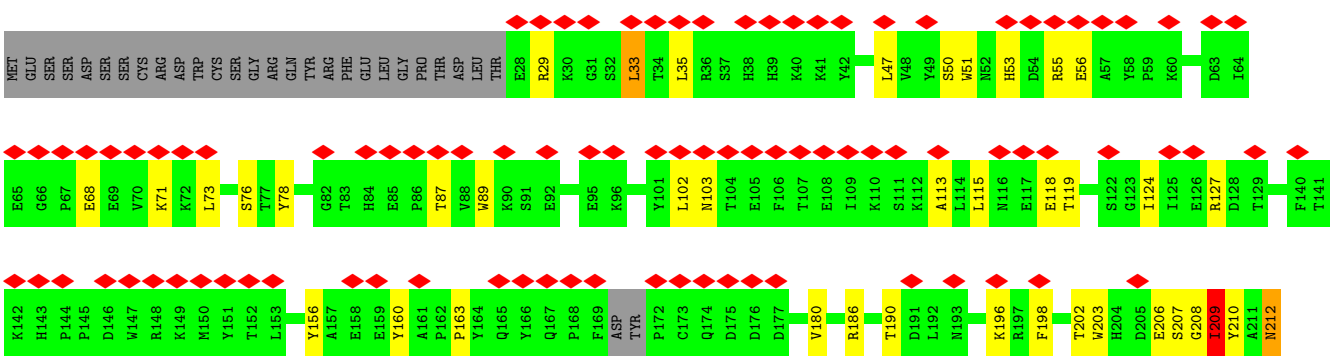

- Molecule 27: Cilia and flagella associated protein 161

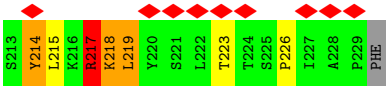
Chain 4Z:




- Molecule 28: Chromosome 1 C9orf135 homolog

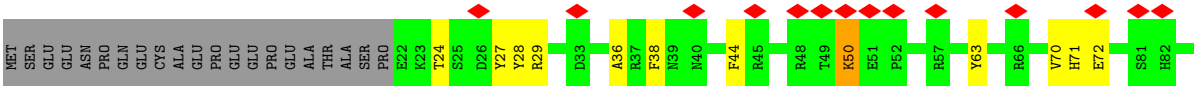
Chain 5B:

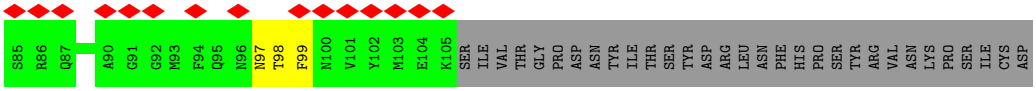





• Molecule 29: Piercer of microtubule wall 1

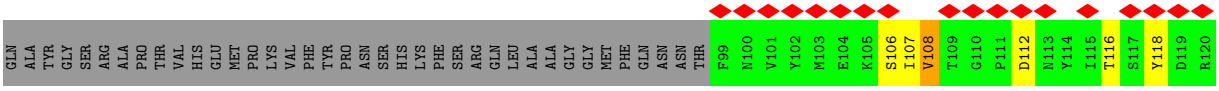
Chain 5D:

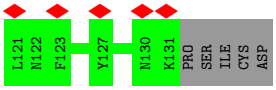



• Molecule 29: Piercer of microtubule wall 1

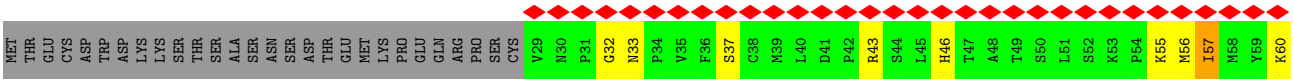
Chain 5E:

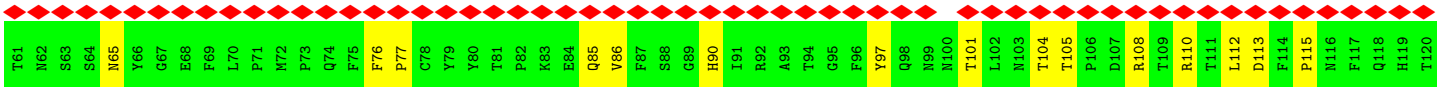



• Molecule 30: Chromosome 1 C15orf65 homolog

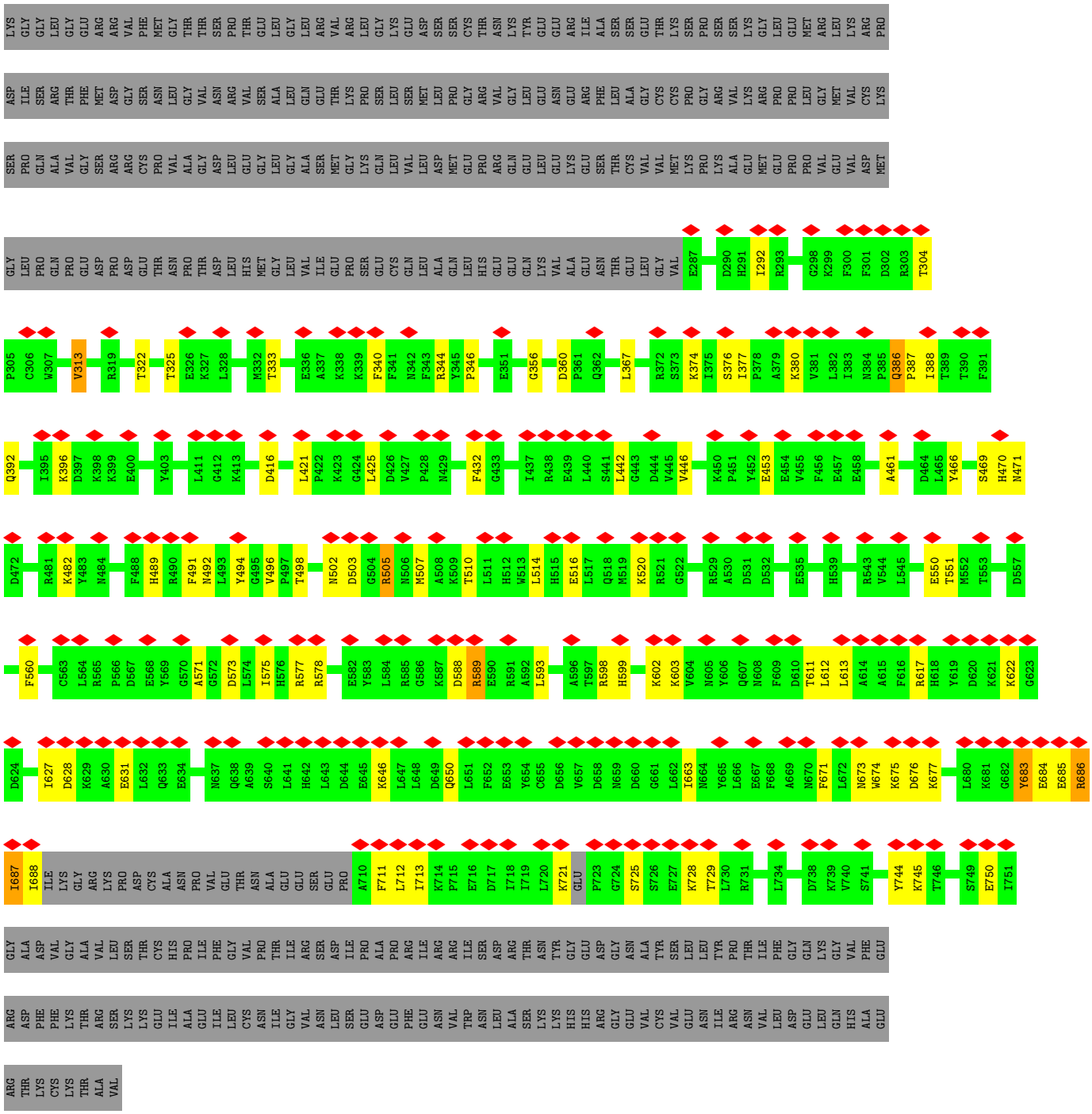
Chain 5G:



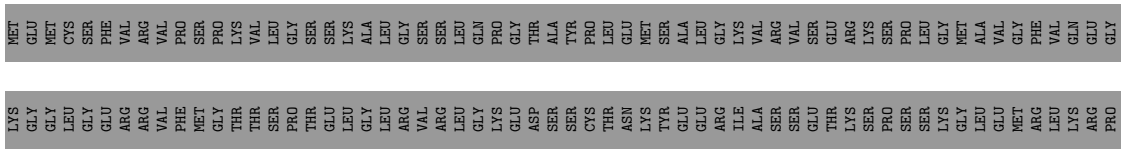
• Molecule 31: EF-hand domain family member B

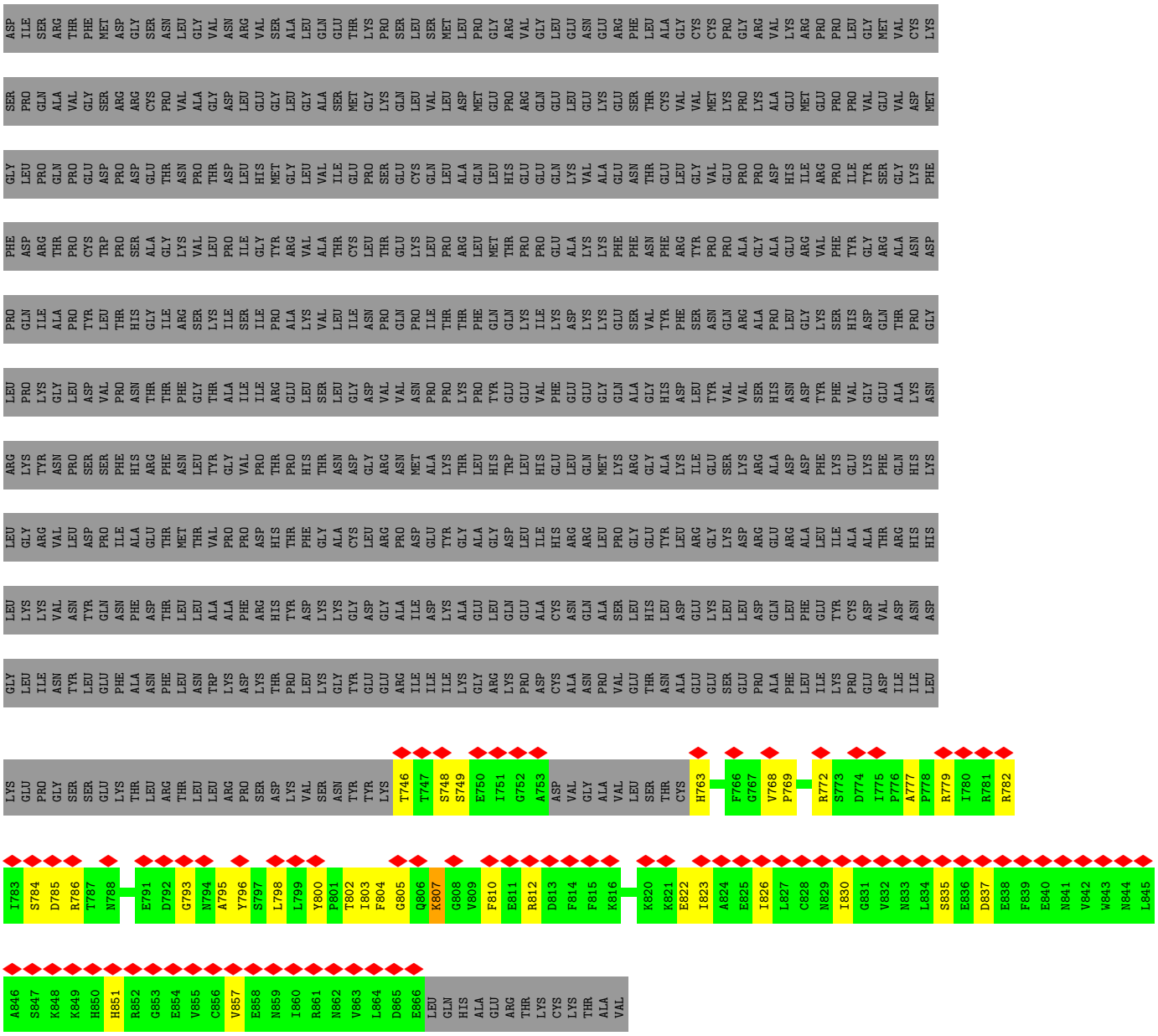
Chain 5I:



• Molecule 31: EF-hand domain family member B

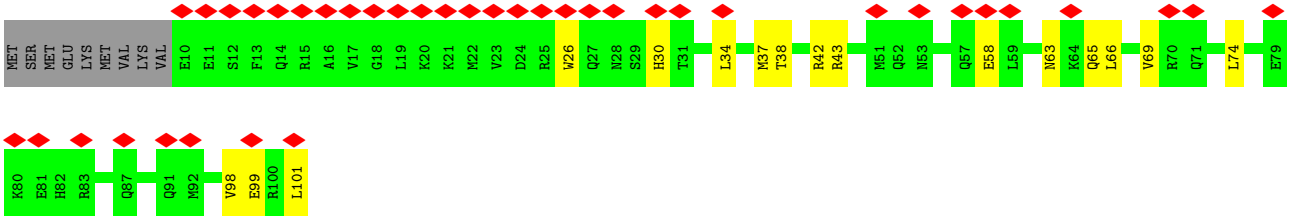
Chain 5J:





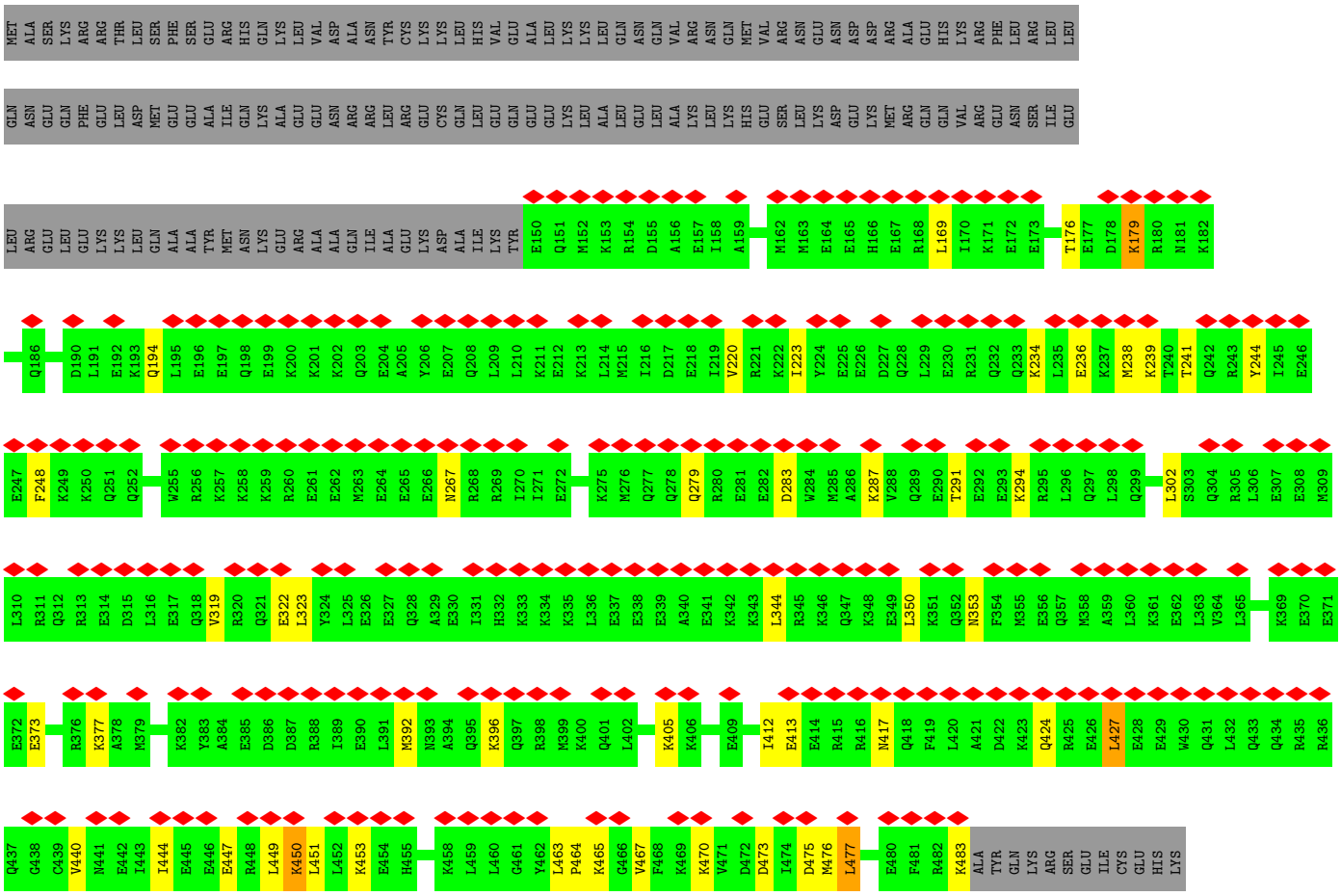
• Molecule 32: Cilia and flagella associated protein 141

Chain 5L:



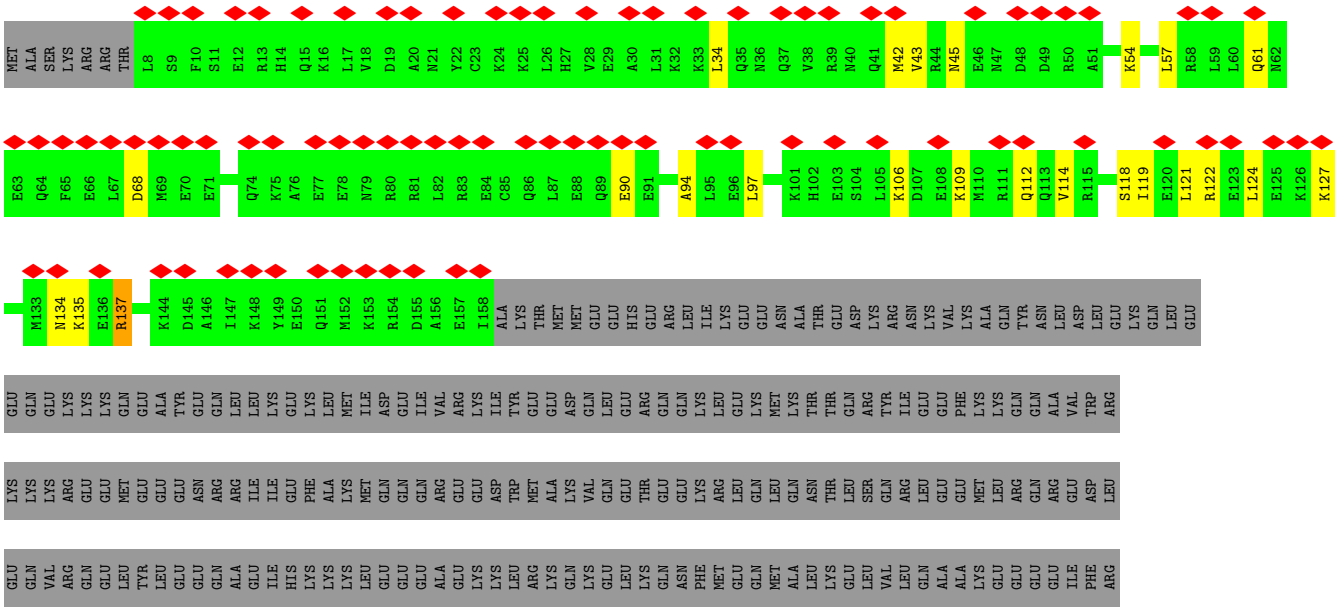
• Molecule 33: Meiosis-specific nuclear structural protein 1

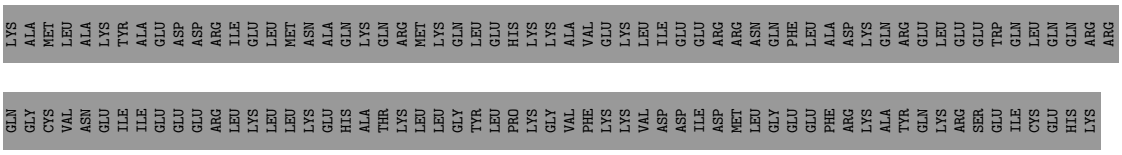
Chain 5N:



• Molecule 33: Meiosis-specific nuclear structural protein 1

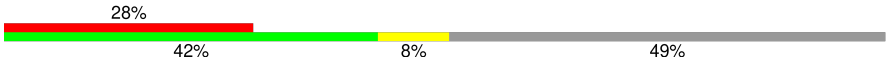
Chain 5O:

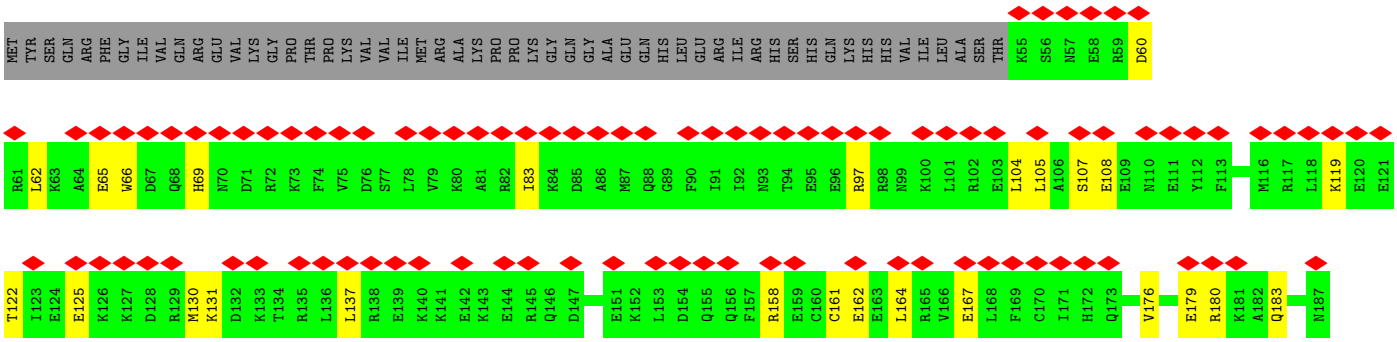




• Molecule 34: Cilia- and flagella-associated protein 53

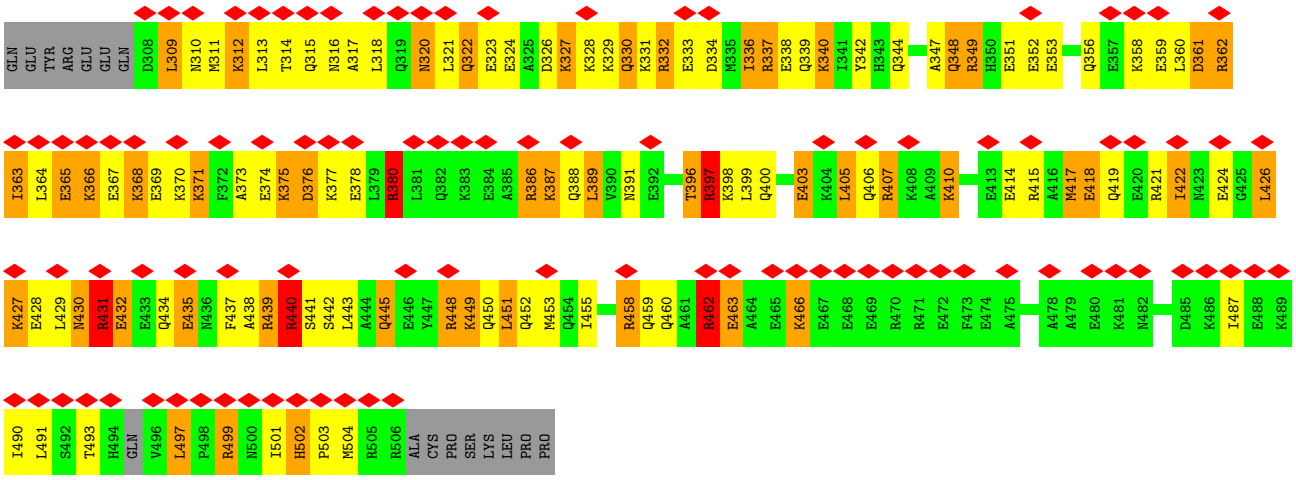
Chain 5Q:



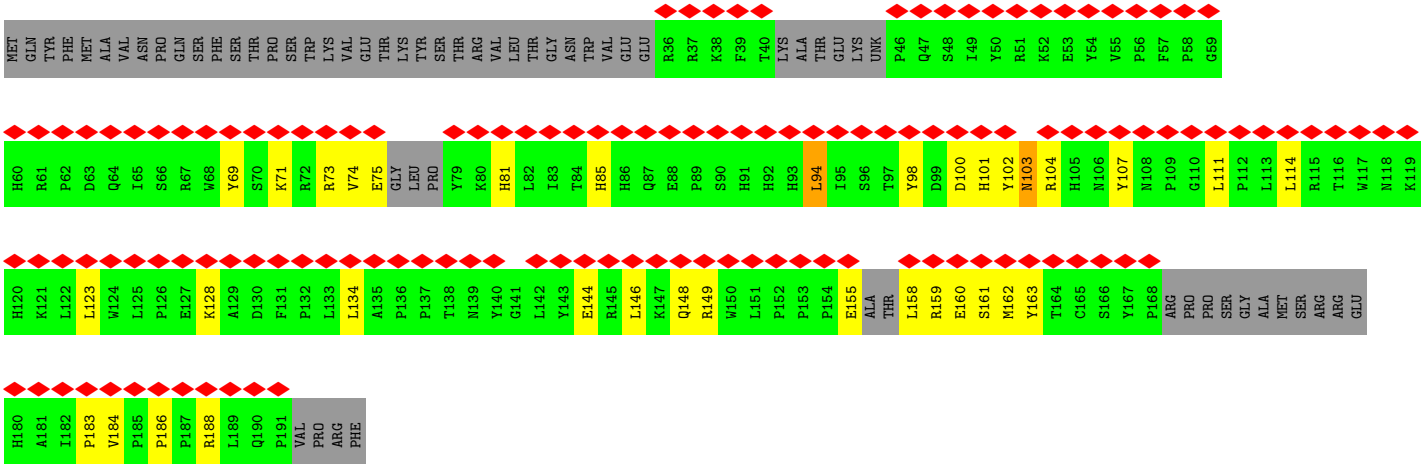
• Molecule 34: Cilia- and flagella-associated protein 53

Chain 5R:



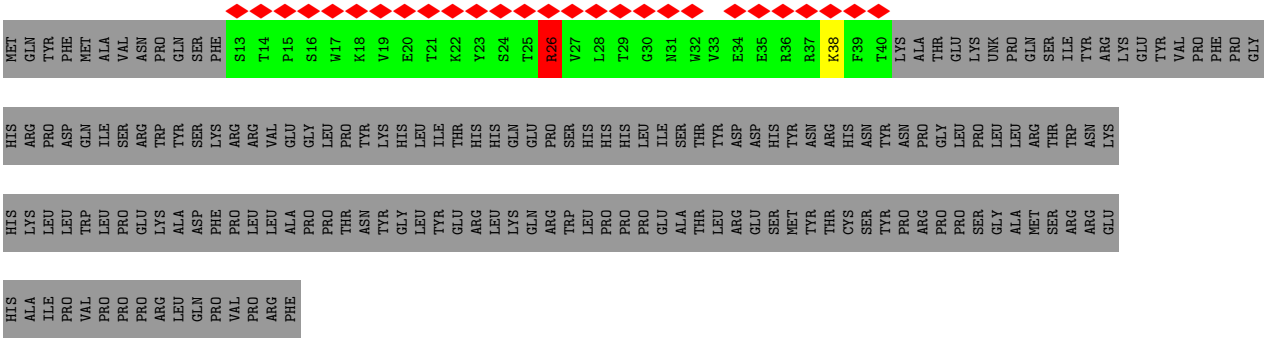

- Molecule 35: CFAP107/C1orf158

Chain 5T:



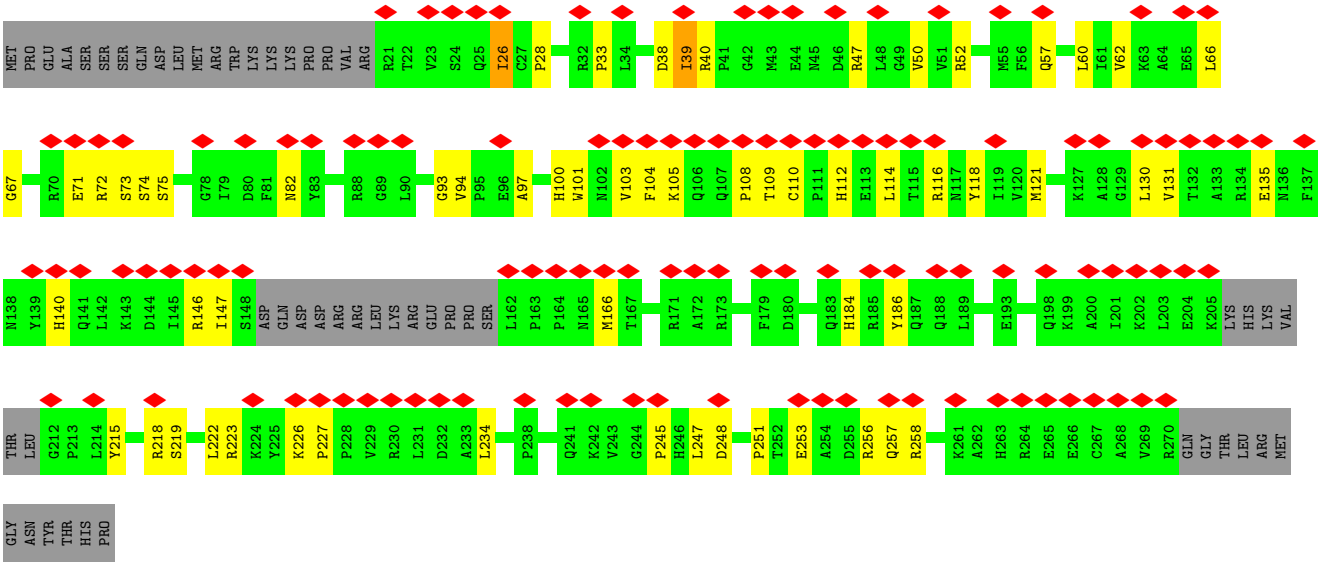

- Molecule 35: CFAP107/C1orf158

Chain 5U:



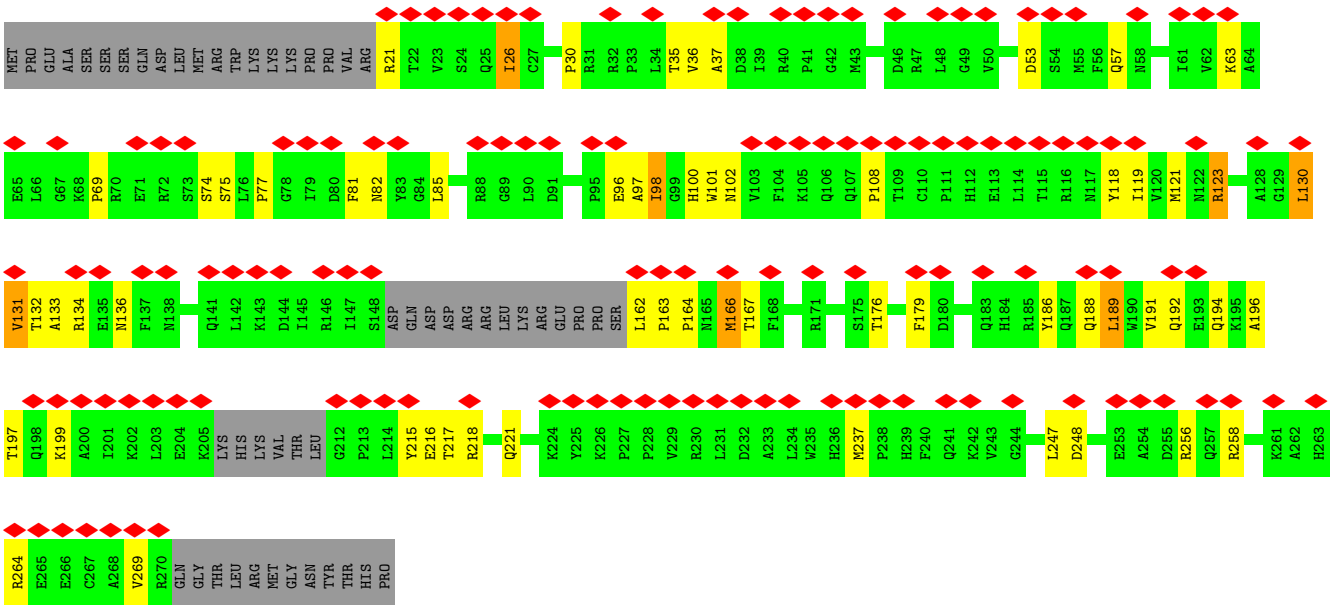

- Molecule 36: Cilia and flagella associated protein 77

Chain 5W:



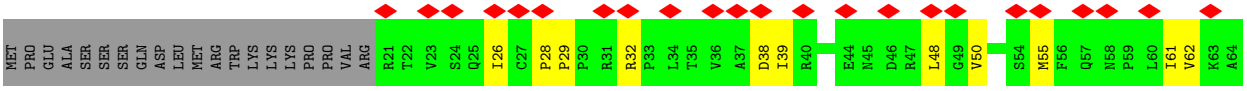

- Molecule 36: Cilia and flagella associated protein 77

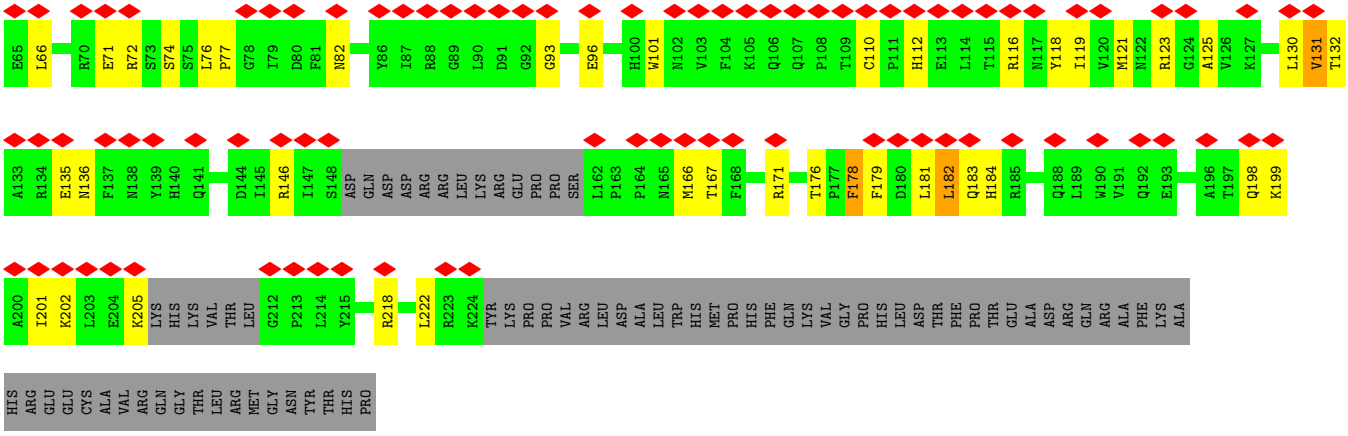
Chain 5X:




- Molecule 36: Cilia and flagella associated protein 77

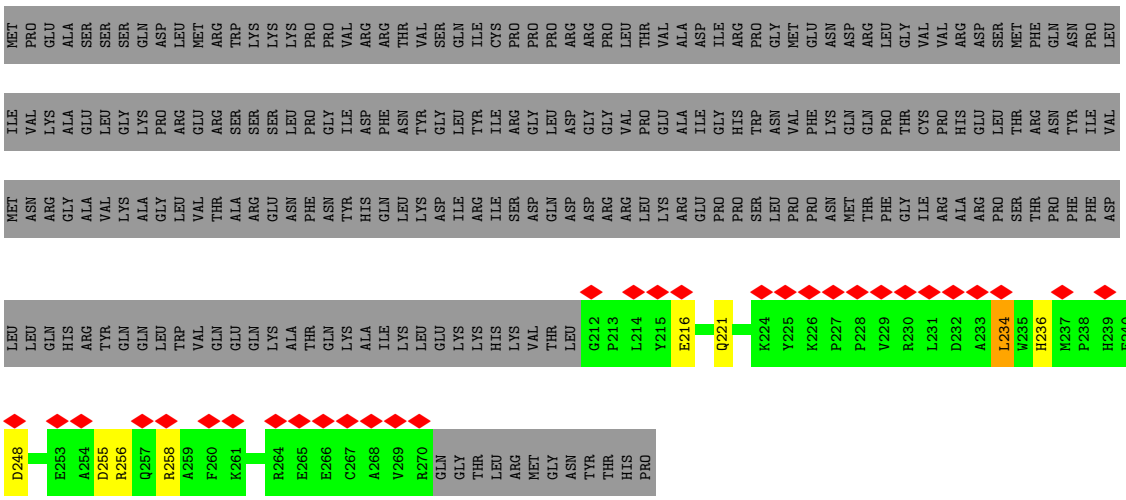
Chain 5Y:





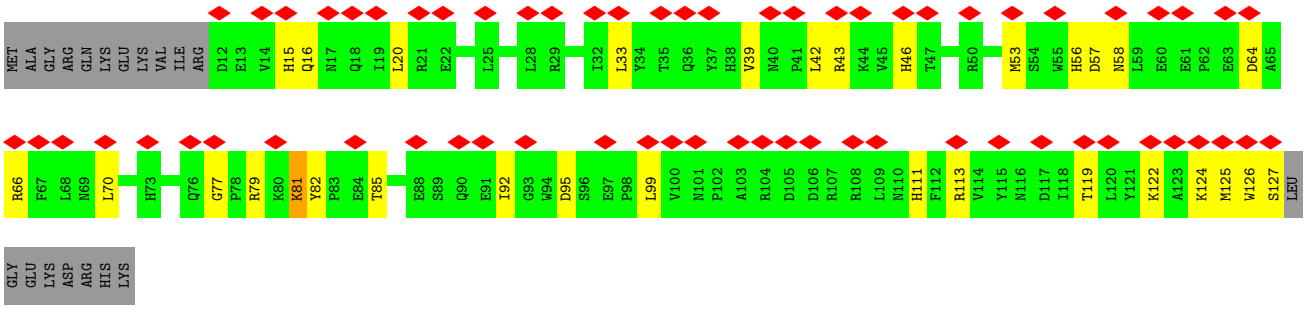

- Molecule 36: Cilia and flagella associated protein 77

Chain 5Z:



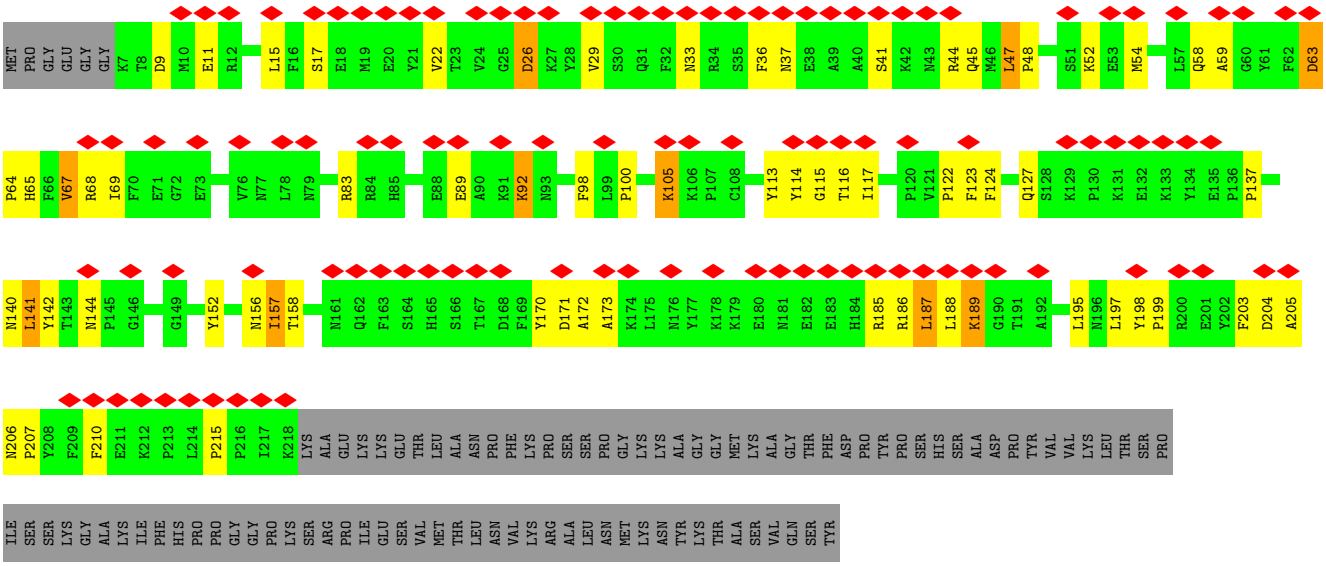

- Molecule 37: Cilia and flagella associated protein 144

Chain 6A:



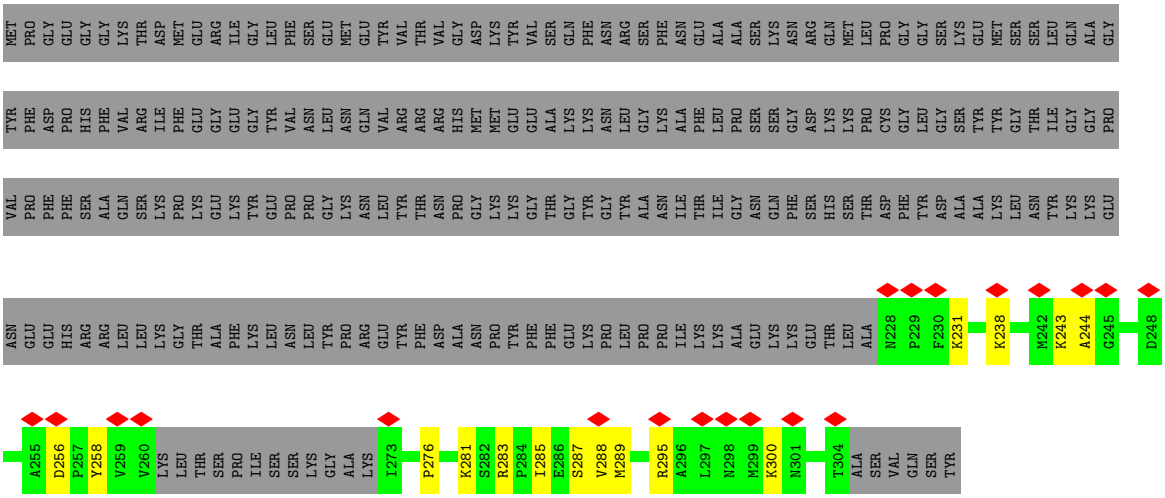

- Molecule 38: Cilia-and flagella-associated protein 96

Chain 6C:



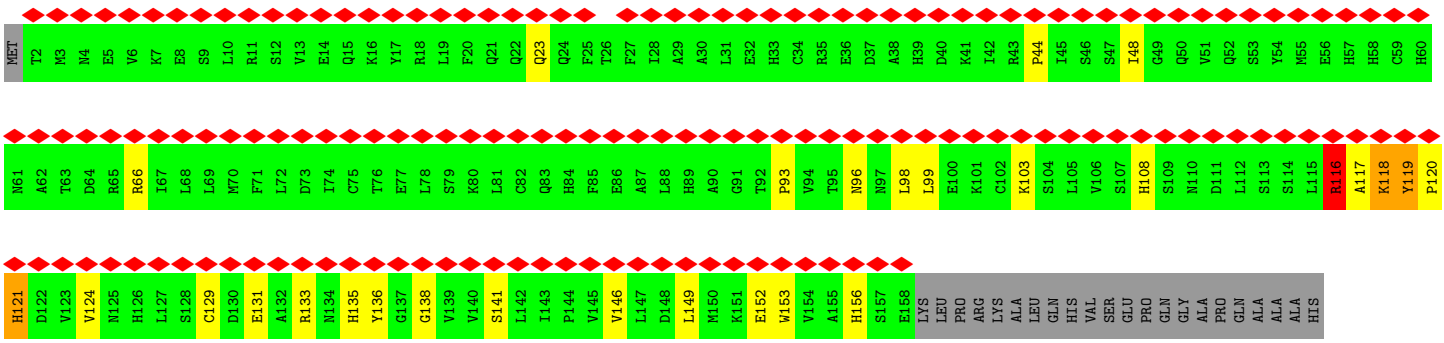

- Molecule 38: Cilia-and flagella-associated protein 96

Chain 6D:




- Molecule 39: Sperm acrosome associated 9

Chain 6F:



ALA PRO CYS GLY THR GLN PRO TRP LEU ARG LYS HIS LYS CYS TRP GLN LEU THR ARG ASP GLY LEU LYS PRO GLY ALA GLY ASP LYS ARG CYS SER LYS PRO PRO TRP ARG PRO PRO GLY GLY LYS LEU

- Molecule 39: Sperm acrosome associated 9

Chain 6G:

MET T2 M3 N4 E5 V6 K7 E8 S9 L10 R11 S12 V13 E14 Q15 K16 Y17 R18 L19 F20 Q21 Q22 Q23 Q24 F25 T26 F27 I28 A29 A30 L31 E32 H33 C34 R35 E36 D37 A38 H39 D40 K41 I42 R43 P44 I45 S46 S47 I48 G49 Q50 V51 Q52 S53 Y54 M55 E56 H57 H58 C59 H60

N61 A62 T63 D64 R65 R66 I67 L68 L69 M70 F71 L72 D73 I74 C75 T76 E77 L78 S79 K80 L81 C82 Q83 H84 F85 E86 A87 L88 H89 A90 G91 T92 P93 V94 T95 N96 N97 L98 L99 E100 K101 C102 K103 S104 L105 V106 S107 H108 S109 N110 D111 L112 S113 S114 L115 R116 A117 K118 Y119 P120

H121 D122 V123 V124 N125 H126 L127 S128 C129 D130 E131 A132 R133 N134 H135 Y136 G137 G138 V139 V140 S141 L142 I143 P144 V145 V146 L147 D148 L149 M150 K151 E152 W153 V154 A155 H156 S157 E158 LYS LEU PRO ARG LYS ALA LEU GLN HIS VAL SER GLU PRO GLN GLY ALA PRO GLN ALA ALA ALA HIS

ALA PRO CYS GLY THR GLN PRO TRP LEU ARG LYS HIS LYS CYS TRP GLN LEU THR ARG ASP GLY LEU LYS PRO GLY ALA GLY ASP LYS ARG CYS SER LYS PRO PRO TRP ARG PRO PRO GLY GLY LYS LEU

- Molecule 39: Sperm acrosome associated 9

Chain 6H:

MET T2 M3 N4 E5 V6 K7 E8 S9 L10 R11 S12 V13 E14 Q15 K16 Y17 R18 L19 F20 Q21 Q22 Q23 Q24 F25 T26 F27 I28 A29 A30 L31 E32 H33 C34 R35 E36 D37 A38 H39 D40 K41 I42 R43 P44 I45 S46 S47 I48 G49 Q50 V51 Q52 S53 Y54 M55 E56 H57 H58 C59 H60

N61 A62 T63 D64 R65 R66 I67 L68 L69 M70 F71 L72 D73 I74 C75 T76 E77 L78 S79 K80 L81 C82 Q83 H84 F85 E86 A87 L88 H89 A90 GLY THR PRO VAL THR ASN ASN LEU L99 E100 K101 C102 K103 S104 L105 V106 S107 H108 S109 N110 D111 L112 S113 S114 L115 ARG ALA LYS TYR PRO

HIS D122 V123 V124 N125 H126 L127 S128 CYS ASP E131 A132 R133 N134 H135 Y136 G137 G138 V139 V140 S141 L142 I143 P144 V145 V146 L147 D148 L149 M150 K151 E152 W153 V154 A155 H156 S157 E158 LYS LEU PRO ARG LYS ALA LEU GLN HIS VAL SER GLU PRO GLN GLY ALA PRO GLN ALA ALA ALA HIS

ALA PRO CYS GLY THR GLN PRO TRP LEU ARG LYS HIS LYS CYS TRP GLN LEU THR ARG ASP GLY LEU LYS PRO GLY ALA GLY ASP LYS ARG CYS SER LYS PRO PRO TRP ARG PRO PRO GLY GLY LYS LEU

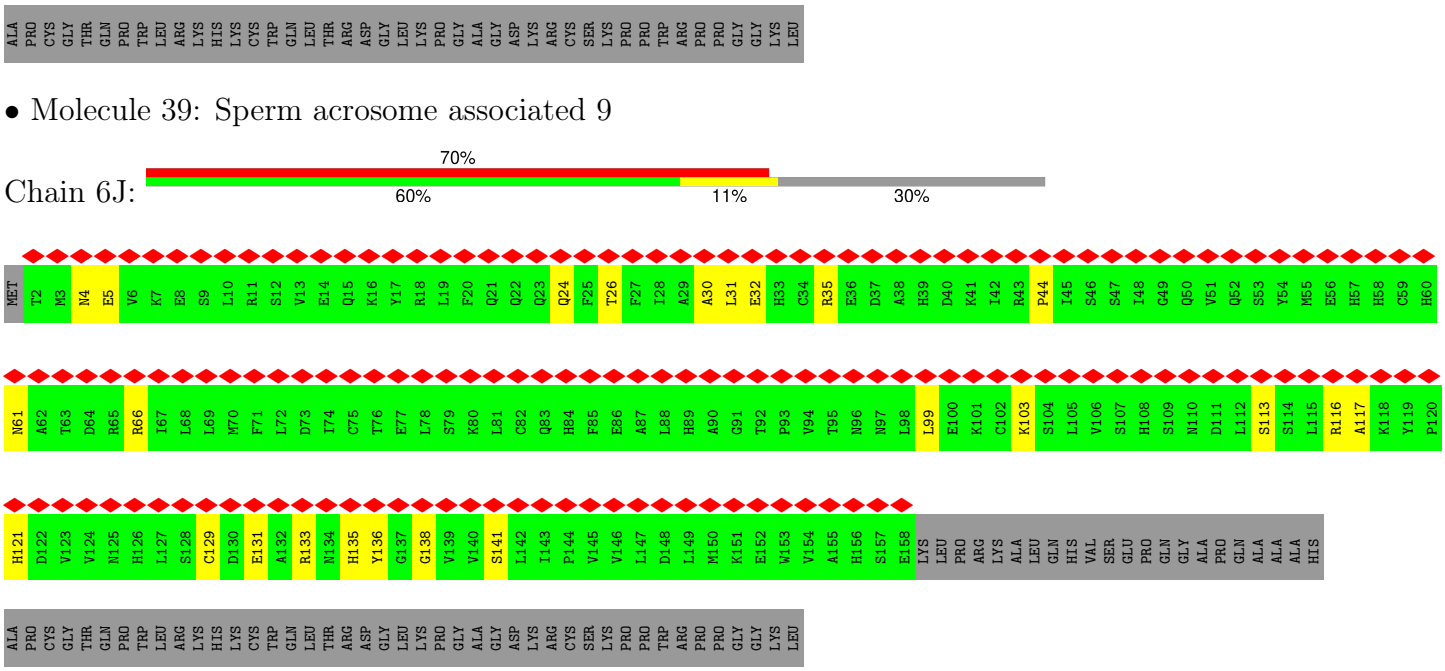
- Molecule 39: Sperm acrosome associated 9

Chain 6I:

MET T2 M3 N4 E5 V6 K7 E8 S9 L10 R11 S12 V13 E14 Q15 K16 Y17 R18 L19 F20 Q21 Q22 Q23 Q24 F25 T26 F27 I28 A29 A30 L31 E32 H33 C34 R35 E36 D37 A38 H39 D40 K41 I42 R43 P44 I45 S46 S47 I48 G49 Q50 V51 Q52 S53 Y64 M55 E56 H57 H58 C59 H60

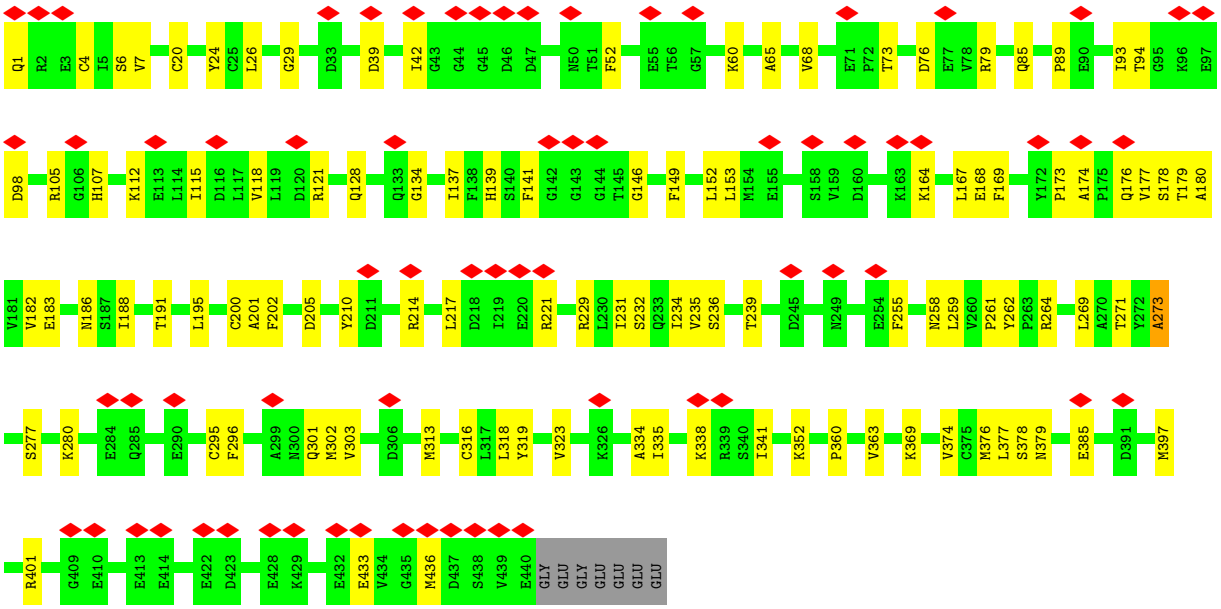
N61 A62 T63 D64 R65 R66 I67 L68 L69 M70 F71 L72 D73 I74 C75 T76 E77 L78 S79 K80 L81 C82 Q83 H84 F85 E86 A87 L88 H89 A90 G91 T92 P93 V94 T95 N96 N97 L98 L99 E100 K101 C102 K103 S104 L105 V106 S107 H108 S109 N110 D111 L112 S113 S114 L115 R116 A117 K118 Y119 P120

H121 D122 V123 V124 N125 H126 L127 S128 C129 D130 E131 A132 R133 N134 H135 Y136 G137 G138 V139 V140 S141 L142 I143 P144 V145 V146 L147 D148 L149 M150 K151 E152 W153 V154 A155 H156 S157 E158 LYS LEU PRO ARG LYS ALA LEU GLN HIS VAL SER GLU PRO GLN GLY ALA PRO GLN ALA ALA ALA HIS


ALA PRO CYS GLY THR GLN PRO TRP LEU ARG LYS HIS LYS CYS TRP GLN LEU THR ARG ASP GLY LEU LYS PRO GLY ALA GLY ASP LYS ARG CYS SER LYS PRO PRO TRP ARG PRO PRO GLY GLY LYS LEU
• Molecule 39: Sperm acrosome associated 9
Chain 6J:
70%
60%
11%
30%
MET T2 M3 N4 E5 V6 K7 E8 S9 L10 R11 S12 V13 E14 Q15 K16 Y17 R18 L19 F20 Q21 Q22 Q23 Q24 F25 T26 F27 I28 A29 A30 L31 E32 H33 C34 R35 E36 D37 A38 H39 D40 K41 I42 R43 P44 I45 S46 S47 I48 G49 Q50 V51 Q52 S53 Y54 M55 E56 H57 H58 C59 H60
N61 A62 T63 D64 R65 R66 I67 L68 L69 M70 F71 L72 D73 I74 C75 T76 E77 L78 S79 K80 L81 C82 Q83 H84 F85 E86 A87 L88 H89 A90 G91 T92 P93 V94 T95 N96 N97 L98 L99 E100 K101 C102 K103 S104 L105 V106 S107 H108 S109 N110 D111 L112 S113 S114 L115 R116 A117 K118 Y119 P120
H121 D122 V123 V124 N125 H126 L127 S128 C129 D130 E131 A132 R133 N134 H135 Y136 G137 G138 V139 V140 S141 L142 I143 P144 V145 V146 L147 D148 L149 M150 K151 E152 W153 V154 A155 H156 S157 E158 LYS LEU PRO ARG LYS ALA LEU GLN HIS VAL SER GLU PRO GLN GLY ALA PRO GLN ALA ALA ALA HIS
ALA PRO CYS GLY THR GLN PRO TRP LEU ARG LYS HIS LYS CYS TRP GLN LEU THR ARG ASP GLY LEU LYS PRO GLY ALA GLY ASP LYS ARG CYS SER LYS PRO PRO TRP ARG PRO PRO GLY GLY LYS LEU
• Molecule 39: Sperm acrosome associated 9
Chain 6K:
69%
58%
13%
30%
MET T2 M3 N4 E5 V6 K7 E8 S9 L10 R11 S12 V13 E14 Q15 K16 Y17 R18 L19 F20 Q21 Q22 Q23 Q24 F25 T26 F27 I28 A29 A30 L31 E32 H33 C34 R35 E36 D37 A38 H39 D40 K41 I42 R43 P44 I45 S46 S47 I48 G49 Q50 V51 Q52 S53 Y54 M55 E56 H57 H58 C59 H60
N61 A62 T63 D64 R65 R66 I67 L68 L69 M70 F71 L72 D73 I74 C75 T76 E77 L78 S79 K80 L81 C82 Q83 H84 F85 E86 A87 L88 H89 A90 G91 T92 P93 V94 T95 N96 N97 L98 L99 E100 K101 C102 K103 S104 L105 V106 S107 H108 S109 N110 D111 L112 S113 S114 L115 R116 A117 K118 Y119 P120
H121 D122 V123 V124 N125 H126 L127 S128 C129 D130 E131 A132 R133 N134 H135 Y136 G137 G138 V139 V140 S141 L142 I143 P144 V145 V146 L147 D148 L149 M150 K151 E152 W153 V154 A155 H156 S157 E158 LYS LEU PRO ARG LYS ALA LEU GLN HIS VAL SER GLU PRO GLN GLY ALA PRO GLN ALA ALA ALA HIS
ALA PRO CYS GLY THR GLN PRO TRP LEU ARG LYS HIS LYS CYS TRP GLN LEU THR ARG ASP GLY LEU LYS PRO GLY ALA GLY ASP LYS ARG CYS SER LYS PRO PRO TRP ARG PRO PRO GLY GLY LYS LEU
• Molecule 39: Sperm acrosome associated 9
Chain 6L:
61%
46%
12%
39%
MET T2 M3 N4 E5 V6 K7 E8 S9 L10 R11 S12 V13 E14 Q15 K16 Y17 R18 L19 F20 Q21 Q22 Q23 Q24 F25 T26 F27 I28 A29 A30 L31 E32 H33 CYS ARG GLU ASP ALA HIS ASP LYS I42 R43 P44 I45 S46 S47 I48 G49 Q50 V51 Q52 S53 Y54 MET GLU HIS HIS CYS HIS
ASN ALA THR ASP ARG ARG I67 L68 L69 M70 F71 L72 D73 I74 C75 T76 E77 L78 S79 K80 L81 C82 Q83 H84 F85 E86 A87 L88 H89 A90 G91 T92 P93 V94 T95 N96 N97 L98 L99 E100 K101 C102 K103 S104 L105 V106 S107 H108 S109 N110 D111 L112 S113 S114 L115 R116 A117 K118 Y119 P120
H121 D122 V123 V124 N125 H126 L127 S128 C129 D130 E131 A132 R133 N134 H135 Y136 G137 G138 V139 V140 S141 L142 I143 P144 V145 V146 L147 D148 L149 M150 K151 E152 W153 V154 A155 H156 S157 E158 LYS LEU PRO ARG LYS ALA LEU GLN HIS VAL SER GLU PRO GLN GLY ALA PRO GLN ALA ALA ALA HIS

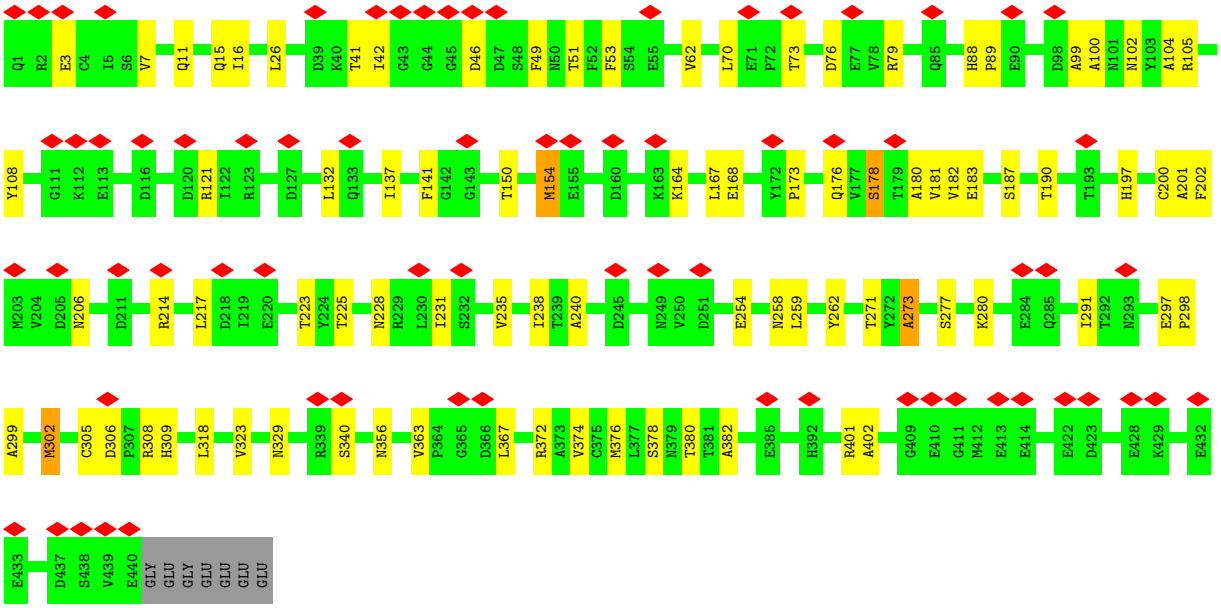
- Molecule 40: Tubulin alpha chain

Chain AA:



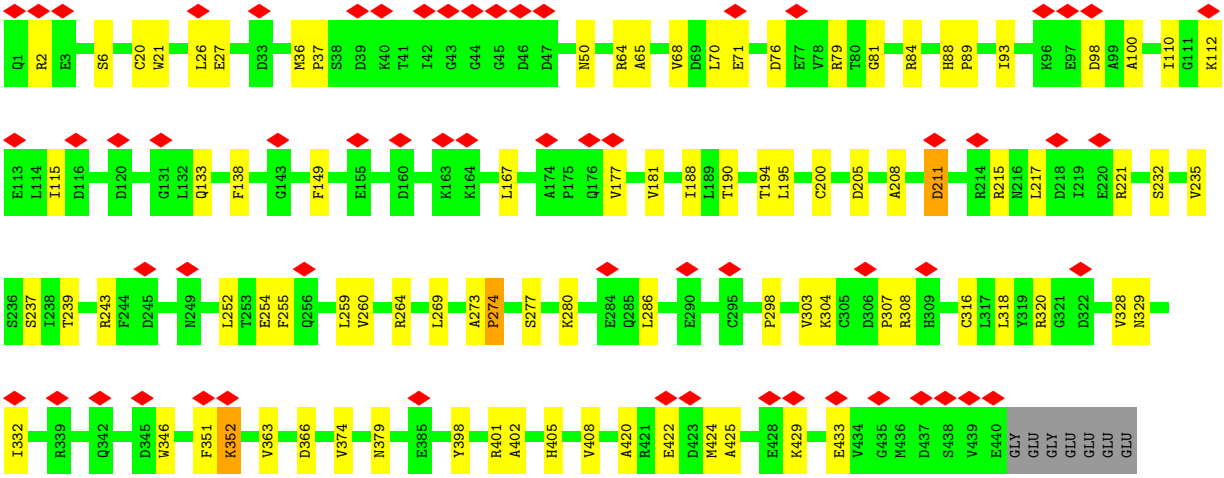

- Molecule 40: Tubulin alpha chain

Chain AE:




- Molecule 40: Tubulin alpha chain

Chain AF:




- Molecule 40: Tubulin alpha chain

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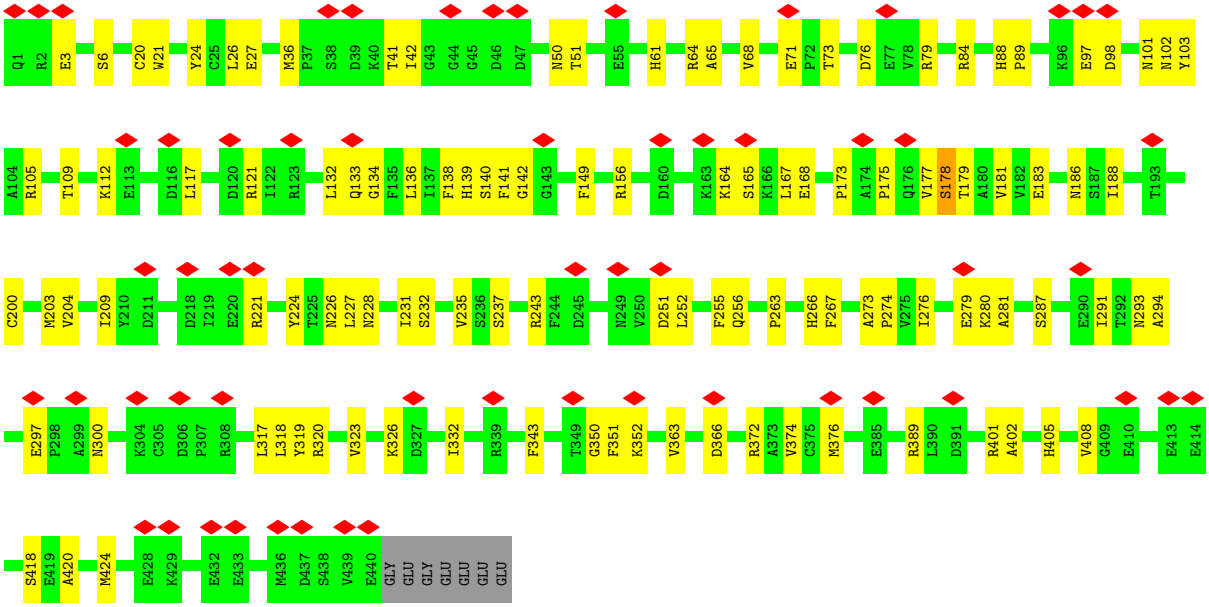
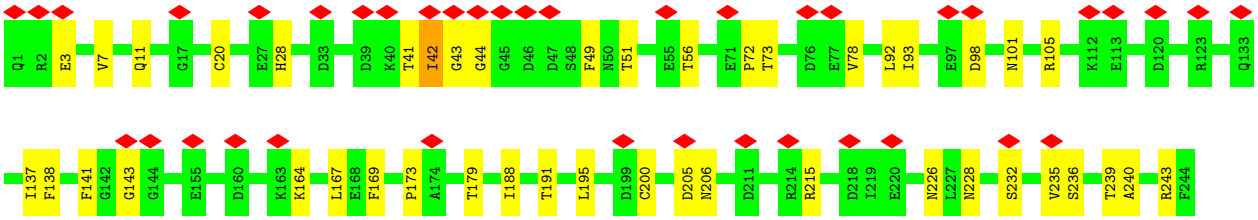
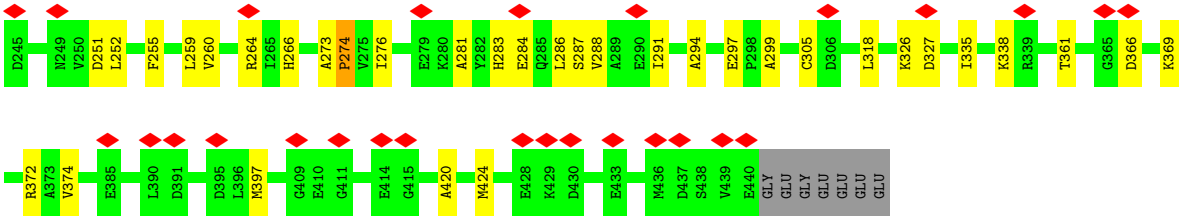



- Molecule 40: Tubulin alpha chain

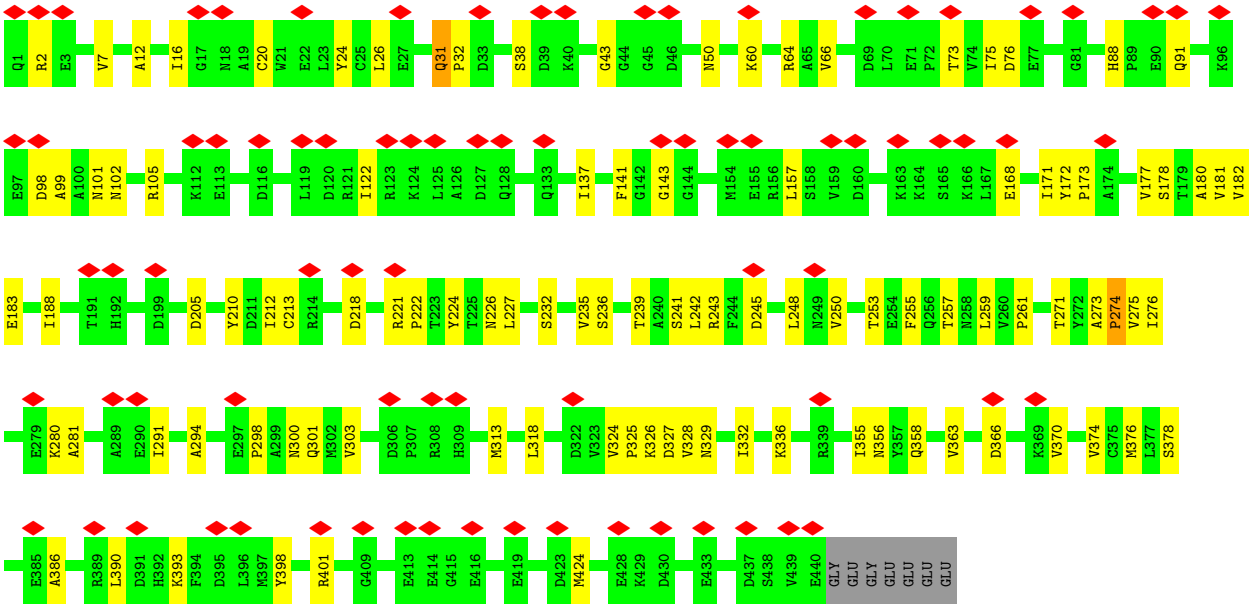
Chain AH:





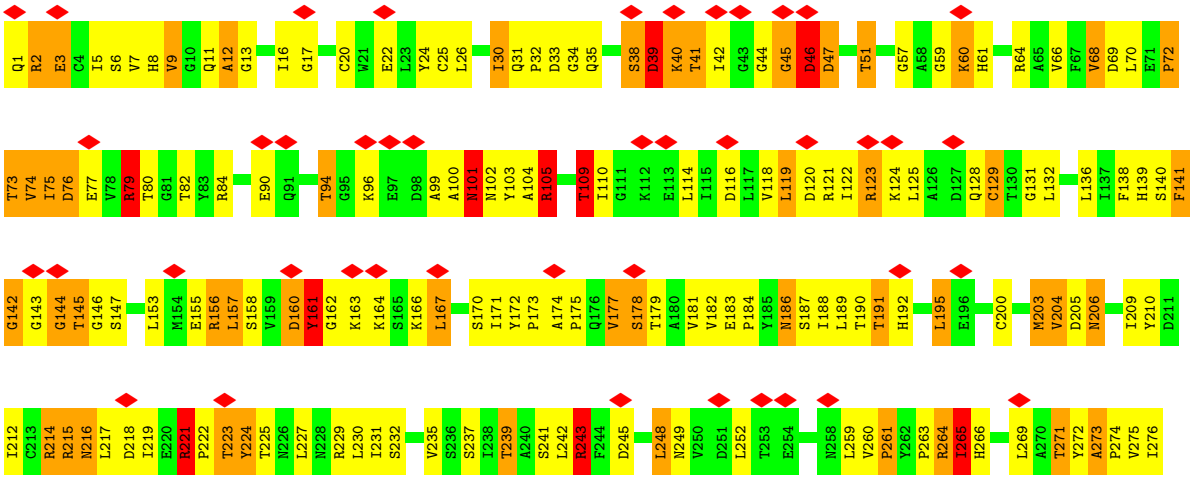

• Molecule 40: Tubulin alpha chain

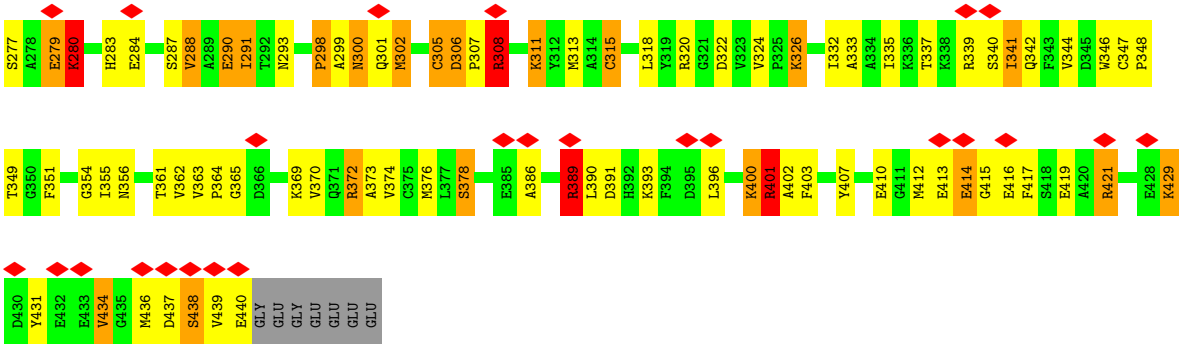
Chain BA:




• Molecule 40: Tubulin alpha chain

Chain BE:






- Molecule 40: Tubulin alpha chain

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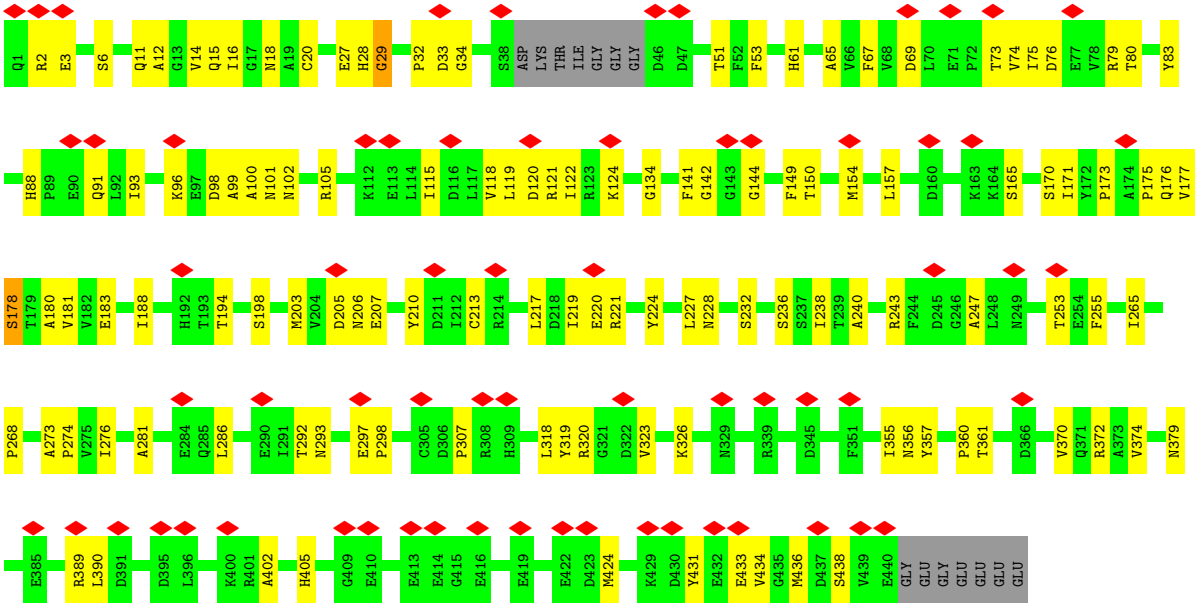


- Molecule 40: Tubulin alpha chain

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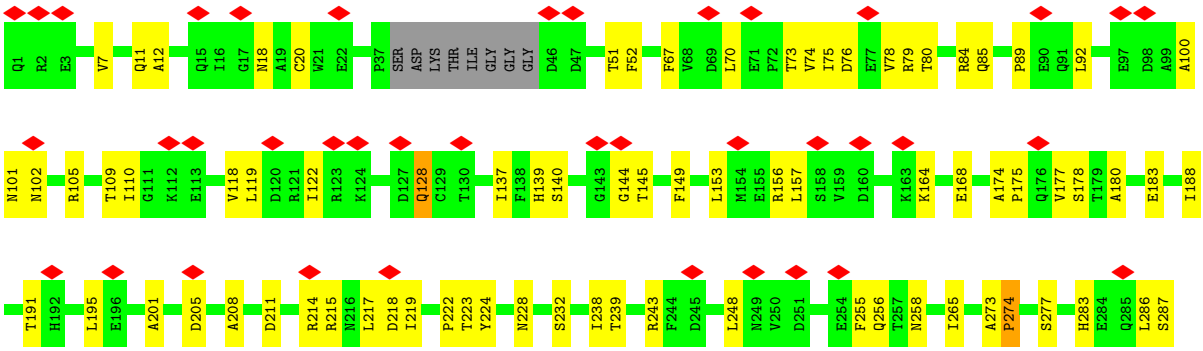
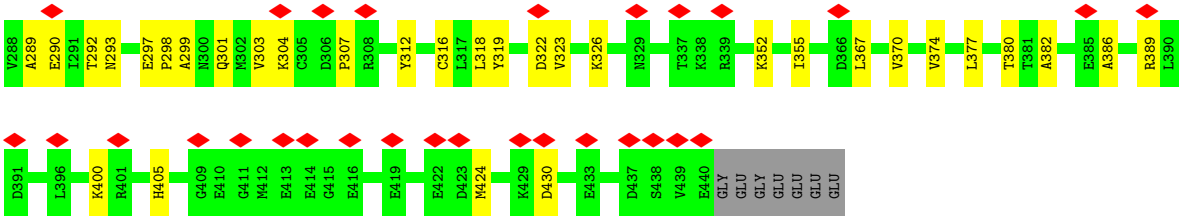
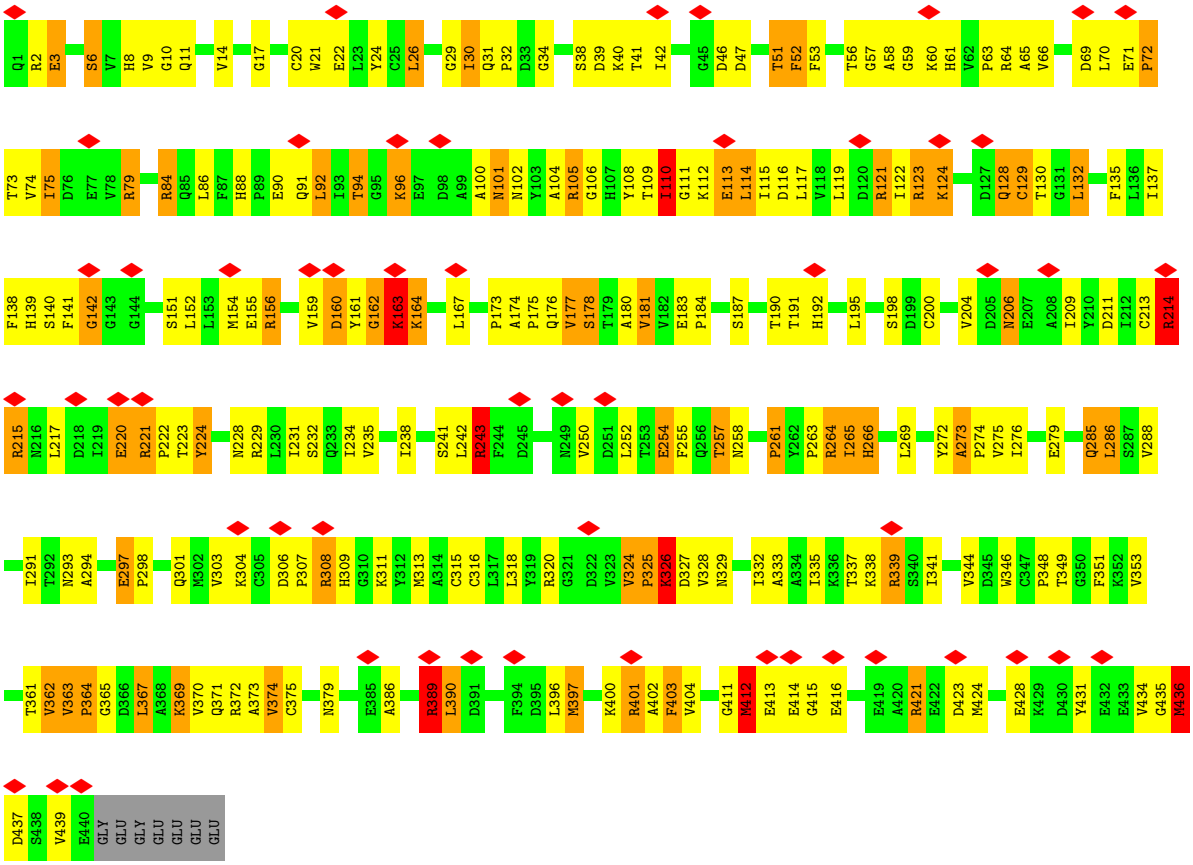




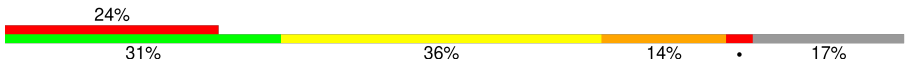

• Molecule 40: Tubulin alpha chain

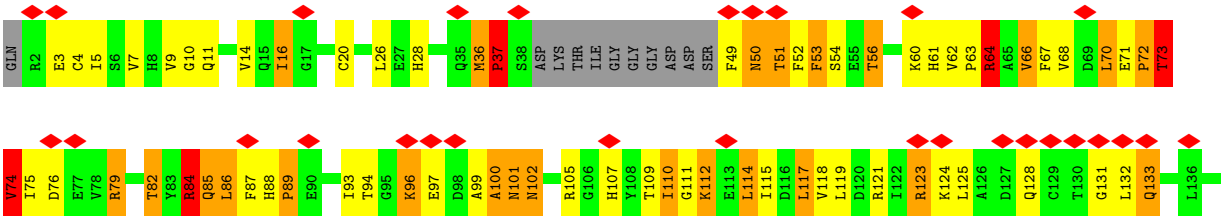
Chain BH:

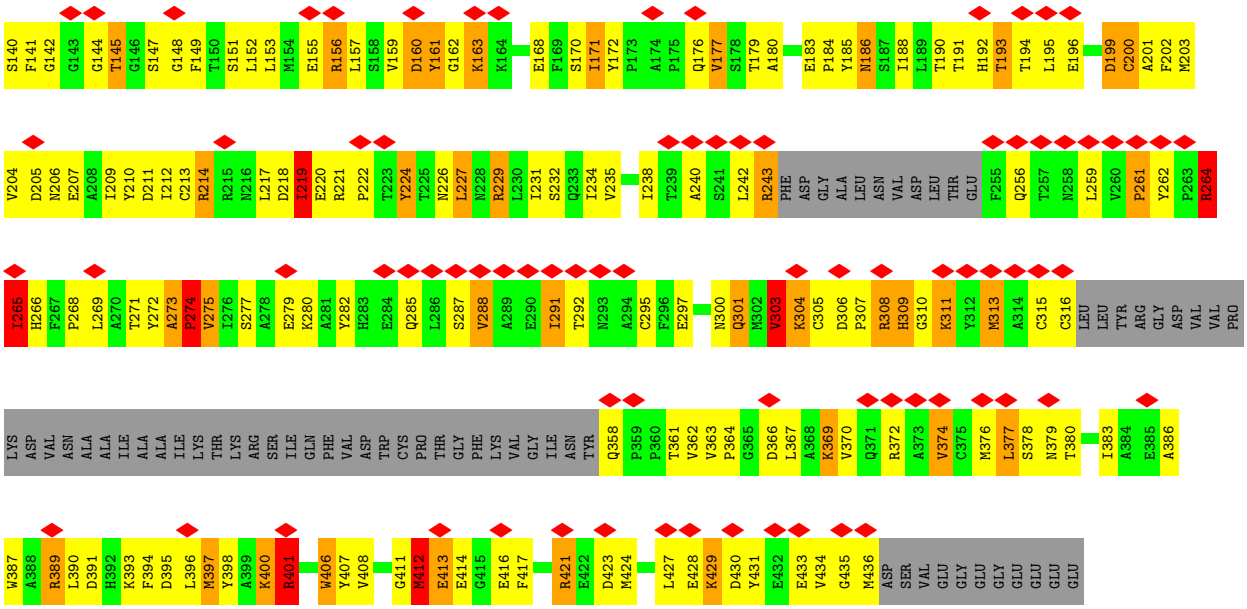



• Molecule 40: Tubulin alpha chain

Chain BI:

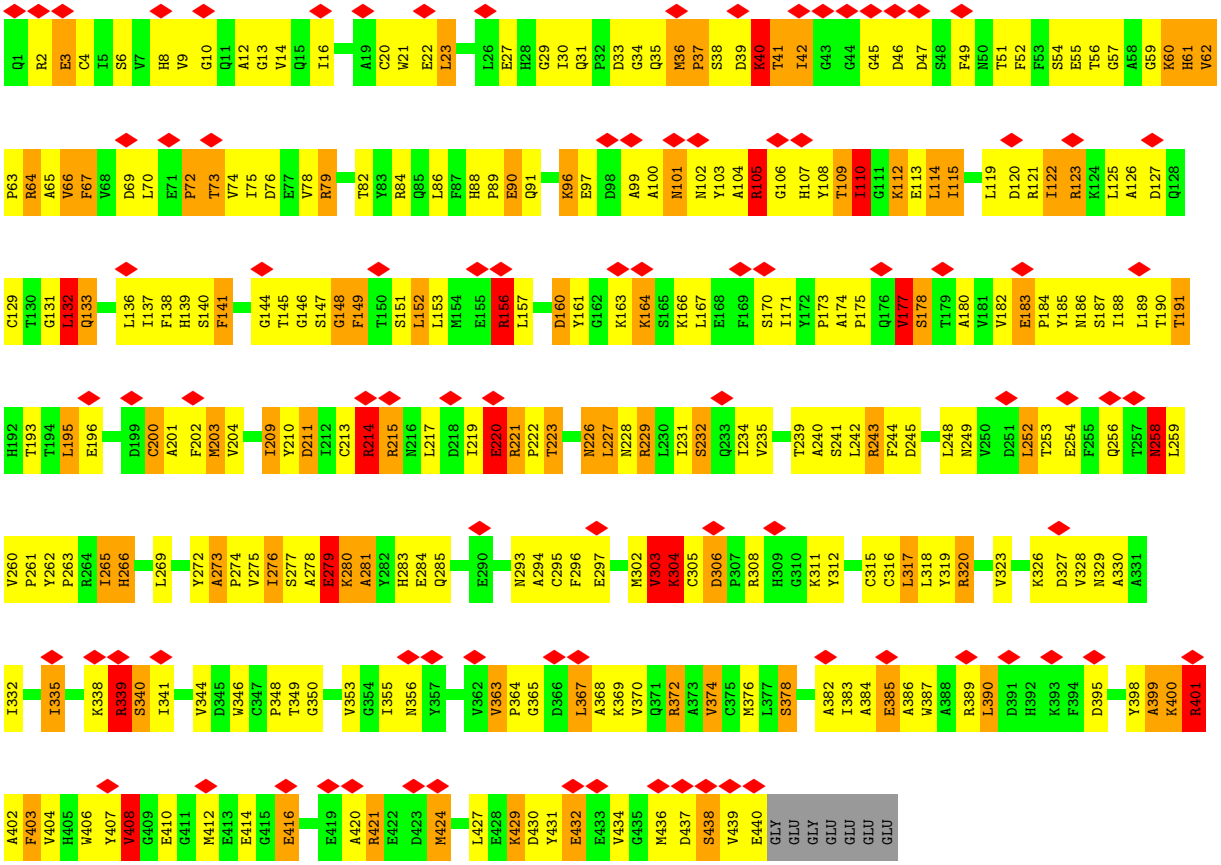




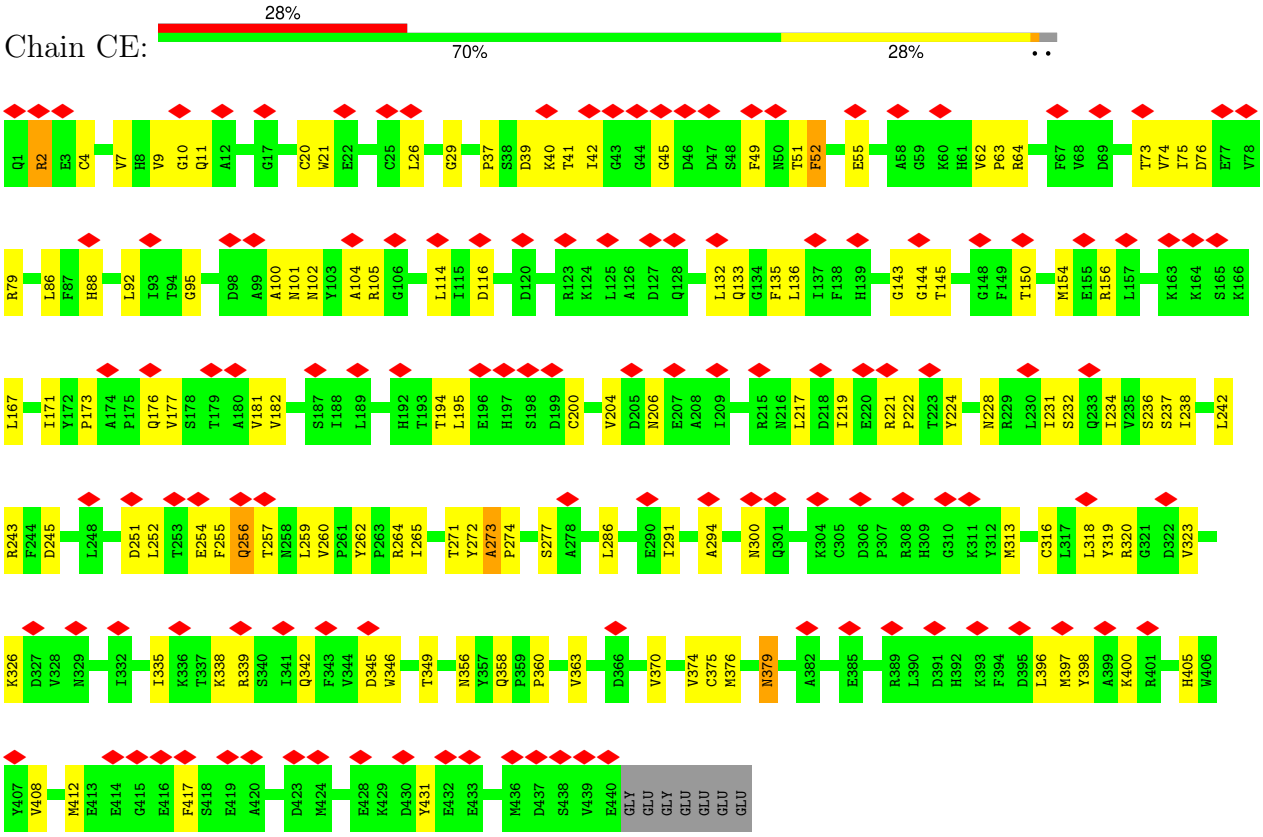

• Molecule 40: Tubulin alpha chain

Chain CA:




• Molecule 40: Tubulin alpha chain

Chain CE:

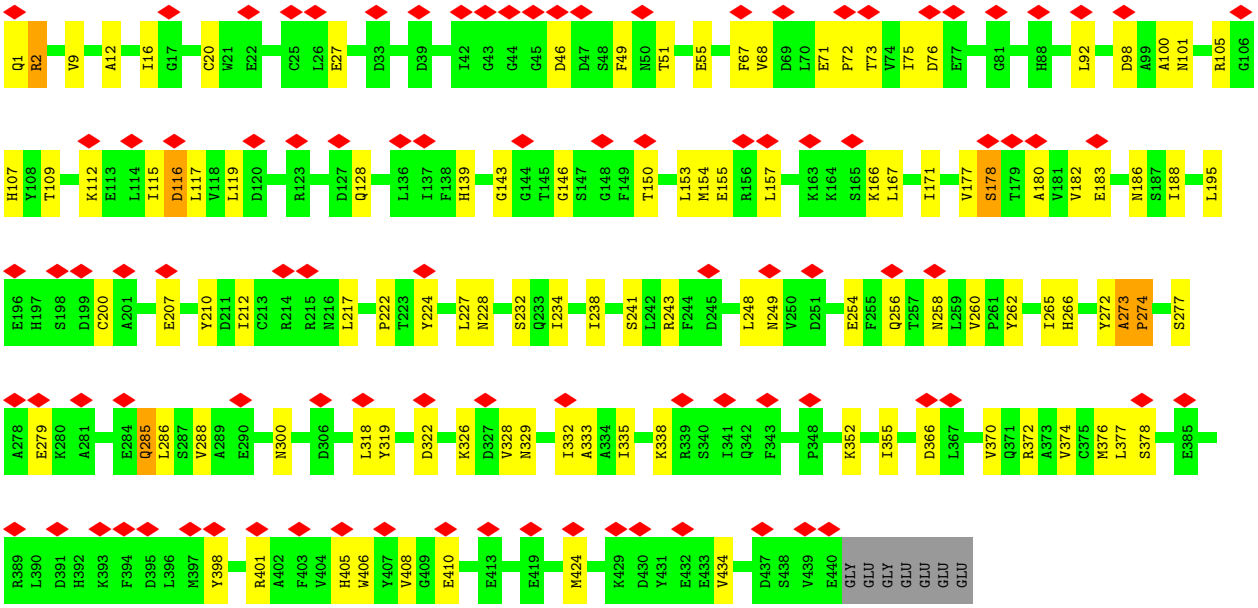



- Molecule 40: Tubulin alpha chain

Chain CF:

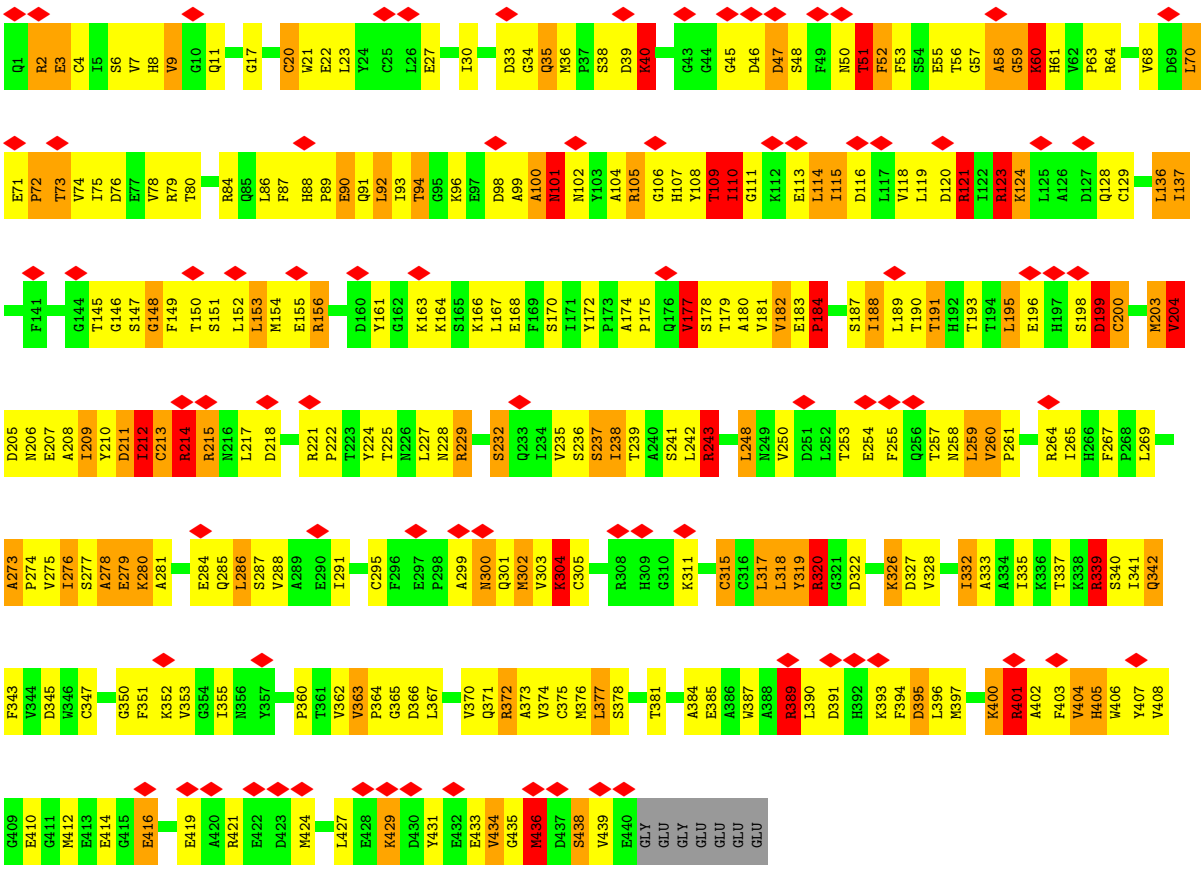
- Molecule 40: Tubulin alpha chain

Chain CG:



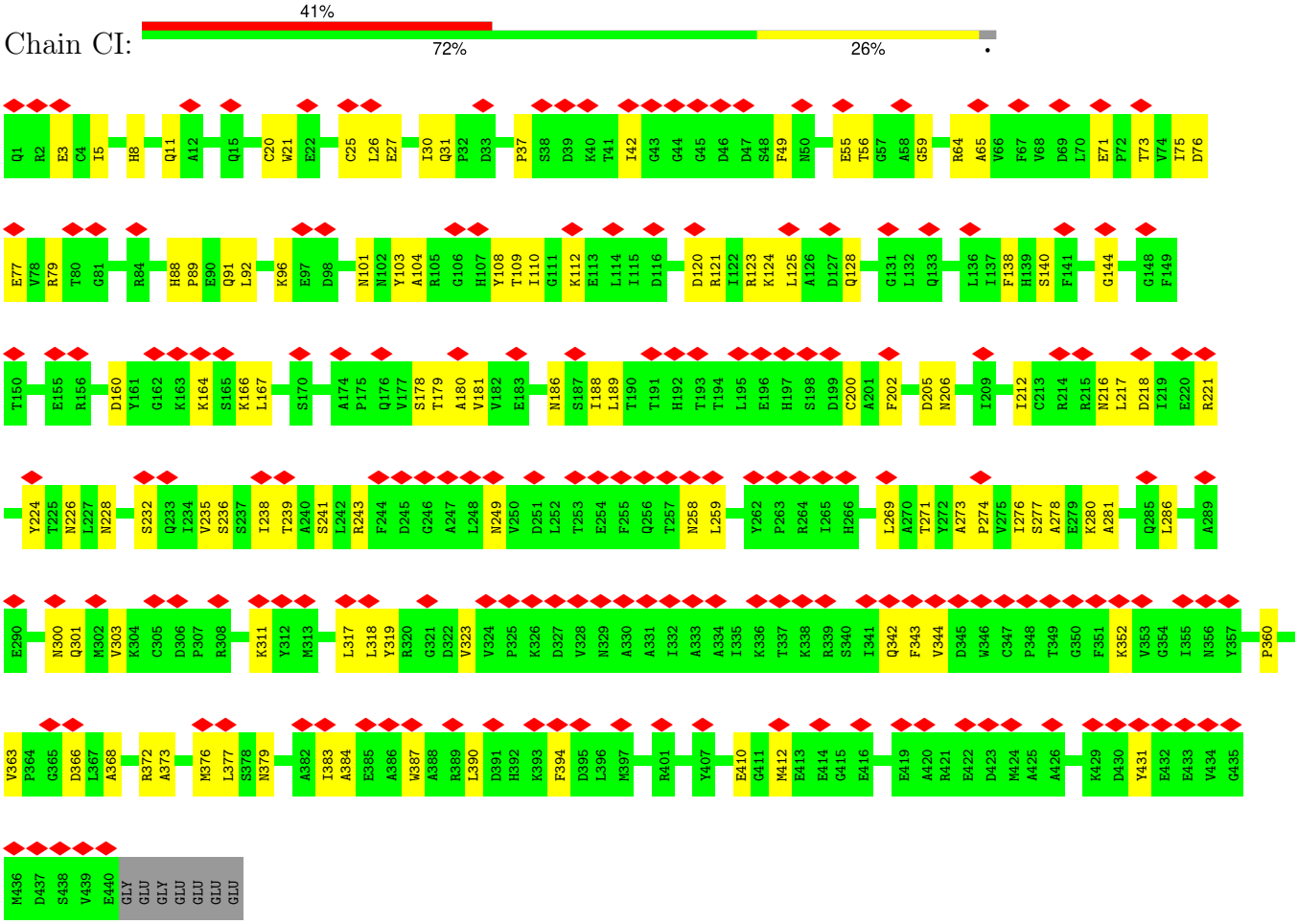

- Molecule 40: Tubulin alpha chain

Chain CH:



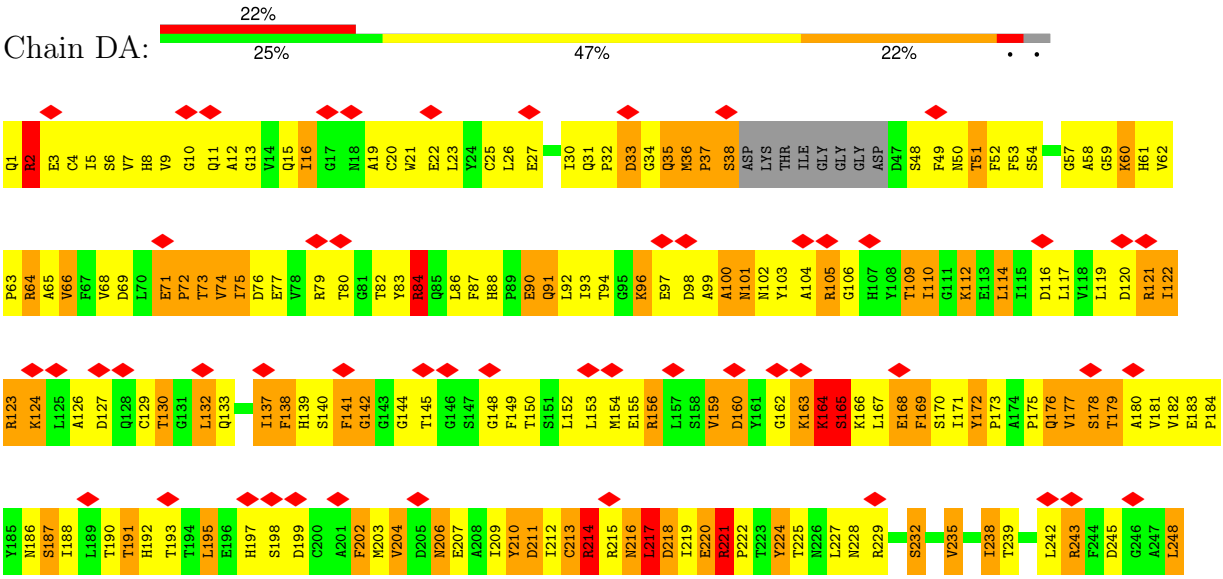
- Molecule 40: Tubulin alpha chain

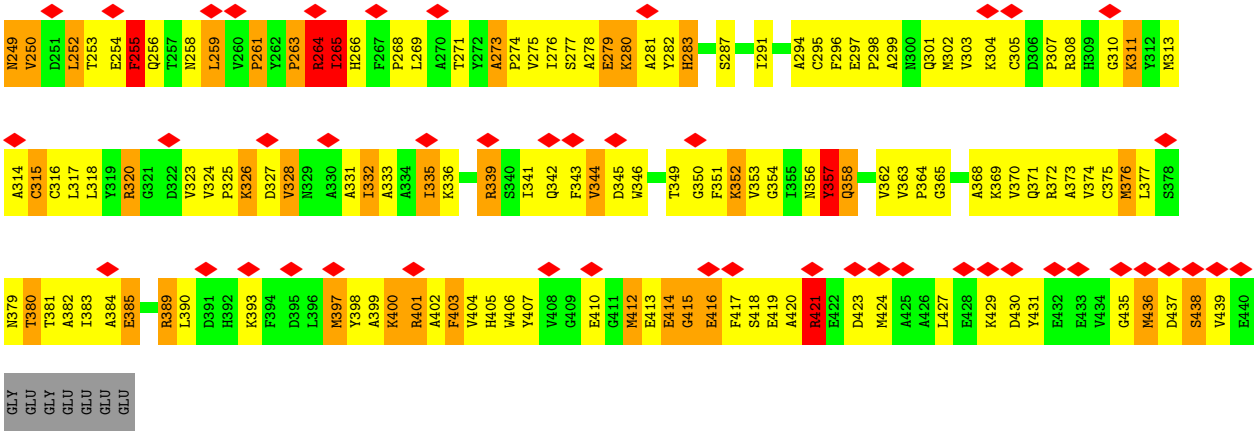
Chain CI:




- Molecule 40: Tubulin alpha chain

Chain DA:






- Molecule 40: Tubulin alpha chain

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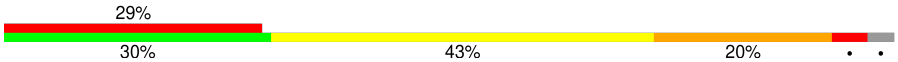
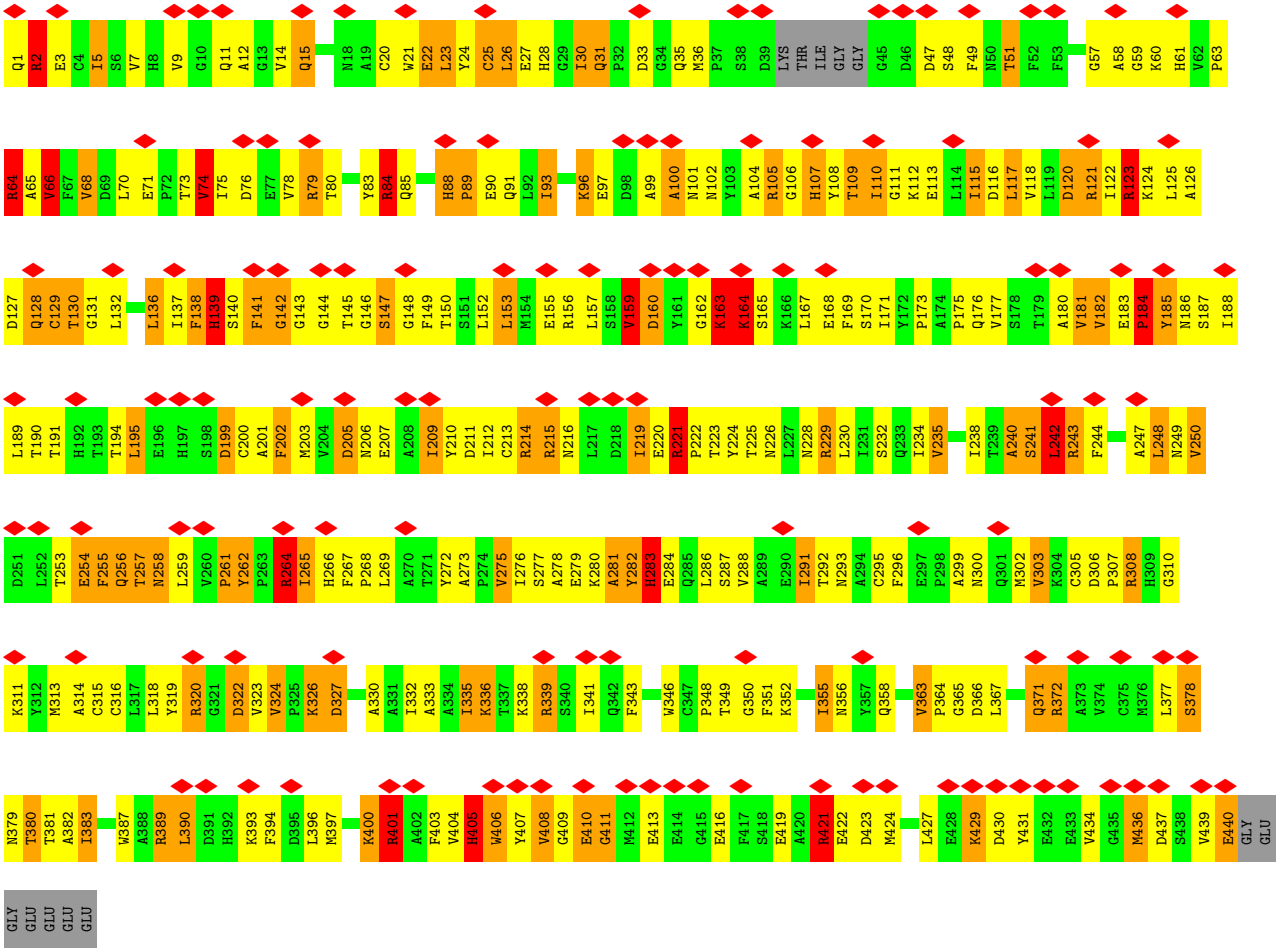
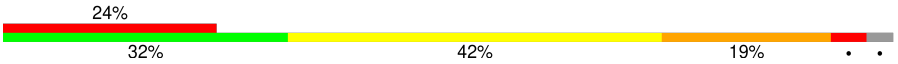
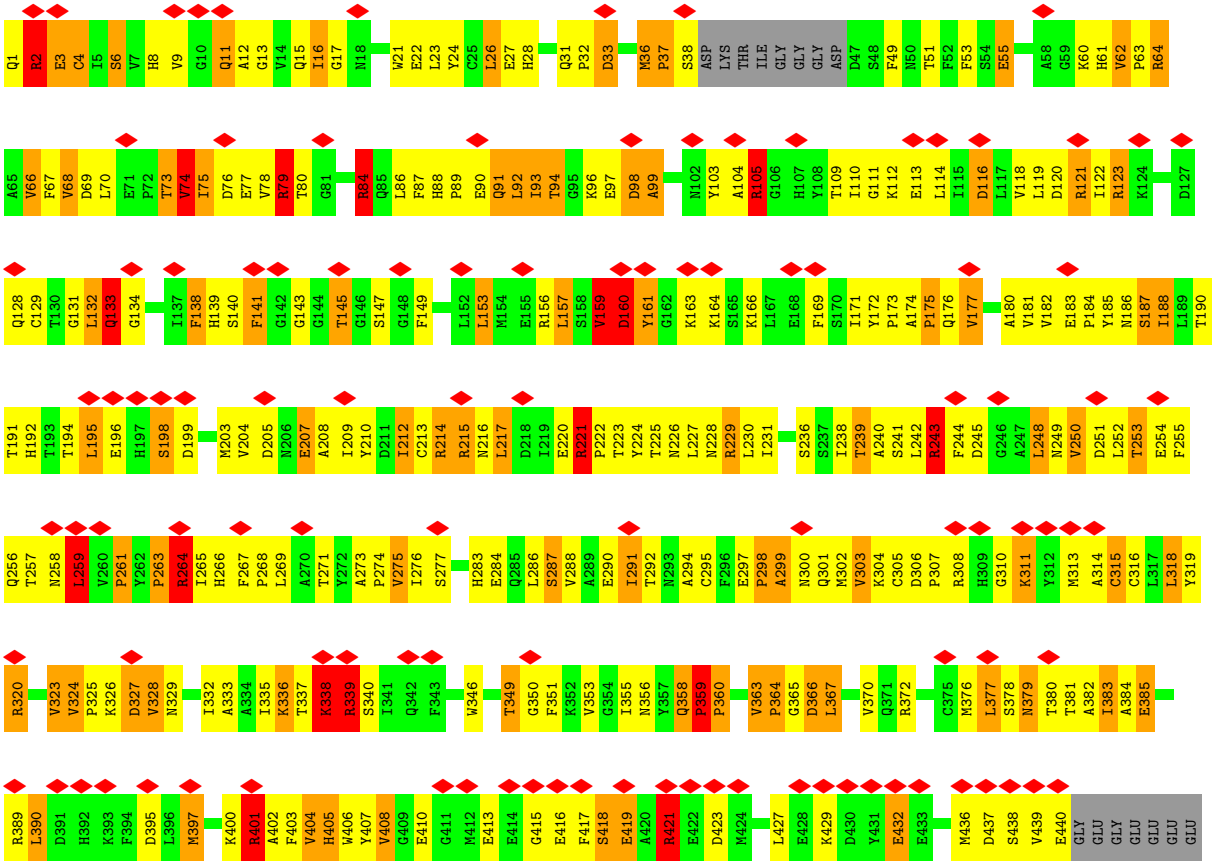



- Molecule 40: Tubulin alpha chain

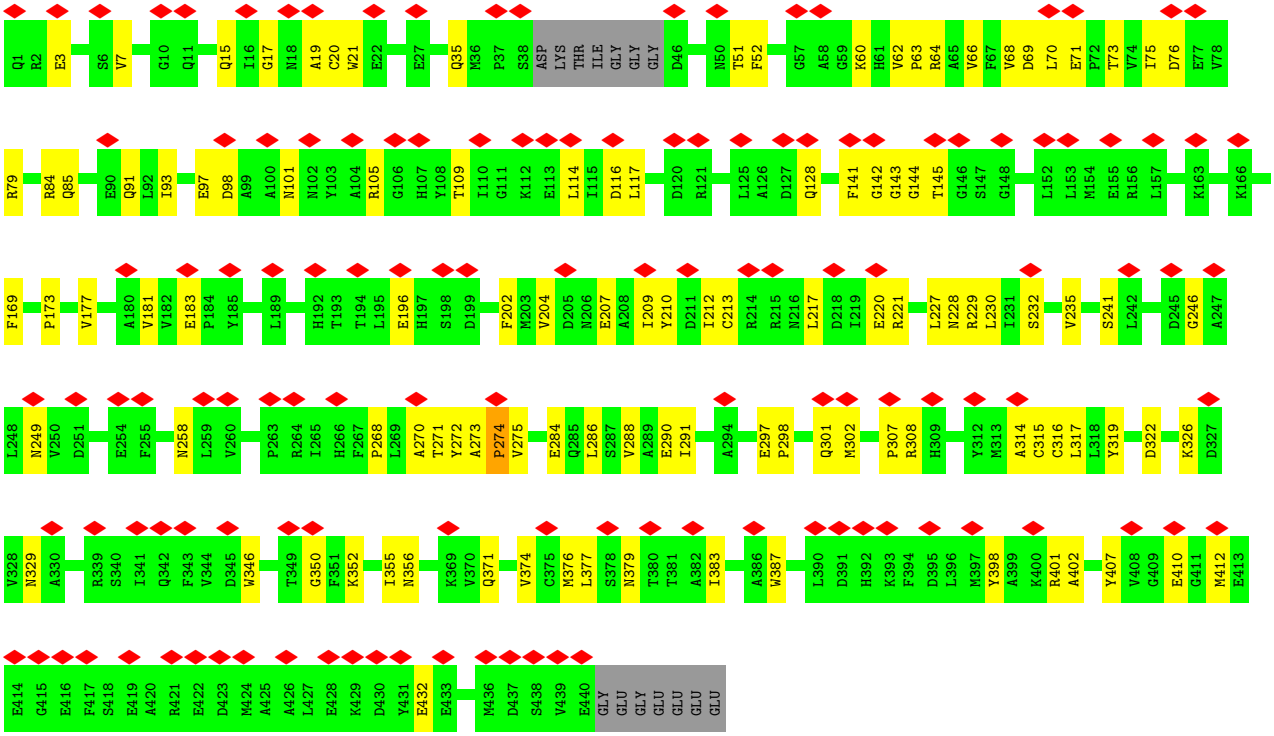
Chain DF:





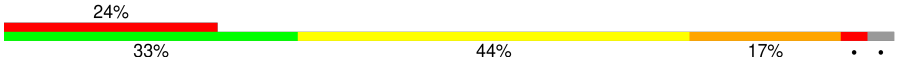
- Molecule 40: Tubulin alpha chain

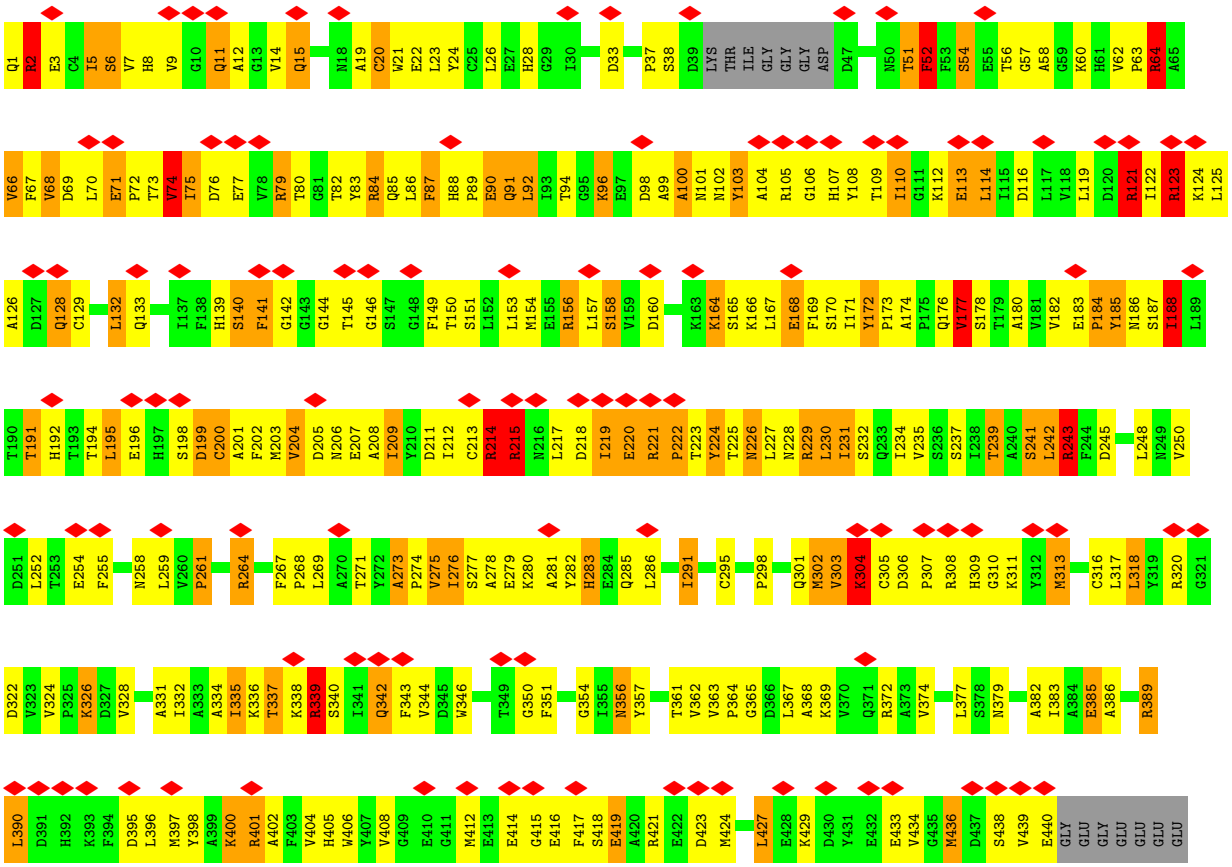
Chain DG:



- Molecule 40: Tubulin alpha chain

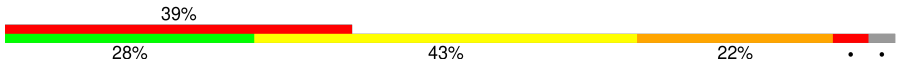
Chain DH:

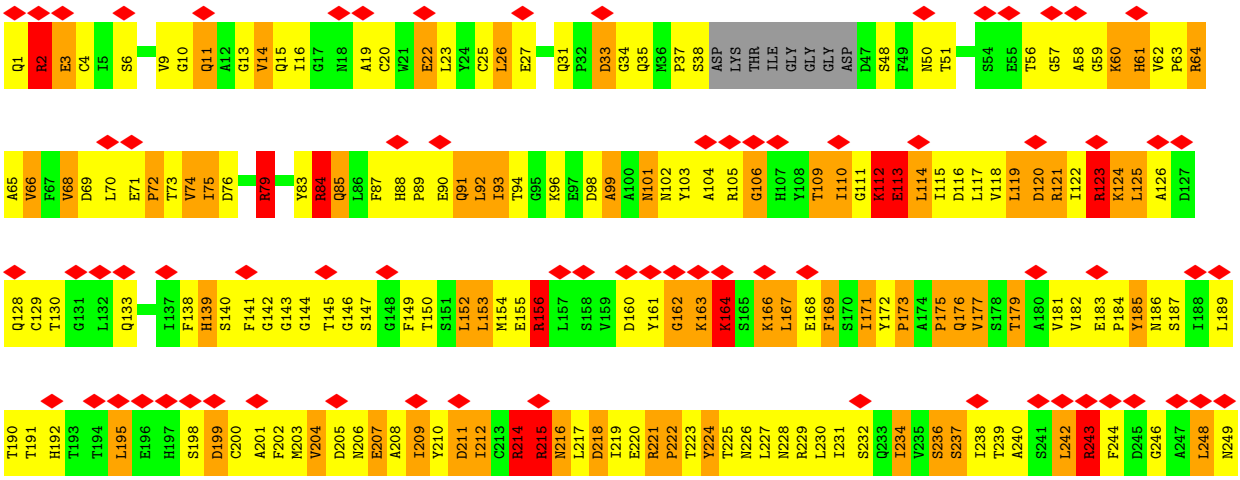


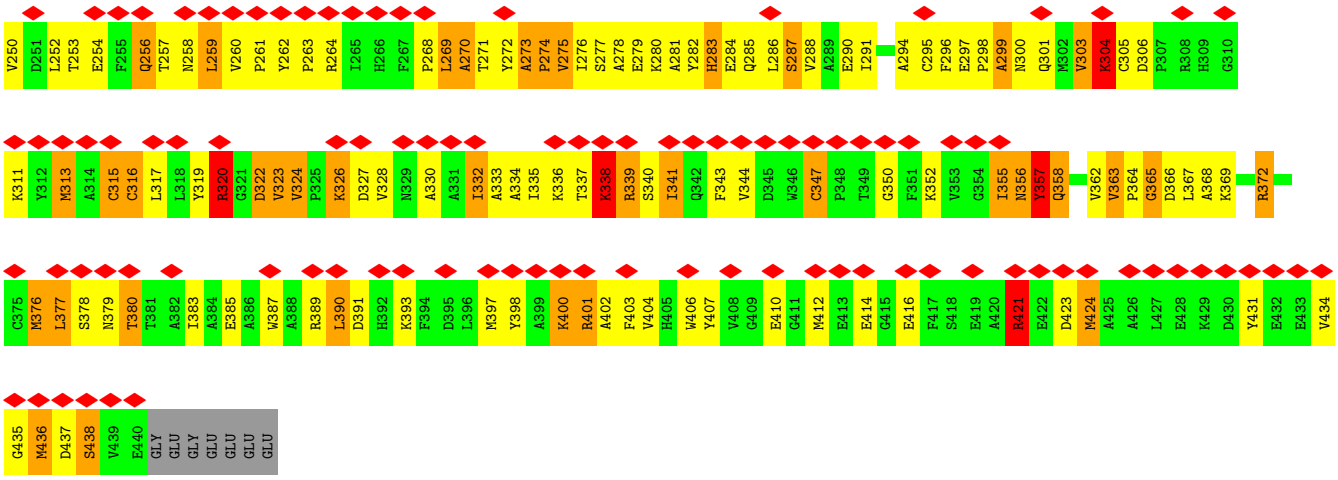




- Molecule 40: Tubulin alpha chain

Chain DI:






- Molecule 40: Tubulin alpha chain

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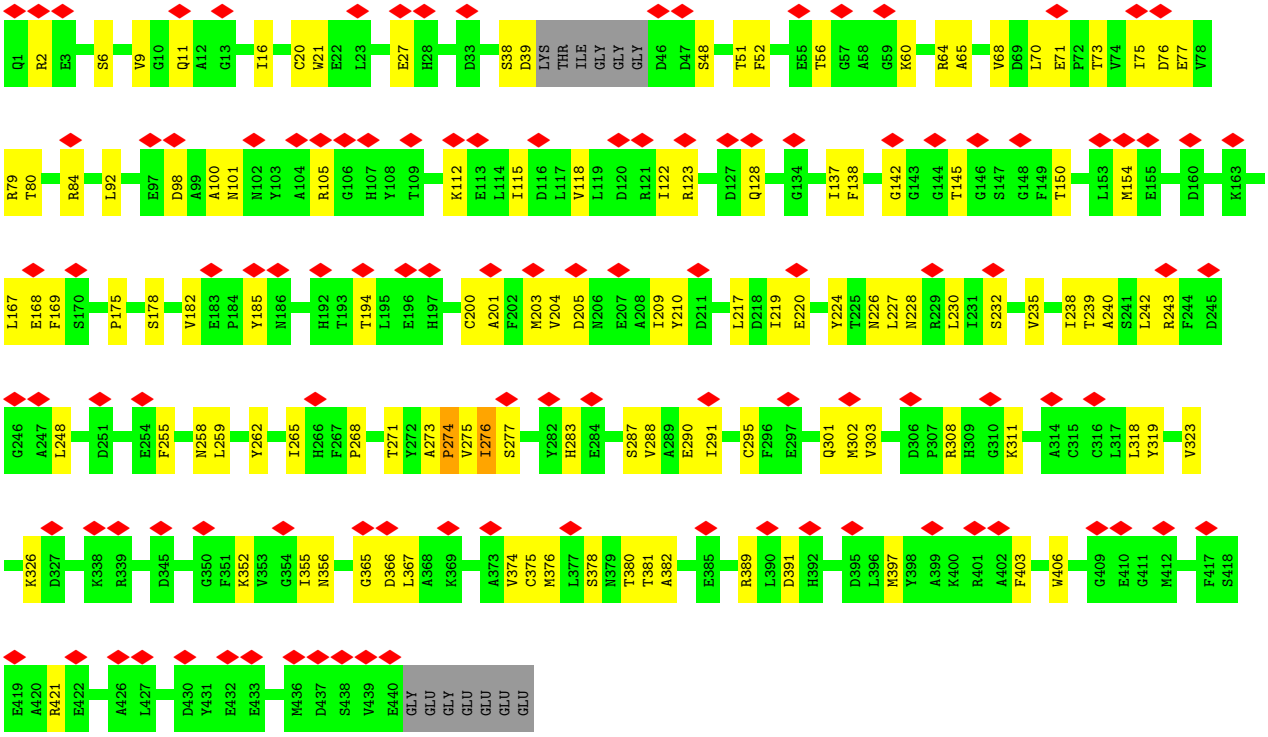
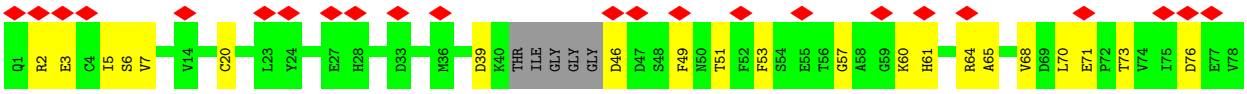


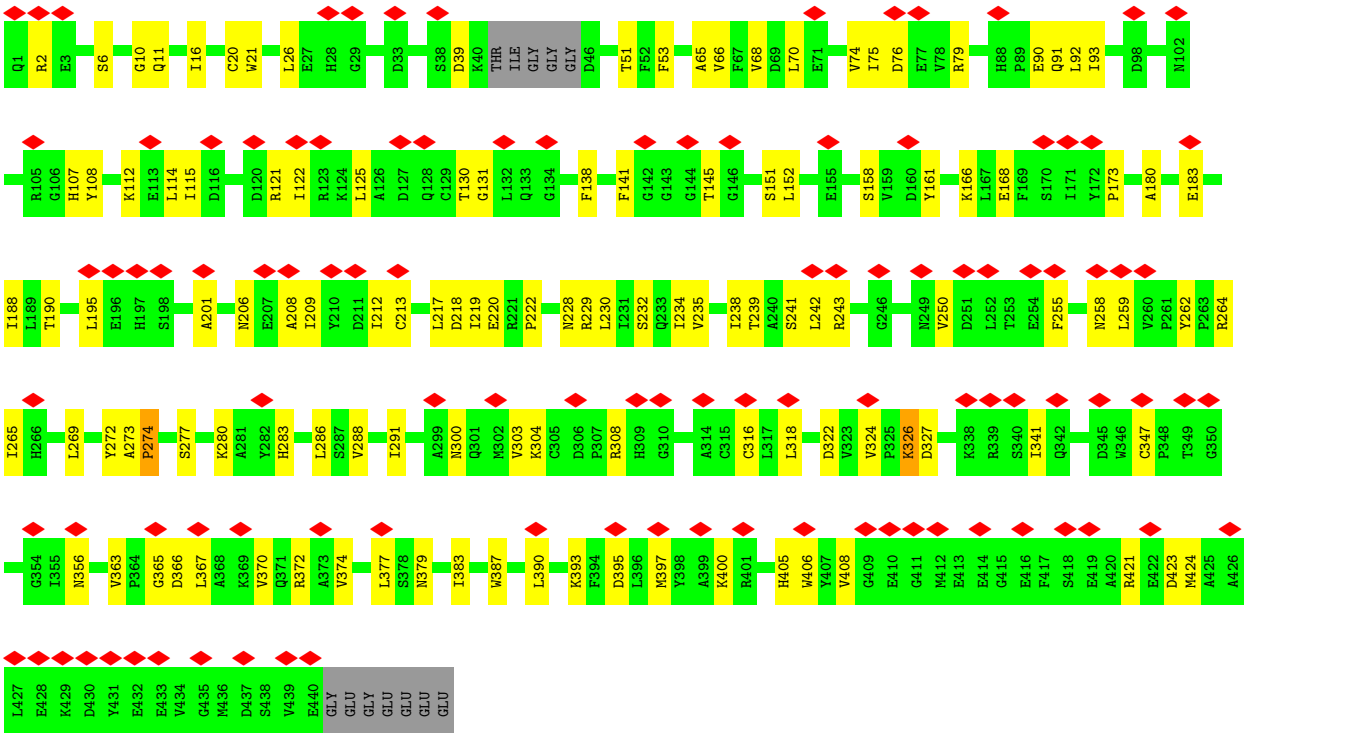

- Molecule 40: Tubulin alpha chain

Chain EE:



- Molecule 40: Tubulin alpha chain

Chain EF:




- Molecule 40: Tubulin alpha chain

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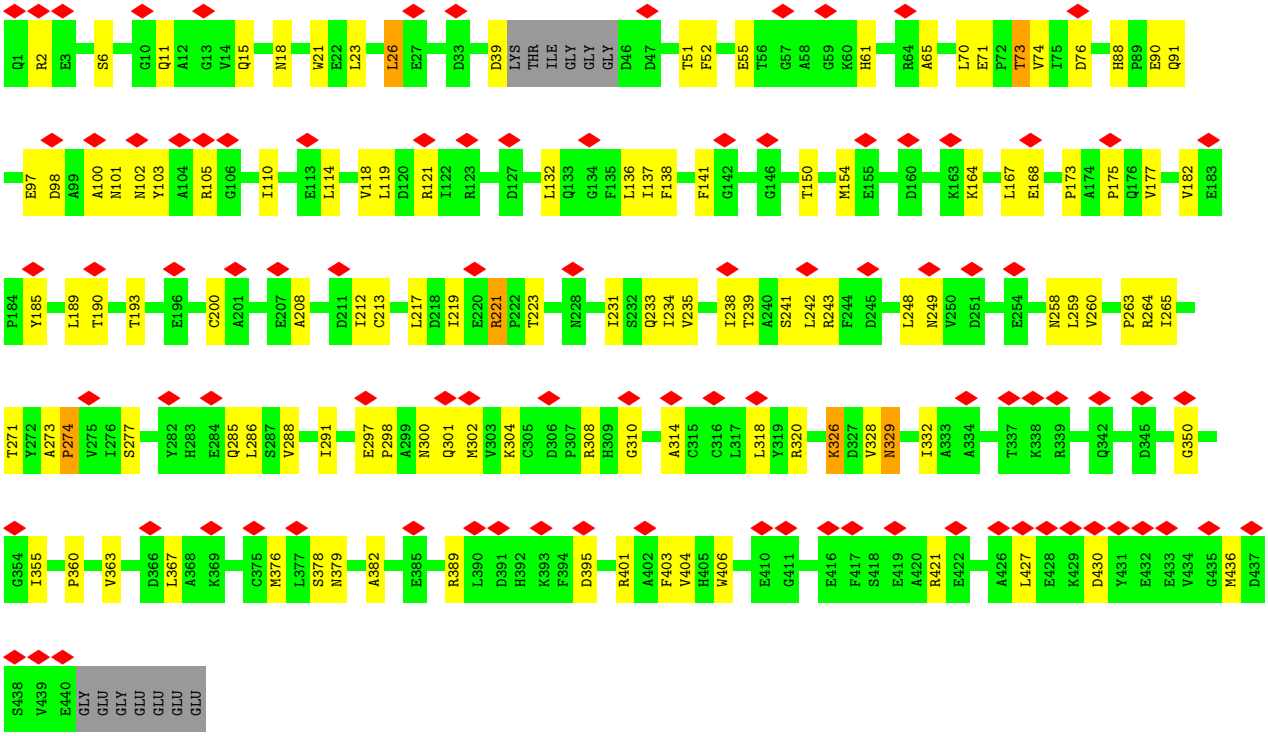
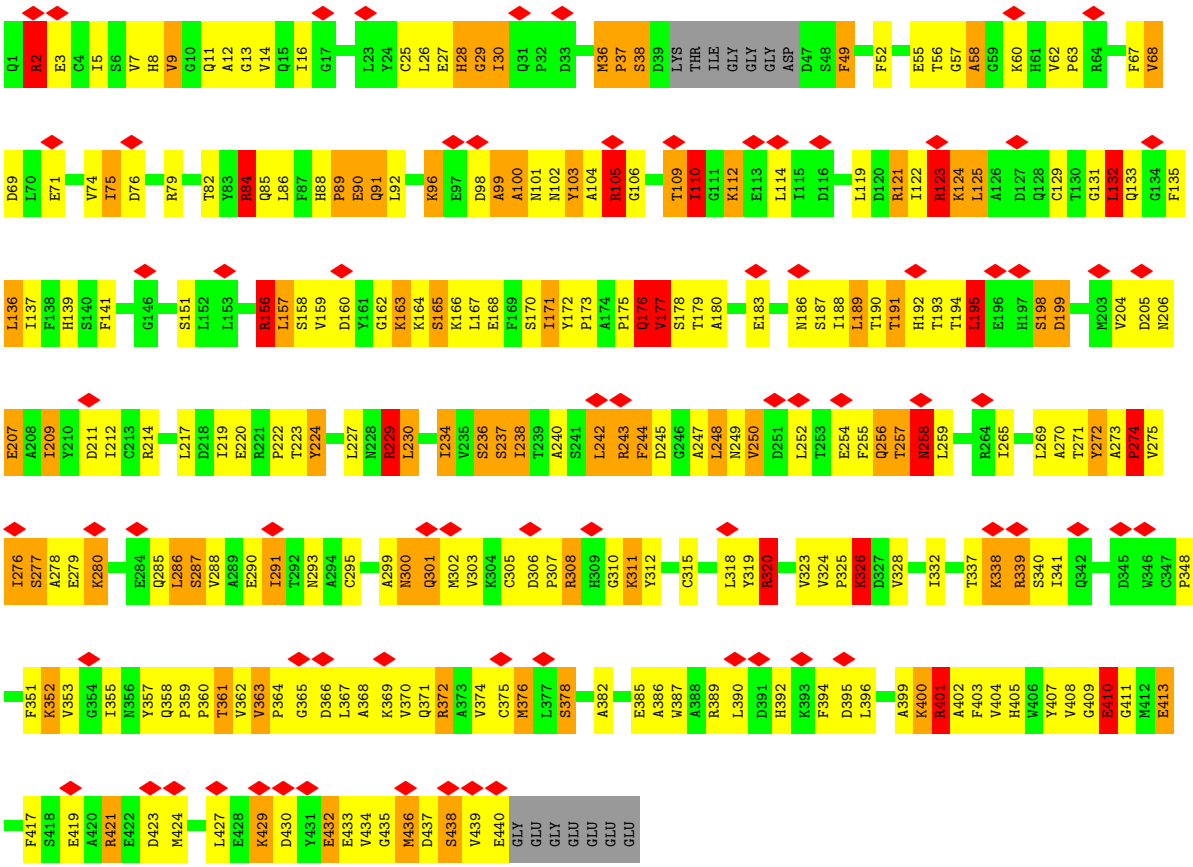


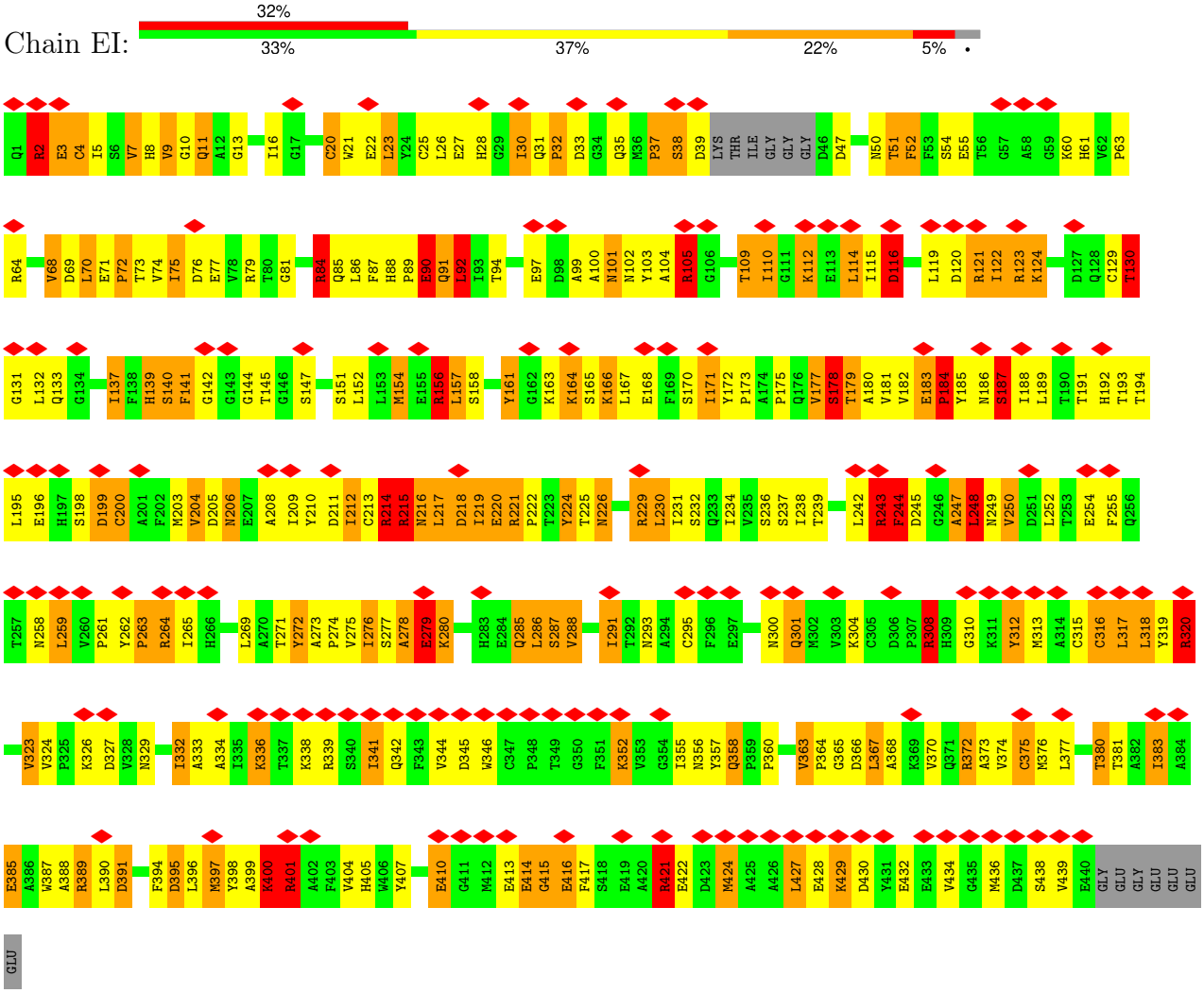

- Molecule 40: Tubulin alpha chain

Chain EH:



• Molecule 40: Tubulin alpha chain

Chain EI:




• Molecule 40: Tubulin alpha chain

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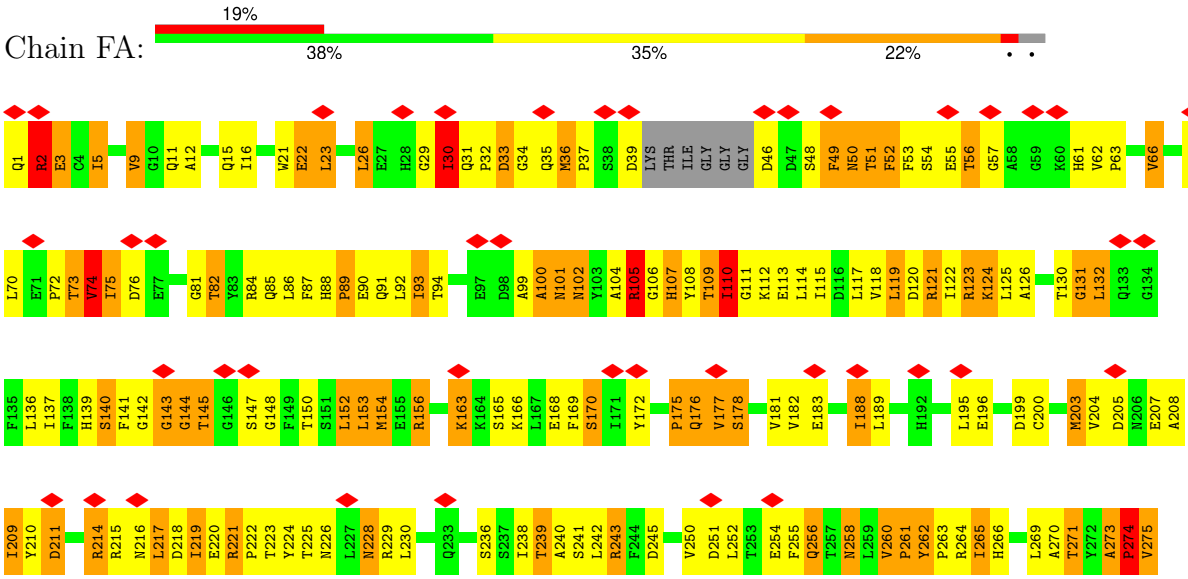

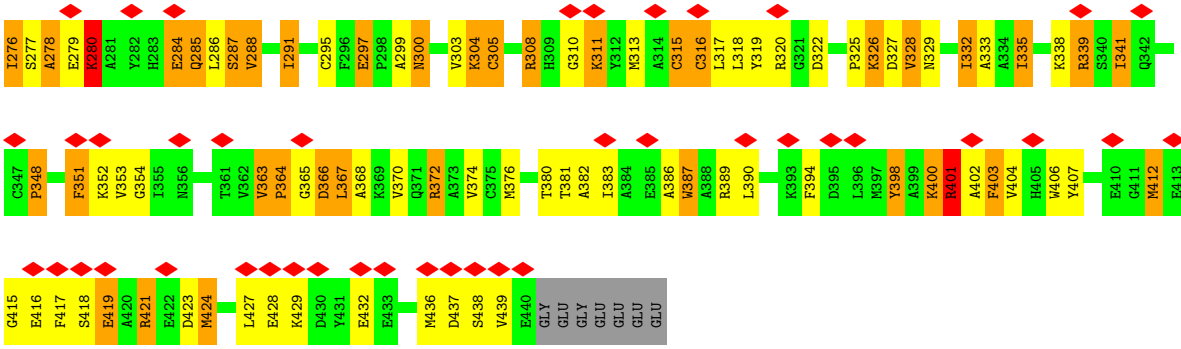


• Molecule 40: Tubulin alpha chain

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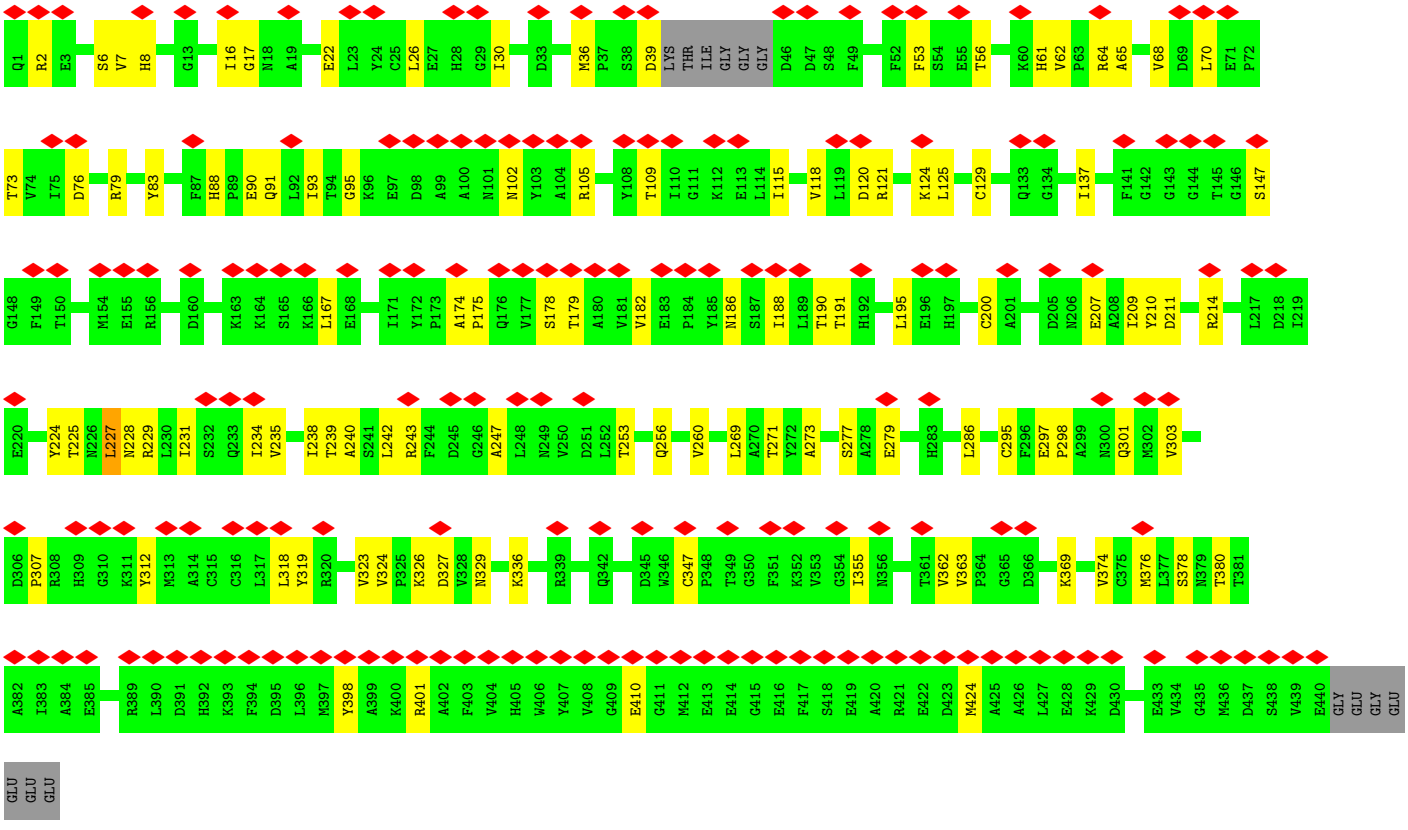
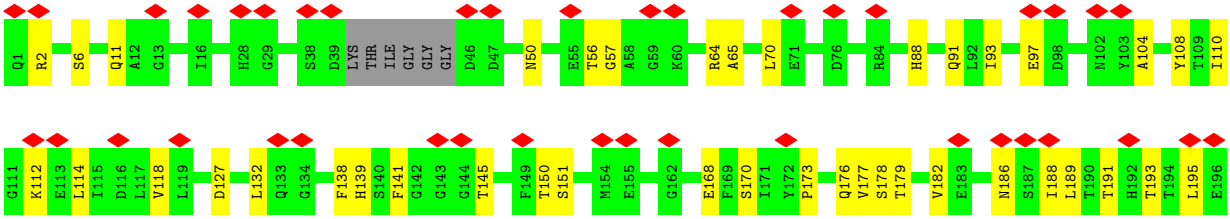
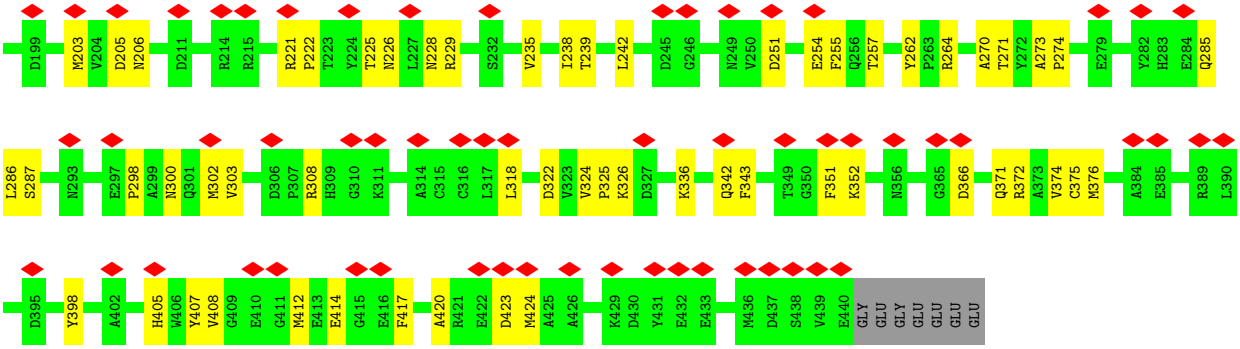



• Molecule 40: Tubulin alpha chain

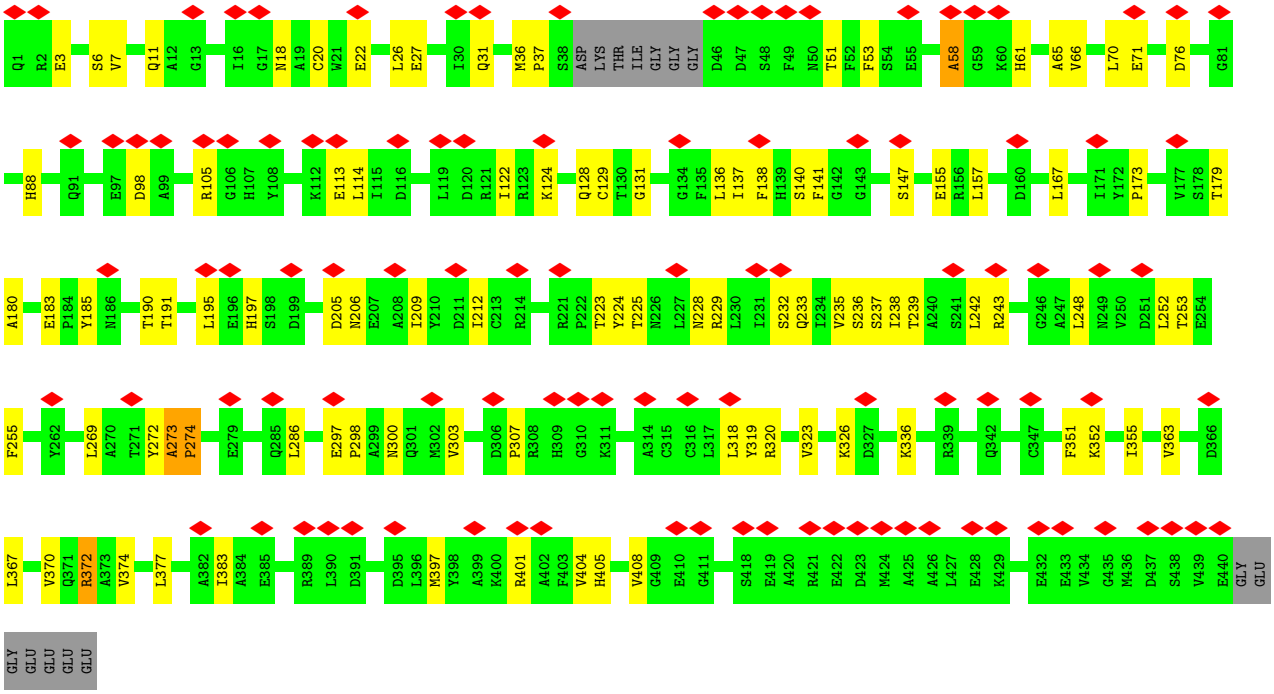
Chain FF:





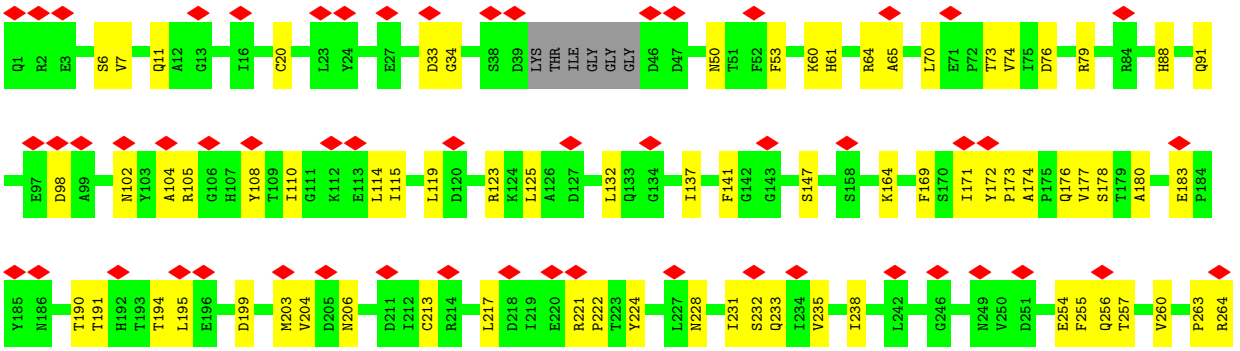

- Molecule 40: Tubulin alpha chain

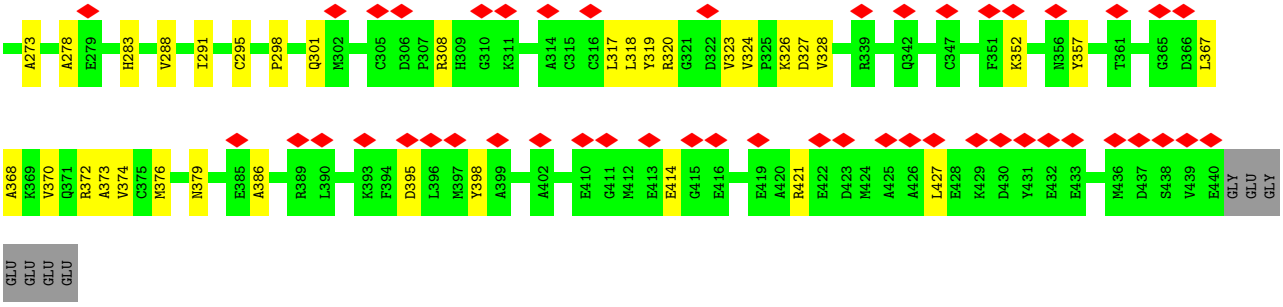
Chain FG:




- Molecule 40: Tubulin alpha chain

Chain FH:






- Molecule 40: Tubulin alpha chain

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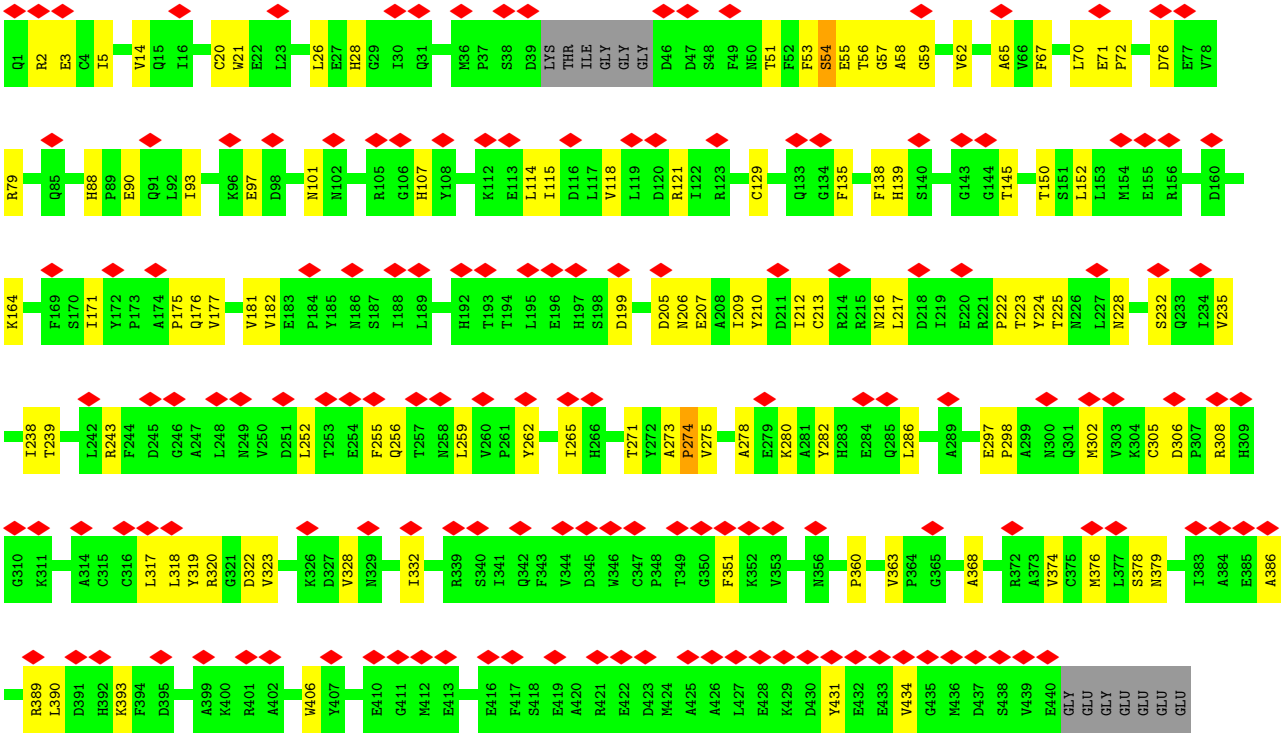


- Molecule 40: Tubulin alpha chain

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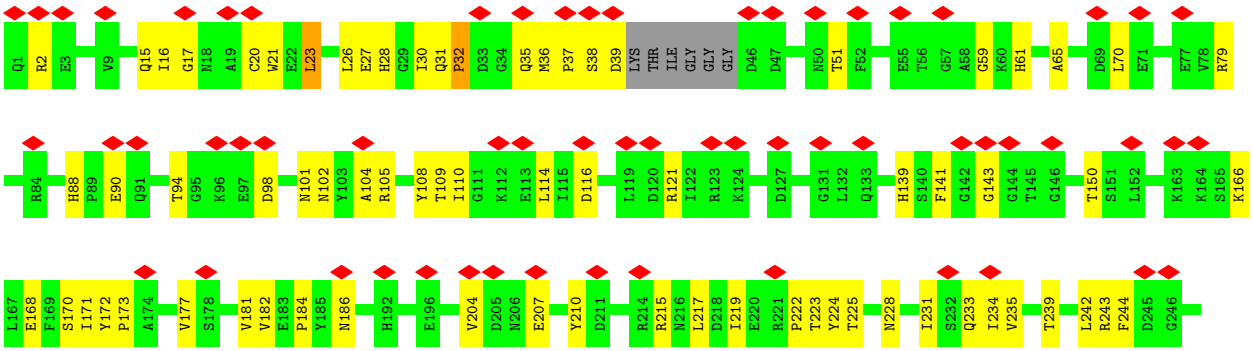
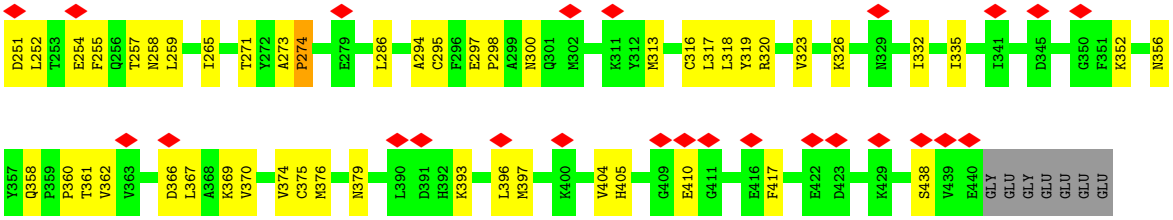
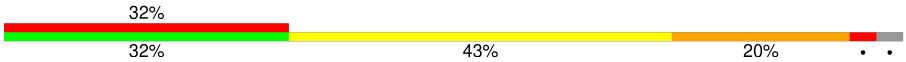
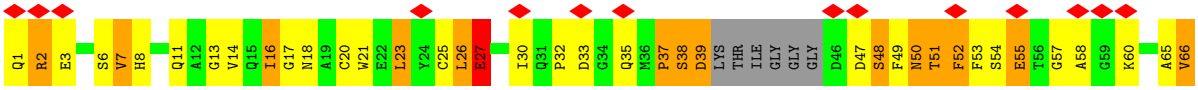


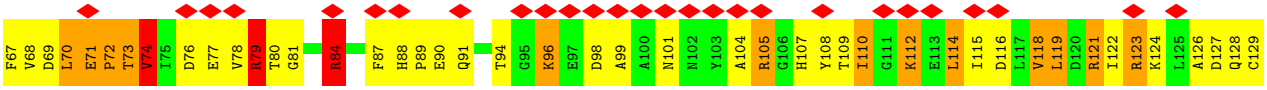


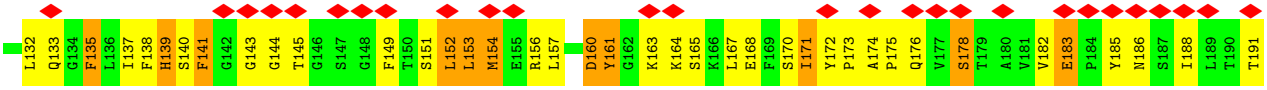

• Molecule 40: Tubulin alpha chain

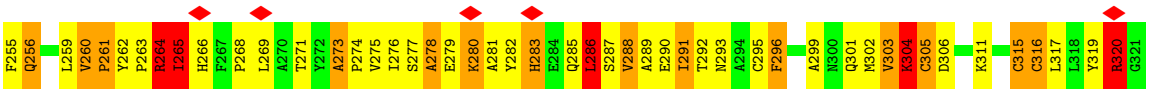
Chain GE:

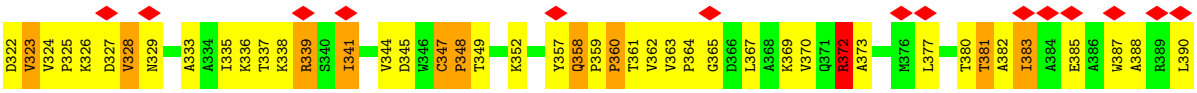


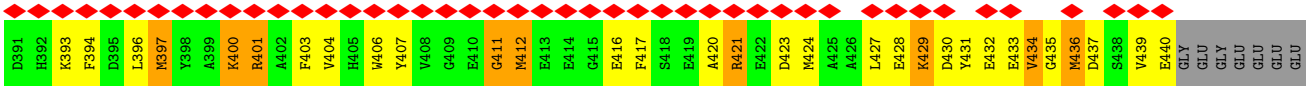



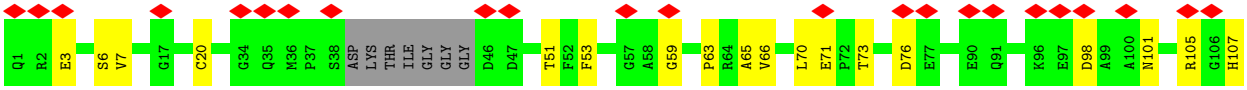


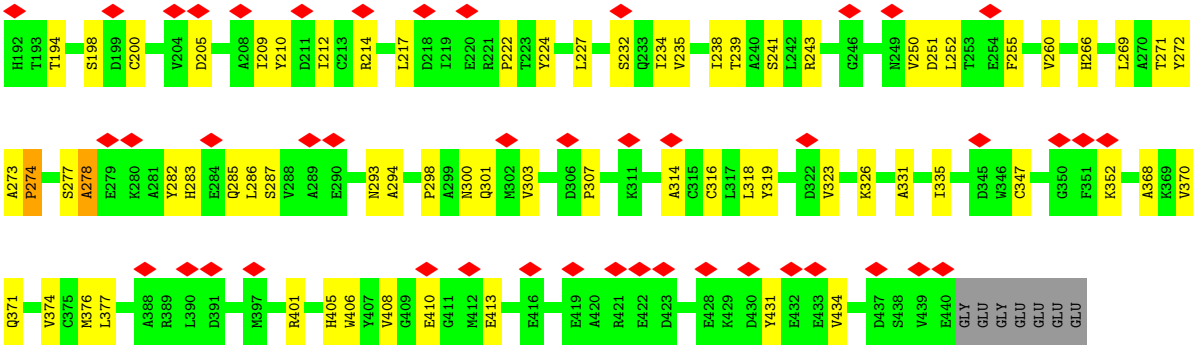




• Molecule 40: Tubulin alpha chain

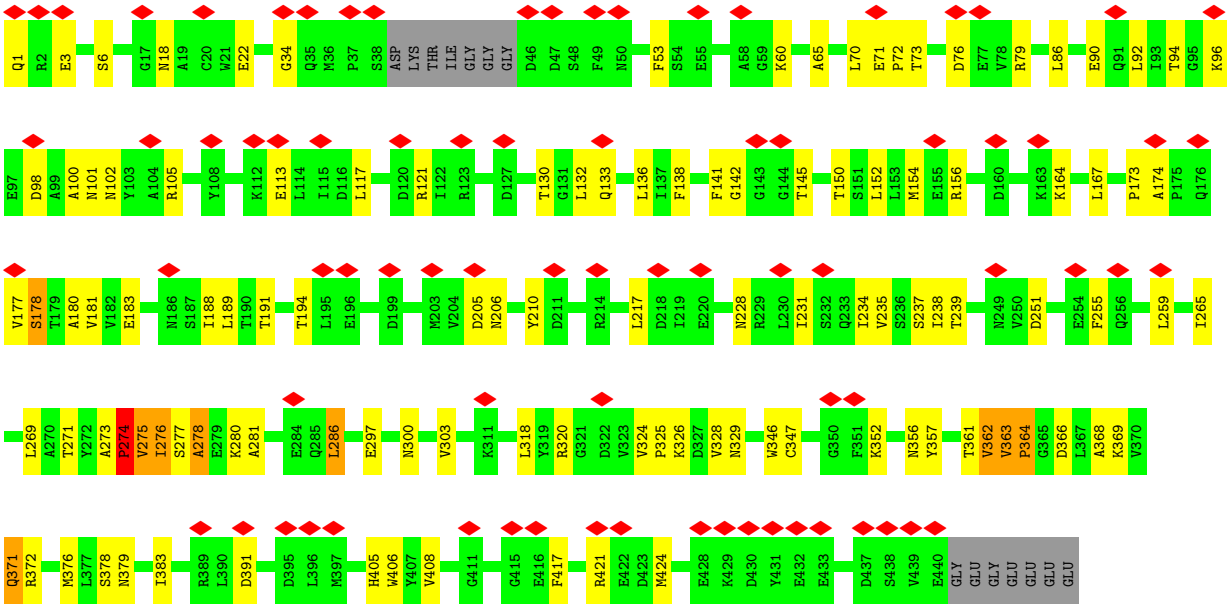
Chain GF:





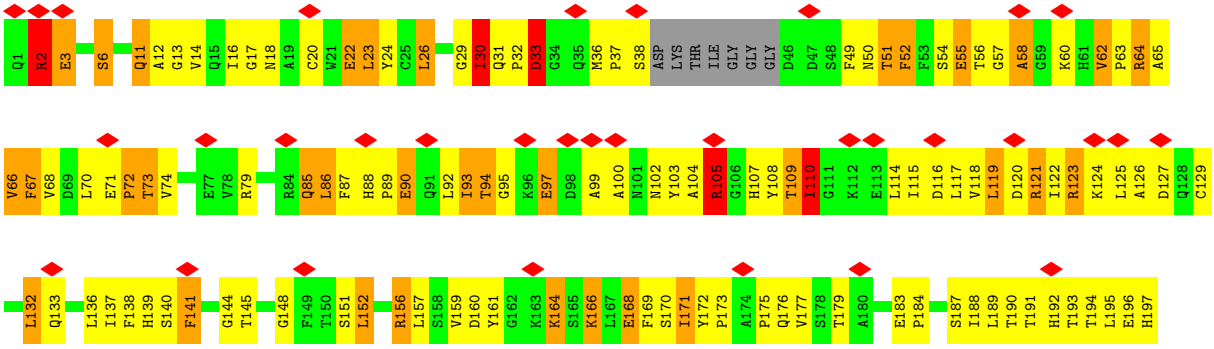

- Molecule 40: Tubulin alpha chain

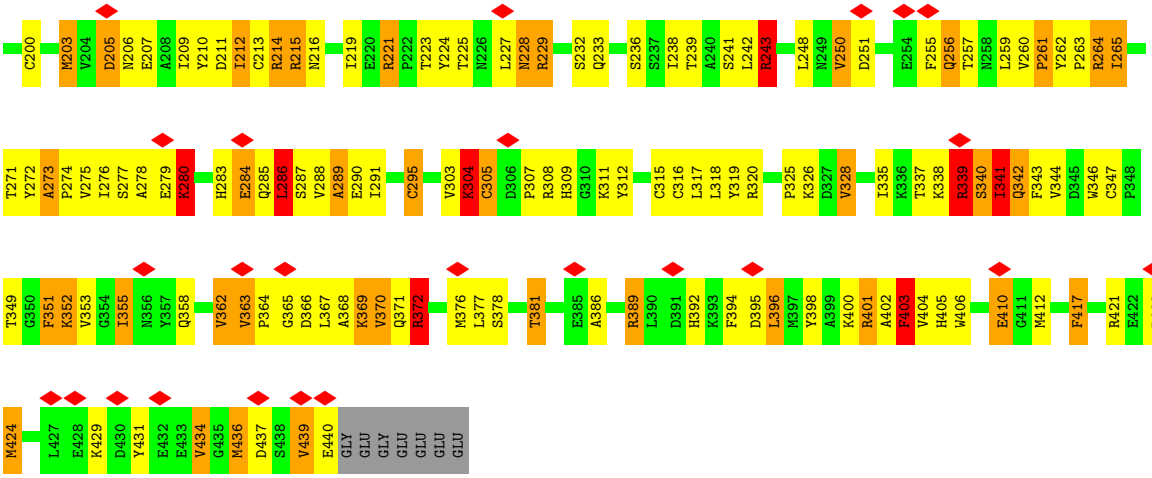
Chain GG:




- Molecule 40: Tubulin alpha chain

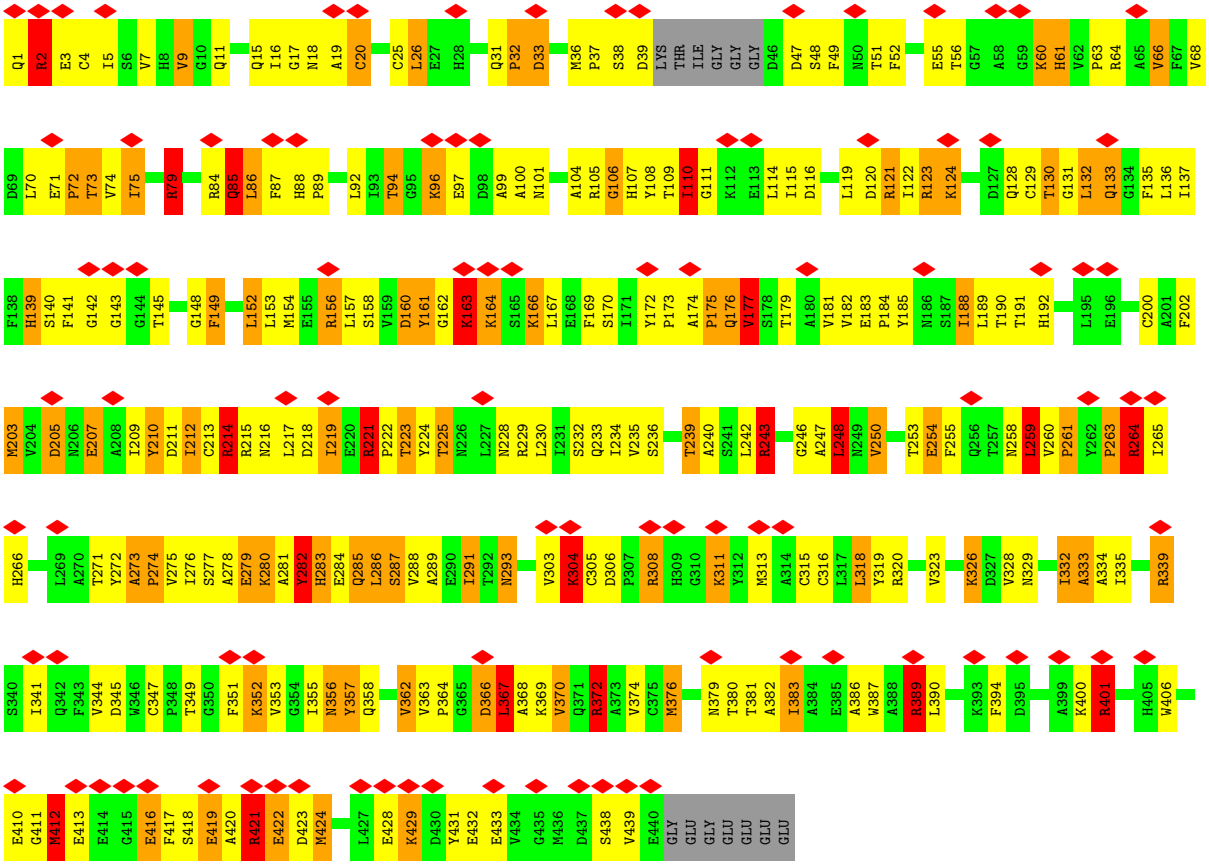
Chain GH:





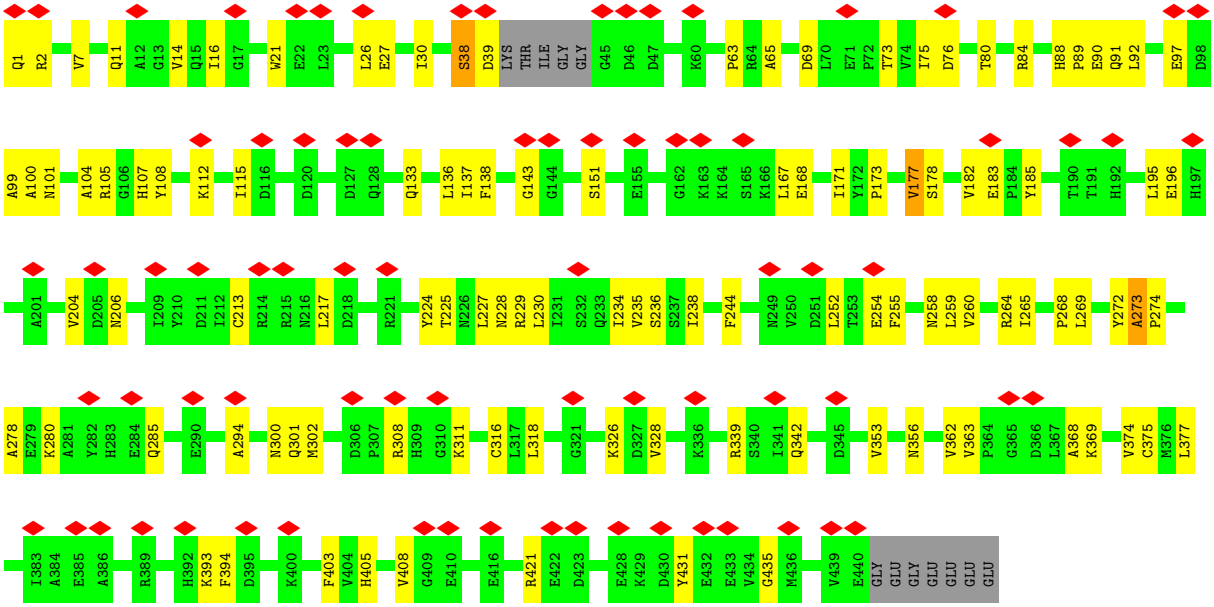

• Molecule 40: Tubulin alpha chain

Chain GI:



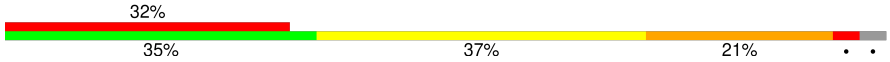

• Molecule 40: Tubulin alpha chain

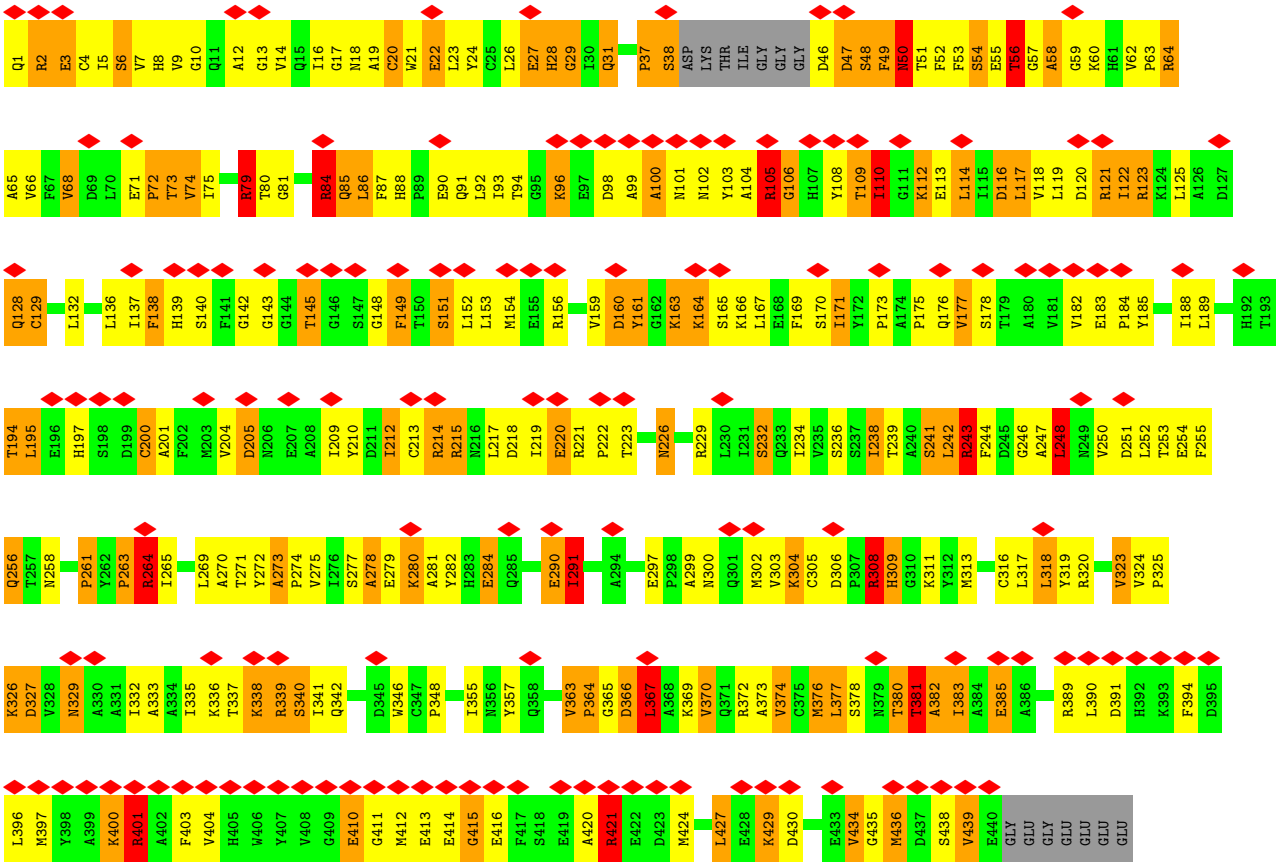
Chain HA:




- Molecule 40: Tubulin alpha chain

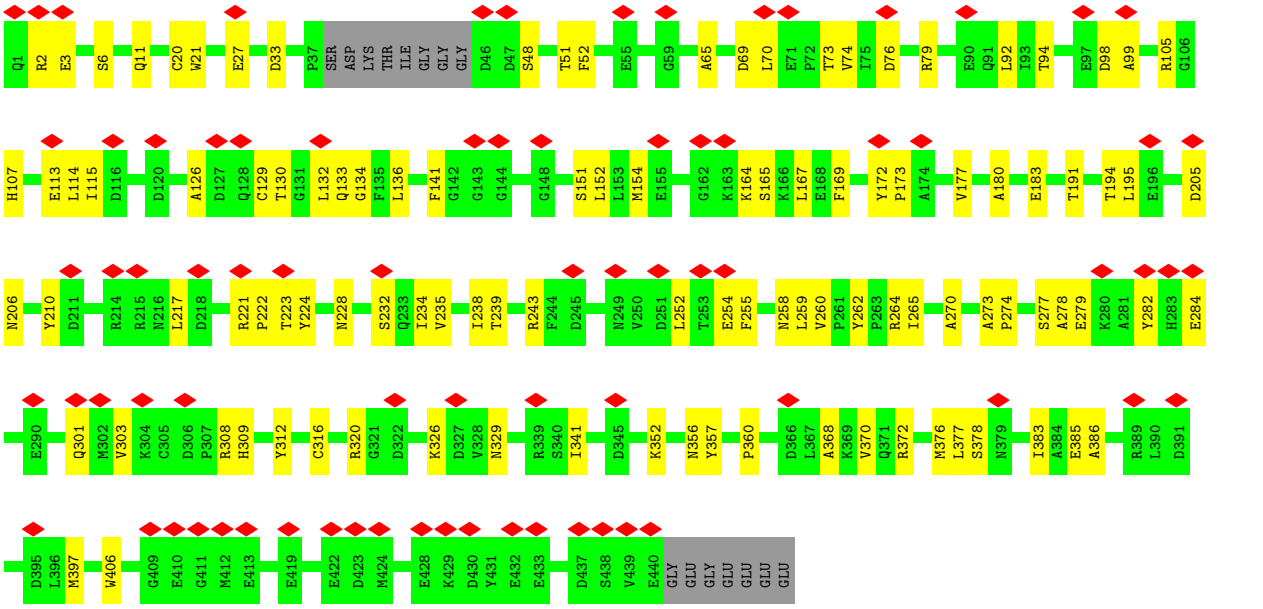
Chain HE:



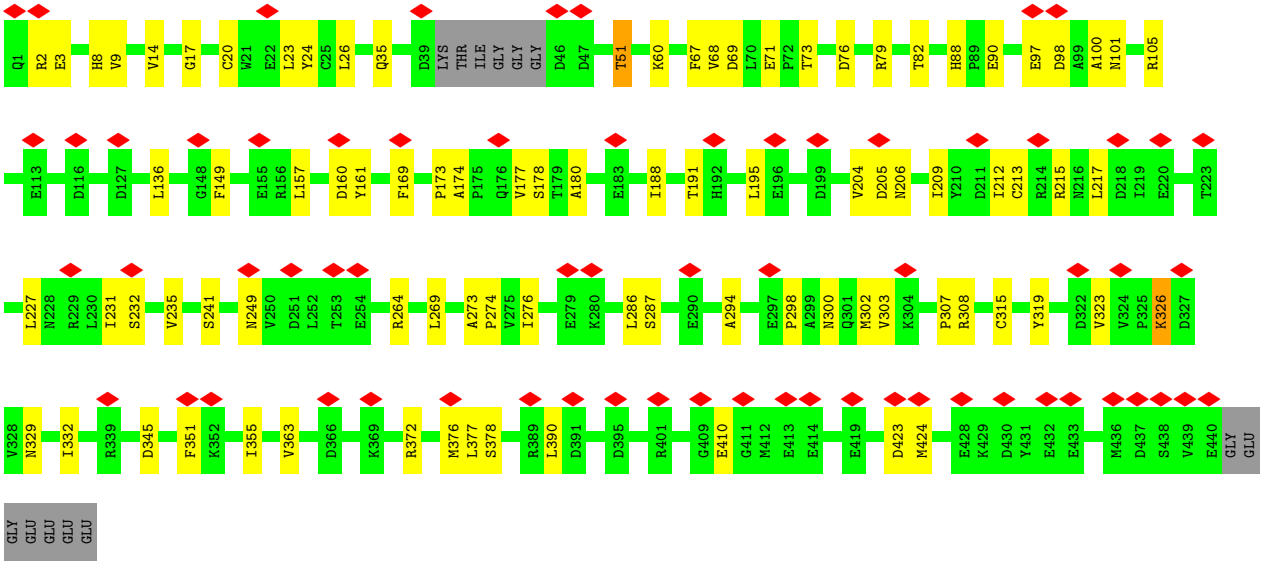

- Molecule 40: Tubulin alpha chain

Chain HF: 17% 73% 24%



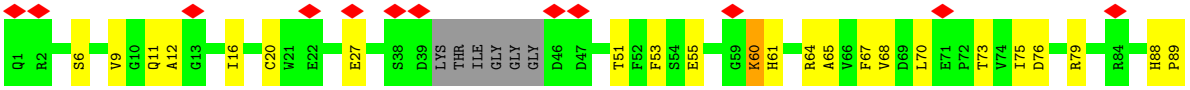

- Molecule 40: Tubulin alpha chain

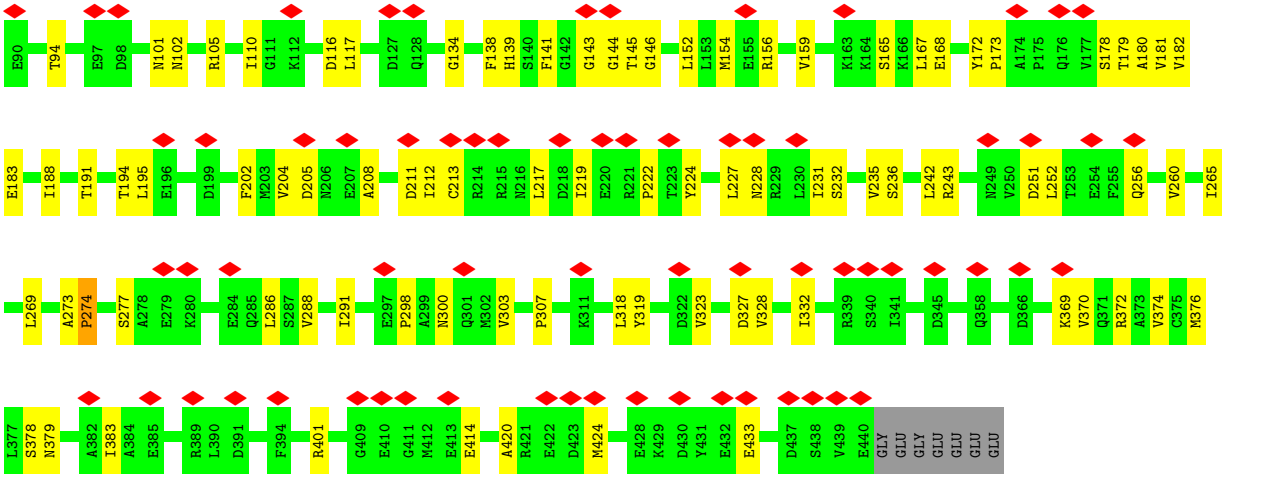
Chain HG: 15% 77% 19%




- Molecule 40: Tubulin alpha chain

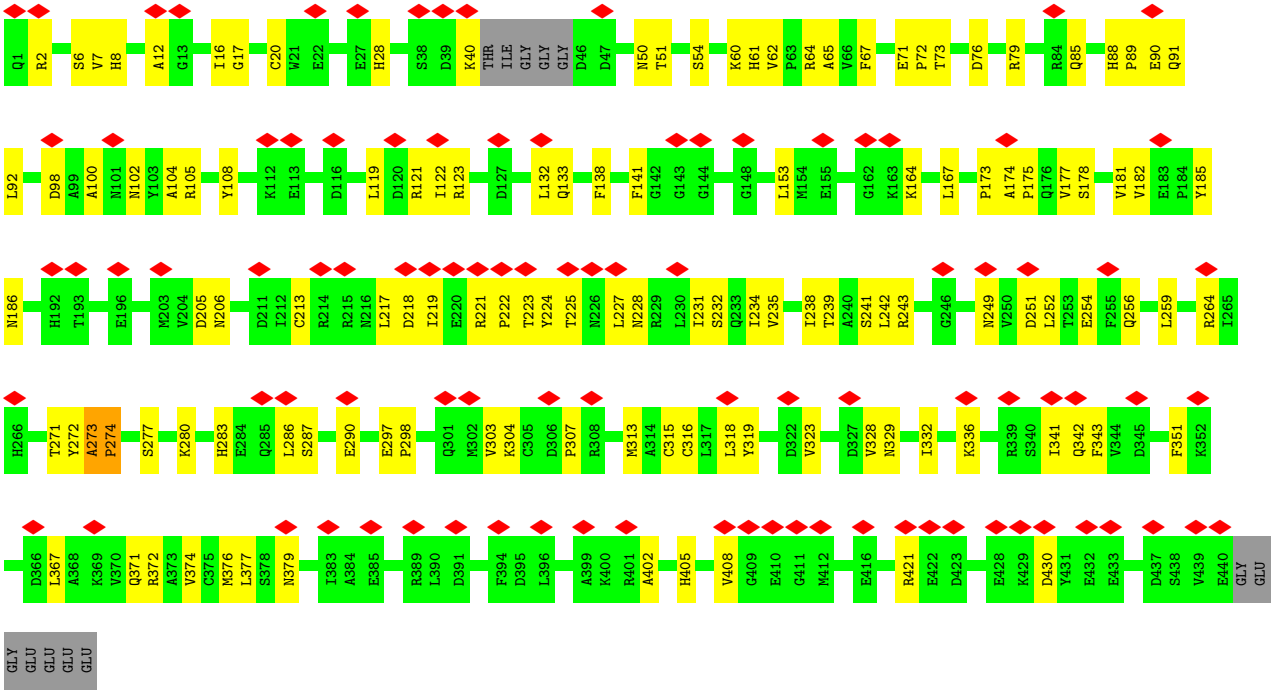
Chain HH: 18% 72% 24%





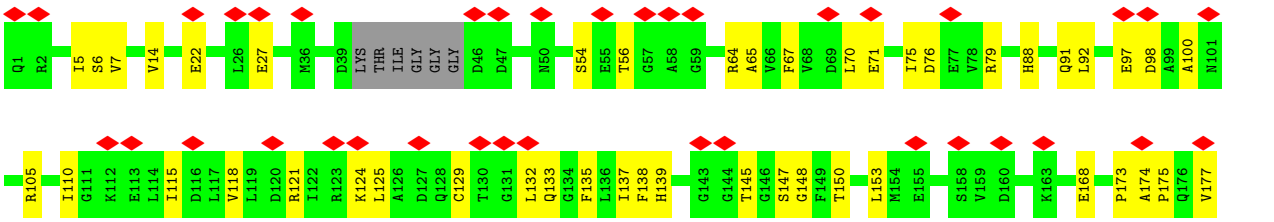

- Molecule 40: Tubulin alpha chain

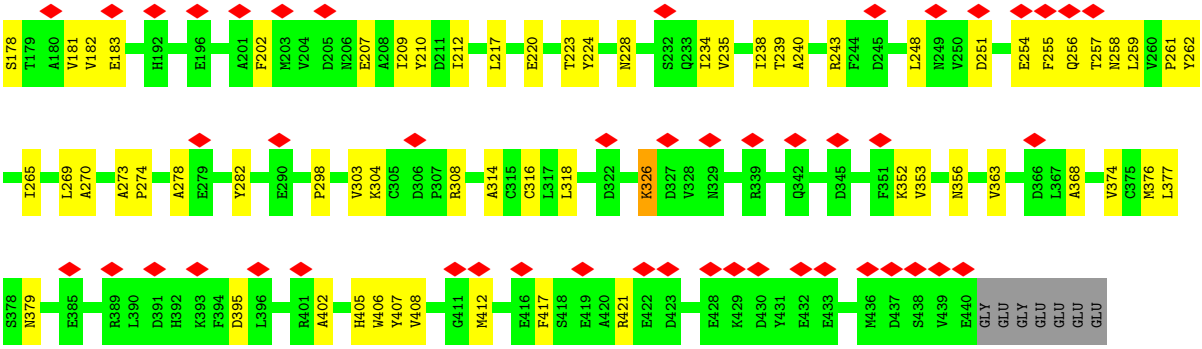
Chain HI:




- Molecule 40: Tubulin alpha chain

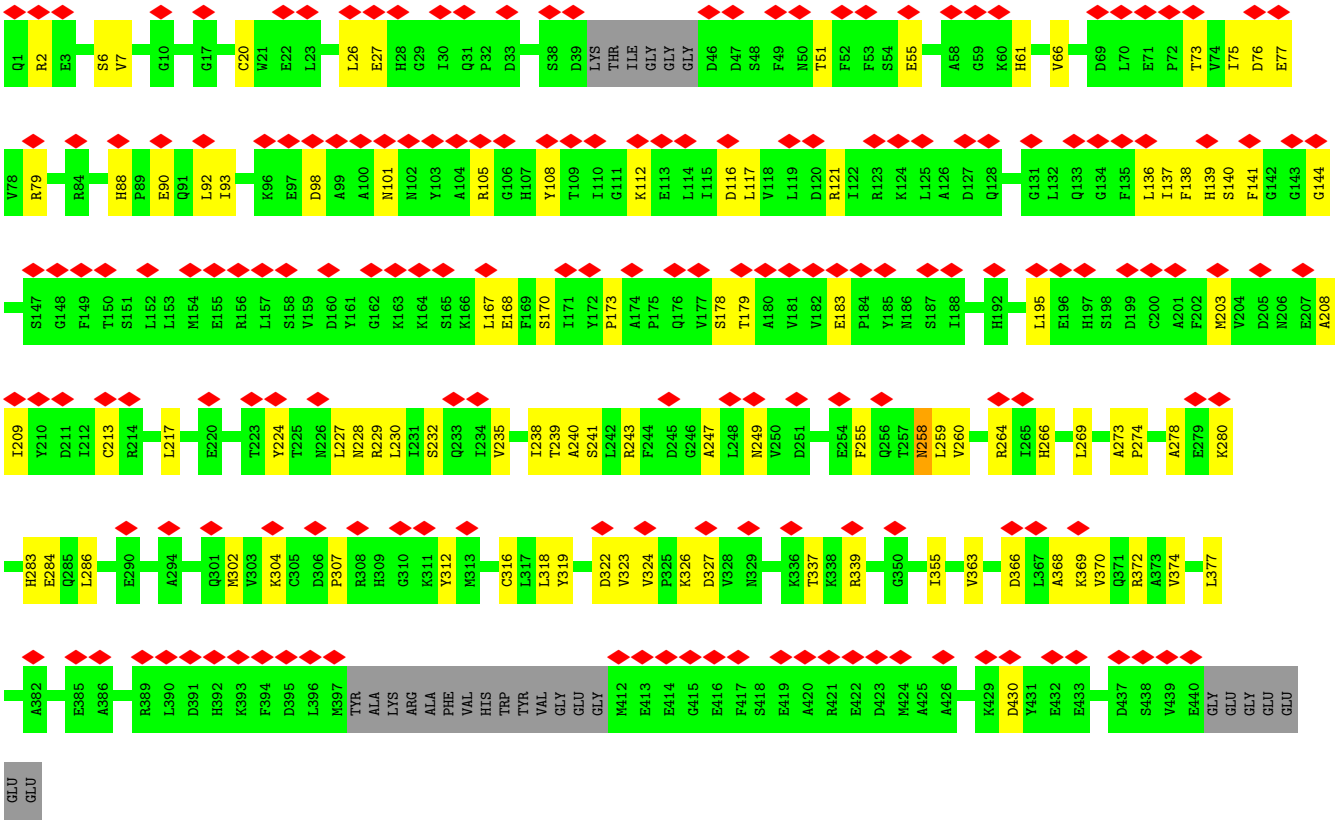
Chain IA:





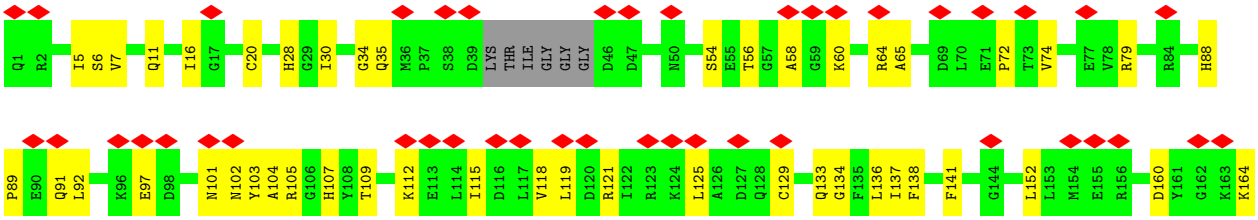

- Molecule 40: Tubulin alpha chain

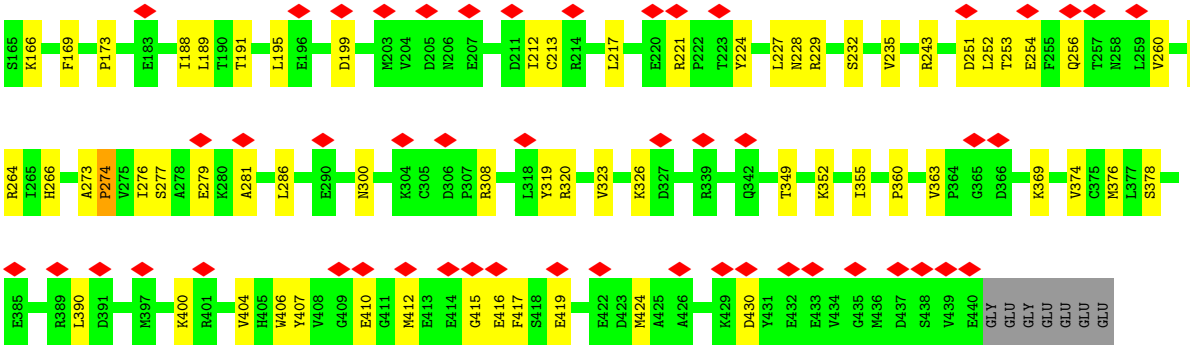
Chain IE:




- Molecule 40: Tubulin alpha chain

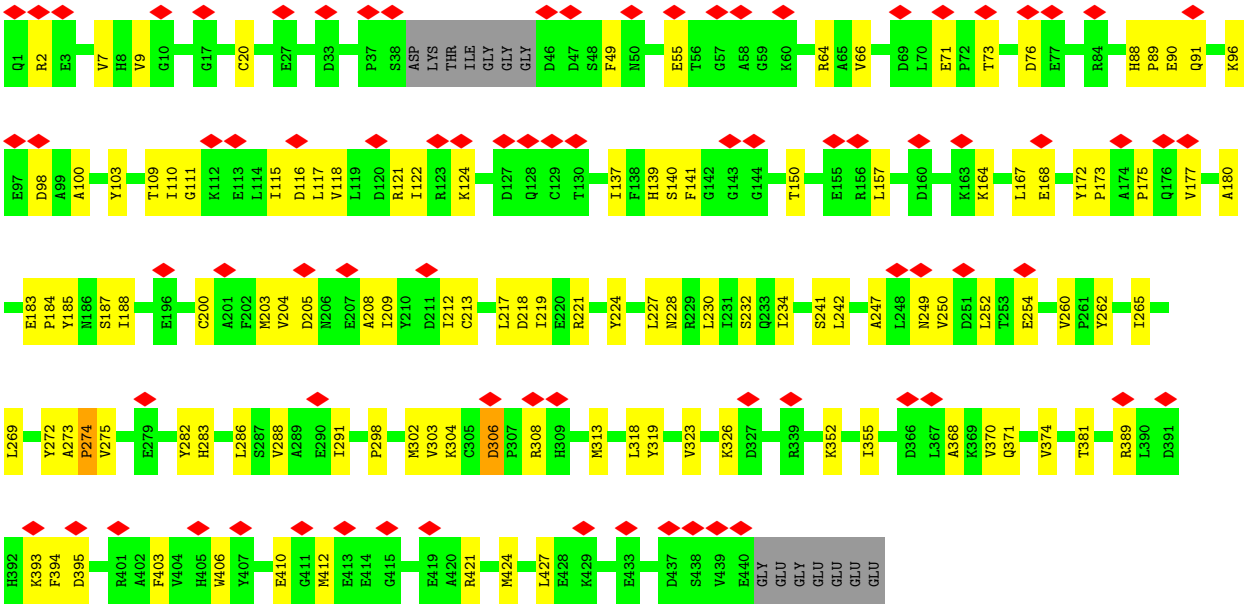
Chain IF:





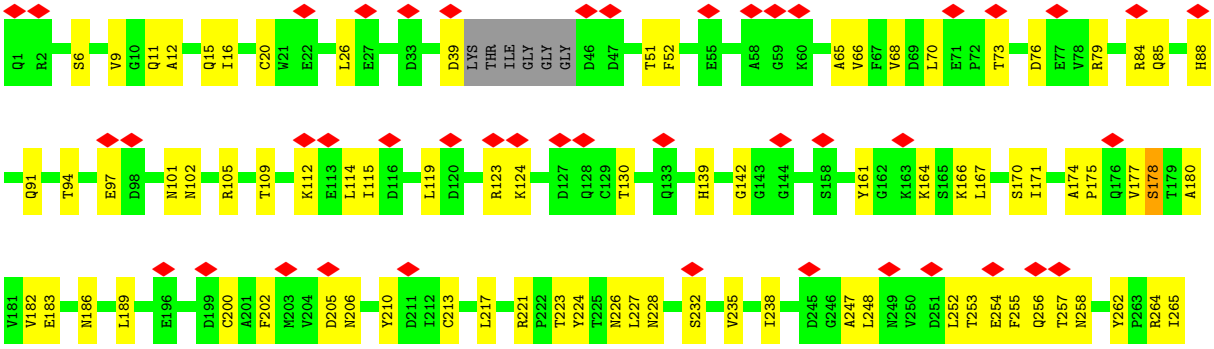

• Molecule 40: Tubulin alpha chain

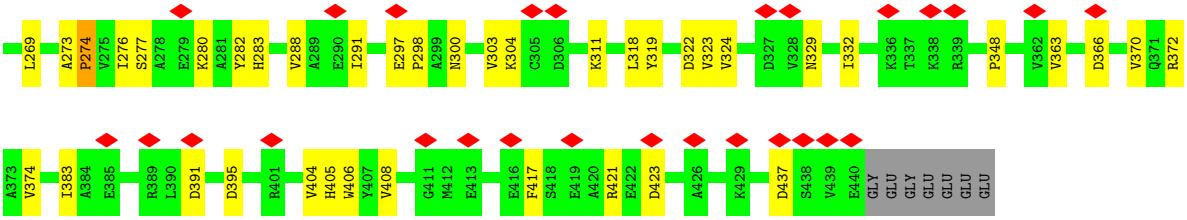
Chain IG:




• Molecule 40: Tubulin alpha chain

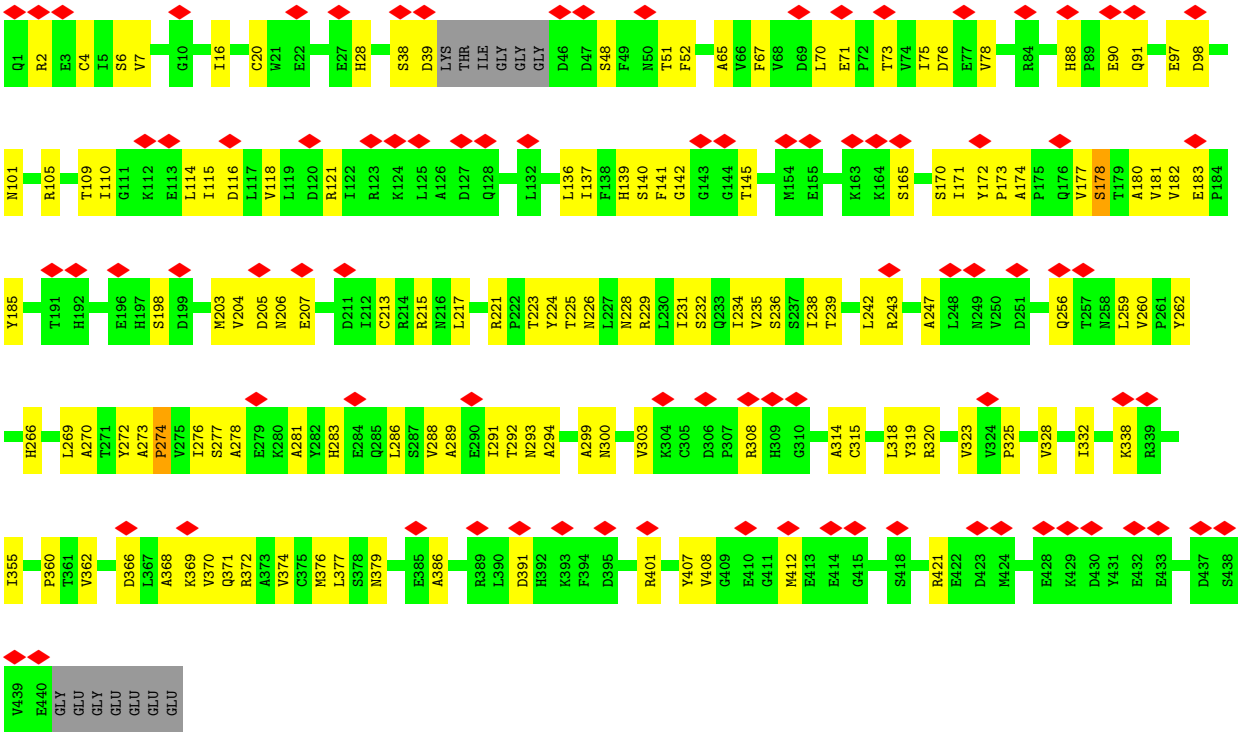
Chain IH:





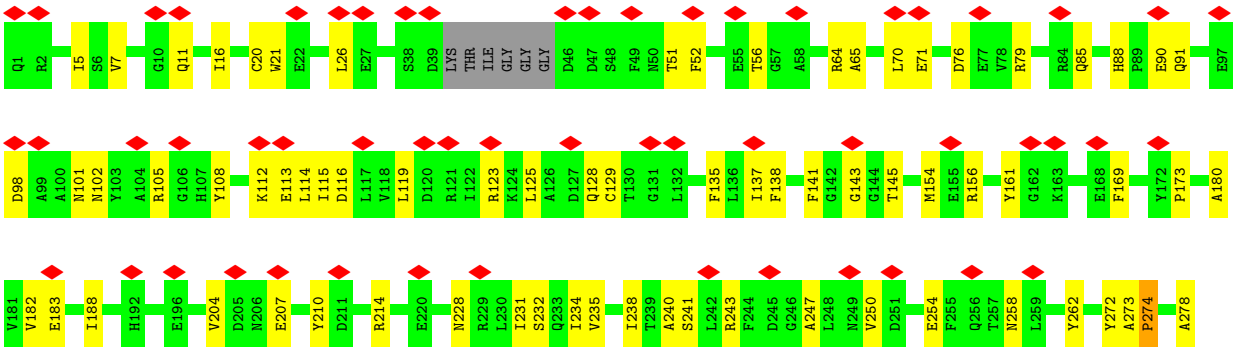

• Molecule 40: Tubulin alpha chain

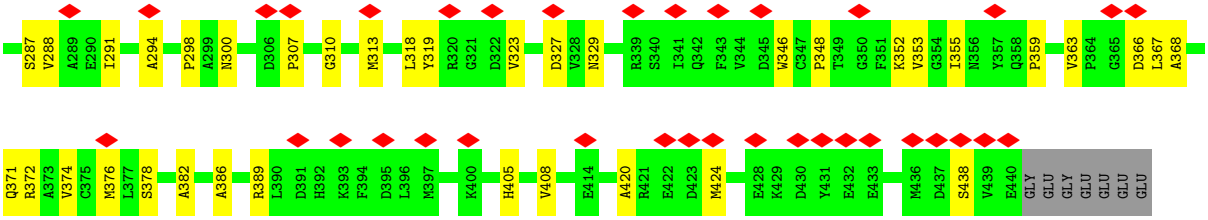
Chain II:




• Molecule 40: Tubulin alpha chain

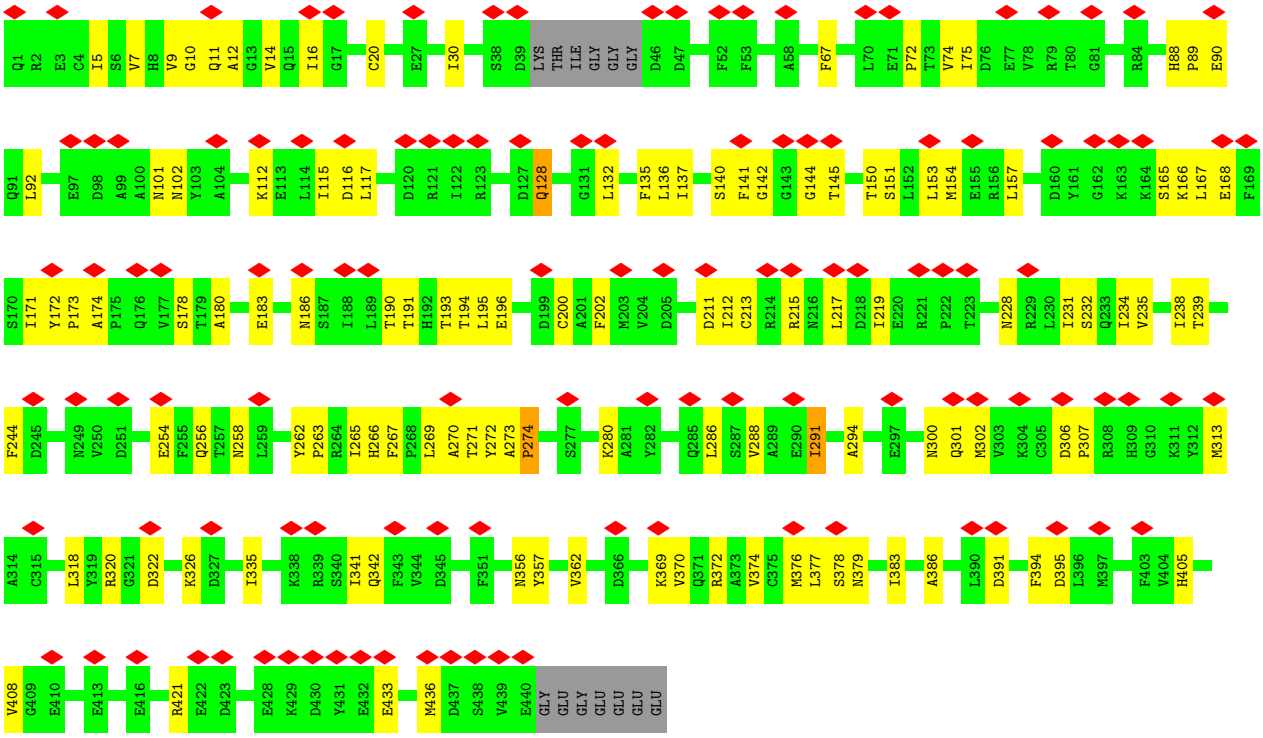
Chain JA:





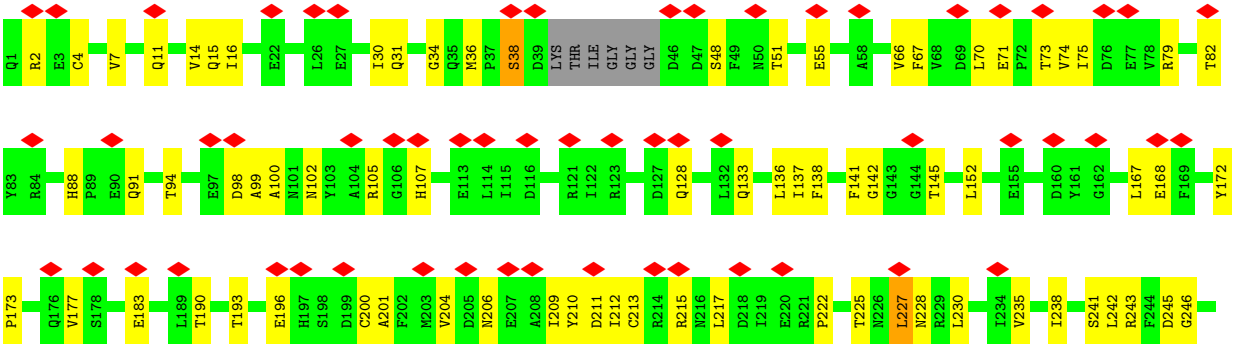

- Molecule 40: Tubulin alpha chain

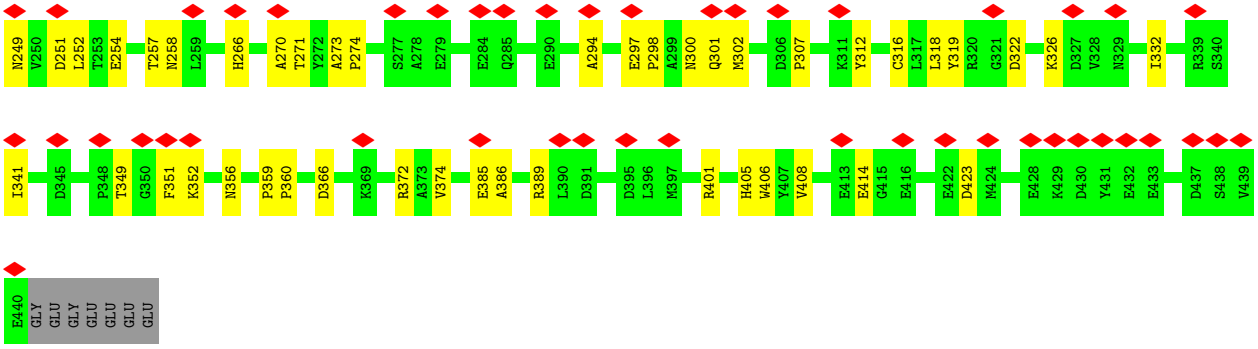
Chain JD:




- Molecule 40: Tubulin alpha chain

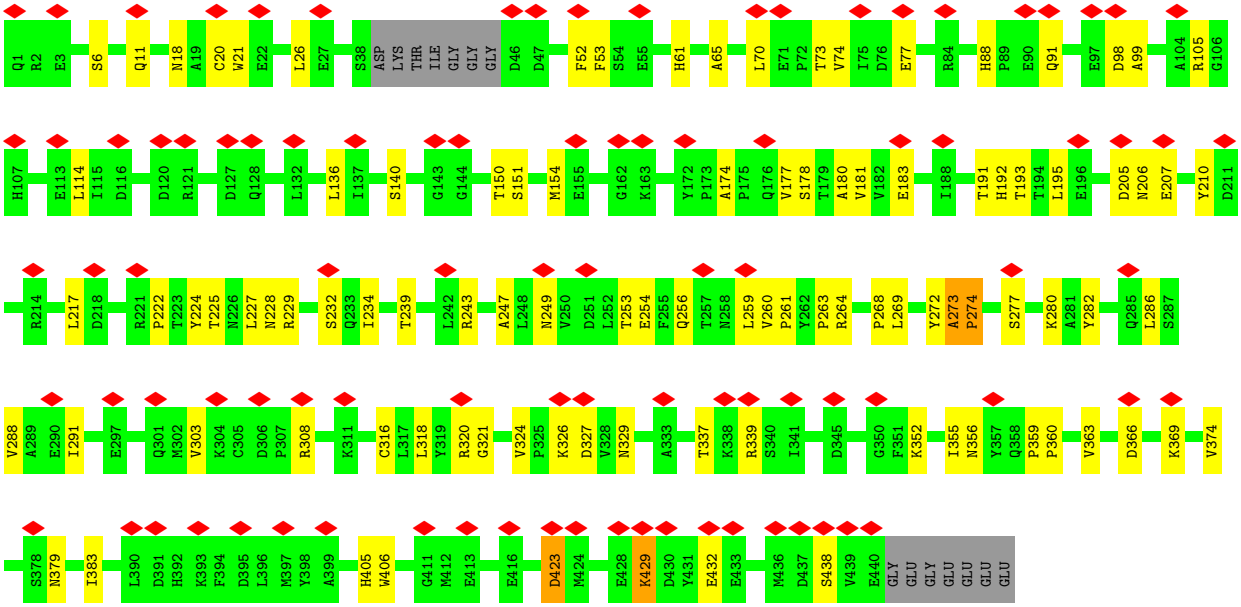
Chain JE:





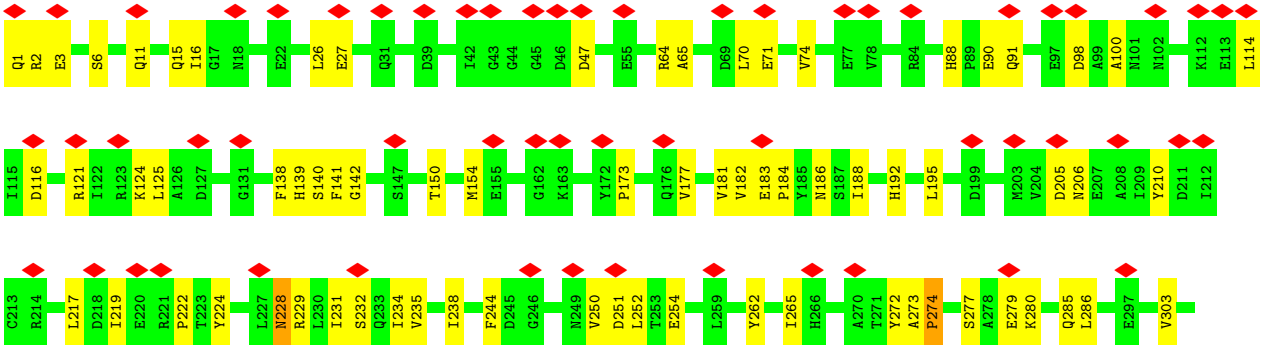

- Molecule 40: Tubulin alpha chain

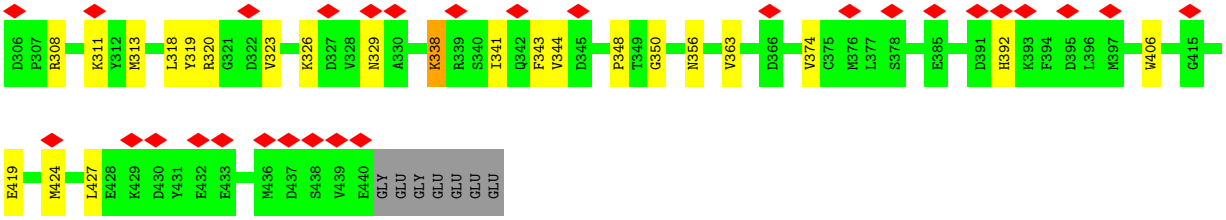
Chain JF:




- Molecule 40: Tubulin alpha chain

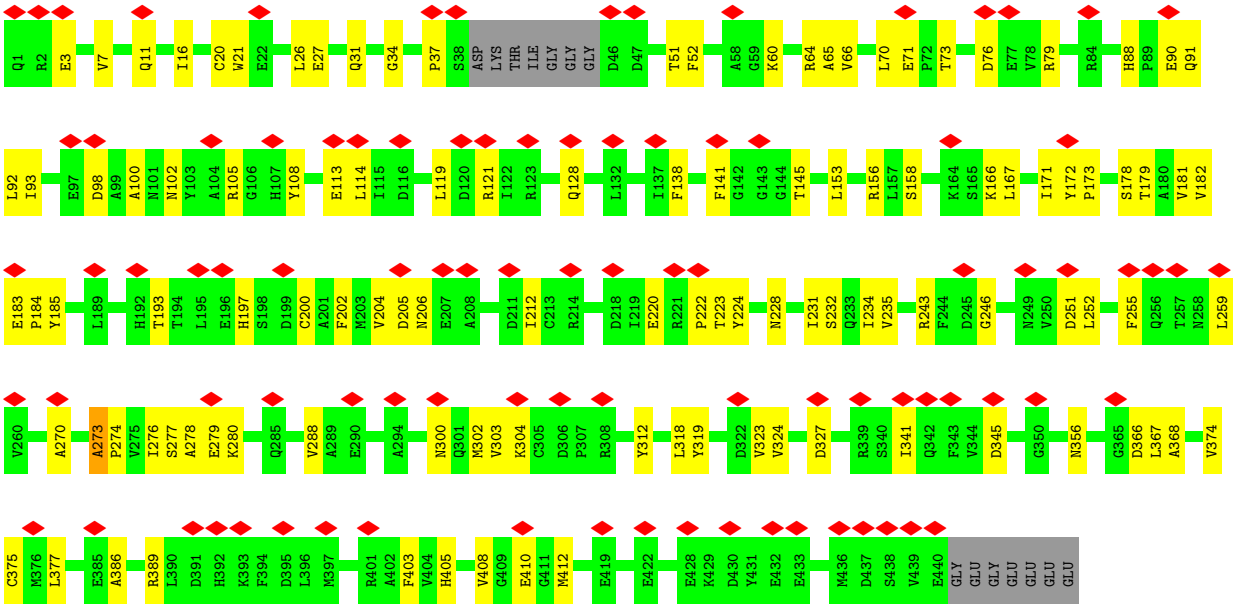
Chain JG:





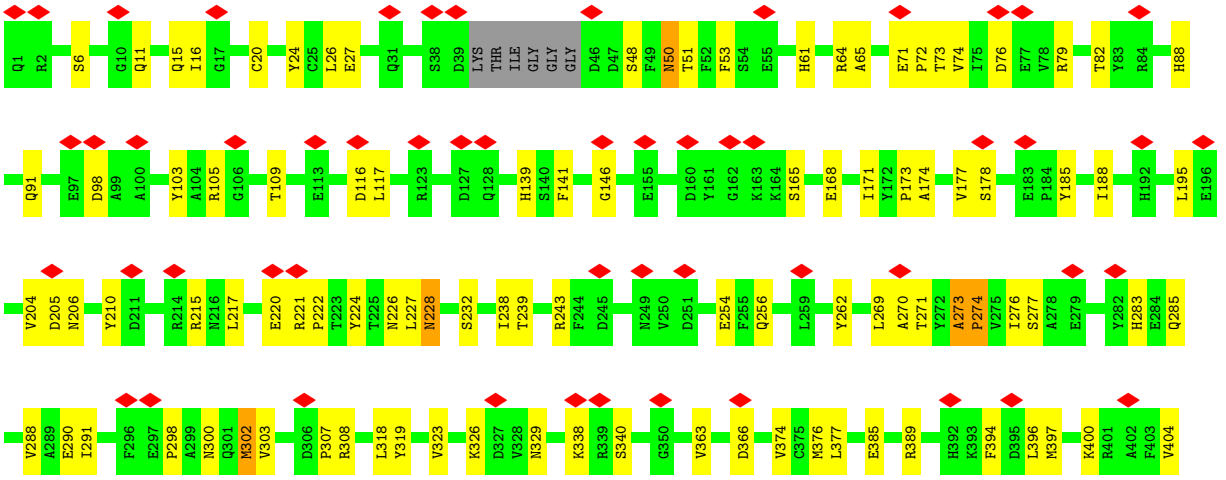

• Molecule 40: Tubulin alpha chain

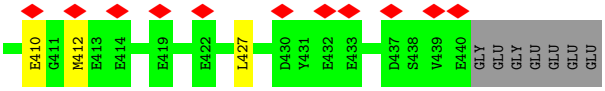
Chain JH:




• Molecule 40: Tubulin alpha chain

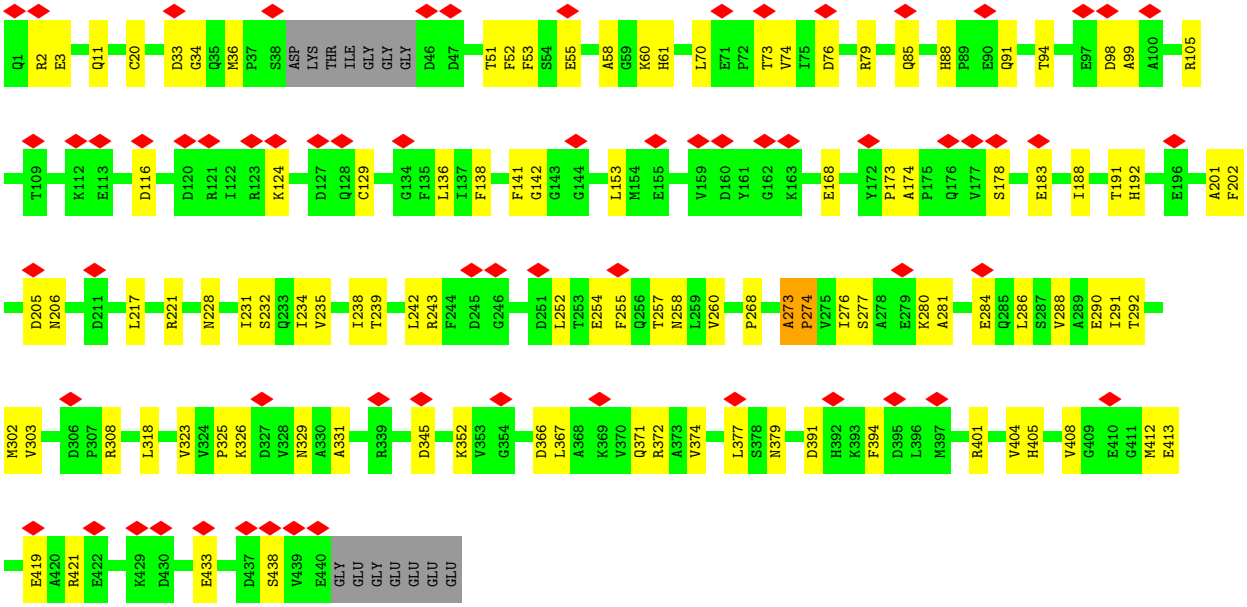
Chain KA:





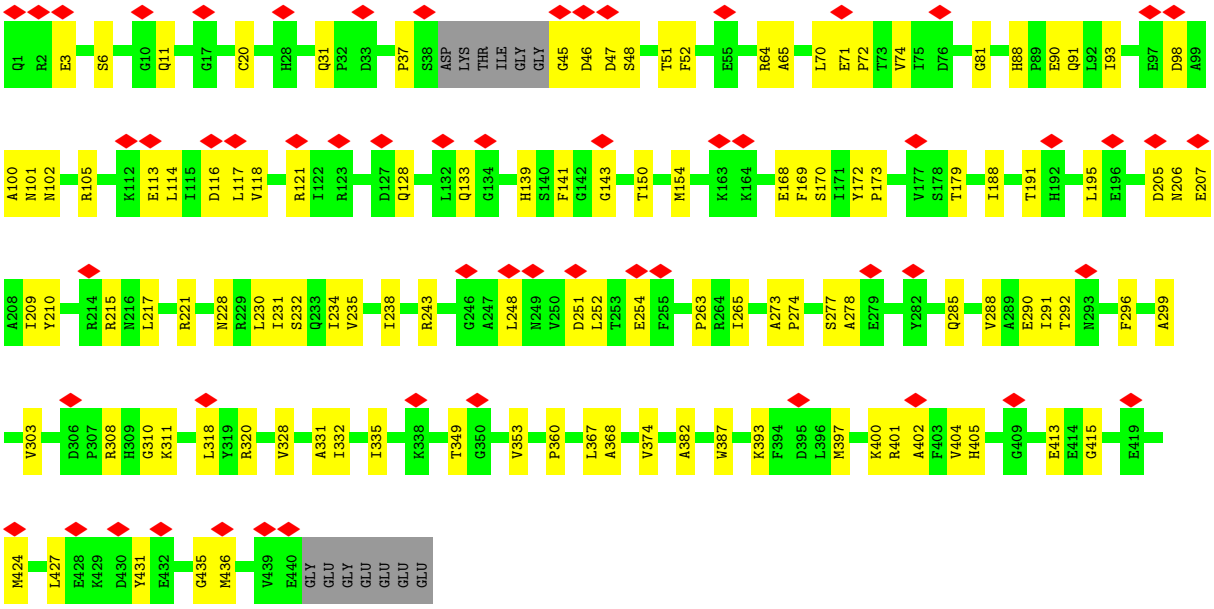

• Molecule 40: Tubulin alpha chain

Chain KD:



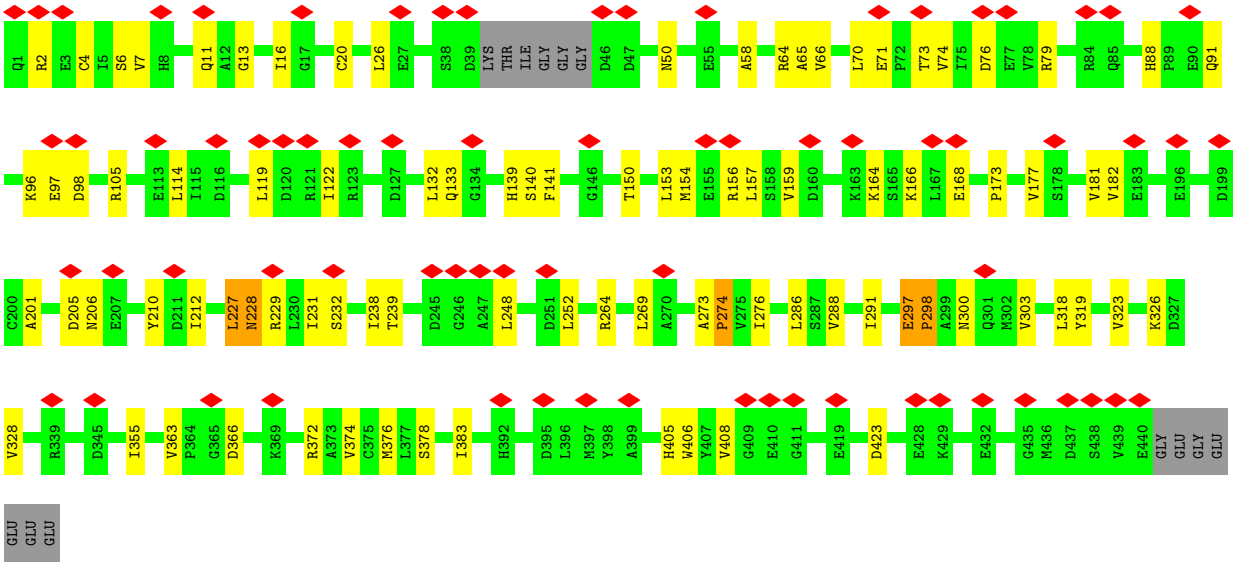

• Molecule 40: Tubulin alpha chain

Chain KE:



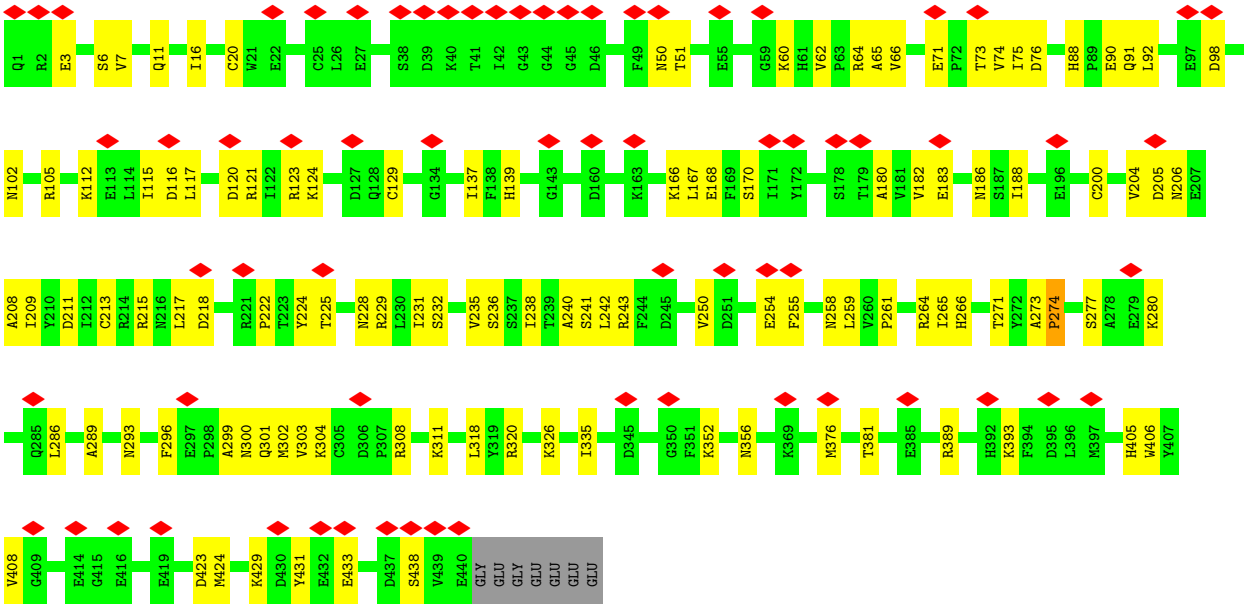

• Molecule 40: Tubulin alpha chain

Chain KF:



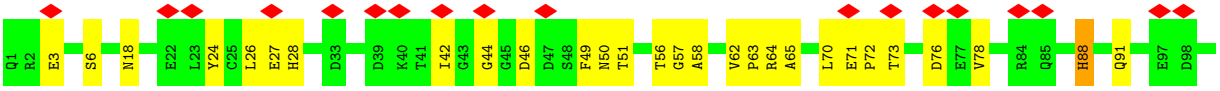

- Molecule 40: Tubulin alpha chain

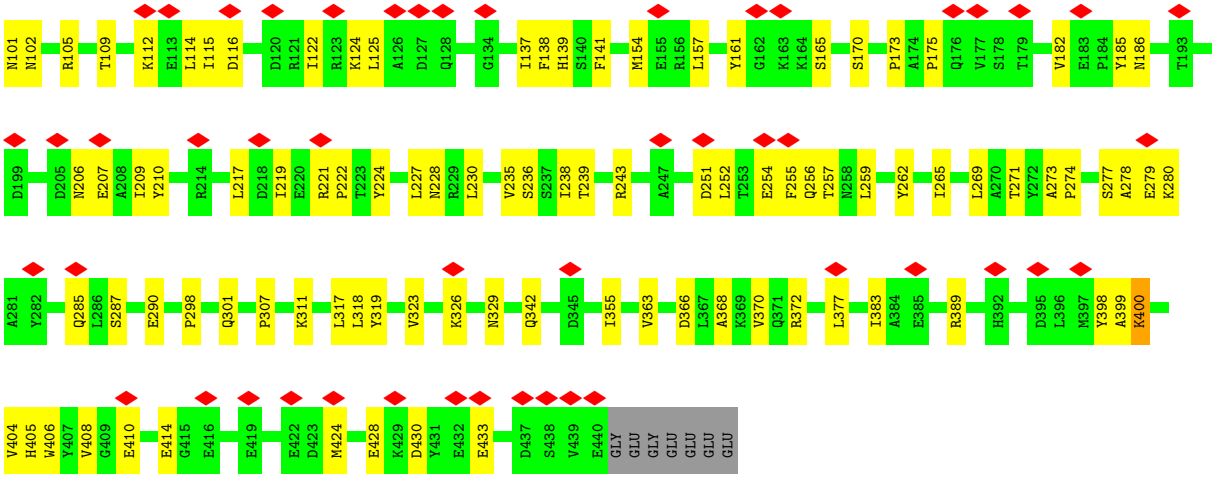
Chain KG:




- Molecule 40: Tubulin alpha chain

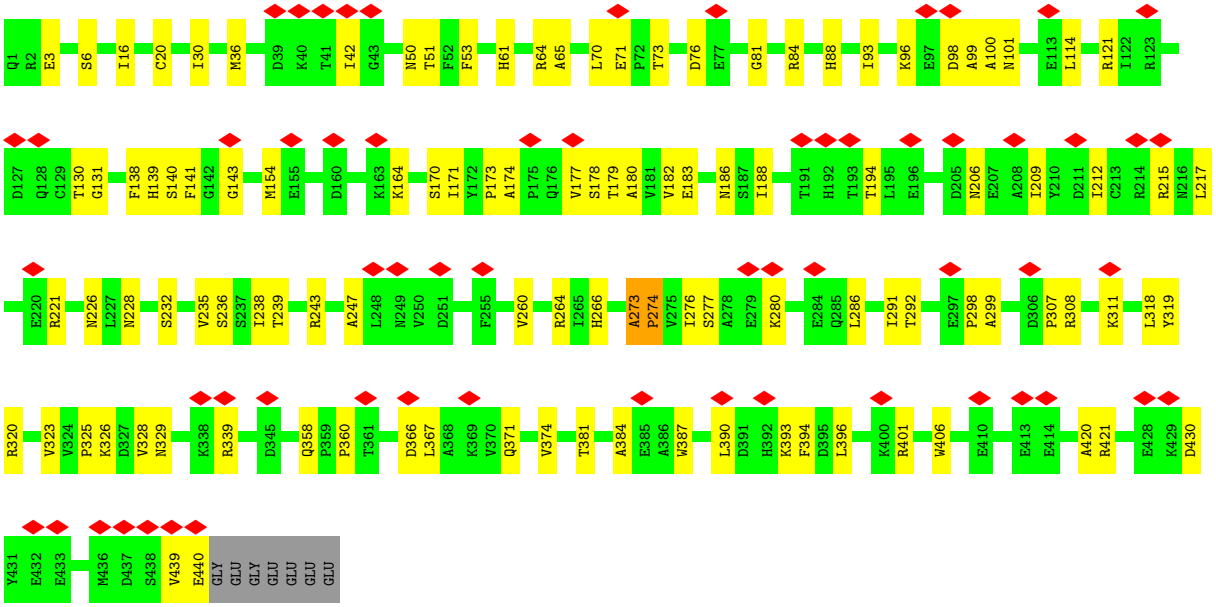
Chain KH:





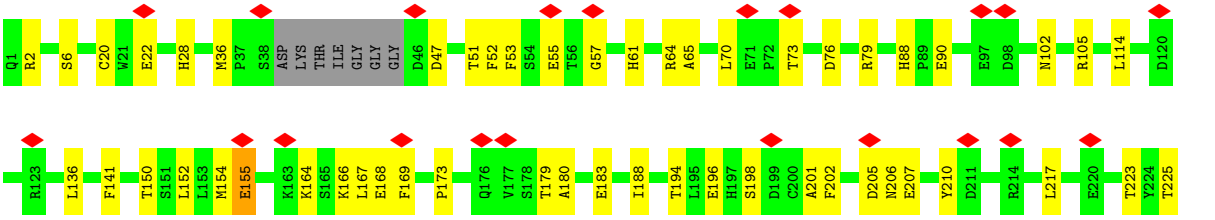

• Molecule 40: Tubulin alpha chain

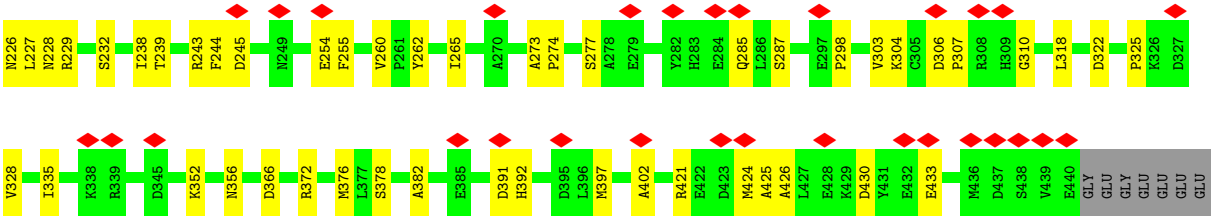
Chain LA:




• Molecule 40: Tubulin alpha chain

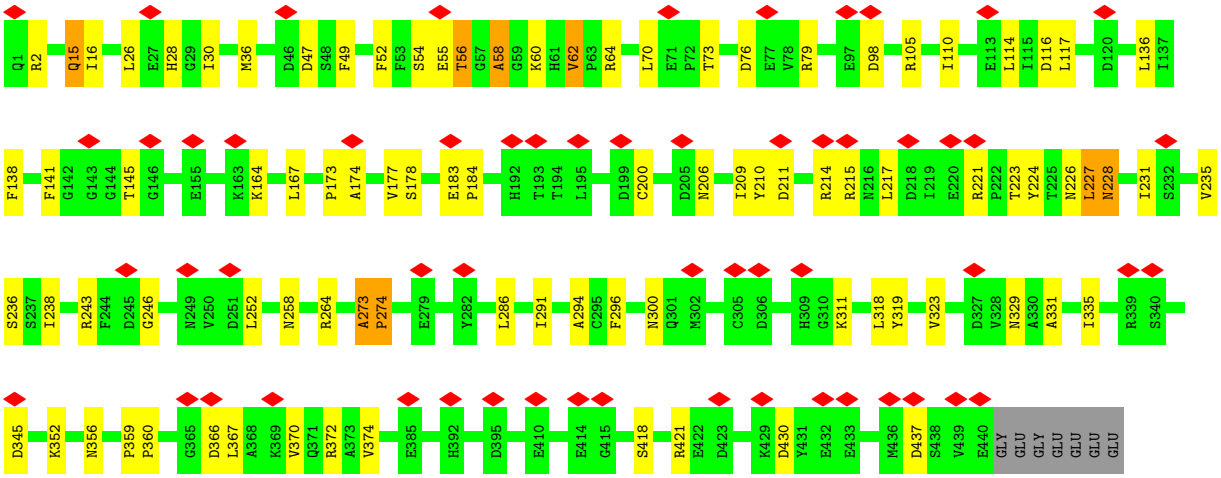
Chain LD:





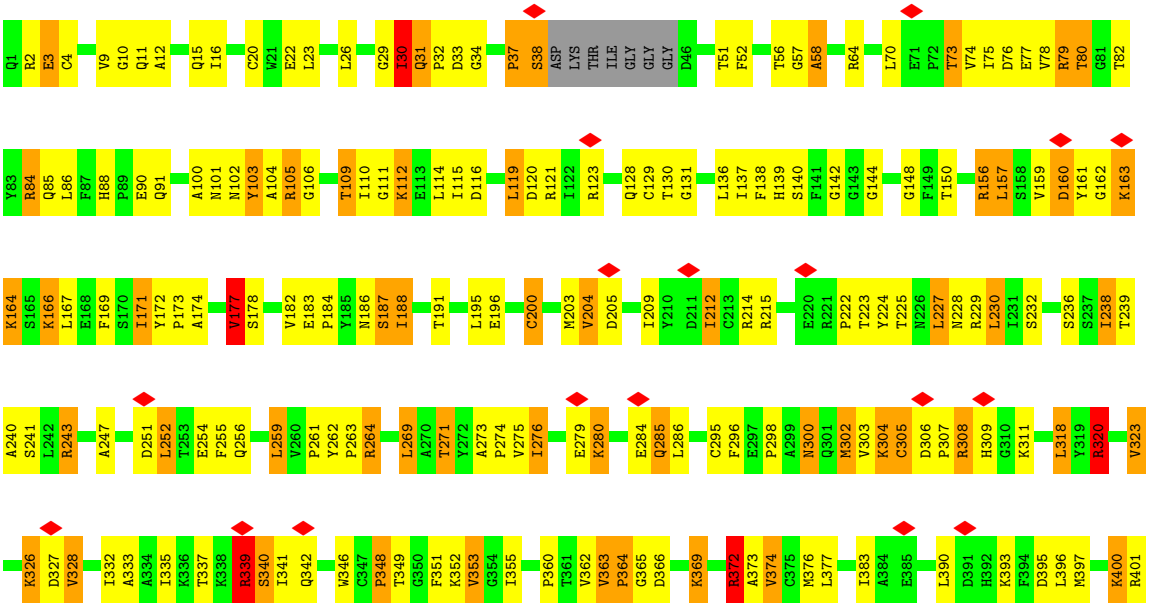

- Molecule 40: Tubulin alpha chain

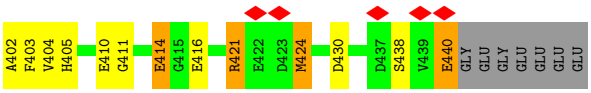
Chain LE:




- Molecule 40: Tubulin alpha chain

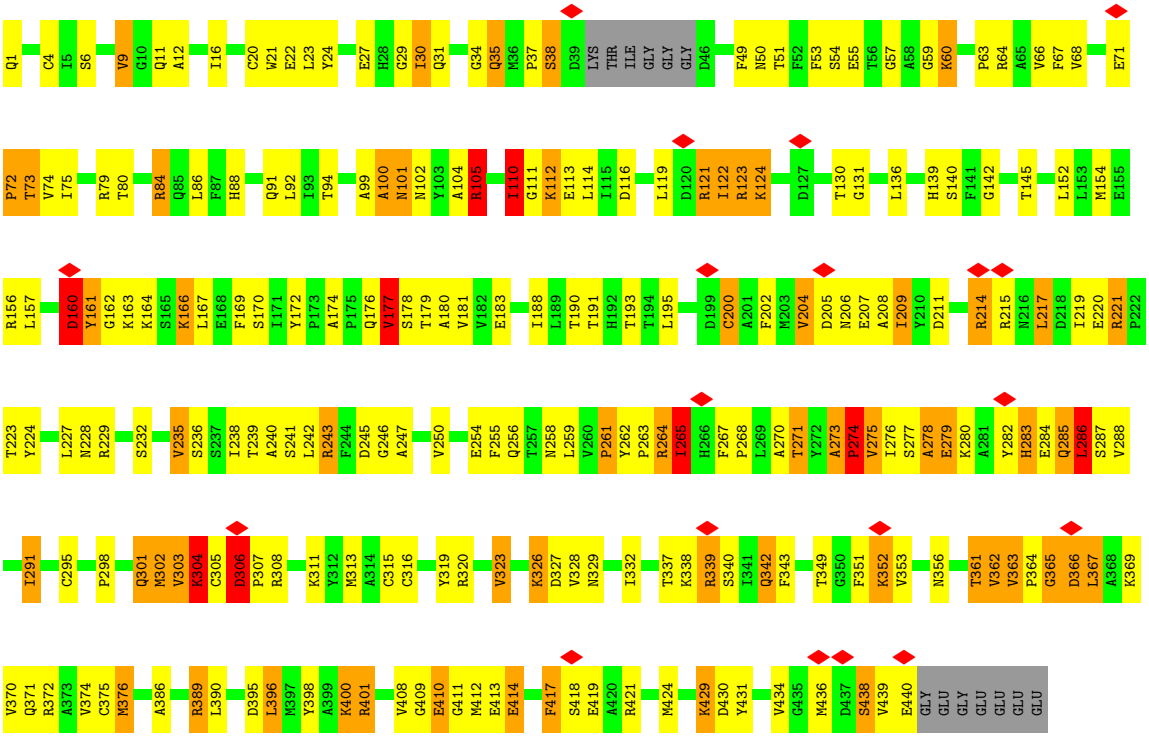
Chain LF:





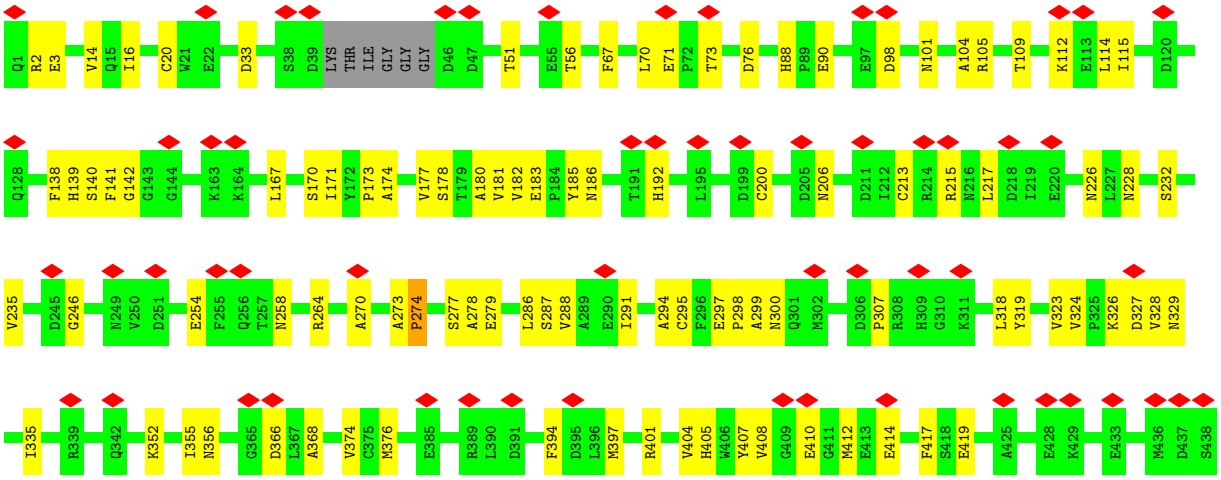

• Molecule 40: Tubulin alpha chain

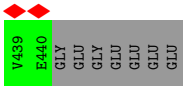
Chain LG:




• Molecule 40: Tubulin alpha chain

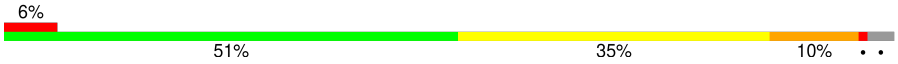
Chain LH:

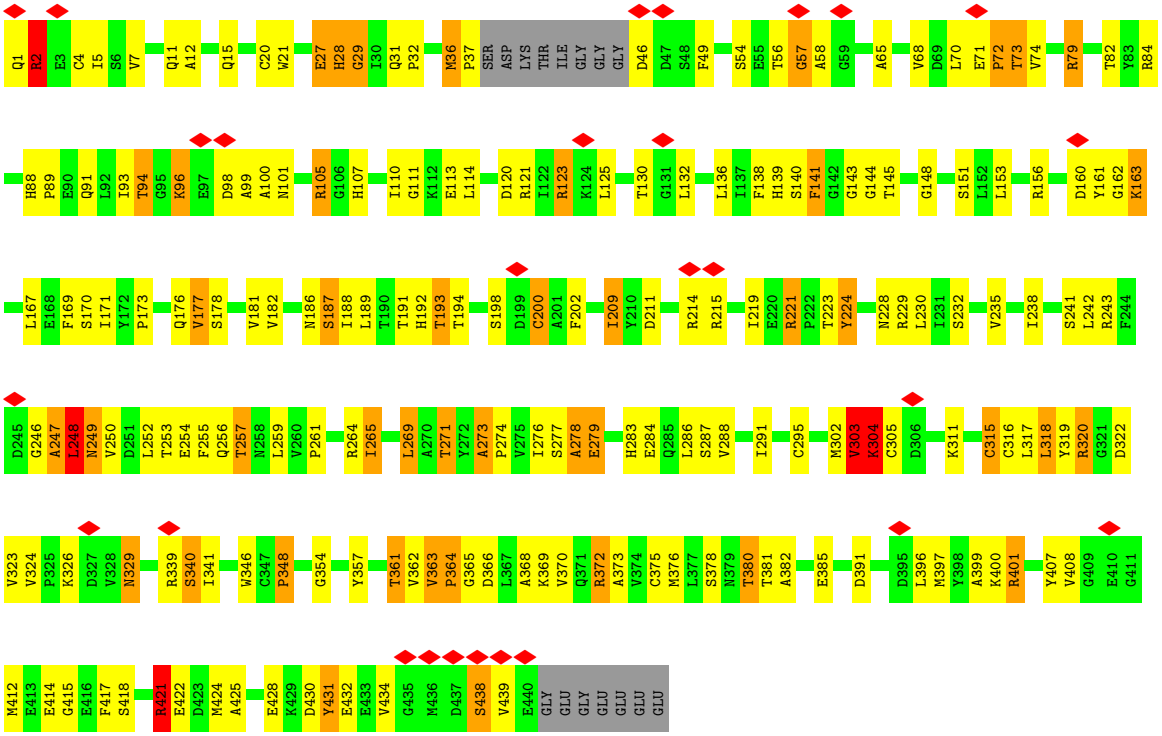





• Molecule 40: Tubulin alpha chain

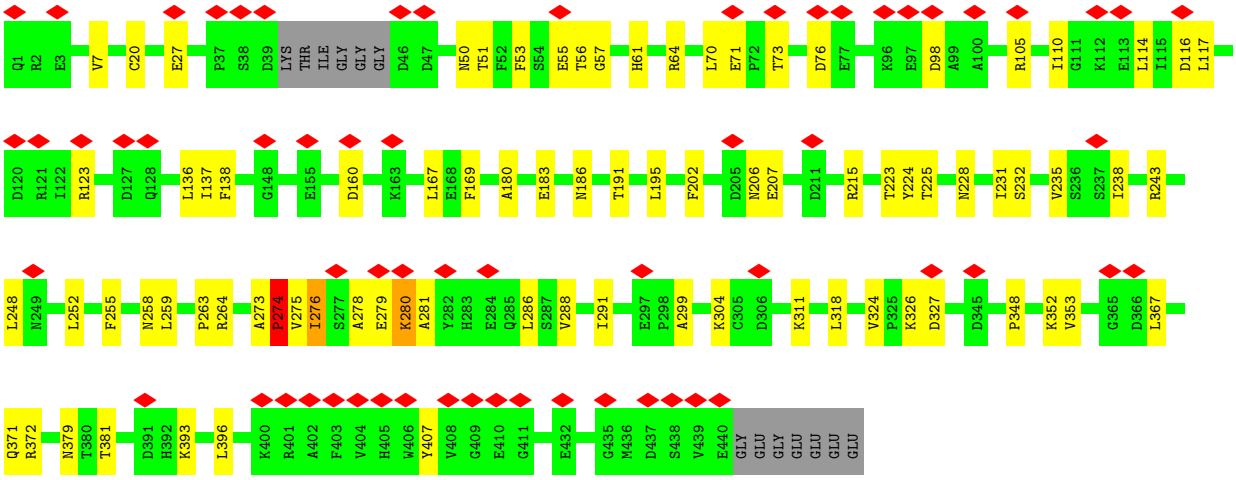
Chain MA:



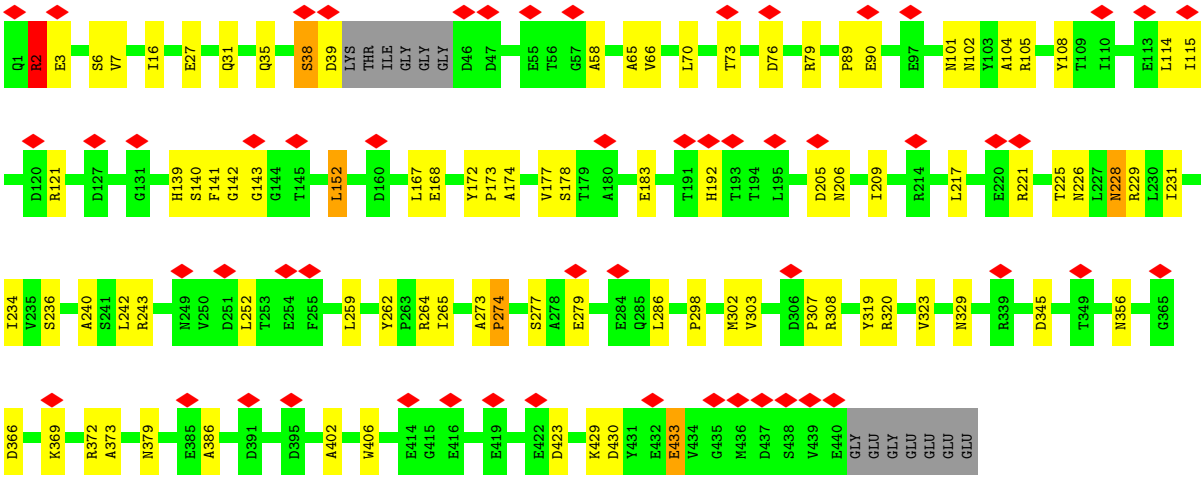

• Molecule 40: Tubulin alpha chain

Chain MD:



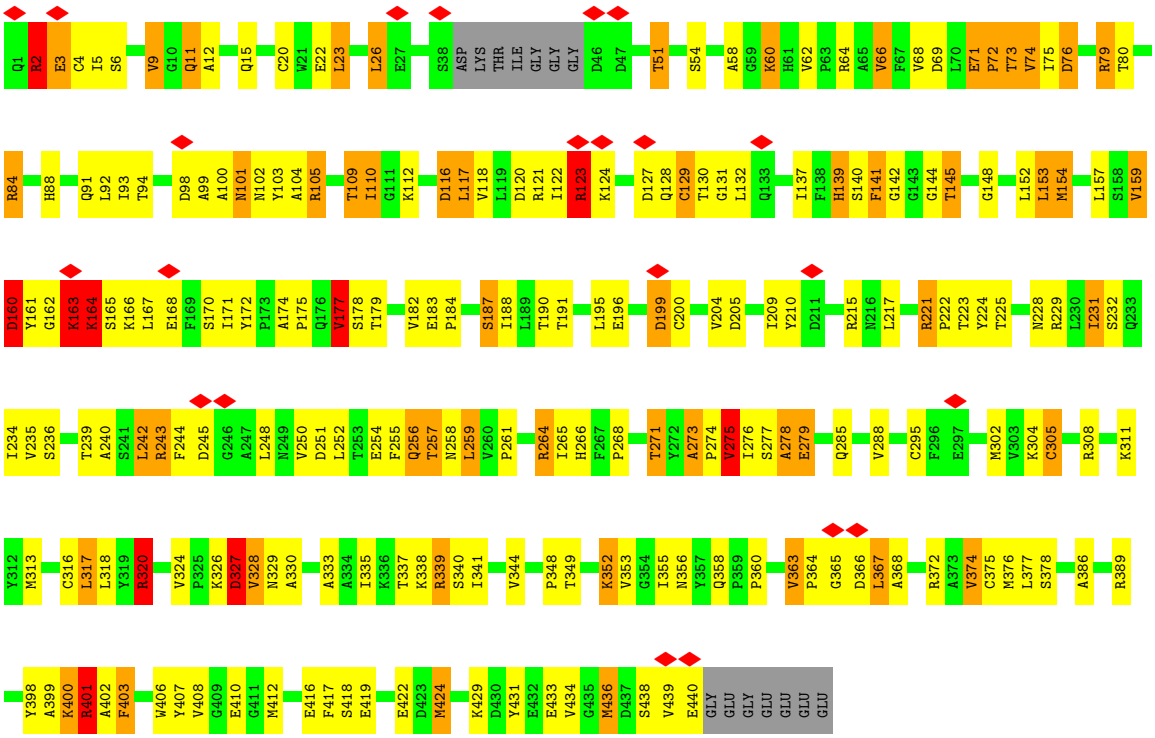

• Molecule 40: Tubulin alpha chain

Chain ME:



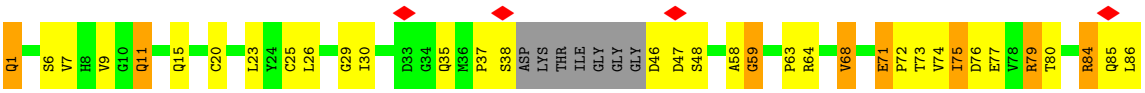

- Molecule 40: Tubulin alpha chain

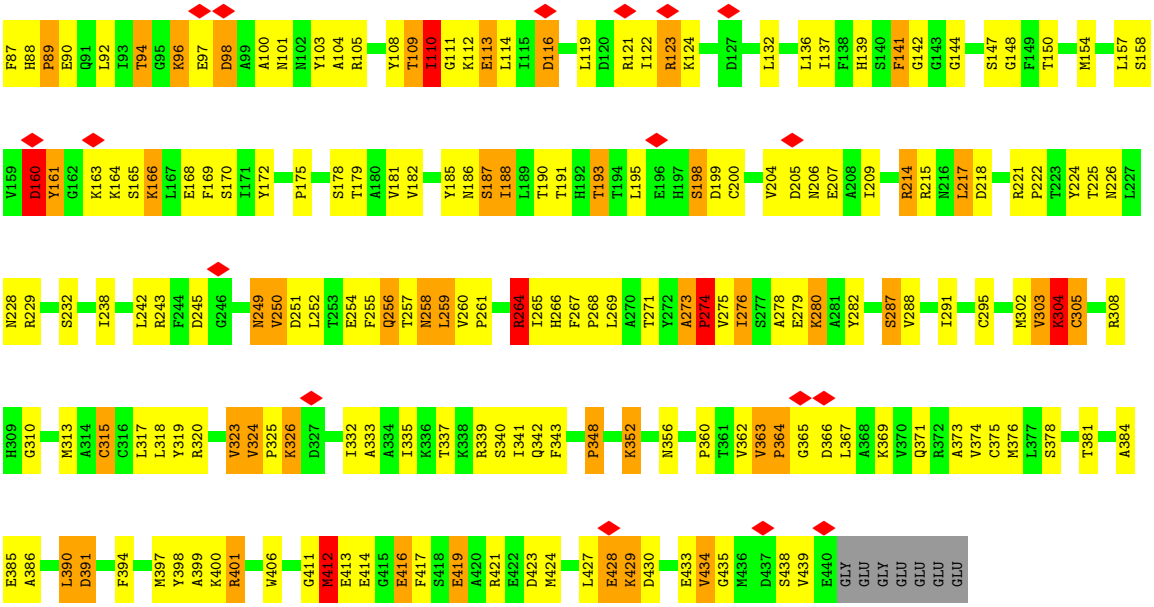
Chain MF:




- Molecule 40: Tubulin alpha chain

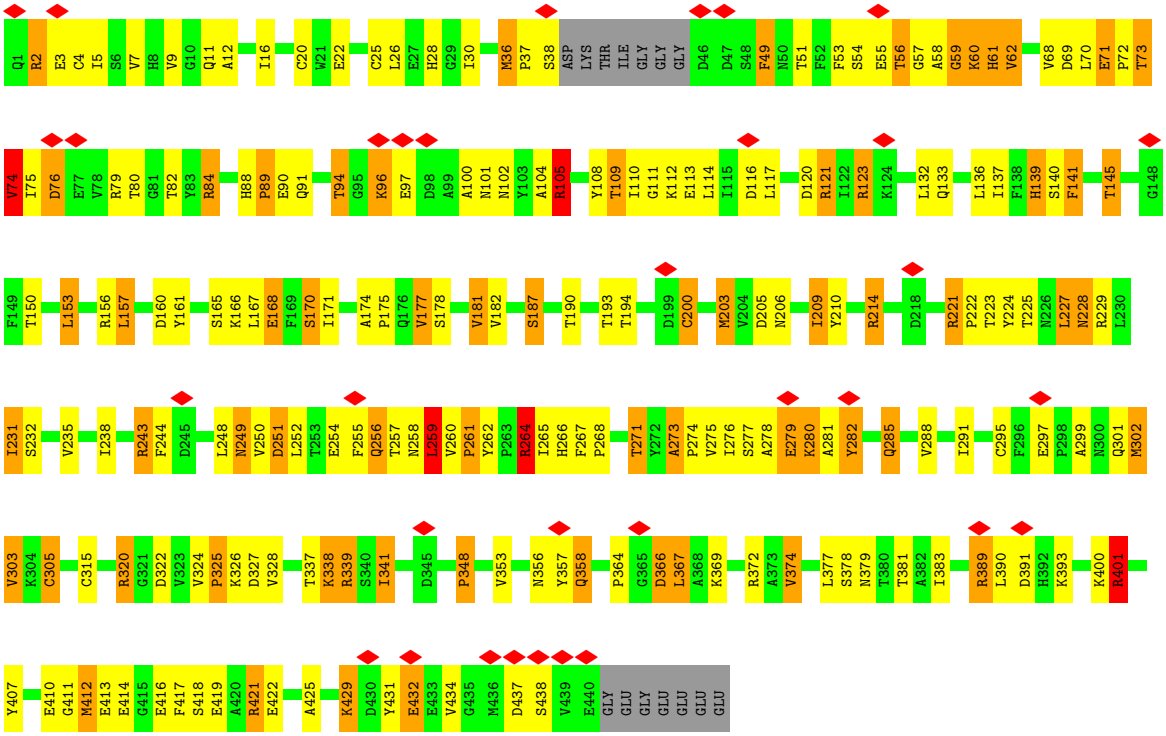
Chain MG:





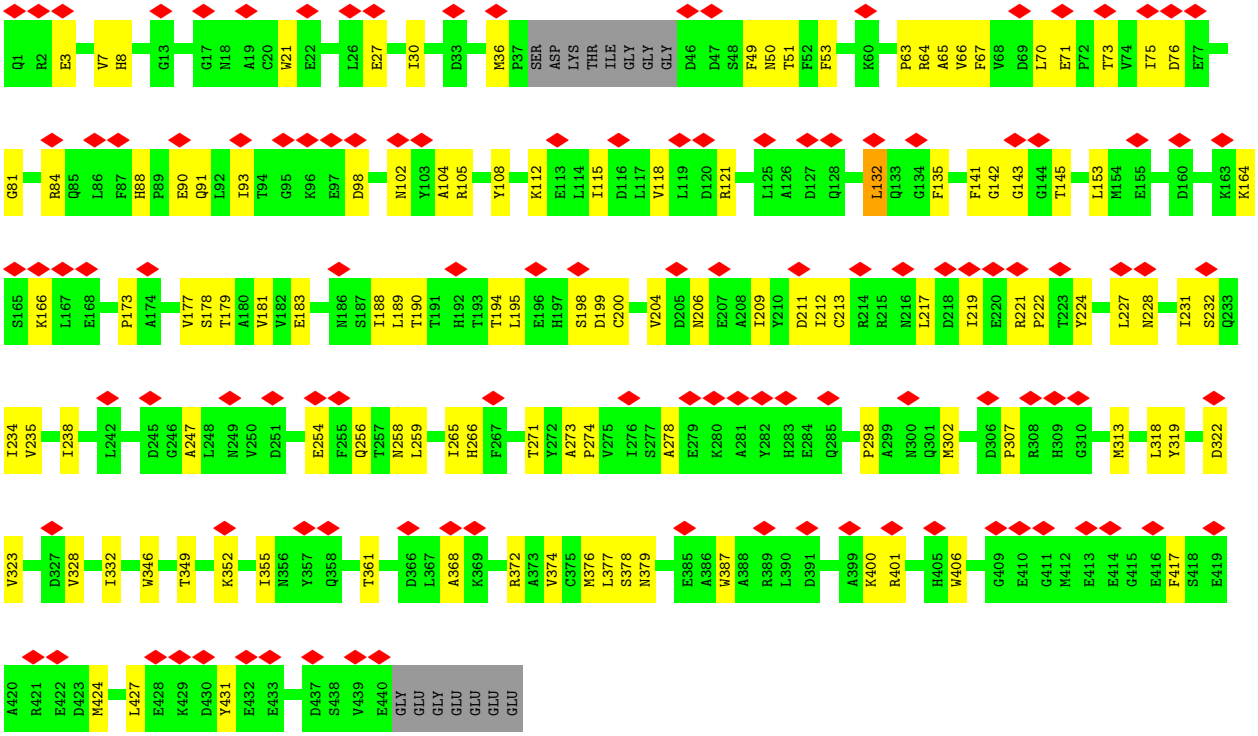

- Molecule 40: Tubulin alpha chain

Chain MH:




- Molecule 40: Tubulin alpha chain

Chain NA:




- Molecule 40: Tubulin alpha chain

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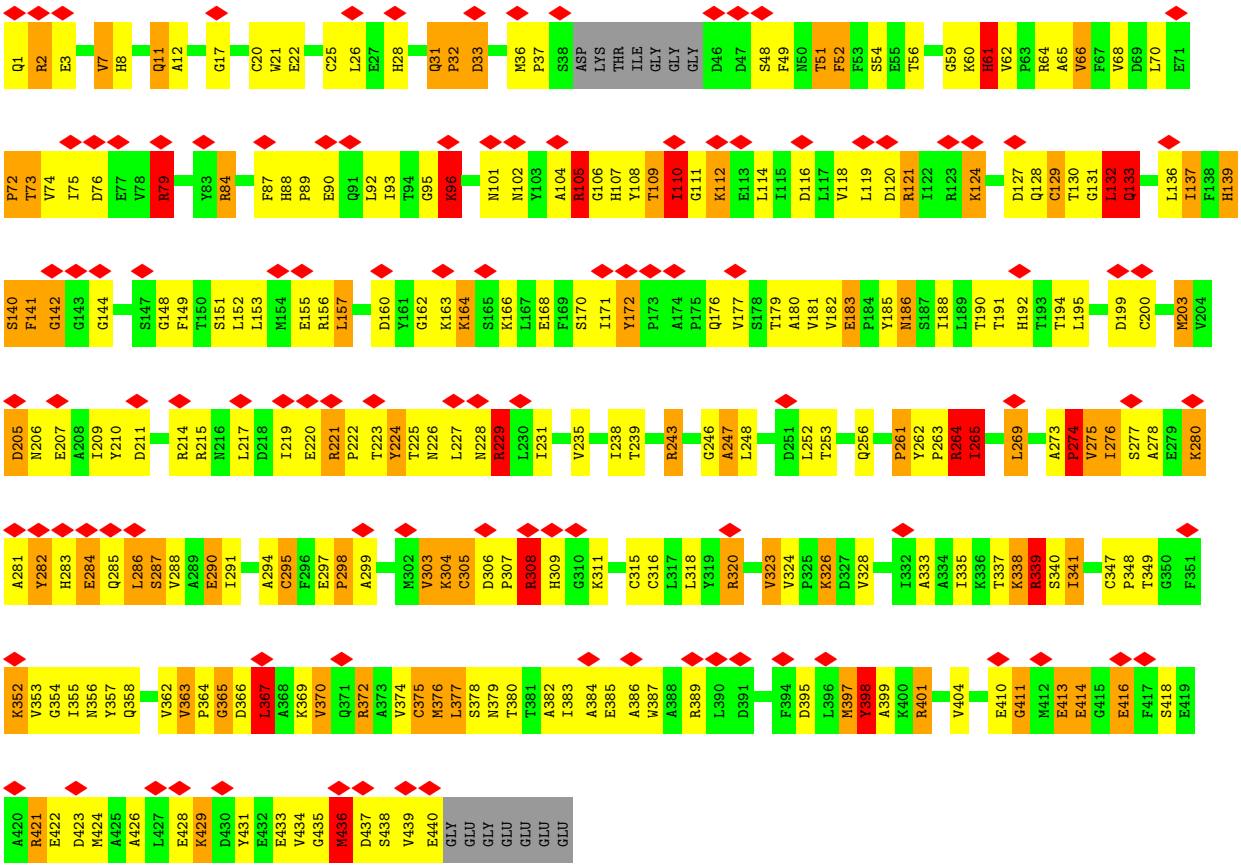
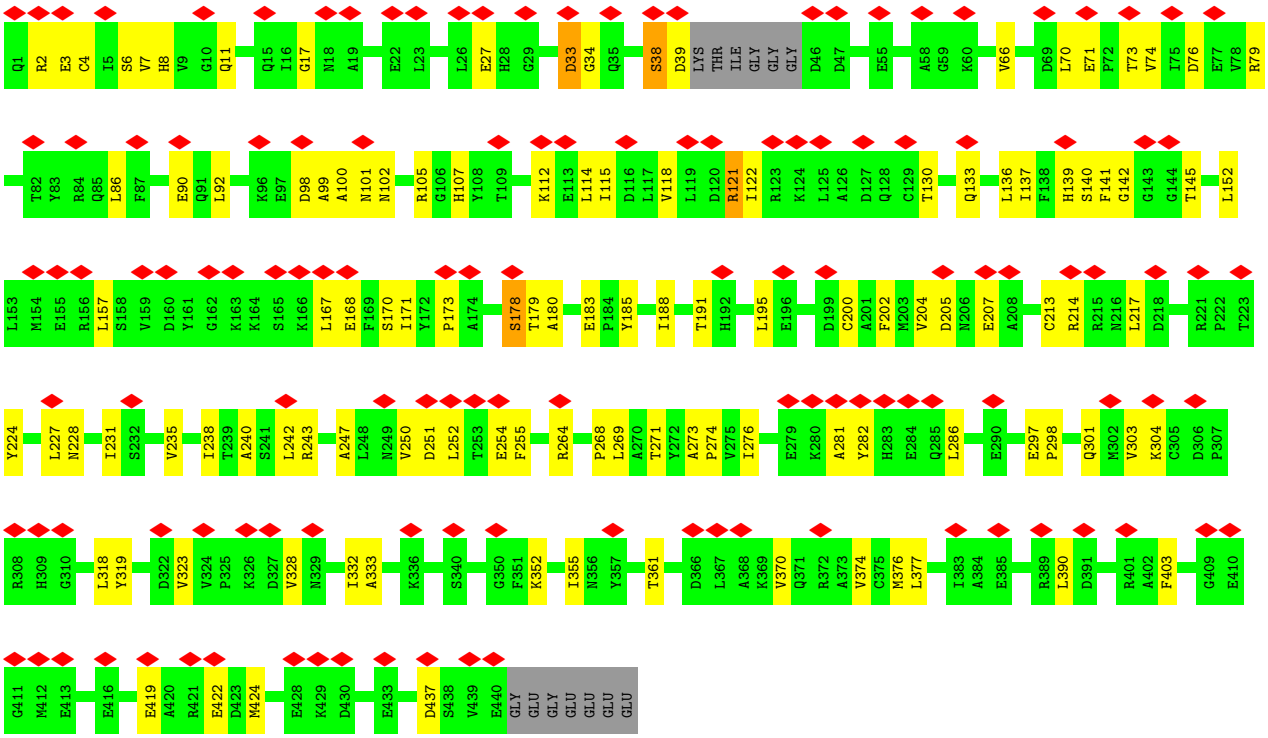


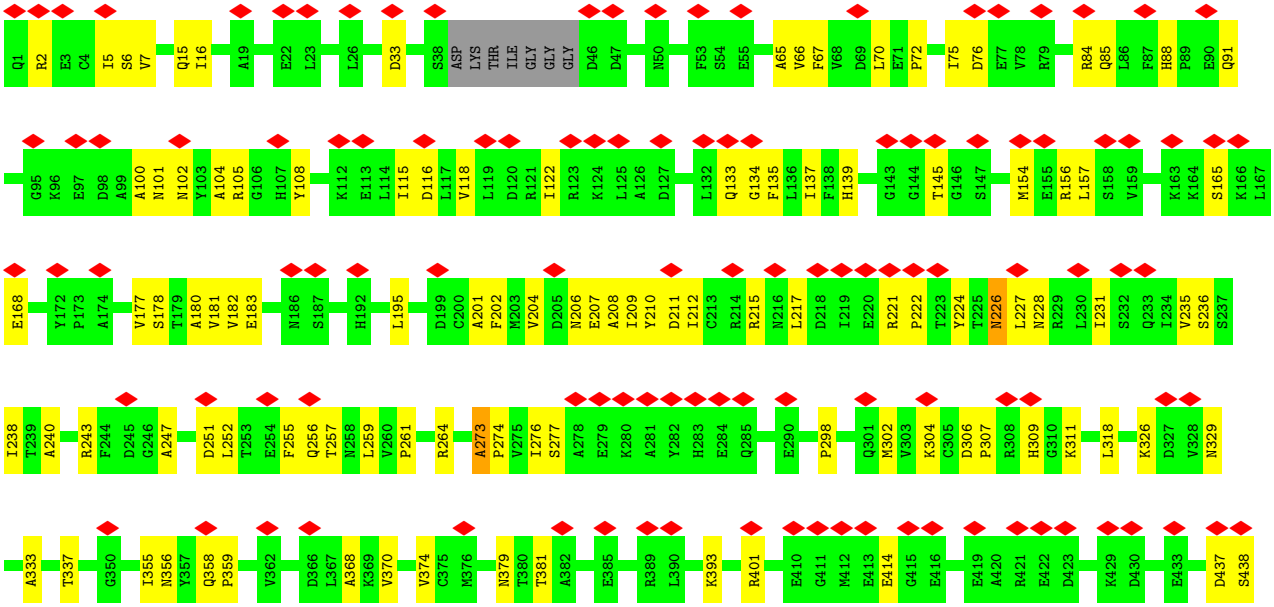
- Molecule 40: Tubulin alpha chain

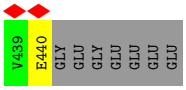
Chain NE:




- Molecule 40: Tubulin alpha chain

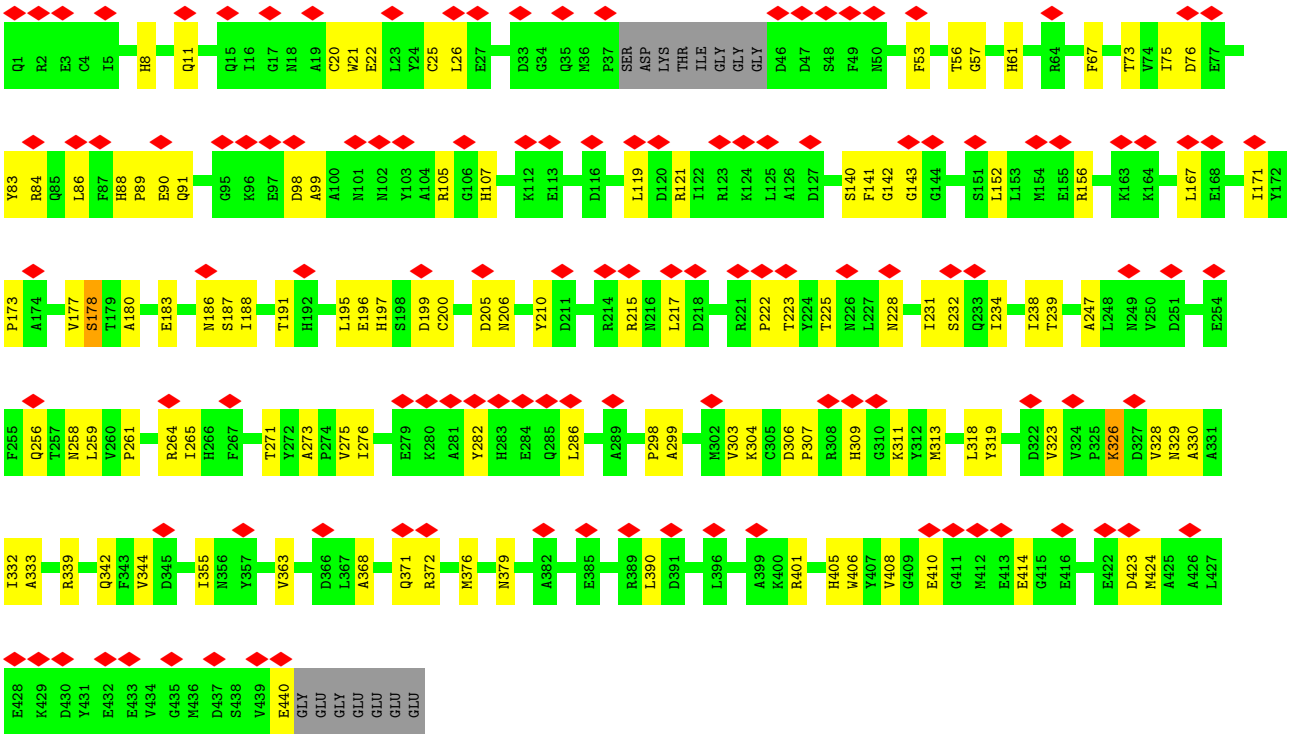
Chain NF:





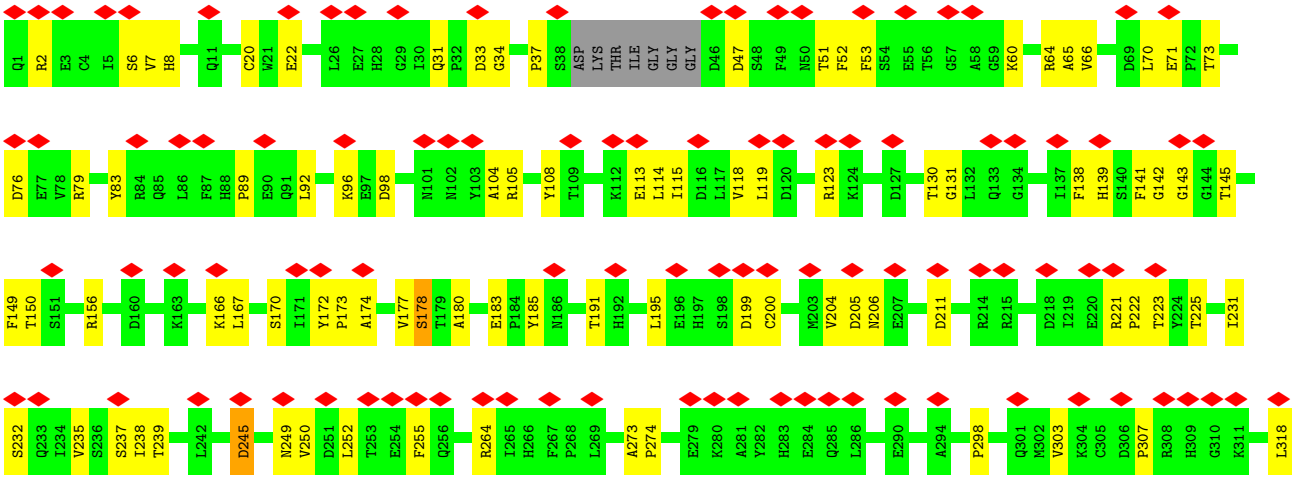

- Molecule 40: Tubulin alpha chain

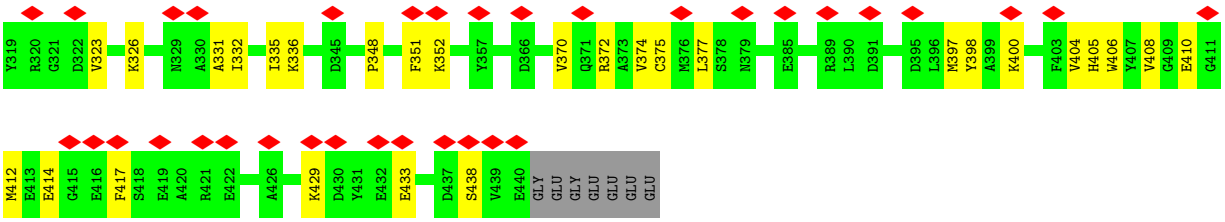
Chain NG:




- Molecule 40: Tubulin alpha chain

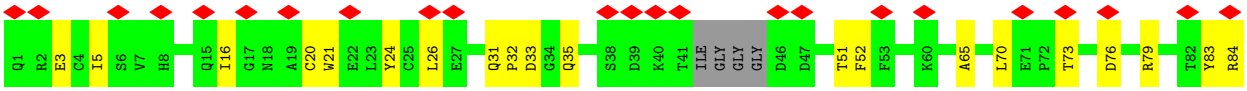
Chain NH:

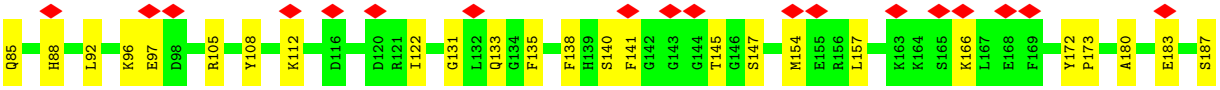


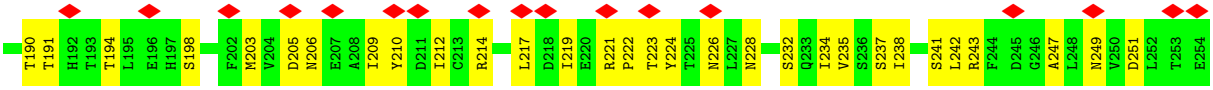


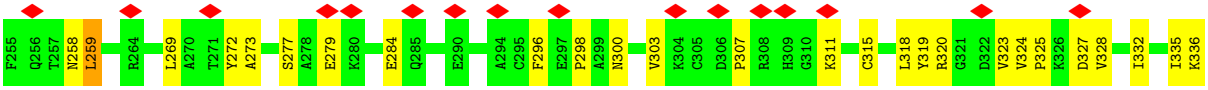

- Molecule 40: Tubulin alpha chain

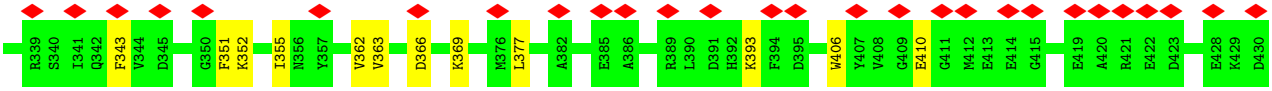
Chain OA:

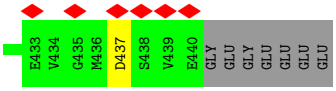


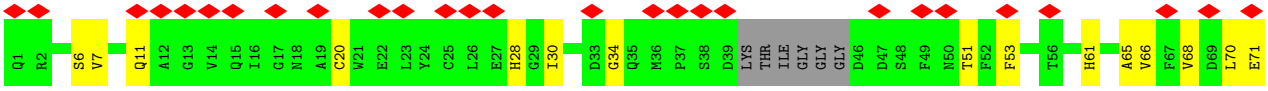



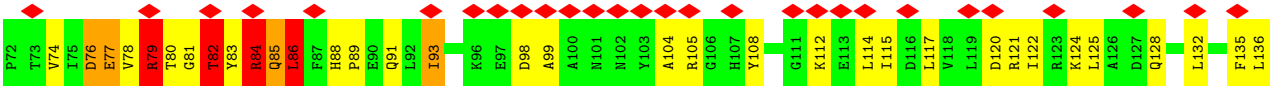



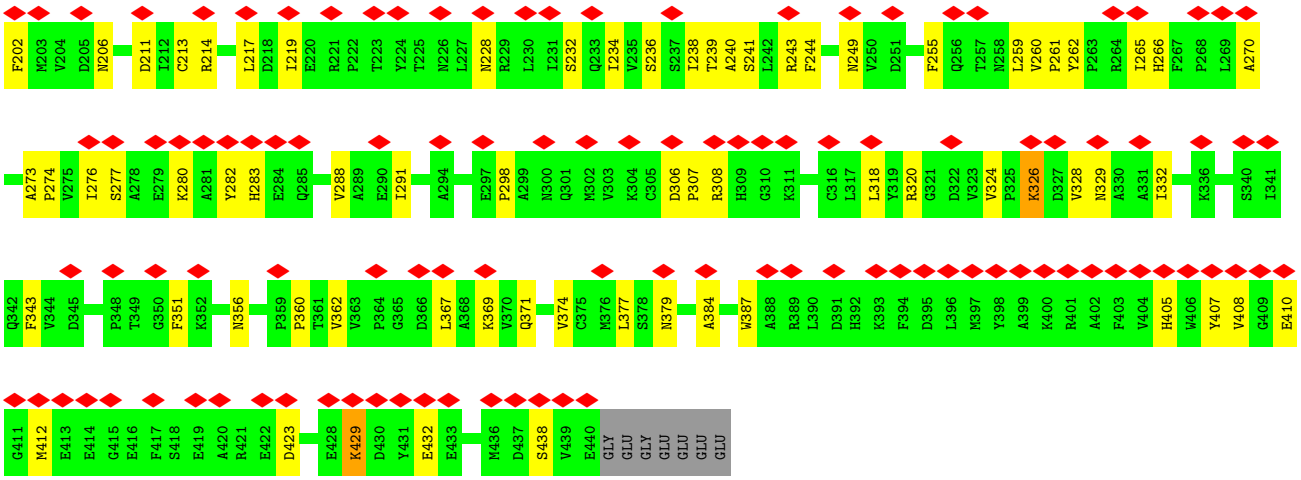




- Molecule 40: Tubulin alpha chain

Chain OD:

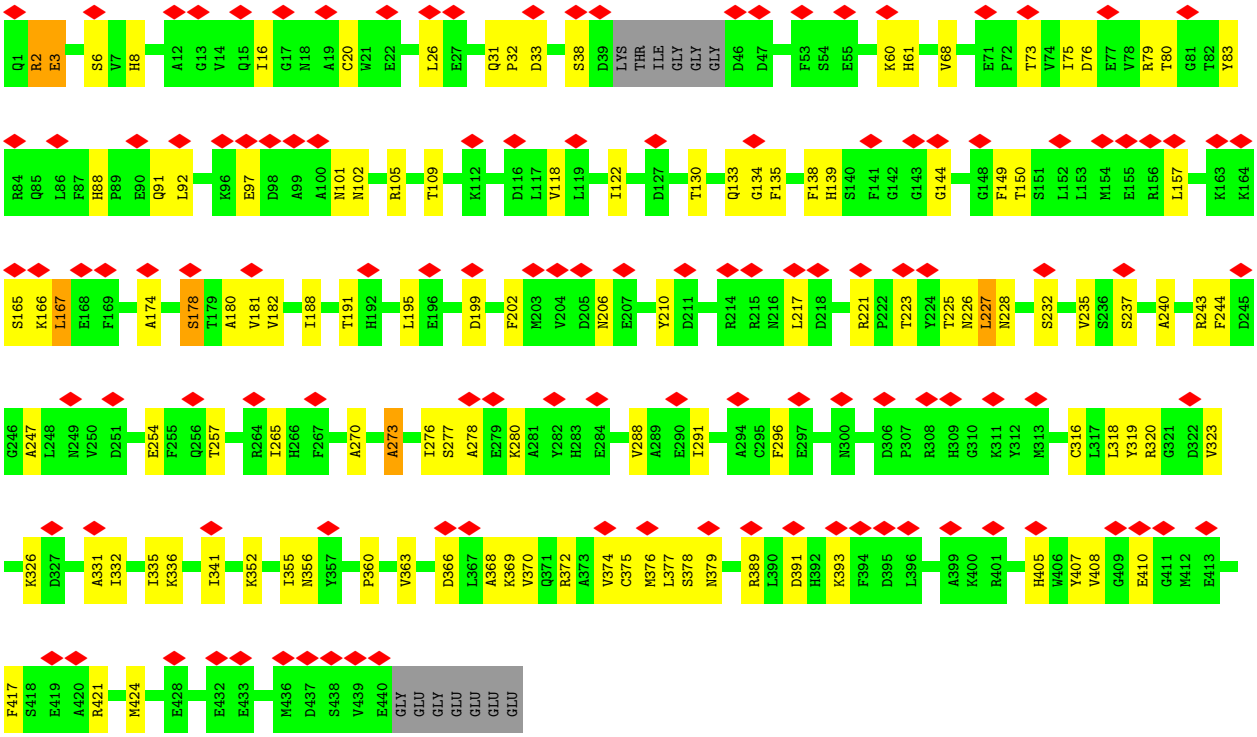




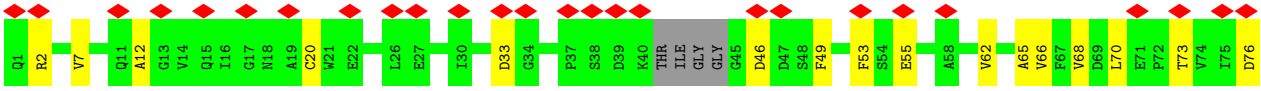

- Molecule 40: Tubulin alpha chain

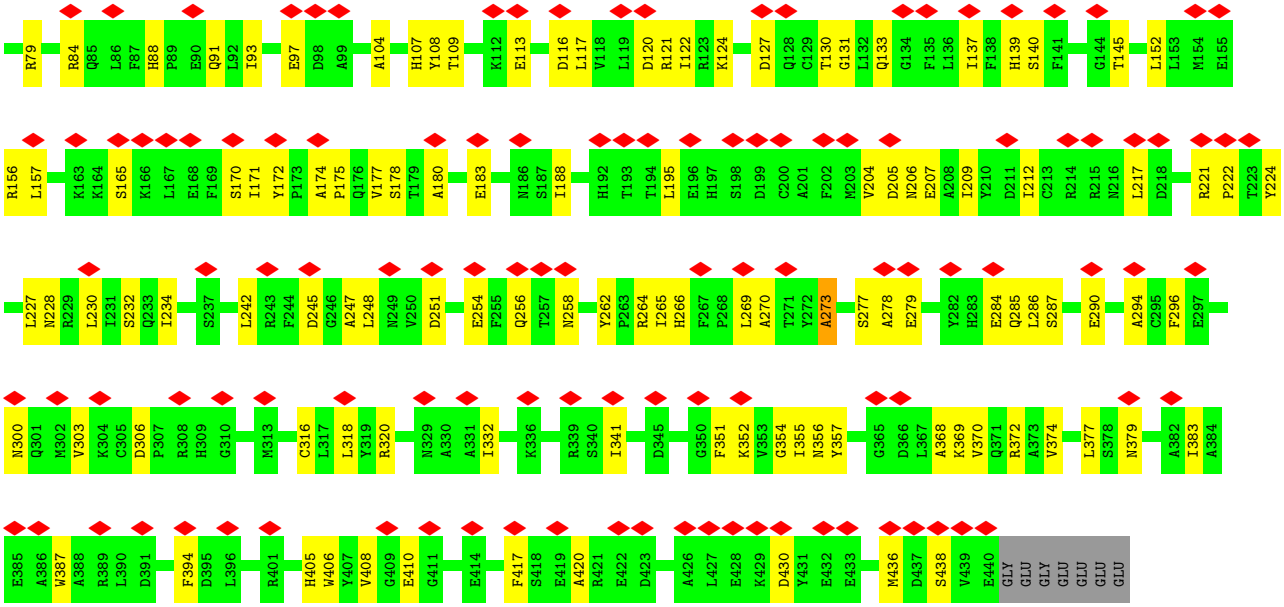
Chain OE:




- Molecule 40: Tubulin alpha chain

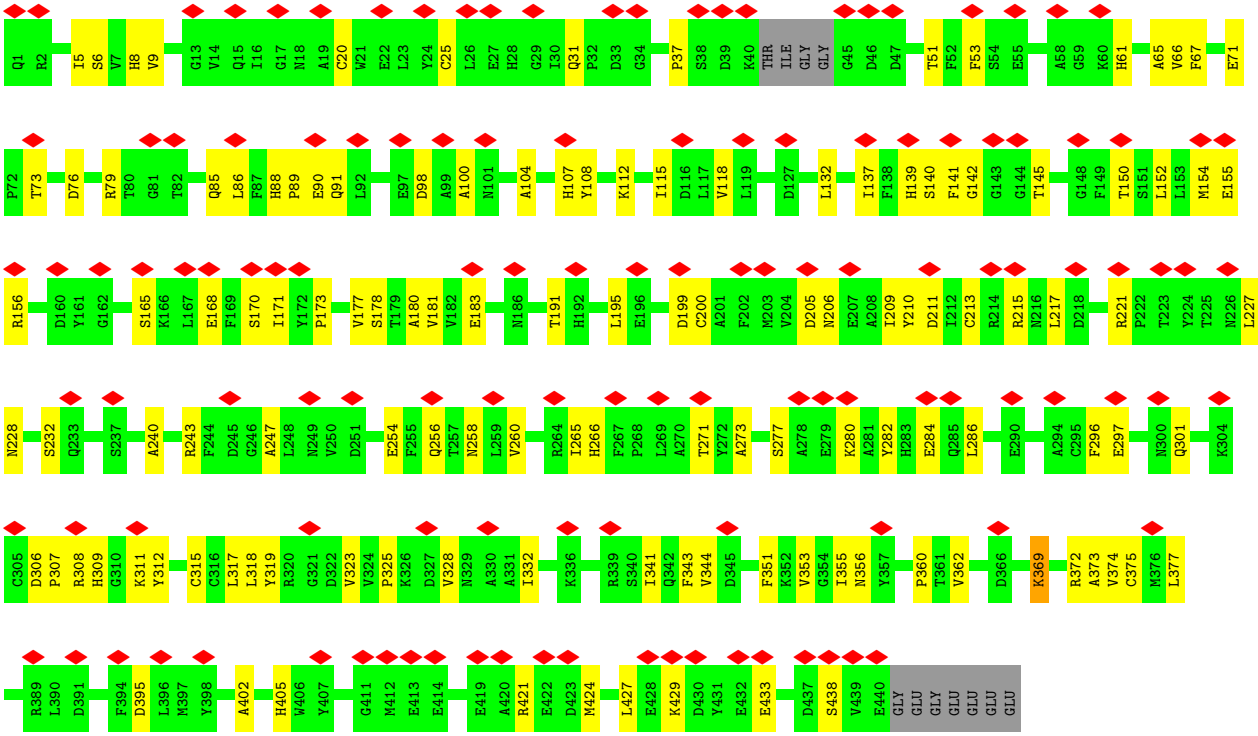
Chain OF:





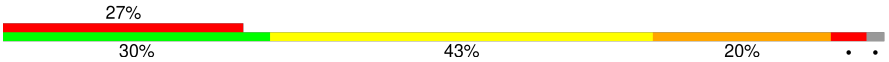

- Molecule 40: Tubulin alpha chain

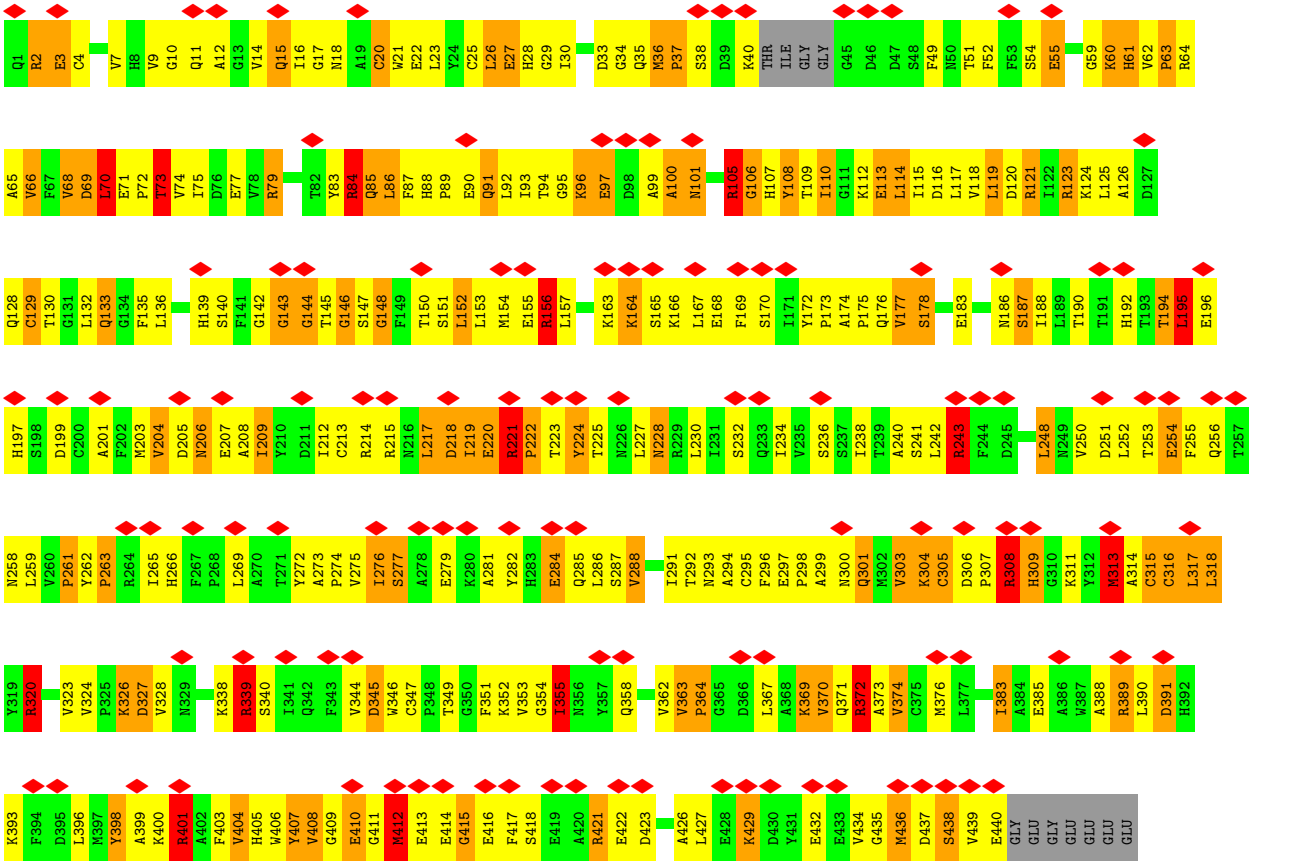
Chain OG:




- Molecule 40: Tubulin alpha chain

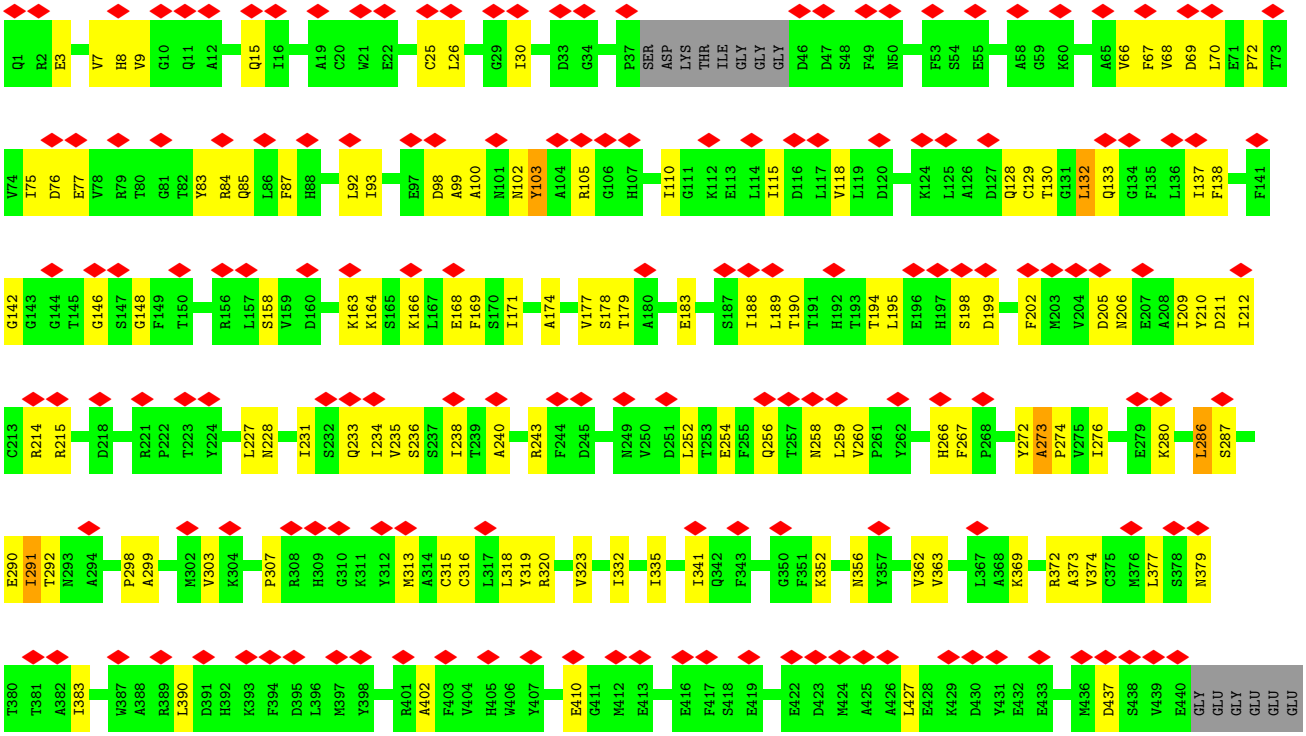
Chain OH:





- Molecule 40: Tubulin alpha chain

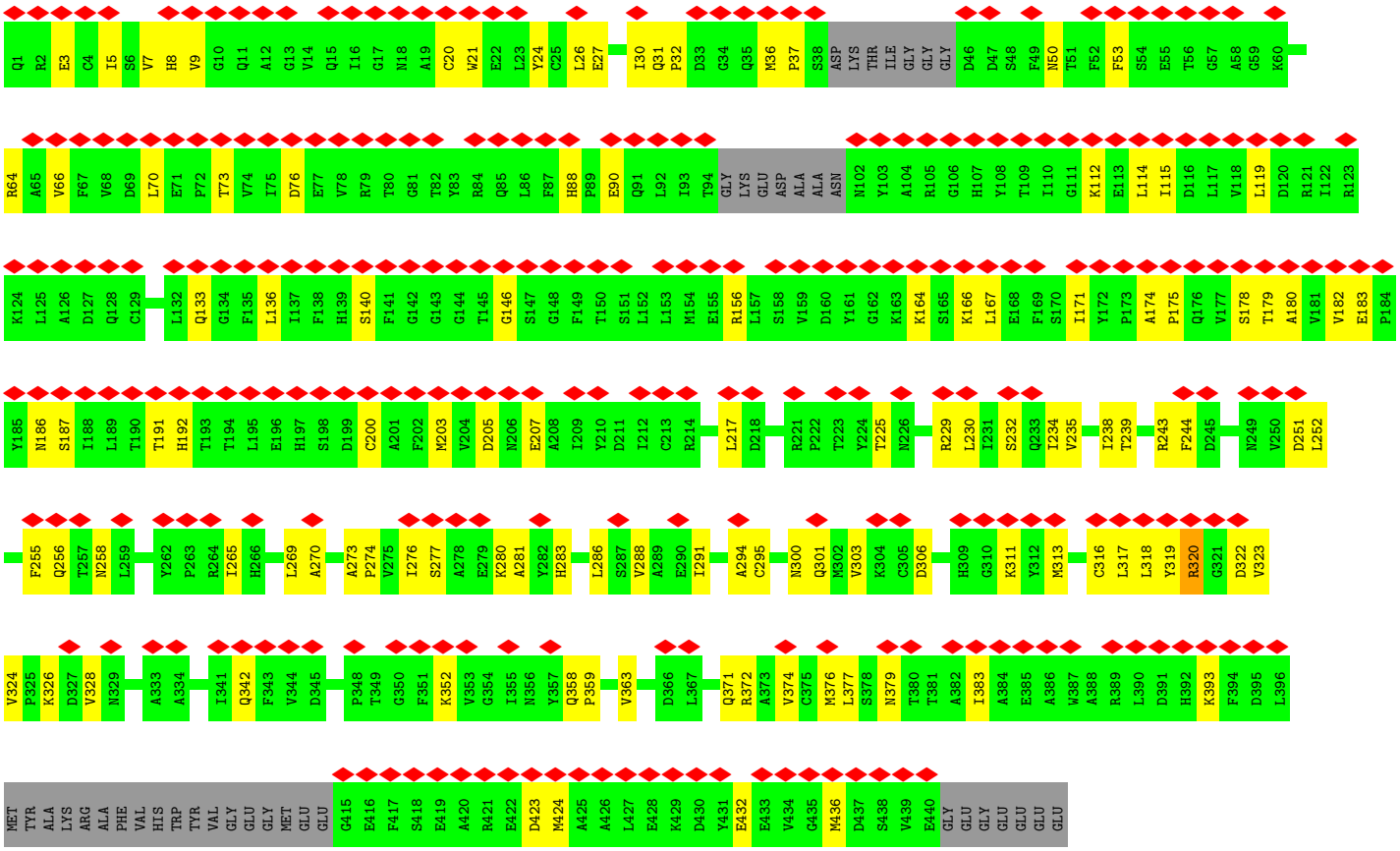
Chain PA:



GLU

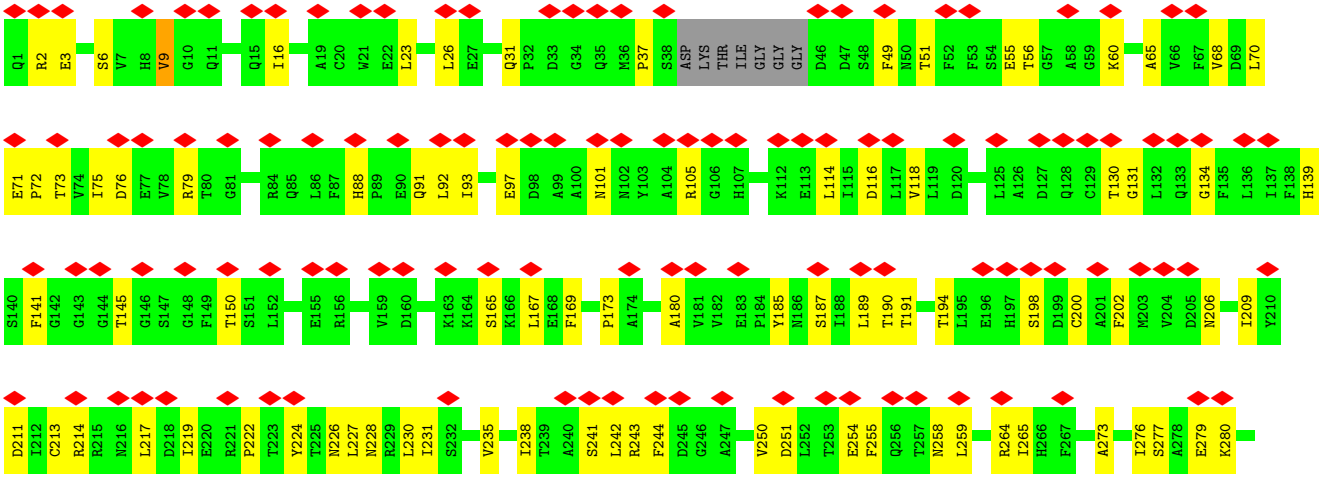
- Molecule 40: Tubulin alpha chain

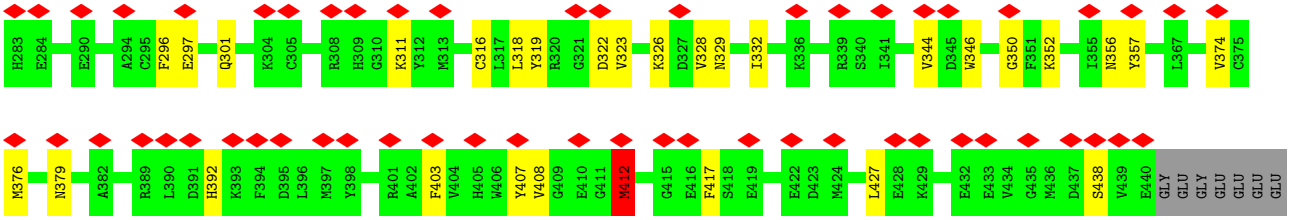
Chain PD:




- Molecule 40: Tubulin alpha chain

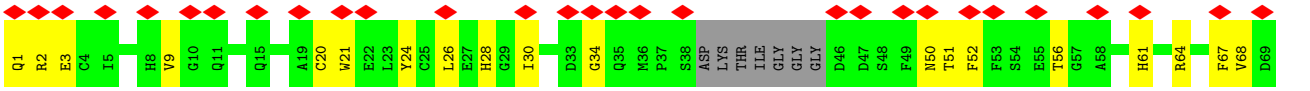
Chain PE:

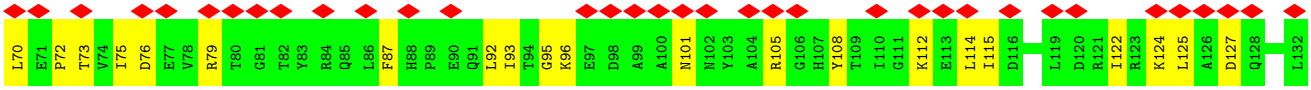


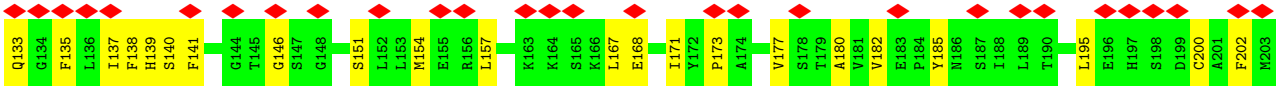


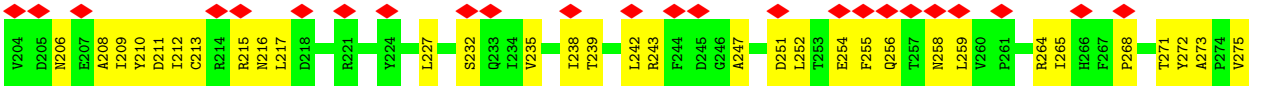

• Molecule 40: Tubulin alpha chain

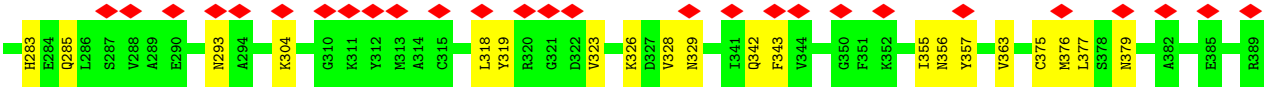
Chain PF:



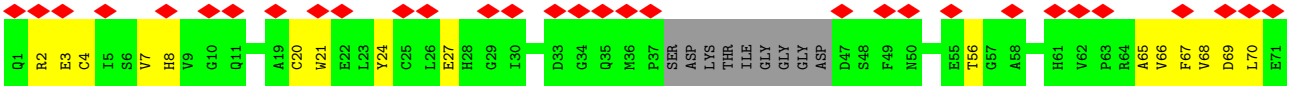



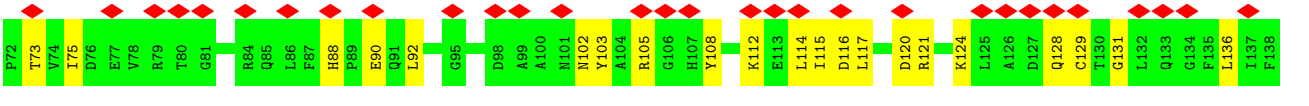



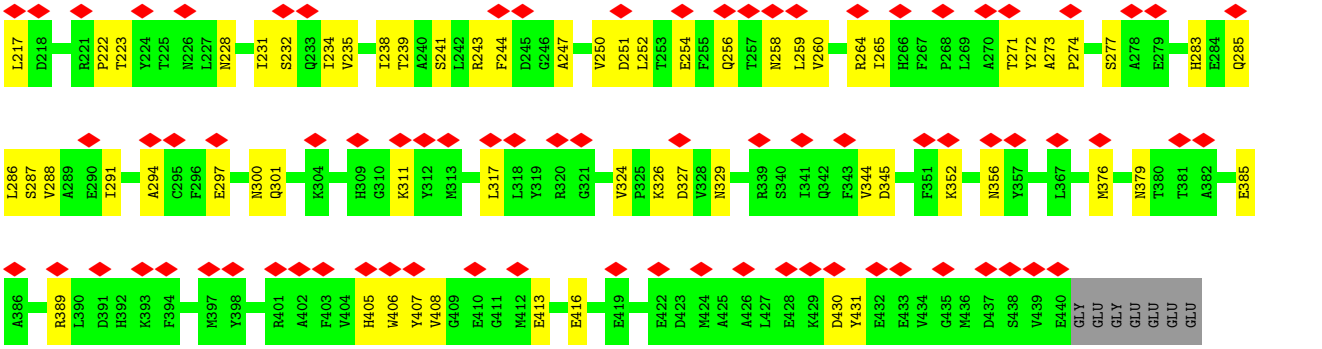



• Molecule 40: Tubulin alpha chain

Chain PG:

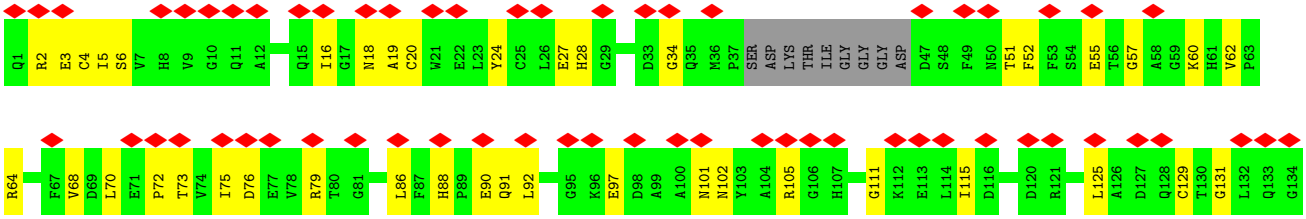




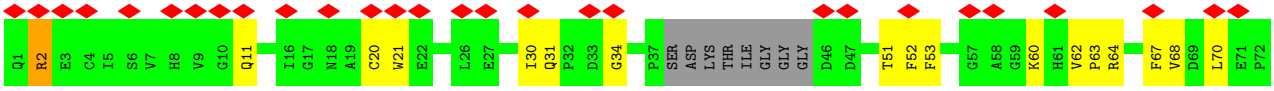

- Molecule 40: Tubulin alpha chain

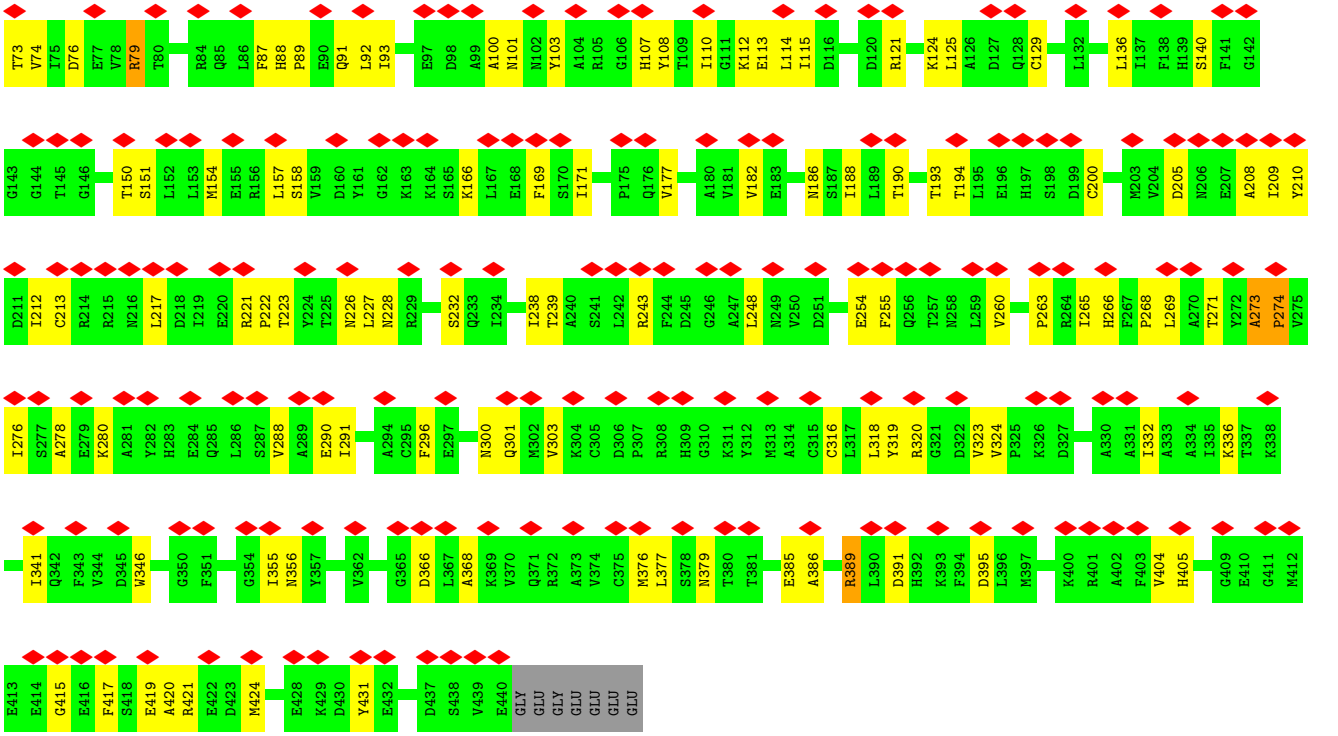
Chain PH:




- Molecule 40: Tubulin alpha chain

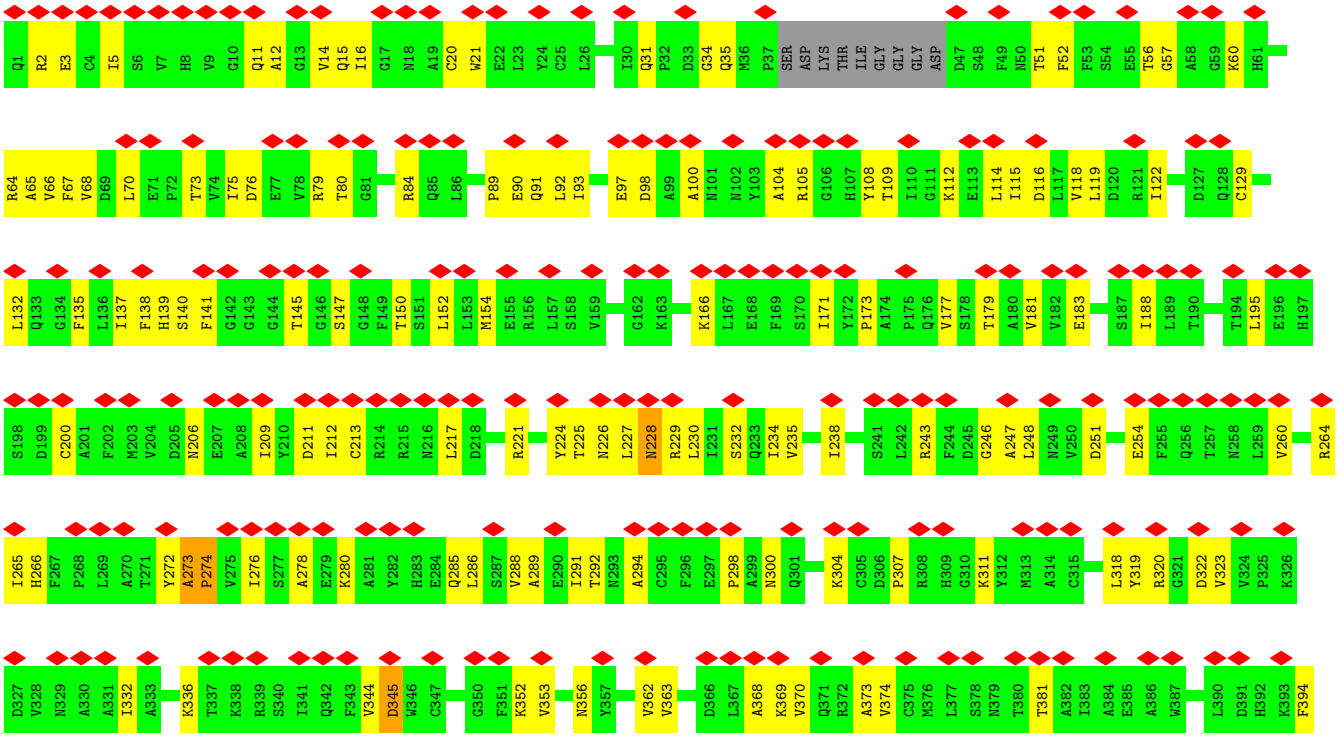
Chain QA:

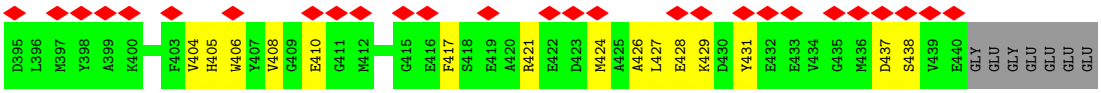





- Molecule 40: Tubulin alpha chain

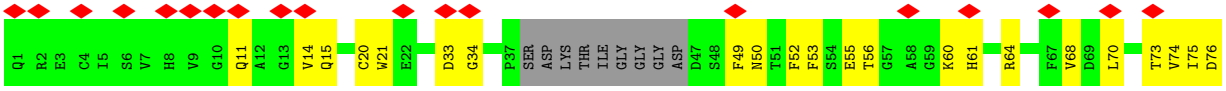
Chain QE:

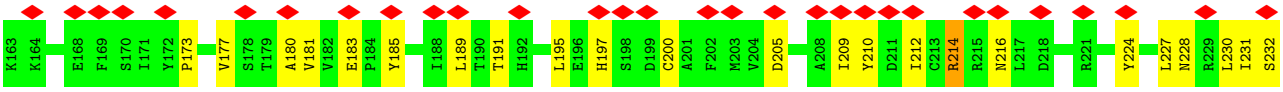


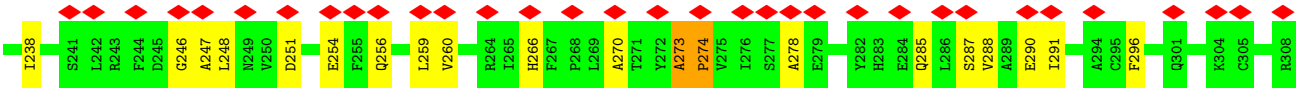


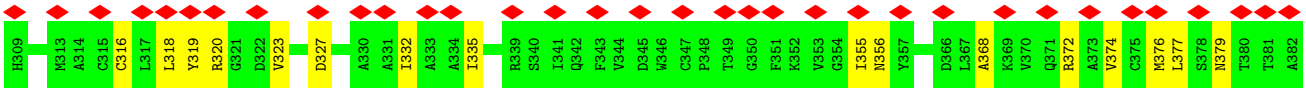

- Molecule 40: Tubulin alpha chain

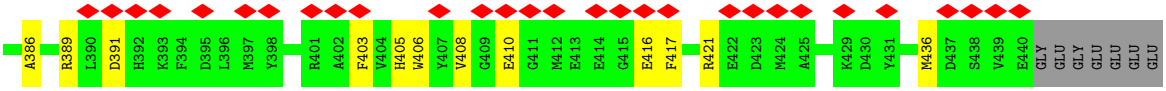
Chain QF:





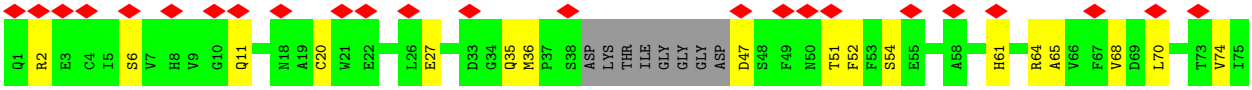



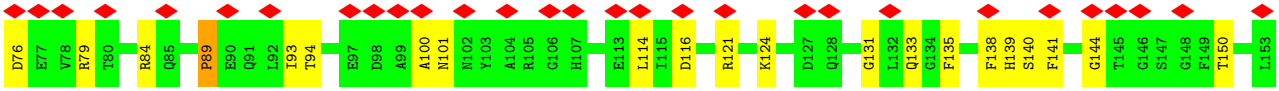



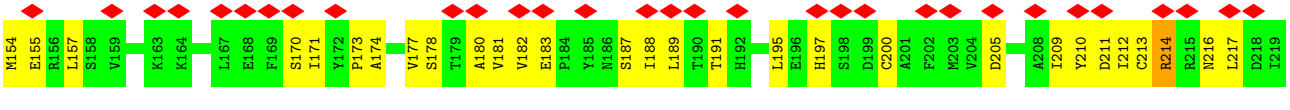



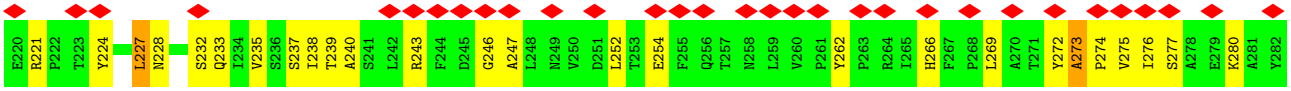

- Molecule 40: Tubulin alpha chain

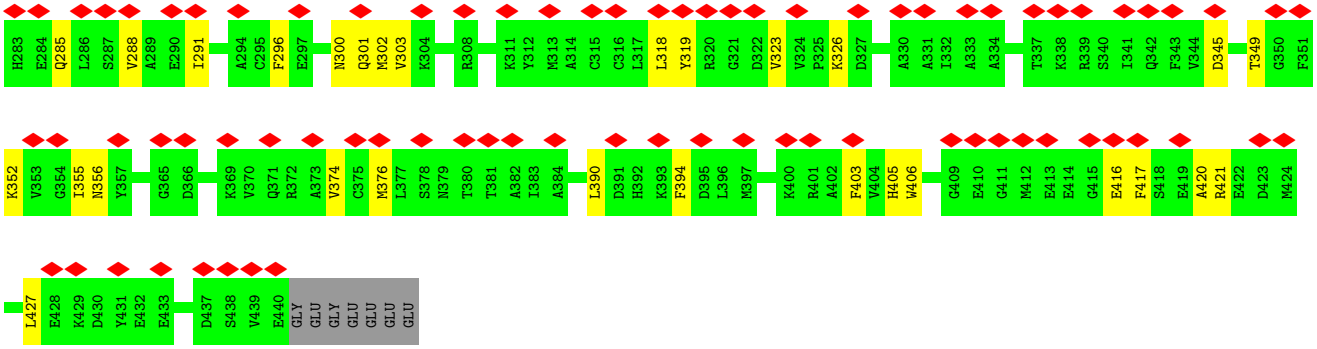
Chain QG:



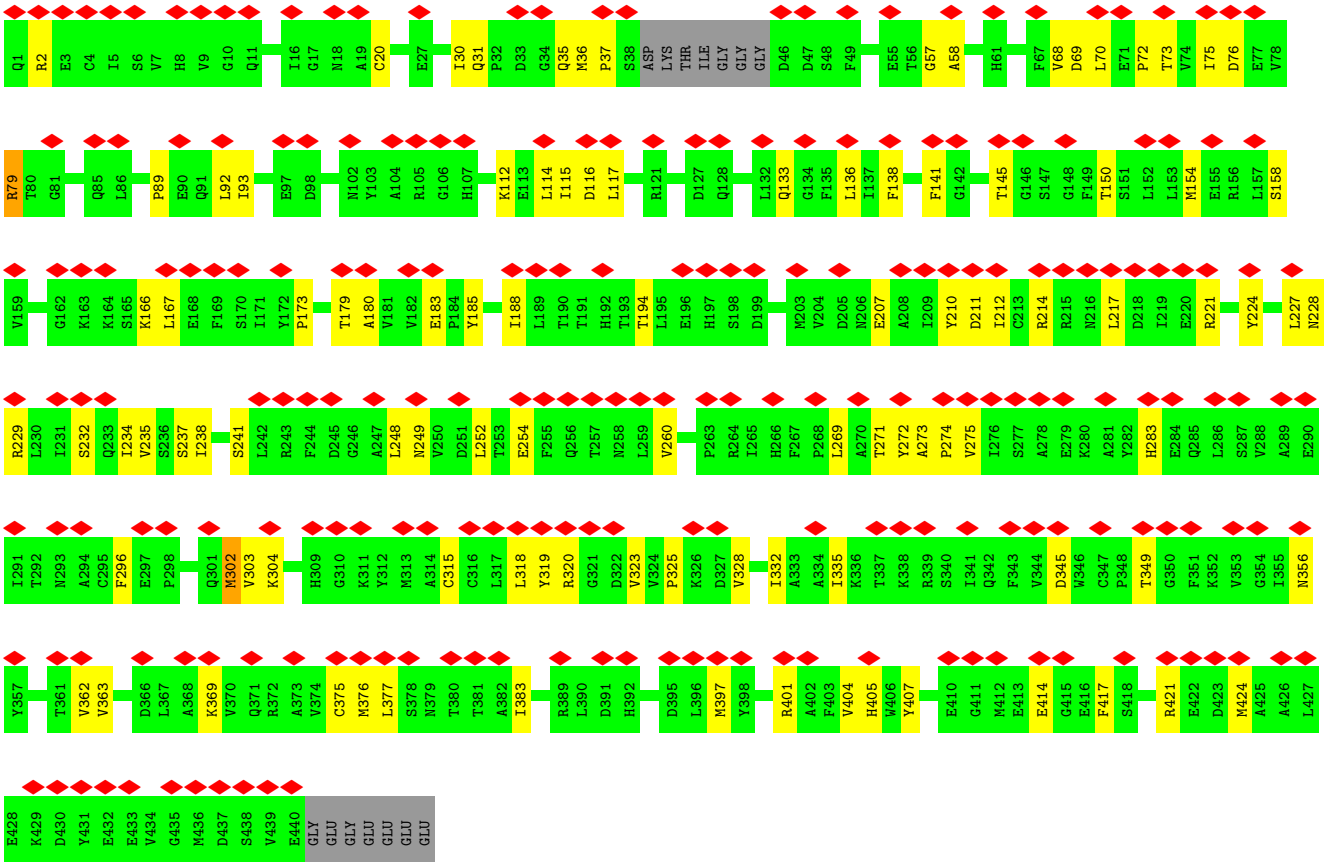





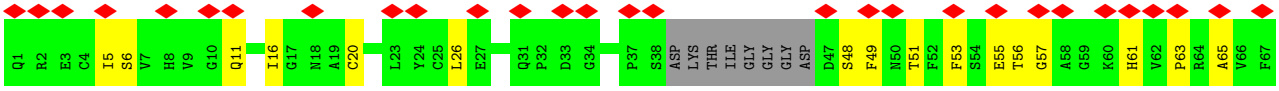

- Molecule 40: Tubulin alpha chain

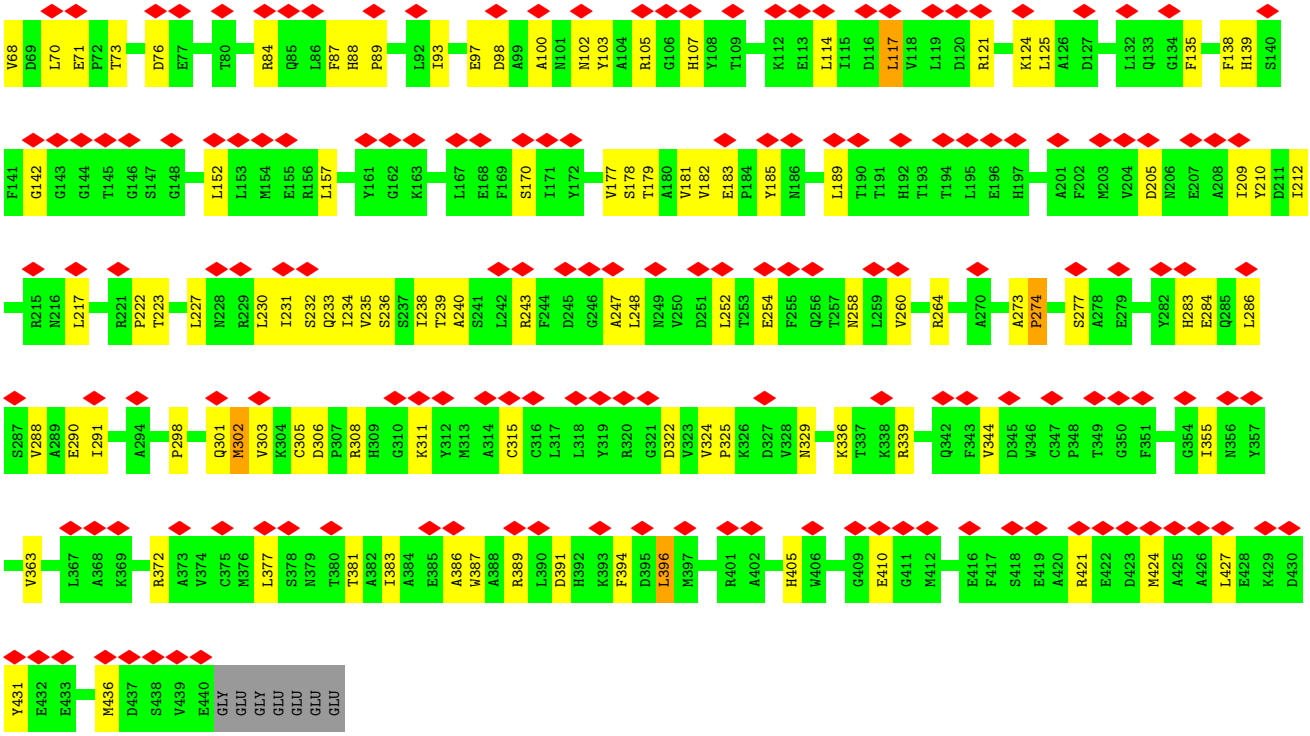
Chain QH:




- Molecule 40: Tubulin alpha chain

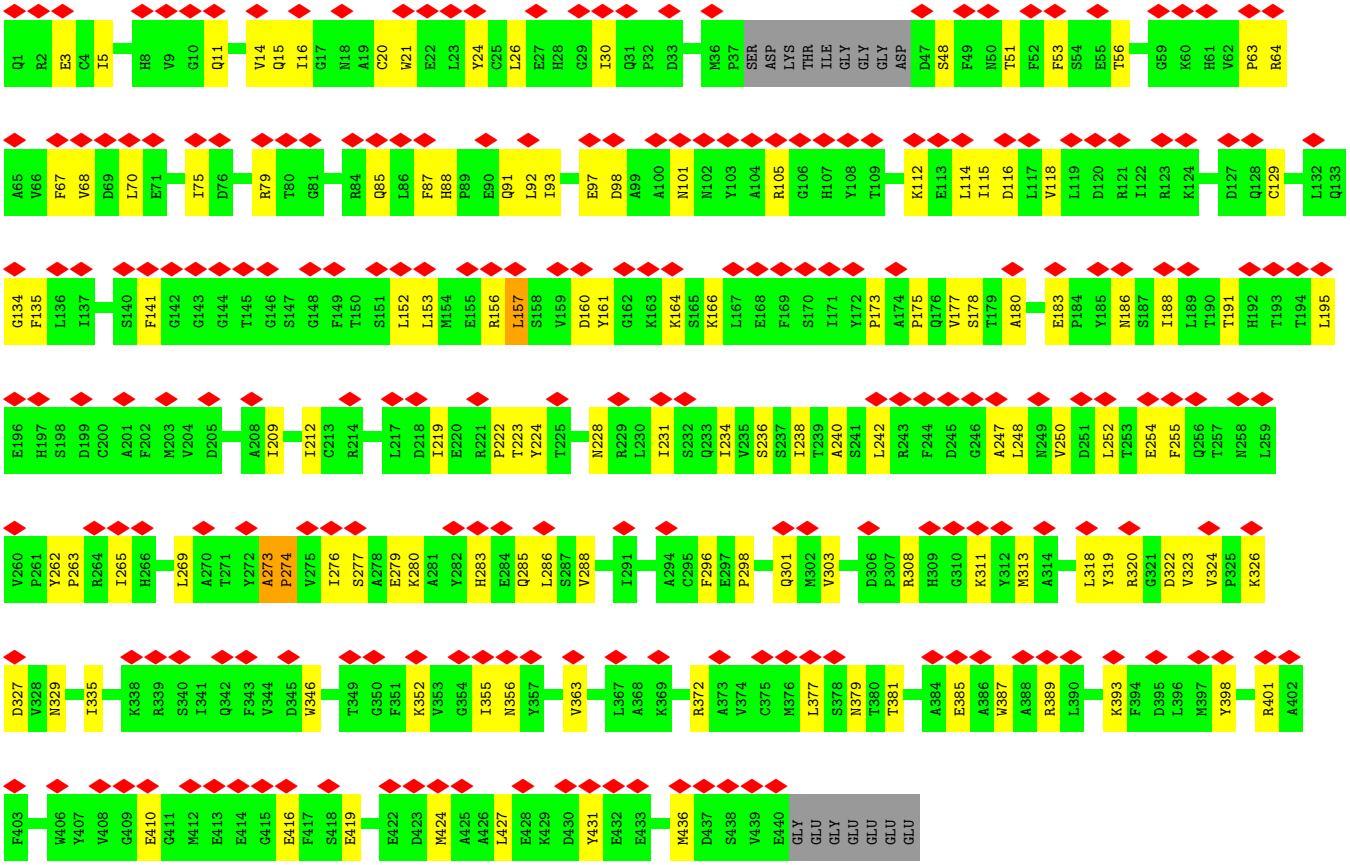
Chain RA:





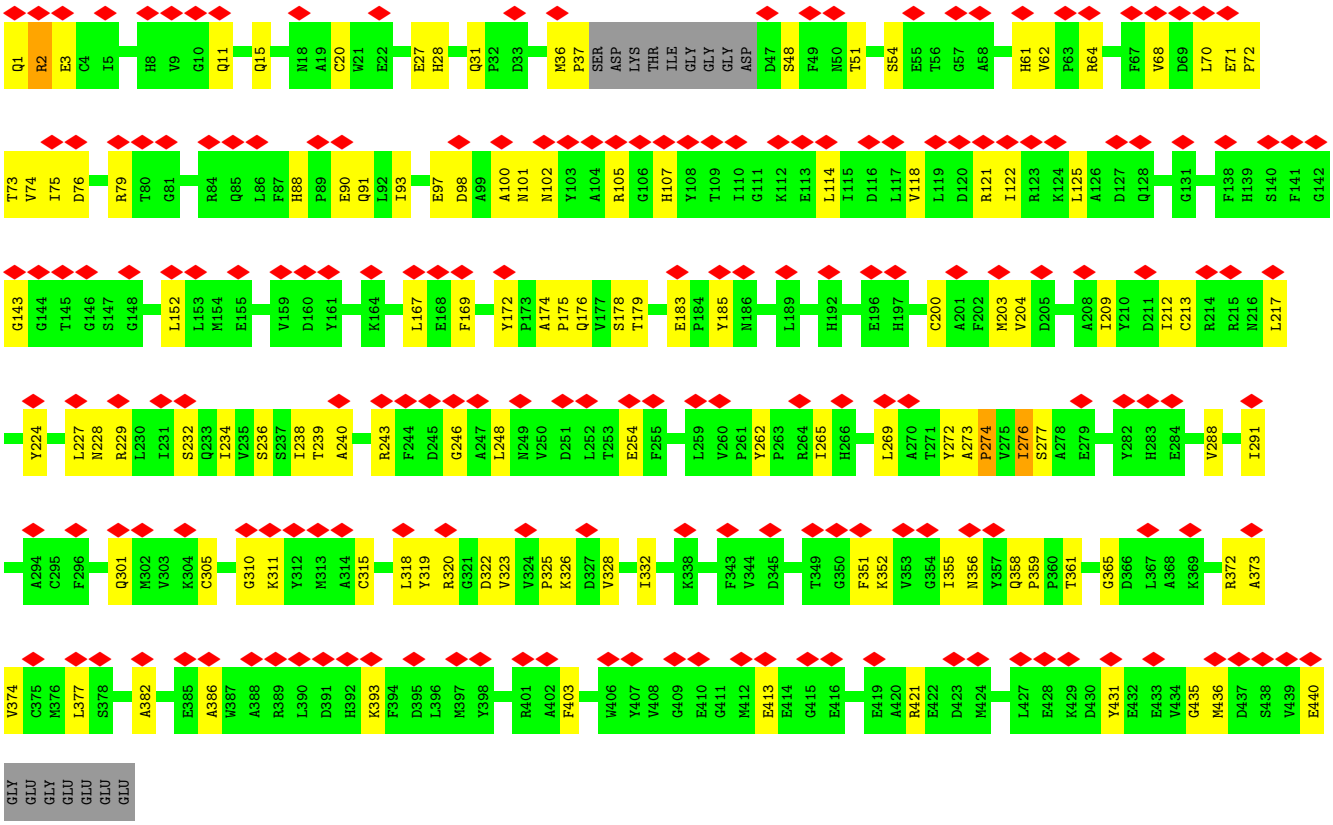
- Molecule 40: Tubulin alpha chain

Chain RE:



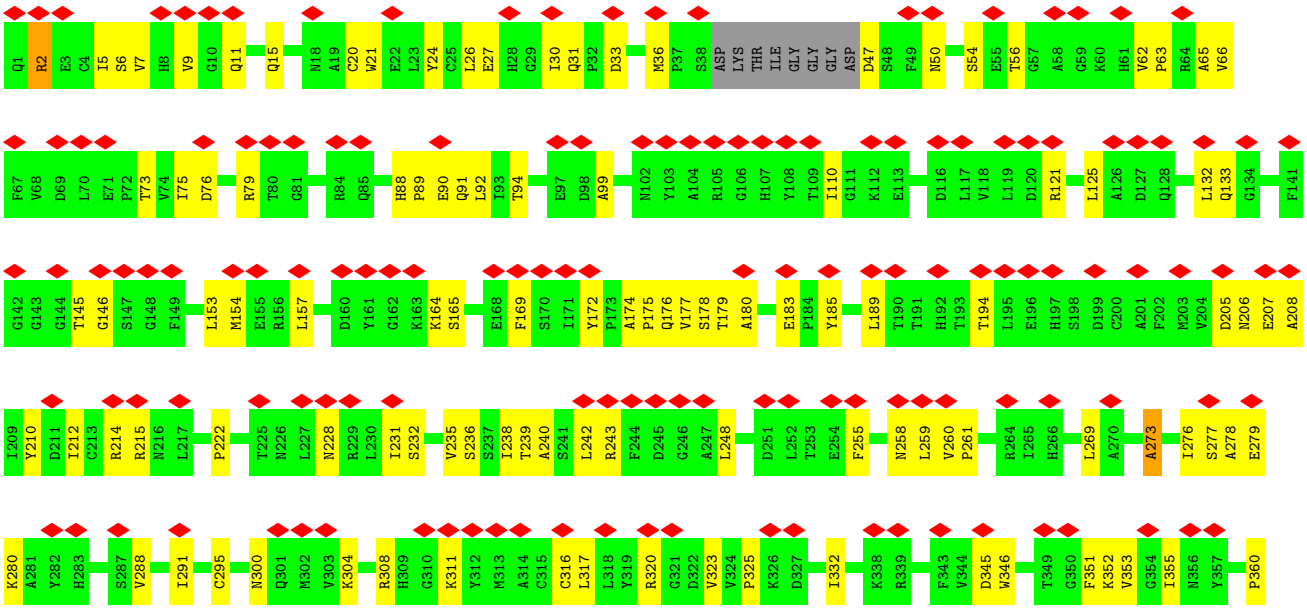
- Molecule 40: Tubulin alpha chain

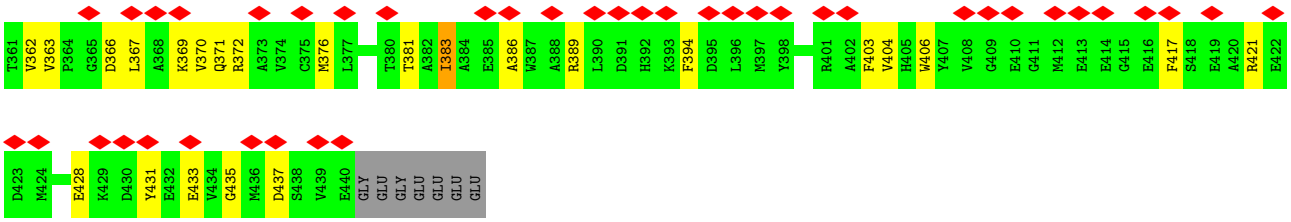
Chain RF:




- Molecule 40: Tubulin alpha chain

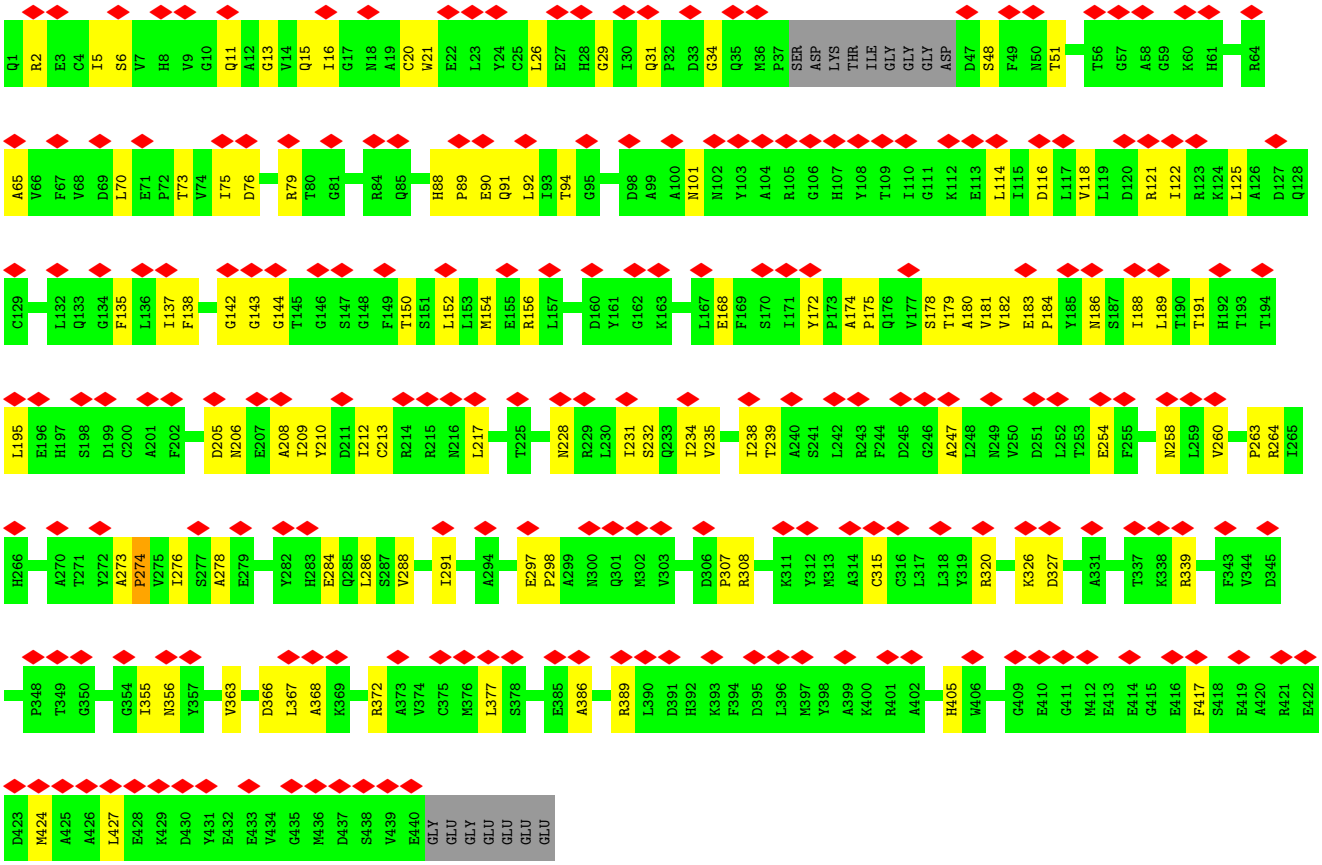
Chain RG:





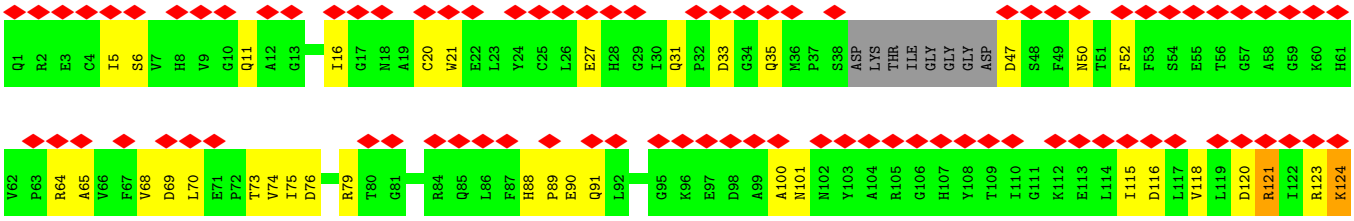

- Molecule 40: Tubulin alpha chain

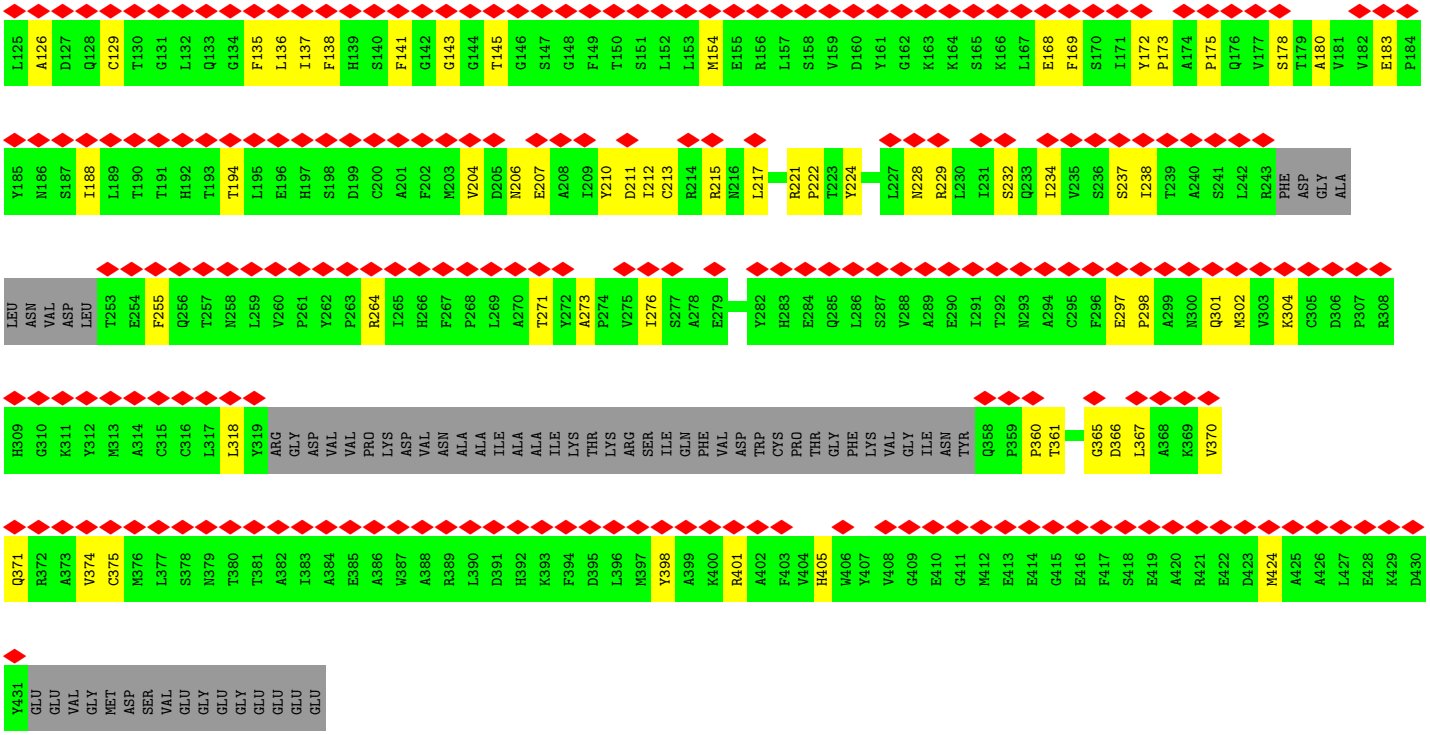
Chain RH:




- Molecule 40: Tubulin alpha chain

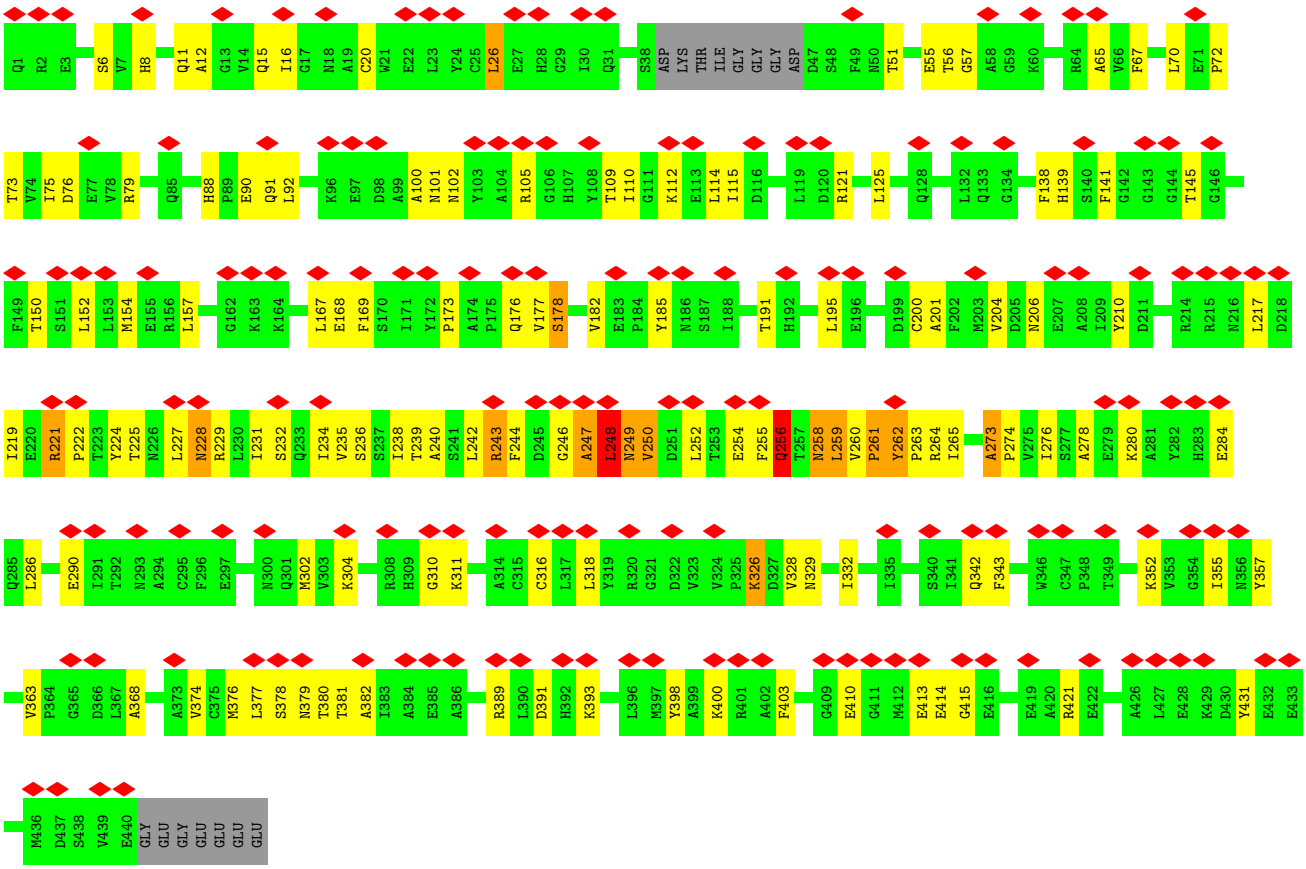
Chain RI:





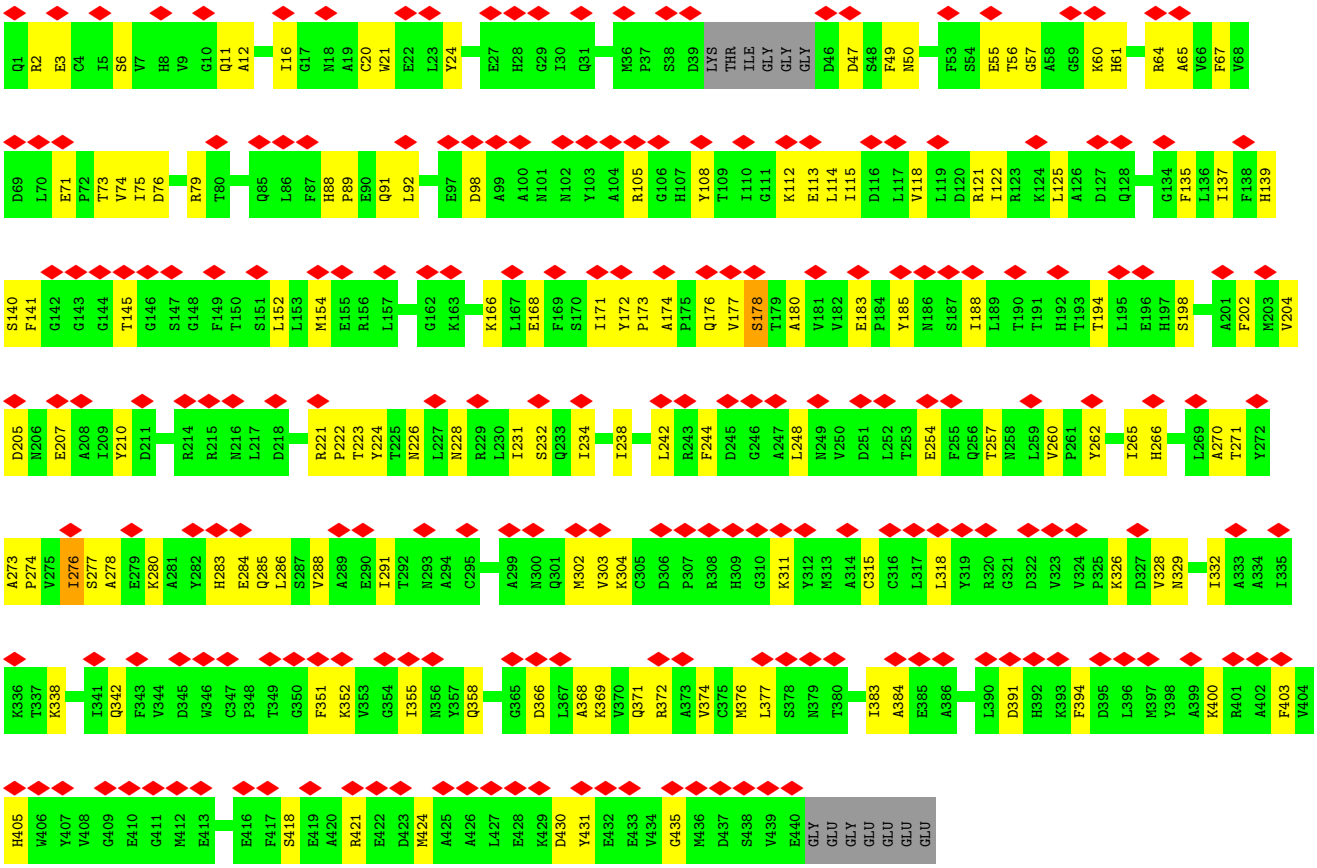

- Molecule 40: Tubulin alpha chain

Chain SA:



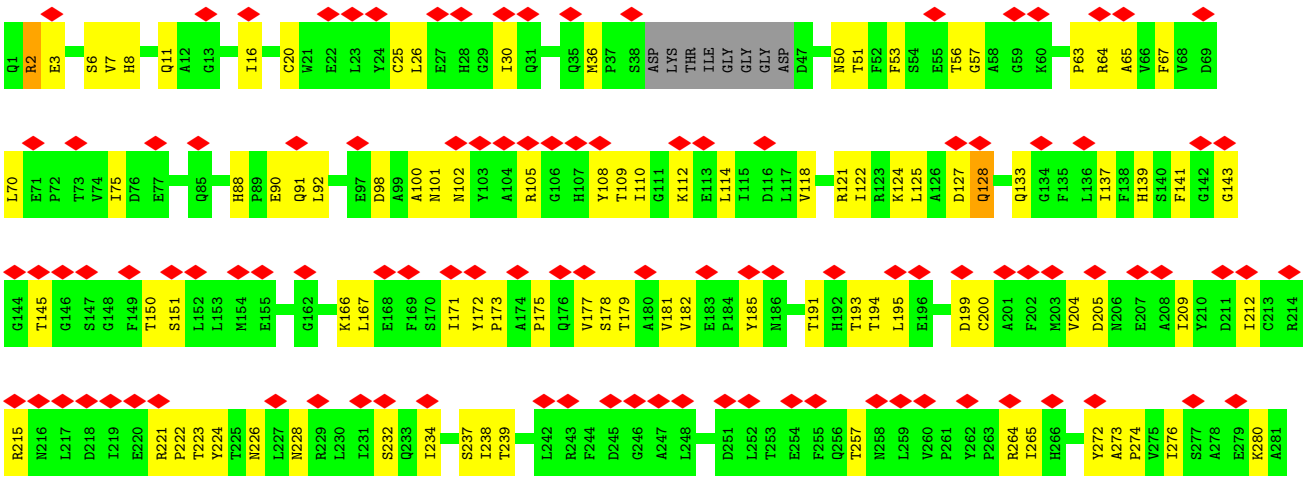
- Molecule 40: Tubulin alpha chain

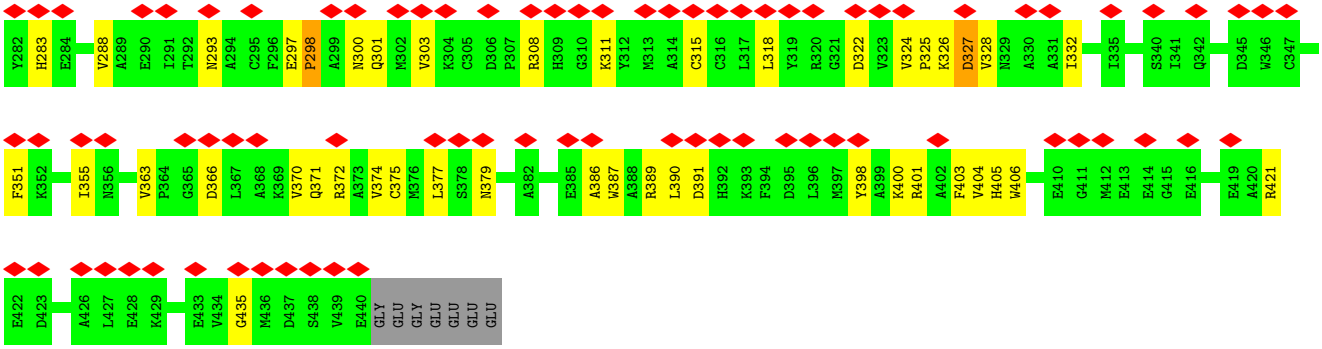
Chain SE:




- Molecule 40: Tubulin alpha chain

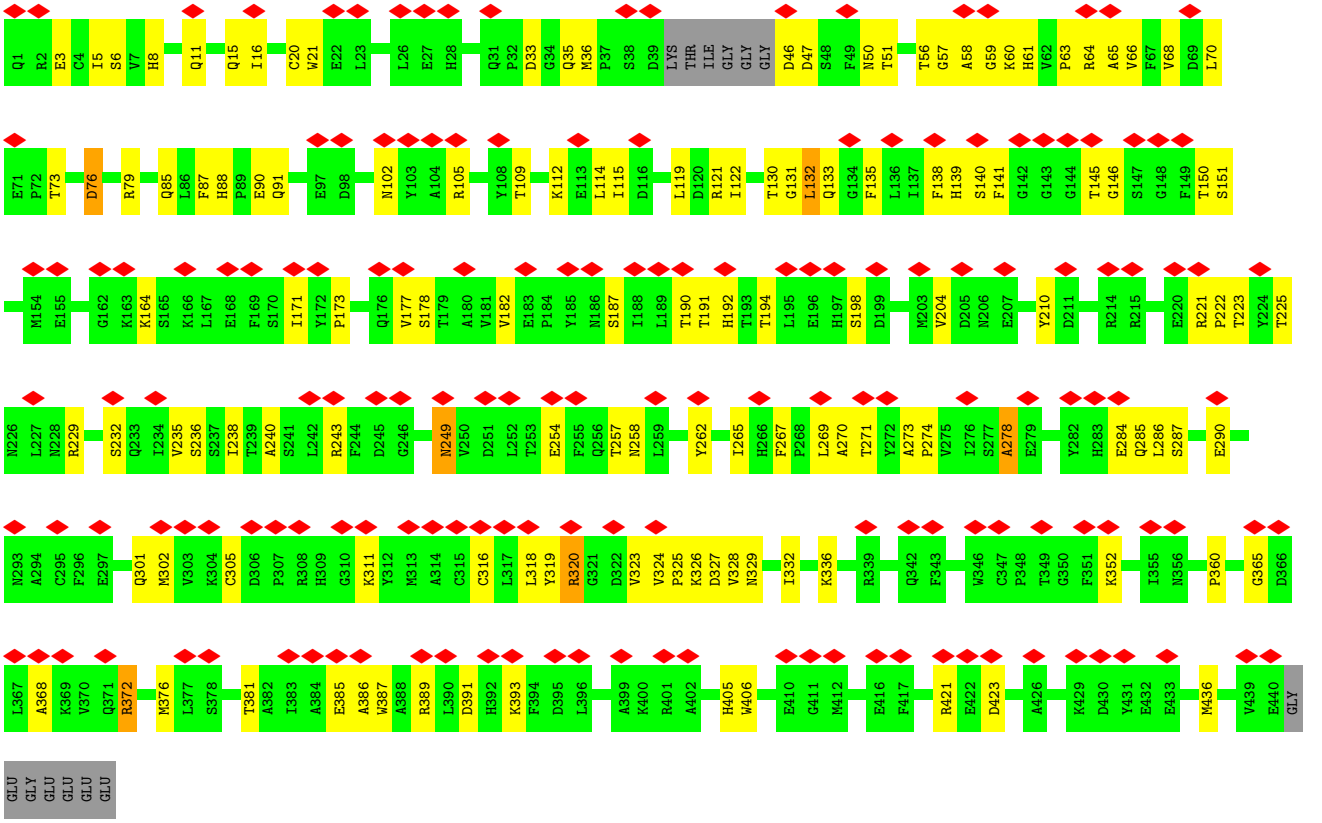
Chain SF:





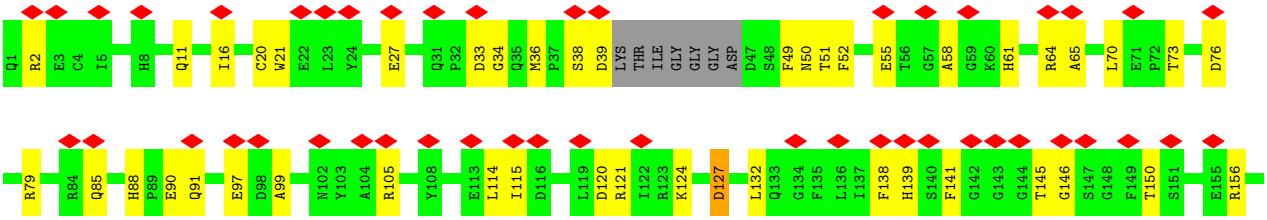

• Molecule 40: Tubulin alpha chain

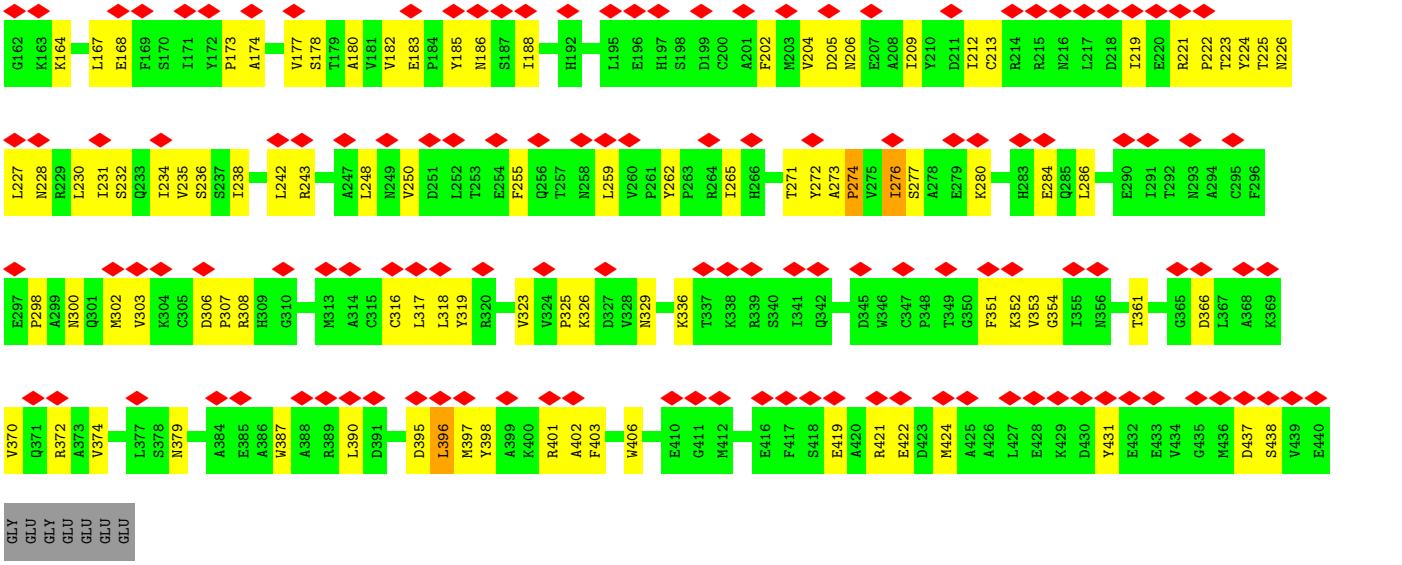
Chain SG:




• Molecule 40: Tubulin alpha chain

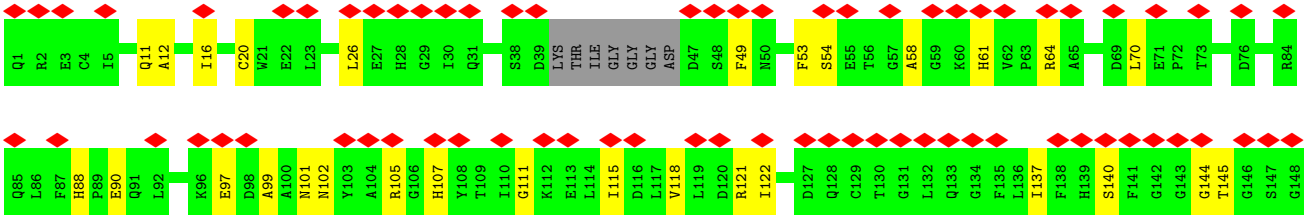
Chain SH:

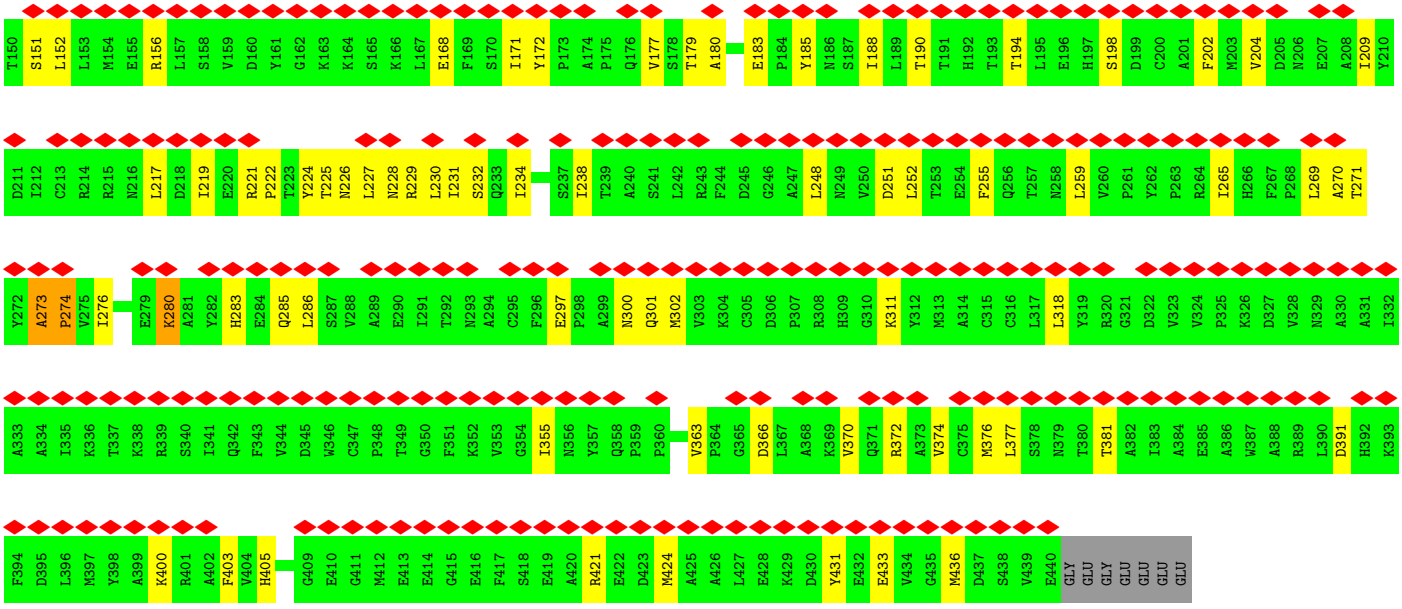





- Molecule 40: Tubulin alpha chain

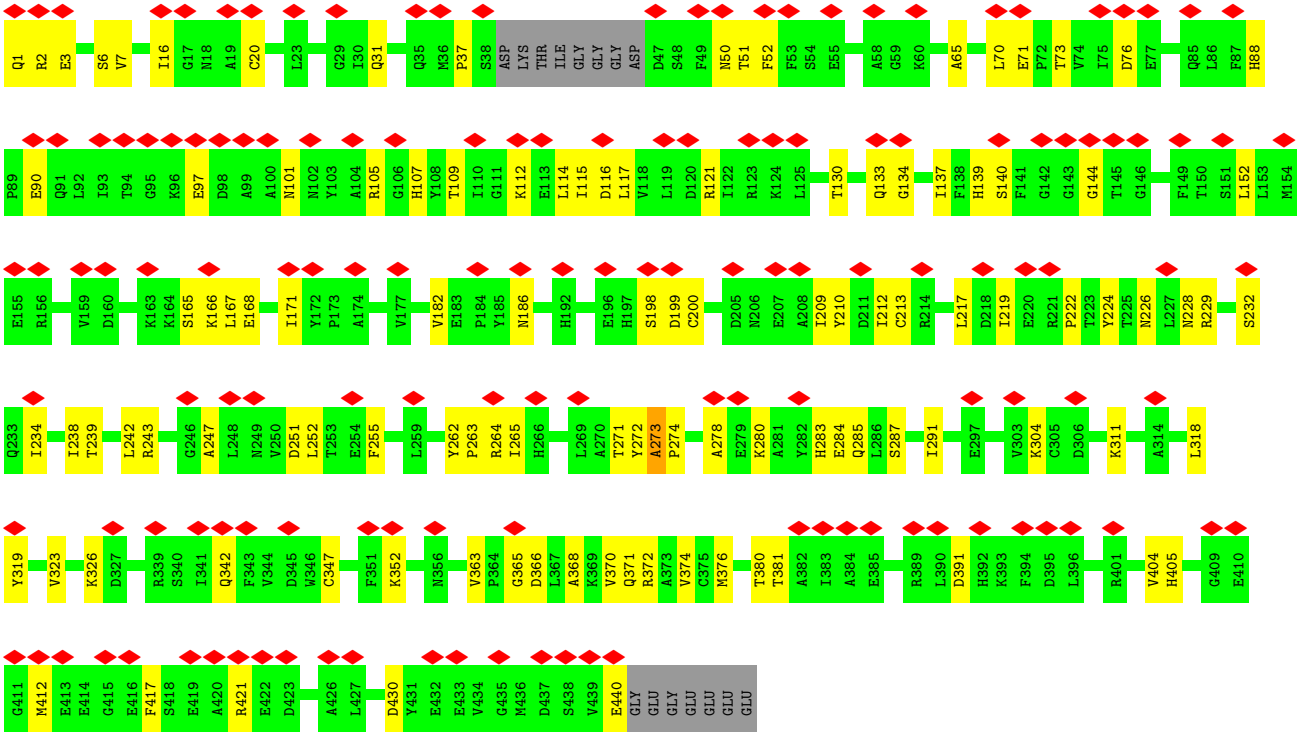
Chain SI:



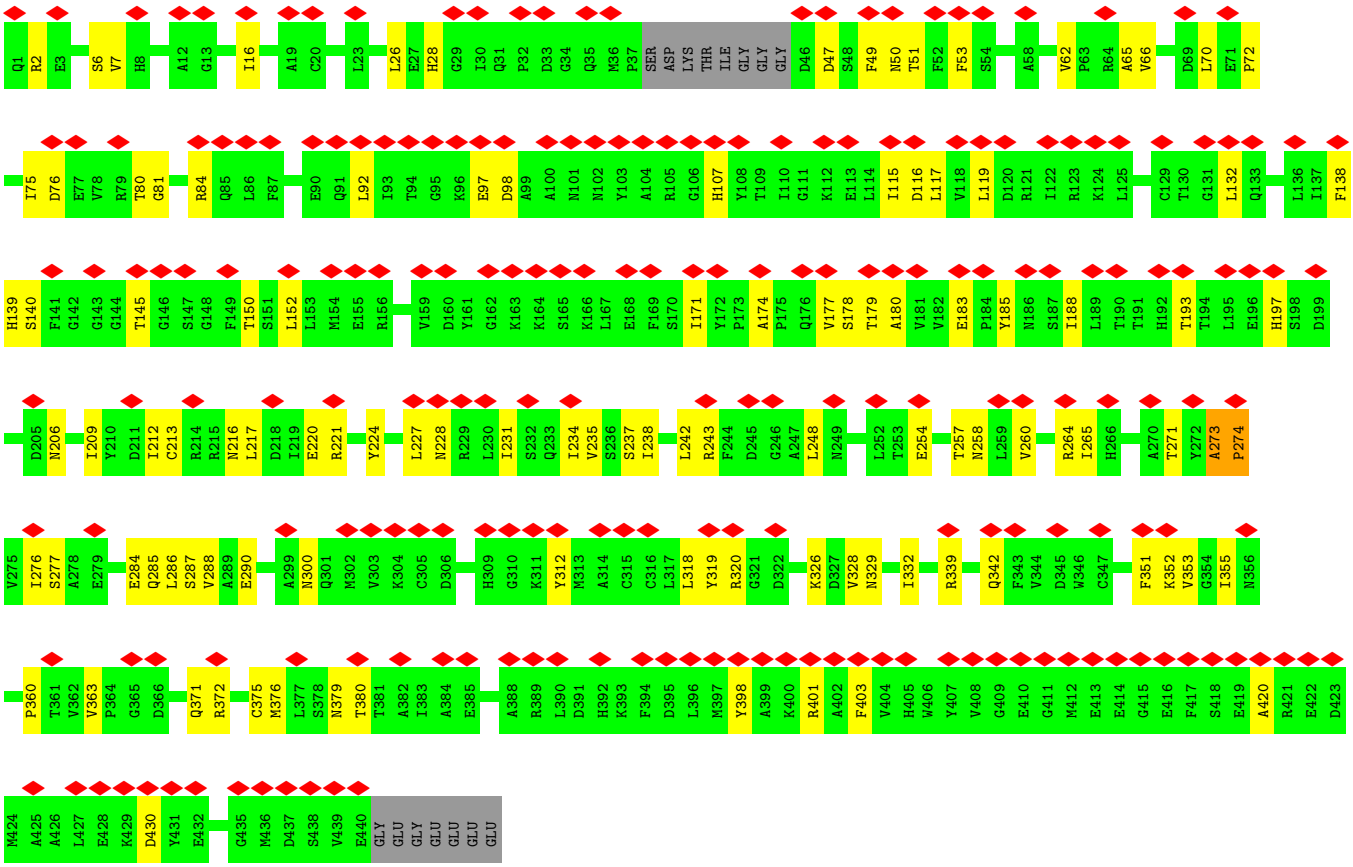

- Molecule 40: Tubulin alpha chain

Chain TA:



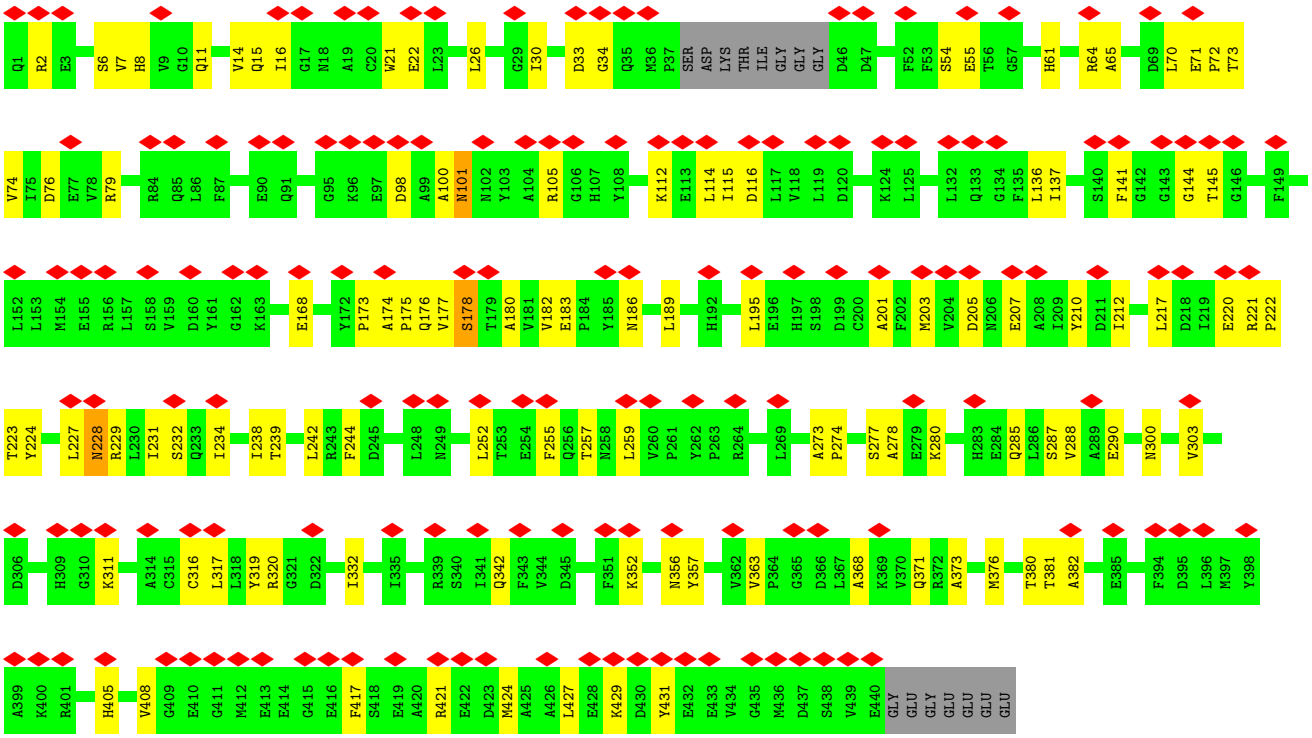

- Molecule 40: Tubulin alpha chain

Chain TE:



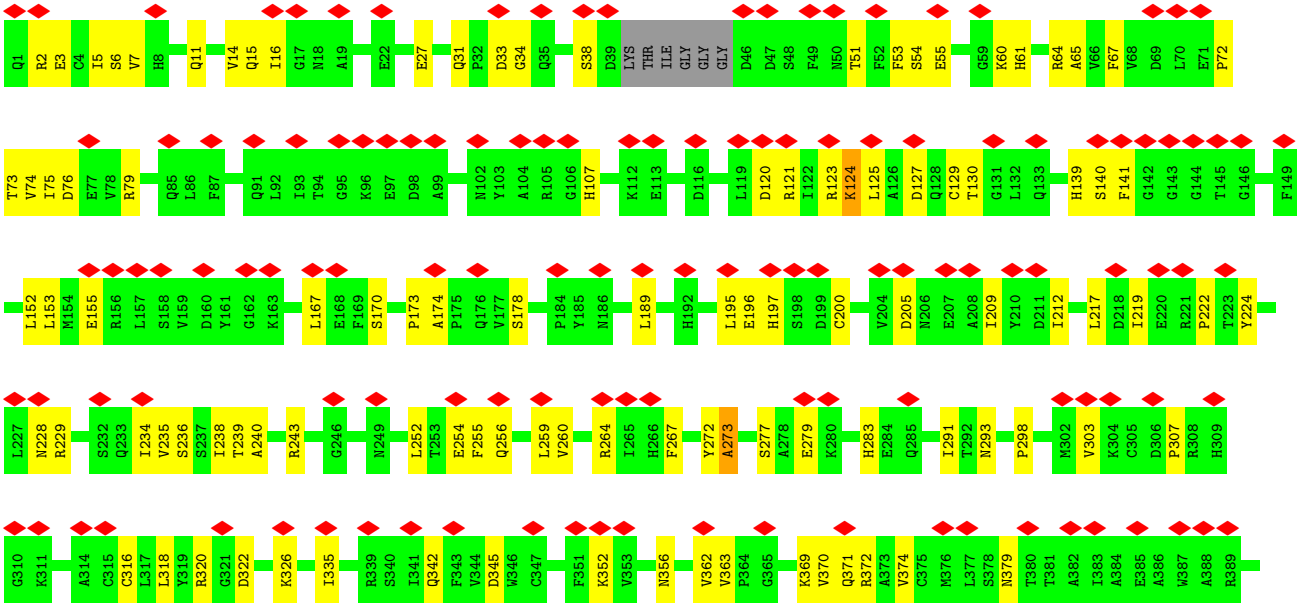
- Molecule 40: Tubulin alpha chain

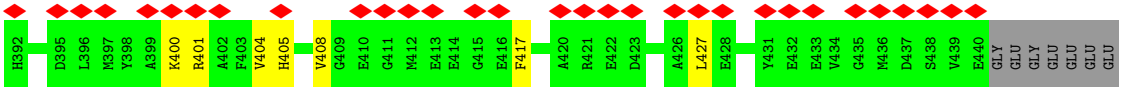
Chain TF:




- Molecule 40: Tubulin alpha chain

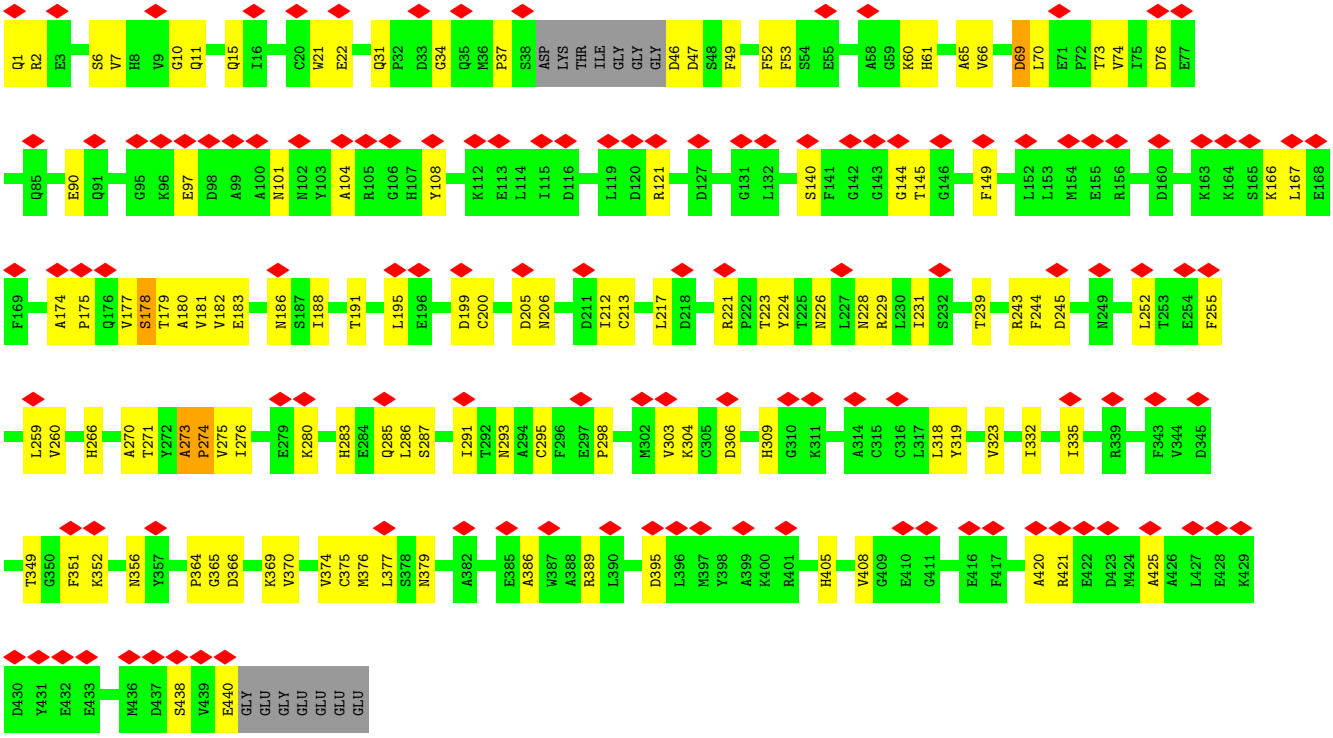
Chain TG:





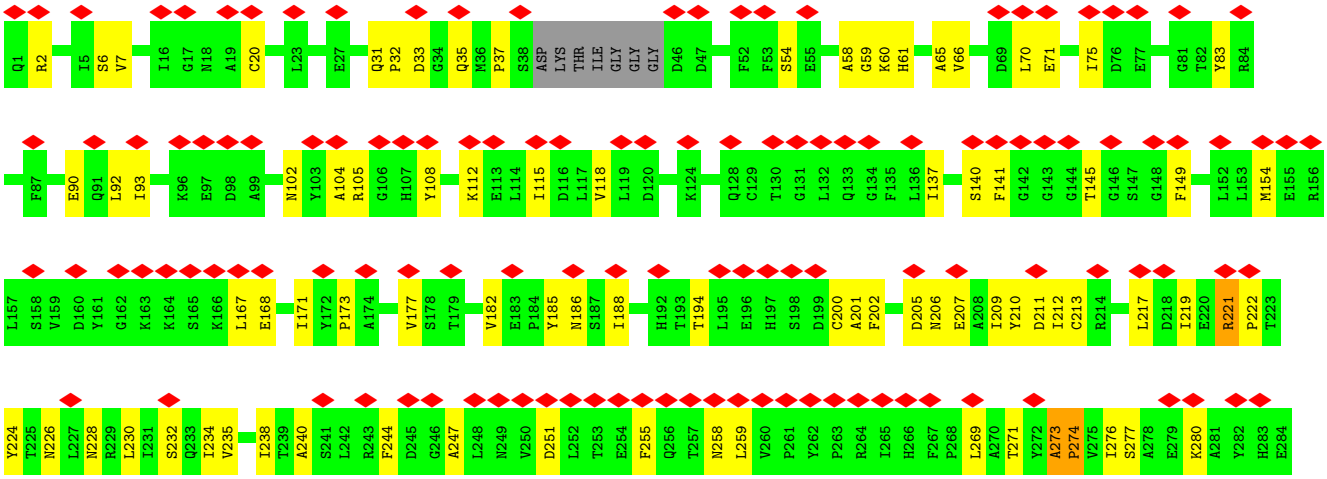

• Molecule 40: Tubulin alpha chain

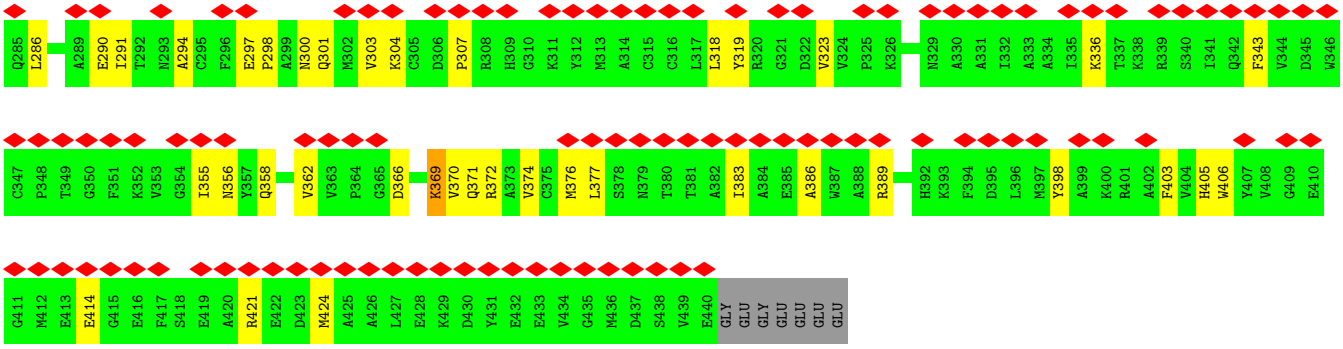
Chain TH:




• Molecule 40: Tubulin alpha chain

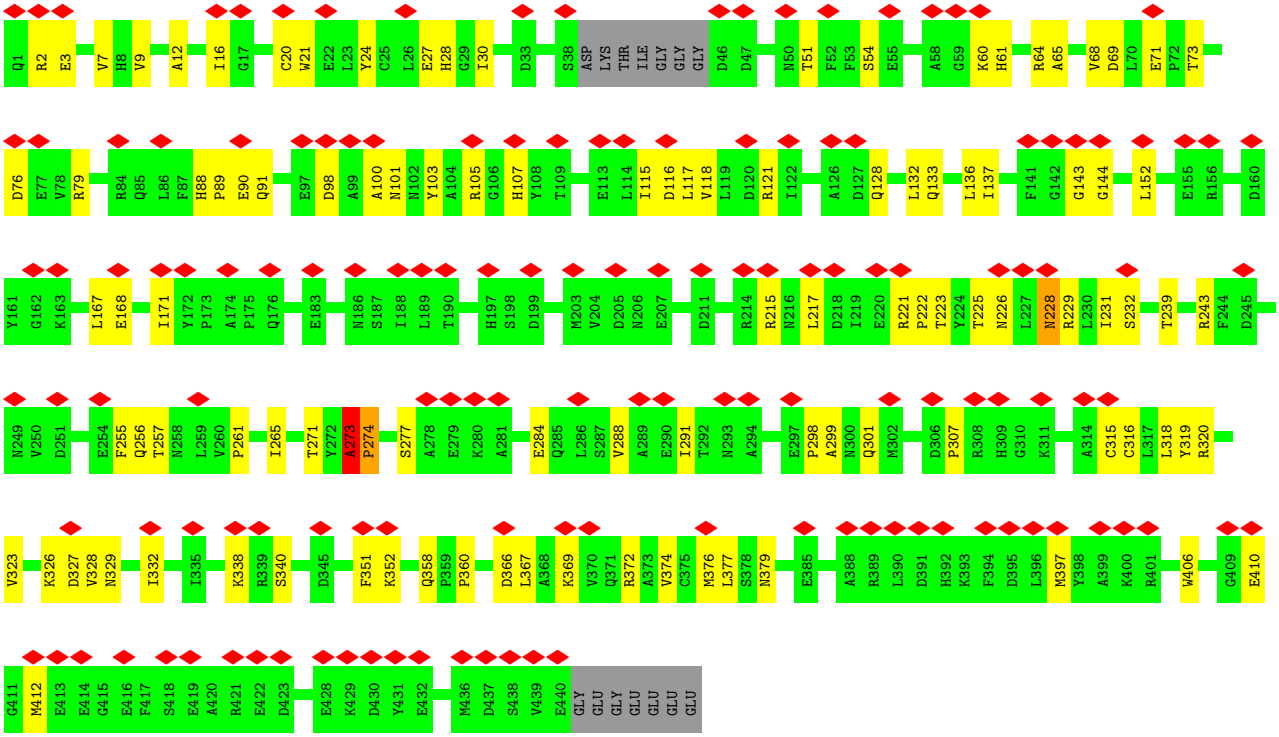
Chain TI:





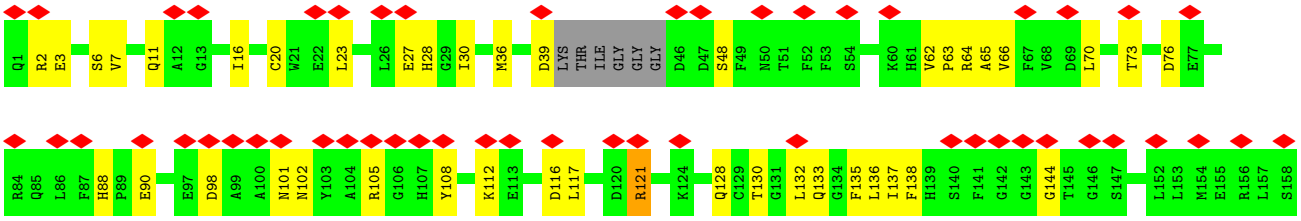

- Molecule 40: Tubulin alpha chain

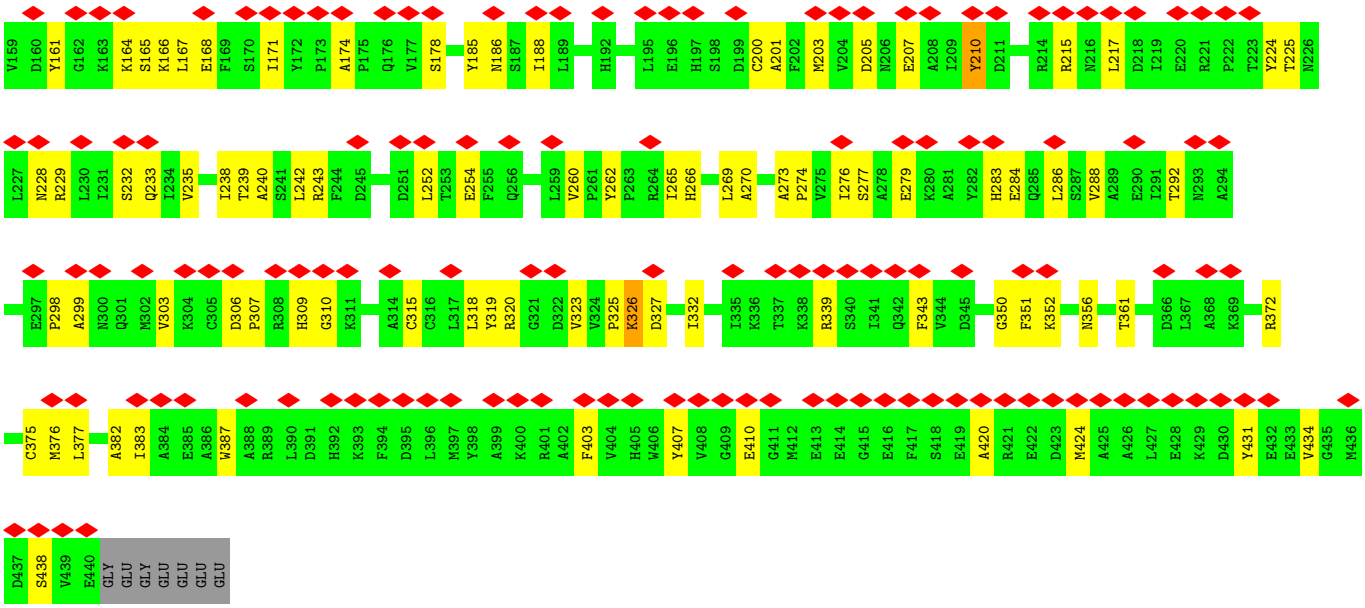
Chain UA:




- Molecule 40: Tubulin alpha chain

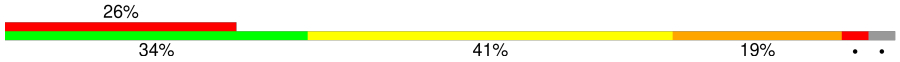
Chain UE:

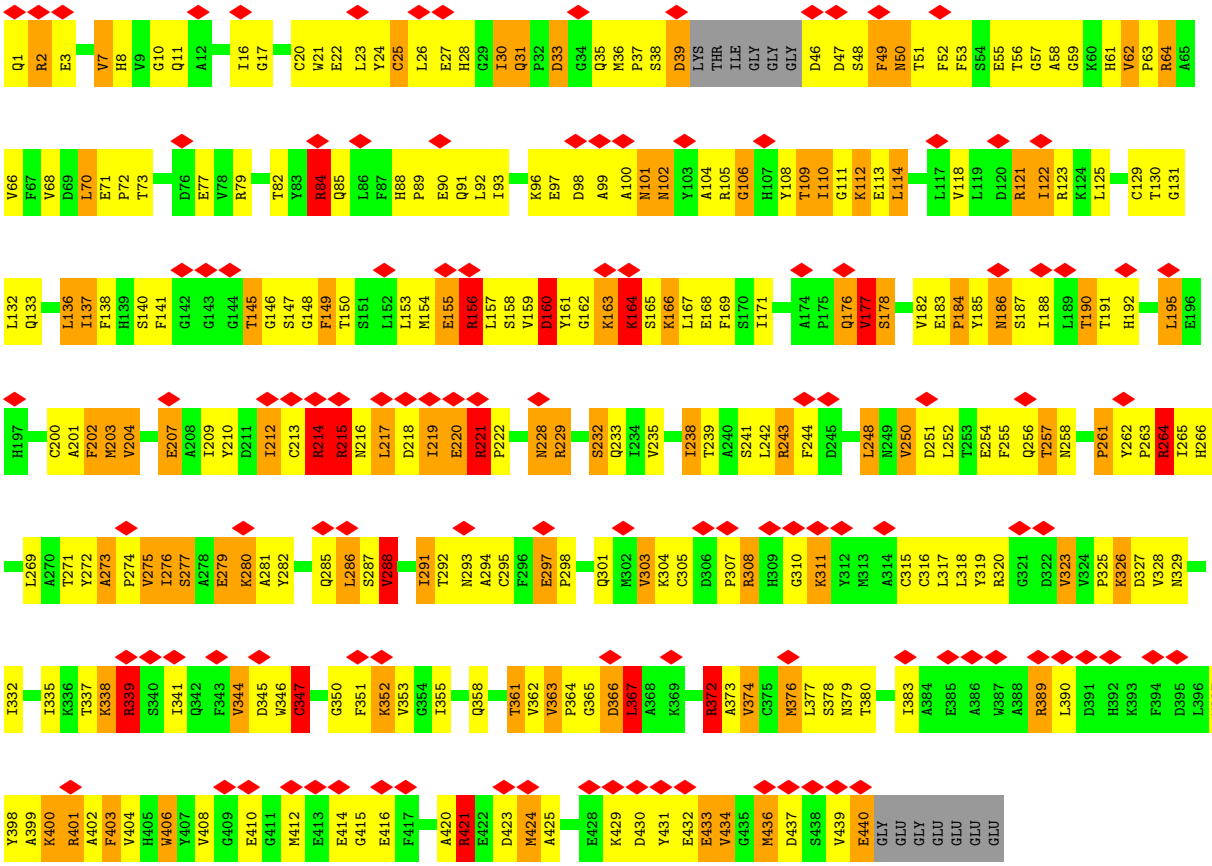





- Molecule 40: Tubulin alpha chain

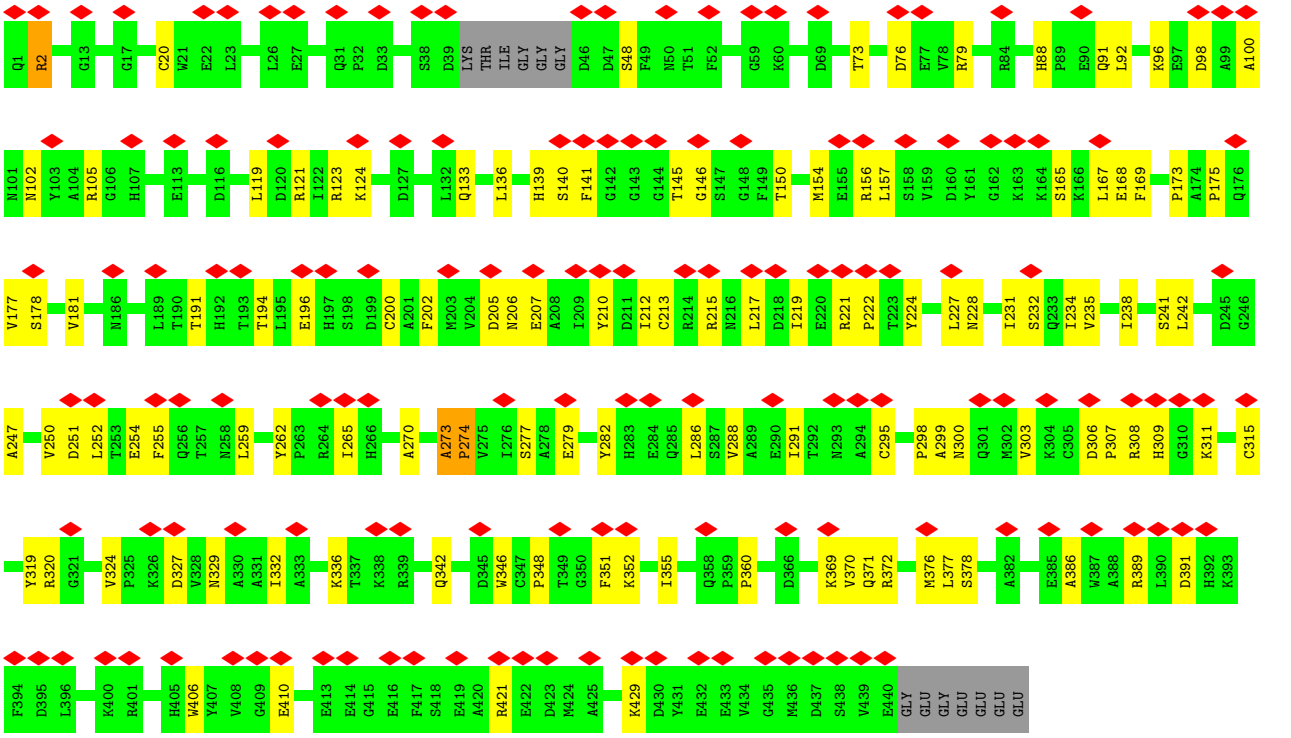
Chain UF:



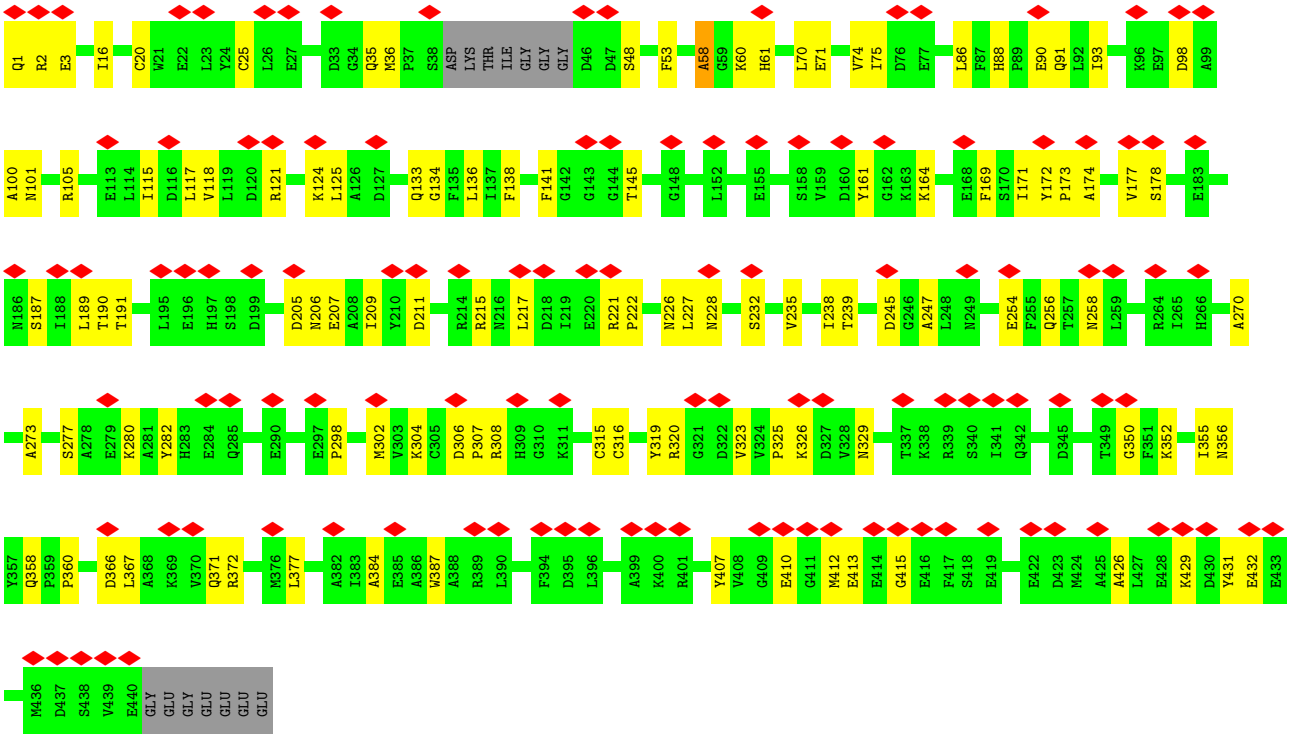

- Molecule 40: Tubulin alpha chain

Chain UG:



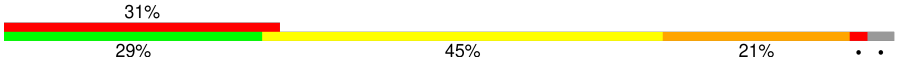

- Molecule 40: Tubulin alpha chain

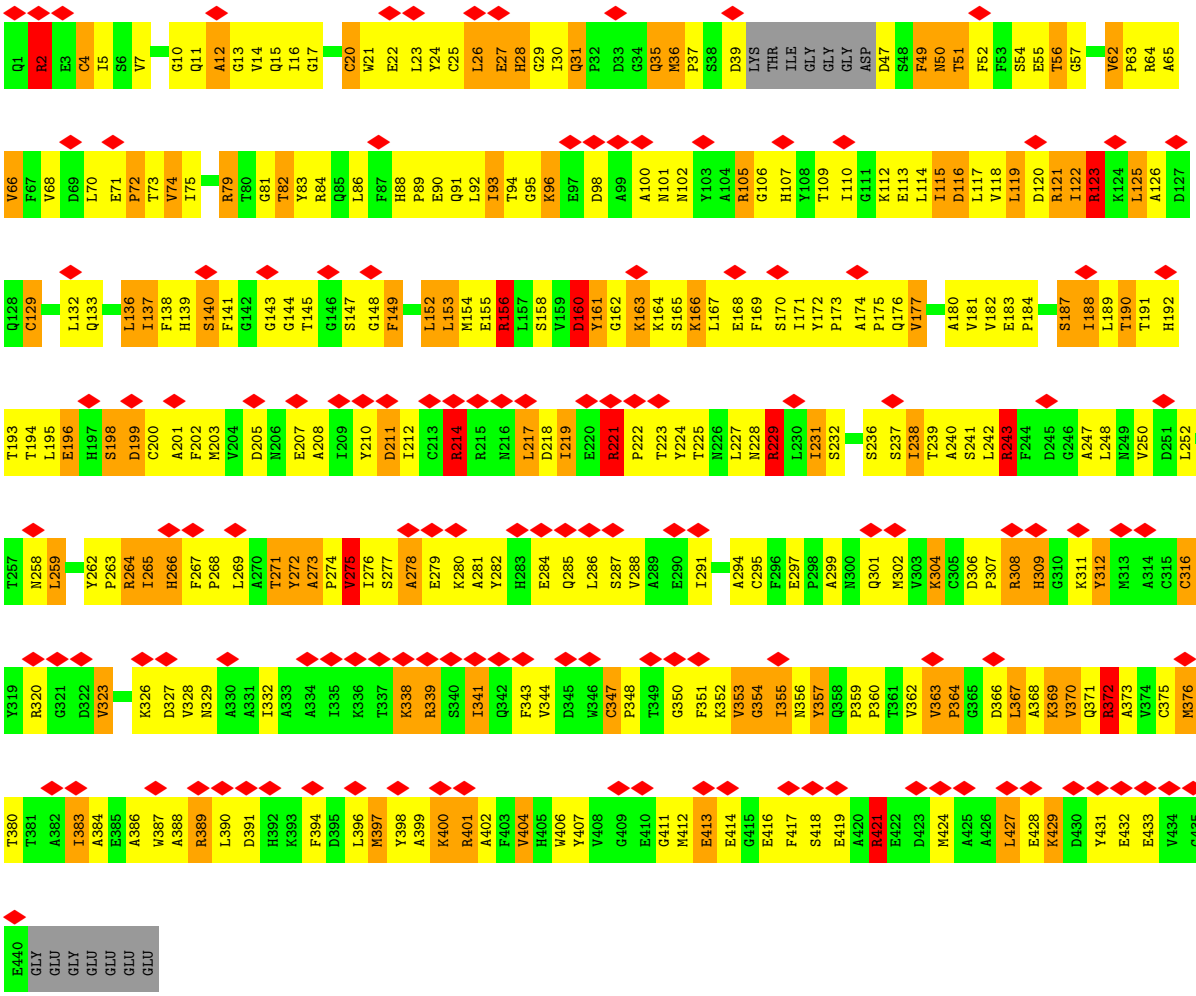
Chain UH:



- Molecule 40: Tubulin alpha chain

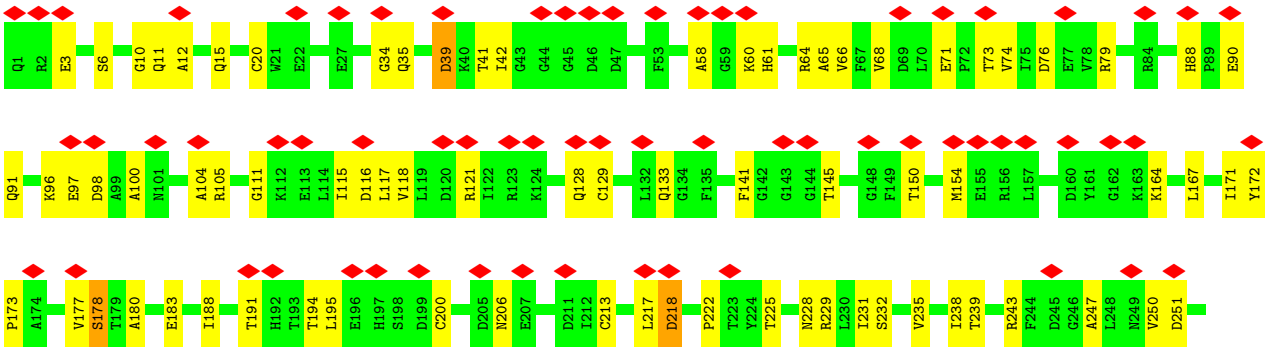
Chain UI:

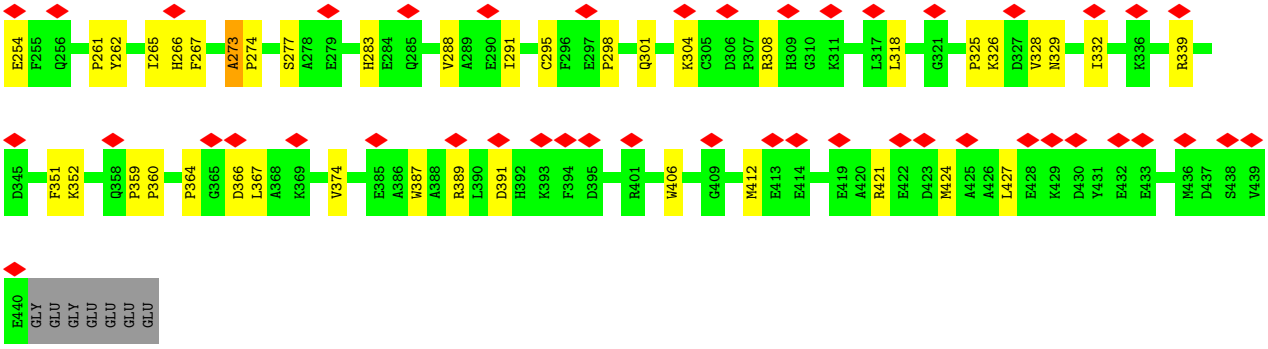



- Molecule 40: Tubulin alpha chain

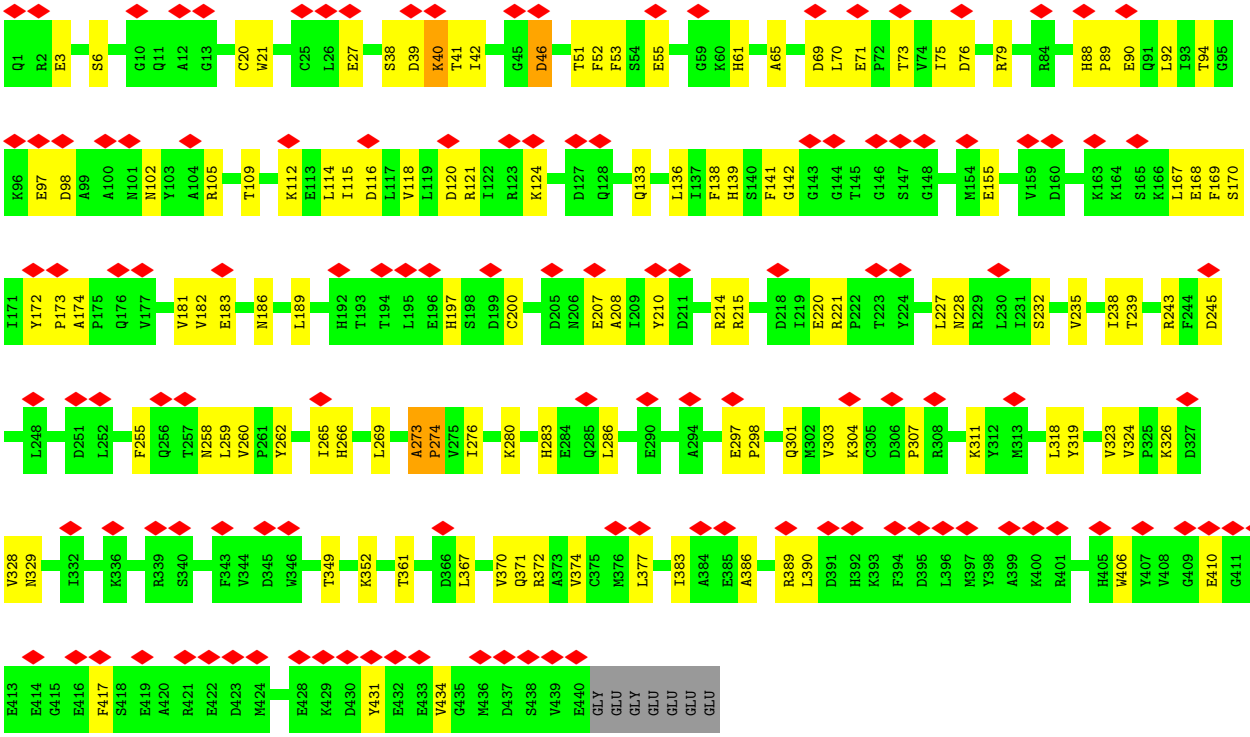
Chain VA:





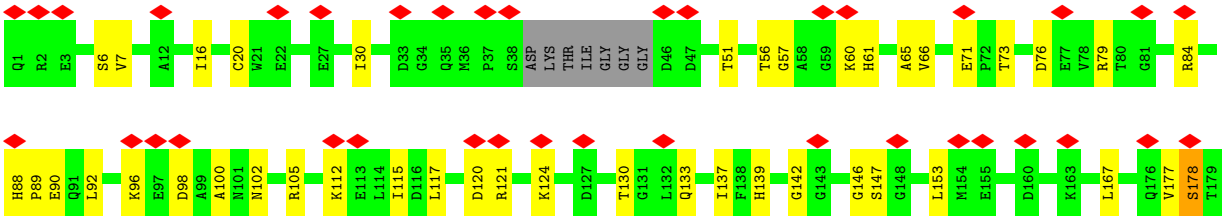

- Molecule 40: Tubulin alpha chain

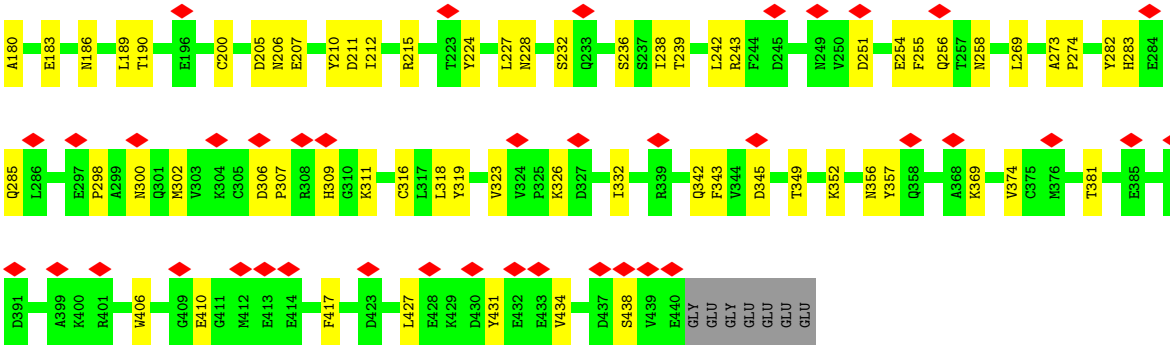
Chain VF:




- Molecule 40: Tubulin alpha chain

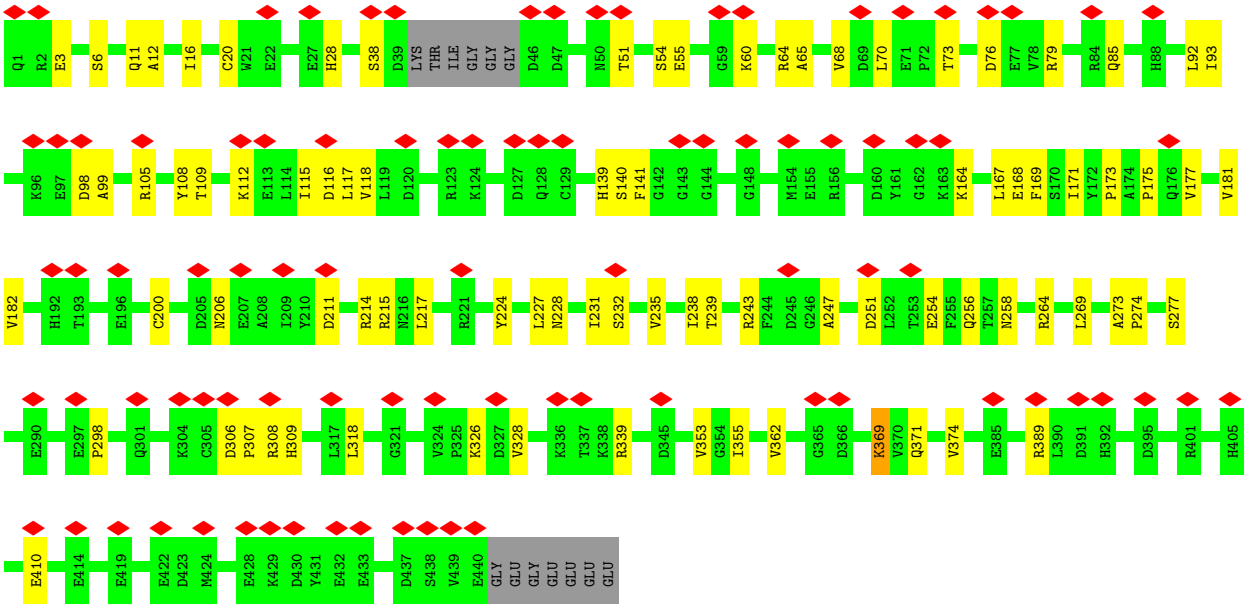
Chain VG:





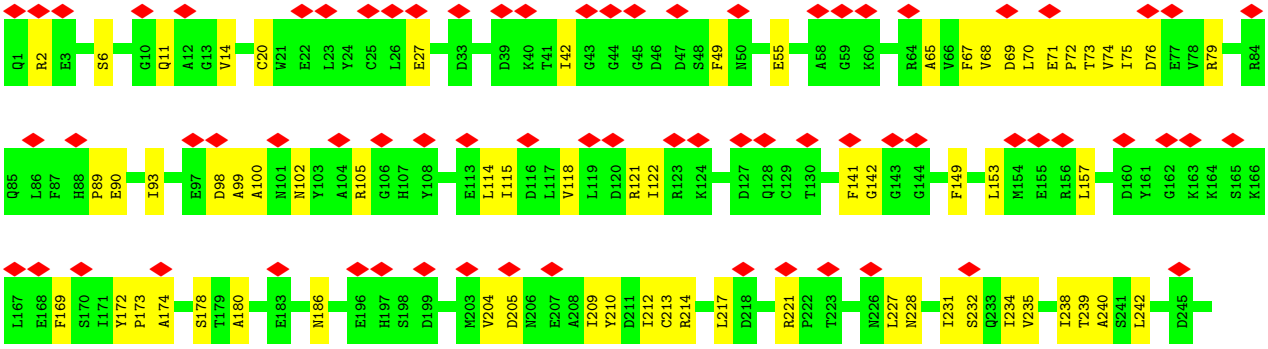

- Molecule 40: Tubulin alpha chain

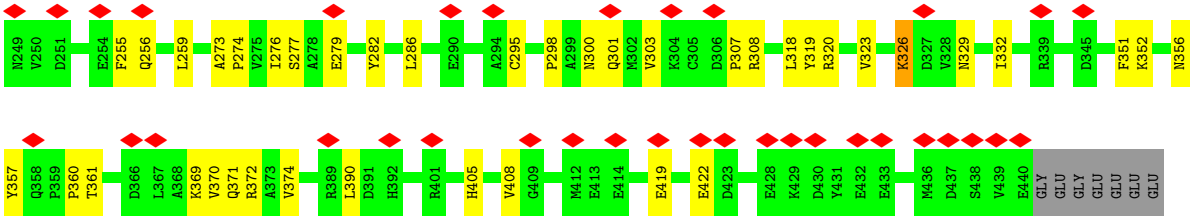
Chain VH:




- Molecule 40: Tubulin alpha chain

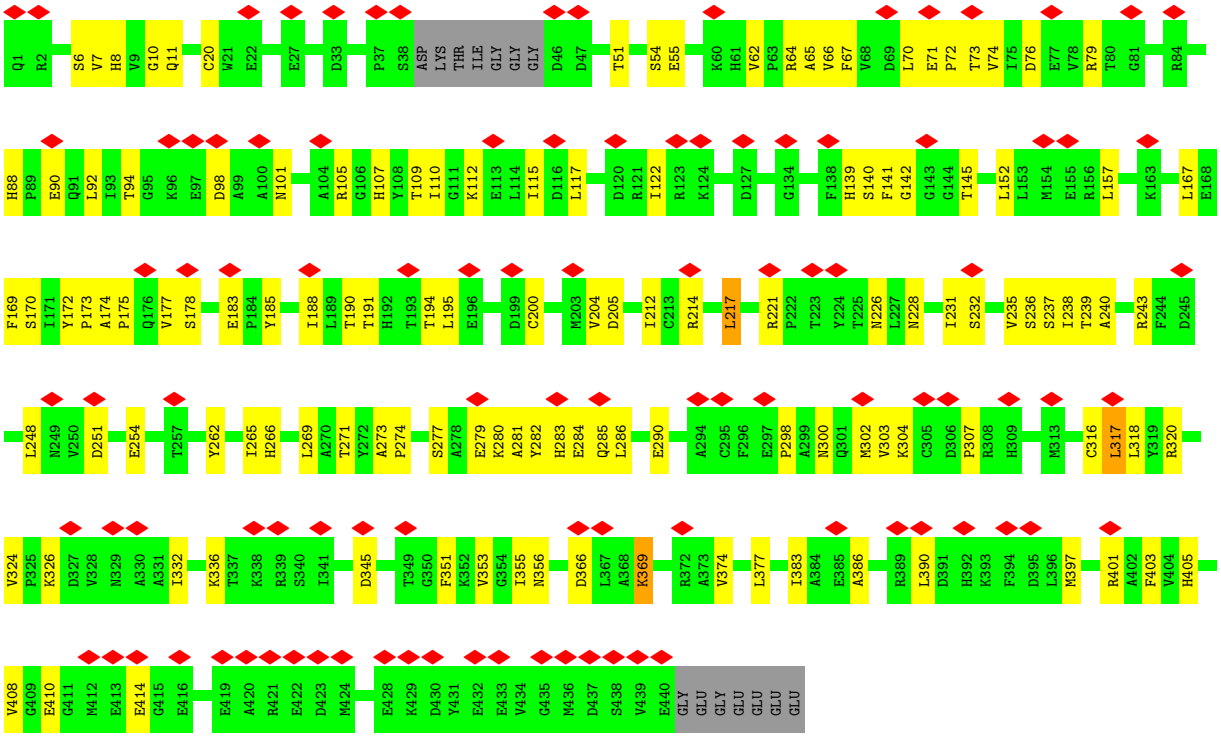
Chain VI:





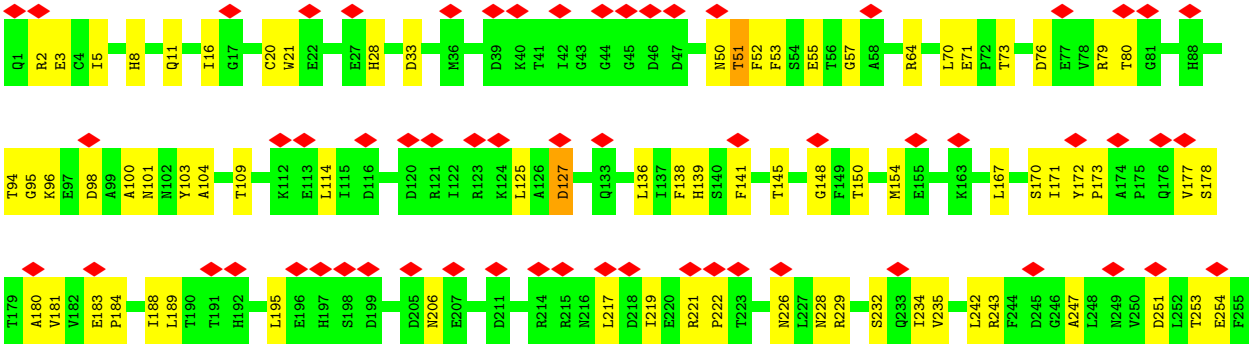

- Molecule 40: Tubulin alpha chain

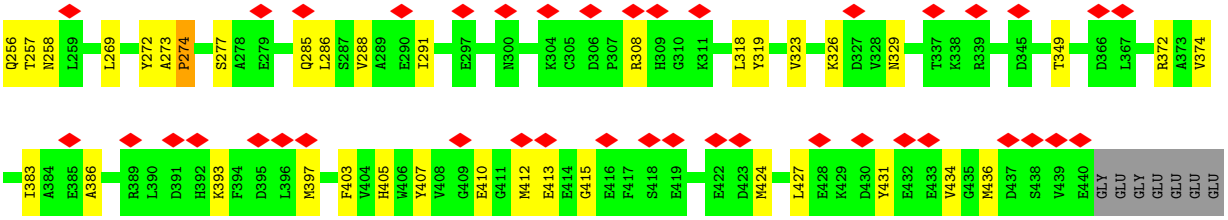
Chain VJ:




- Molecule 40: Tubulin alpha chain

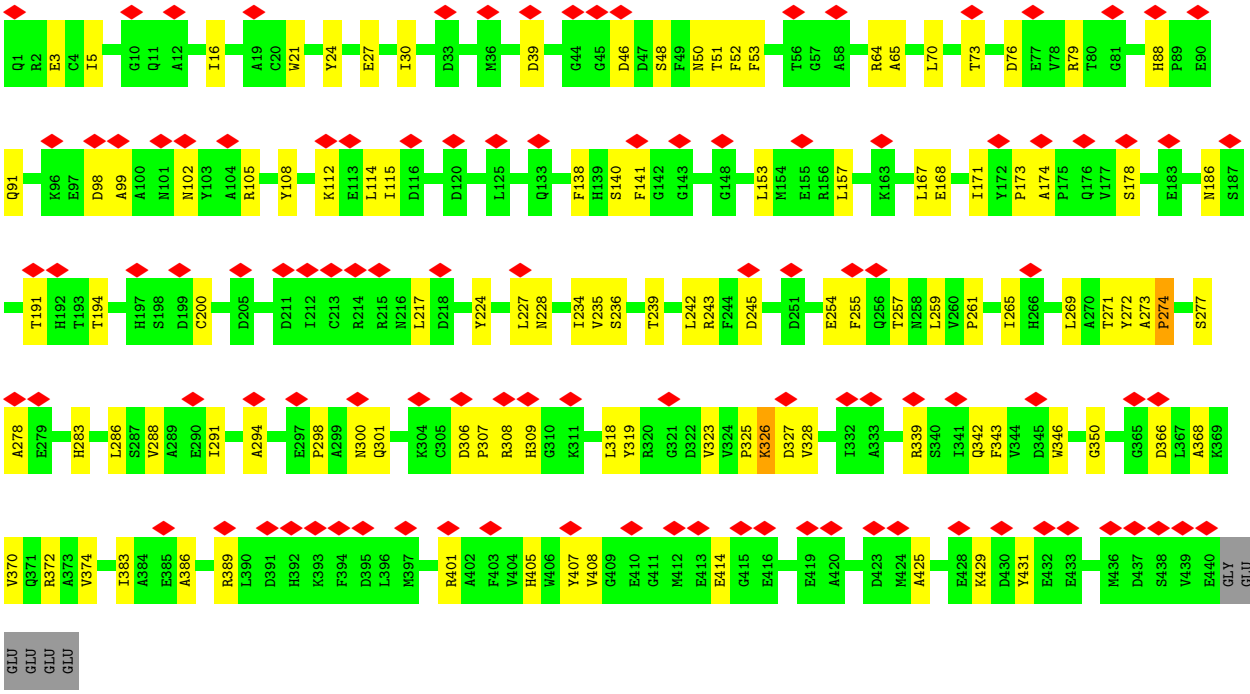
Chain WA:





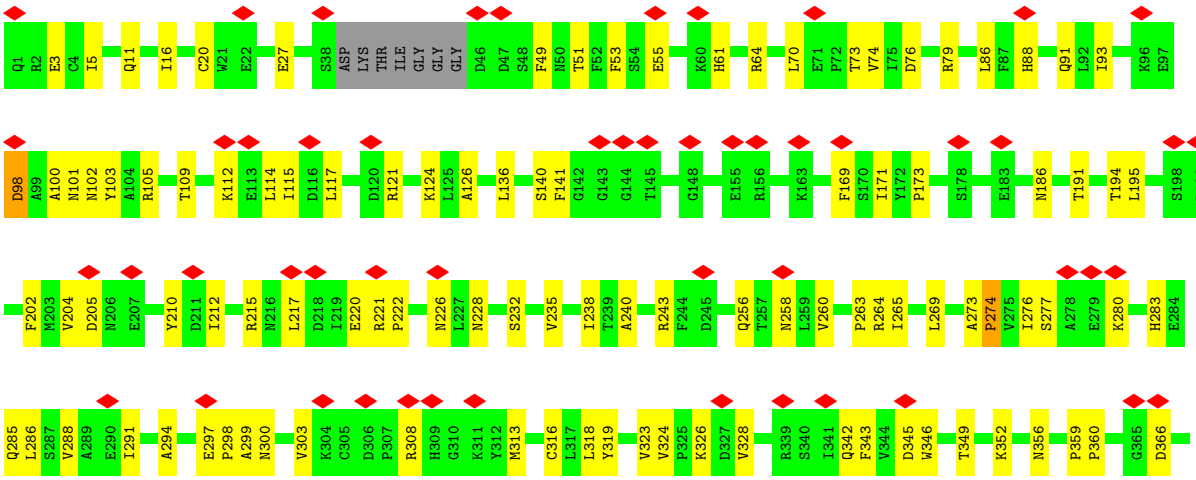

• Molecule 40: Tubulin alpha chain

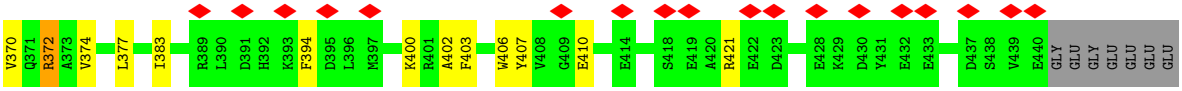
Chain WE:




• Molecule 40: Tubulin alpha chain

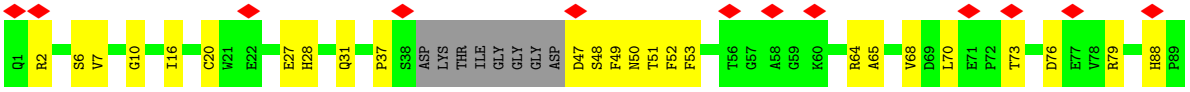
Chain WF:

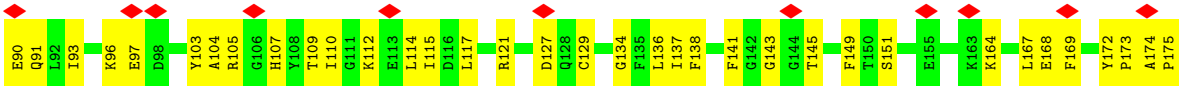


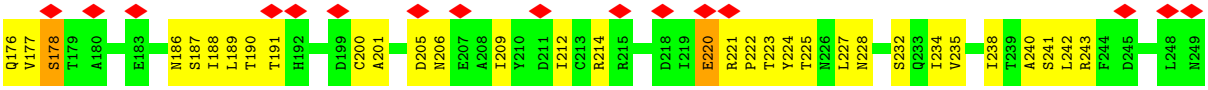


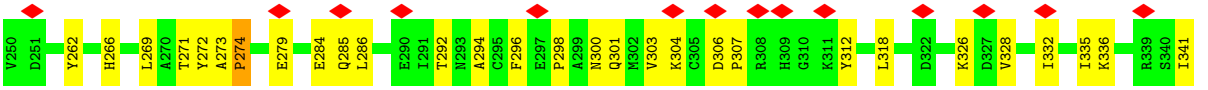

• Molecule 40: Tubulin alpha chain

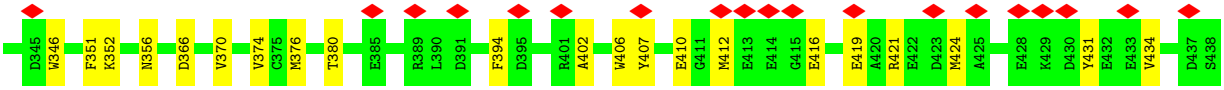
Chain WG:

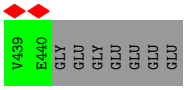


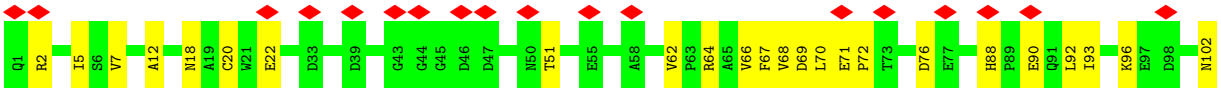



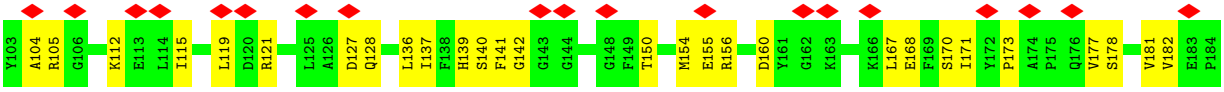



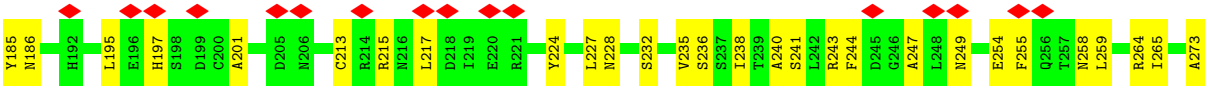



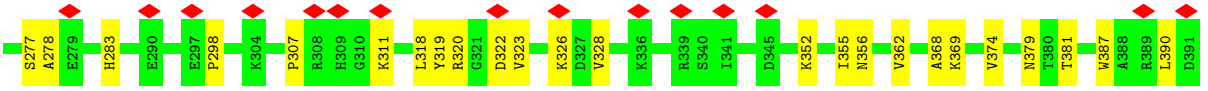

• Molecule 40: Tubulin alpha chain

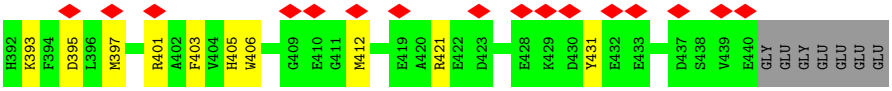
Chain WH:



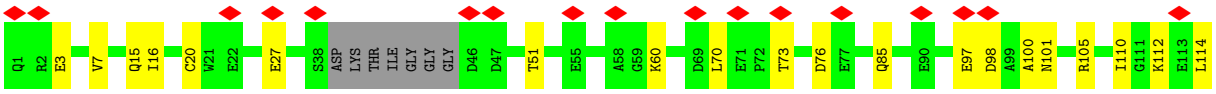



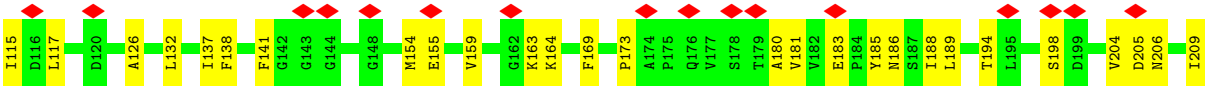



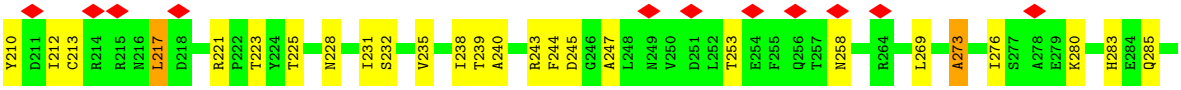


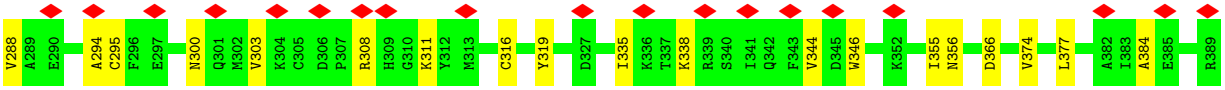

- Molecule 40: Tubulin alpha chain

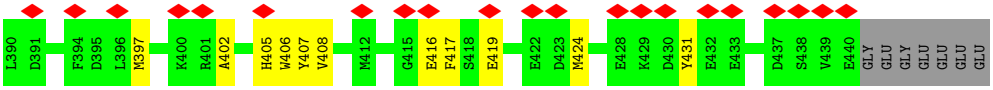
Chain WI:



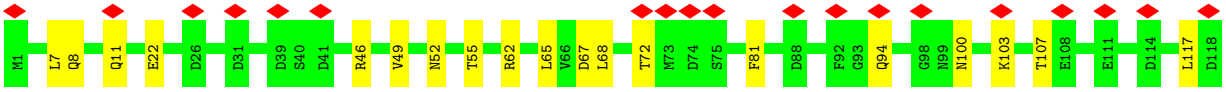



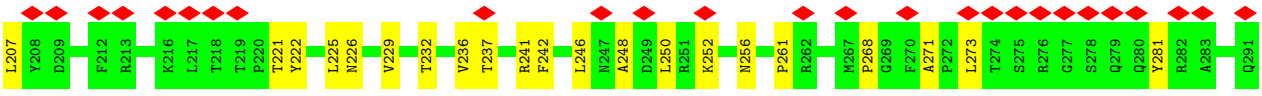



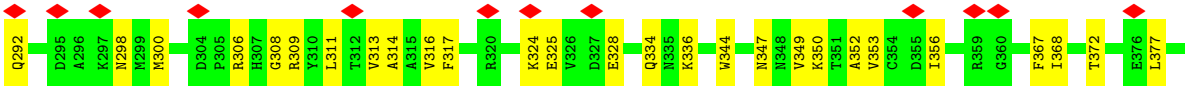



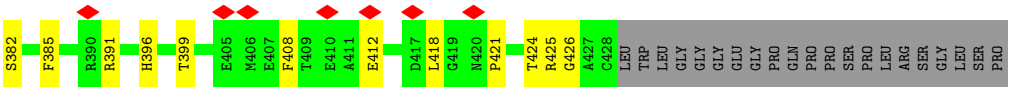

- Molecule 41: Tubulin beta chain

Chain AB:



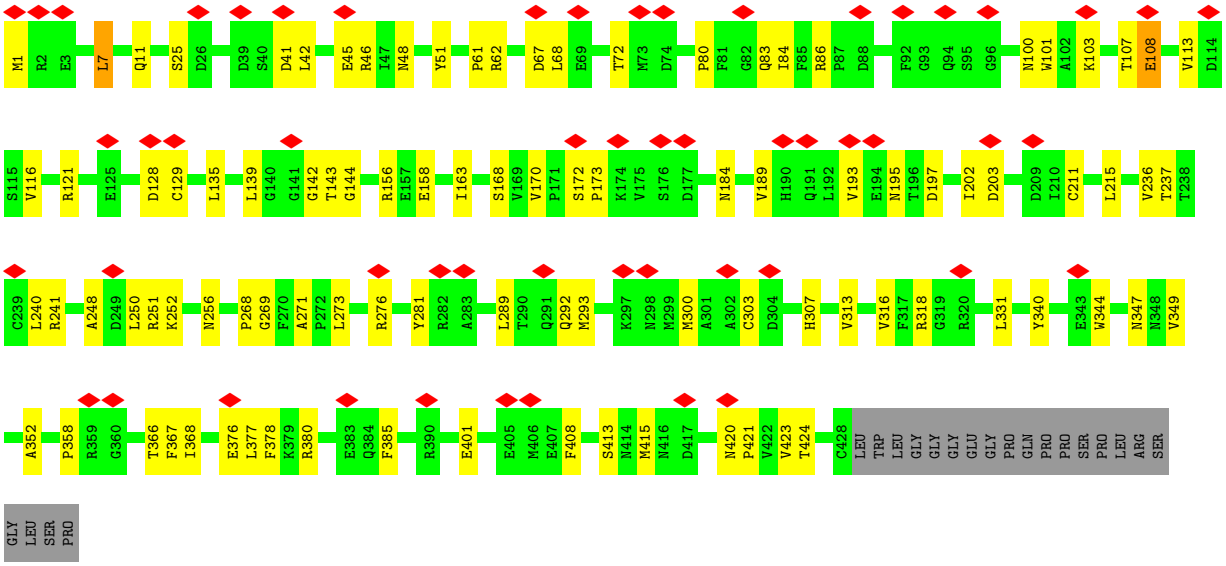


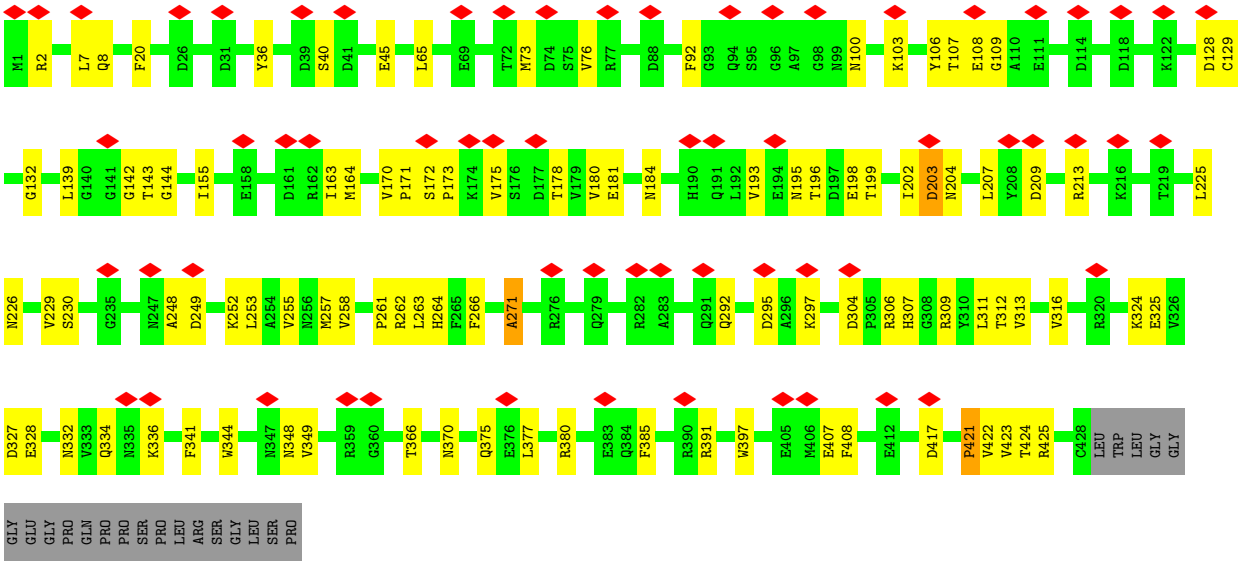

- Molecule 41: Tubulin beta chain

Chain AL: 12% 74% 21% 5%



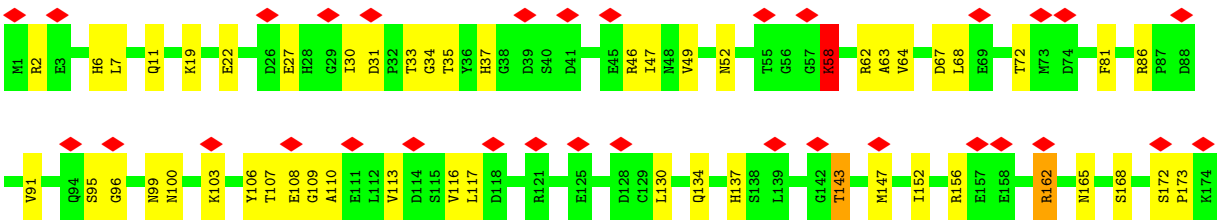

- Molecule 41: Tubulin beta chain

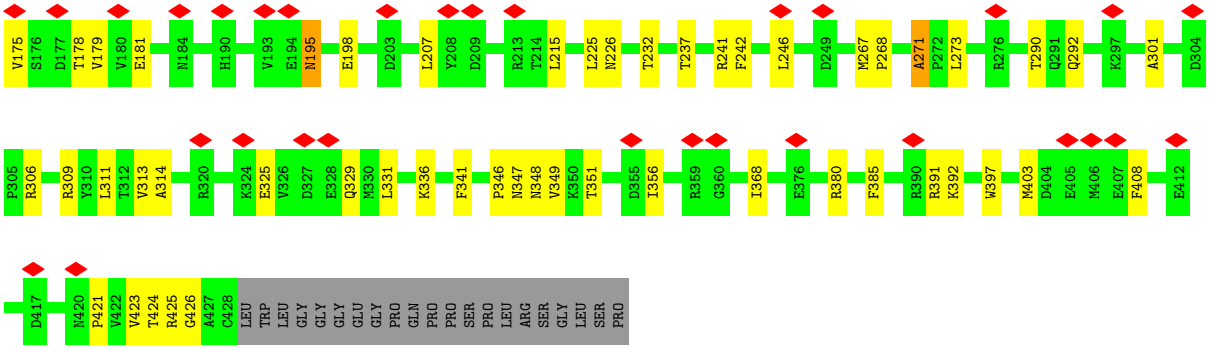
Chain AM: 14% 73% 22% • 5%




- Molecule 41: Tubulin beta chain

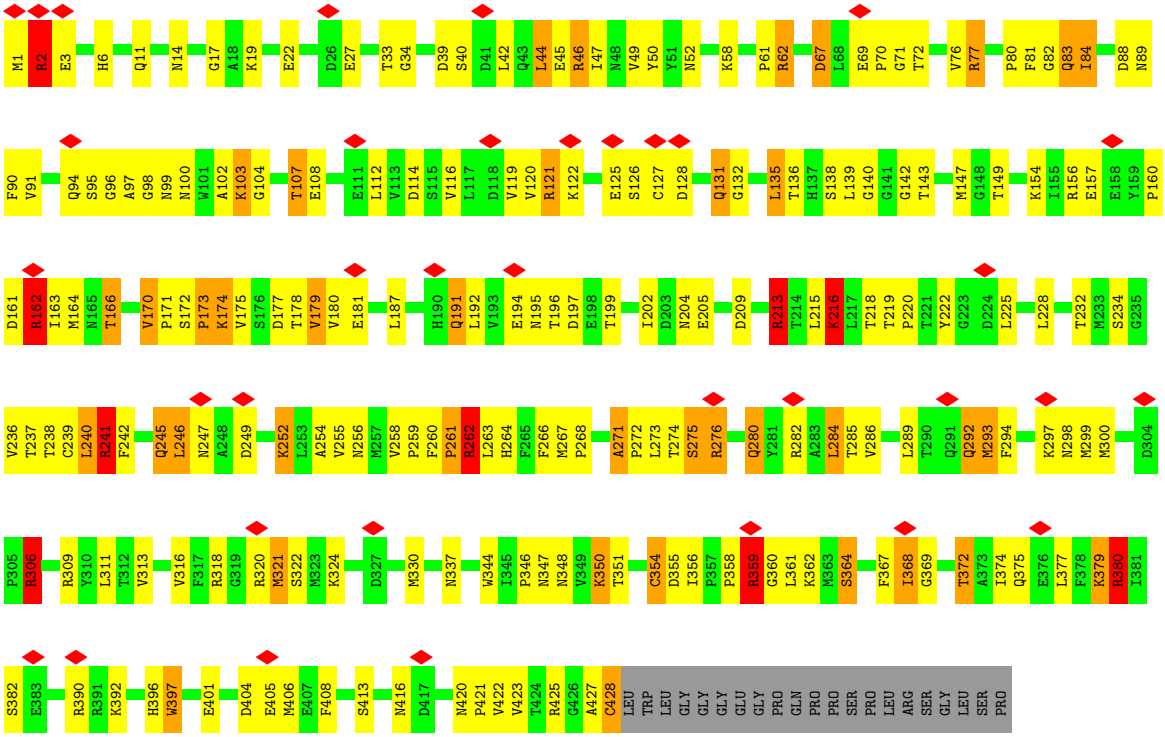
Chain AN: 14% 72% 22% • 5%





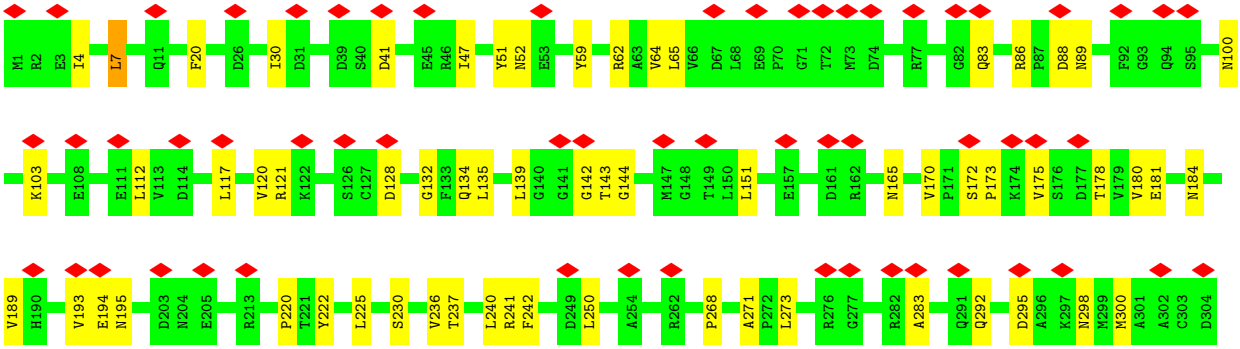

- Molecule 41: Tubulin beta chain

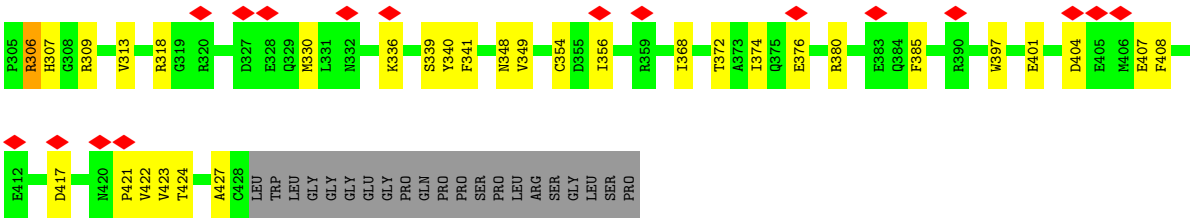
Chain AO:




- Molecule 41: Tubulin beta chain

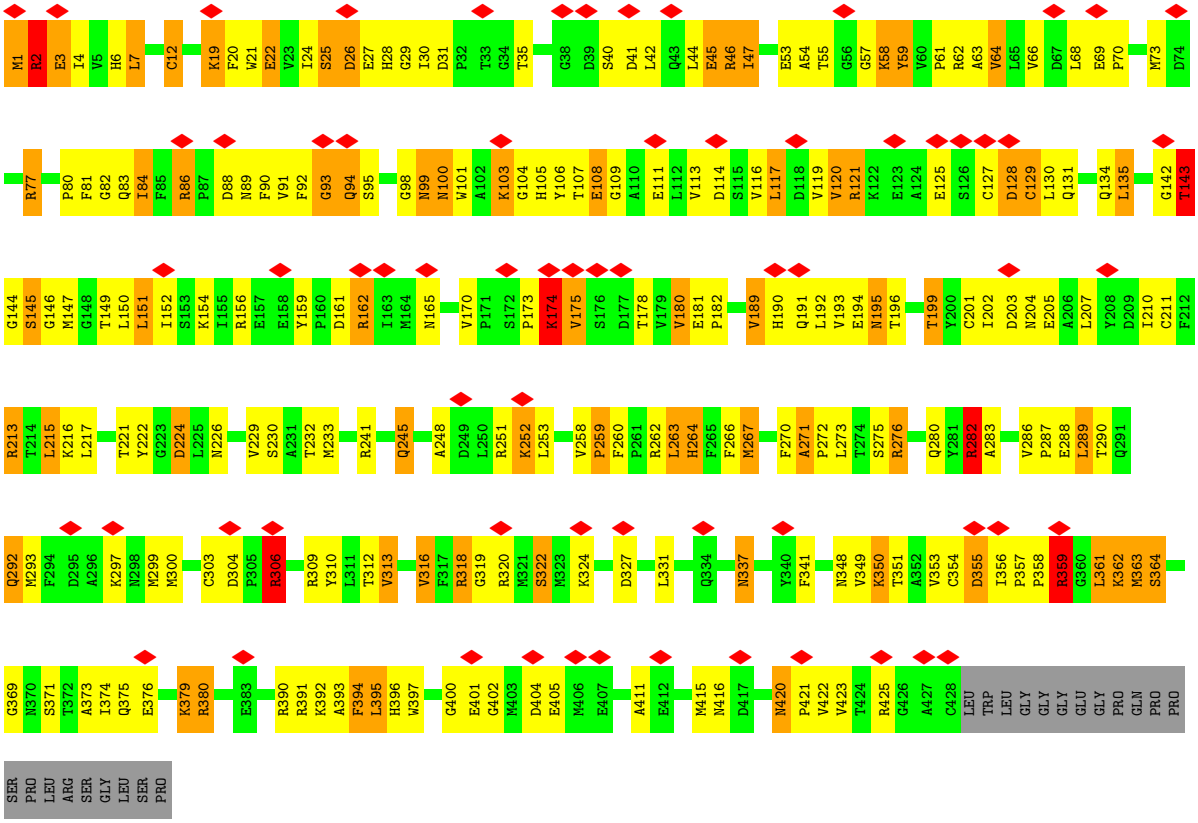
Chain AP:





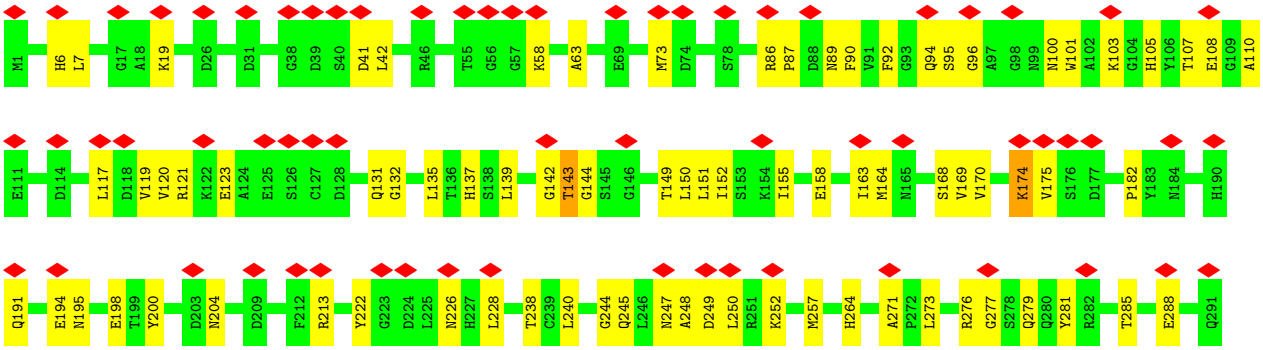

• Molecule 41: Tubulin beta chain

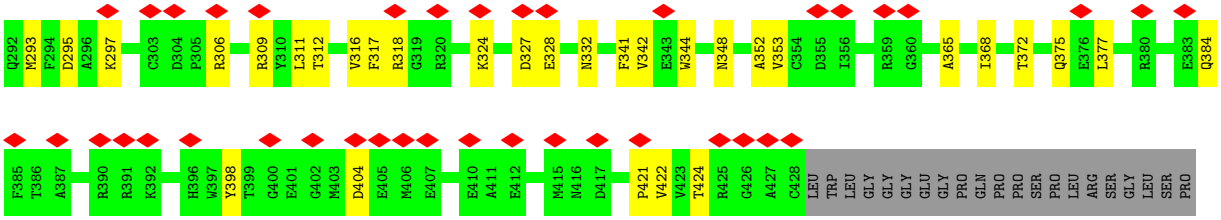
Chain BB:




• Molecule 41: Tubulin beta chain

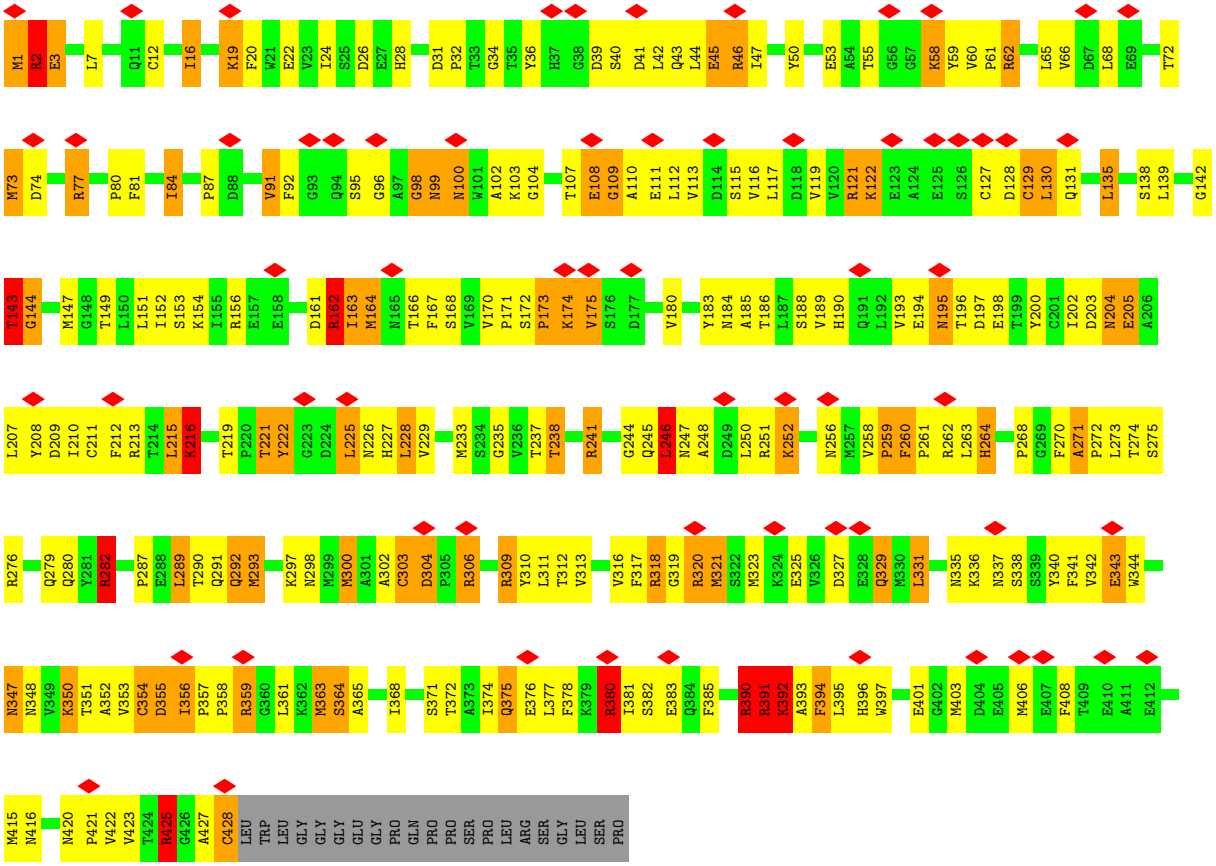
Chain BL:





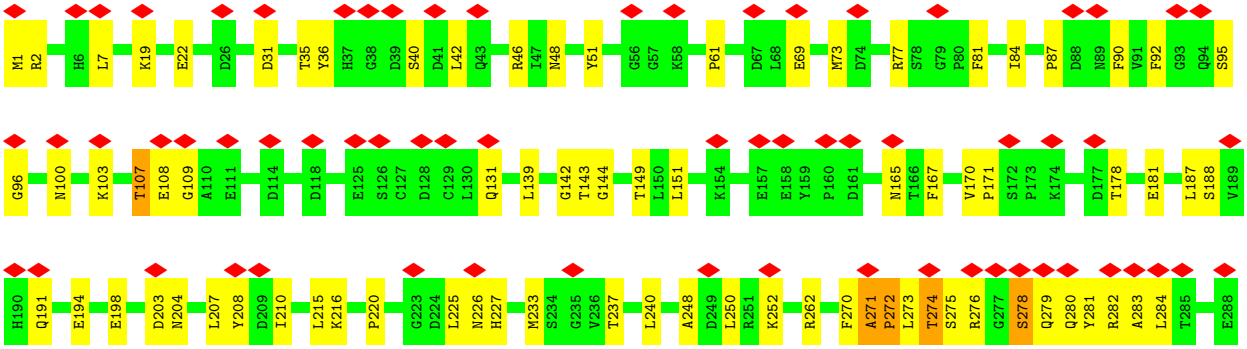

• Molecule 41: Tubulin beta chain

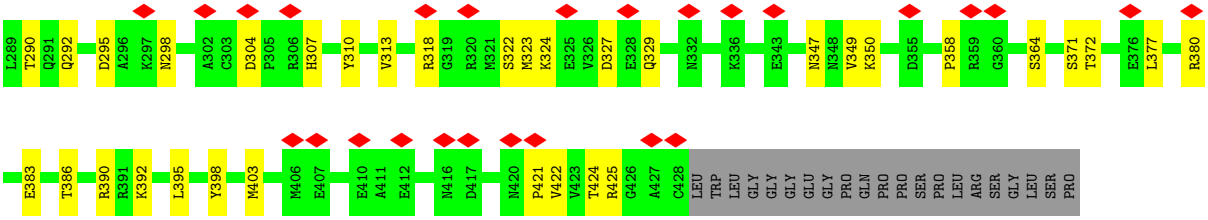
Chain BM:




• Molecule 41: Tubulin beta chain

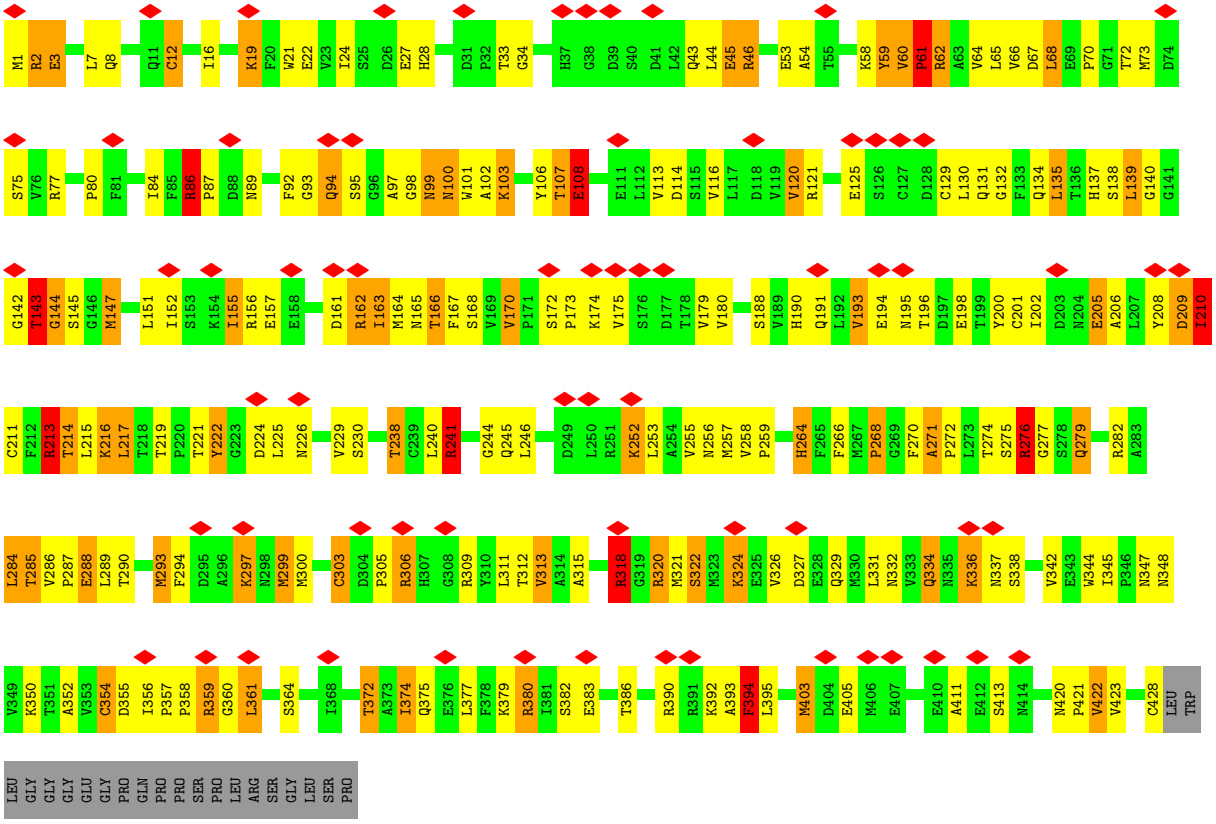
Chain BN:





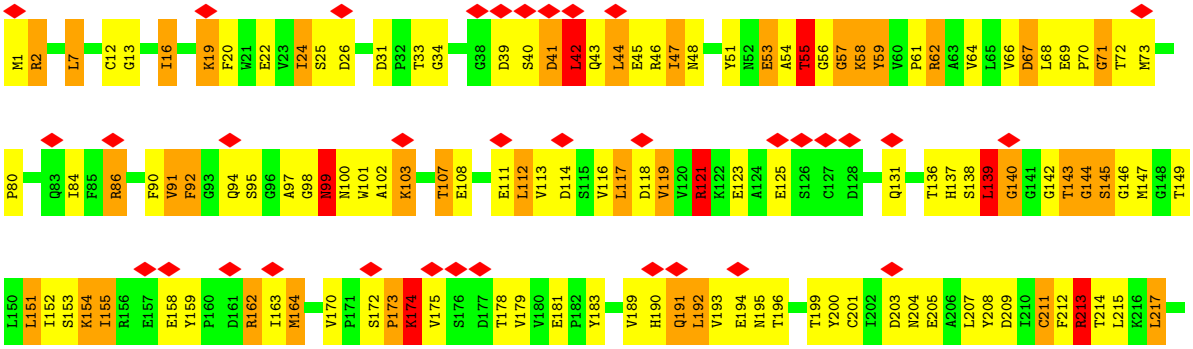

• Molecule 41: Tubulin beta chain

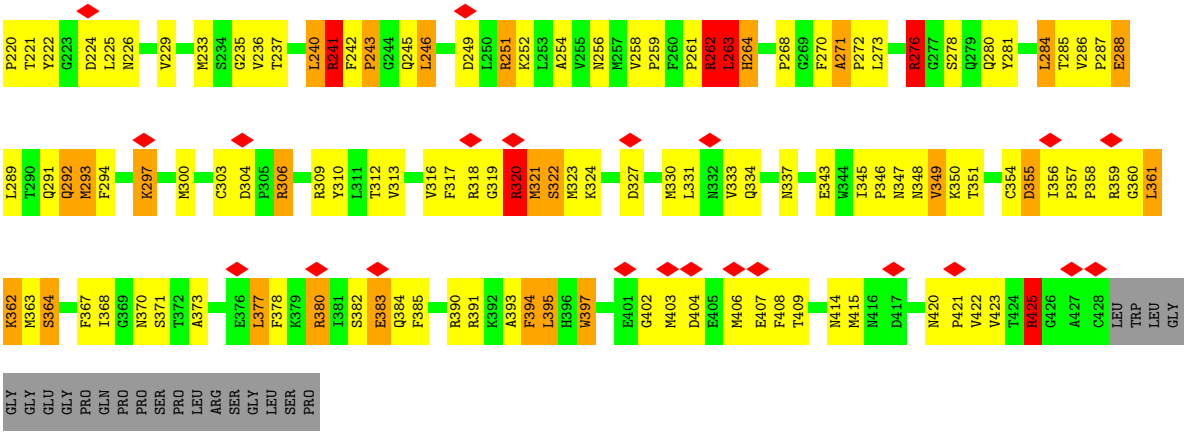
Chain BO:




• Molecule 41: Tubulin beta chain

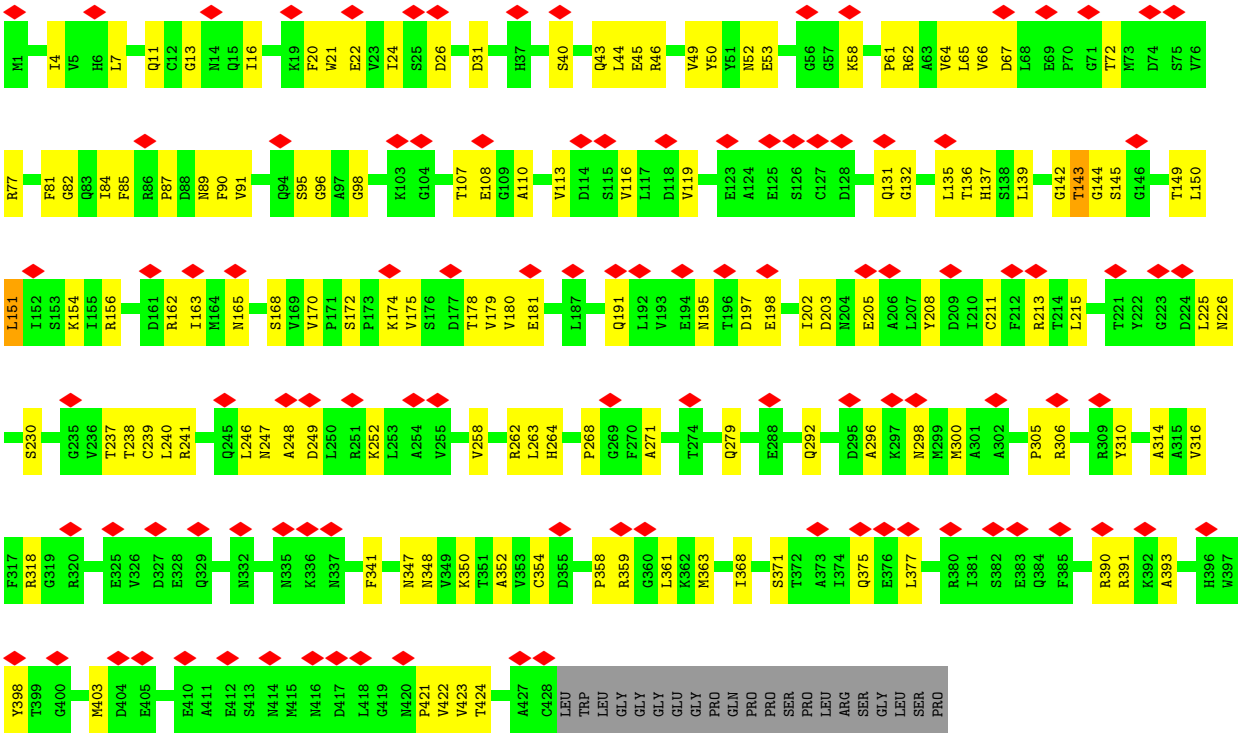
Chain BP:





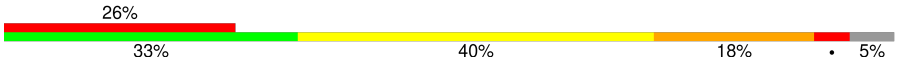

- Molecule 41: Tubulin beta chain

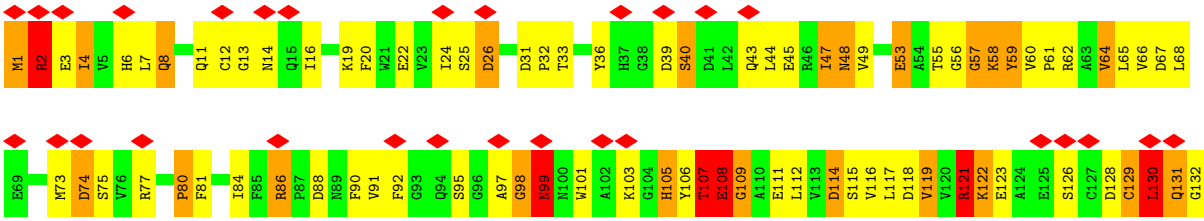
Chain CB:

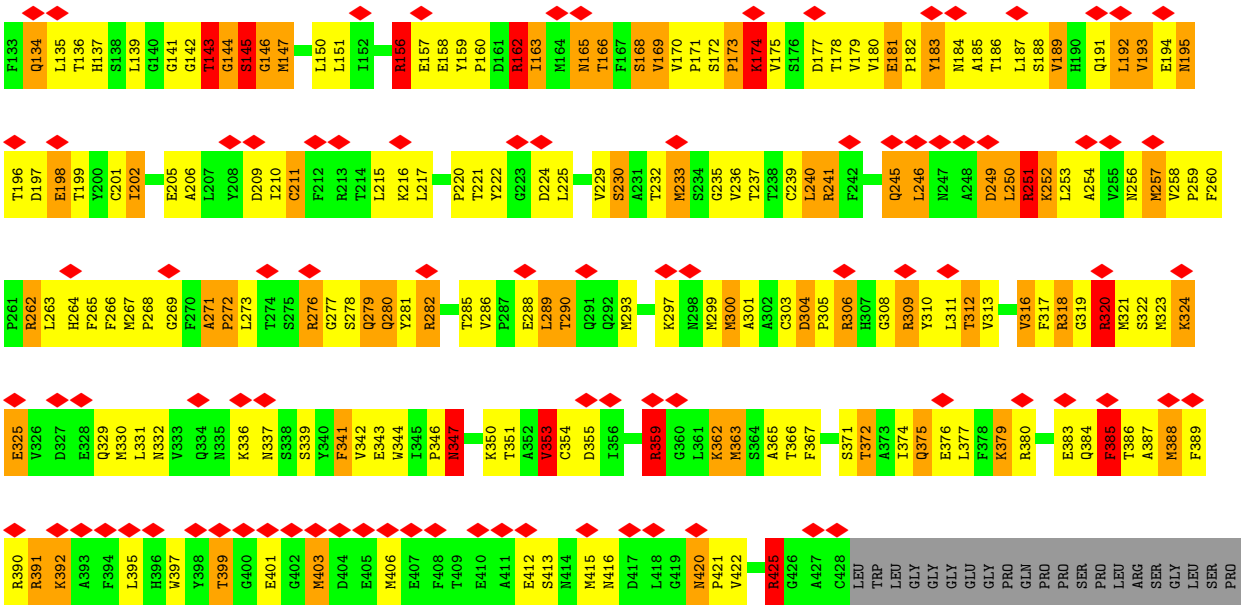



- Molecule 41: Tubulin beta chain

Chain CL:

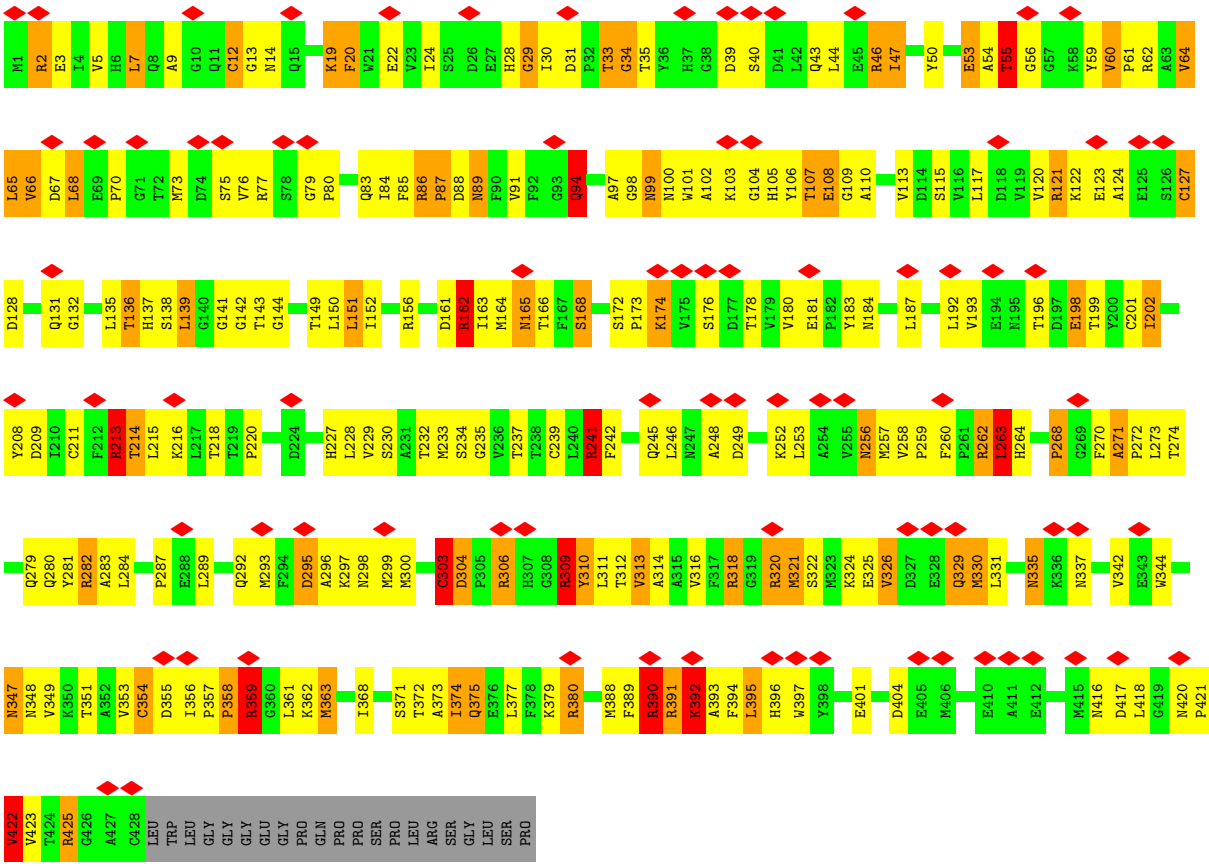




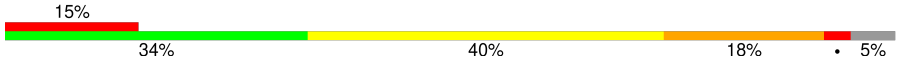

- Molecule 41: Tubulin beta chain

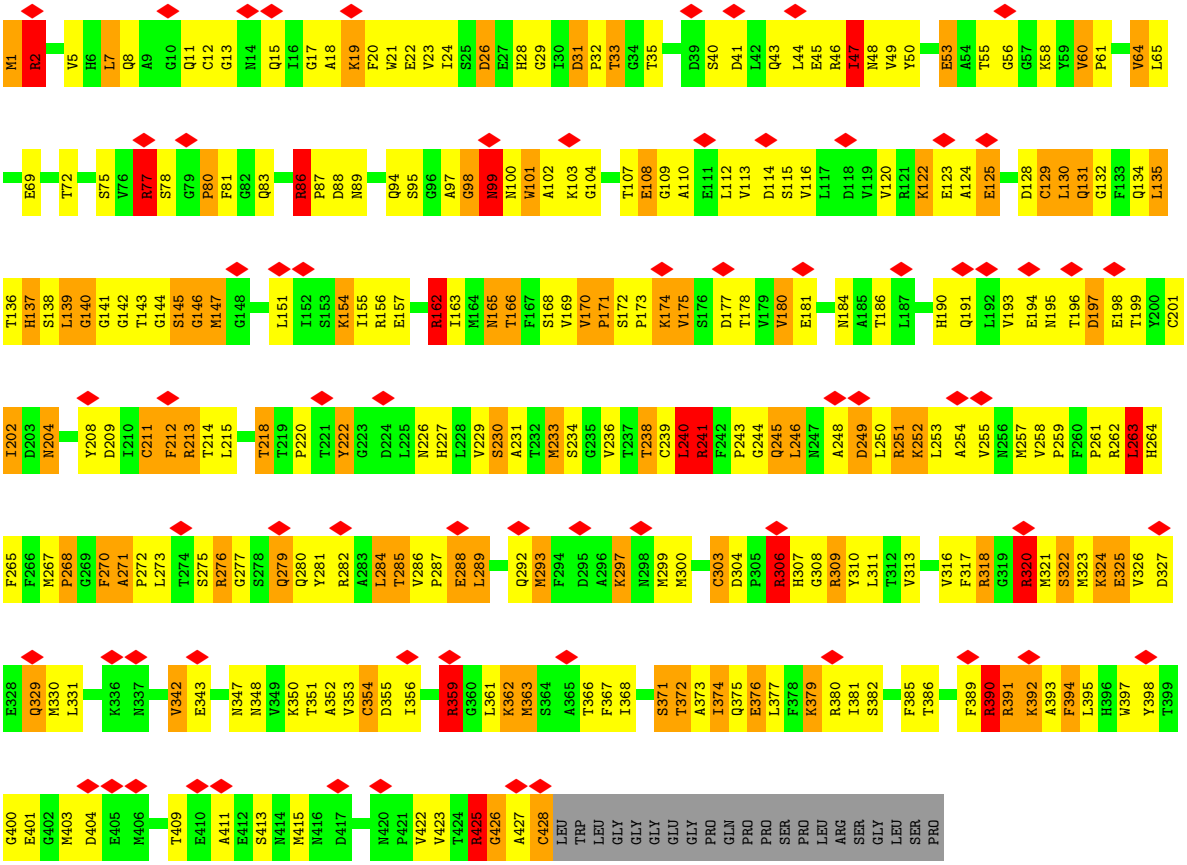
Chain CM:




- Molecule 41: Tubulin beta chain

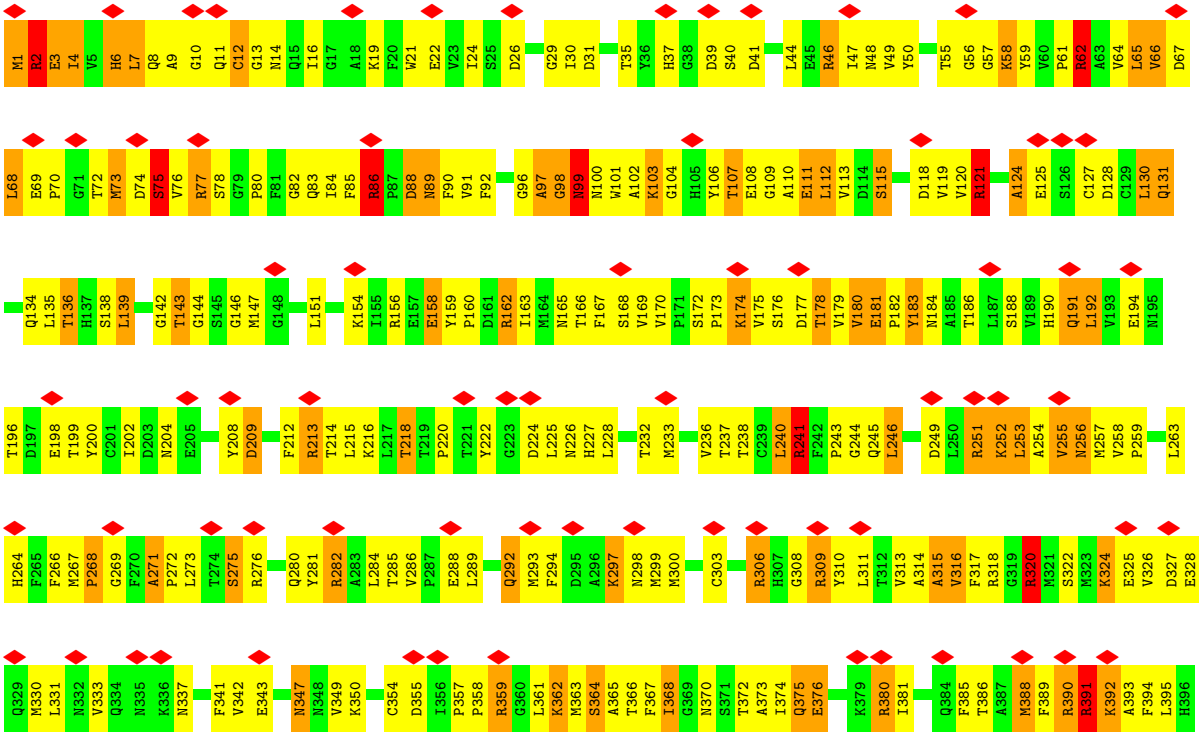
Chain CN:

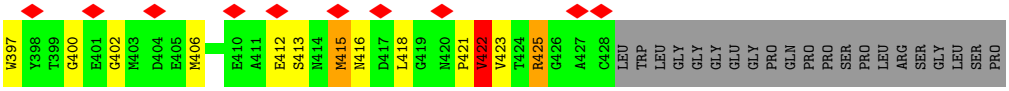




• Molecule 41: Tubulin beta chain

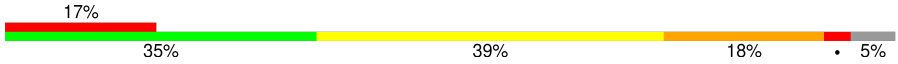
Chain CO:

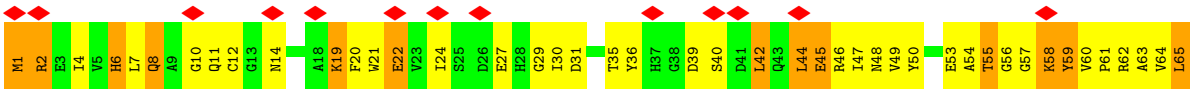


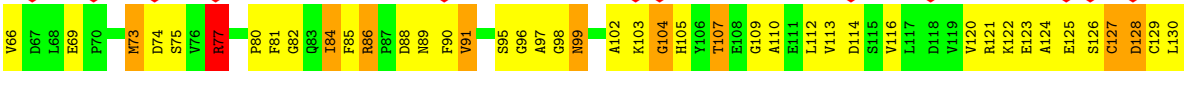


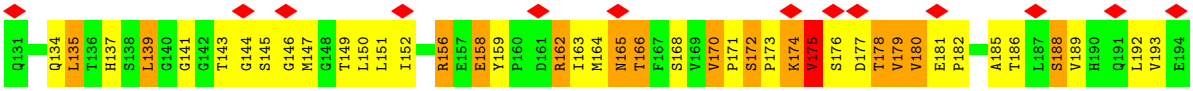

- Molecule 41: Tubulin beta chain

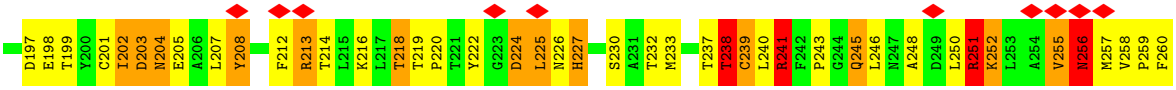
Chain CP:

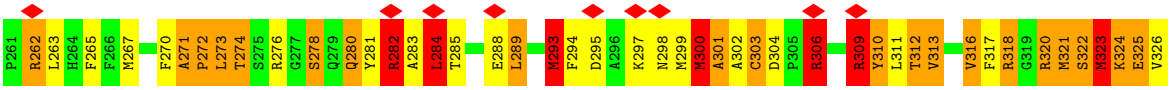


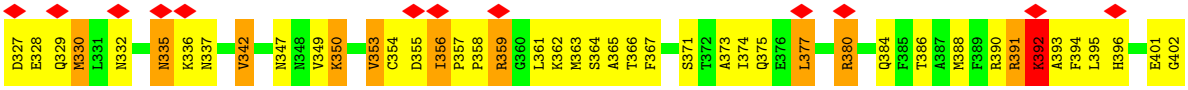



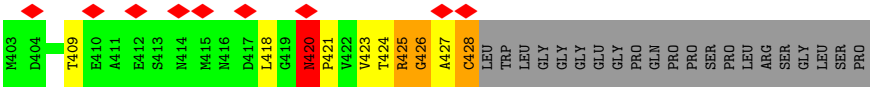



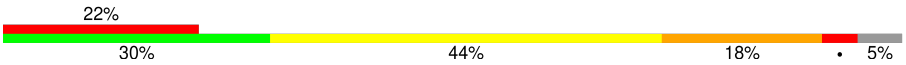



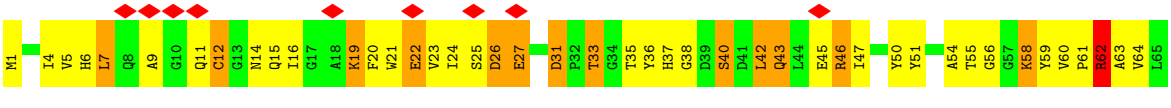



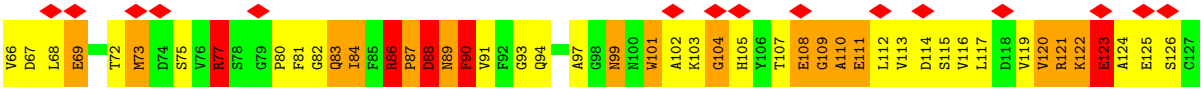



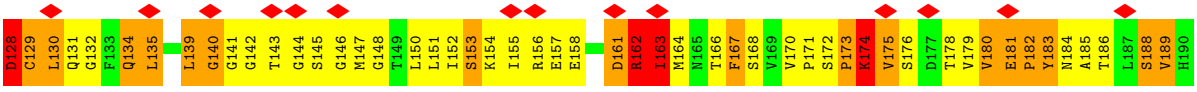

- Molecule 41: Tubulin beta chain

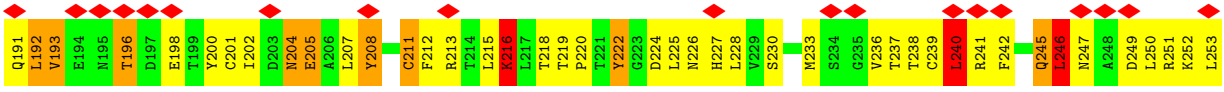
Chain DB:

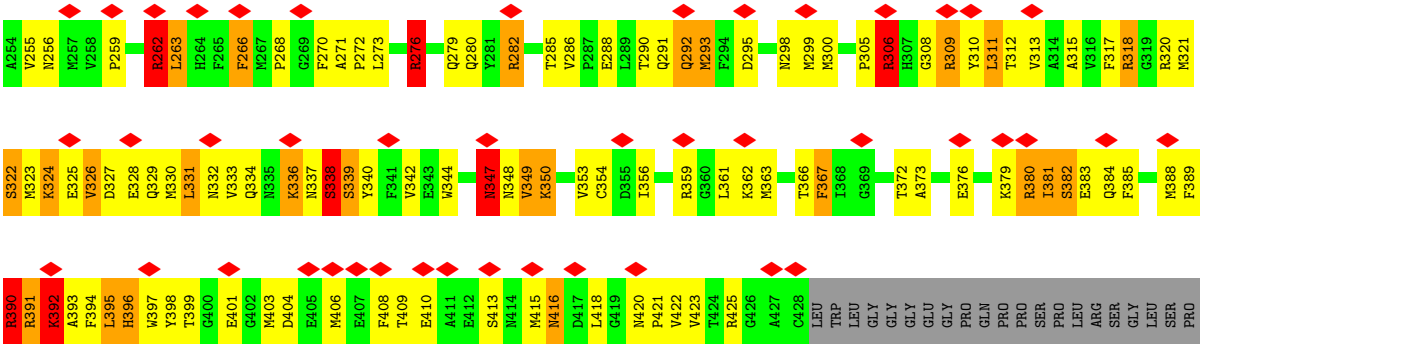


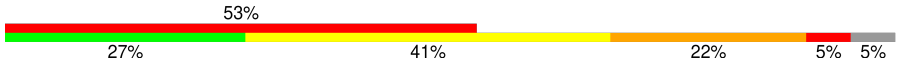



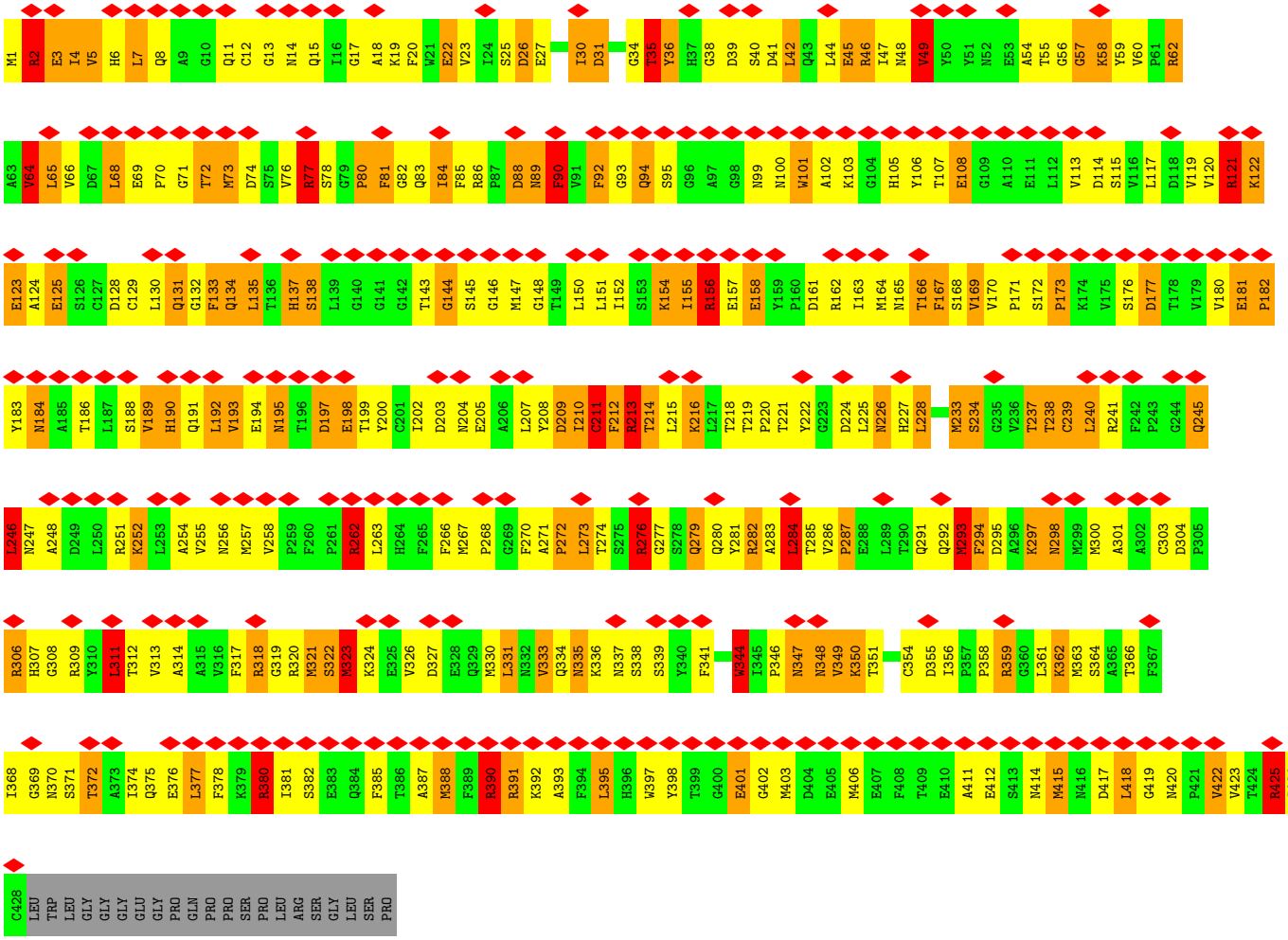






- Molecule 41: Tubulin beta chain

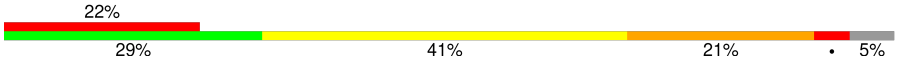
Chain DL:

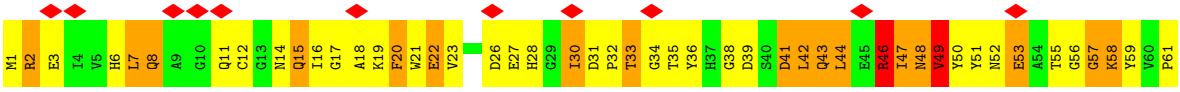


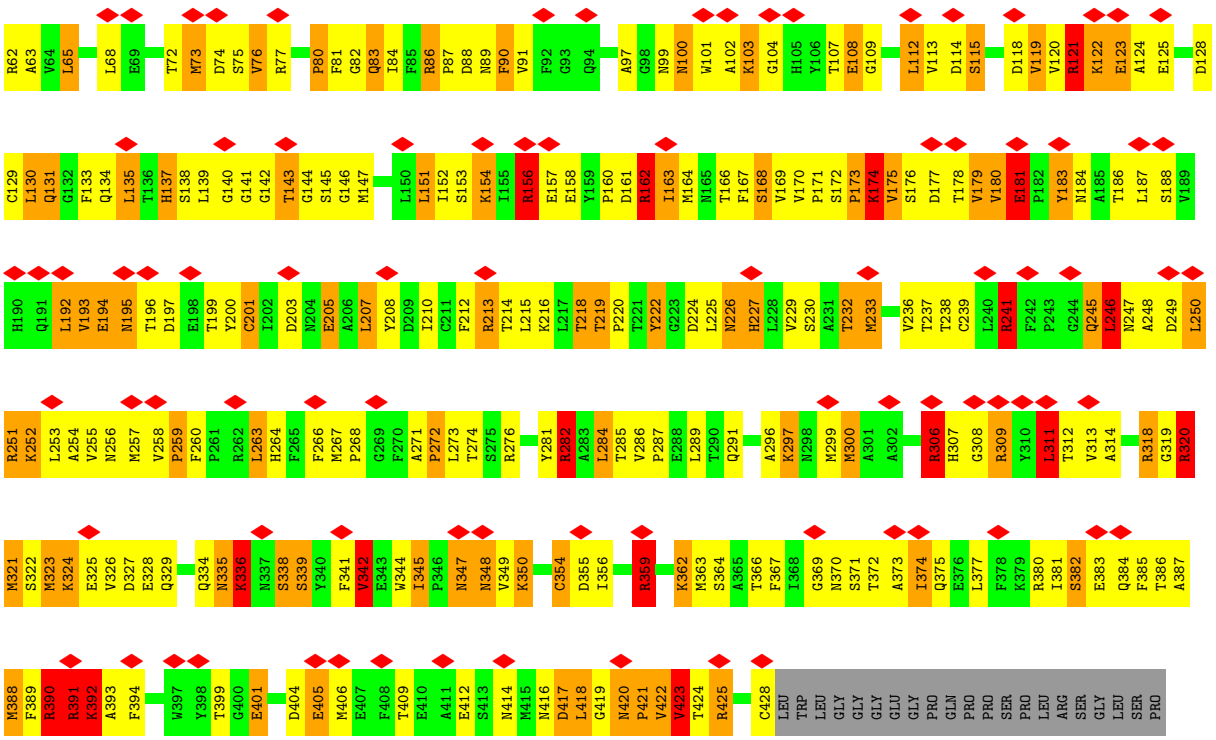




- Molecule 41: Tubulin beta chain

Chain DM:

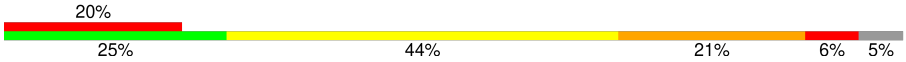


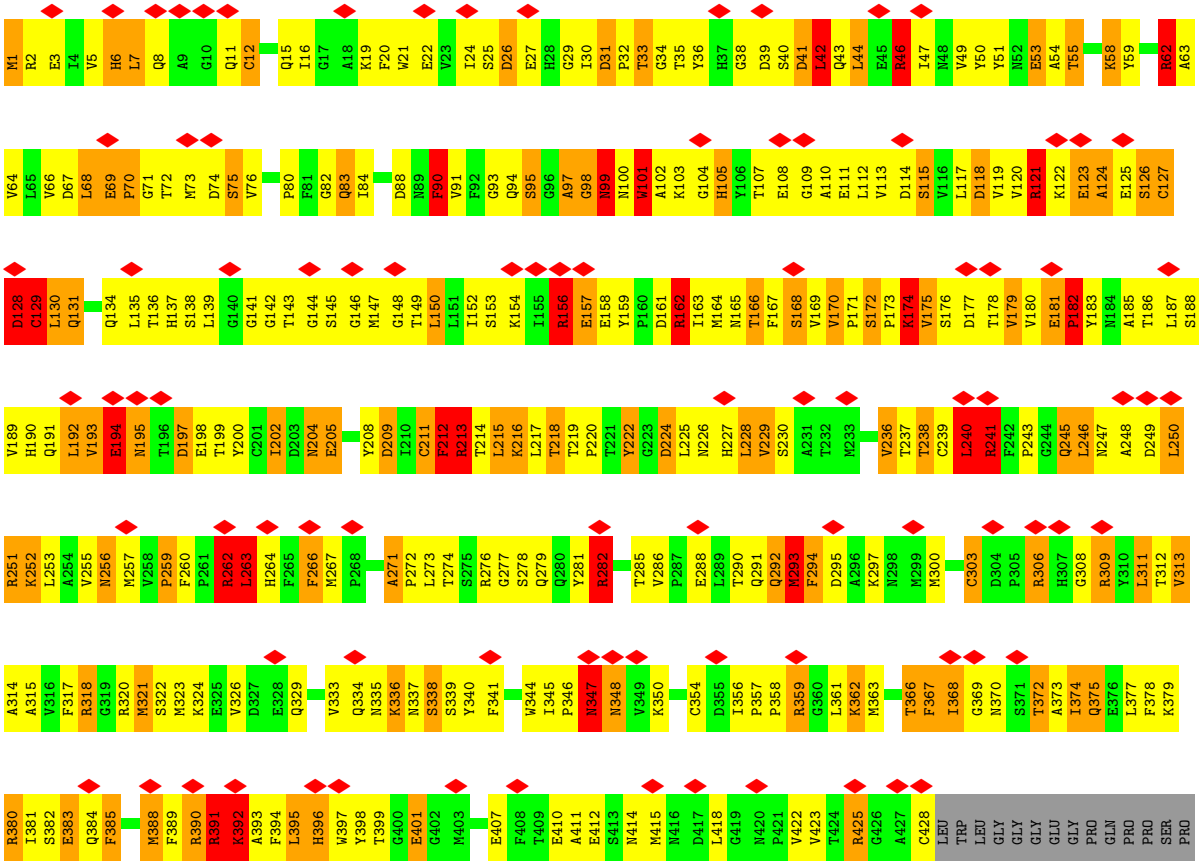





- Molecule 41: Tubulin beta chain

Chain DN:

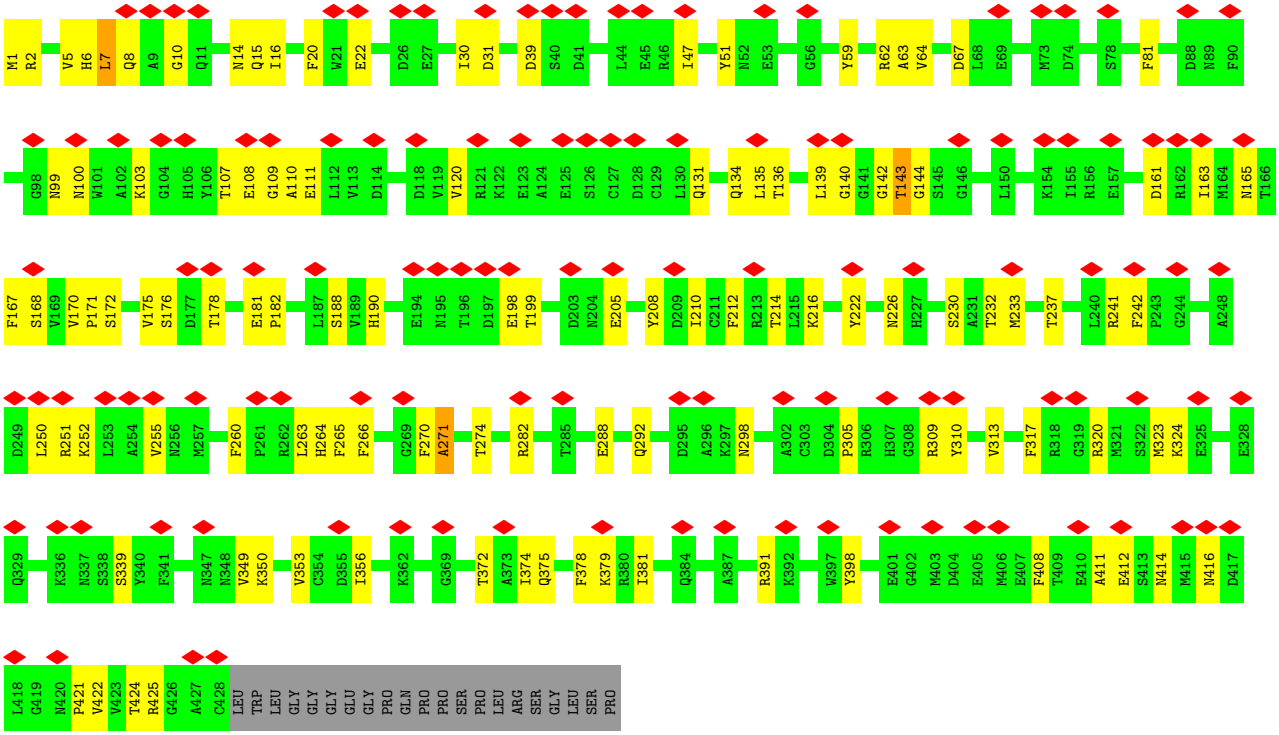


LEU ARG SER GLY LEU SER PRO

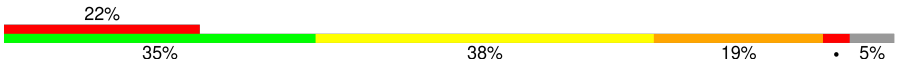
- Molecule 41: Tubulin beta chain

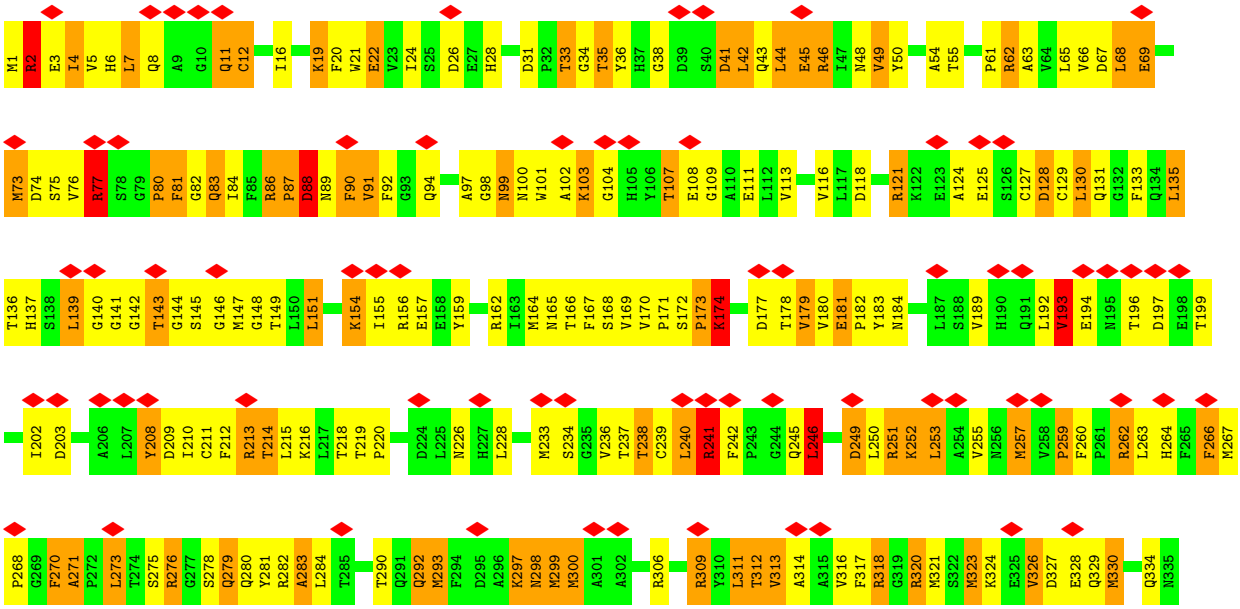
Chain DO:

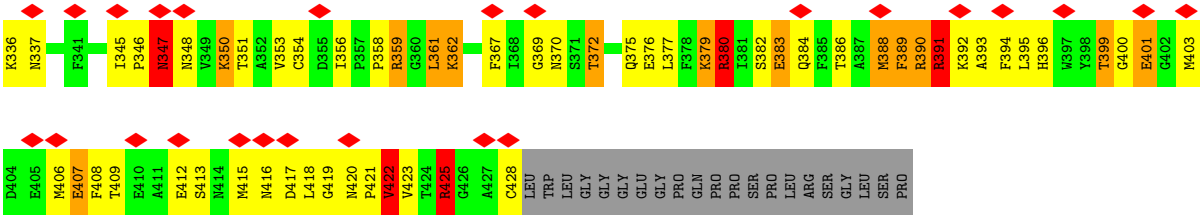



- Molecule 41: Tubulin beta chain

Chain DP:

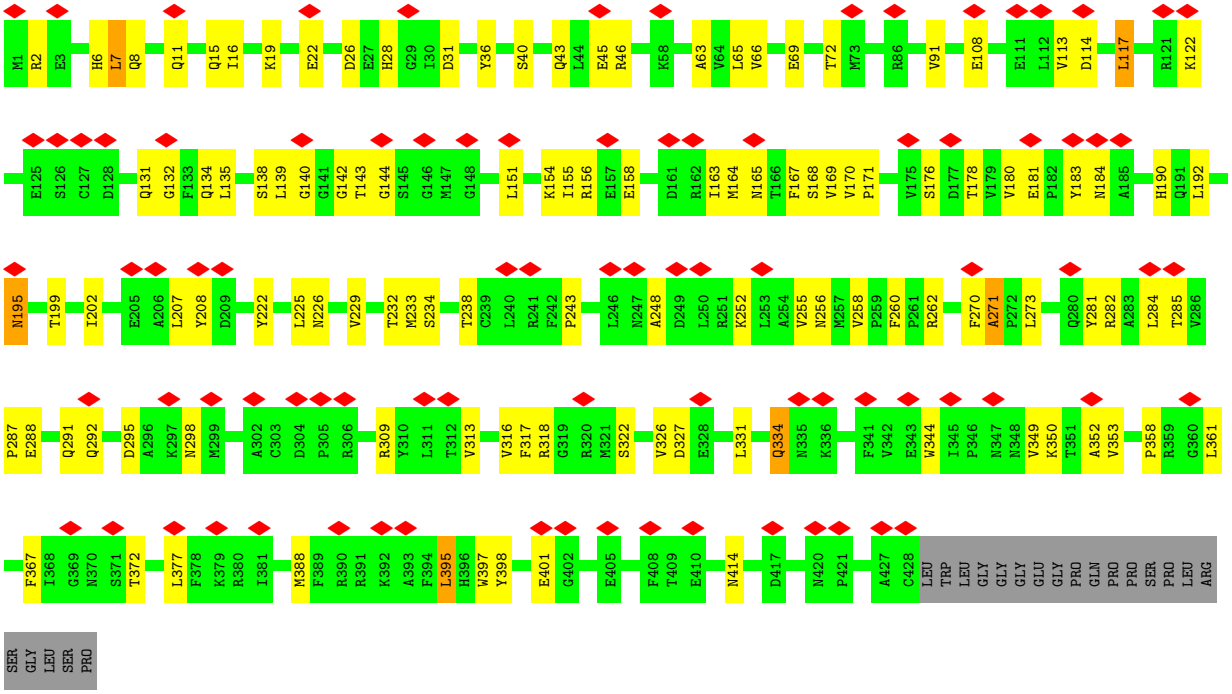




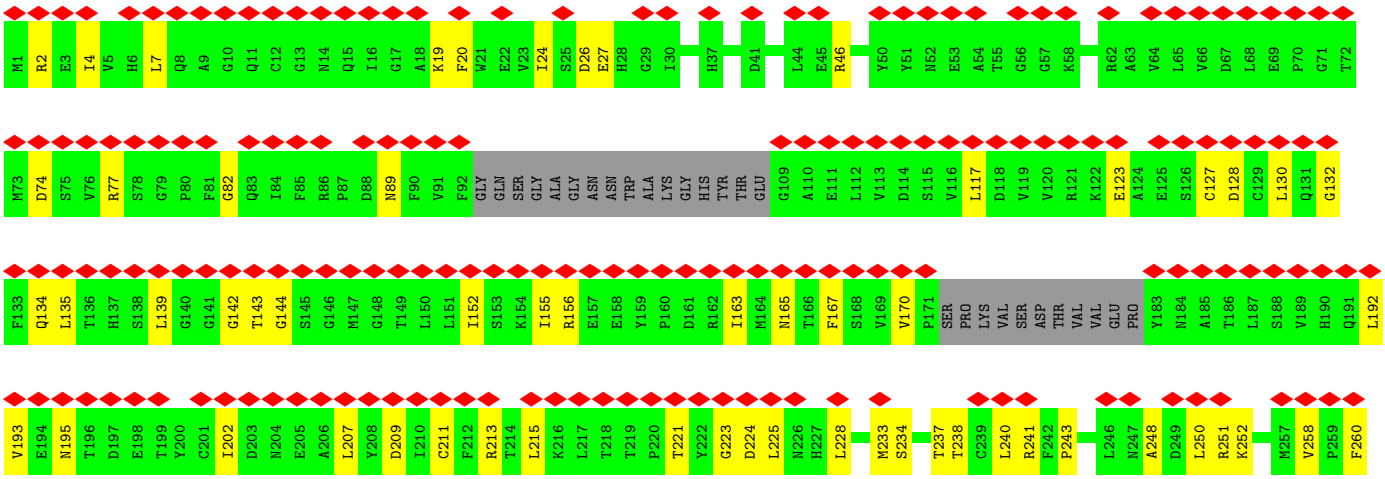

• Molecule 41: Tubulin beta chain

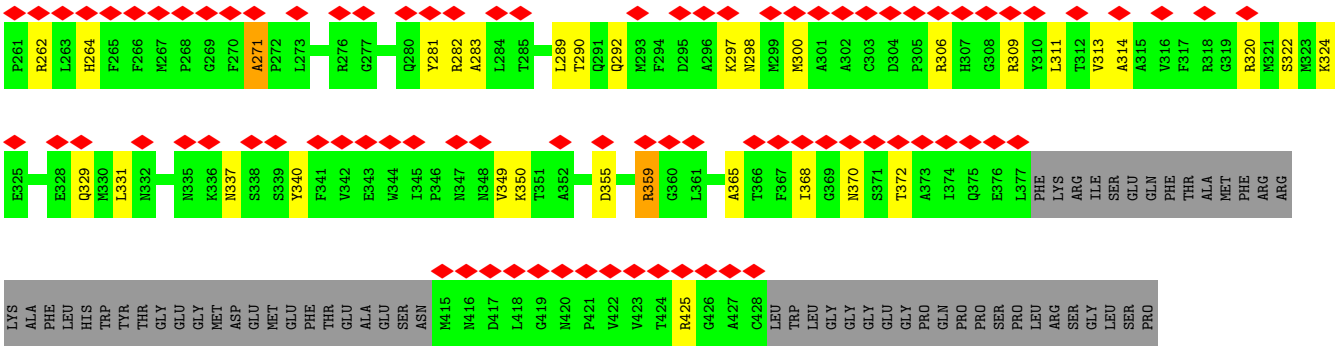
Chain EB:




• Molecule 41: Tubulin beta chain

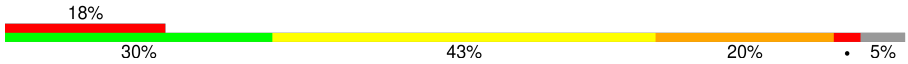
Chain EL:

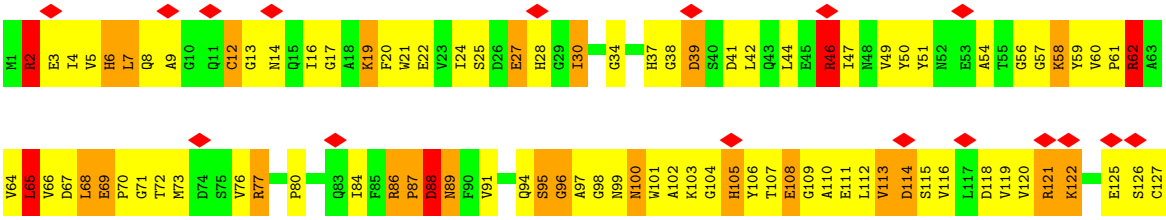


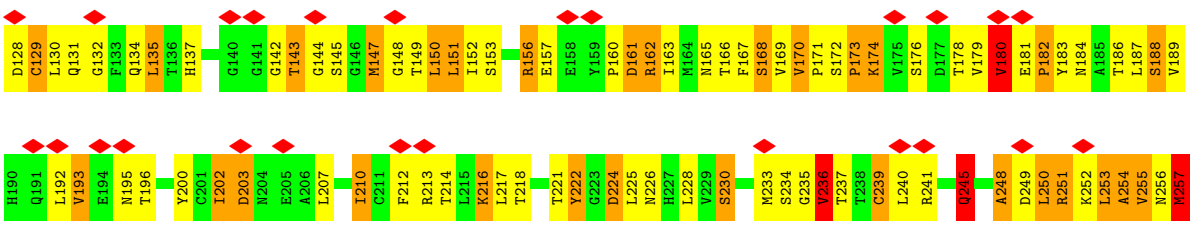


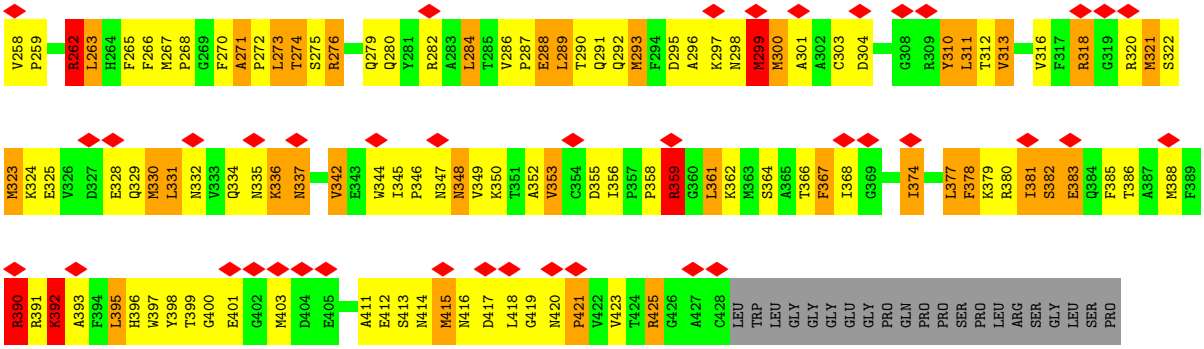

- Molecule 41: Tubulin beta chain

Chain EM:



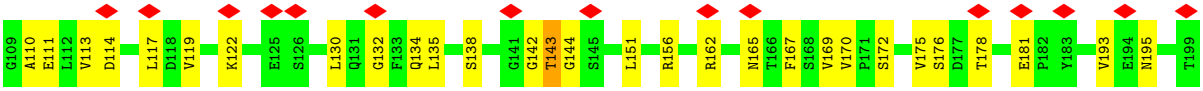



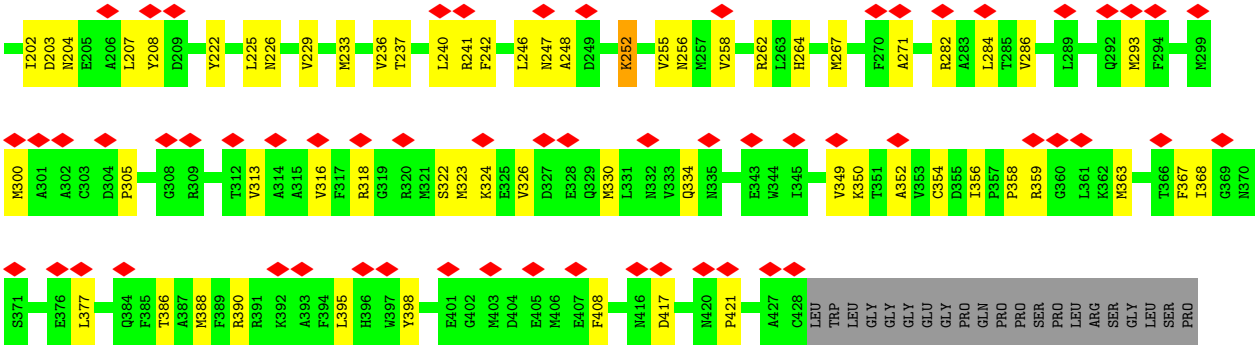




- Molecule 41: Tubulin beta chain

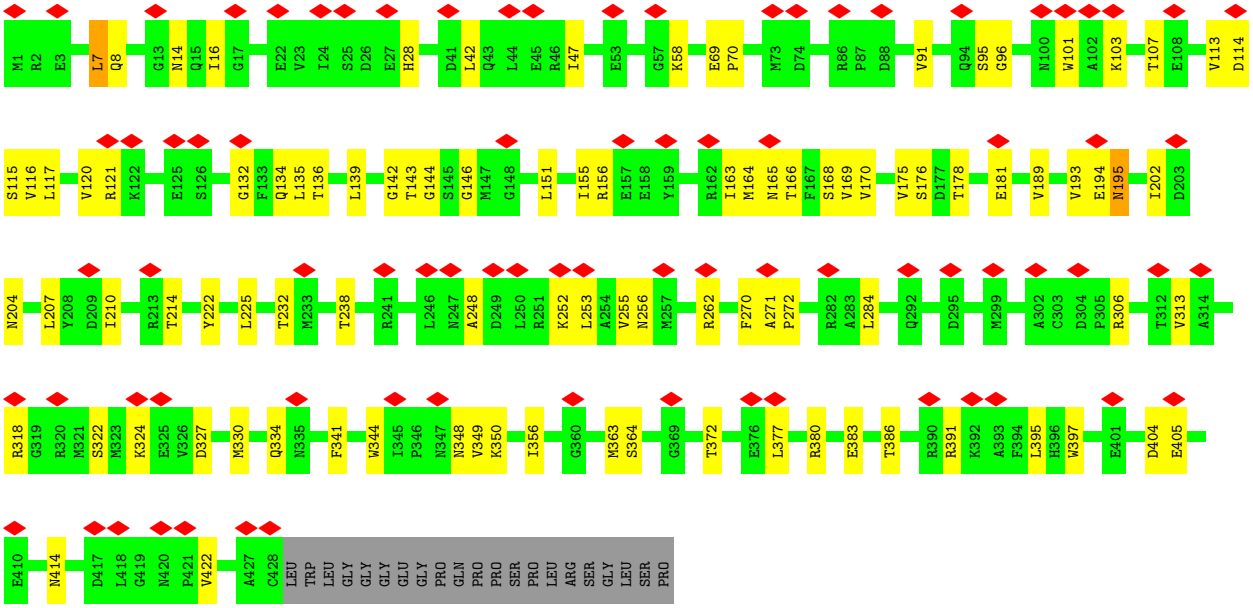
Chain EN:





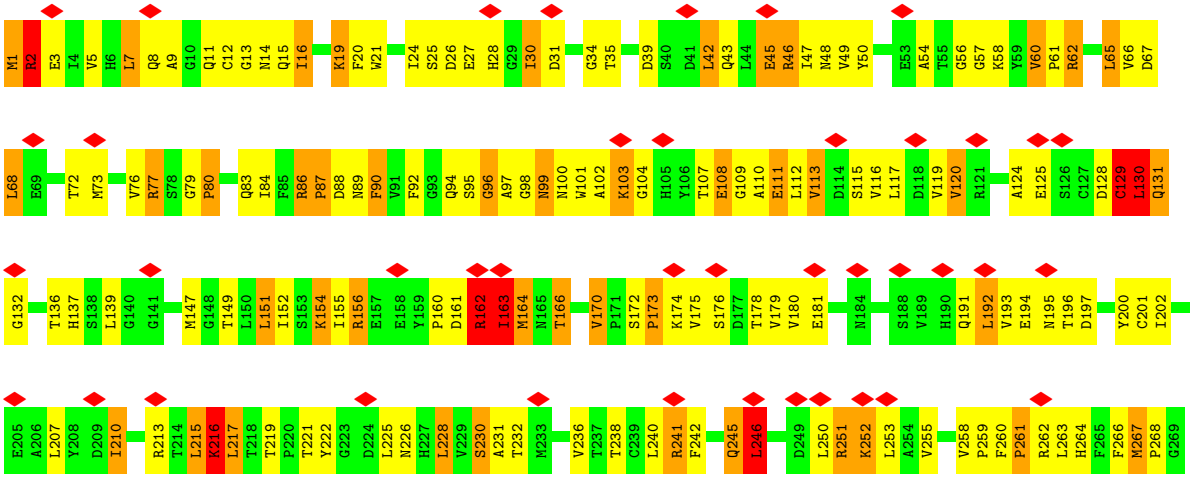

• Molecule 41: Tubulin beta chain

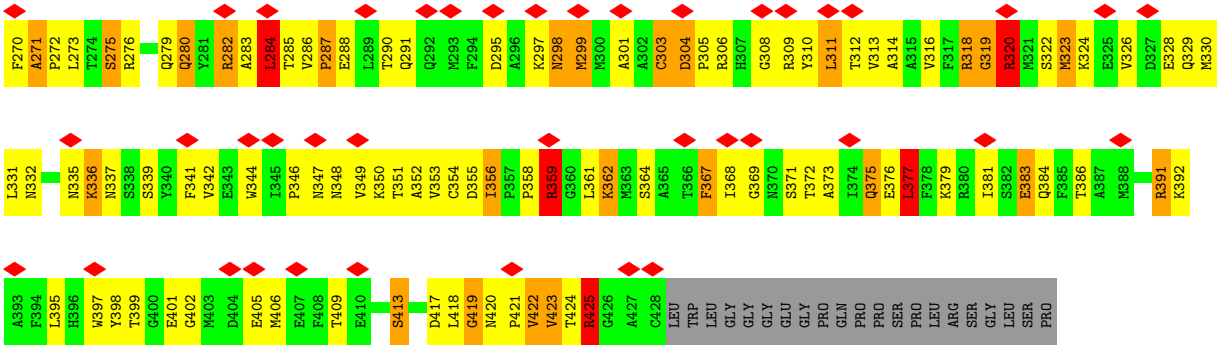
Chain EO:




• Molecule 41: Tubulin beta chain

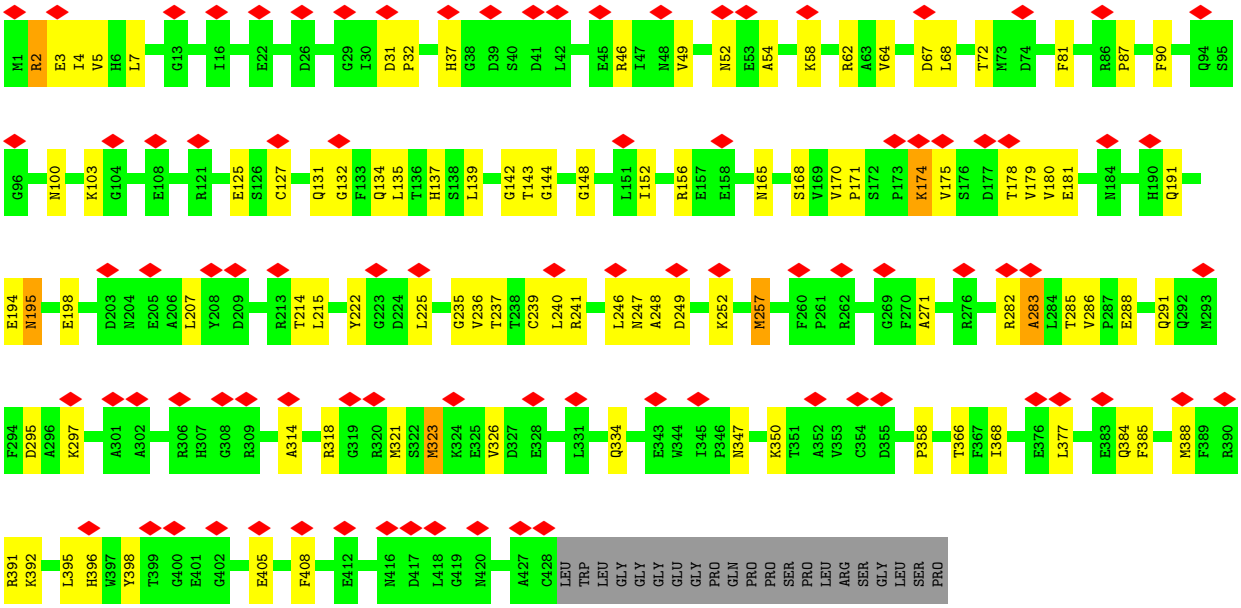
Chain EP:





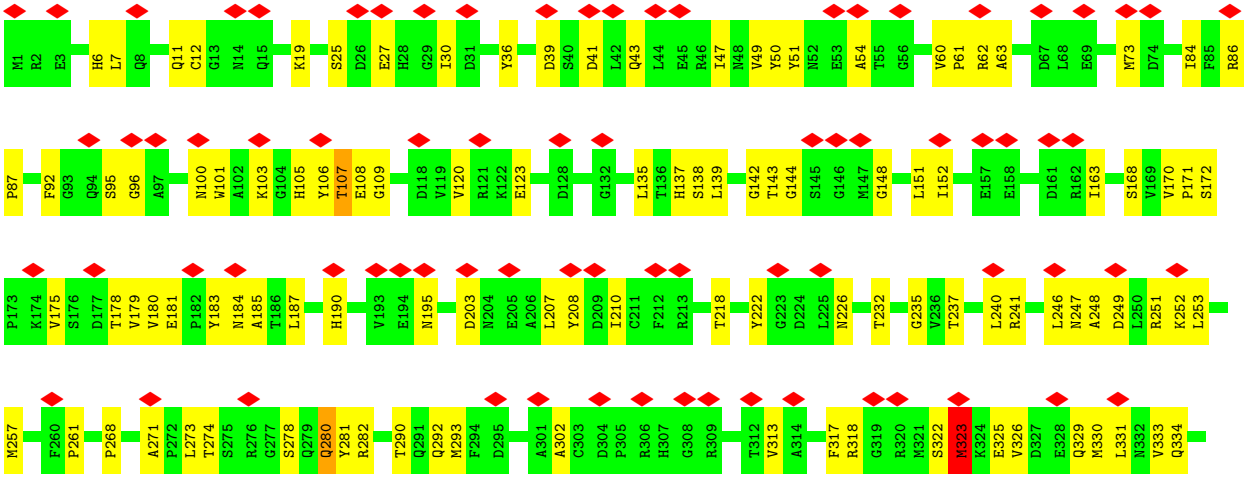

- Molecule 41: Tubulin beta chain

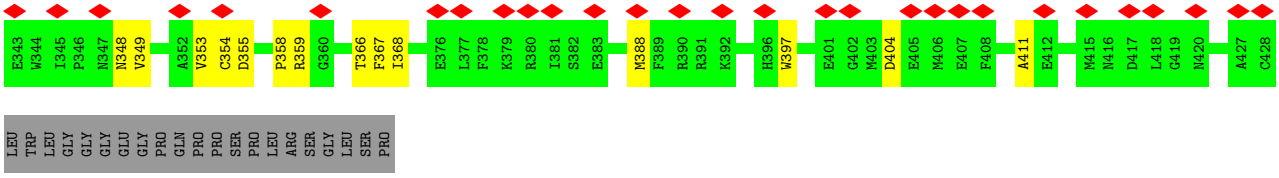
Chain FB:




- Molecule 41: Tubulin beta chain

Chain FM:






• Molecule 41: Tubulin beta chain

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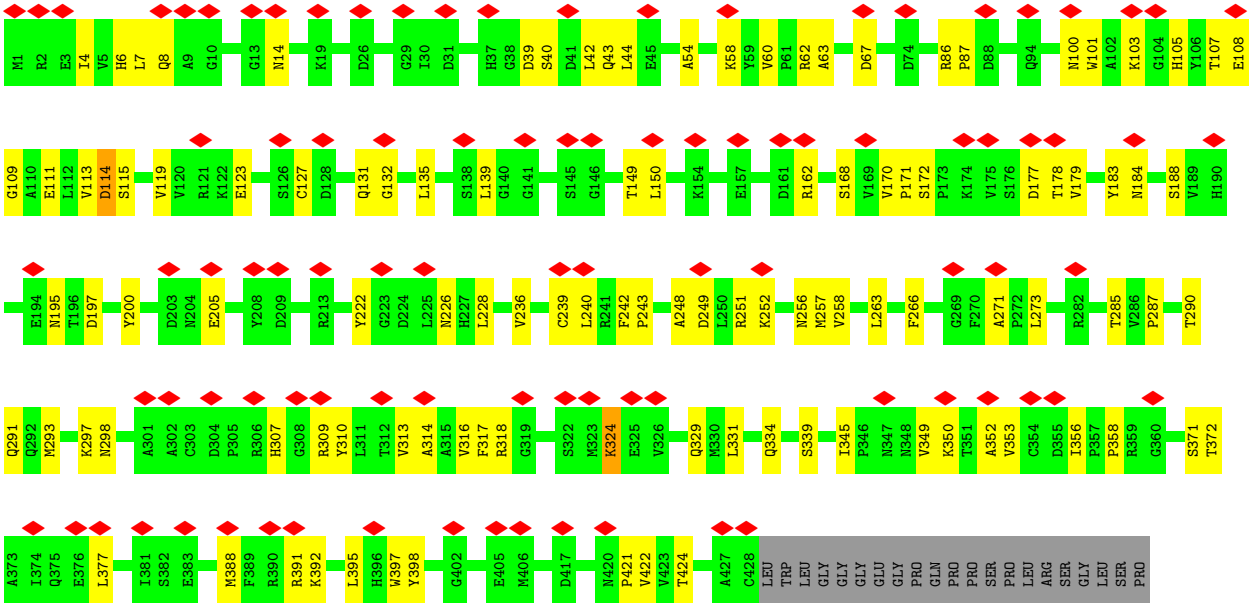
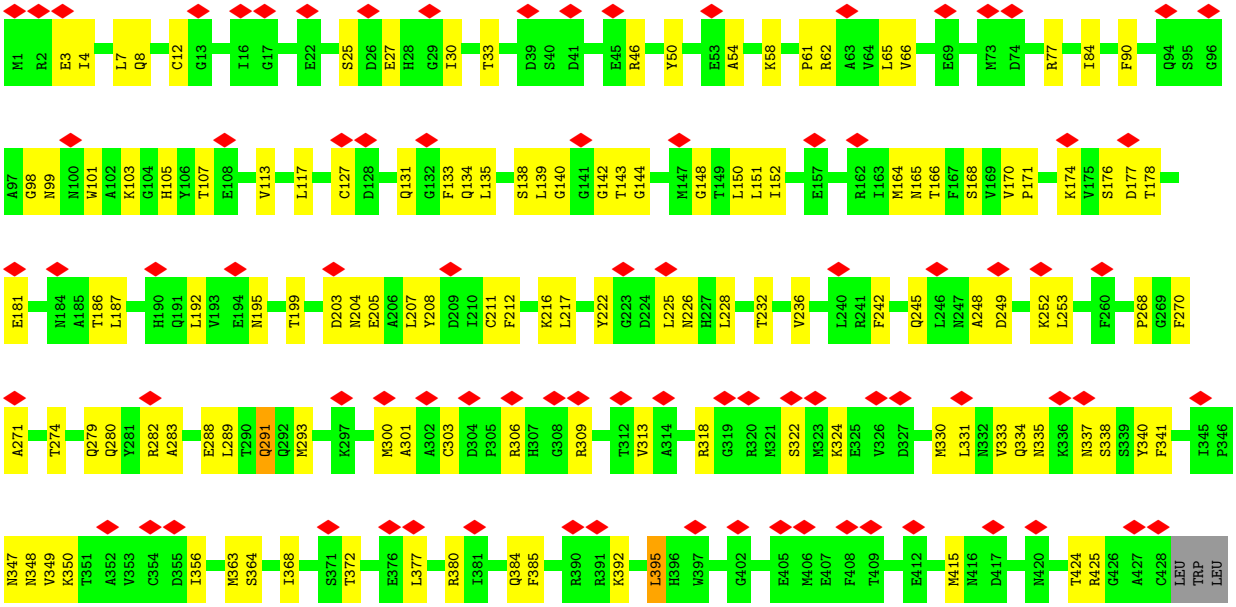
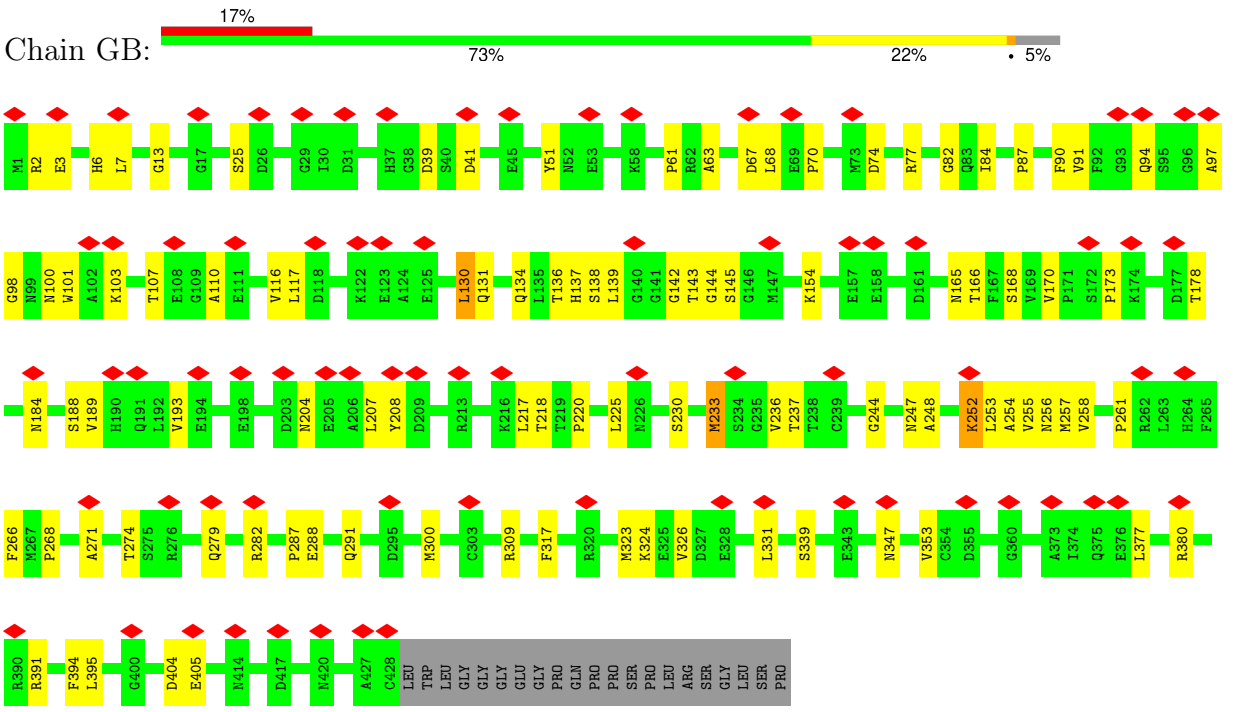



• Molecule 41: Tubulin beta chain

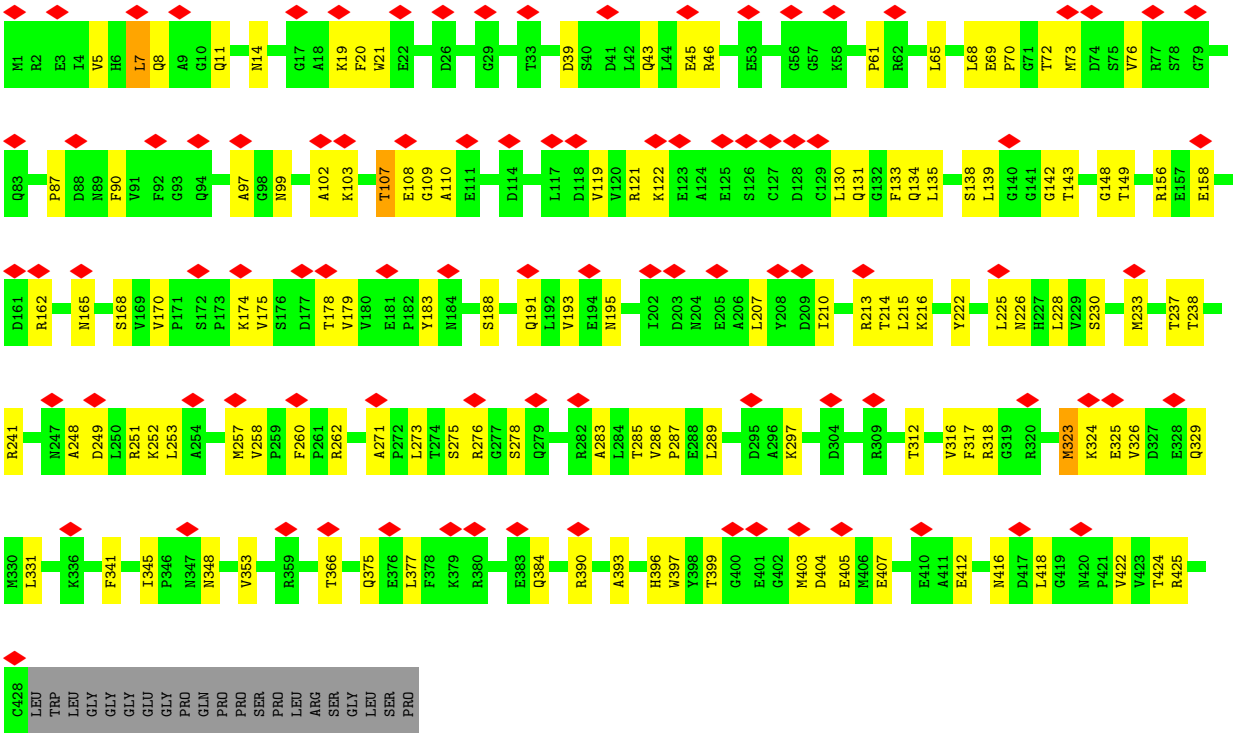
Chain FO:



GLY GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER GLY LEU SER PRO
• Molecule 41: Tubulin beta chain
Chain FP:
25%
68%
26%
5%
M1 R2 H6 L7 Q8 A9 G10 Q11 C12 G13 I16 G17 E22 D26 E27 H28 G29 I30 D31 G34 T35 D39 S40 D41 L42 Q43 L44 E45 R46 Y51 N52 E53 A54 K58 Y59 V60 A63 E69 T72 M73 D74 F81 G82 Q83 R86 P87 D88
N89 F90 V91 F92 S95 G96 N99 G104 E108 D114 L117 K122 E123 S126 C127 Q131 G132 F133 Q134 L135 L139 G140 G141 G142 T143 G144 S145 G146 M147 G148 T149 L150 L151 I152 R156 E157 E158 R162 I163 M164 N165 S168 V169 V170 P171 S172
V175 S176 D177 T178 V179 V180 E181 P182 Y183 N184 S188 V189 H190 Q191 E194 N195 D203 N204 E205 A206 L207 Y208 D209 I210 C211 F212 R213 T214 L215 T221 Y222 G223 D224 L225 N226 H227 L228 V229 S230 S234 G235 T238 C239 L240 R241 Q245 L246 N247 A248 D249 L250 R251 K252
L253 A254 V255 F260 P261 R262 G269 F270 A271 P272 L273 T274 S275 R276 Y281 R282 A283 Q291 Q292 M293 F294 D295 A296 K297 N298 M299 M300 A301 A302 C303 D304 P305 R306 R309 A314 A315 V316 F317 R318 G319 R320 M321 S322 M323 K324 E325 E328 M332 V333 Q334 Y340
E343 P346 N347 N348 A352 V353 C354 D355 R359 G360 L361 S364 A365 T366 F367 I368 E376 L377 F378 K379 R380 I381 M388 F389 R390 L395 H396 W397 Y398 E401 G402 M403 D404 F408 T409 E410 M416 D417 L418 G419 N420 P421 V422 R425 G426 A427 C428 LEU
TRP LEU GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER GLY LEU SER PRO

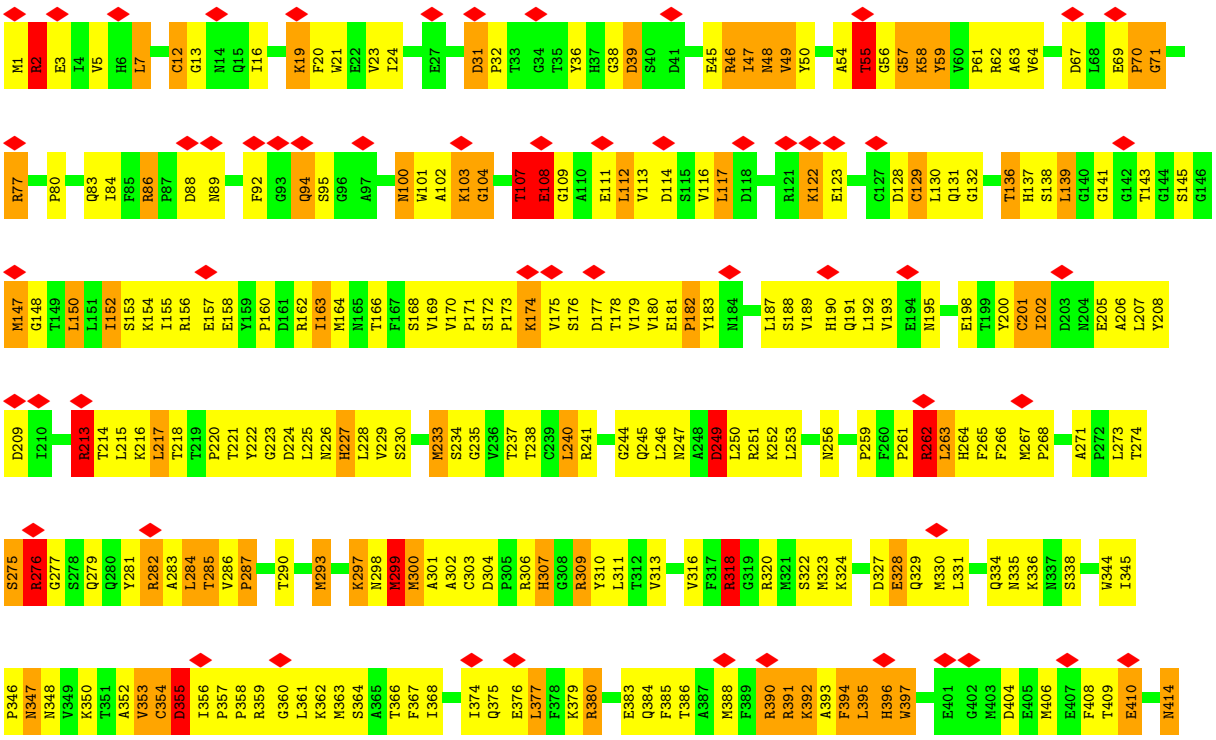

• Molecule 41: Tubulin beta chain
Chain GB:
17%
73%
22%
5%
M1 R2 E3 H6 L7 G13 G17 S25 D26 G29 I30 D31 H37 G38 D39 S40 D41 E45 Y51 N52 E53 K58 P61 R62 A63 D67 L68 E69 P70 M73 D74 R77 G82 Q83 I84 P87 F90 V91 F92 G93 Q94 S95 G96 A97
G98 N99 N100 W101 A102 K103 T107 E108 G109 A110 E111 V116 L117 D118 K122 E123 A124 E125 L130 Q131 Q134 L135 T136 H137 S138 L139 G140 G141 G142 T143 G144 S145 G146 M147 K154 E157 E158 D161 N165 T166 F167 S168 V169 V170 P171 S172 P173 K174 D177 T178
N184 S188 V189 H190 Q191 L192 V193 E194 E198 D203 N204 E205 A206 L207 Y208 D209 R213 K216 L217 T218 T219 P220 L225 N226 S230 M233 S234 G235 V236 T237 T238 C239 G244 N247 A248 K252 L253 A254 V255 N256 M257 V258 P261 R262 L263 H264 F265
F266 M267 P268 A271 T274 S275 R276 Q279 R282 P287 E288 Q291 D295 M300 C303 R309 F317 R320 M323 K324 E325 V326 D327 E328 L331 S339 E343 N347 V353 C354 D355 G360 A373 I374 Q375 E376 L377 R380
R390 R391 F394 L395 G400 D404 E405 N414 D417 N420 A427 C428 LEU TRP LEU GLY GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER GLY LEU SER PRO
• Molecule 41: Tubulin beta chain

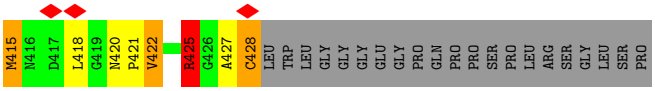
Chain GM:




• Molecule 41: Tubulin beta chain

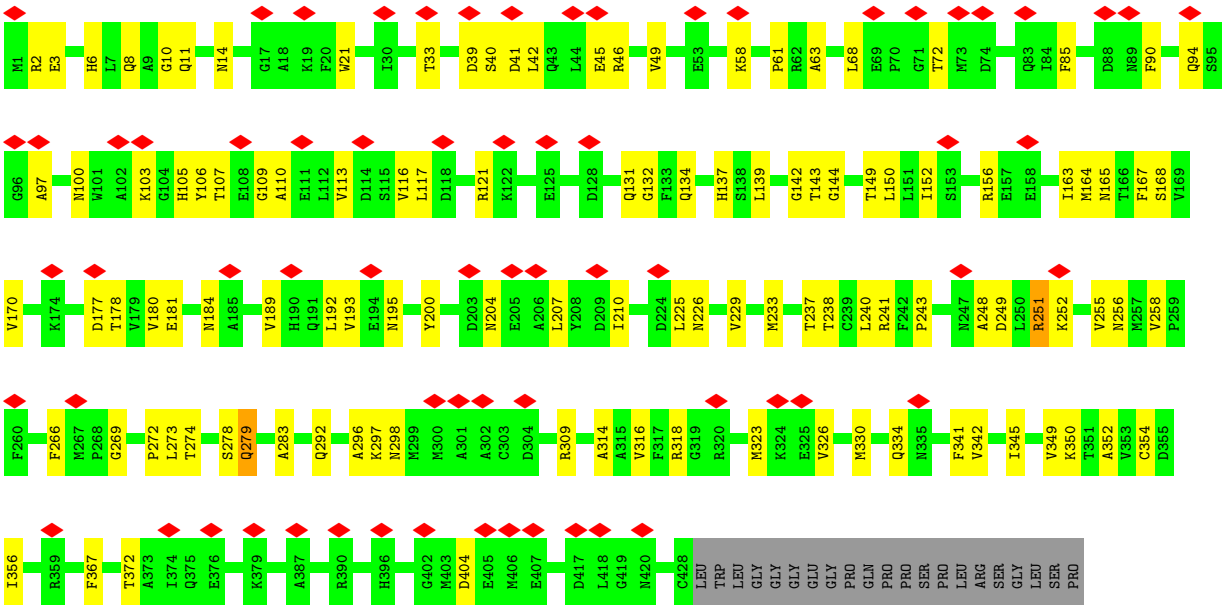
Chain GN:





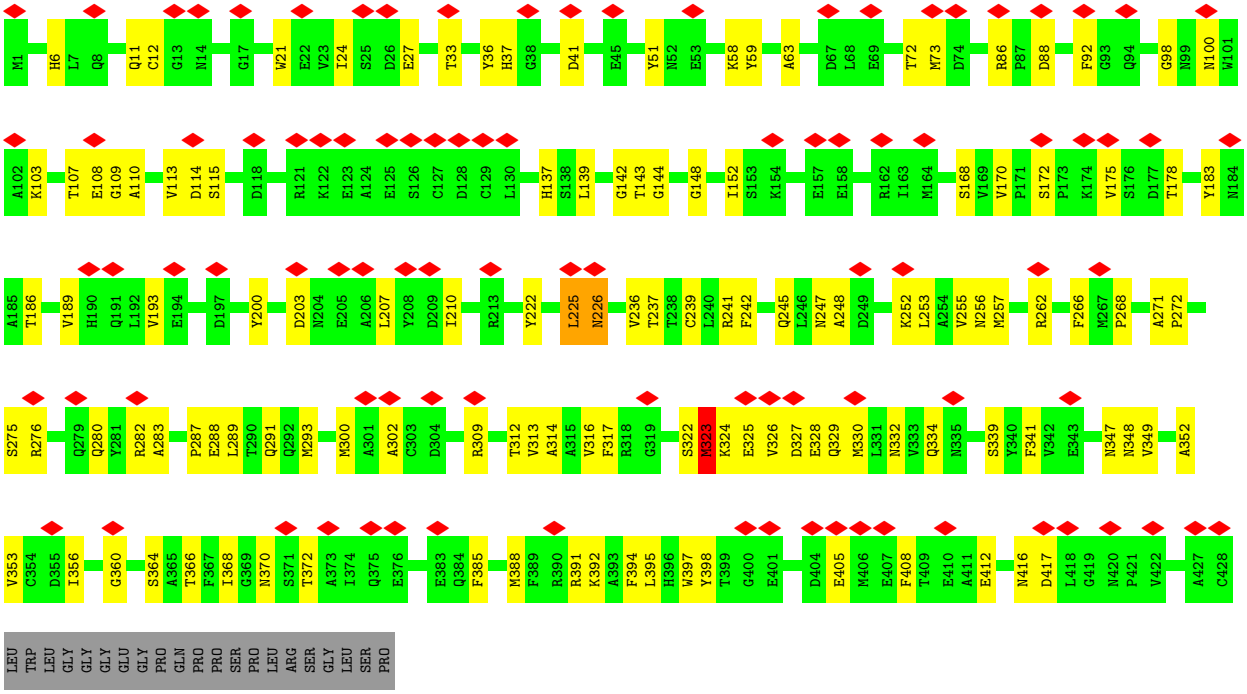

• Molecule 41: Tubulin beta chain

Chain GO:



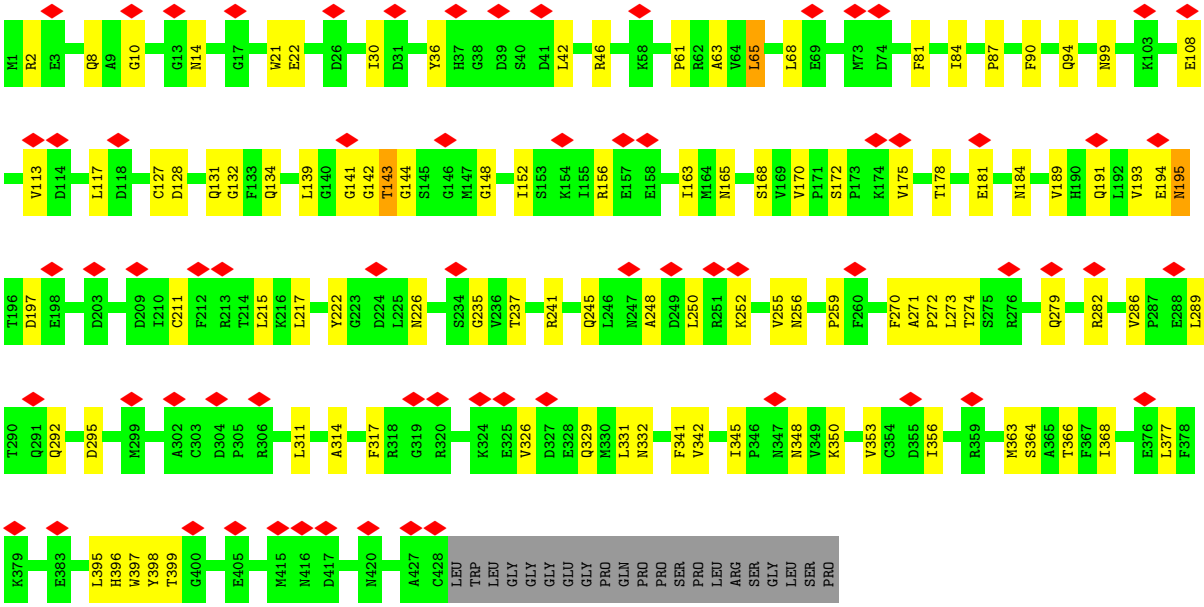

• Molecule 41: Tubulin beta chain

Chain GP:



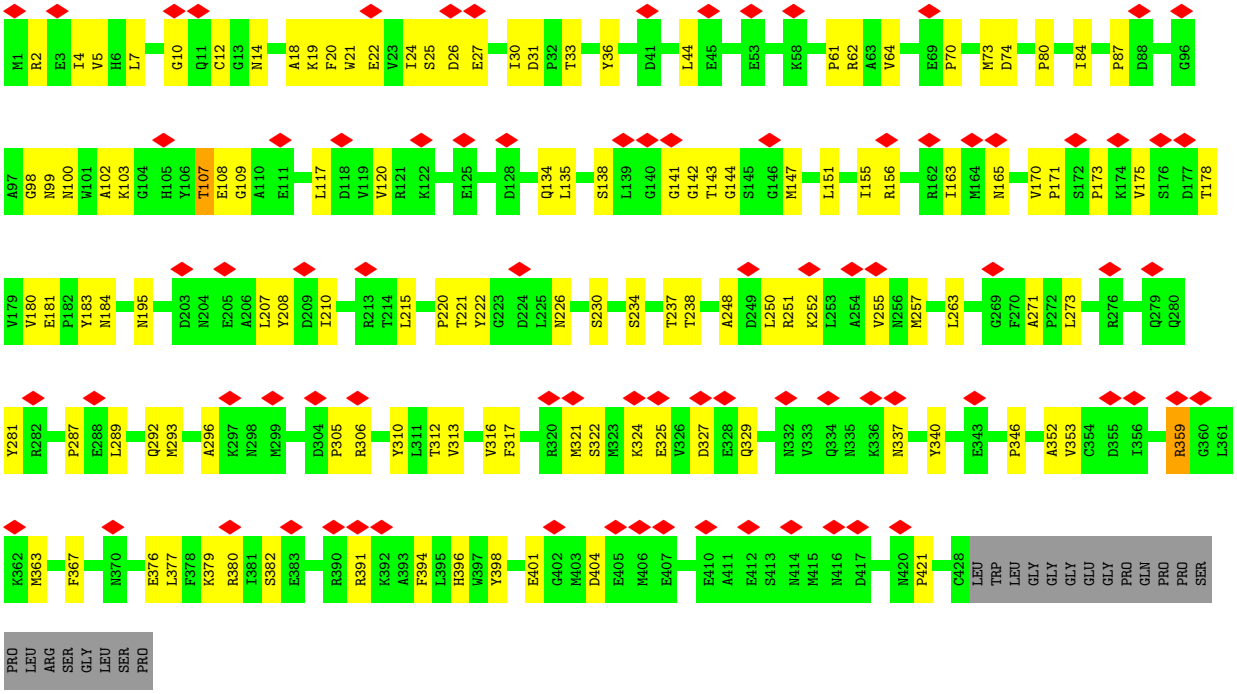
• Molecule 41: Tubulin beta chain

Chain HB:



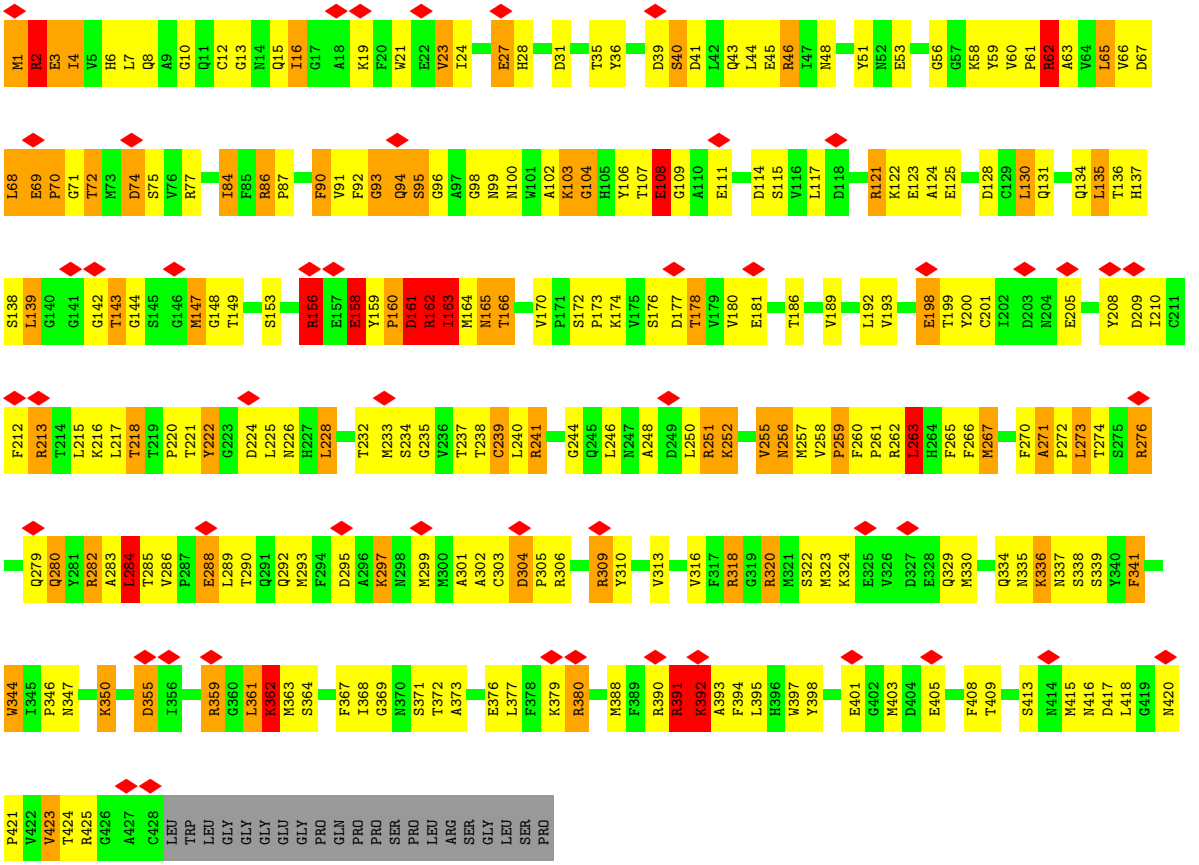

• Molecule 41: Tubulin beta chain

Chain HM:



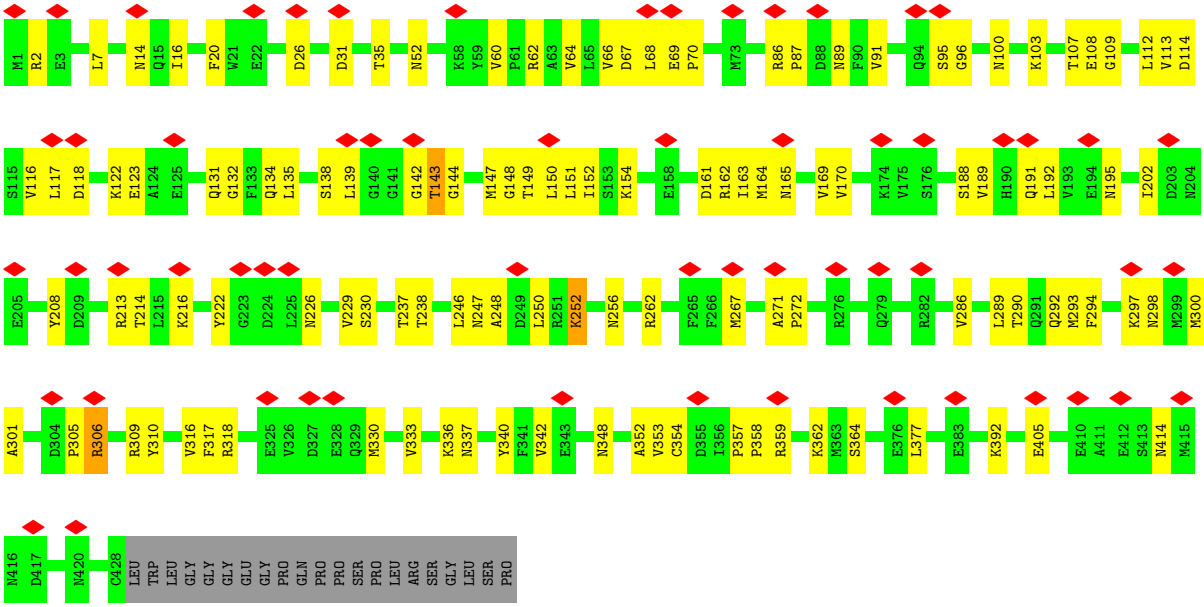

• Molecule 41: Tubulin beta chain

Chain HN:



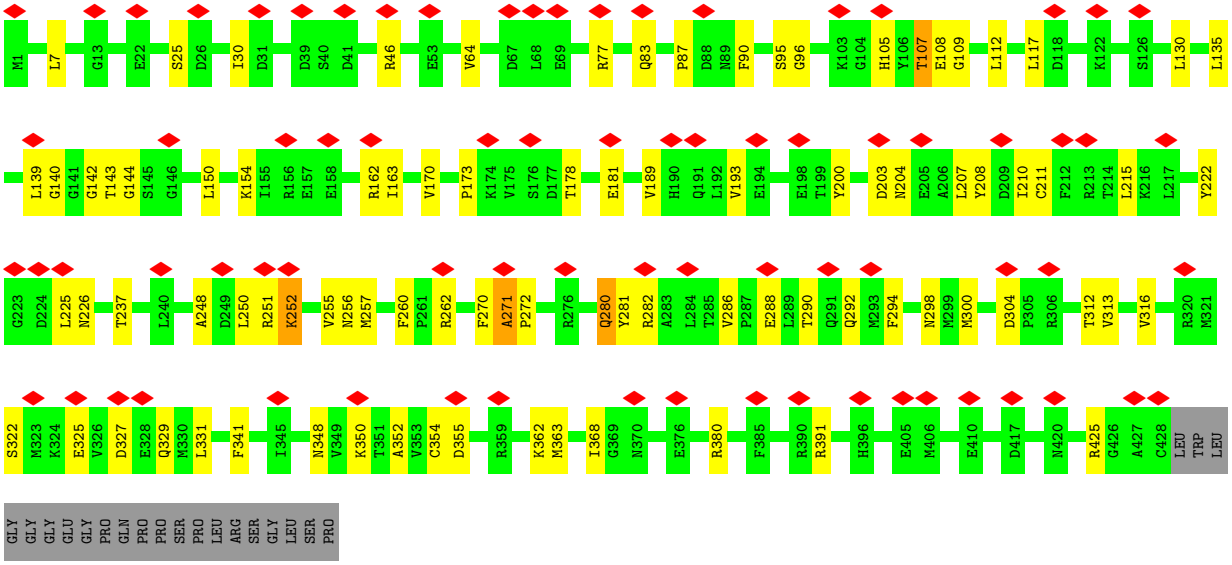

- Molecule 41: Tubulin beta chain

Chain HO:



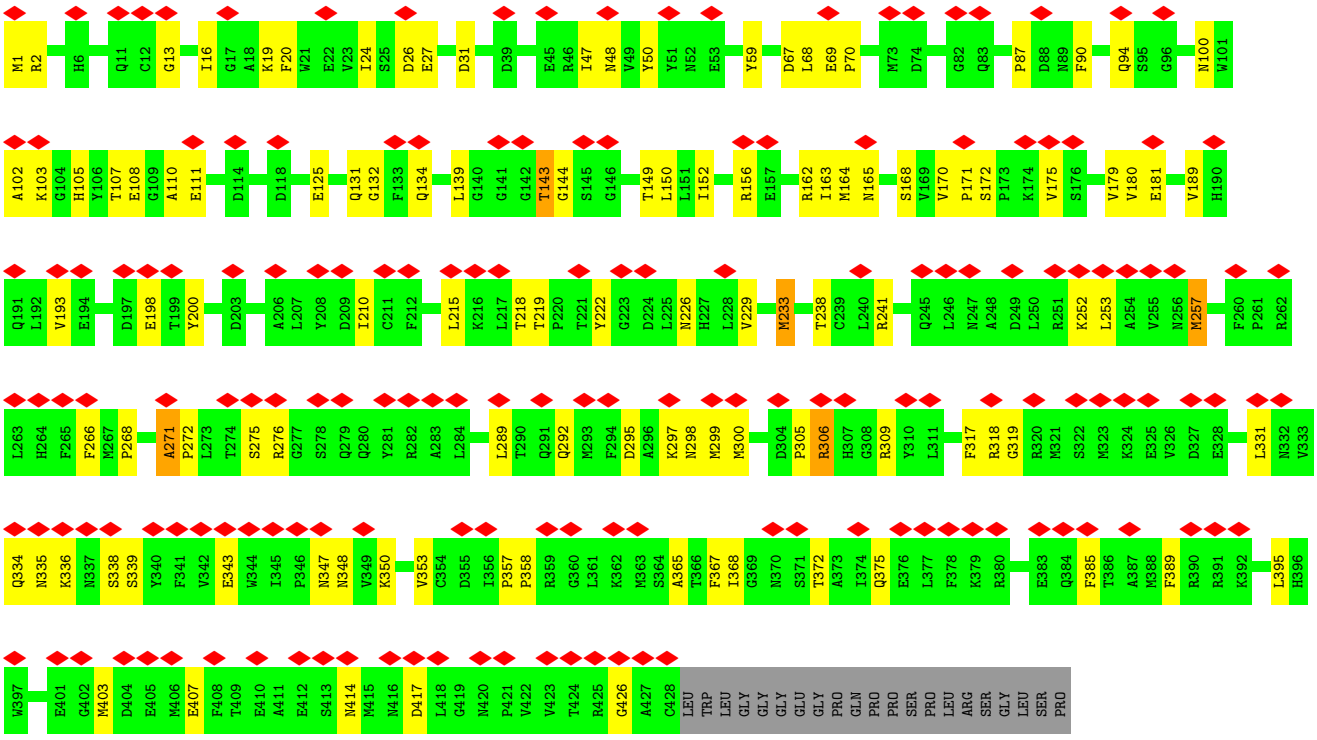

- Molecule 41: Tubulin beta chain

Chain HP:



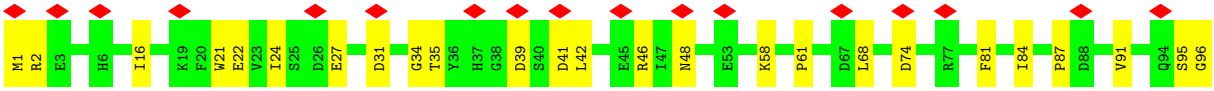

- Molecule 41: Tubulin beta chain

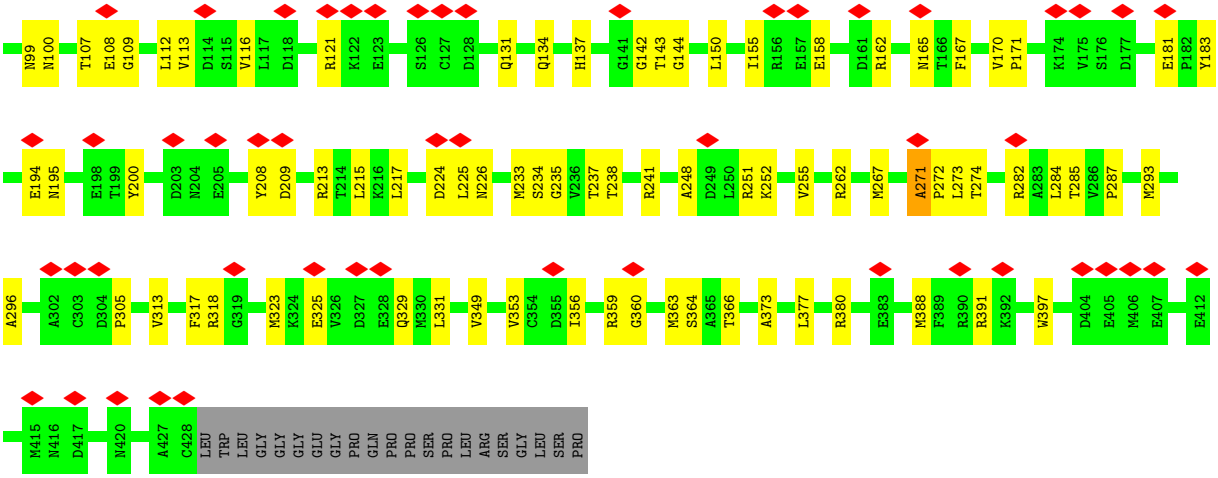
Chain HQ:




- Molecule 41: Tubulin beta chain

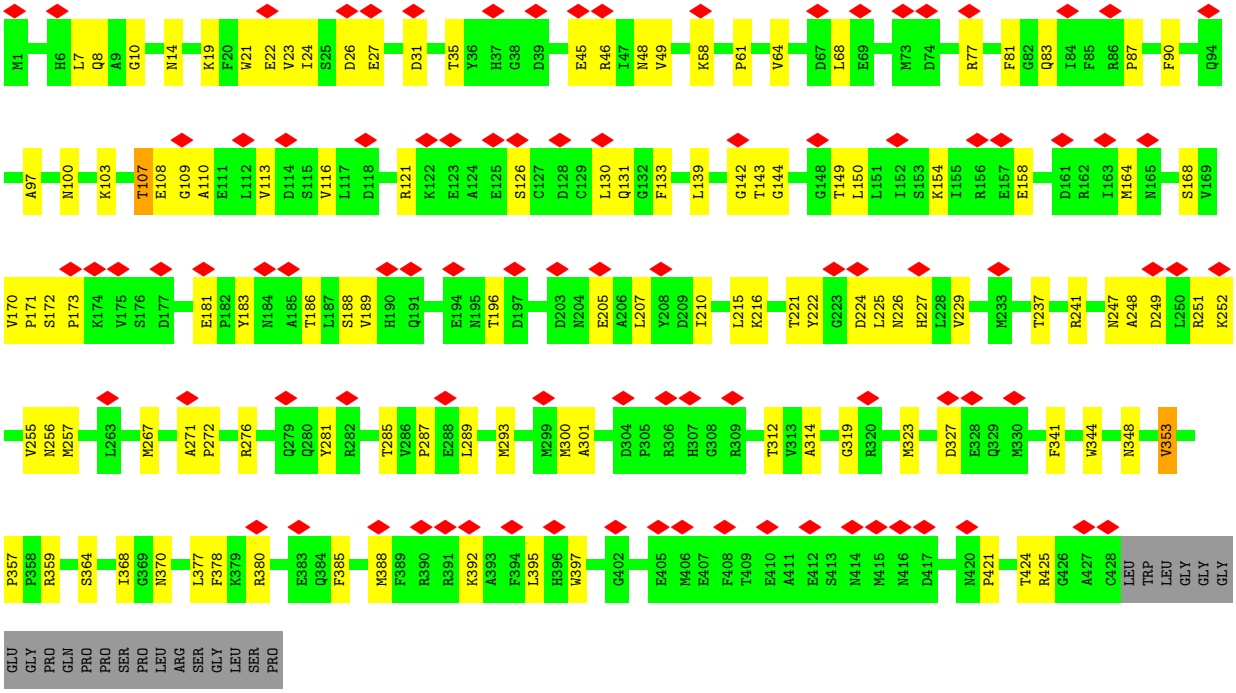
Chain IB:





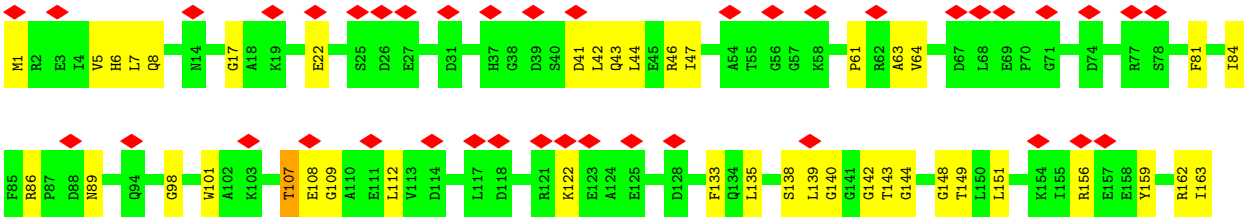

- Molecule 41: Tubulin beta chain

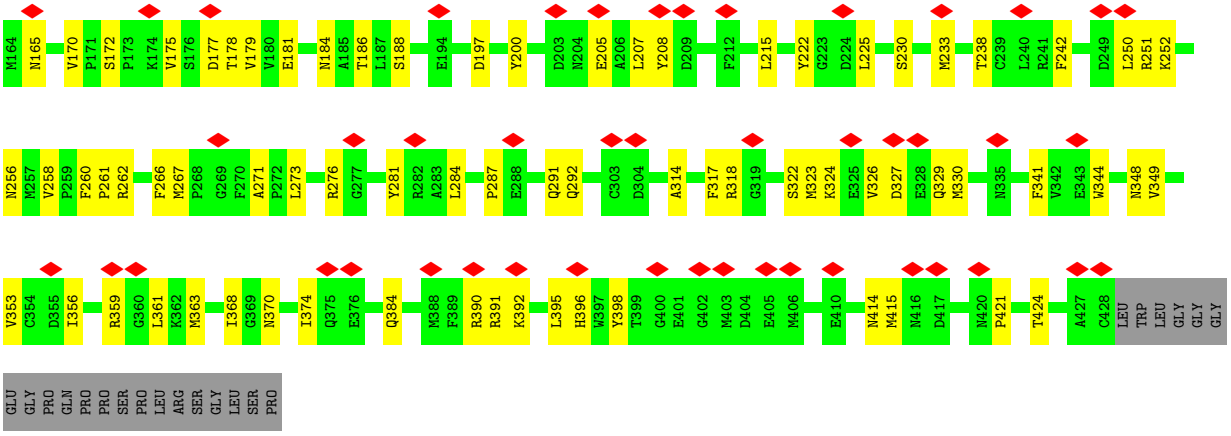
Chain IM:




- Molecule 41: Tubulin beta chain

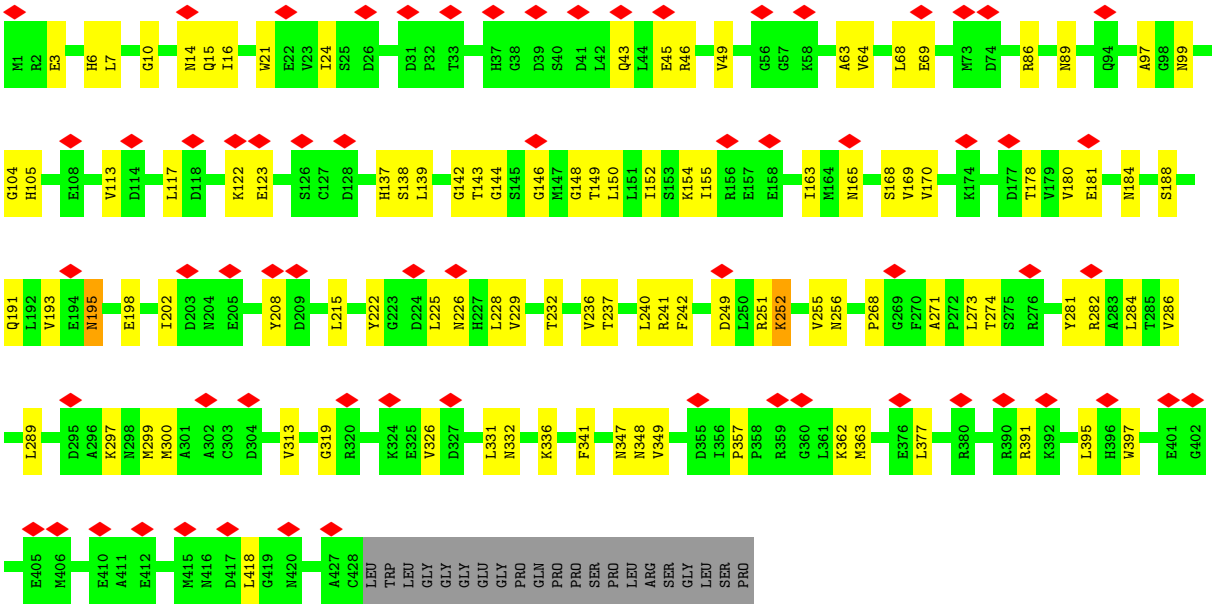
Chain IN:





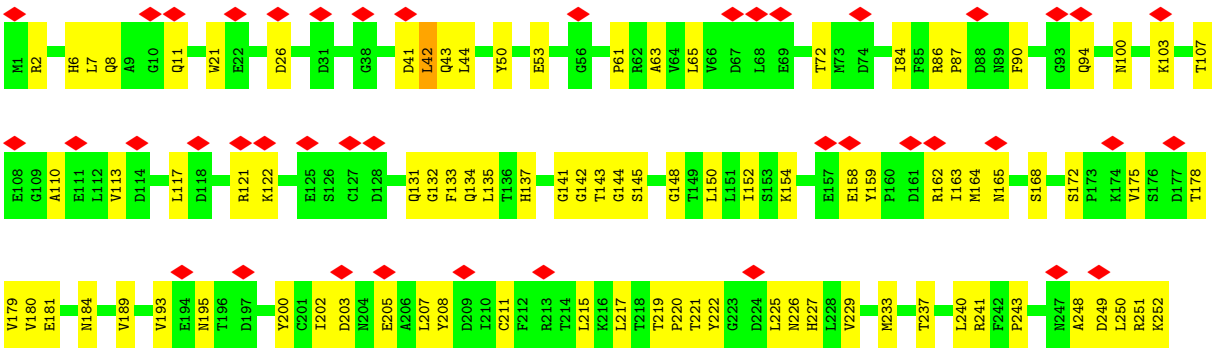

- Molecule 41: Tubulin beta chain

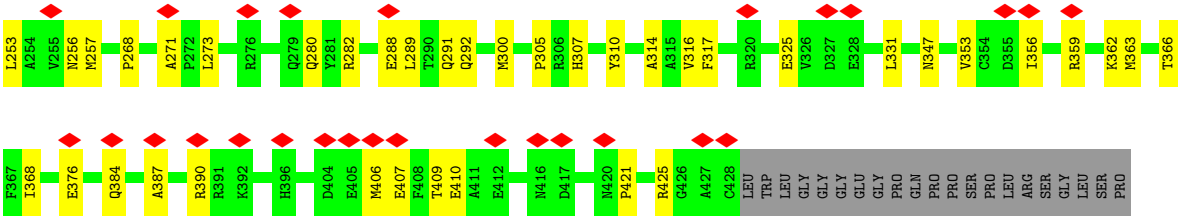
Chain IO:




- Molecule 41: Tubulin beta chain

Chain IP:



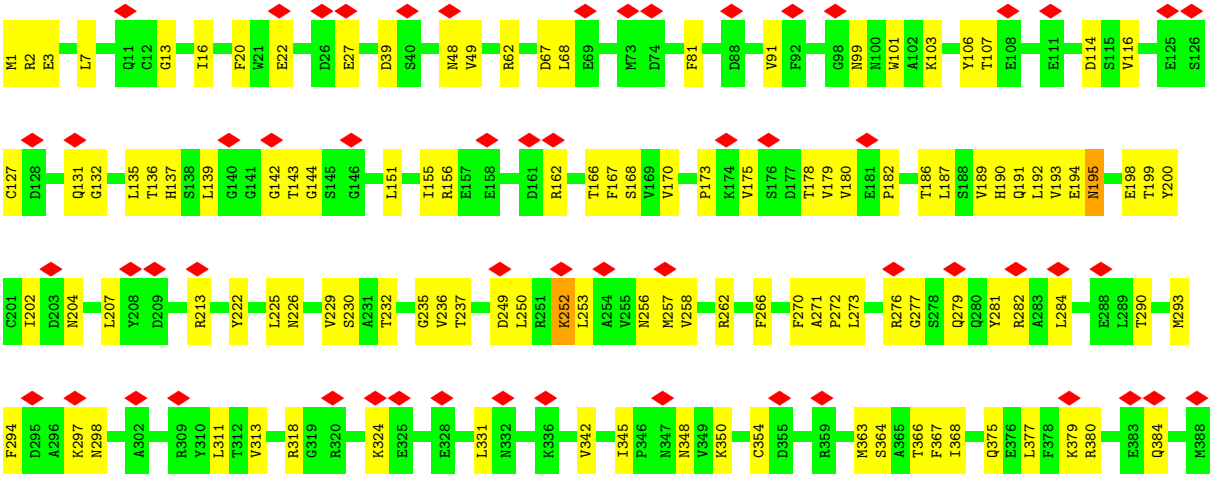


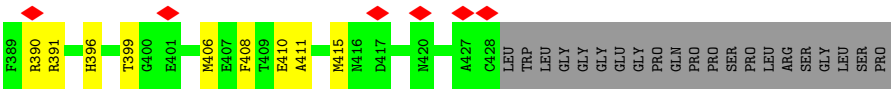

• Molecule 41: Tubulin beta chain

Chain IQ:

• Molecule 41: Tubulin beta chain

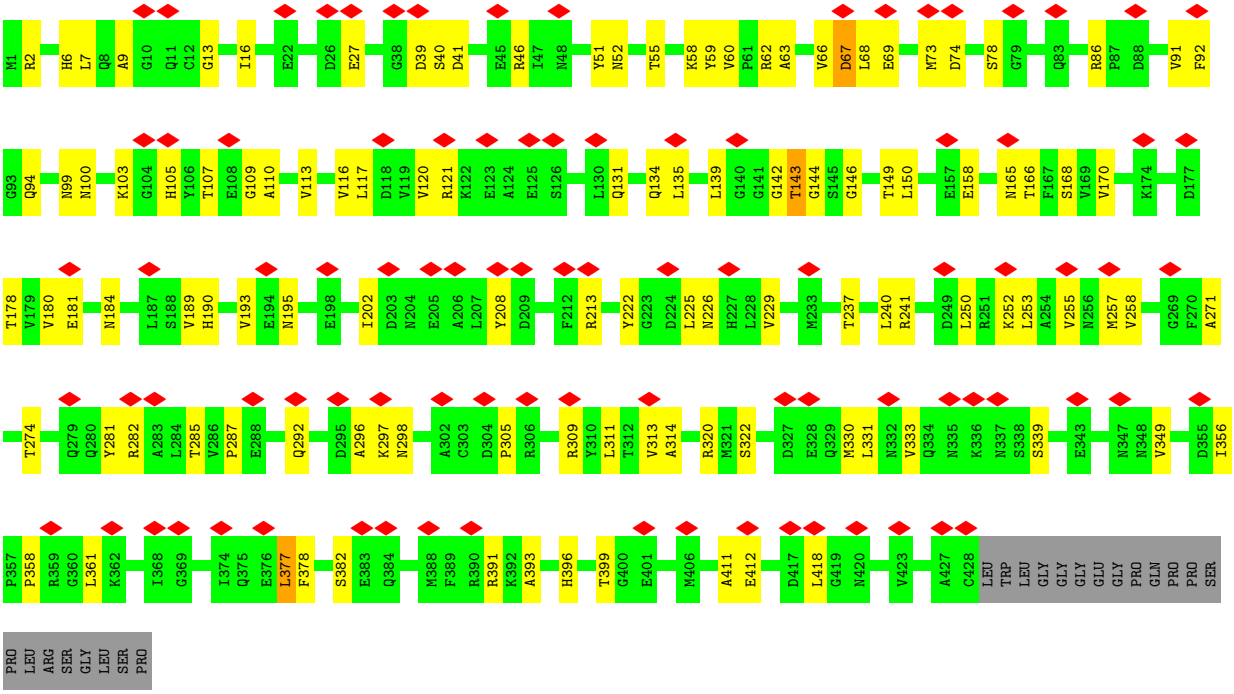
Chain JB:





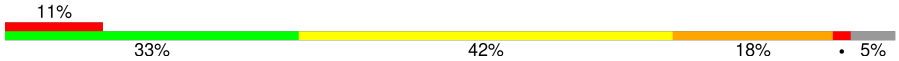

- Molecule 41: Tubulin beta chain

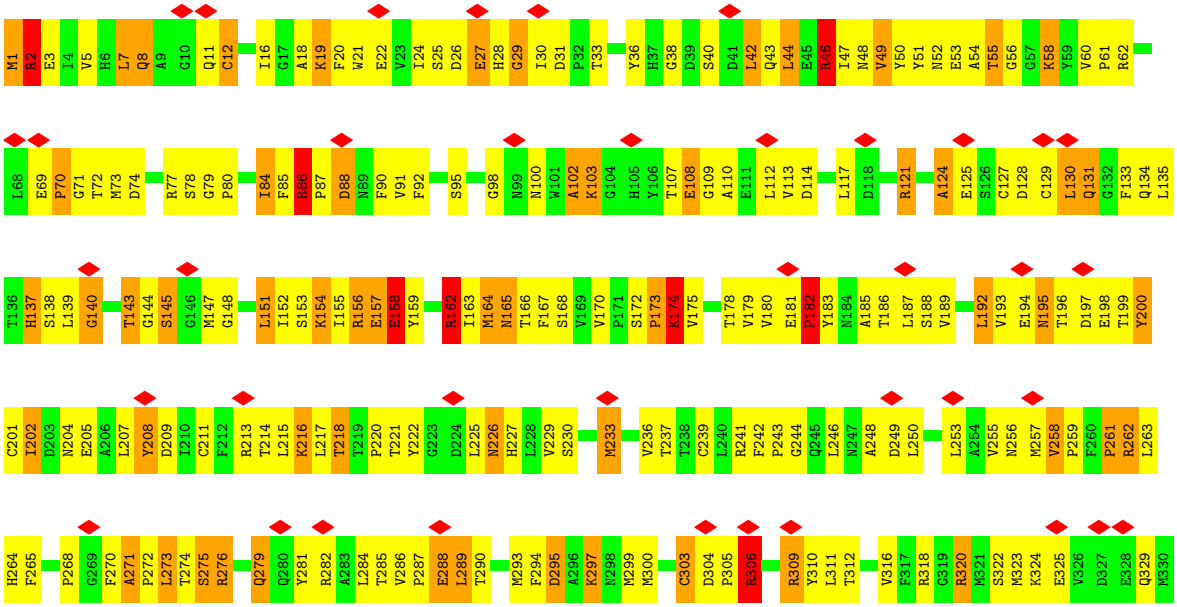
Chain JL:

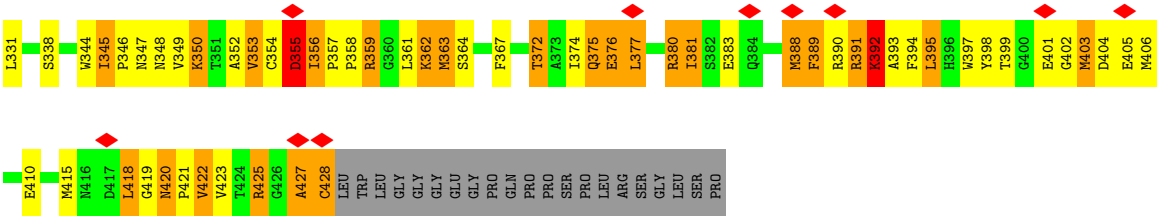



- Molecule 41: Tubulin beta chain

Chain JM:






• Molecule 41: Tubulin beta chain

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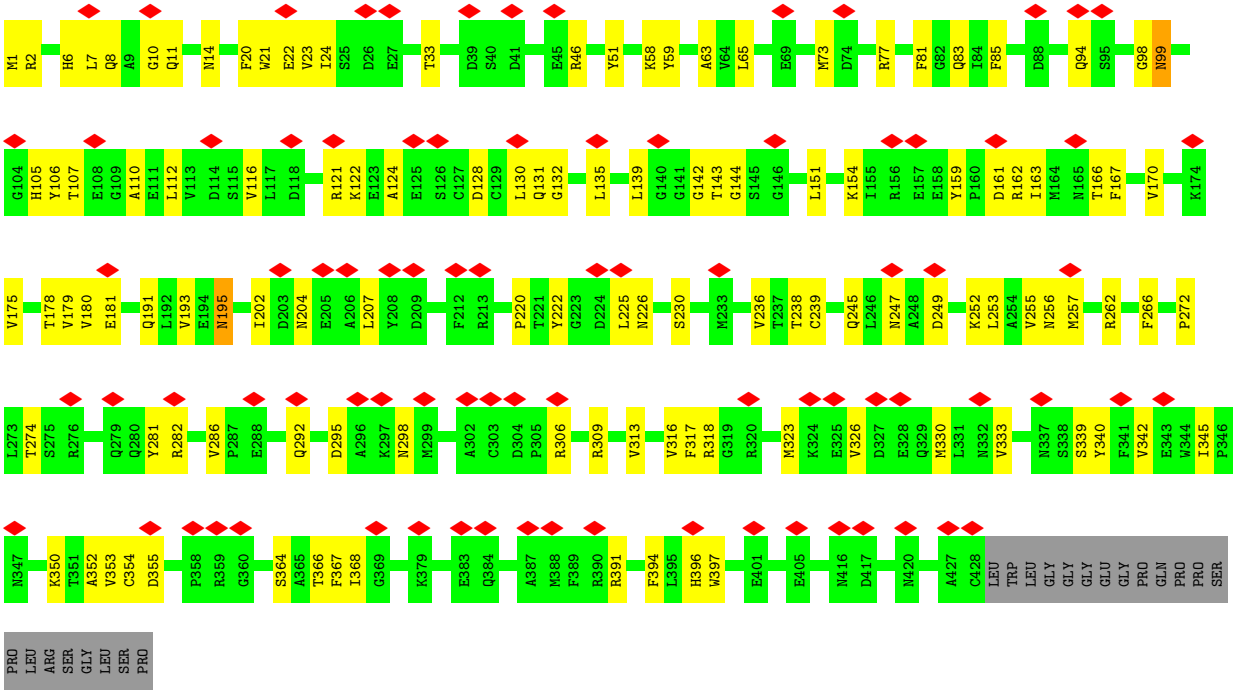
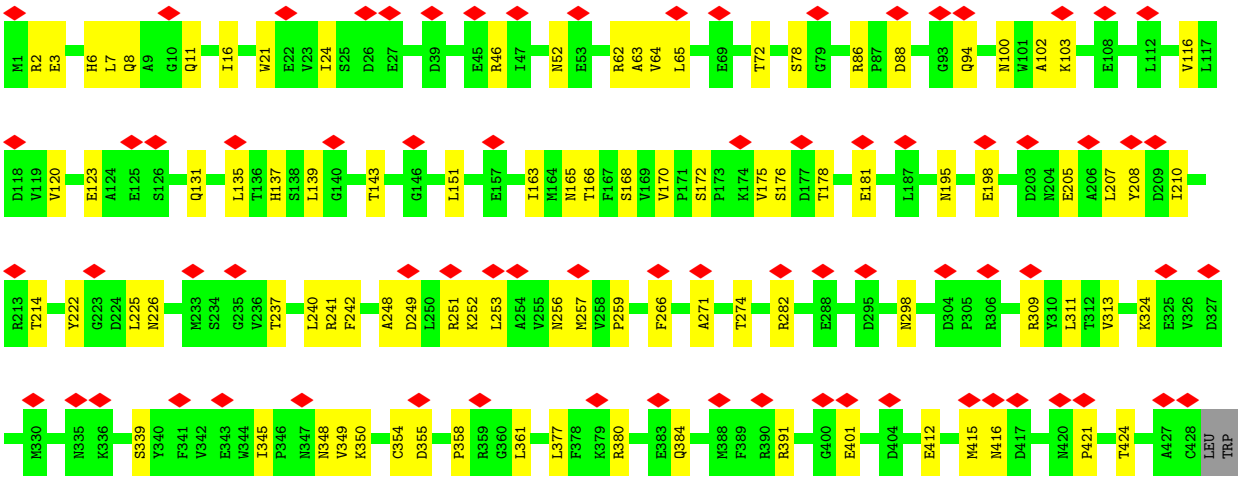


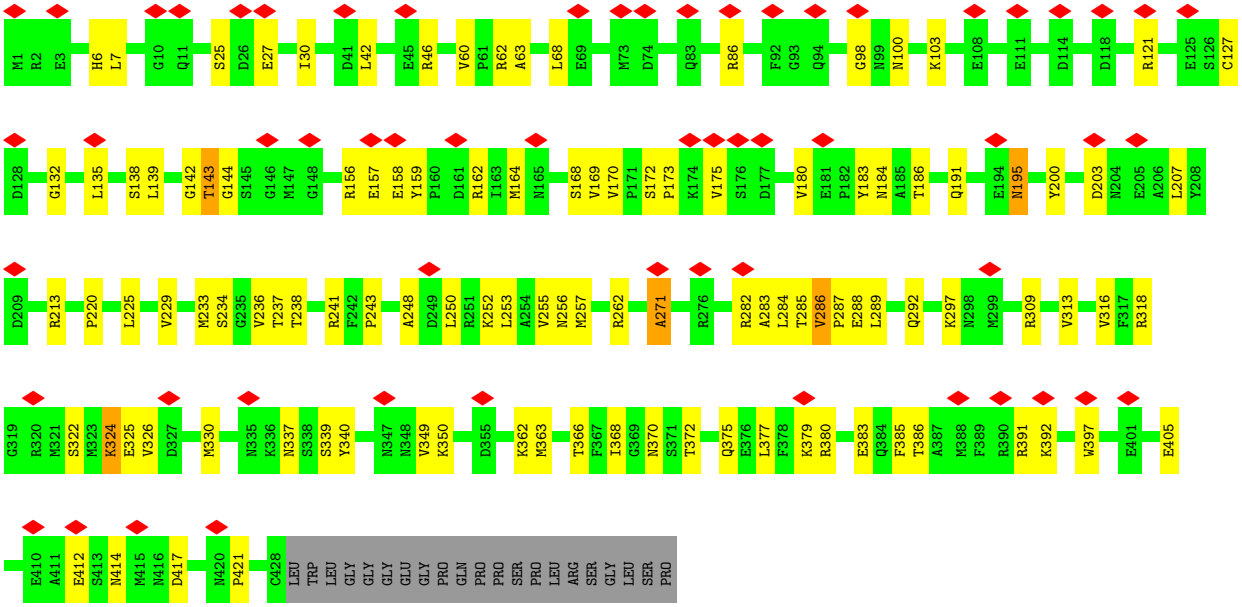

• Molecule 41: Tubulin beta chain

Chain JO:



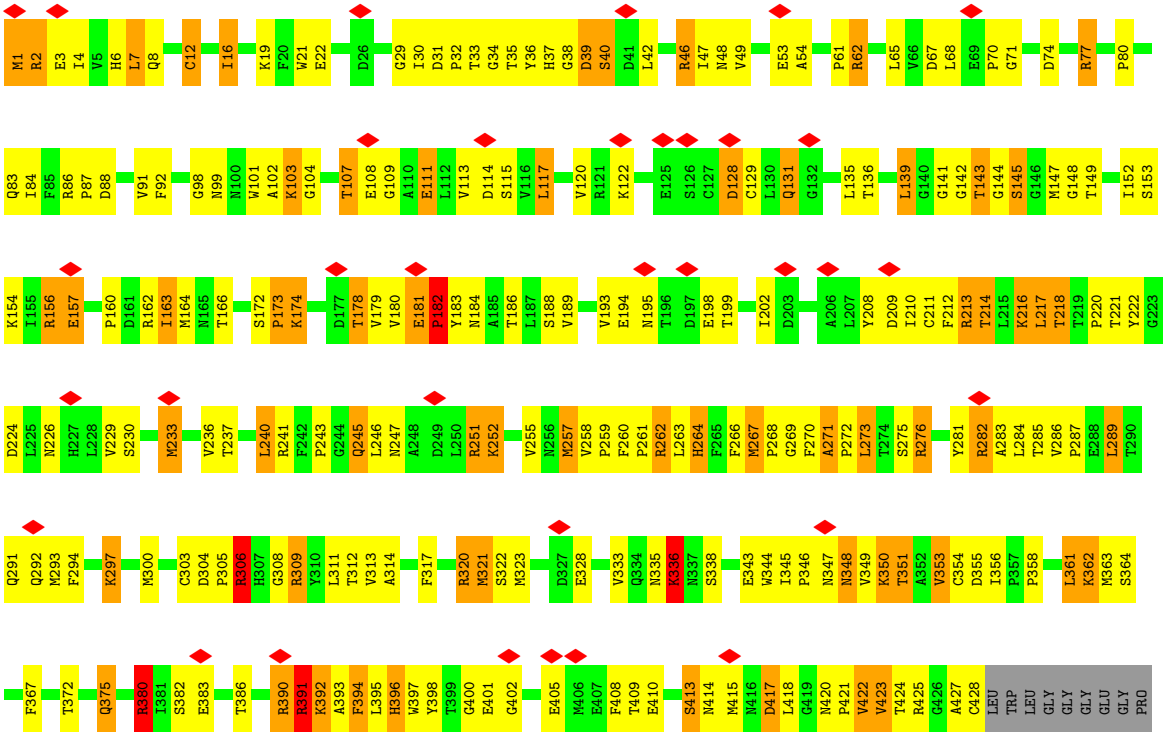
- Molecule 41: Tubulin beta chain

Chain KB:



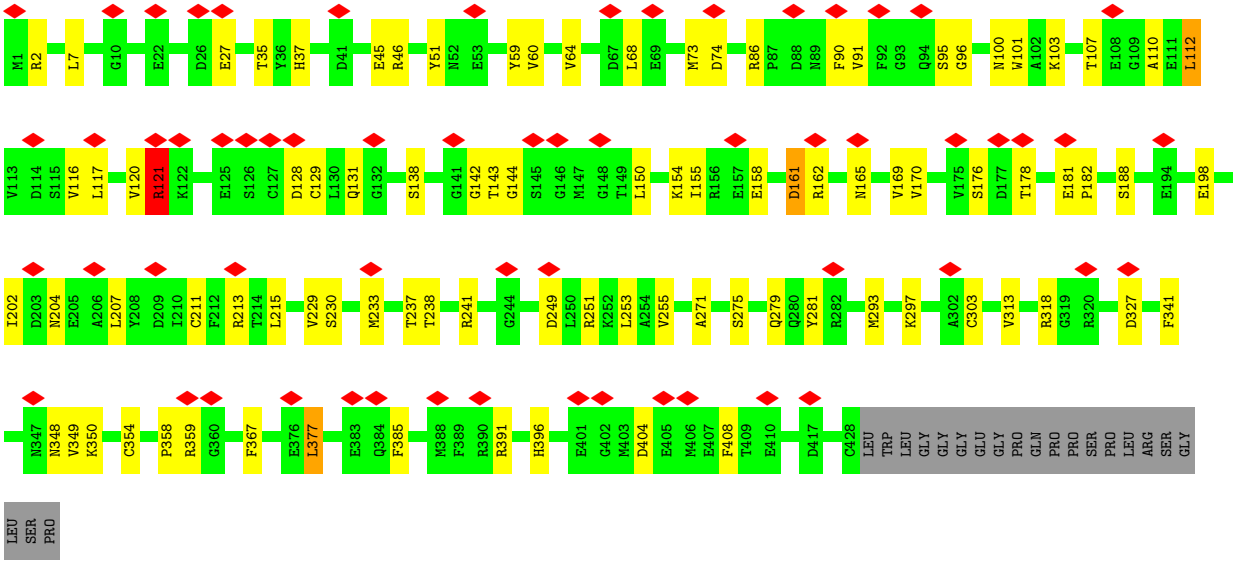

- Molecule 41: Tubulin beta chain

Chain KL:



• Molecule 41: Tubulin beta chain

Chain KM:




• Molecule 41: Tubulin beta chain

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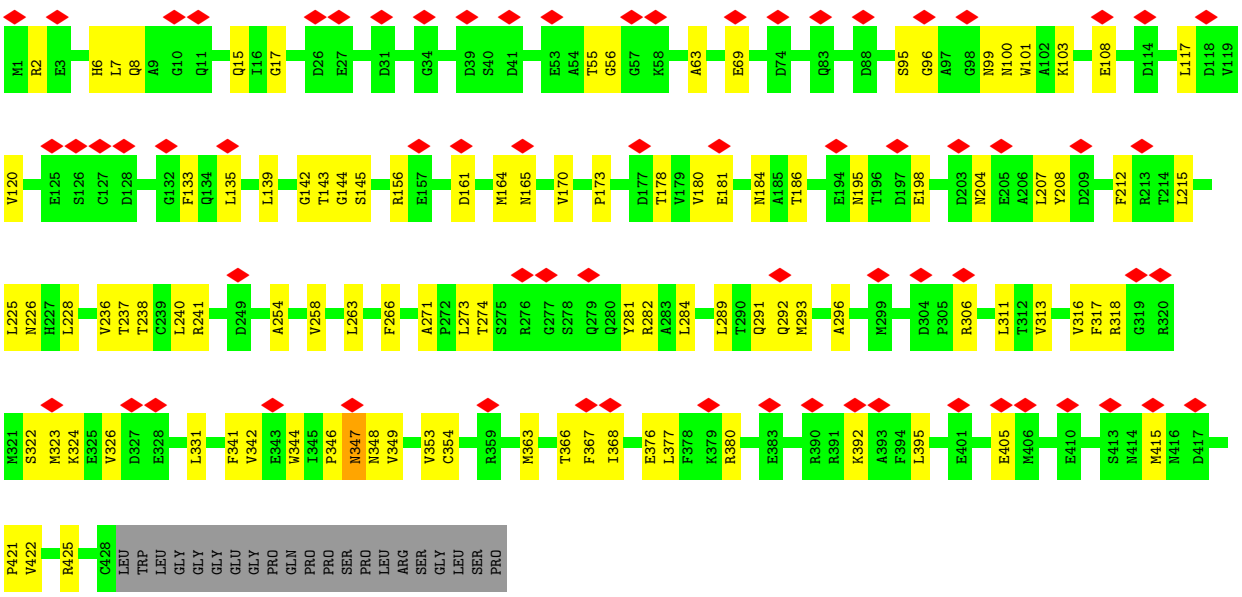
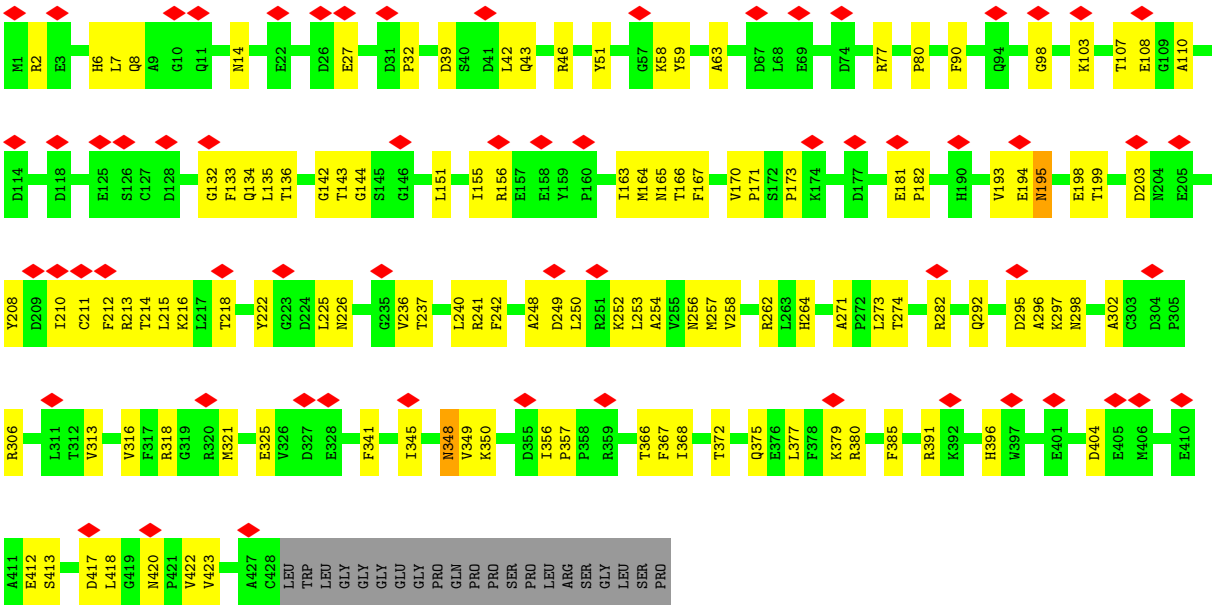


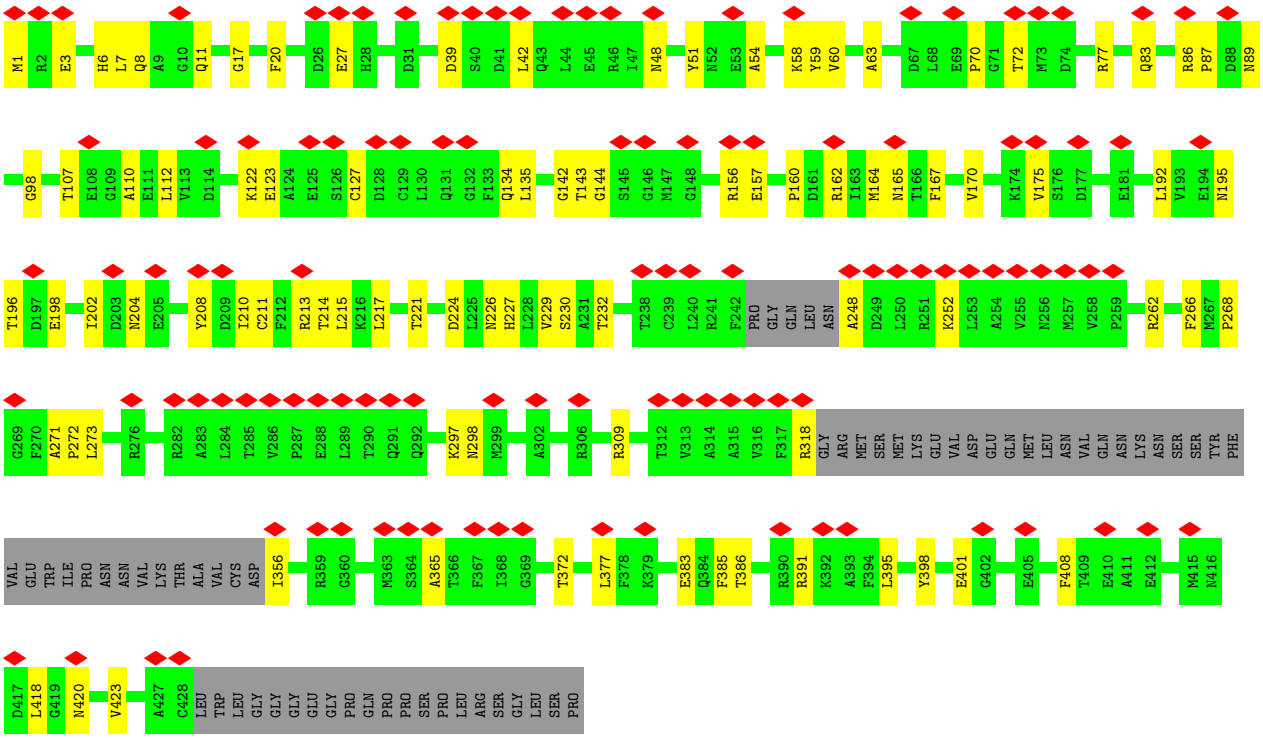

• Molecule 41: Tubulin beta chain

Chain KO:



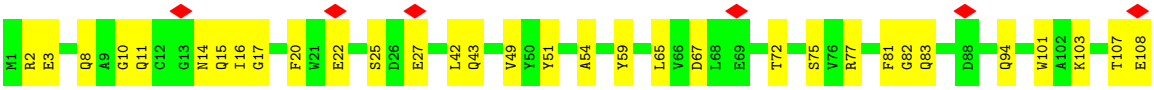

- Molecule 41: Tubulin beta chain

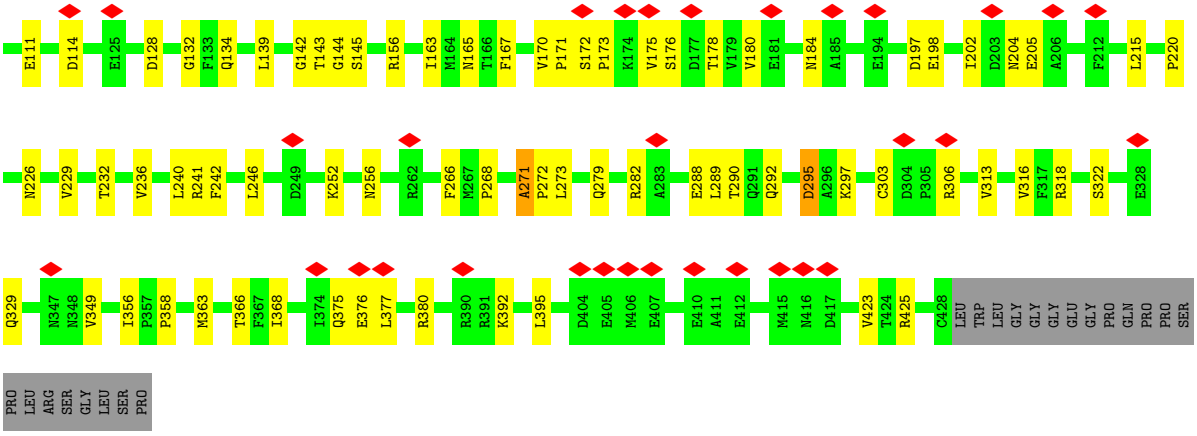
Chain KP:




- Molecule 41: Tubulin beta chain

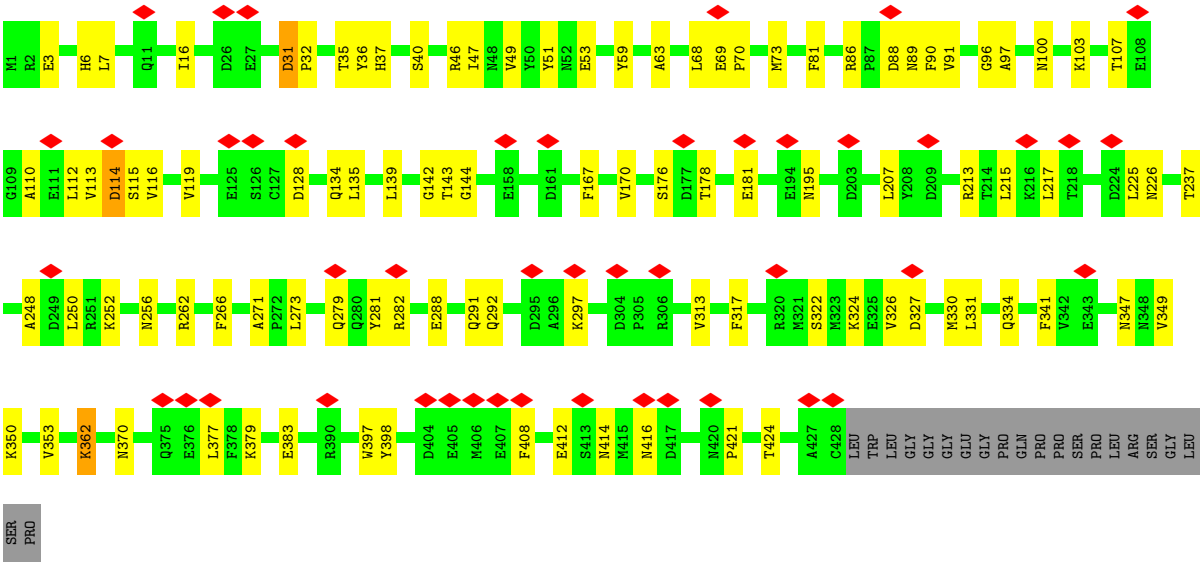
Chain LB:





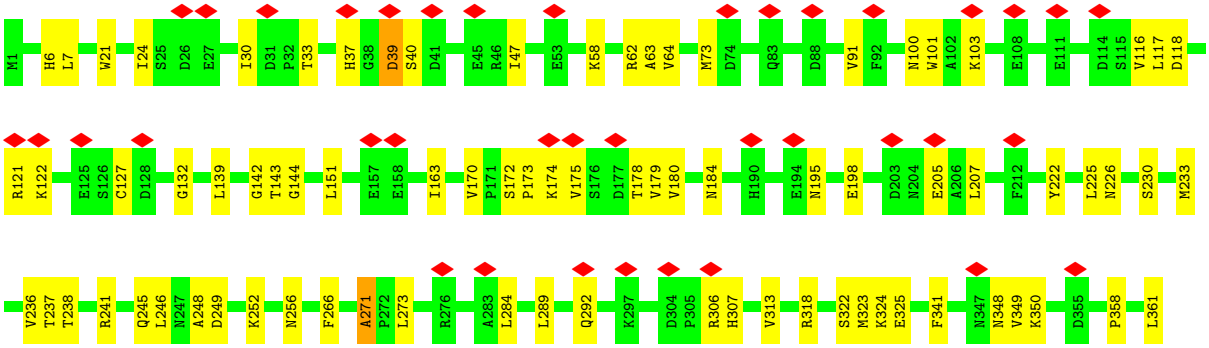

- Molecule 41: Tubulin beta chain

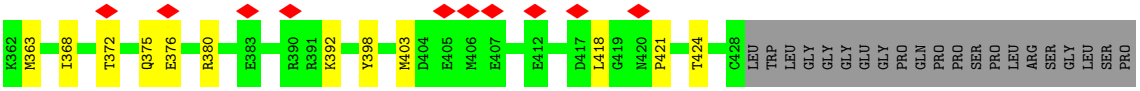
Chain LL:




- Molecule 41: Tubulin beta chain

Chain LM:






- Molecule 41: Tubulin beta chain

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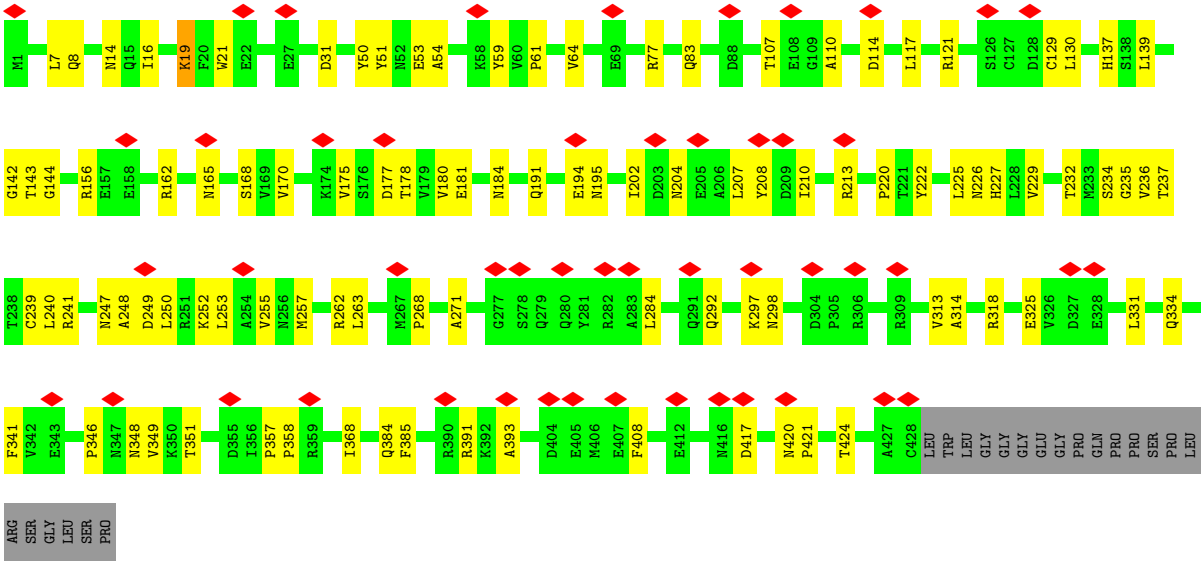


- Molecule 41: Tubulin beta chain

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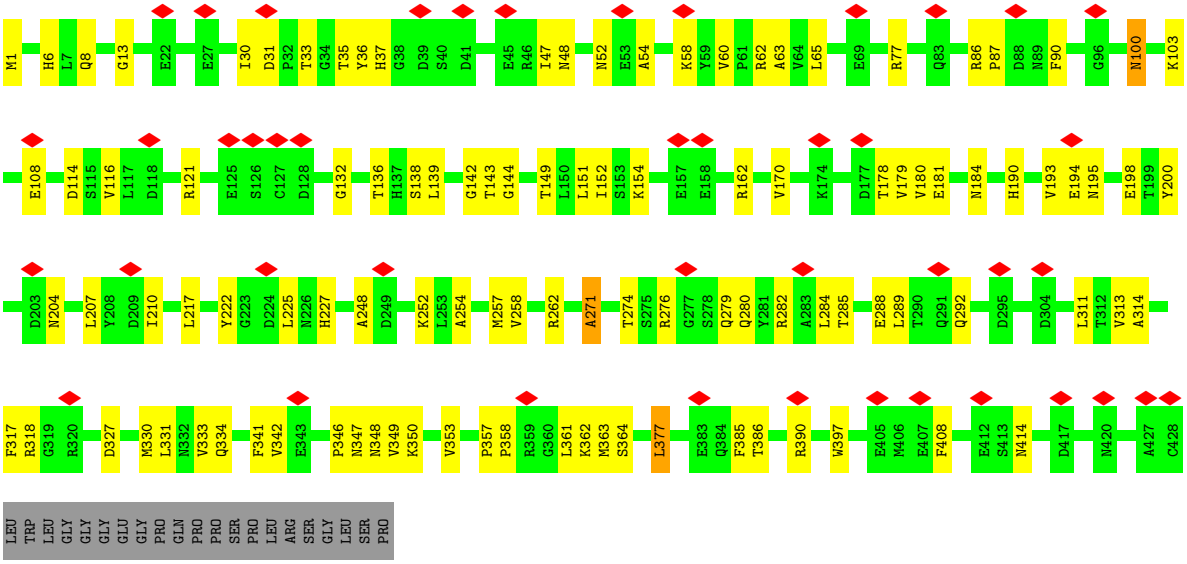


- Molecule 41: Tubulin beta chain

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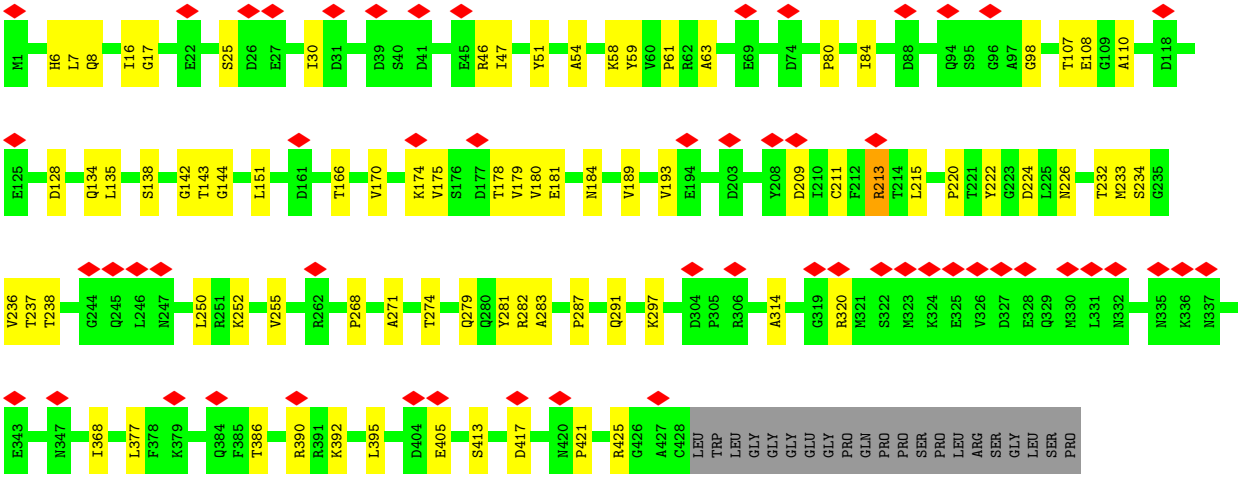
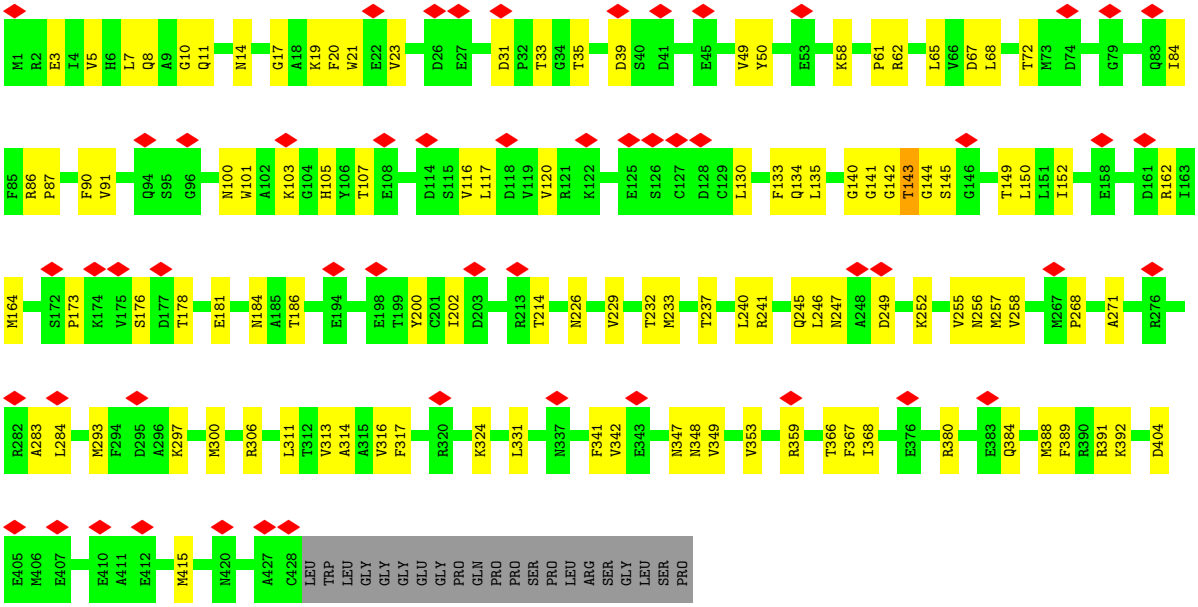


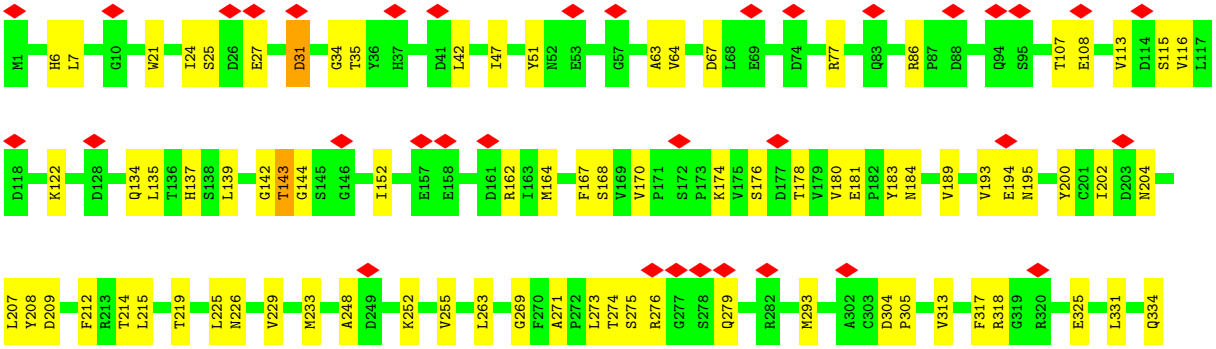

• Molecule 41: Tubulin beta chain

Chain MB:



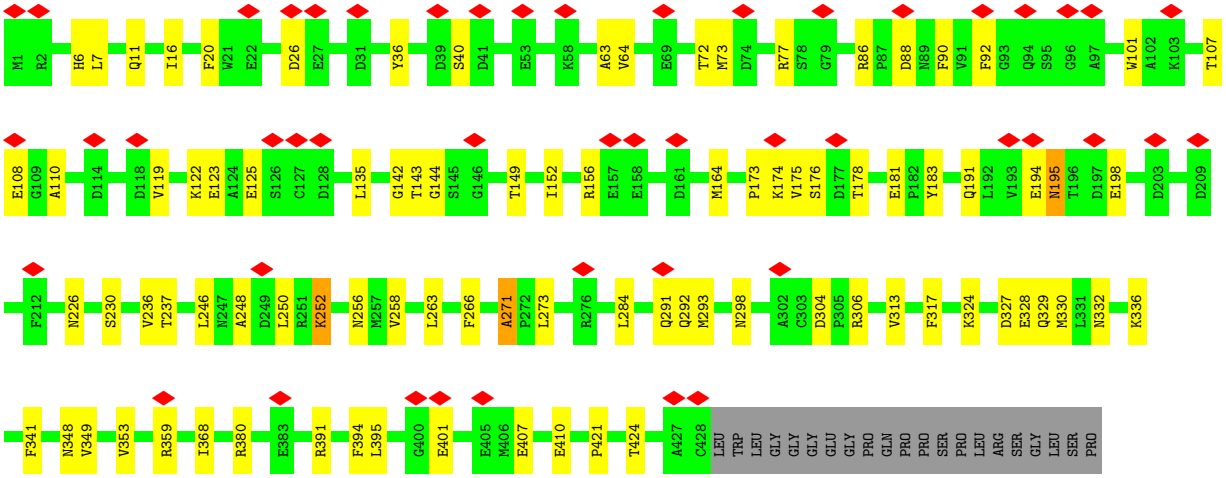

• Molecule 41: Tubulin beta chain

Chain ML:



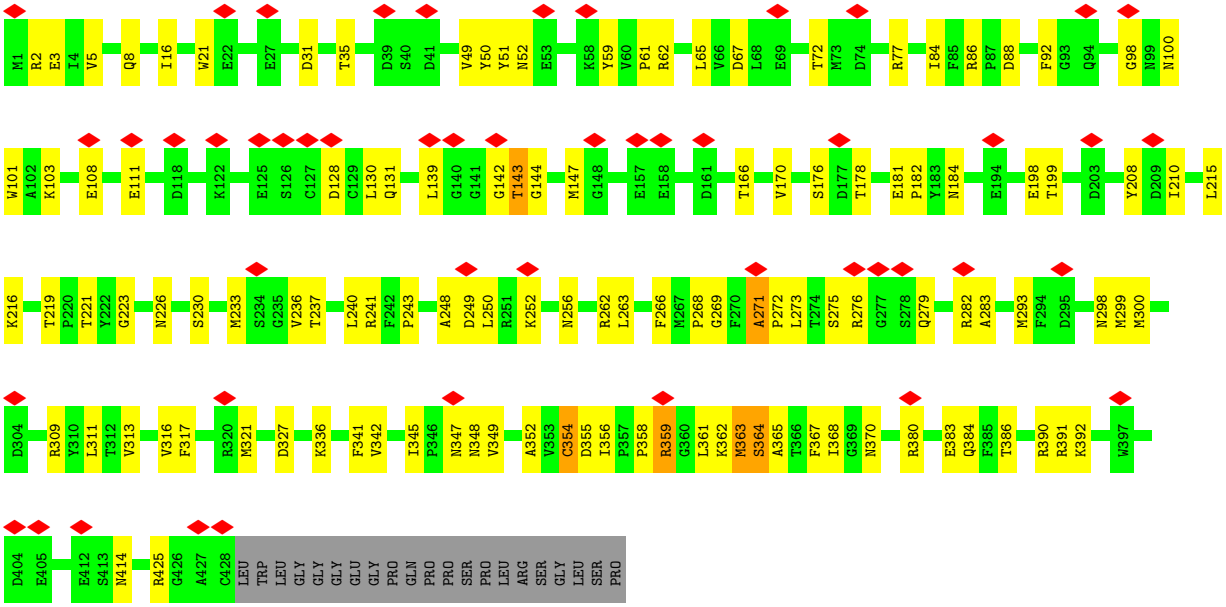
• Molecule 41: Tubulin beta chain

Chain MM:



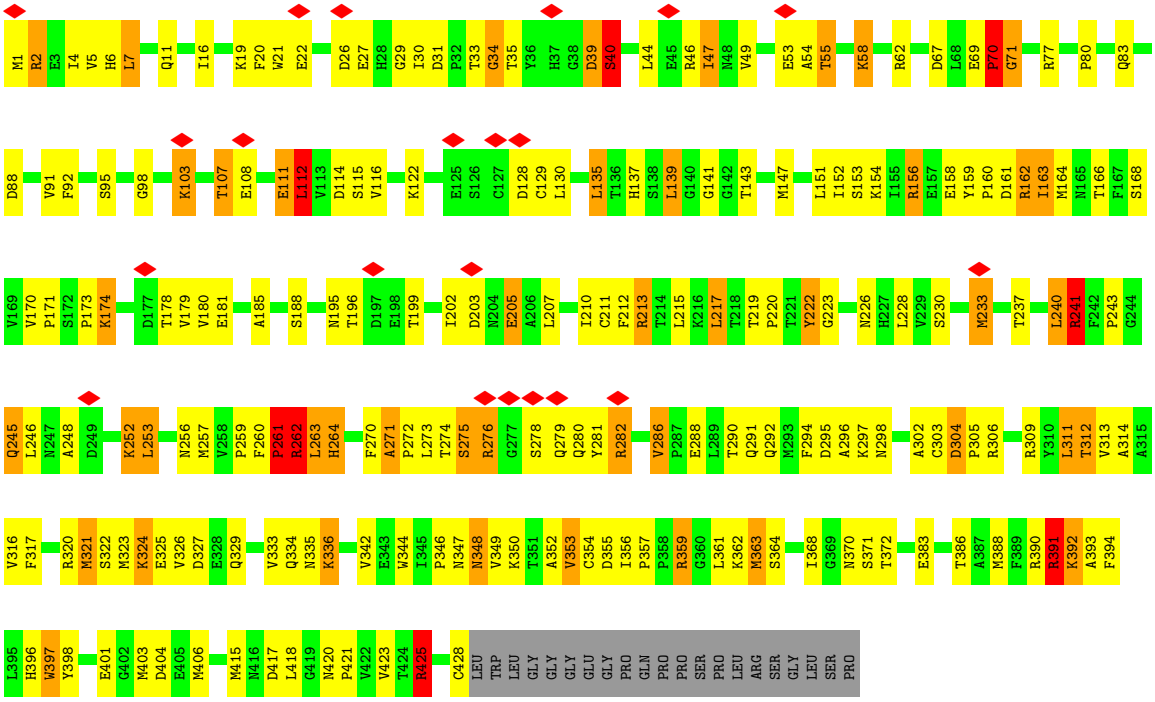

• Molecule 41: Tubulin beta chain

Chain MN:




• Molecule 41: Tubulin beta chain

Chain MO:




• Molecule 41: Tubulin beta chain

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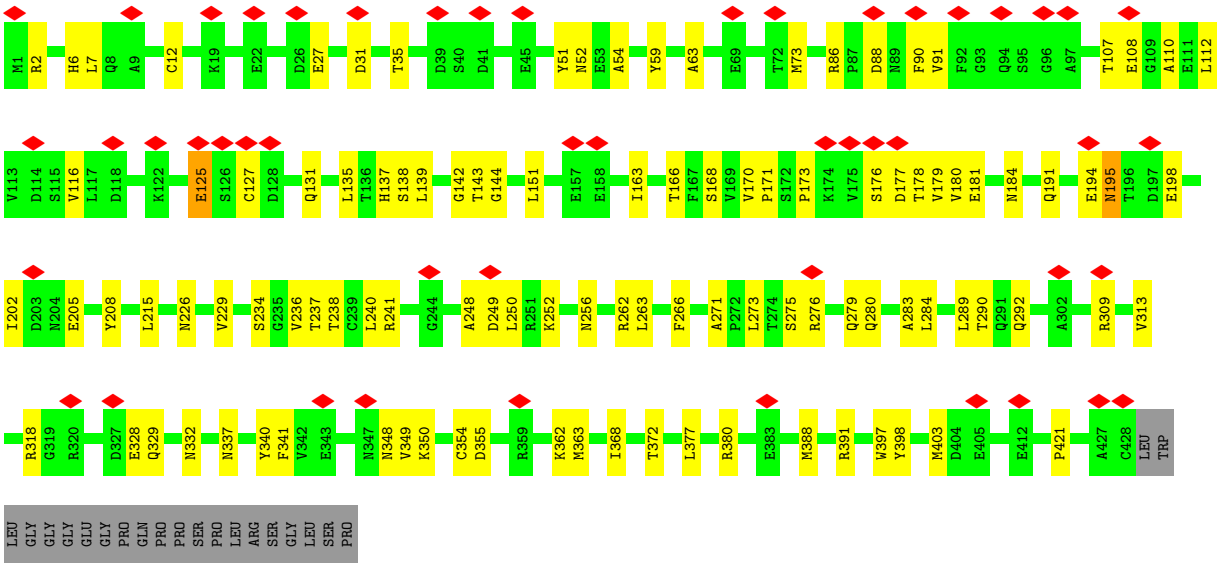
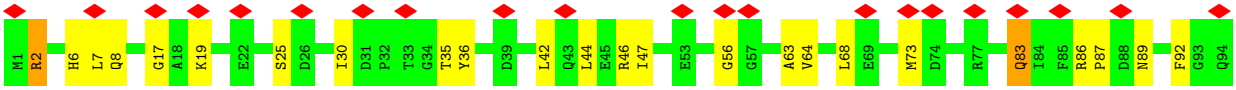
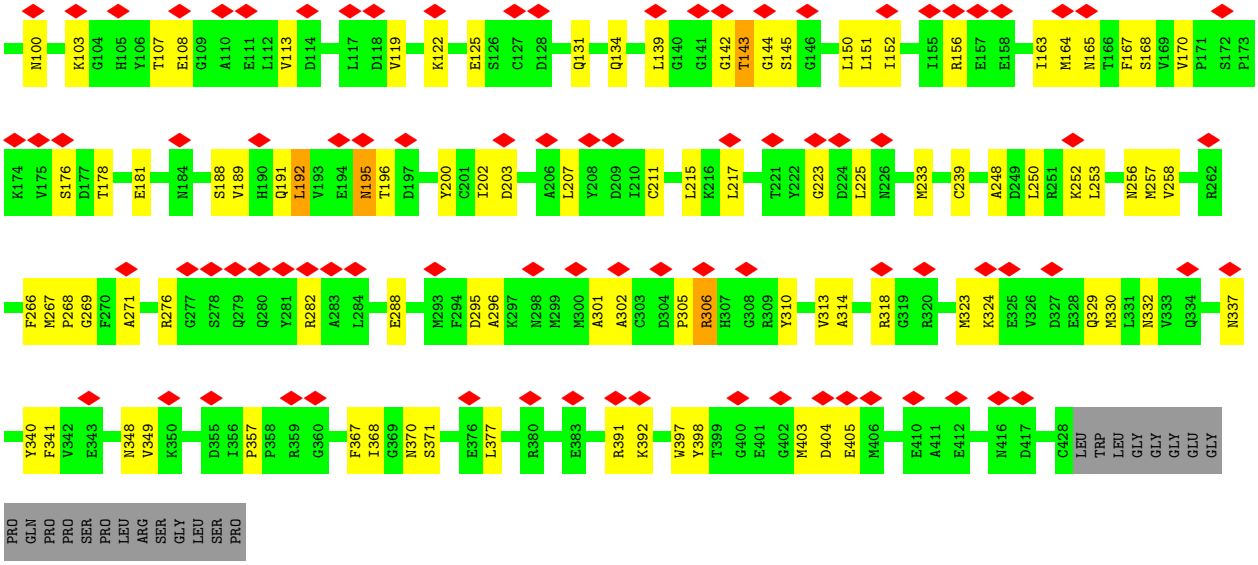



• Molecule 41: Tubulin beta chain

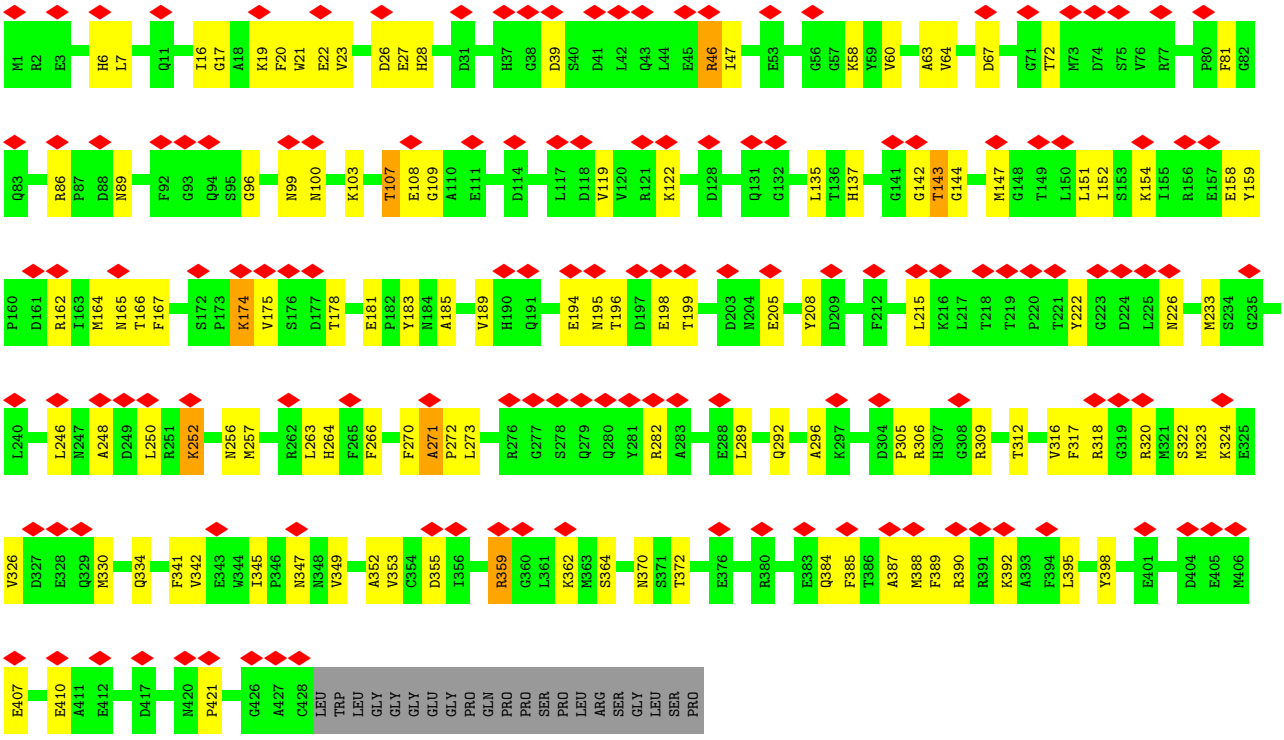
Chain NB:





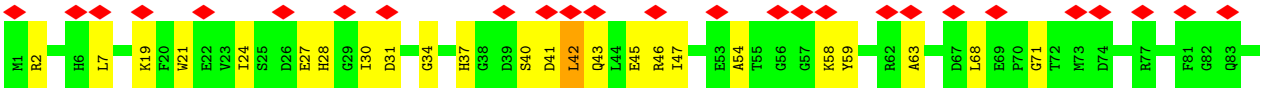

- Molecule 41: Tubulin beta chain

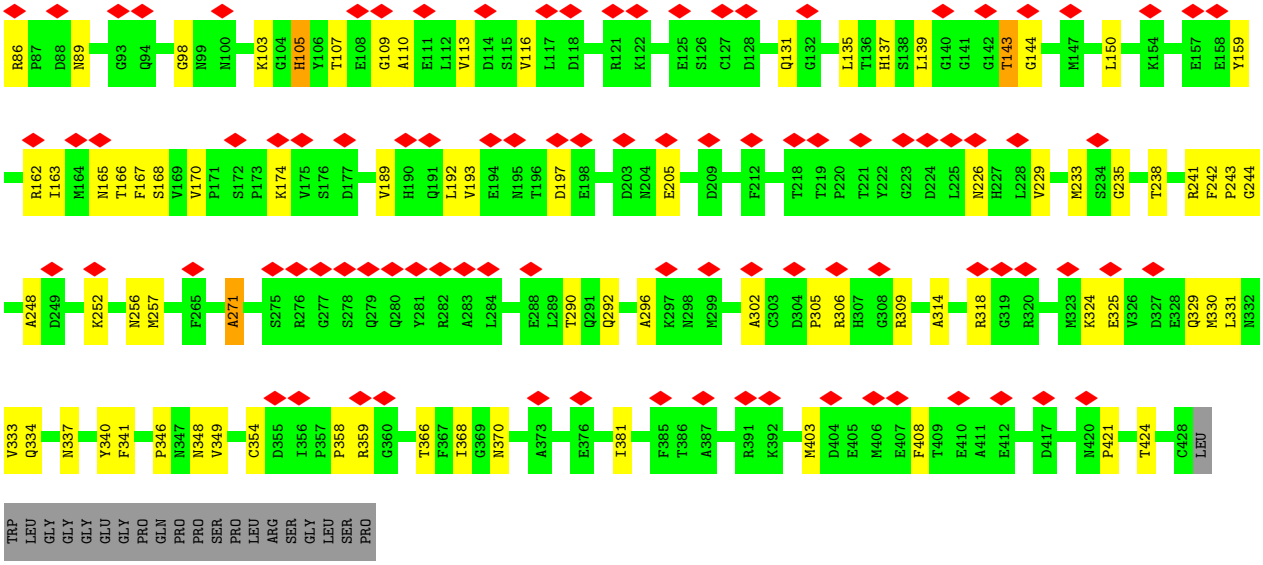
Chain NL:




- Molecule 41: Tubulin beta chain

Chain NM:






- Molecule 41: Tubulin beta chain

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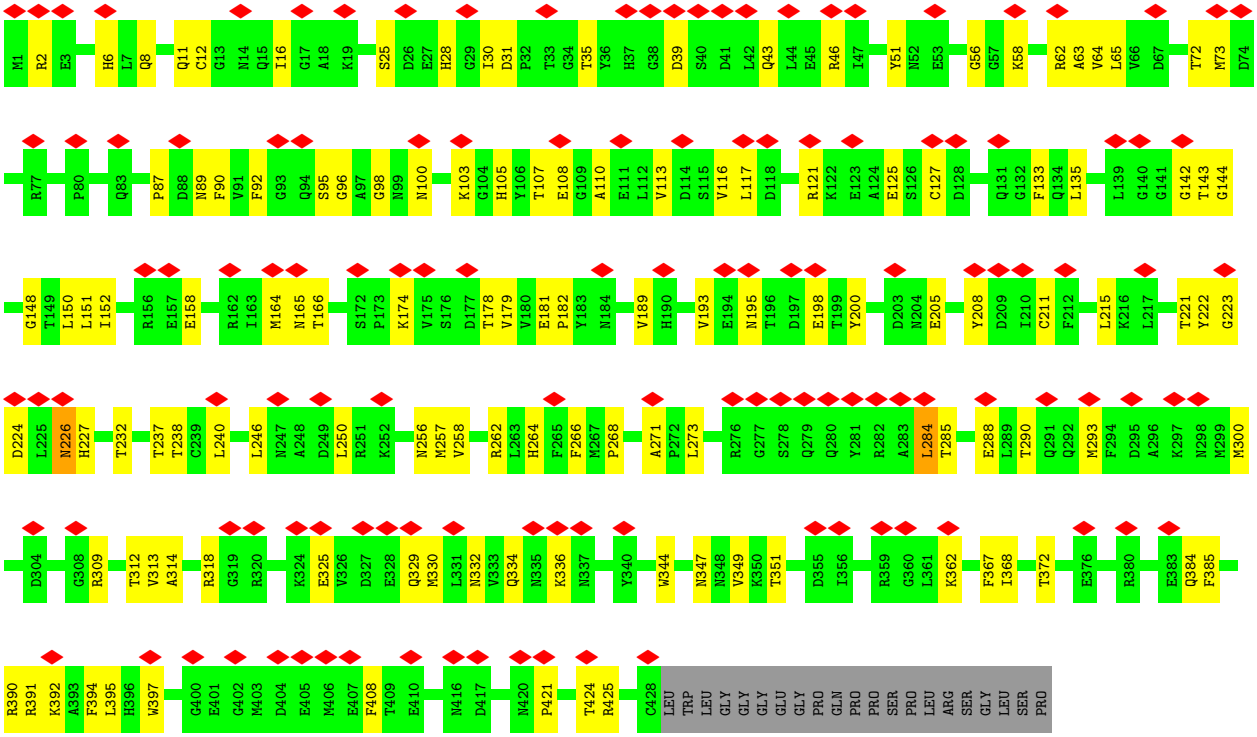


- Molecule 41: Tubulin beta chain

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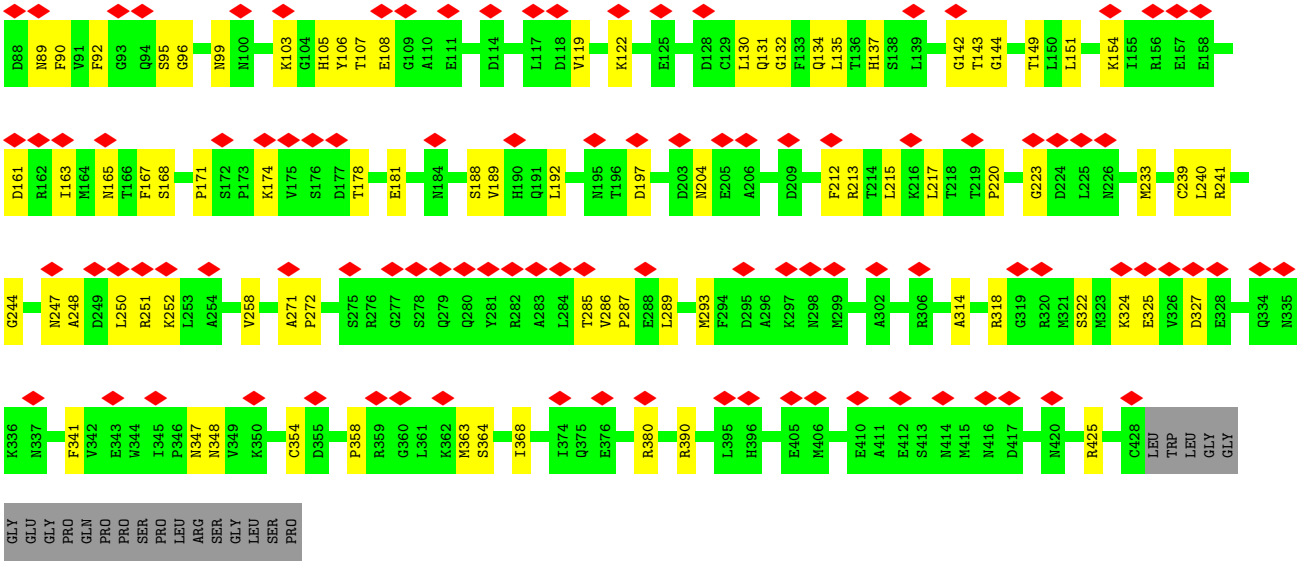
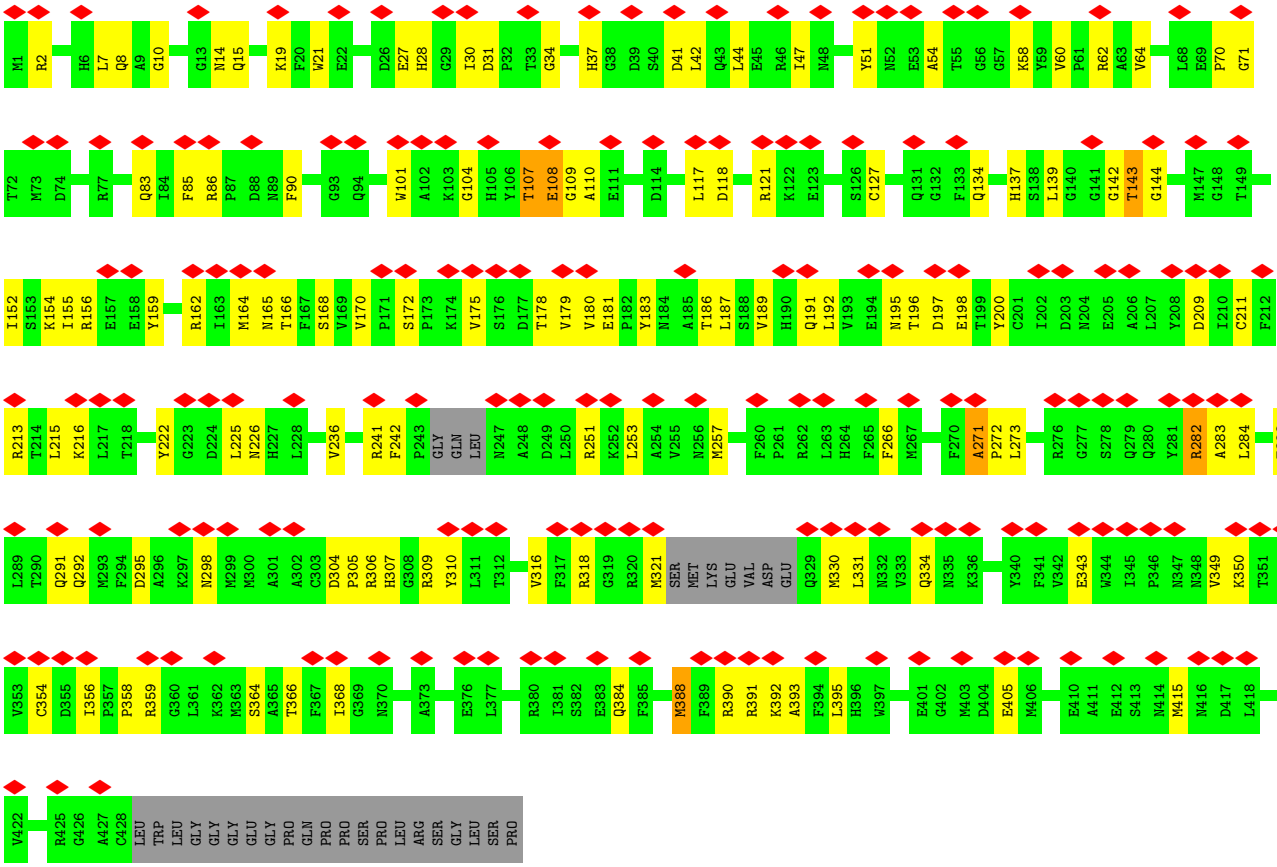


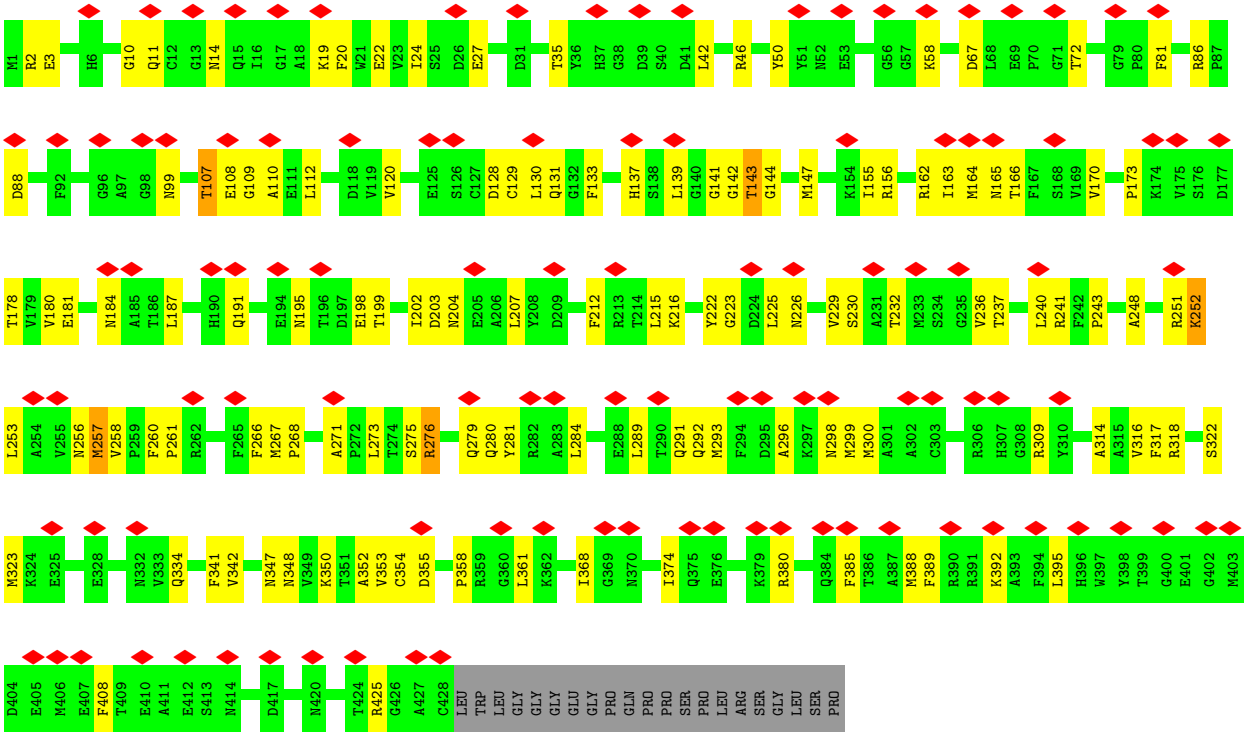

- Molecule 41: Tubulin beta chain

Chain NP:



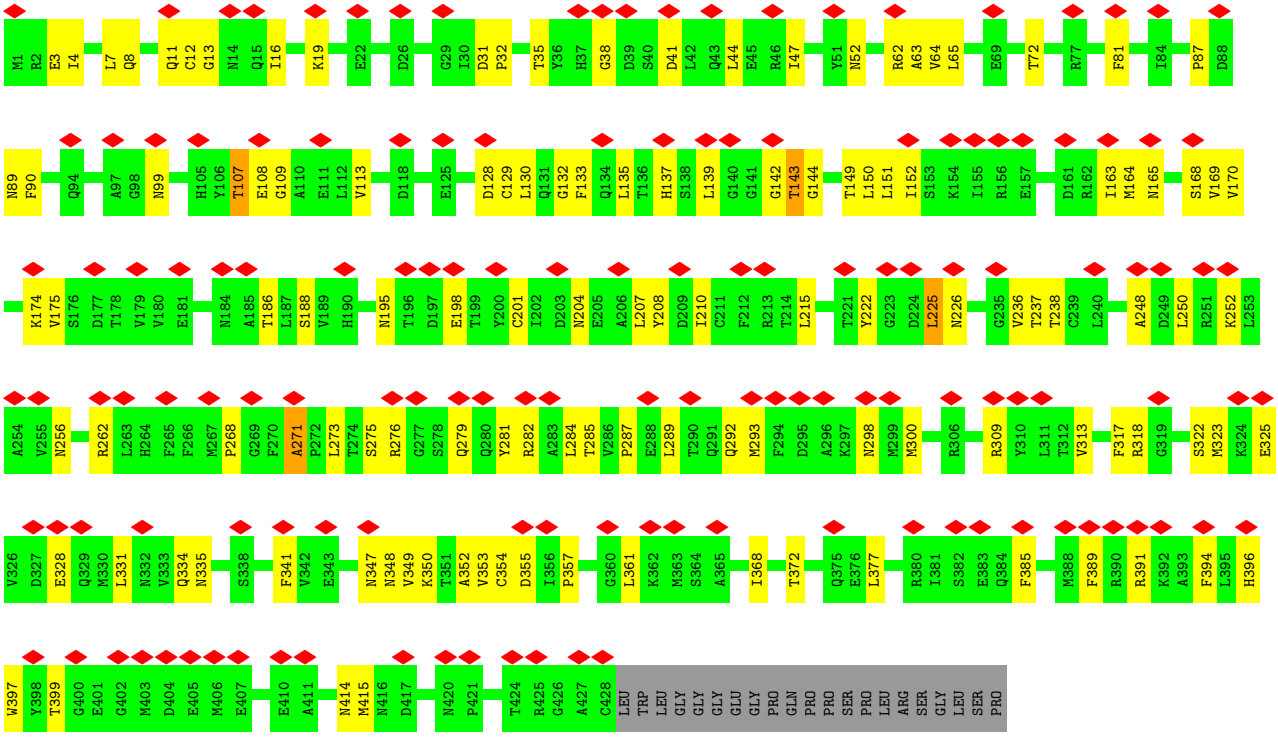

- Molecule 41: Tubulin beta chain

Chain OB:



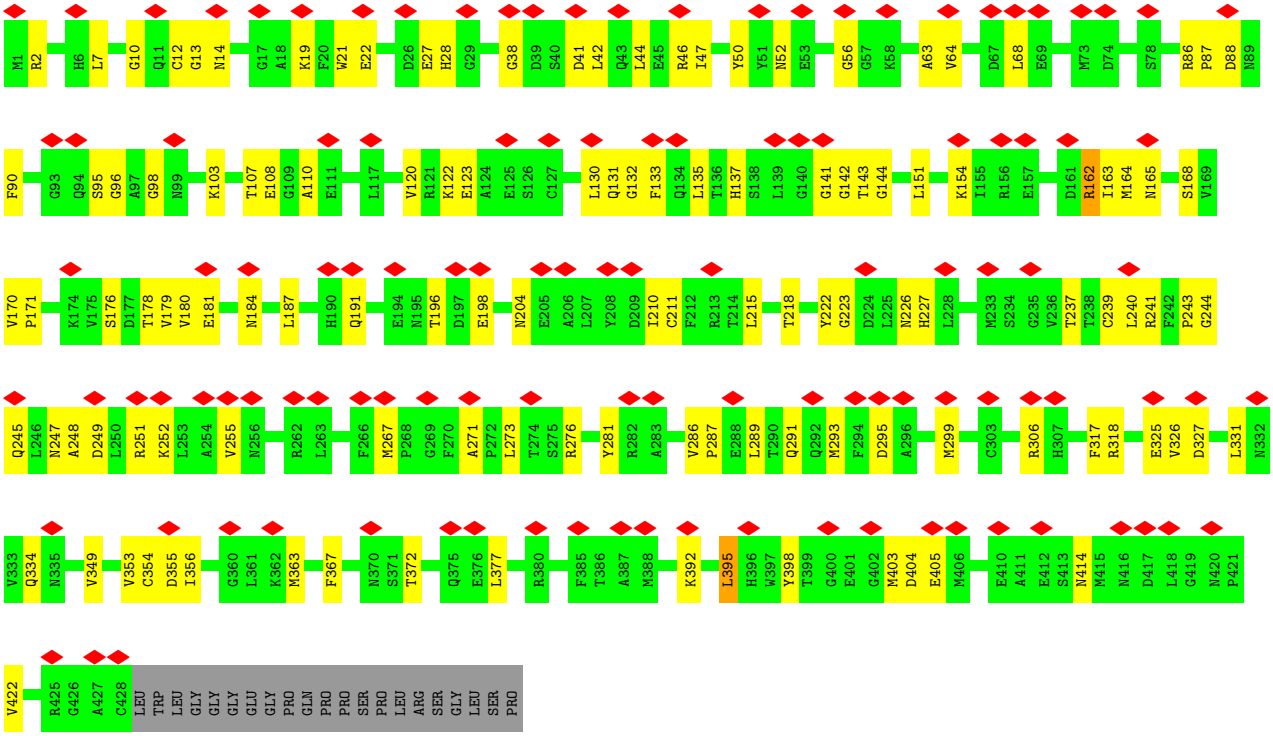

- Molecule 41: Tubulin beta chain

Chain OL:



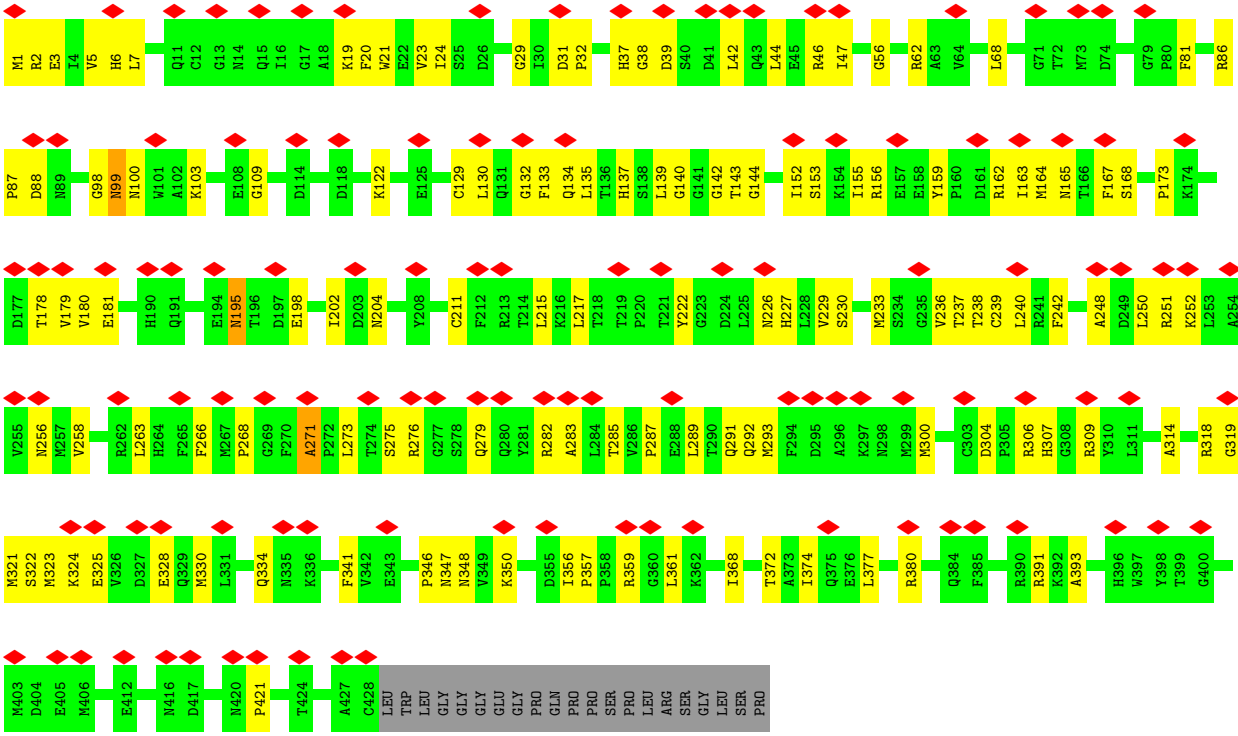

- Molecule 41: Tubulin beta chain

Chain OM:




- Molecule 41: Tubulin beta chain

Chain ON:




- Molecule 41: Tubulin beta chain

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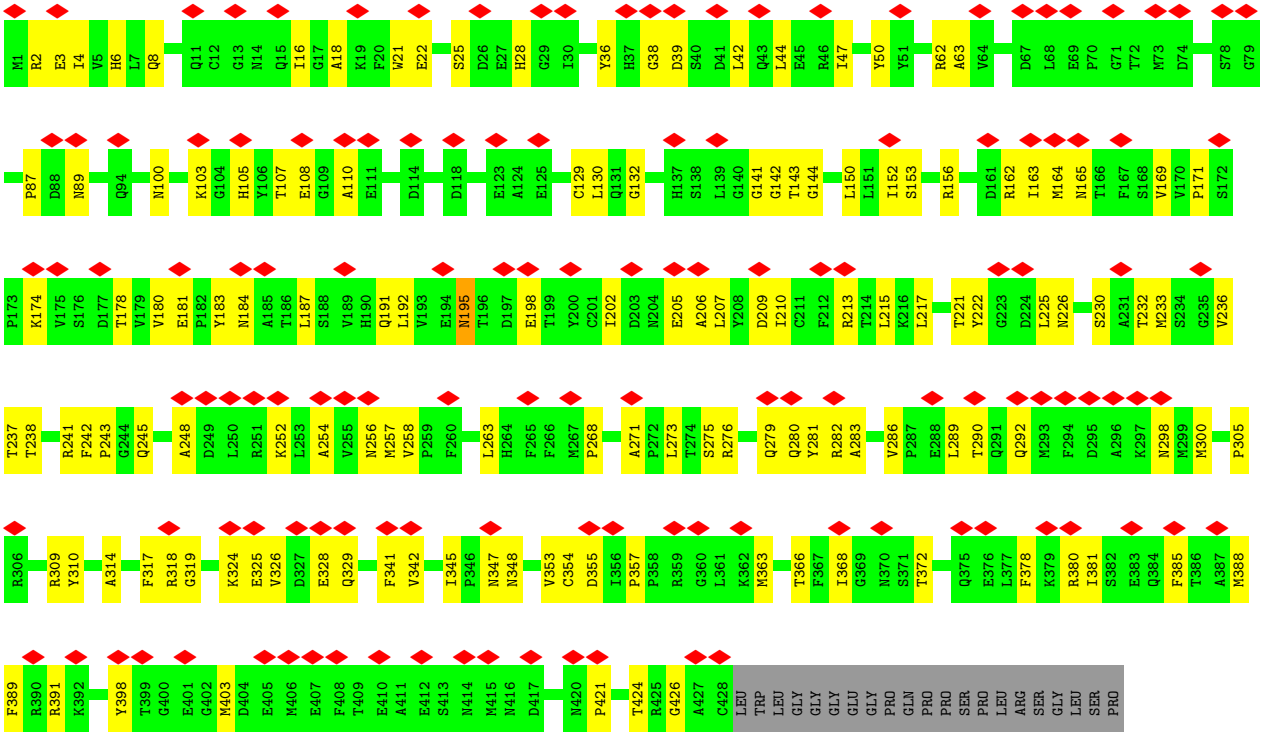
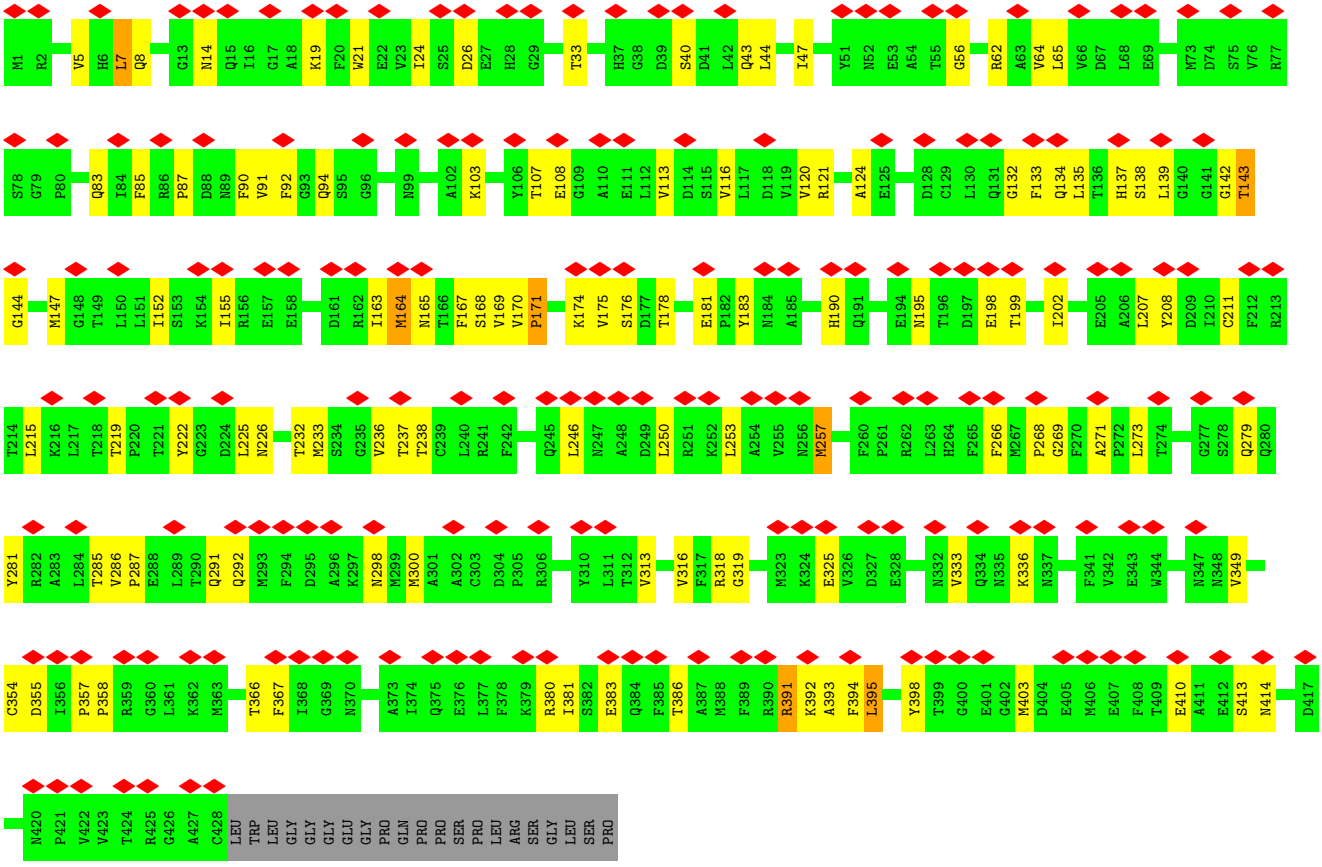


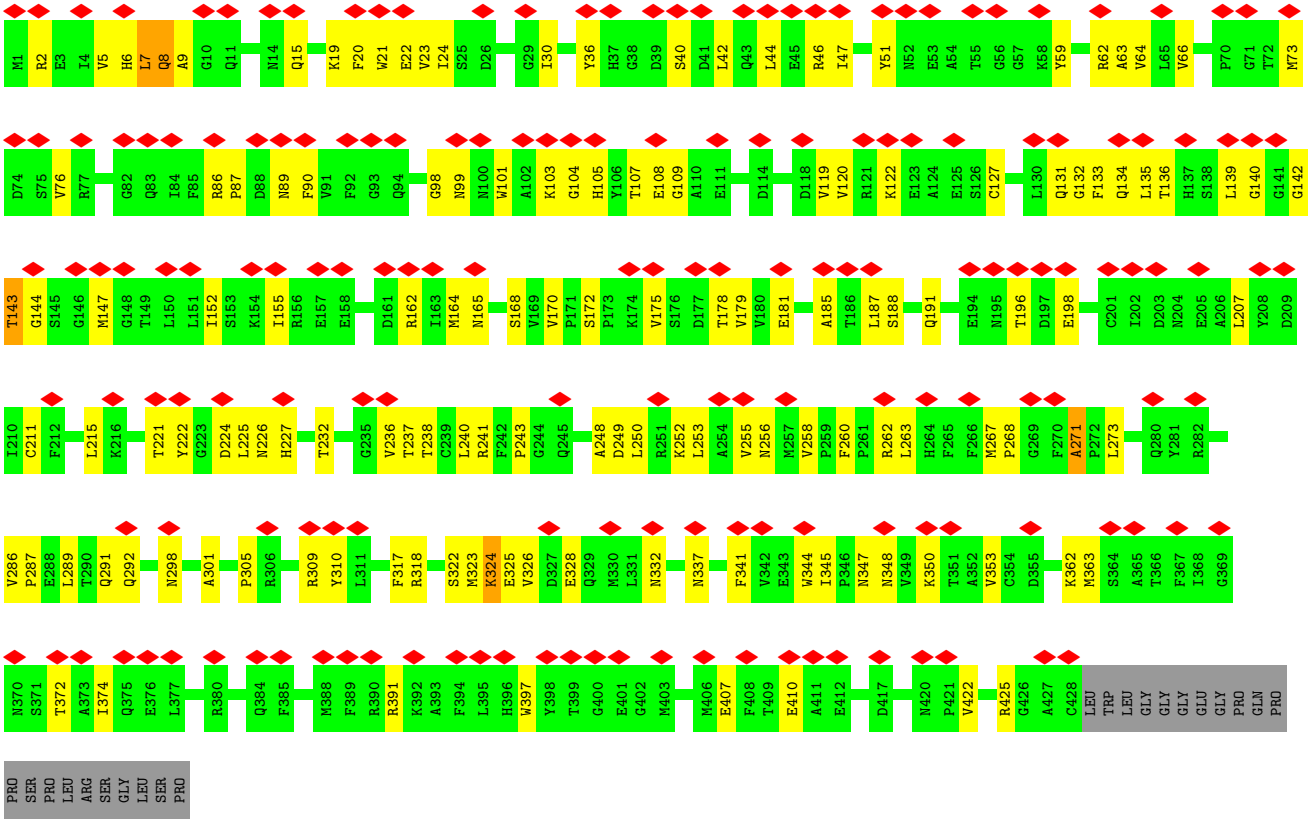

- Molecule 41: Tubulin beta chain

Chain OP:



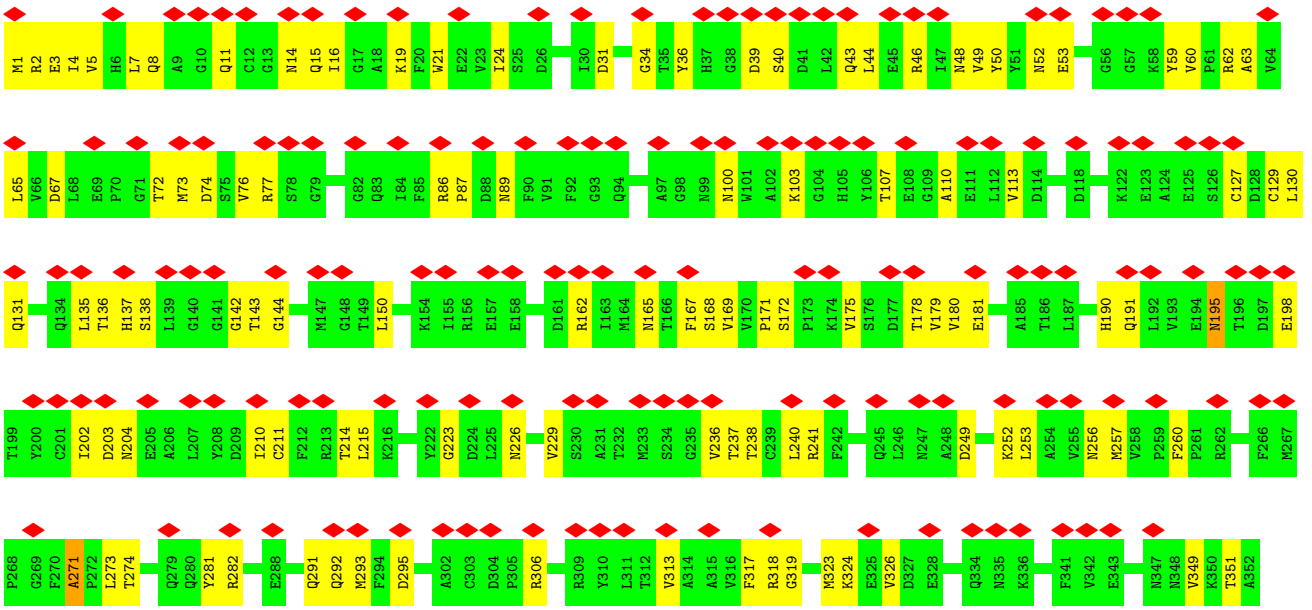
- Molecule 41: Tubulin beta chain

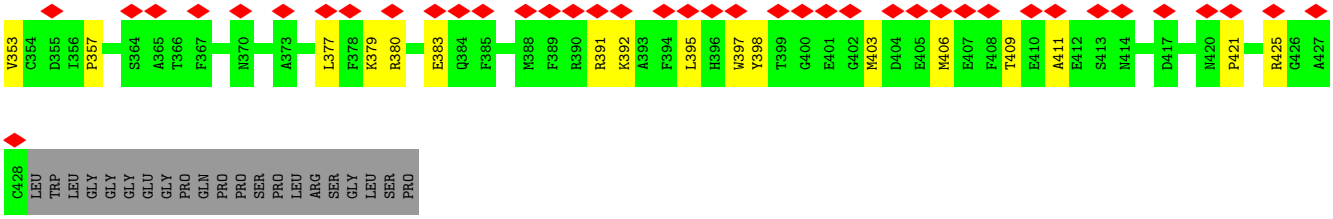
Chain PB:




- Molecule 41: Tubulin beta chain

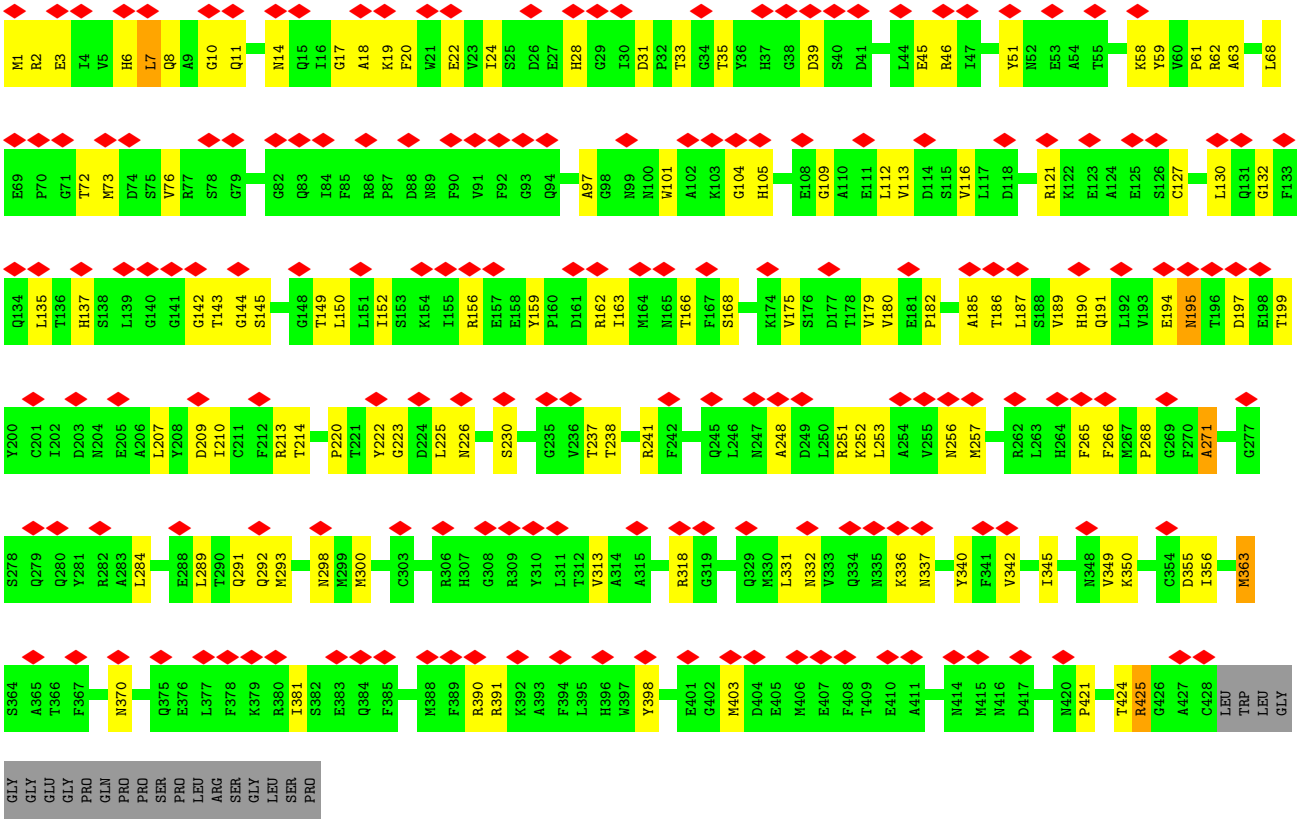
Chain PL:





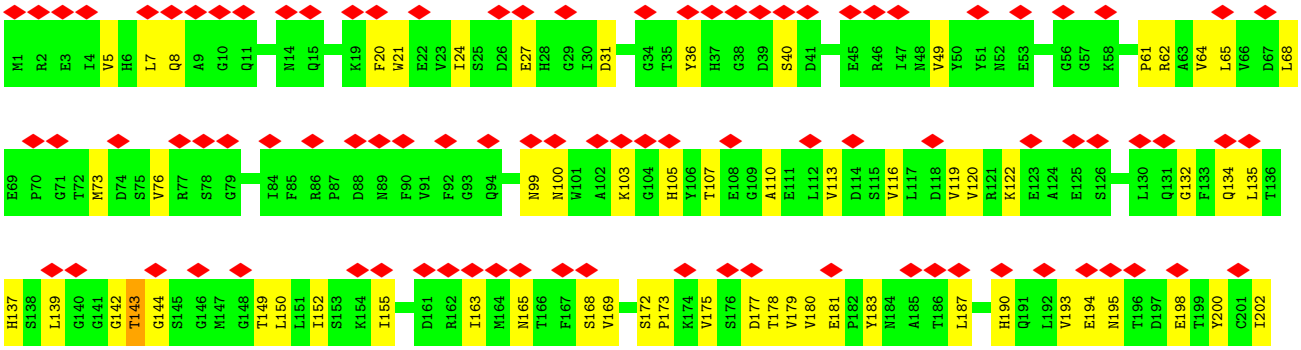

- Molecule 41: Tubulin beta chain

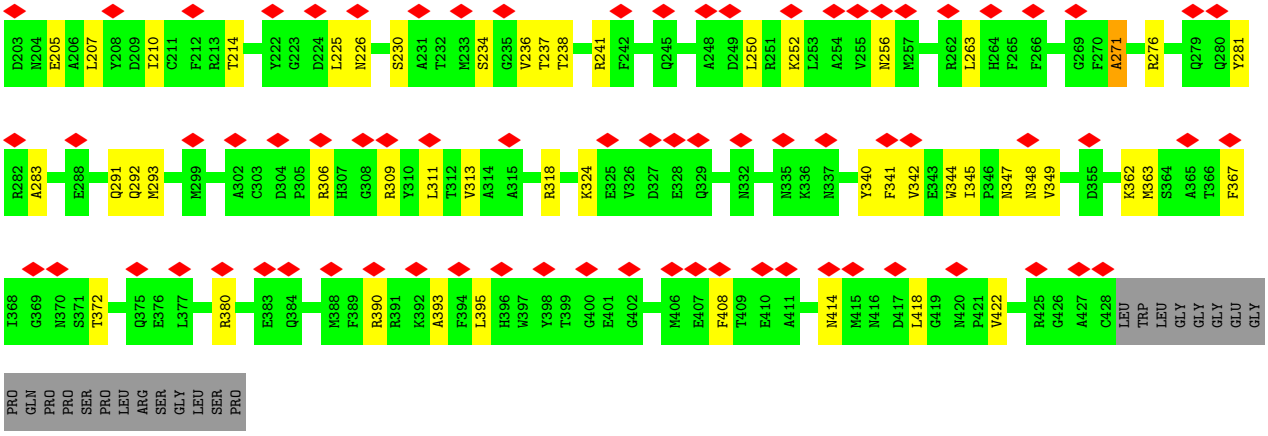
Chain PM:




- Molecule 41: Tubulin beta chain

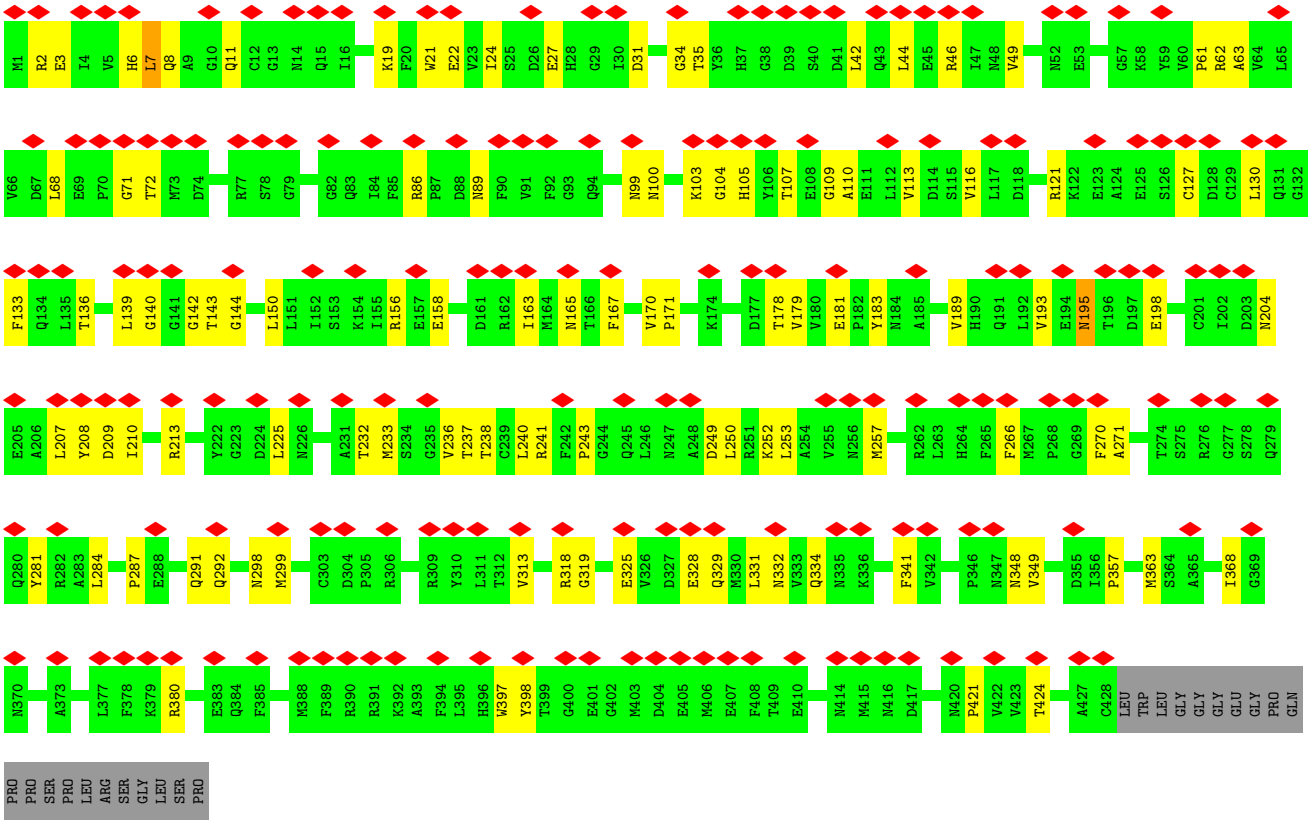
Chain PN:





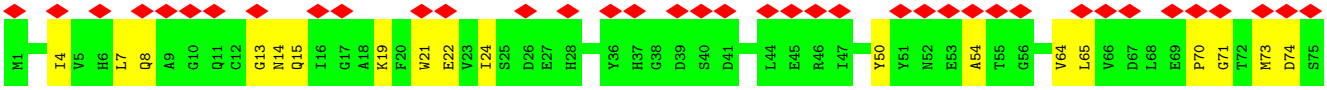

• Molecule 41: Tubulin beta chain

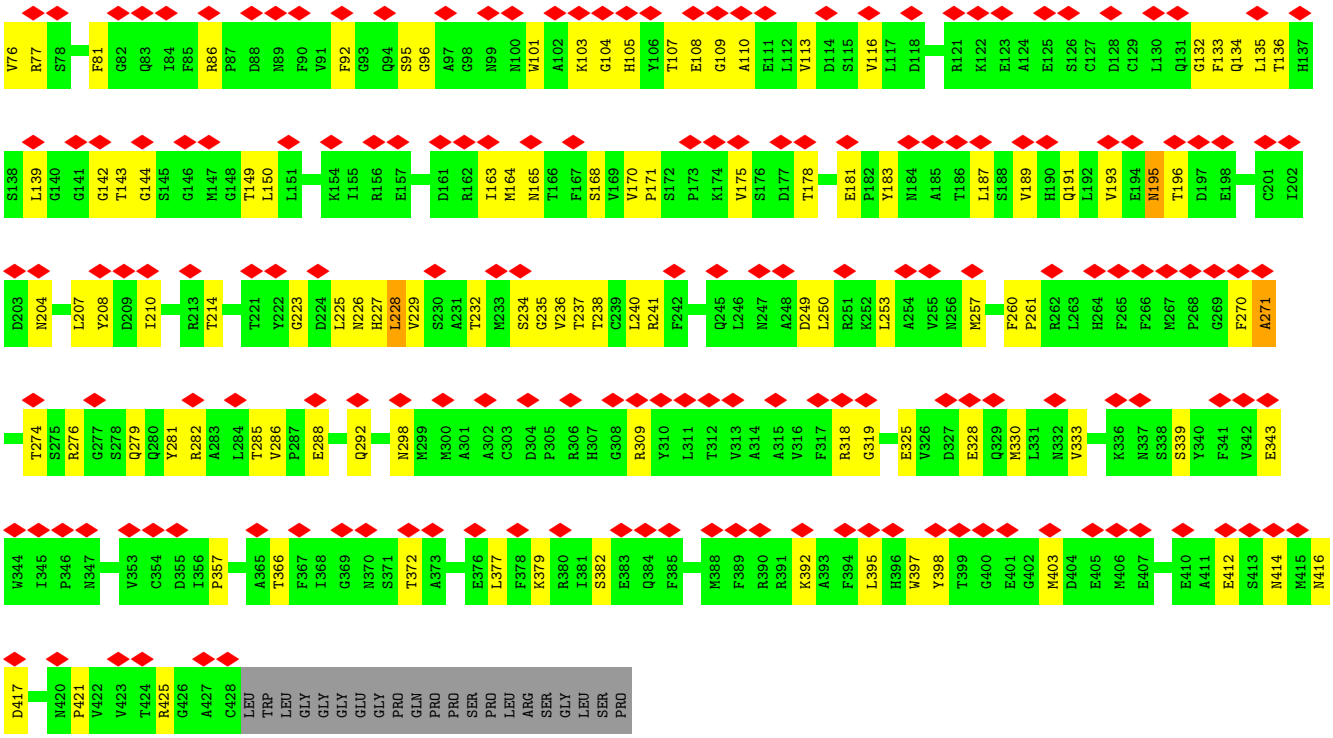
Chain PO:




• Molecule 41: Tubulin beta chain

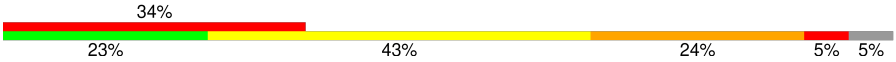
Chain PP:

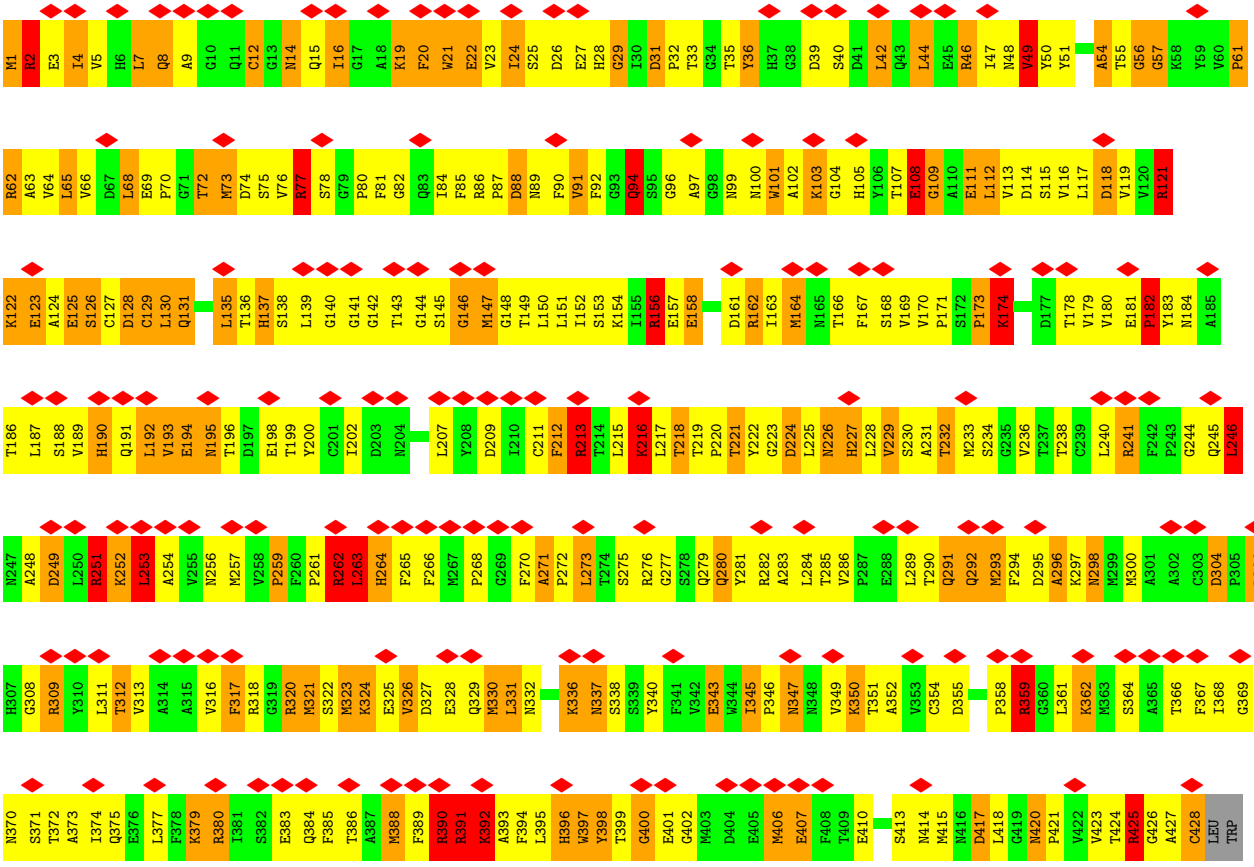





- Molecule 41: Tubulin beta chain

Chain QB:

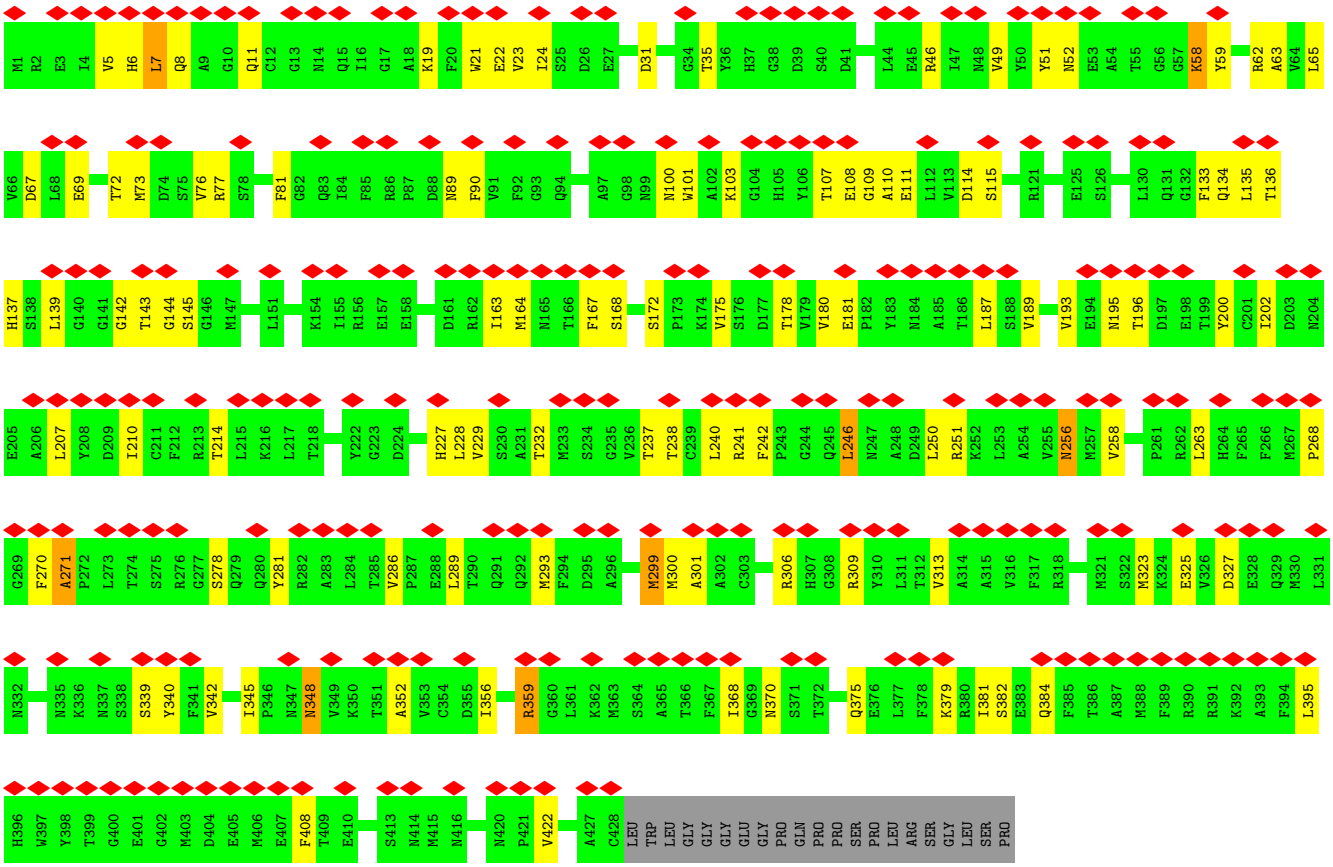


LEU GLY GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER GLY LEU SER PRO

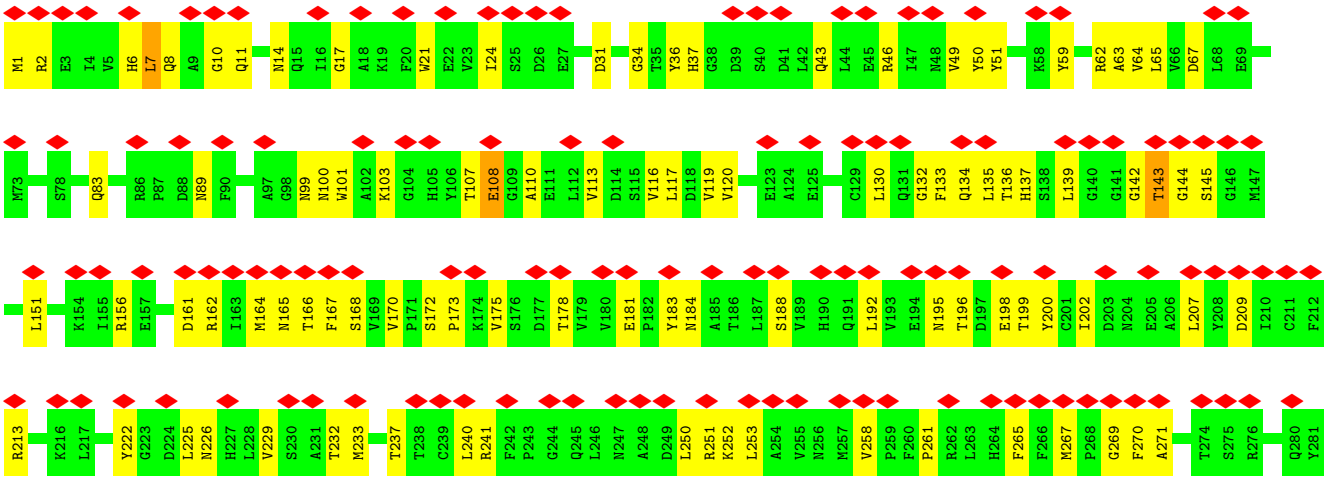
- Molecule 41: Tubulin beta chain

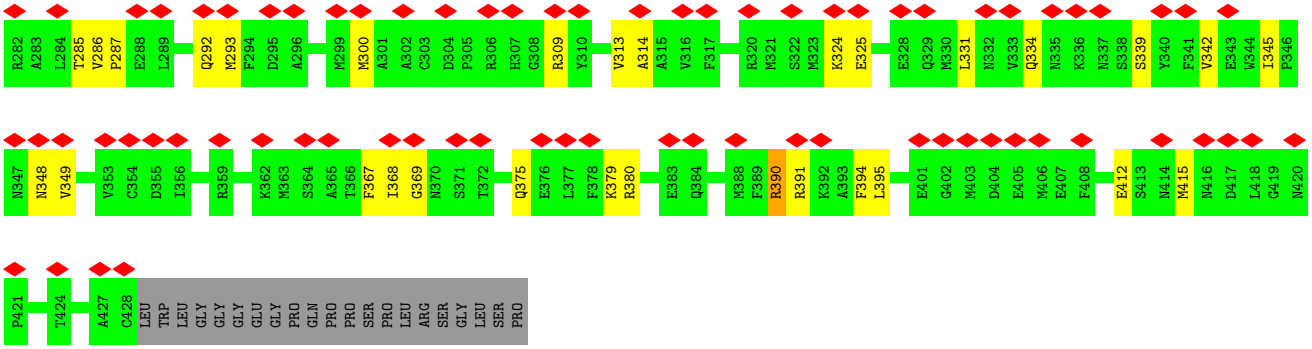
Chain QL:




- Molecule 41: Tubulin beta chain

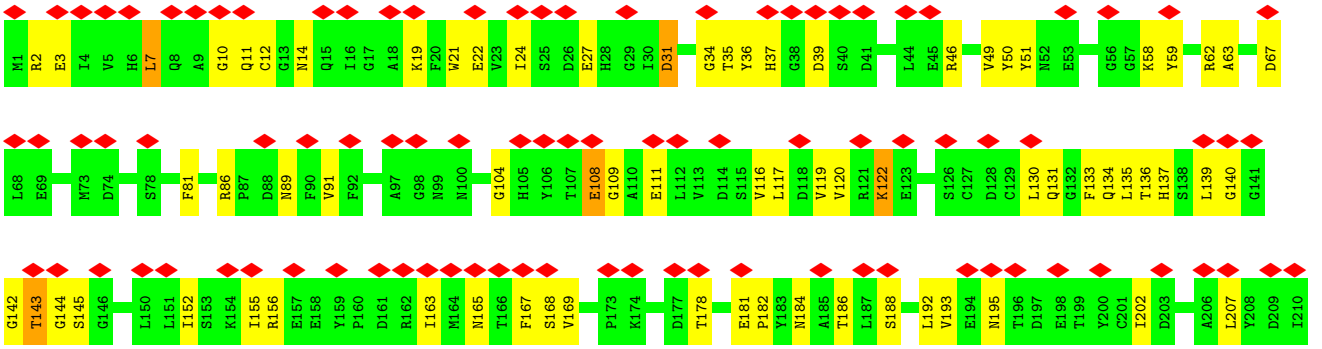
Chain QM:





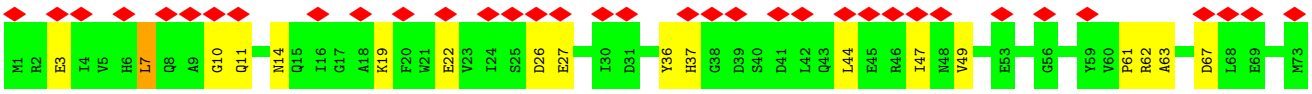

- Molecule 41: Tubulin beta chain

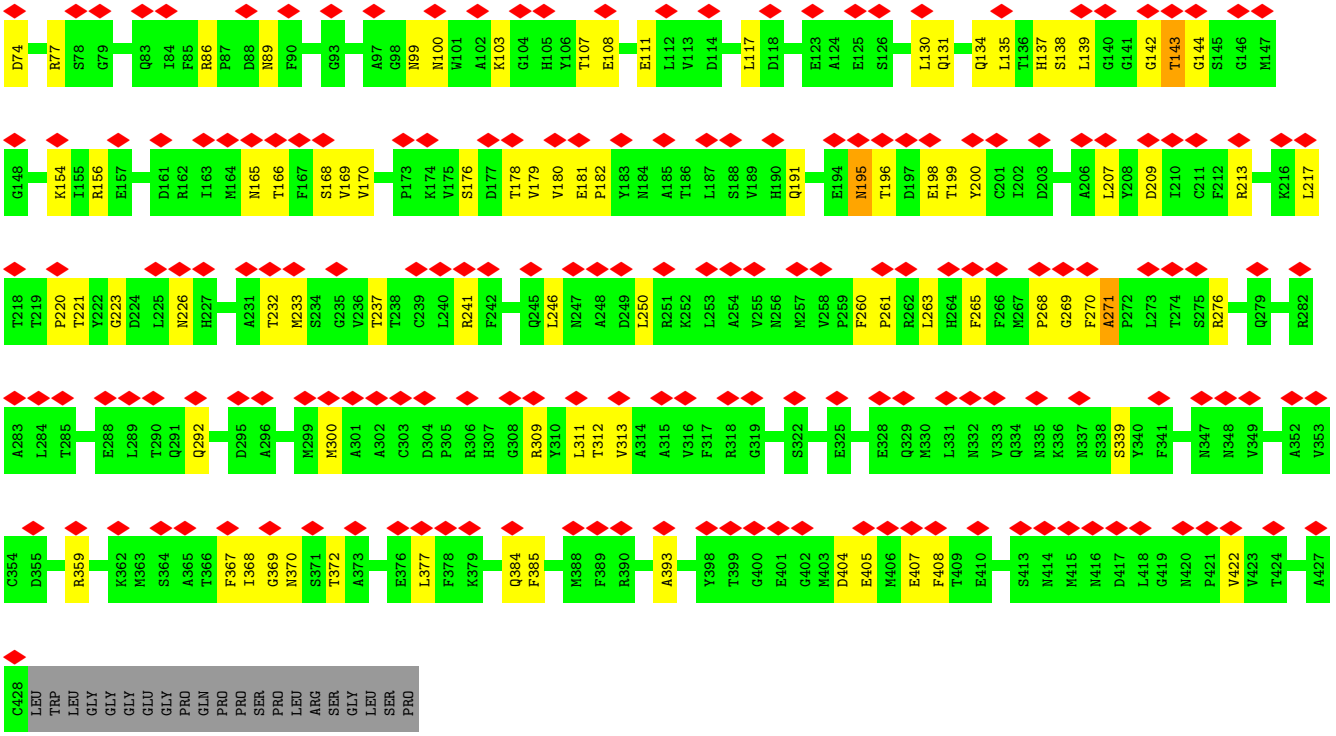
Chain QN: 45% 67% 27% • 5%




- Molecule 41: Tubulin beta chain

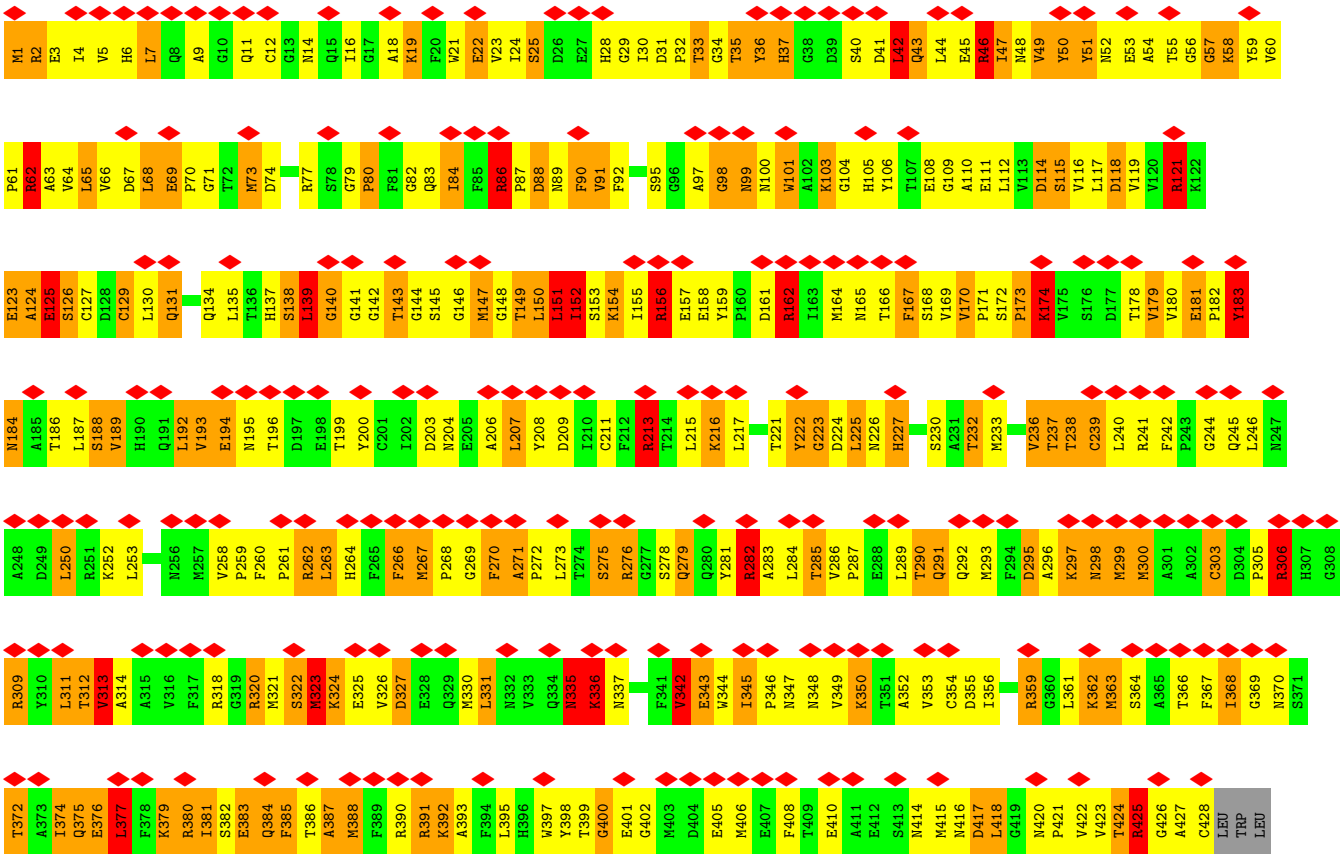
Chain QO: 48% 72% 22% • 5%






- Molecule 41: Tubulin beta chain

Chain QP:



GLY GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER GLY LEU SER PRO

- Molecule 41: Tubulin beta chain

Chain RB: 42% 69% 25% • 5%

M1 R2 E3 L7 Q8 A9 G10 Q11 C12 G13 I16 W21 E22 V23 I24 S25 D26 E27 H28 G29 I30 D31 P32 T33 G34 D39 S40 D41 L44 E45 R46 I47 Y51 N52 E53 A54 T55 G56 G57 K58 Y59 V60 P61 R62 A63 V64 L65 V66 D67 L68 E69 M73 D74

S75 V76 F81 G82 Q83 I84 F85 R86 P87 D88 N89 F90 V91 F92 G93 Q94 G98 N99 N100 W101 A102 K103 G104 H105 Y106 T107 E108 G109 L112 V113 D114 S115 V116 L117 D118 V119 V120 R121 K122 E125 S126 C127 D128 C129 L130 Q131 G132 F133 Q134 L135 T136 H137 S138 L139 G140 G141

G142 T143 G144 S145 G146 M147 G148 L151 I152 S153 K154 I155 R156 E157 E158 Y159 P160 D161 R162 I163 M164 N165 T166 F167 S168 V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 Y183 N184 A185 T186 L187 S188 V189 H190 Q191 L192 V193 E194 N195 T196 D197 E198 T199 I202 D203

N204 E205 A206 L207 Y208 R213 Y222 G223 D224 L225 N226 H227 L228 V229 S230 A231 T232 M233 T238 C239 L240 R241 F242 P243 G244 Q245 L246 N247 A248 D249 L250 R251 K252 L253 N256 M257 V258 R262 L263 H264 F265 F266 G269 F270 A271 R276 Q279 R282 A283 L284 T285

L289 T290 Q291 Q292 M293 F294 N298 M299 M300 A301 A302 C303 D304 P305 R306 H307 G308 R309 T312 V313 A314 A315 V316 F317 R318 G319 R320 M321 S322 M323 K324 E325 V326 D327 E328 Q329 M330 L331 N332 V333 Q334 N335 S338 F341 I345 P346 N347 N348 V349 K350 T351 A352 V353 C354

D355 R359 K362 M363 S364 A365 T366 F367 I368 G369 N370 S371 T372 A373 I374 L377 F378 K379 R380 I381 S382 E383 Q384 F385 T386 A387 M388 R391 K392 A393 W397 Y398 E401 G402 M403 D404 E405 M406 E410 S413 N414 M415 N416 D417 L418 G419 N420 P421 V422 V423 T424

A427 C428 LEU TRP LEU GLY GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER GLY LEU SER PRO

- Molecule 41: Tubulin beta chain

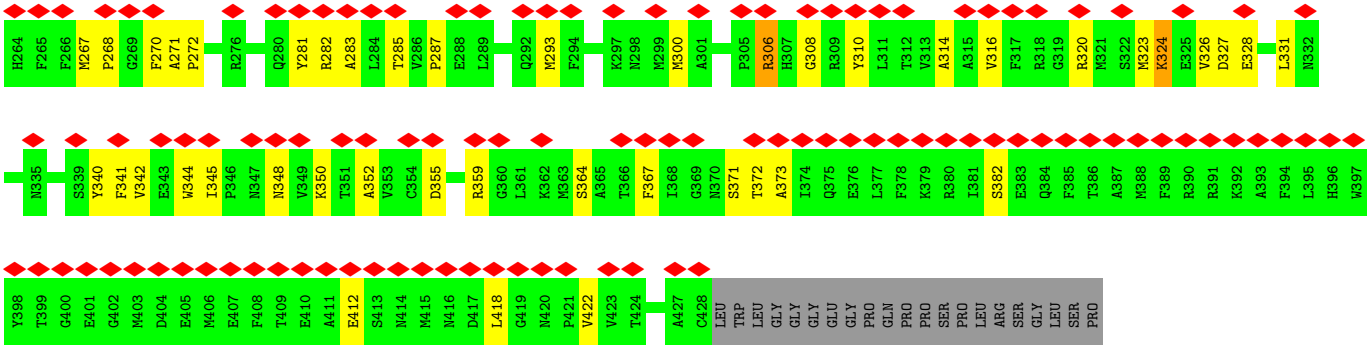
Chain RL: 64% 71% 23% • 5%

M1 R2 E3 I4 V5 H6 L7 Q8 A9 G10 Q11 C12 G13 N14 Q15 I16 G17 E22 V23 I24 S25 D26 E27 I30 D31 P32 T33 G34 T35 D39 S40 D41 L44 E45 R46 I47 N48 V49 Y50 Y51 N52 E53 A54 T55 G56 G57 K58 Y59 R62 A63 V64 L65 V66 D67 L68

E69 P70 G71 T72 M73 D74 S75 V76 R77 S78 Q83 I84 F85 R86 P87 D88 N89 F90 V91 F92 G93 Q94 S95 G96 A97 G98 N99 N100 W101 A102 K103 G104 H105 Y106 T107 E108 G109 A110 E111 L112 V113 D114 S115 V116 L117 D118 V119 V120 R121 K122 E123 A124 E125 S126 C127 D128 C129 L130

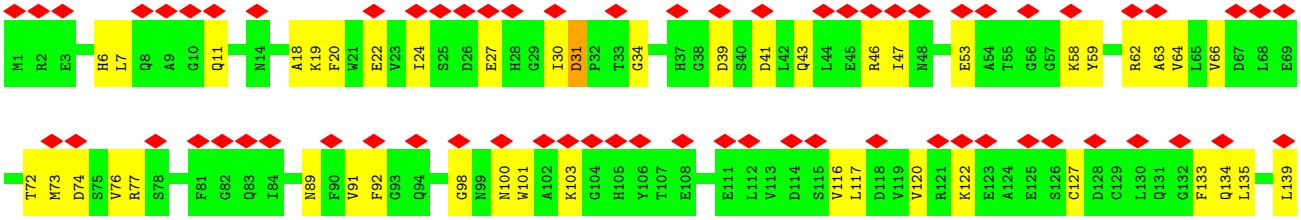
F133 Q134 L135 T136 H137 S138 L139 G140 G141 G142 T143 G144 S145 G146 M147 G148 T149 L150 L151 I152 S153 K154 I155 R156 E157 E158 Y159 R162 I163 M164 N165 T166 F167 S168 V169 V170 P171 S172 P173 K174 V175 S176 D177 T178 V179 V180 E181 P182 Y183 N184 A185 T186 L187 S188 V189 H190 Q191 L192 V193

E194 N195 T199 Y200 C201 I202 D203 N204 E205 A206 L207 Y208 D209 I210 R213 T214 L215 K216 L217 P220 T221 Y222 G223 D224 L225 N226 H227 L228 A231 T232 M233 S234 G235 L240 R241 F242 P243 G244 N247 A248 D249 L250 R251 K252 L253 N256 M257 V258 P259 F260 P261 R262 L263



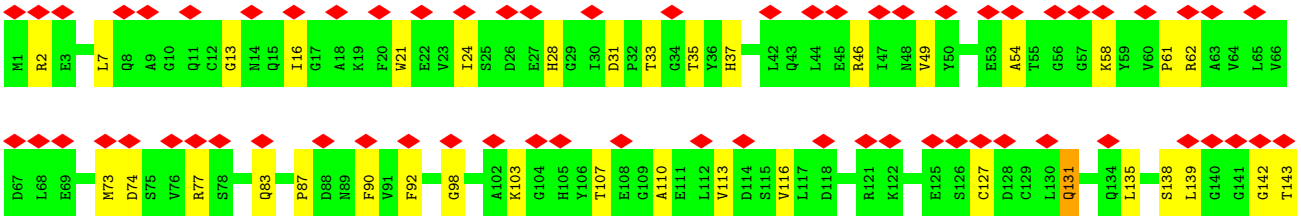

- Molecule 41: Tubulin beta chain

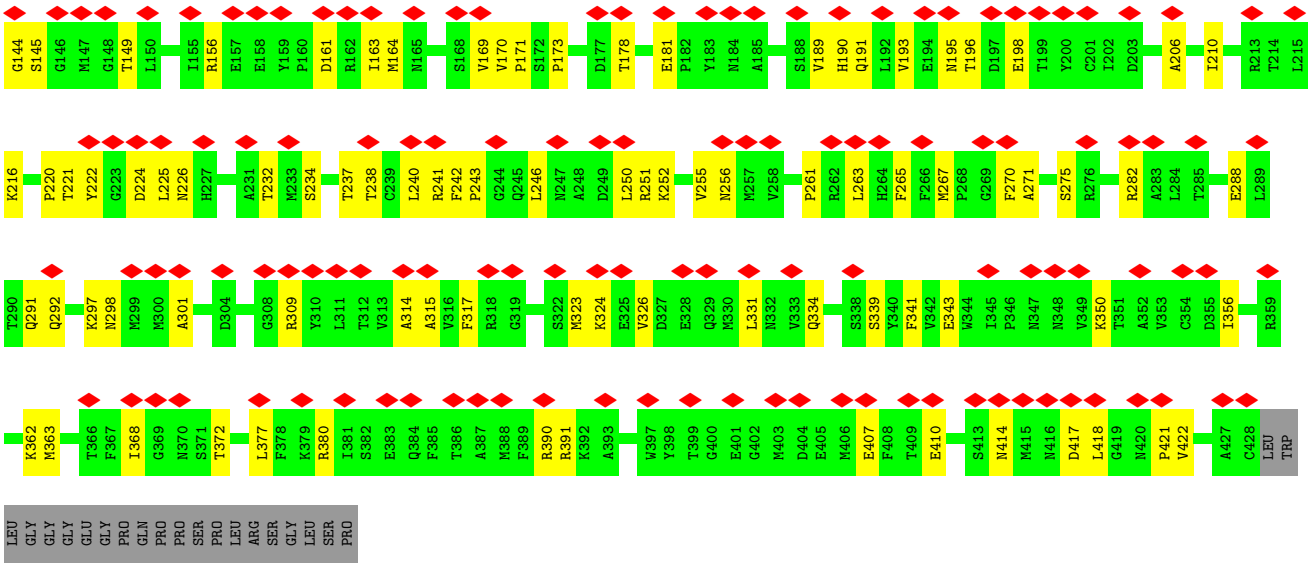
Chain RM:




- Molecule 41: Tubulin beta chain

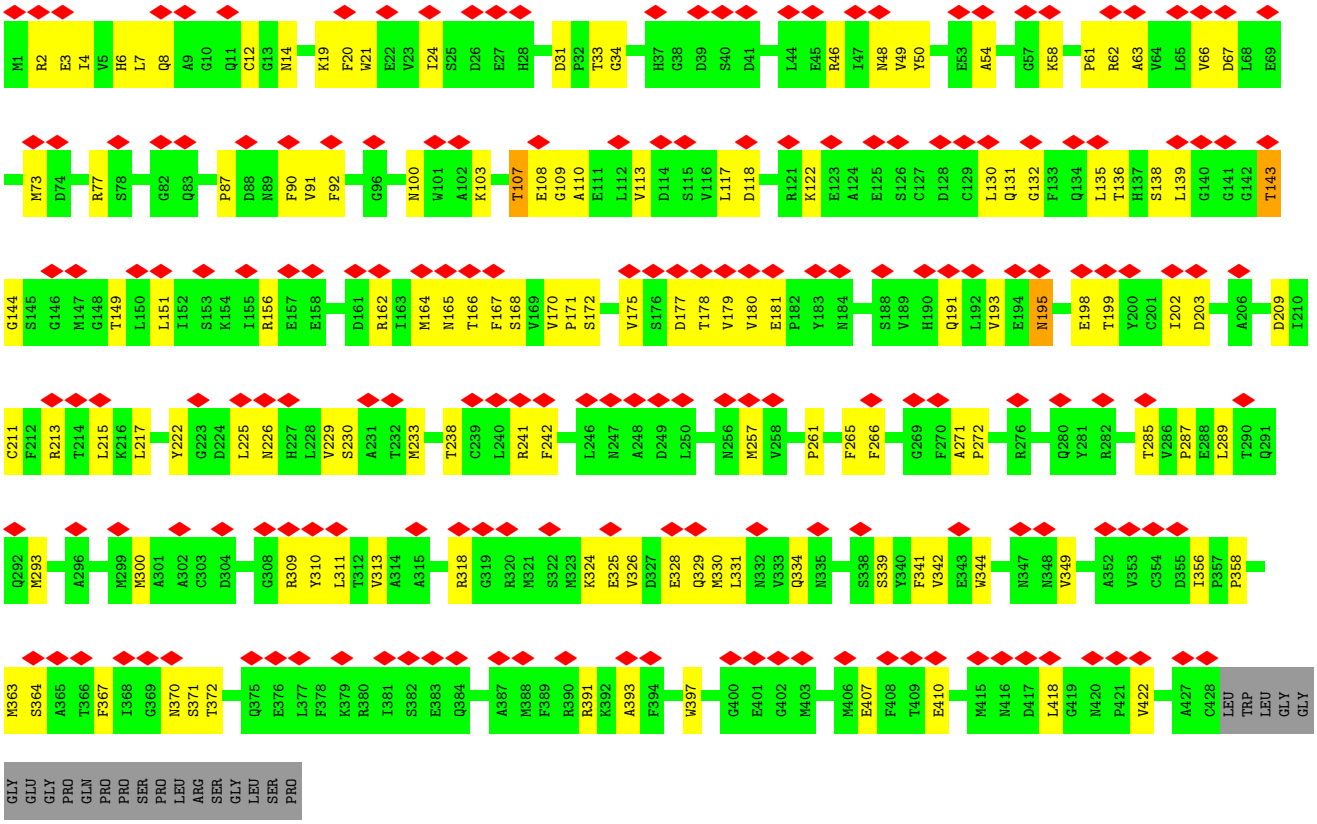
Chain RN:





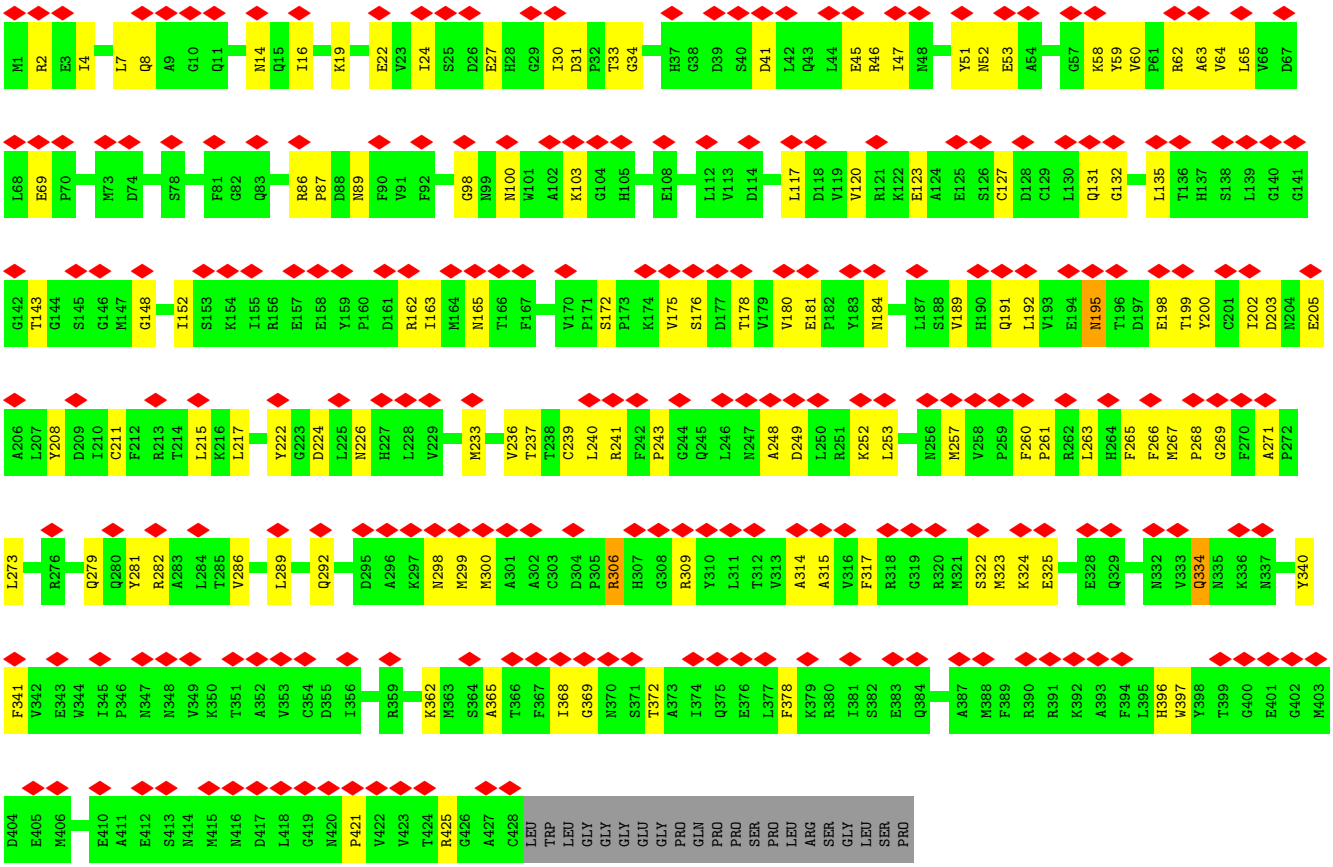

- Molecule 41: Tubulin beta chain

Chain RO:



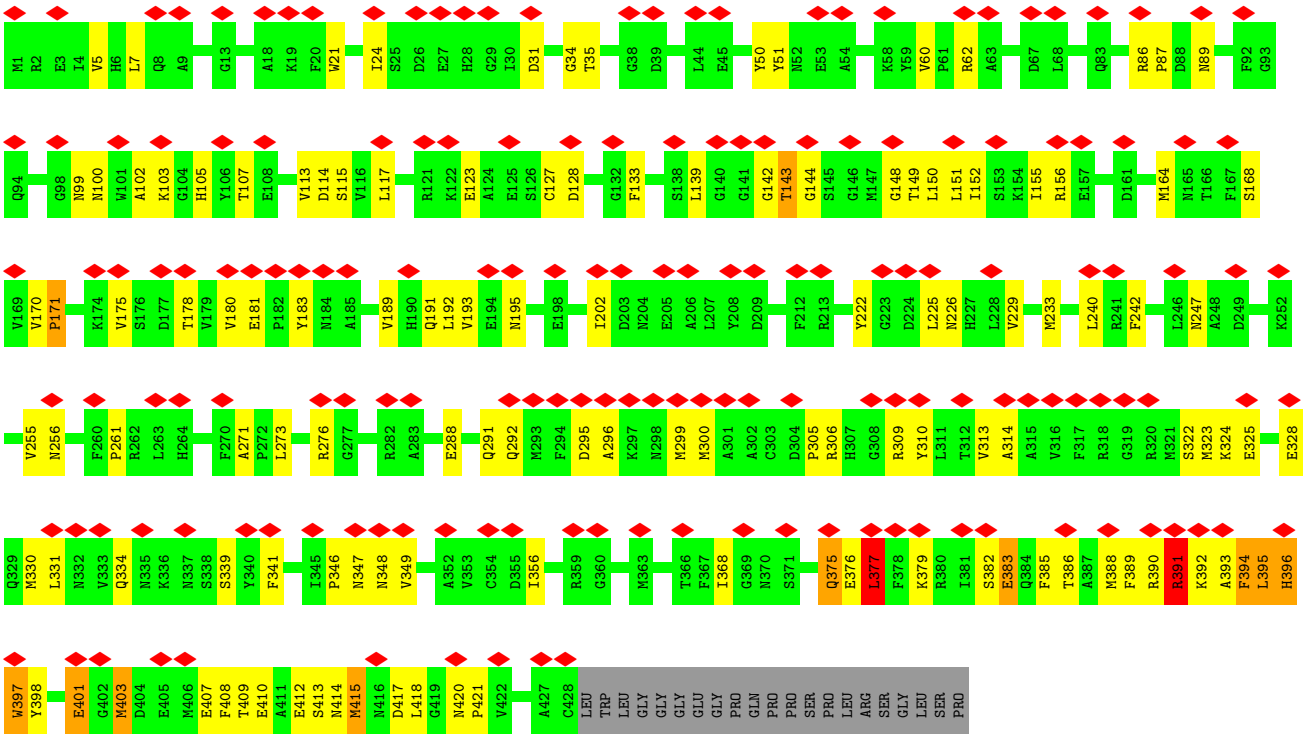

- Molecule 41: Tubulin beta chain

Chain RP:



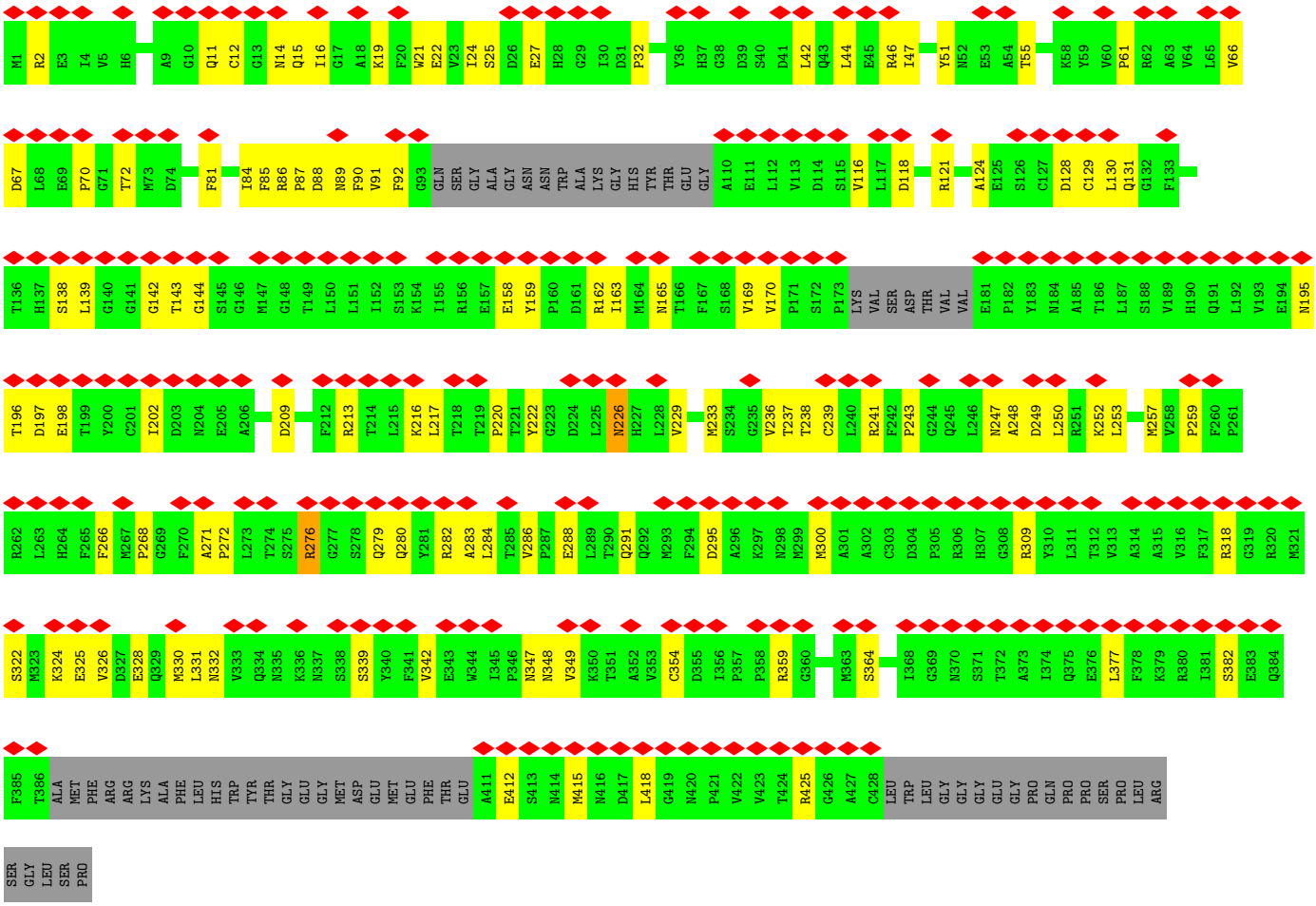

- Molecule 41: Tubulin beta chain

Chain SB:



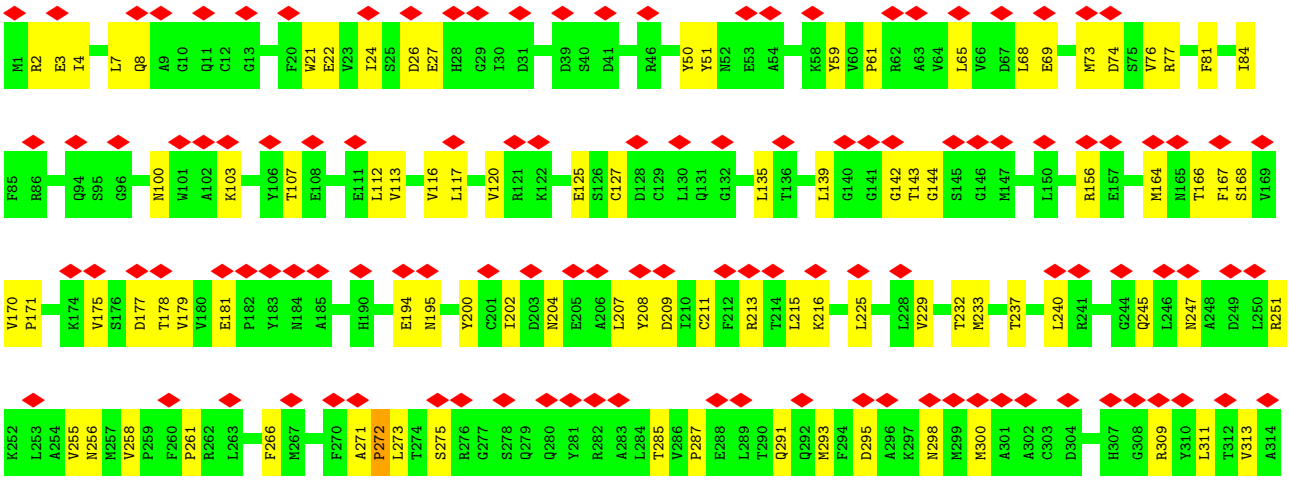
- Molecule 41: Tubulin beta chain

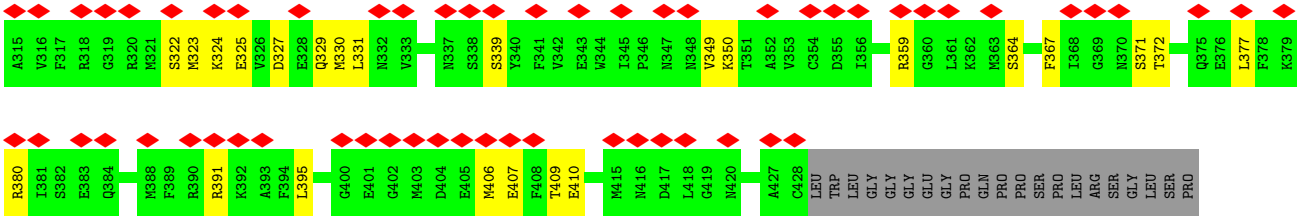
Chain SL:




- Molecule 41: Tubulin beta chain

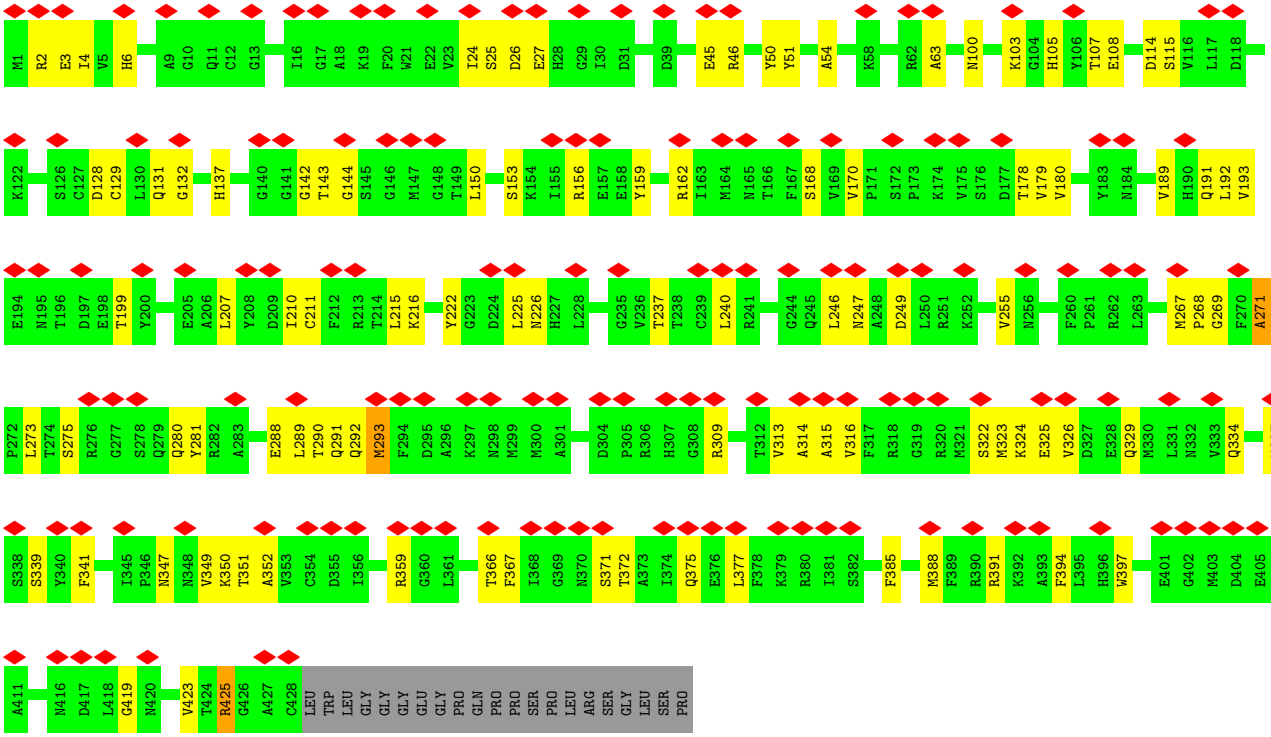
Chain SM:





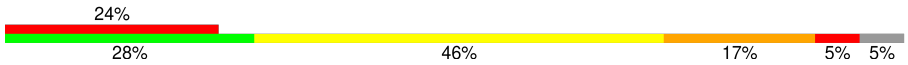

• Molecule 41: Tubulin beta chain

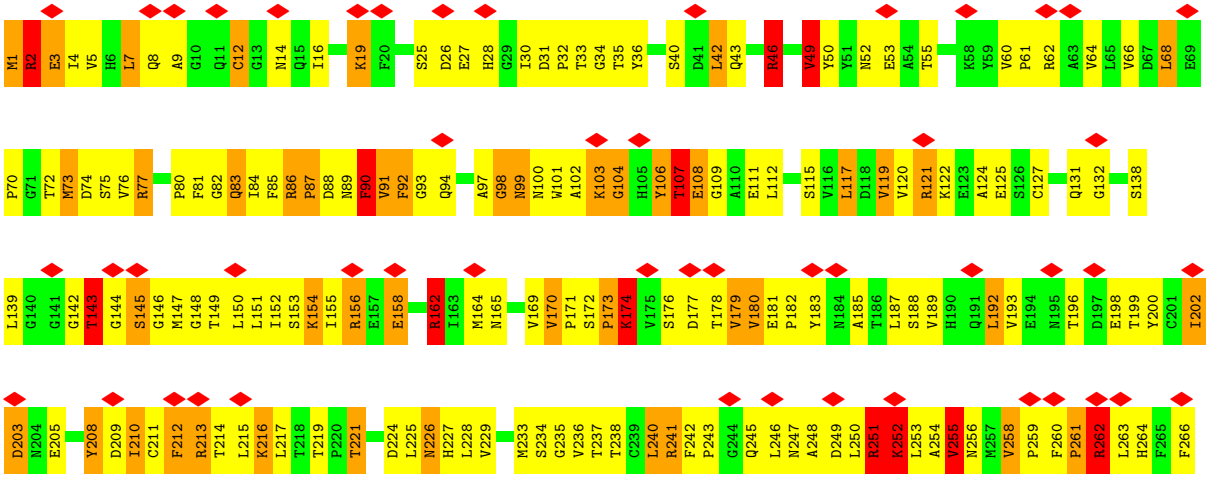
Chain SN:

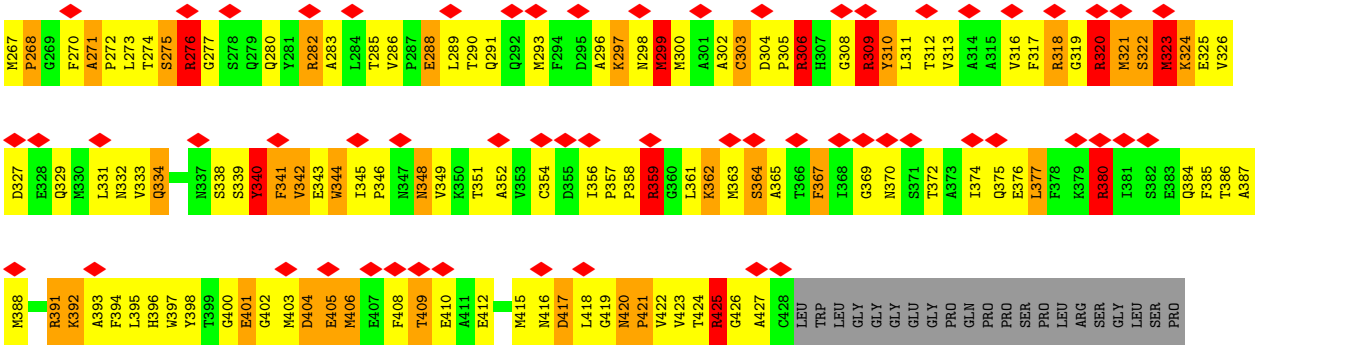



• Molecule 41: Tubulin beta chain

Chain SO:

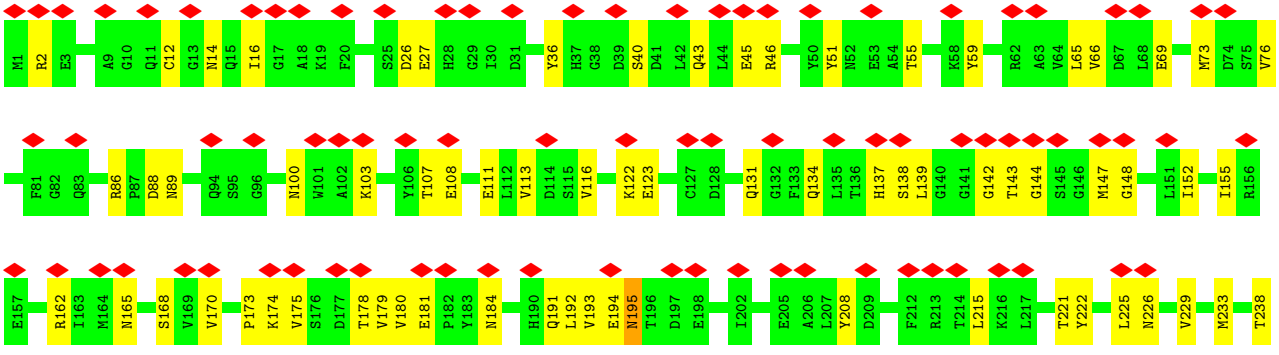


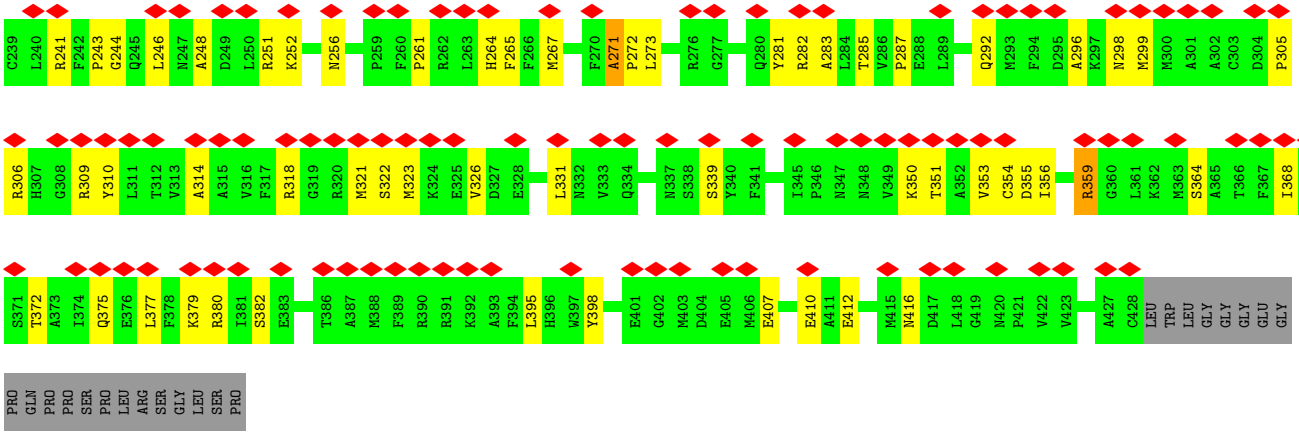






- Molecule 41: Tubulin beta chain

Chain SP:



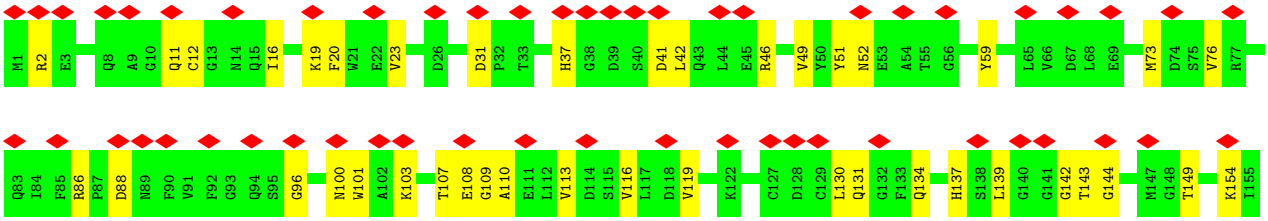



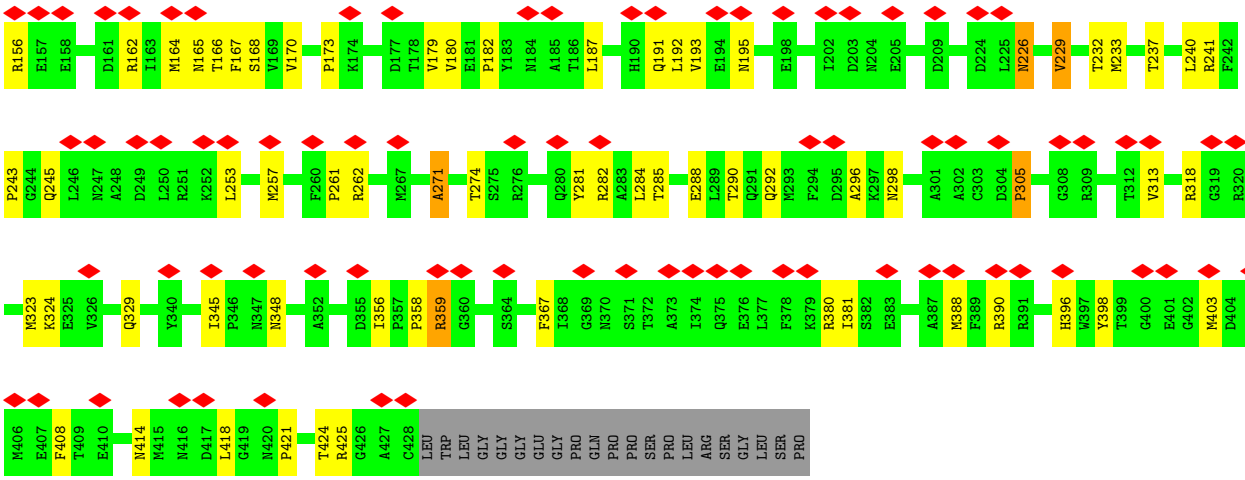




- Molecule 41: Tubulin beta chain

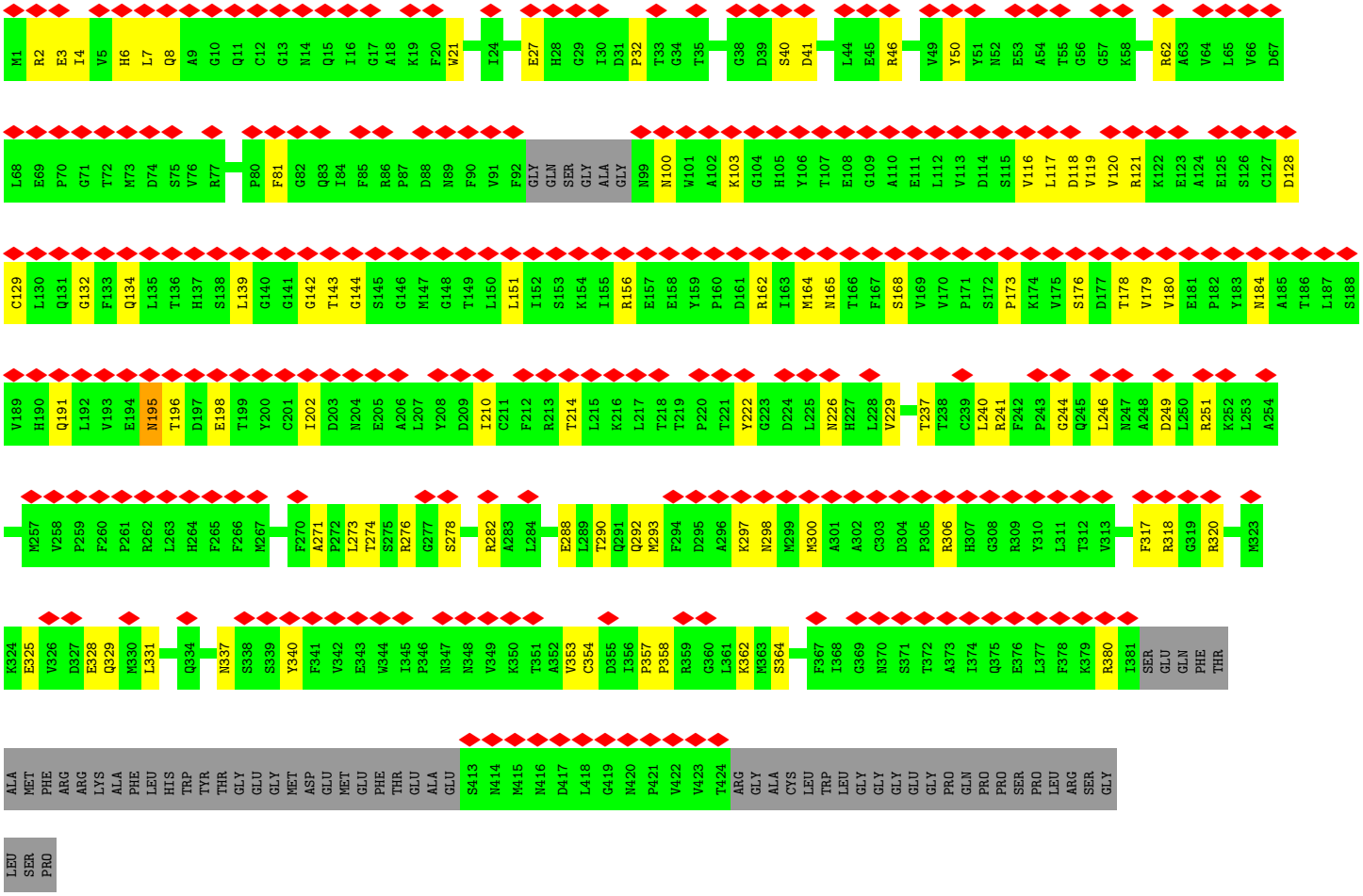
Chain TB:





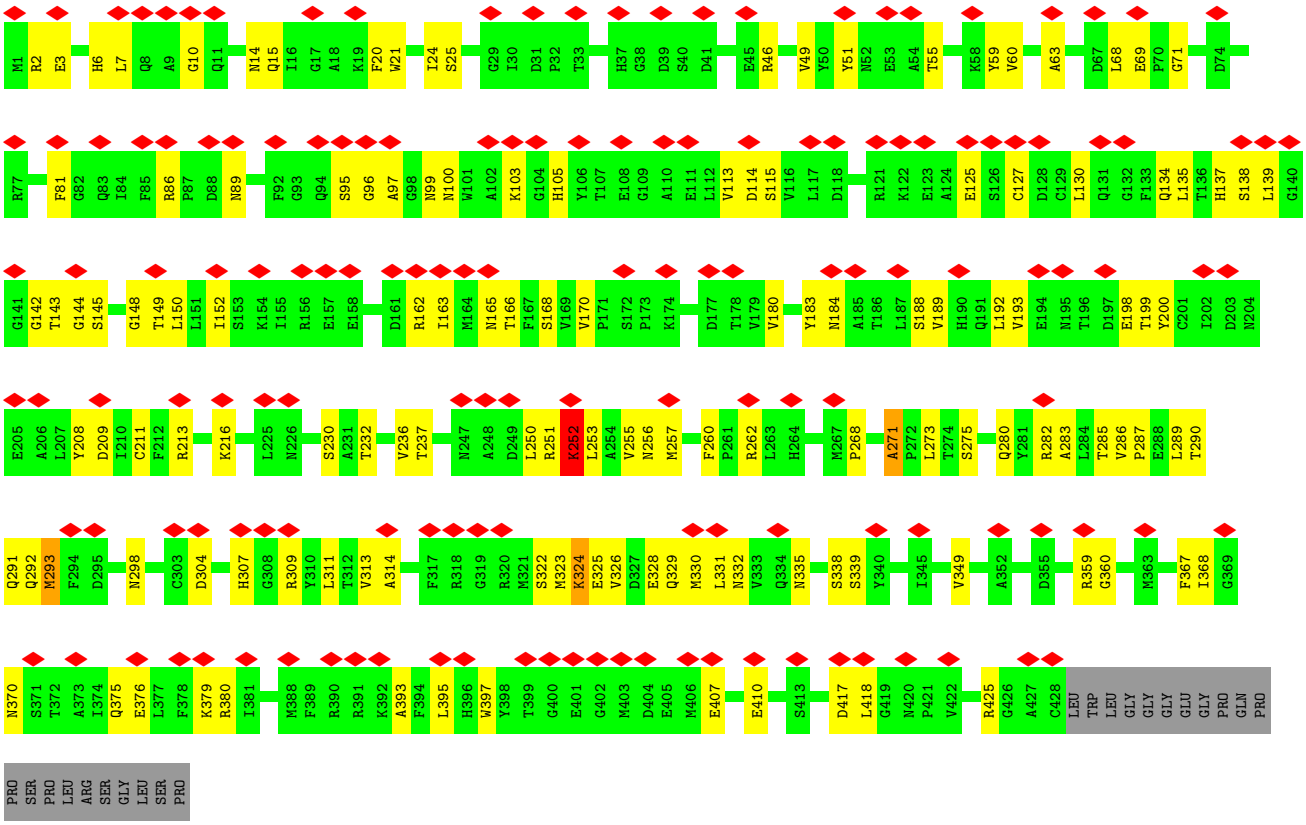

- Molecule 41: Tubulin beta chain

Chain TL:



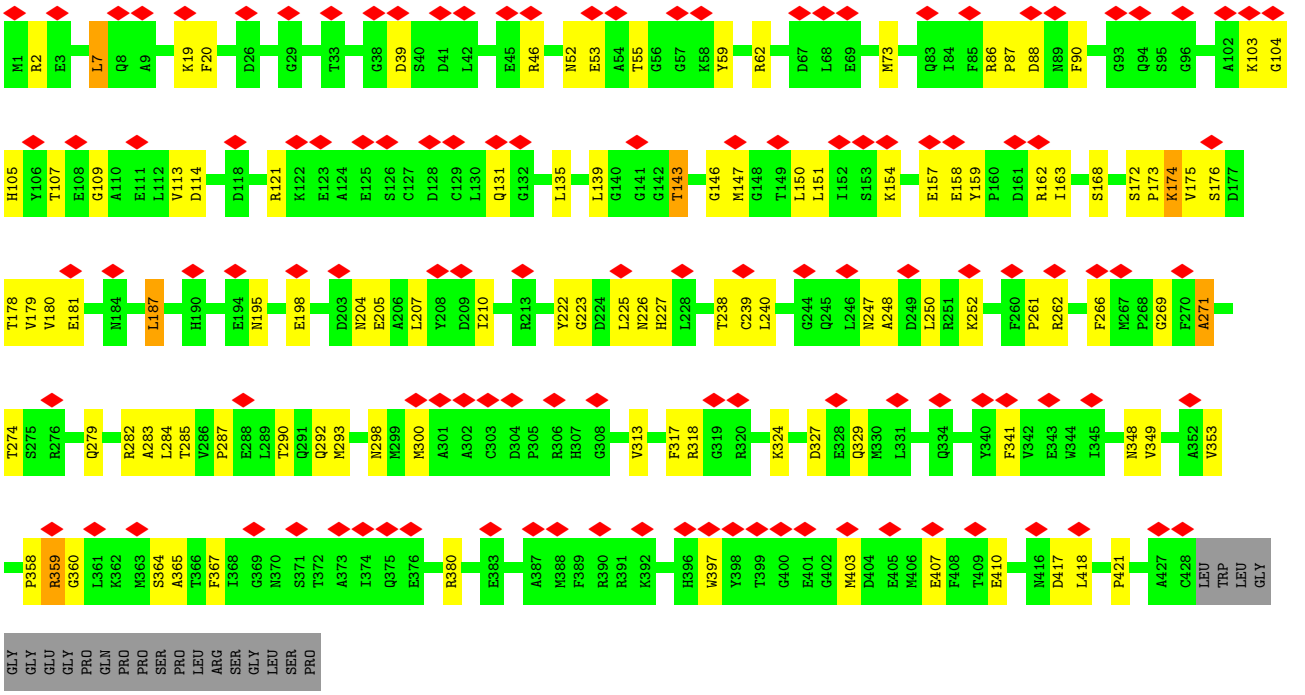

- Molecule 41: Tubulin beta chain

Chain TM:



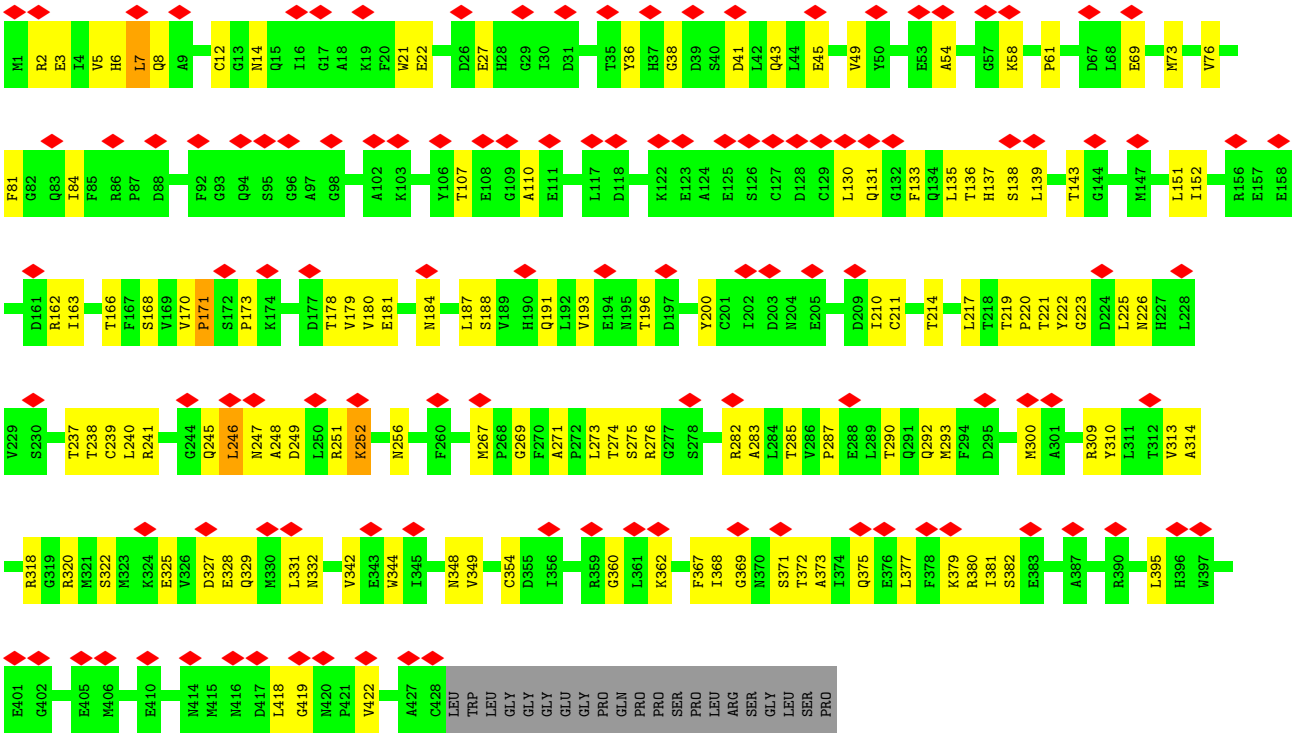

- Molecule 41: Tubulin beta chain

Chain TN:



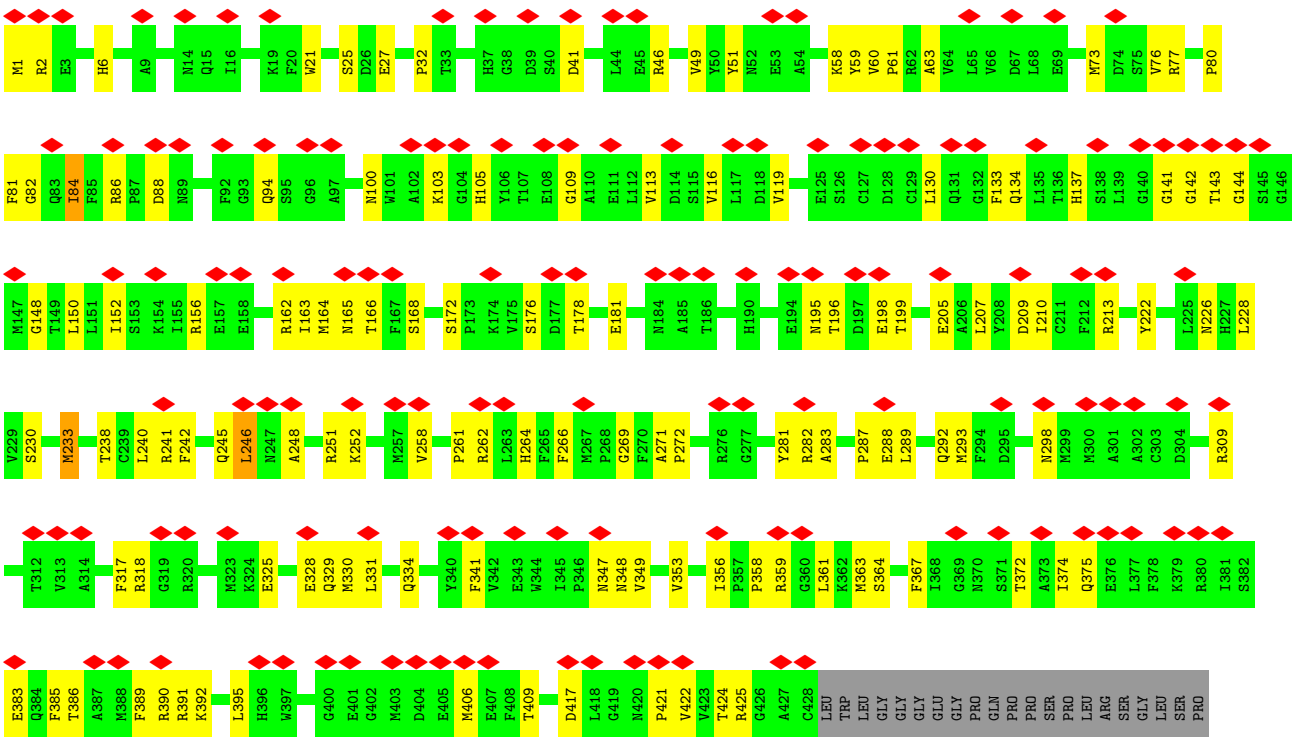

- Molecule 41: Tubulin beta chain

Chain TO:



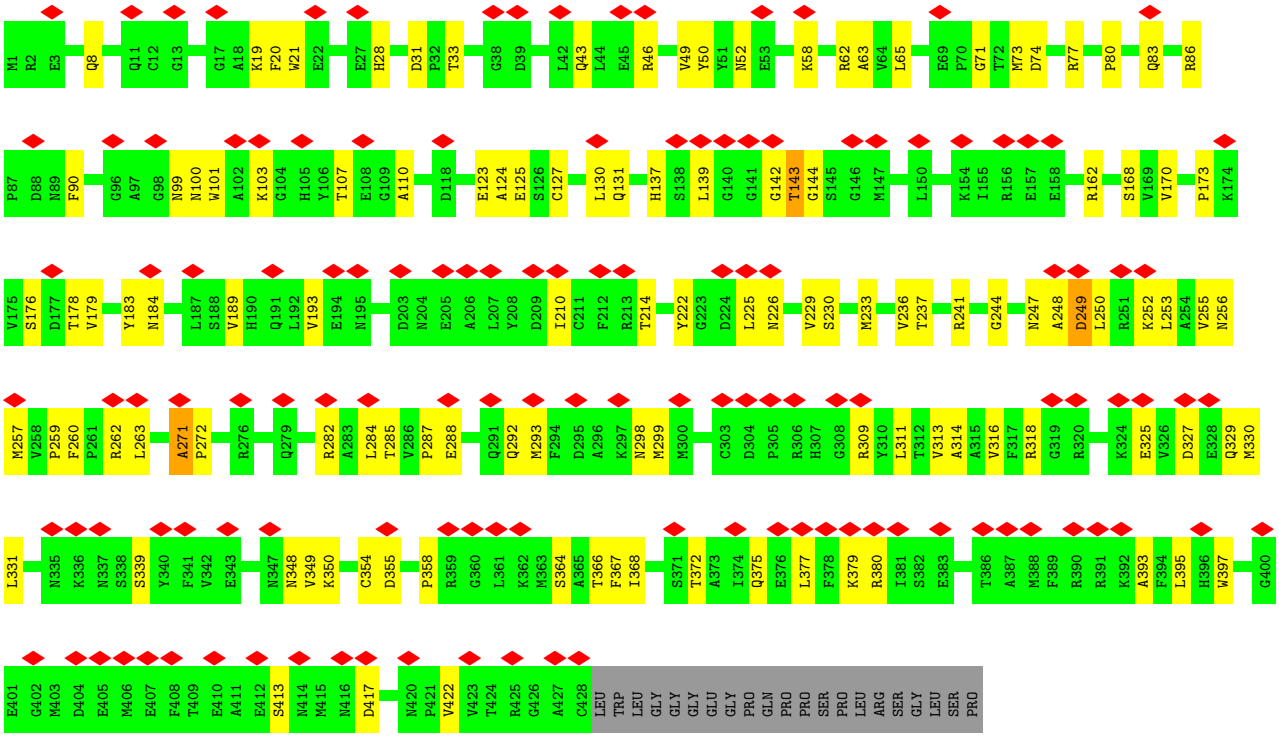

• Molecule 41: Tubulin beta chain

Chain TP:



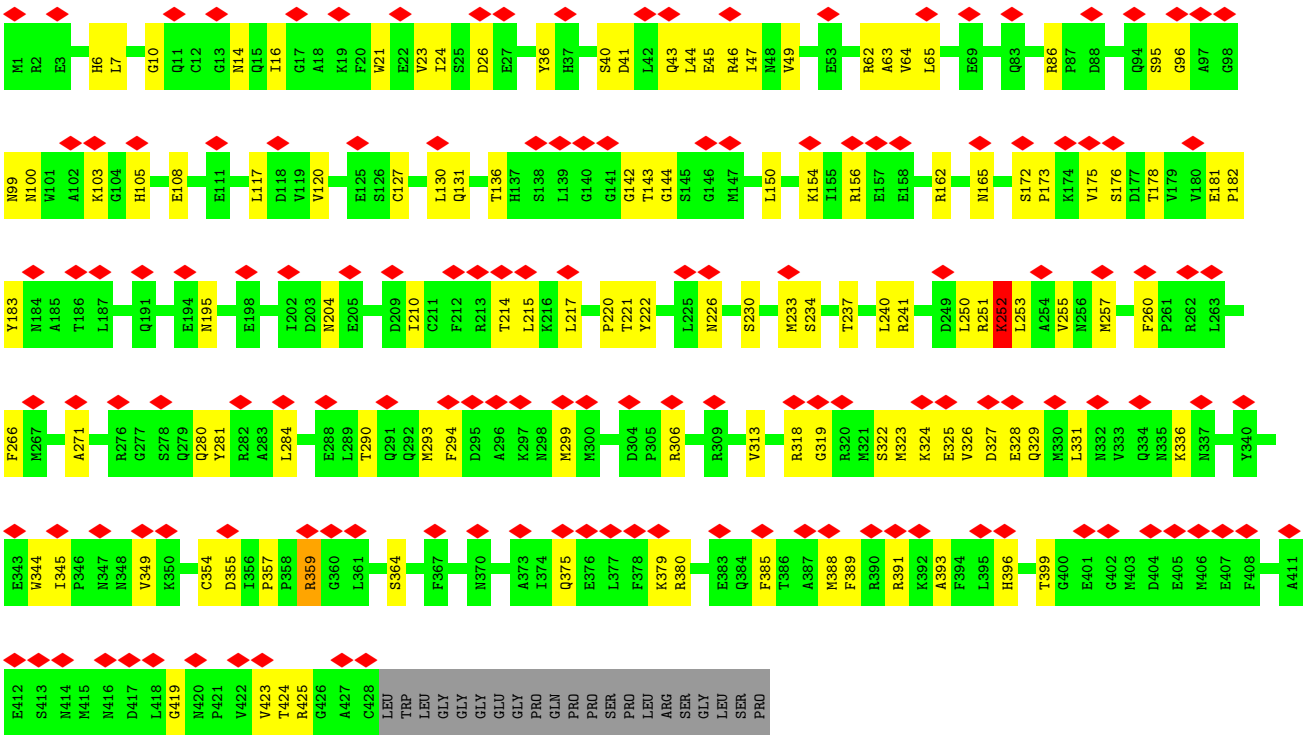

• Molecule 41: Tubulin beta chain

Chain UB:



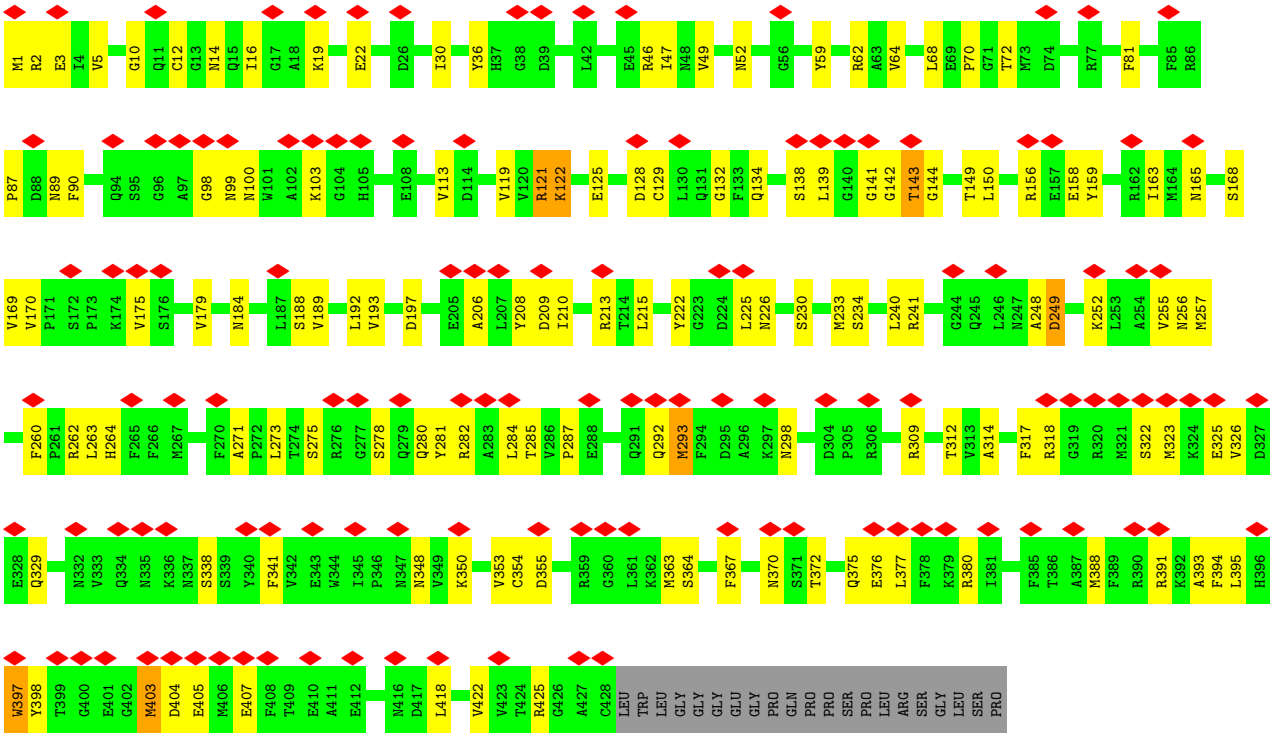

- Molecule 41: Tubulin beta chain

Chain UM:



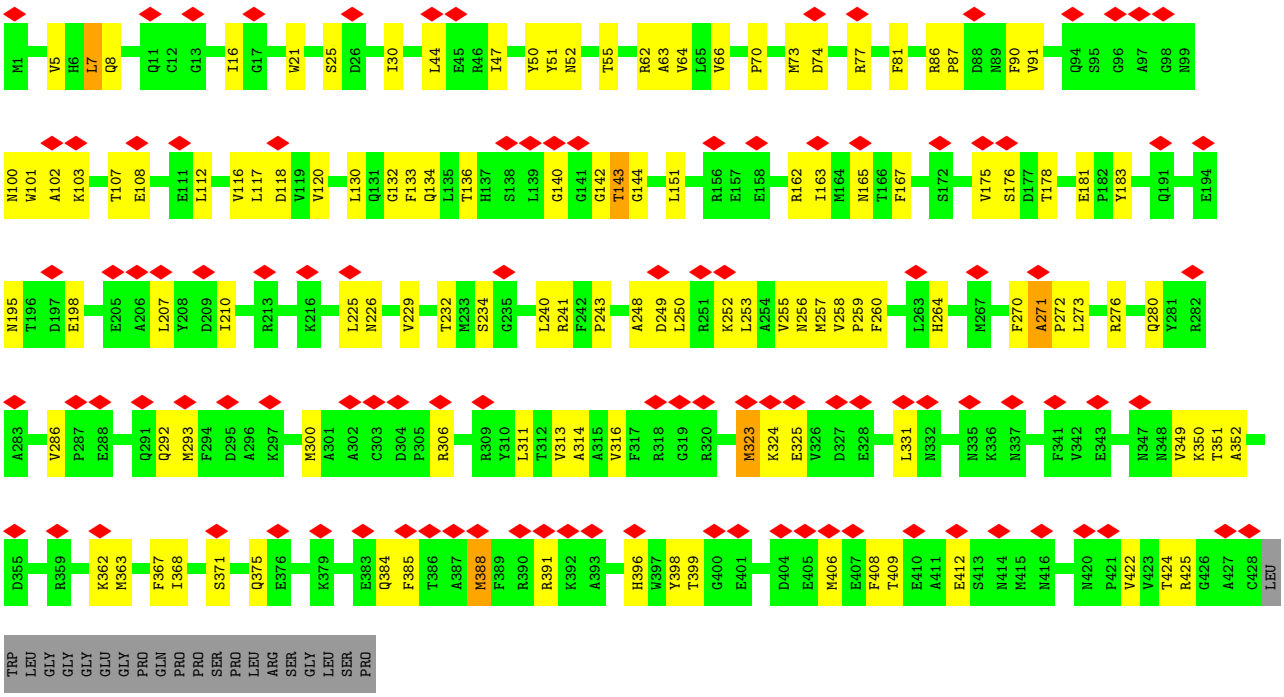

- Molecule 41: Tubulin beta chain

Chain UN: 29% 64% 30% • 5%



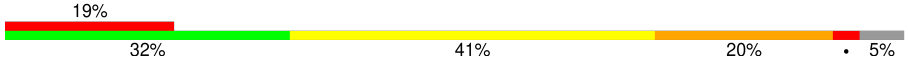

• Molecule 41: Tubulin beta chain

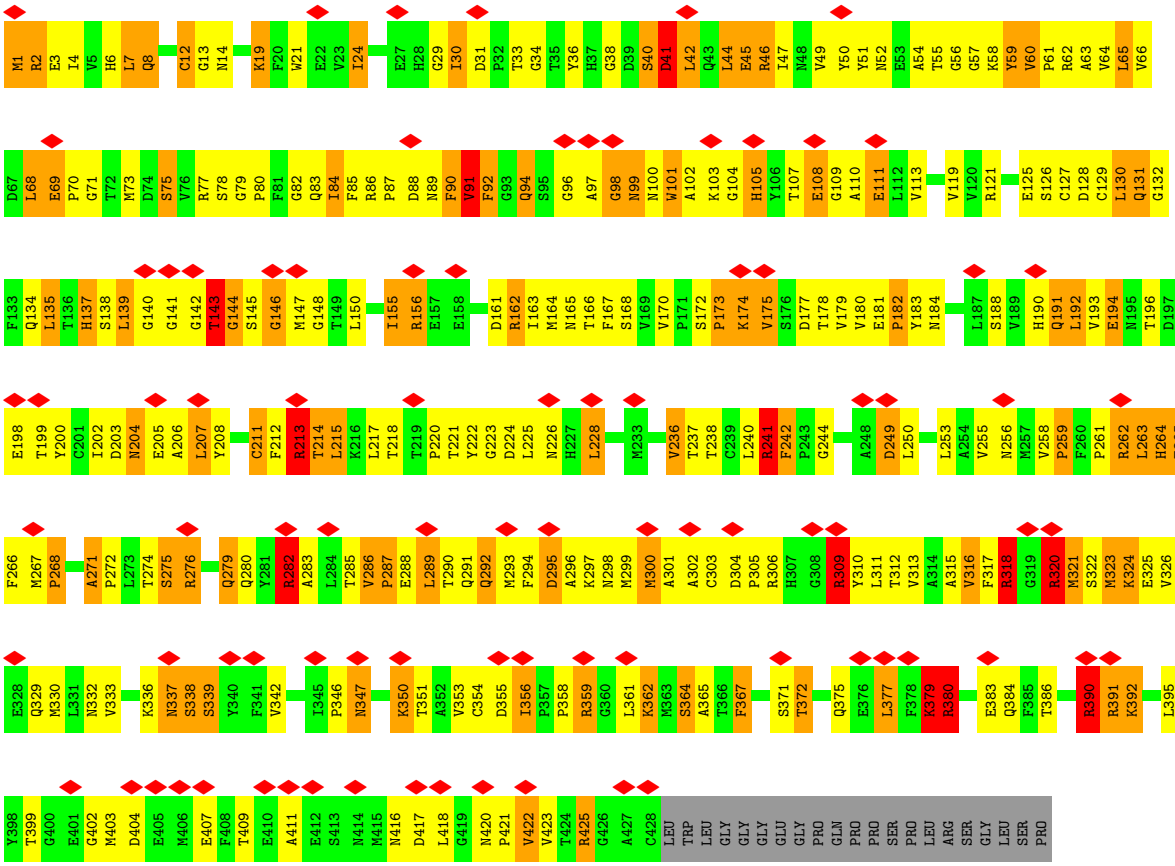
Chain UO: 23% 68% 26% • 5%




• Molecule 41: Tubulin beta chain

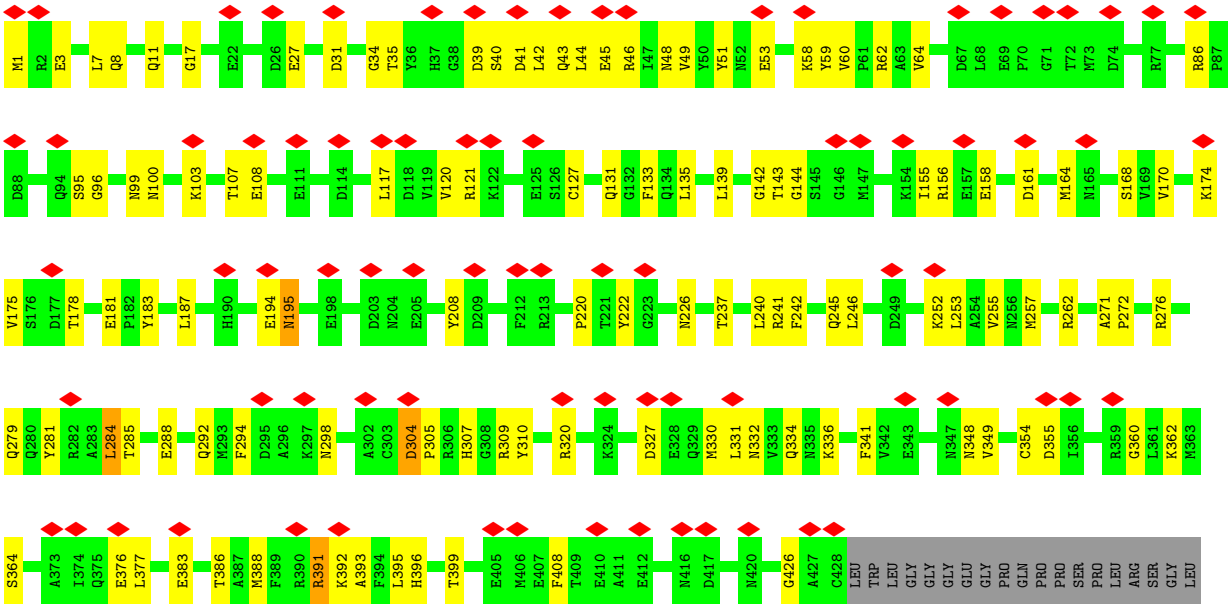
Chain UP:




- Molecule 41: Tubulin beta chain

Chain VB:



SER PRO

• Molecule 41: Tubulin beta chain

Chain VN:

M1 R2 H6 L7 Q8 A9 G10 Q11 C12 G13 N14 Q15 F20 W21 E22 S25 D26 E27 H28 D31 P32 T33 H37 G38 D39 S40 D41 L42 E45 R46 I47 N48 Y51 K58 A63 V66 D67 L68 E69 R77 F81 R86 P87 D88 V91

Q94 N100 K103 T107 E108 G109 A110 E111 D114 D118 R121 K122 E123 A124 E125 D128 C129 Q134 L135 G141 G142 T143 G144 S145 G146 M147 G148 T149 L150 L151 I152 S153 K154 I155 R156 E157 E158 D161 N165 T166 F167 P171 S172 P173 K174 V175 S176 D177

T178 V179 V180 E181 N184 S188 V189 H190 E194 N195 Y200 L207 Y208 D209 I210 C211 F212 L215 Y222 G223 D224 L225 N226 S230 M233 S234 G235 V236 T237 T238 R241 F242 P243 D249 L250 R251 K252 L253 A254 V255 F266 M267 P268 G269 F270 A271 P272 L273

R276 Q280 Y281 R282 V286 P287 E288 L289 T290 Q291 Q292 D295 N298 M299 M300 C303 D304 P305 R306 R309 A314 R318 G319 R320 K324 D327 E328 Q329 M330 L331 N337 F341 V342 E343 N347 N348 V349 C354 D355 I356 R359 G360 M363

T366 F367 I368 Q375 E376 R380 I381 S382 E383 Q384 F385 R390 R391 K392 W397 G400 E401 G402 M403 D404 E405 M406 E407 E410 A411 E412 S413 N414 M415 N416 D417 N420 A427 C428 LEU TRP LEU GLY GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER

GLY LEU SER PRO

• Molecule 41: Tubulin beta chain

Chain VO:

M1 I4 V5 H6 L7 G10 Q11 C12 G13 N14 Q15 I16 K19 F20 W21 E22 D26 D39 S40 D41 E45 R46 I47 N48 N52 E53 A54 T55 K58 P61 R62 A63 V64 L65 V66 D67 L68 E69 T72 M73 D74 F81 G82 Q83 I84 F85 R86 P87 D88

V91 Q94 S95 G96 A97 G98 N99 K103 T107 E108 G109 A110 E111 L112 V113 D114 S115 V116 L117 D118 K122 E125 S126 C127 D128 C129 G132 F133 Q134 L135 S138 G142 T143 G144 S145 G146 L151 K154 I155 R156 E157 P160 D161 M164 N165 T166 F167

K174 V175 S176 D177 T178 V179 V180 E181 N184 L187 S188 V189 L192 V193 E194 N195 T196 D203 N204 E205 A206 L207 Y208 D209 I210 R213 T214 L215 T221 Y222 G223 D224 V229 T232 M233 T237 R241 D249 L250 R251 K252 V255 F260 P261 R262 L263

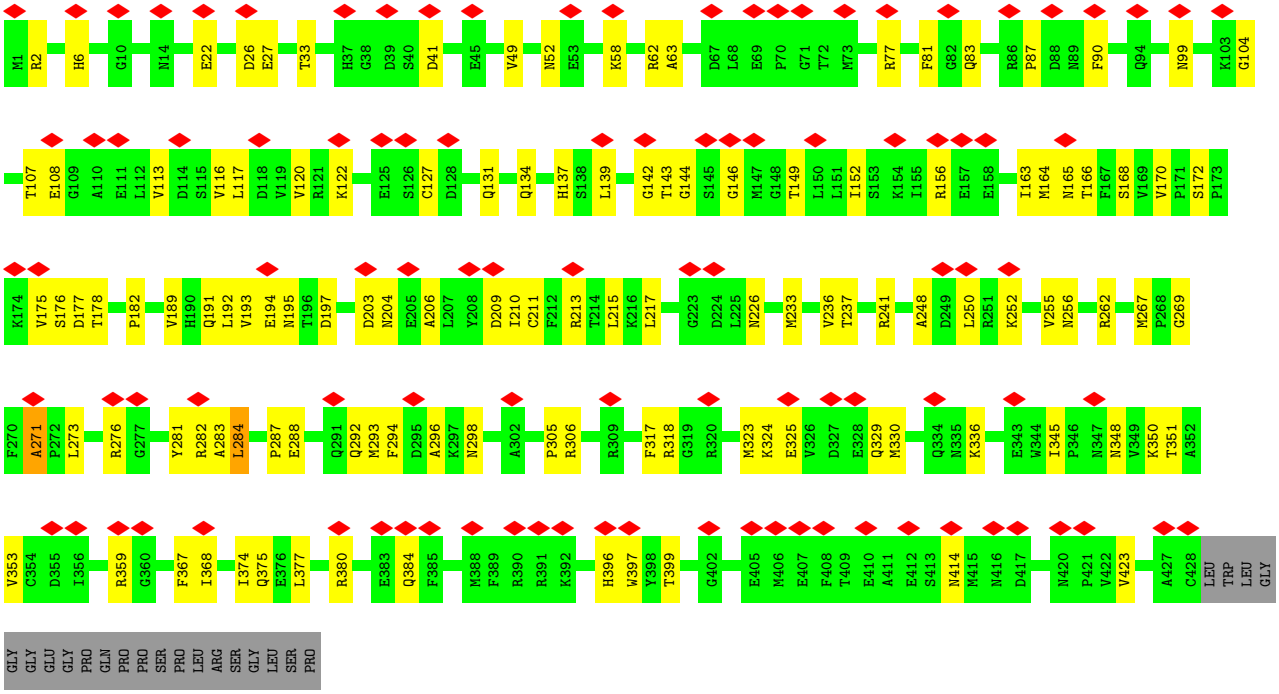
P268 A271 P272 L273 T274 S275 R276 G277 S278 Y281 R282 A283 L284 T290 Q291 Q292 D295 A296 K297 M300 C303 D304 P305 R306 H307 G308 R309 Y310 A314 A315 V316 F317 R320 M323 K324 E325 V326 D327 E328 Q329 M330 L331 N332 V333 Q334 N335 K336 F341 V342

E343 N347 N348 V349 K350 V353 C354 D355 L361 A365 I368 Q375 E376 L377 F378 K379 R380 E383 R391 K392 A393 H396 T399 G402 E405 M406 E407 E410 A411 E412 N416 D417 L418 G419 N420 P421 V422 V423 T424 R425 G426 A427 C428 LEU TRP LEU

GLY GLY GLY GLU GLY PRO GLN PRO PRO SER SER PRO LEU ARG SER GLY LEU SER PRO

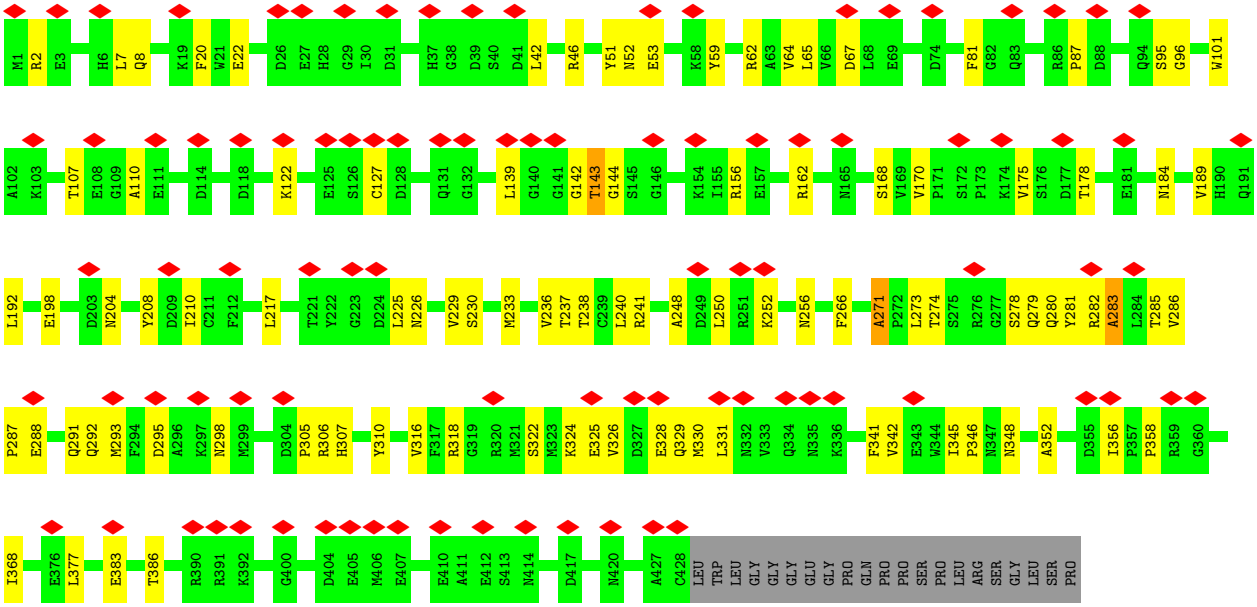
• Molecule 41: Tubulin beta chain

Chain VP: 23% 68% 27% 5%



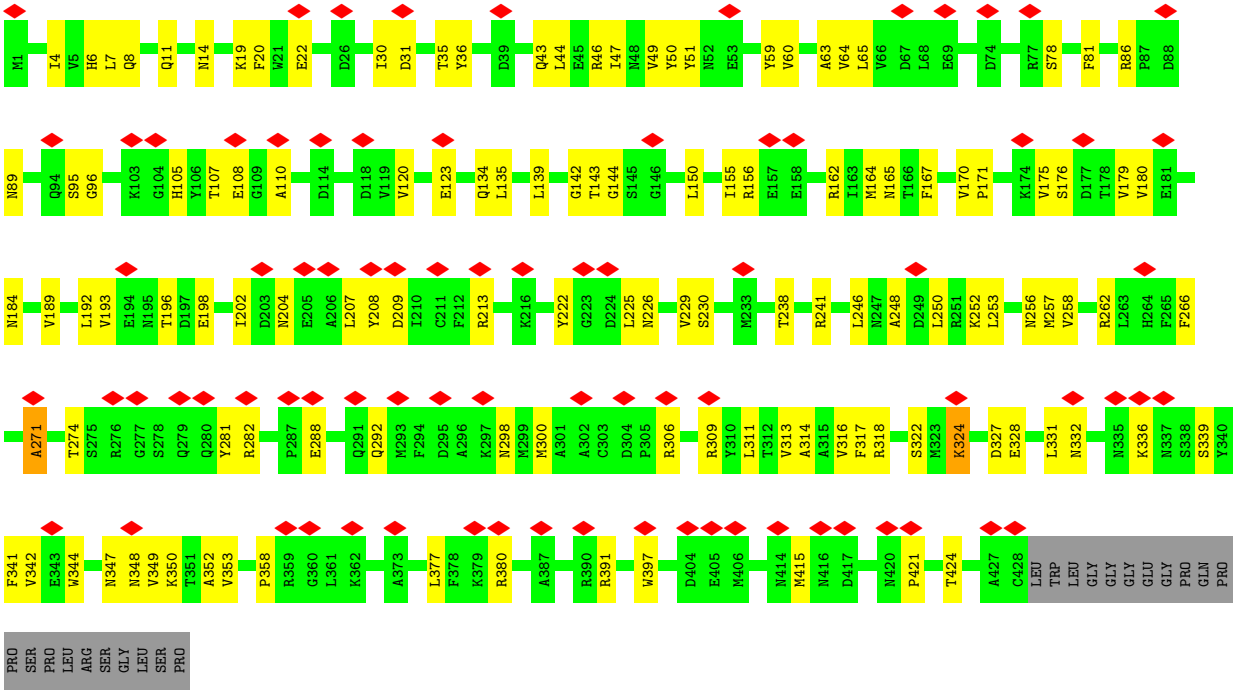

• Molecule 41: Tubulin beta chain

Chain VQ: 21% 73% 22% • 5%



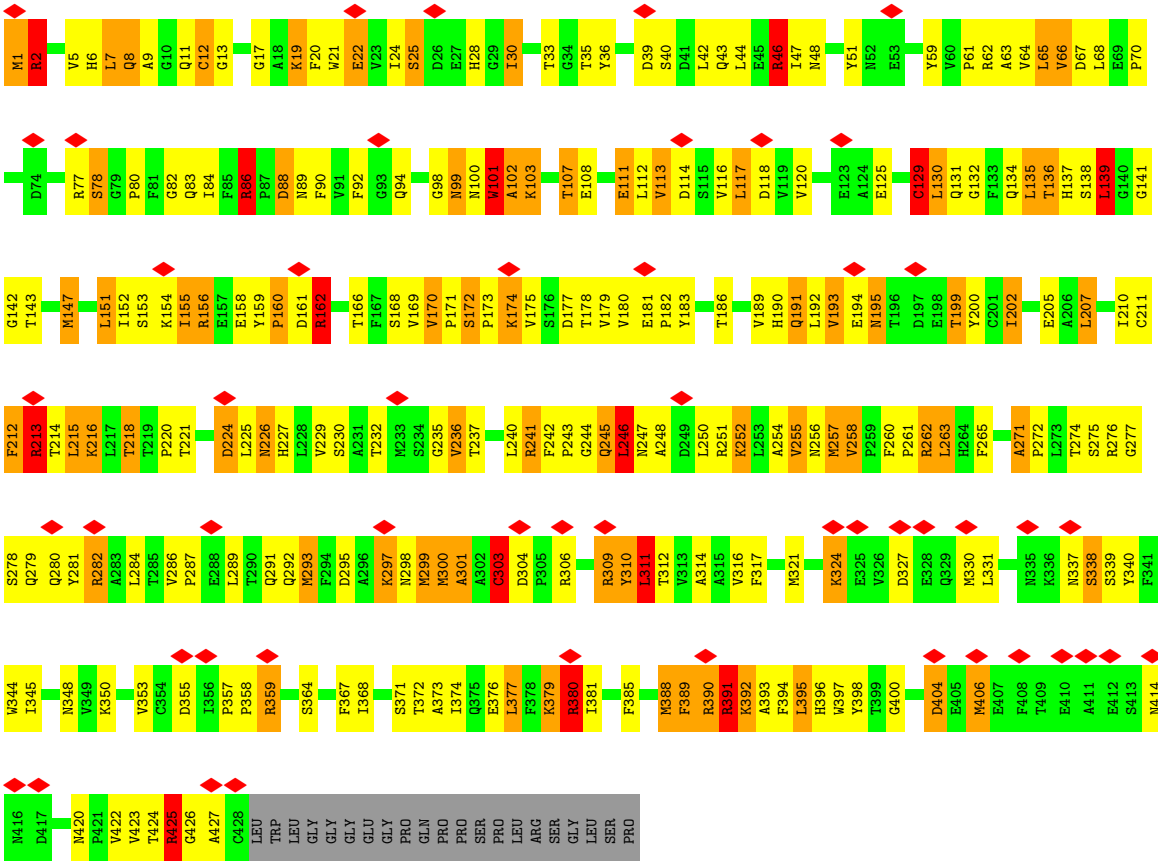

• Molecule 41: Tubulin beta chain

Chain WB: 18% 67% 28% 5%



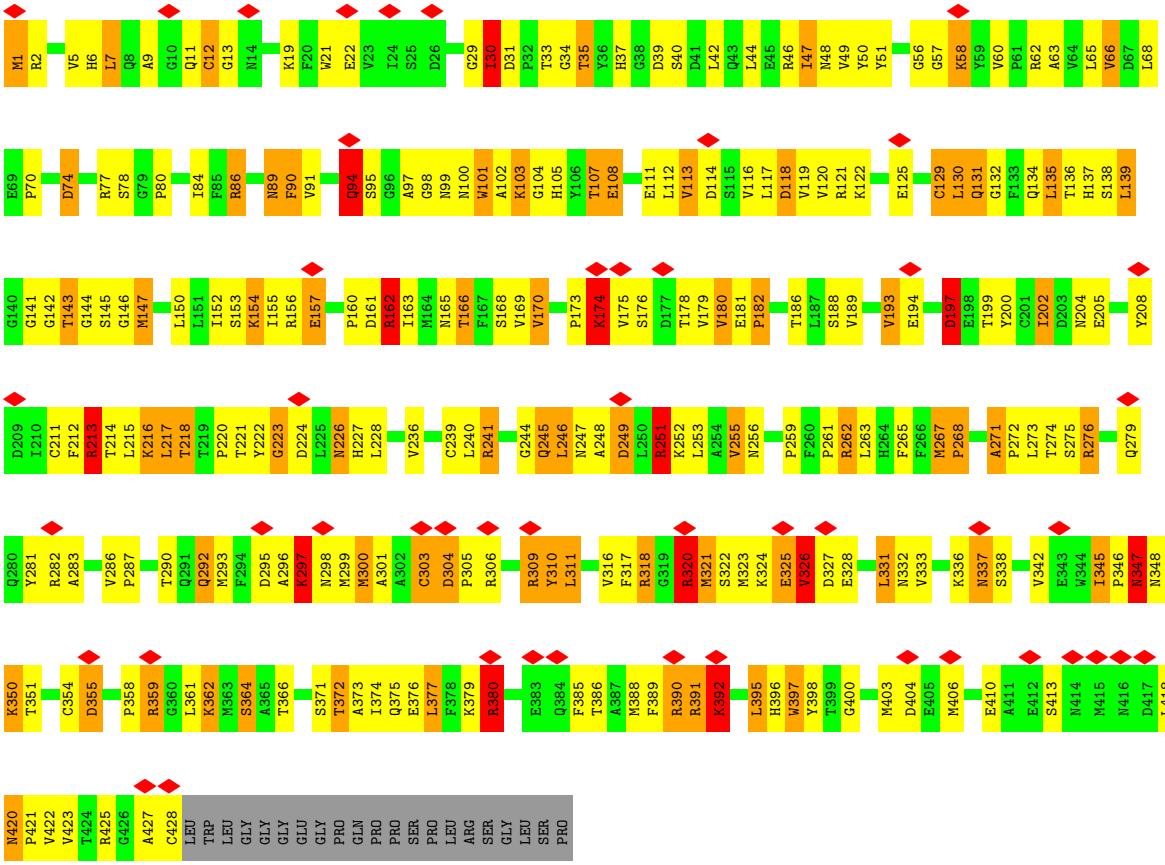
- Molecule 41: Tubulin beta chain

Chain WM:



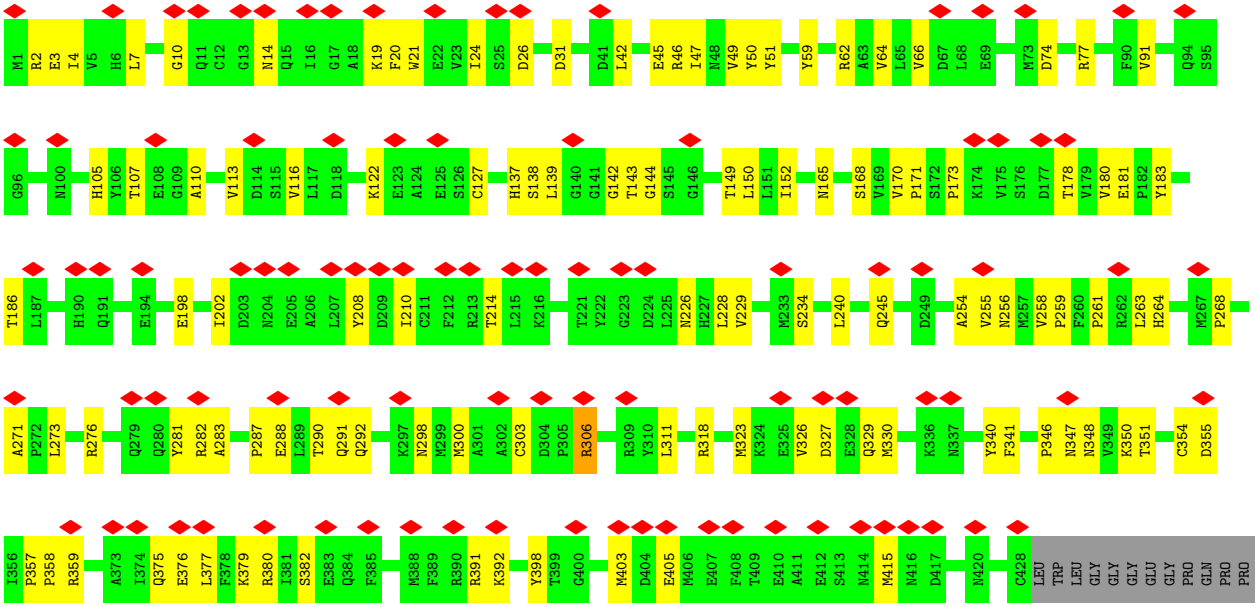
- Molecule 41: Tubulin beta chain

Chain WN:




- Molecule 41: Tubulin beta chain

Chain WO:



SER PRO LEU ARG SER GLY LEU SER PRO

- Molecule 41: Tubulin beta chain

Chain WP: 17% 73% 22% 5%

M1 R2 H6 Q11 F20 W21 E22 D26 E27 I30 T33 Y36 D39 S40 D41 L42 Q43 L44 I47 Y50 Y51 N52 E53 K58 Y59 R62 A63 L68 E69 D74 R77 F81 N89 Q94 S95 G96 N99 K103 G104 H105

Y106 T107 E108 G109 A110 D114 D118 V119 E123 C127 G132 F133 Q134 G140 G141 G142 T143 G144 S145 G146 L150 K154 R162 I163 M164 N165 P173 K174 V175 S176 D177 T178 V179 V180 E181 N184 L187 H190 E194 N195 E198 D203 N204 E205

A206 I210 C211 F212 R213 T214 L215 K216 L217 P220 T221 Y222 G223 D224 L225 N226 V229 M233 T238 C239 L240 P243 C244 Q245 A248 D249 L250 R251 K252 V255 N256 M257 V258 R262 A271 P272 L273 T274 Y281 R282 T285 V286 P287 E288 Q291 Q292 M293

K297 R306 H307 G308 R309 Y310 L311 T312 V313 V316 F317 R318 S322 M323 K324 E325 V326 D327 E328 Q329 M330 L331 N332 V333 Q334 N335 K336 N337 S338 S339 Y340 F341 V342 E343 W344 N347 N348 V349 A352 D355 I356 P357 P358 K362 F367 Q375 E376 R380

L395 G400 D404 E405 M406 E407 E410 A411 E412 N416 D417 N420 P421 V422 V423 T424 A427 C428 LEU TRP LEU GLY GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER GLY LEU SER PRO

- Molecule 41: Tubulin beta chain

Chain WQ: 29% 73% 21% 6%

M1 R2 E3 I4 V5 H6 L7 Q8 A9 G10 N14 K19 E22 D26 E27 D31 D39 S40 D41 L42 Q43 V49 Y50 Y51 Y59 A63 V64 L65 V66 D67 L68 E69 P70 G71 T72 M73 R77 S78 Q83 R86 P87 D88 F92 G93 Q94 S95

G98 N99 N100 K103 G104 H105 Y106 T107 E108 G109 A110 E111 L112 V113 D114 L117 D118 R121 F133 Q134 L135 T136 L139 G140 G141 G142 T143 G144 S145 G146 L150 L151 I155 R156 E157 E158 Y159 R162 I163 M164 F167 S168 V169 V170 K174 V175 S176 D177 T178

E181 V189 H190 Q191 L192 V193 E194 E198 C201 I202 D203 N204 E205 D209 I210 C211 F212 R213 Y222 G223 D224 L225 N226 M233 S234 G235 L240 R241 F242 P243 G244 Q245 L246 N247 A248 D249 L253 M257 R262 L263 H264 F265 F266 M267 A271 P272 L273 T274 S275

R276 G277 S278 Q279 R282 A283 E288 L289 Q292 M293 K297 N298 M299 M300 A301 A302 C303 D304 P305 R306 H307 G308 R309 Y310 L311 T312 V313 R318 G319 R320 M321 SER MET LYS GLU VAL ASP GLU Q329 M330 L331 N332 V333 Q334 N335 K336 M337 F341 V342 E343 W344 I345 P346 N347

N348 V349 D355 P358 R359 G360 M363 S364 F367 I368 T372 E376 L377 F378 K379 R380 E383 Q384 F385 M388 F389 R390 R391 K392 A393 F394 L395 H396 T399 G400 E401 G402 M403 D404 E405 M406 E407 F408 T409 E410 A411 E412 S413 N414 M415 N416 D417 M420 P421

A427 C428 LEU TRP LEU GLY GLY GLY GLU GLY PRO GLN PRO PRO SER PRO LEU ARG SER GLY LEU SER PRO

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 113809 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 2.382 | Depositor |
| Minimum map value | 0.000 | Depositor |
| Average map value | 0.011 | Depositor |
| Map value standard deviation | 0.079 | Depositor |
| Recommended contour level | 0.35 | Depositor |
| Map size (Å) | 686.08, 686.08, 686.08 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.34, 1.34, 1.34 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 1A | 0.30 | 0/4550 | 0.63 | 2/6154 (0.0%) |
| 1 | 1B | 0.27 | 0/1148 | 0.60 | 1/1555 (0.1%) |
| 2 | 1C | 0.35 | 0/1727 | 0.74 | 0/2313 |
| 2 | 1D | 0.35 | 0/1727 | 0.70 | 1/2313 (0.0%) |
| 3 | 1F | 0.31 | 0/1400 | 0.61 | 0/1875 |
| 3 | 1G | 0.61 | 0/1400 | 0.59 | 0/1875 |
| 4 | 1H | 0.39 | 0/1644 | 0.76 | 1/2193 (0.0%) |
| 4 | 1I | 0.34 | 0/729 | 0.82 | 1/967 (0.1%) |
| 4 | 1J | 0.34 | 0/981 | 0.76 | 1/1313 (0.1%) |
| 5 | 1L | 0.38 | 0/1316 | 0.78 | 1/1760 (0.1%) |
| 5 | 1M | 0.33 | 0/2106 | 0.73 | 2/2823 (0.1%) |
| 5 | 1N | 0.33 | 0/875 | 0.70 | 0/1175 |
| 6 | 1P | 0.30 | 0/724 | 0.62 | 0/974 |
| 6 | 1Q | 0.29 | 0/694 | 0.58 | 0/935 |
| 7 | 1S | 0.35 | 0/4812 | 0.66 | 0/6518 |
| 7 | 1T | 0.65 | 0/4812 | 0.66 | 0/6518 |
| 7 | 1U | 0.33 | 0/4812 | 0.67 | 1/6518 (0.0%) |
| 8 | 1W | 0.36 | 0/2736 | 0.79 | 1/3616 (0.0%) |
| 8 | 1X | 0.50 | 0/2305 | 0.80 | 2/3061 (0.1%) |
| 8 | 1Y | 0.32 | 0/1339 | 0.68 | 0/1784 |
| 8 | 1Z | 0.36 | 0/1690 | 0.76 | 0/2237 |
| 9 | 2B | 0.39 | 0/3244 | 0.75 | 1/4299 (0.0%) |
| 9 | 2C | 0.36 | 0/671 | 0.75 | 1/890 (0.1%) |
| 10 | 2E | 0.34 | 0/954 | 0.66 | 1/1289 (0.1%) |
| 10 | 2F | 0.37 | 1/954 (0.1%) | 0.69 | 2/1289 (0.2%) |
| 10 | 2G | 0.29 | 0/954 | 0.65 | 1/1289 (0.1%) |
| 11 | 2I | 0.52 | 1/2068 (0.0%) | 0.63 | 1/2777 (0.0%) |
| 11 | 2J | 0.32 | 0/2071 | 0.66 | 1/2780 (0.0%) |
| 11 | 2K | 0.43 | 0/1985 | 0.58 | 0/2656 |
| 12 | 2M | 0.30 | 0/1810 | 0.63 | 1/2447 (0.0%) |
| 12 | 2N | 0.33 | 0/1810 | 0.69 | 1/2447 (0.0%) |
| 12 | 2O | 0.43 | 0/1810 | 0.68 | 2/2447 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 12 | 2P | 0.32 | 0/1810 | 0.64 | 0/2447 |
| 12 | 2Q | 0.33 | 0/1810 | 0.67 | 1/2447 (0.0%) |
| 12 | 2R | 0.32 | 0/1810 | 0.68 | 3/2447 (0.1%) |
| 13 | 2T | 0.63 | 0/1573 | 0.66 | 0/2122 |
| 13 | 2U | 0.60 | 0/1573 | 0.67 | 0/2122 |
| 13 | 2V | 0.60 | 0/1573 | 0.65 | 0/2122 |
| 13 | 2W | 0.60 | 0/1573 | 0.66 | 0/2122 |
| 13 | 2X | 0.65 | 0/1573 | 0.68 | 0/2122 |
| 14 | 3A | 0.29 | 0/951 | 0.62 | 0/1294 |
| 14 | 3B | 0.31 | 0/951 | 0.71 | 2/1294 (0.2%) |
| 14 | 3C | 0.32 | 0/951 | 0.61 | 0/1294 |
| 15 | 3E | 0.31 | 0/3254 | 0.60 | 1/4383 (0.0%) |
| 15 | 3F | 0.34 | 0/3279 | 0.64 | 3/4418 (0.1%) |
| 15 | 3G | 0.29 | 0/1102 | 0.57 | 0/1477 |
| 15 | 3H | 0.31 | 0/2481 | 0.62 | 0/3342 |
| 16 | 3J | 0.33 | 0/3272 | 0.62 | 2/4409 (0.0%) |
| 16 | 3K | 0.31 | 0/2583 | 0.64 | 2/3471 (0.1%) |
| 16 | 3L | 0.30 | 0/3272 | 0.61 | 1/4409 (0.0%) |
| 16 | 3M | 0.28 | 0/955 | 0.64 | 0/1294 |
| 17 | 3O | 0.40 | 0/3220 | 0.65 | 4/4342 (0.1%) |
| 17 | 3P | 0.66 | 0/3220 | 0.61 | 0/4342 |
| 17 | 3Q | 0.65 | 0/1066 | 0.61 | 0/1436 |
| 17 | 3R | 0.62 | 0/2179 | 0.58 | 0/2941 |
| 18 | 3T | 0.32 | 0/3334 | 0.64 | 4/4495 (0.1%) |
| 18 | 3U | 0.34 | 0/3339 | 0.68 | 2/4502 (0.0%) |
| 18 | 3V | 0.29 | 0/1433 | 0.54 | 0/1934 |
| 18 | 3W | 0.30 | 0/2140 | 0.65 | 0/2881 |
| 19 | 3Y | 0.34 | 0/3013 | 0.65 | 2/4026 (0.0%) |
| 19 | 3Z | 0.44 | 0/198 | 0.56 | 0/266 |
| 20 | 4A | 0.63 | 0/1494 | 0.59 | 0/1989 |
| 20 | 4B | 0.64 | 0/951 | 0.60 | 0/1273 |
| 21 | 4D | 0.44 | 0/3944 | 0.67 | 3/5339 (0.1%) |
| 21 | 4E | 0.44 | 0/3944 | 0.63 | 2/5339 (0.0%) |
| 21 | 4F | 0.43 | 0/3944 | 0.64 | 0/5339 |
| 22 | 4H | 0.33 | 0/2970 | 0.67 | 2/4009 (0.0%) |
| 22 | 4I | 0.38 | 0/5138 | 0.65 | 1/6912 (0.0%) |
| 22 | 4J | 0.40 | 0/5169 | 0.74 | 10/6956 (0.1%) |
| 22 | 4K | 0.50 | 0/2015 | 0.67 | 1/2698 (0.0%) |
| 23 | 4M | 0.66 | 0/1374 | 0.67 | 0/1862 |
| 23 | 4N | 0.68 | 1/1364 (0.1%) | 0.63 | 0/1851 |
| 23 | 4P | 0.68 | 1/729 (0.1%) | 0.62 | 0/981 |
| 23 | 4Q | 0.69 | 0/1103 | 0.64 | 0/1490 |
| 23 | 4R | 0.67 | 0/1362 | 0.64 | 0/1843 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 24 | 4O | 0.69 | 0/726 | 0.70 | 1/978 (0.1%) |
| 25 | 4T | 0.36 | 0/1360 | 0.70 | 1/1847 (0.1%) |
| 26 | 4V | 0.33 | 0/3009 | 0.72 | 3/4063 (0.1%) |
| 26 | 4W | 0.35 | 0/3009 | 0.72 | 3/4063 (0.1%) |
| 27 | 4Y | 0.31 | 0/2195 | 0.64 | 2/2970 (0.1%) |
| 27 | 4Z | 0.30 | 0/2212 | 0.71 | 4/2995 (0.1%) |
| 28 | 5B | 0.36 | 0/1671 | 0.68 | 3/2267 (0.1%) |
| 29 | 5D | 0.30 | 0/720 | 0.68 | 0/974 |
| 29 | 5E | 0.31 | 0/288 | 0.73 | 0/390 |
| 30 | 5G | 0.29 | 0/729 | 0.64 | 0/996 |
| 31 | 5I | 0.36 | 0/3672 | 0.72 | 1/4968 (0.0%) |
| 31 | 5J | 0.32 | 0/915 | 0.66 | 0/1234 |
| 32 | 5L | 0.34 | 0/749 | 0.73 | 0/1010 |
| 33 | 5N | 0.36 | 0/2907 | 0.73 | 3/3851 (0.1%) |
| 33 | 5O | 0.36 | 0/1286 | 0.72 | 1/1707 (0.1%) |
| 34 | 5Q | 0.36 | 0/2231 | 0.75 | 2/2965 (0.1%) |
| 34 | 5R | 0.64 | 0/1681 | 0.64 | 0/2226 |
| 35 | 5T | 0.30 | 0/1164 | 0.65 | 1/1592 (0.1%) |
| 35 | 5U | 0.31 | 0/229 | 0.75 | 0/312 |
| 36 | 5W | 0.33 | 0/1917 | 0.78 | 0/2595 |
| 36 | 5X | 0.33 | 0/1917 | 0.79 | 4/2595 (0.2%) |
| 36 | 5Y | 0.30 | 0/1521 | 0.79 | 2/2056 (0.1%) |
| 36 | 5Z | 0.34 | 0/504 | 0.76 | 1/682 (0.1%) |
| 37 | 6A | 0.32 | 0/1019 | 0.82 | 0/1382 |
| 38 | 6C | 0.41 | 0/1746 | 0.81 | 2/2348 (0.1%) |
| 38 | 6D | 0.31 | 0/511 | 0.67 | 0/690 |
| 39 | 6F | 0.30 | 0/1290 | 0.53 | 0/1743 |
| 39 | 6G | 0.30 | 0/1290 | 0.53 | 0/1743 |
| 39 | 6H | 0.30 | 0/1153 | 0.65 | 0/1551 |
| 39 | 6I | 0.26 | 0/1290 | 0.56 | 0/1743 |
| 39 | 6J | 0.24 | 0/1290 | 0.50 | 0/1743 |
| 39 | 6K | 0.28 | 0/1290 | 0.58 | 0/1743 |
| 39 | 6L | 0.39 | 0/1115 | 0.60 | 1/1506 (0.1%) |
| 40 | AA | 0.31 | 0/3520 | 0.61 | 1/4778 (0.0%) |
| 40 | AE | 0.32 | 0/3520 | 0.61 | 1/4778 (0.0%) |
| 40 | AF | 0.33 | 0/3520 | 0.63 | 4/4778 (0.1%) |
| 40 | AG | 0.32 | 0/3520 | 0.60 | 0/4778 |
| 40 | AH | 0.31 | 0/3520 | 0.59 | 0/4778 |
| 40 | BA | 0.32 | 0/3520 | 0.62 | 2/4778 (0.0%) |
| 40 | BE | 0.66 | 0/3520 | 0.66 | 0/4778 |
| 40 | BF | 0.35 | 0/3475 | 0.67 | 1/4717 (0.0%) |
| 40 | BG | 0.66 | 3/3469 (0.1%) | 0.94 | 7/4709 (0.1%) |
| 40 | BH | 0.66 | 0/3520 | 0.66 | 0/4778 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 40 | BI | 0.66 | 0/2998 | 0.66 | 0/4064 |
| 40 | CA | 0.66 | 0/3520 | 0.67 | 0/4778 |
| 40 | CE | 0.33 | 0/3516 | 0.67 | 1/4774 (0.0%) |
| 40 | CF | 0.35 | 0/3520 | 0.67 | 2/4778 (0.0%) |
| 40 | CG | 0.33 | 0/3520 | 0.67 | 2/4778 (0.0%) |
| 40 | CH | 0.66 | 0/3520 | 0.68 | 0/4778 |
| 40 | CI | 0.32 | 0/3520 | 0.64 | 0/4778 |
| 40 | DA | 0.66 | 0/3467 | 0.67 | 0/4706 |
| 40 | DE | 0.65 | 0/3487 | 0.66 | 0/4733 |
| 40 | DF | 0.65 | 0/3467 | 0.67 | 0/4706 |
| 40 | DG | 0.31 | 0/3475 | 0.64 | 1/4717 (0.0%) |
| 40 | DH | 0.66 | 0/3475 | 0.69 | 0/4717 |
| 40 | DI | 0.66 | 0/3467 | 0.66 | 0/4706 |
| 40 | EA | 0.33 | 0/3483 | 0.62 | 1/4728 (0.0%) |
| 40 | EE | 0.31 | 0/3492 | 0.64 | 0/4739 |
| 40 | EF | 0.33 | 0/3492 | 0.63 | 0/4739 |
| 40 | EG | 0.36 | 1/3483 (0.0%) | 0.69 | 3/4728 (0.1%) |
| 40 | EH | 0.66 | 0/3475 | 0.67 | 0/4717 |
| 40 | EI | 0.66 | 0/3483 | 0.65 | 0/4728 |
| 40 | FA | 0.65 | 0/3483 | 0.67 | 0/4728 |
| 40 | FE | 0.30 | 0/3483 | 0.65 | 2/4728 (0.0%) |
| 40 | FF | 0.34 | 0/3483 | 0.65 | 1/4728 (0.0%) |
| 40 | FG | 0.32 | 0/3475 | 0.65 | 2/4717 (0.0%) |
| 40 | FH | 0.33 | 0/3483 | 0.64 | 1/4728 (0.0%) |
| 40 | FI | 0.36 | 0/3479 | 0.67 | 2/4724 (0.0%) |
| 40 | GA | 0.37 | 0/3483 | 0.66 | 0/4728 |
| 40 | GE | 0.66 | 0/3483 | 0.65 | 0/4728 |
| 40 | GF | 0.32 | 0/3475 | 0.65 | 0/4717 |
| 40 | GG | 0.38 | 0/3475 | 0.66 | 4/4717 (0.1%) |
| 40 | GH | 0.65 | 0/3475 | 0.66 | 0/4717 |
| 40 | GI | 0.66 | 0/3483 | 0.66 | 0/4728 |
| 40 | HA | 0.32 | 0/3487 | 0.67 | 1/4733 (0.0%) |
| 40 | HE | 0.66 | 0/3475 | 0.63 | 0/4717 |
| 40 | HF | 0.30 | 0/3469 | 0.63 | 1/4709 (0.0%) |
| 40 | HG | 0.34 | 0/3479 | 0.68 | 1/4723 (0.0%) |
| 40 | HH | 0.32 | 0/3483 | 0.65 | 3/4728 (0.1%) |
| 40 | HI | 0.33 | 0/3492 | 0.65 | 0/4739 |
| 40 | IA | 0.35 | 0/3483 | 0.69 | 1/4728 (0.0%) |
| 40 | IE | 0.31 | 0/3356 | 0.61 | 0/4554 |
| 40 | IF | 0.32 | 0/3483 | 0.65 | 1/4728 (0.0%) |
| 40 | IG | 0.33 | 0/3475 | 0.67 | 3/4717 (0.1%) |
| 40 | IH | 0.35 | 0/3483 | 0.63 | 0/4728 |
| 40 | II | 0.33 | 0/3483 | 0.65 | 0/4728 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 40 | JA | 0.33 | 0/3483 | 0.65 | 0/4728 |
| 40 | JD | 0.32 | 0/3483 | 0.68 | 3/4728 (0.1%) |
| 40 | JE | 0.34 | 0/3483 | 0.66 | 2/4728 (0.0%) |
| 40 | JF | 0.32 | 0/3475 | 0.63 | 2/4717 (0.0%) |
| 40 | JG | 0.32 | 0/3520 | 0.63 | 0/4778 |
| 40 | JH | 0.30 | 0/3475 | 0.60 | 1/4717 (0.0%) |
| 40 | KA | 0.32 | 0/3483 | 0.64 | 1/4728 (0.0%) |
| 40 | KD | 0.33 | 0/3475 | 0.62 | 3/4717 (0.1%) |
| 40 | KE | 0.31 | 0/3479 | 0.60 | 0/4722 |
| 40 | KF | 0.63 | 5/3483 (0.1%) | 0.74 | 5/4728 (0.1%) |
| 40 | KG | 0.32 | 0/3520 | 0.65 | 2/4778 (0.0%) |
| 40 | KH | 0.33 | 0/3520 | 0.64 | 1/4778 (0.0%) |
| 40 | LA | 0.32 | 0/3520 | 0.59 | 0/4778 |
| 40 | LD | 0.31 | 0/3475 | 0.61 | 1/4717 (0.0%) |
| 40 | LE | 0.33 | 0/3520 | 0.65 | 3/4778 (0.1%) |
| 40 | LF | 0.66 | 0/3475 | 0.68 | 0/4717 |
| 40 | LG | 0.66 | 0/3483 | 0.68 | 0/4728 |
| 40 | LH | 0.33 | 0/3483 | 0.61 | 1/4728 (0.0%) |
| 40 | MA | 0.66 | 0/3469 | 0.67 | 0/4709 |
| 40 | MD | 0.33 | 0/3483 | 0.61 | 3/4728 (0.1%) |
| 40 | ME | 0.33 | 1/3483 (0.0%) | 0.63 | 3/4728 (0.1%) |
| 40 | MF | 0.66 | 0/3475 | 0.68 | 0/4717 |
| 40 | MG | 0.66 | 0/3475 | 0.67 | 0/4717 |
| 40 | MH | 0.66 | 0/3475 | 0.67 | 0/4717 |
| 40 | NA | 0.32 | 0/3469 | 0.64 | 2/4709 (0.0%) |
| 40 | ND | 0.65 | 0/3475 | 0.64 | 0/4717 |
| 40 | NE | 0.32 | 0/3479 | 0.68 | 3/4723 (0.1%) |
| 40 | NF | 0.31 | 0/3475 | 0.60 | 0/4717 |
| 40 | NG | 0.33 | 0/3469 | 0.66 | 0/4709 |
| 40 | NH | 0.32 | 0/3475 | 0.66 | 3/4717 (0.1%) |
| 40 | OA | 0.33 | 0/3499 | 0.65 | 0/4749 |
| 40 | OD | 0.34 | 0/3483 | 0.67 | 1/4728 (0.0%) |
| 40 | OE | 0.32 | 0/3483 | 0.66 | 2/4728 (0.0%) |
| 40 | OF | 0.33 | 0/3496 | 0.66 | 2/4744 (0.0%) |
| 40 | OG | 0.32 | 0/3492 | 0.67 | 0/4740 |
| 40 | OH | 0.66 | 0/3496 | 0.68 | 0/4744 |
| 40 | PA | 0.36 | 0/3469 | 0.69 | 3/4709 (0.1%) |
| 40 | PD | 0.31 | 0/3265 | 0.67 | 5/4432 (0.1%) |
| 40 | PE | 0.32 | 0/3475 | 0.64 | 3/4717 (0.1%) |
| 40 | PF | 0.31 | 0/3475 | 0.67 | 0/4717 |
| 40 | PG | 0.32 | 0/3461 | 0.67 | 1/4698 (0.0%) |
| 40 | PH | 0.30 | 0/3461 | 0.64 | 1/4698 (0.0%) |
| 40 | QA | 0.32 | 0/3469 | 0.65 | 3/4709 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 40 | QE | 0.33 | 0/3461 | 0.65 | 1/4698 (0.0%) |
| 40 | QF | 0.32 | 0/3461 | 0.63 | 0/4698 |
| 40 | QG | 0.33 | 0/3467 | 0.68 | 4/4706 (0.1%) |
| 40 | QH | 0.33 | 0/3475 | 0.69 | 4/4717 (0.1%) |
| 40 | RA | 0.32 | 0/3467 | 0.68 | 4/4706 (0.1%) |
| 40 | RE | 0.32 | 0/3461 | 0.67 | 2/4698 (0.0%) |
| 40 | RF | 0.33 | 0/3461 | 0.70 | 1/4698 (0.0%) |
| 40 | RG | 0.33 | 0/3467 | 0.69 | 3/4706 (0.1%) |
| 40 | RH | 0.31 | 0/3461 | 0.65 | 1/4698 (0.0%) |
| 40 | RI | 0.32 | 0/3029 | 0.66 | 2/4108 (0.0%) |
| 40 | SA | 0.35 | 0/3467 | 0.67 | 2/4706 (0.0%) |
| 40 | SE | 0.34 | 0/3483 | 0.70 | 1/4728 (0.0%) |
| 40 | SF | 0.35 | 0/3467 | 0.73 | 3/4706 (0.1%) |
| 40 | SG | 0.34 | 0/3483 | 0.71 | 2/4728 (0.0%) |
| 40 | SH | 0.35 | 0/3475 | 0.69 | 4/4717 (0.1%) |
| 40 | SI | 0.30 | 0/3475 | 0.64 | 2/4717 (0.0%) |
| 40 | TA | 0.32 | 0/3467 | 0.65 | 0/4706 |
| 40 | TE | 0.31 | 0/3469 | 0.67 | 2/4709 (0.0%) |
| 40 | TF | 0.32 | 0/3469 | 0.68 | 0/4709 |
| 40 | TG | 0.34 | 0/3483 | 0.67 | 0/4728 |
| 40 | TH | 0.34 | 0/3475 | 0.69 | 3/4717 (0.1%) |
| 40 | TI | 0.31 | 0/3475 | 0.63 | 0/4717 |
| 40 | UA | 0.33 | 0/3475 | 0.69 | 5/4717 (0.1%) |
| 40 | UE | 0.32 | 0/3483 | 0.67 | 4/4728 (0.1%) |
| 40 | UF | 0.65 | 0/3483 | 0.66 | 0/4728 |
| 40 | UG | 0.35 | 0/3483 | 0.67 | 0/4728 |
| 40 | UH | 0.33 | 0/3475 | 0.68 | 1/4717 (0.0%) |
| 40 | UI | 0.66 | 0/3475 | 0.66 | 0/4717 |
| 40 | VA | 0.33 | 0/3520 | 0.67 | 3/4778 (0.1%) |
| 40 | VF | 0.32 | 0/3520 | 0.63 | 0/4778 |
| 40 | VG | 0.34 | 0/3475 | 0.68 | 3/4717 (0.1%) |
| 40 | VH | 0.31 | 0/3483 | 0.63 | 1/4728 (0.0%) |
| 40 | VI | 0.33 | 0/3520 | 0.65 | 1/4778 (0.0%) |
| 40 | VJ | 0.36 | 0/3475 | 0.71 | 3/4717 (0.1%) |
| 40 | WA | 0.32 | 0/3520 | 0.67 | 2/4778 (0.0%) |
| 40 | WE | 0.32 | 0/3520 | 0.62 | 0/4778 |
| 40 | WF | 0.33 | 0/3475 | 0.64 | 2/4717 (0.0%) |
| 40 | WG | 0.35 | 0/3467 | 0.67 | 5/4706 (0.1%) |
| 40 | WH | 0.33 | 0/3520 | 0.65 | 1/4778 (0.0%) |
| 40 | WI | 0.34 | 0/3475 | 0.65 | 2/4717 (0.0%) |
| 41 | AB | 0.30 | 0/3415 | 0.60 | 0/4628 |
| 41 | AL | 0.31 | 0/3415 | 0.63 | 2/4628 (0.0%) |
| 41 | AM | 0.34 | 1/3415 (0.0%) | 0.67 | 7/4628 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 41 | AN | 0.33 | 0/3415 | 0.63 | 0/4628 |
| 41 | AO | 0.66 | 0/3415 | 0.66 | 0/4628 |
| 41 | AP | 0.33 | 1/3415 (0.0%) | 0.65 | 5/4628 (0.1%) |
| 41 | BB | 0.65 | 0/3415 | 0.67 | 0/4628 |
| 41 | BL | 0.33 | 1/3415 (0.0%) | 0.66 | 2/4628 (0.0%) |
| 41 | BM | 0.66 | 0/3415 | 0.67 | 0/4628 |
| 41 | BN | 0.34 | 0/3415 | 0.70 | 3/4628 (0.1%) |
| 41 | BO | 0.66 | 0/3415 | 0.67 | 0/4628 |
| 41 | BP | 0.66 | 0/3415 | 0.69 | 1/4628 (0.0%) |
| 41 | CB | 0.33 | 0/3415 | 0.70 | 5/4628 (0.1%) |
| 41 | CL | 0.65 | 0/3415 | 0.67 | 0/4628 |
| 41 | CM | 0.66 | 0/3415 | 0.68 | 0/4628 |
| 41 | CN | 0.65 | 0/3415 | 0.69 | 0/4628 |
| 41 | CO | 0.65 | 0/3415 | 0.69 | 0/4628 |
| 41 | CP | 0.66 | 0/3415 | 0.67 | 0/4628 |
| 41 | DB | 0.66 | 0/3415 | 0.69 | 1/4628 (0.0%) |
| 41 | DL | 0.66 | 0/3415 | 0.67 | 1/4628 (0.0%) |
| 41 | DM | 0.65 | 0/3415 | 0.69 | 0/4628 |
| 41 | DN | 0.65 | 0/3415 | 0.68 | 0/4628 |
| 41 | DO | 0.33 | 0/3415 | 0.72 | 4/4628 (0.1%) |
| 41 | DP | 0.65 | 0/3411 | 0.67 | 0/4623 |
| 41 | EB | 0.33 | 0/3415 | 0.71 | 6/4628 (0.1%) |
| 41 | EL | 0.32 | 0/2882 | 0.67 | 3/3905 (0.1%) |
| 41 | EM | 0.65 | 0/3415 | 0.68 | 0/4628 |
| 41 | EN | 0.33 | 0/3415 | 0.68 | 3/4628 (0.1%) |
| 41 | EO | 0.31 | 0/3415 | 0.66 | 1/4628 (0.0%) |
| 41 | EP | 0.65 | 0/3415 | 0.70 | 0/4628 |
| 41 | FB | 0.33 | 1/3415 (0.0%) | 0.66 | 2/4628 (0.0%) |
| 41 | FM | 0.33 | 0/3415 | 0.68 | 2/4628 (0.0%) |
| 41 | FN | 0.37 | 1/3415 (0.0%) | 0.71 | 5/4628 (0.1%) |
| 41 | FO | 0.34 | 0/3415 | 0.69 | 3/4628 (0.1%) |
| 41 | FP | 0.34 | 0/3415 | 0.72 | 4/4628 (0.1%) |
| 41 | GB | 0.33 | 0/3415 | 0.66 | 6/4628 (0.1%) |
| 41 | GM | 0.33 | 0/3415 | 0.71 | 3/4628 (0.1%) |
| 41 | GN | 0.65 | 0/3415 | 0.67 | 0/4628 |
| 41 | GO | 0.37 | 0/3409 | 0.72 | 2/4621 (0.0%) |
| 41 | GP | 0.34 | 0/3415 | 0.71 | 5/4628 (0.1%) |
| 41 | HB | 0.33 | 1/3415 (0.0%) | 0.65 | 1/4628 (0.0%) |
| 41 | HM | 0.32 | 0/3415 | 0.66 | 1/4628 (0.0%) |
| 41 | HN | 0.64 | 0/3415 | 0.66 | 0/4628 |
| 41 | HO | 0.33 | 0/3415 | 0.67 | 1/4628 (0.0%) |
| 41 | HP | 0.32 | 0/3415 | 0.71 | 3/4628 (0.1%) |
| 41 | HQ | 0.34 | 0/3415 | 0.70 | 5/4628 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 41 | IB | 0.32 | 0/3415 | 0.65 | 1/4628 (0.0%) |
| 41 | IM | 0.33 | 0/3415 | 0.67 | 1/4628 (0.0%) |
| 41 | IN | 0.33 | 0/3415 | 0.65 | 1/4628 (0.0%) |
| 41 | IO | 0.32 | 0/3415 | 0.68 | 3/4628 (0.1%) |
| 41 | IP | 0.33 | 0/3415 | 0.65 | 3/4628 (0.1%) |
| 41 | IQ | 0.32 | 0/3415 | 0.68 | 2/4628 (0.0%) |
| 41 | JB | 0.33 | 0/3415 | 0.68 | 1/4628 (0.0%) |
| 41 | JL | 0.34 | 0/3415 | 0.71 | 2/4628 (0.0%) |
| 41 | JM | 0.65 | 0/3415 | 0.67 | 0/4628 |
| 41 | JN | 0.33 | 0/3415 | 0.69 | 3/4628 (0.1%) |
| 41 | JO | 0.31 | 0/3415 | 0.65 | 1/4628 (0.0%) |
| 41 | KB | 0.33 | 0/3415 | 0.65 | 2/4628 (0.0%) |
| 41 | KL | 0.65 | 0/3415 | 0.68 | 0/4628 |
| 41 | KM | 0.33 | 0/3415 | 0.68 | 4/4628 (0.1%) |
| 41 | KN | 0.31 | 0/3415 | 0.63 | 1/4628 (0.0%) |
| 41 | KO | 0.33 | 0/3415 | 0.67 | 0/4628 |
| 41 | KP | 0.32 | 0/3073 | 0.63 | 1/4162 (0.0%) |
| 41 | LB | 0.31 | 0/3415 | 0.63 | 3/4628 (0.1%) |
| 41 | LL | 0.34 | 0/3415 | 0.64 | 4/4628 (0.1%) |
| 41 | LM | 0.31 | 0/3415 | 0.64 | 3/4628 (0.1%) |
| 41 | LN | 0.31 | 0/3415 | 0.61 | 1/4628 (0.0%) |
| 41 | LO | 0.32 | 0/3415 | 0.66 | 1/4628 (0.0%) |
| 41 | LP | 0.30 | 0/3415 | 0.63 | 0/4628 |
| 41 | MB | 0.32 | 0/3415 | 0.65 | 2/4628 (0.0%) |
| 41 | ML | 0.32 | 0/3415 | 0.64 | 2/4628 (0.0%) |
| 41 | MM | 0.34 | 1/3415 (0.0%) | 0.66 | 3/4628 (0.1%) |
| 41 | MN | 0.33 | 0/3415 | 0.61 | 0/4628 |
| 41 | MO | 0.66 | 0/3415 | 0.67 | 0/4628 |
| 41 | MP | 0.32 | 0/3415 | 0.64 | 2/4628 (0.0%) |
| 41 | NB | 0.32 | 0/3415 | 0.69 | 5/4628 (0.1%) |
| 41 | NL | 0.36 | 1/3415 (0.0%) | 0.71 | 2/4628 (0.0%) |
| 41 | NM | 0.31 | 0/3415 | 0.66 | 1/4628 (0.0%) |
| 41 | NN | 0.35 | 0/3415 | 0.69 | 3/4628 (0.1%) |
| 41 | NO | 0.32 | 0/3415 | 0.68 | 0/4628 |
| 41 | NP | 0.31 | 0/3336 | 0.67 | 1/4520 (0.0%) |
| 41 | OB | 0.32 | 0/3415 | 0.68 | 5/4628 (0.1%) |
| 41 | OL | 0.37 | 1/3415 (0.0%) | 0.74 | 4/4628 (0.1%) |
| 41 | OM | 0.34 | 0/3415 | 0.72 | 1/4628 (0.0%) |
| 41 | ON | 0.32 | 0/3415 | 0.67 | 3/4628 (0.1%) |
| 41 | OO | 0.34 | 0/3415 | 0.66 | 1/4628 (0.0%) |
| 41 | OP | 0.35 | 0/3415 | 0.71 | 8/4628 (0.2%) |
| 41 | PB | 0.34 | 0/3415 | 0.67 | 1/4628 (0.0%) |
| 41 | PL | 0.32 | 0/3415 | 0.66 | 0/4628 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 41 | PM | 0.33 | 0/3415 | 0.68 | 4/4628 (0.1%) |
| 41 | PN | 0.33 | 1/3415 (0.0%) | 0.66 | 1/4628 (0.0%) |
| 41 | PO | 0.31 | 0/3415 | 0.68 | 4/4628 (0.1%) |
| 41 | PP | 0.33 | 0/3415 | 0.70 | 2/4628 (0.0%) |
| 41 | QB | 0.65 | 0/3415 | 0.67 | 0/4628 |
| 41 | QL | 0.32 | 0/3415 | 0.68 | 5/4628 (0.1%) |
| 41 | QM | 0.34 | 0/3415 | 0.71 | 4/4628 (0.1%) |
| 41 | QN | 0.32 | 0/3415 | 0.69 | 5/4628 (0.1%) |
| 41 | QO | 0.41 | 2/3415 (0.1%) | 0.79 | 5/4628 (0.1%) |
| 41 | QP | 0.66 | 0/3400 | 0.68 | 0/4609 |
| 41 | RB | 0.34 | 0/3415 | 0.69 | 3/4628 (0.1%) |
| 41 | RL | 0.33 | 0/3415 | 0.68 | 2/4628 (0.0%) |
| 41 | RM | 0.33 | 0/3415 | 0.71 | 3/4628 (0.1%) |
| 41 | RN | 0.31 | 0/3415 | 0.68 | 2/4628 (0.0%) |
| 41 | RO | 0.34 | 0/3415 | 0.70 | 0/4628 |
| 41 | RP | 0.32 | 0/3415 | 0.68 | 0/4628 |
| 41 | SB | 0.35 | 0/3415 | 0.67 | 1/4628 (0.0%) |
| 41 | SL | 0.31 | 0/3024 | 0.67 | 0/4097 |
| 41 | SM | 0.33 | 1/3415 (0.0%) | 0.66 | 1/4628 (0.0%) |
| 41 | SN | 0.35 | 1/3415 (0.0%) | 0.73 | 4/4628 (0.1%) |
| 41 | SO | 0.65 | 0/3415 | 0.67 | 0/4628 |
| 41 | SP | 0.34 | 0/3415 | 0.69 | 1/4628 (0.0%) |
| 41 | TB | 0.35 | 1/3415 (0.0%) | 0.72 | 4/4628 (0.1%) |
| 41 | TL | 0.30 | 0/3083 | 0.66 | 0/4182 |
| 41 | TM | 0.34 | 0/3415 | 0.75 | 7/4628 (0.2%) |
| 41 | TN | 0.33 | 0/3415 | 0.71 | 4/4628 (0.1%) |
| 41 | TO | 0.34 | 0/3415 | 0.73 | 4/4628 (0.1%) |
| 41 | TP | 0.33 | 0/3415 | 0.71 | 3/4628 (0.1%) |
| 41 | UB | 0.33 | 0/3415 | 0.67 | 4/4628 (0.1%) |
| 41 | UM | 0.33 | 0/3415 | 0.70 | 3/4628 (0.1%) |
| 41 | UN | 0.37 | 0/3415 | 0.76 | 7/4628 (0.2%) |
| 41 | UO | 0.37 | 0/3415 | 0.73 | 4/4628 (0.1%) |
| 41 | UP | 0.65 | 0/3415 | 0.66 | 0/4628 |
| 41 | VB | 0.32 | 0/3415 | 0.68 | 5/4628 (0.1%) |
| 41 | VN | 0.32 | 0/3415 | 0.64 | 0/4628 |
| 41 | VO | 0.33 | 0/3415 | 0.70 | 4/4628 (0.1%) |
| 41 | VP | 0.32 | 0/3415 | 0.67 | 2/4628 (0.0%) |
| 41 | VQ | 0.33 | 0/3415 | 0.63 | 1/4628 (0.0%) |
| 41 | WB | 0.33 | 0/3415 | 0.67 | 3/4628 (0.1%) |
| 41 | WM | 0.65 | 0/3415 | 0.68 | 0/4628 |
| 41 | WN | 0.65 | 0/3415 | 0.67 | 0/4628 |
| 41 | WO | 0.32 | 0/3415 | 0.67 | 1/4628 (0.0%) |
| 41 | WP | 0.34 | 0/3415 | 0.65 | 1/4628 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 41 | WQ | 0.31 | 0/3358 | 0.69 | 4/4551 (0.1%) |
| All | All | 0.42 | 29/1130564 (0.0%) | 0.67 | 567/1531441 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | 1A | 0 | 3 |
| 3 | 1F | 0 | 1 |
| 5 | 1L | 0 | 4 |
| 5 | 1M | 0 | 1 |
| 5 | 1N | 0 | 1 |
| 7 | 1S | 0 | 3 |
| 7 | 1T | 0 | 19 |
| 7 | 1U | 0 | 3 |
| 8 | 1W | 0 | 1 |
| 8 | 1X | 0 | 7 |
| 9 | 2B | 0 | 2 |
| 10 | 2G | 0 | 2 |
| 11 | 2I | 0 | 6 |
| 11 | 2K | 0 | 1 |
| 12 | 2N | 0 | 1 |
| 12 | 2O | 0 | 1 |
| 12 | 2P | 0 | 1 |
| 12 | 2Q | 0 | 1 |
| 13 | 2T | 0 | 13 |
| 13 | 2U | 0 | 12 |
| 13 | 2V | 0 | 13 |
| 13 | 2W | 0 | 11 |
| 13 | 2X | 0 | 13 |
| 14 | 3C | 0 | 1 |
| 15 | 3E | 0 | 1 |
| 17 | 3O | 0 | 7 |
| 17 | 3P | 0 | 27 |
| 17 | 3Q | 0 | 8 |
| 17 | 3R | 0 | 8 |
| 18 | 3U | 0 | 1 |
| 19 | 3Y | 0 | 3 |
| 19 | 3Z | 0 | 1 |
| 20 | 4A | 0 | 18 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 20 | 4B | 0 | 8 |
| 21 | 4D | 0 | 7 |
| 21 | 4E | 0 | 5 |
| 21 | 4F | 0 | 6 |
| 22 | 4H | 0 | 3 |
| 22 | 4I | 0 | 6 |
| 22 | 4J | 0 | 4 |
| 22 | 4K | 0 | 5 |
| 23 | 4M | 0 | 6 |
| 23 | 4N | 0 | 5 |
| 23 | 4P | 0 | 4 |
| 23 | 4Q | 0 | 6 |
| 23 | 4R | 0 | 8 |
| 24 | 4O | 0 | 5 |
| 25 | 4T | 0 | 4 |
| 26 | 4V | 0 | 2 |
| 26 | 4W | 0 | 1 |
| 27 | 4Z | 0 | 1 |
| 28 | 5B | 0 | 1 |
| 29 | 5D | 0 | 1 |
| 30 | 5G | 0 | 1 |
| 31 | 5I | 0 | 3 |
| 33 | 5N | 0 | 1 |
| 33 | 5O | 0 | 1 |
| 34 | 5R | 0 | 15 |
| 35 | 5U | 0 | 1 |
| 36 | 5W | 0 | 2 |
| 36 | 5X | 0 | 1 |
| 38 | 6C | 0 | 5 |
| 38 | 6D | 0 | 1 |
| 39 | 6F | 0 | 1 |
| 39 | 6G | 0 | 2 |
| 39 | 6H | 0 | 1 |
| 39 | 6L | 0 | 3 |
| 40 | AA | 0 | 1 |
| 40 | AE | 0 | 1 |
| 40 | AF | 0 | 1 |
| 40 | AG | 0 | 1 |
| 40 | AH | 0 | 1 |
| 40 | BA | 0 | 1 |
| 40 | BE | 0 | 19 |
| 40 | BF | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 40 | BG | 0 | 1 |
| 40 | BH | 0 | 18 |
| 40 | BI | 0 | 15 |
| 40 | CA | 0 | 16 |
| 40 | CE | 0 | 1 |
| 40 | CF | 0 | 2 |
| 40 | CG | 0 | 1 |
| 40 | CH | 0 | 16 |
| 40 | CI | 0 | 2 |
| 40 | DA | 0 | 17 |
| 40 | DE | 0 | 18 |
| 40 | DF | 0 | 17 |
| 40 | DH | 0 | 15 |
| 40 | DI | 0 | 19 |
| 40 | EA | 0 | 1 |
| 40 | EE | 0 | 2 |
| 40 | EF | 0 | 2 |
| 40 | EG | 0 | 2 |
| 40 | EH | 0 | 12 |
| 40 | EI | 0 | 19 |
| 40 | FA | 0 | 19 |
| 40 | FF | 0 | 1 |
| 40 | FG | 0 | 3 |
| 40 | FI | 0 | 1 |
| 40 | GE | 0 | 14 |
| 40 | GF | 0 | 1 |
| 40 | GH | 0 | 16 |
| 40 | GI | 0 | 19 |
| 40 | HA | 0 | 2 |
| 40 | HE | 0 | 20 |
| 40 | HF | 0 | 1 |
| 40 | HG | 0 | 2 |
| 40 | HH | 0 | 1 |
| 40 | HI | 0 | 1 |
| 40 | IA | 0 | 2 |
| 40 | IE | 0 | 1 |
| 40 | IF | 0 | 1 |
| 40 | IG | 0 | 2 |
| 40 | IH | 0 | 1 |
| 40 | II | 0 | 1 |
| 40 | JA | 0 | 1 |
| 40 | JD | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 40 | JE | 0 | 1 |
| 40 | JF | 0 | 1 |
| 40 | JG | 0 | 3 |
| 40 | JH | 0 | 1 |
| 40 | KA | 0 | 3 |
| 40 | KD | 0 | 1 |
| 40 | KE | 0 | 1 |
| 40 | KF | 0 | 2 |
| 40 | KG | 0 | 1 |
| 40 | KH | 0 | 2 |
| 40 | LA | 0 | 1 |
| 40 | LD | 0 | 1 |
| 40 | LE | 0 | 4 |
| 40 | LF | 0 | 16 |
| 40 | LG | 0 | 18 |
| 40 | LH | 0 | 1 |
| 40 | MA | 0 | 13 |
| 40 | ME | 0 | 2 |
| 40 | MF | 0 | 16 |
| 40 | MG | 0 | 15 |
| 40 | MH | 0 | 18 |
| 40 | NA | 0 | 2 |
| 40 | ND | 0 | 18 |
| 40 | NE | 0 | 2 |
| 40 | NF | 0 | 1 |
| 40 | NG | 0 | 2 |
| 40 | NH | 0 | 1 |
| 40 | OA | 0 | 3 |
| 40 | OD | 0 | 4 |
| 40 | OE | 0 | 2 |
| 40 | OF | 0 | 1 |
| 40 | OG | 0 | 1 |
| 40 | OH | 0 | 18 |
| 40 | PA | 0 | 1 |
| 40 | PD | 0 | 1 |
| 40 | PE | 0 | 3 |
| 40 | PF | 0 | 1 |
| 40 | PG | 0 | 1 |
| 40 | PH | 0 | 1 |
| 40 | QA | 0 | 1 |
| 40 | QE | 0 | 2 |
| 40 | QF | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 40 | QG | 0 | 3 |
| 40 | QH | 0 | 1 |
| 40 | RA | 0 | 1 |
| 40 | RE | 0 | 1 |
| 40 | RF | 0 | 1 |
| 40 | RG | 0 | 2 |
| 40 | RH | 0 | 1 |
| 40 | RI | 0 | 3 |
| 40 | SA | 0 | 5 |
| 40 | SE | 0 | 2 |
| 40 | SF | 0 | 1 |
| 40 | SG | 0 | 1 |
| 40 | SH | 0 | 2 |
| 40 | SI | 0 | 2 |
| 40 | TA | 0 | 1 |
| 40 | TE | 0 | 1 |
| 40 | TF | 0 | 3 |
| 40 | TG | 0 | 1 |
| 40 | TH | 0 | 1 |
| 40 | TI | 0 | 2 |
| 40 | UA | 0 | 2 |
| 40 | UE | 0 | 2 |
| 40 | UF | 0 | 17 |
| 40 | UG | 0 | 1 |
| 40 | UH | 0 | 1 |
| 40 | UI | 0 | 17 |
| 40 | VA | 0 | 1 |
| 40 | VF | 0 | 1 |
| 40 | VG | 0 | 1 |
| 40 | VH | 0 | 2 |
| 40 | VI | 0 | 2 |
| 40 | VJ | 0 | 1 |
| 40 | WA | 0 | 1 |
| 40 | WE | 0 | 2 |
| 40 | WF | 0 | 1 |
| 40 | WG | 0 | 1 |
| 40 | WH | 0 | 2 |
| 40 | WI | 0 | 1 |
| 41 | AB | 0 | 2 |
| 41 | AL | 0 | 1 |
| 41 | AM | 0 | 1 |
| 41 | AN | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 41 | AO | 0 | 15 |
| 41 | AP | 0 | 1 |
| 41 | BB | 0 | 20 |
| 41 | BL | 0 | 1 |
| 41 | BM | 0 | 20 |
| 41 | BN | 0 | 4 |
| 41 | BO | 0 | 18 |
| 41 | BP | 0 | 18 |
| 41 | CB | 0 | 1 |
| 41 | CL | 0 | 19 |
| 41 | CM | 0 | 19 |
| 41 | CN | 0 | 19 |
| 41 | CO | 0 | 20 |
| 41 | CP | 0 | 19 |
| 41 | DB | 0 | 18 |
| 41 | DL | 0 | 16 |
| 41 | DM | 0 | 20 |
| 41 | DN | 0 | 18 |
| 41 | DO | 0 | 3 |
| 41 | DP | 0 | 23 |
| 41 | EB | 0 | 2 |
| 41 | EL | 0 | 2 |
| 41 | EM | 0 | 17 |
| 41 | EN | 0 | 1 |
| 41 | EO | 0 | 2 |
| 41 | EP | 0 | 17 |
| 41 | FB | 0 | 3 |
| 41 | FM | 0 | 3 |
| 41 | FN | 0 | 1 |
| 41 | FO | 0 | 1 |
| 41 | FP | 0 | 3 |
| 41 | GB | 0 | 1 |
| 41 | GM | 0 | 3 |
| 41 | GN | 0 | 19 |
| 41 | GP | 0 | 4 |
| 41 | HB | 0 | 1 |
| 41 | HM | 0 | 2 |
| 41 | HN | 0 | 20 |
| 41 | HO | 0 | 1 |
| 41 | HP | 0 | 2 |
| 41 | HQ | 0 | 1 |
| 41 | IB | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 41 | IM | 0 | 3 |
| 41 | IN | 0 | 2 |
| 41 | IO | 0 | 1 |
| 41 | IP | 0 | 1 |
| 41 | IQ | 0 | 1 |
| 41 | JB | 0 | 1 |
| 41 | JL | 0 | 2 |
| 41 | JM | 0 | 17 |
| 41 | JO | 0 | 2 |
| 41 | KB | 0 | 1 |
| 41 | KL | 0 | 16 |
| 41 | KM | 0 | 3 |
| 41 | KN | 0 | 2 |
| 41 | KO | 0 | 1 |
| 41 | KP | 0 | 1 |
| 41 | LB | 0 | 1 |
| 41 | LL | 0 | 1 |
| 41 | LM | 0 | 1 |
| 41 | LN | 0 | 1 |
| 41 | LO | 0 | 1 |
| 41 | LP | 0 | 2 |
| 41 | MB | 0 | 1 |
| 41 | ML | 0 | 1 |
| 41 | MM | 0 | 2 |
| 41 | MN | 0 | 2 |
| 41 | MO | 0 | 16 |
| 41 | MP | 0 | 2 |
| 41 | NB | 0 | 2 |
| 41 | NL | 0 | 4 |
| 41 | NM | 0 | 1 |
| 41 | NN | 0 | 2 |
| 41 | NO | 0 | 2 |
| 41 | NP | 0 | 2 |
| 41 | OB | 0 | 3 |
| 41 | OL | 0 | 2 |
| 41 | OM | 0 | 2 |
| 41 | ON | 0 | 1 |
| 41 | OO | 0 | 1 |
| 41 | OP | 0 | 3 |
| 41 | PB | 0 | 1 |
| 41 | PL | 0 | 1 |
| 41 | PM | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 41 | PN | 0 | 2 |
| 41 | PO | 0 | 1 |
| 41 | PP | 0 | 1 |
| 41 | QB | 0 | 19 |
| 41 | QL | 0 | 1 |
| 41 | QO | 0 | 1 |
| 41 | QP | 0 | 18 |
| 41 | RB | 0 | 4 |
| 41 | RL | 0 | 1 |
| 41 | RM | 0 | 2 |
| 41 | RO | 0 | 2 |
| 41 | RP | 0 | 1 |
| 41 | SB | 0 | 3 |
| 41 | SL | 0 | 2 |
| 41 | SM | 0 | 1 |
| 41 | SN | 0 | 2 |
| 41 | SO | 0 | 20 |
| 41 | SP | 0 | 3 |
| 41 | TB | 0 | 1 |
| 41 | TL | 0 | 1 |
| 41 | TM | 0 | 2 |
| 41 | TN | 0 | 1 |
| 41 | TO | 0 | 3 |
| 41 | TP | 0 | 1 |
| 41 | UB | 0 | 2 |
| 41 | UM | 0 | 2 |
| 41 | UN | 0 | 2 |
| 41 | UO | 0 | 1 |
| 41 | UP | 0 | 18 |
| 41 | VB | 0 | 1 |
| 41 | VN | 0 | 1 |
| 41 | VO | 0 | 2 |
| 41 | VP | 0 | 1 |
| 41 | VQ | 0 | 2 |
| 41 | WB | 0 | 1 |
| 41 | WM | 0 | 19 |
| 41 | WN | 0 | 19 |
| 41 | WO | 0 | 1 |
| 41 | WP | 0 | 1 |
| 41 | WQ | 0 | 1 |
| All | All | 0 | 1619 |

All (29) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 40 | BG | 298 | PRO | CG-CD | -27.70 | 0.59 | 1.50 |
| 40 | KF | 298 | PRO | CB-CG | 20.07 | 2.50 | 1.50 |
| 40 | KF | 298 | PRO | CG-CD | -18.29 | 0.90 | 1.50 |
| 40 | BG | 298 | PRO | CB-CG | 14.73 | 2.23 | 1.50 |
| 41 | QO | 61 | PRO | CG-CD | -12.65 | 1.08 | 1.50 |
| 40 | BG | 297 | GLU | C-N | 10.38 | 1.53 | 1.34 |
| 40 | KF | 297 | GLU | C-N | 10.15 | 1.53 | 1.34 |
| 40 | KF | 298 | PRO | N-CD | 10.12 | 1.62 | 1.47 |
| 40 | KF | 298 | PRO | CA-CB | -8.71 | 1.36 | 1.53 |
| 11 | 2I | 83 | PRO | CB-CG | 7.98 | 1.89 | 1.50 |
| 41 | MM | 194 | GLU | CA-CB | 7.34 | 1.70 | 1.53 |
| 41 | FN | 324 | LYS | CB-CG | -7.21 | 1.33 | 1.52 |
| 41 | AM | 421 | PRO | CG-CD | -6.66 | 1.28 | 1.50 |
| 40 | EG | 263 | PRO | CG-CD | -6.57 | 1.28 | 1.50 |
| 41 | FB | 194 | GLU | CA-CB | 6.39 | 1.68 | 1.53 |
| 41 | QO | 61 | PRO | CB-CG | -6.36 | 1.18 | 1.50 |
| 41 | PN | 194 | GLU | CA-CB | 6.09 | 1.67 | 1.53 |
| 41 | TB | 229 | VAL | CB-CG1 | -6.04 | 1.40 | 1.52 |
| 40 | ME | 2 | ARG | CA-CB | 5.86 | 1.66 | 1.53 |
| 41 | BL | 194 | GLU | CA-CB | 5.82 | 1.66 | 1.53 |
| 23 | 4N | 270 | GLY | C-O | -5.75 | 1.14 | 1.23 |
| 23 | 4P | 270 | GLY | C-O | -5.75 | 1.14 | 1.23 |
| 41 | SM | 194 | GLU | CA-CB | 5.70 | 1.66 | 1.53 |
| 41 | OL | 208 | TYR | CD2-CE2 | -5.64 | 1.30 | 1.39 |
| 10 | 2F | 148 | VAL | C-N | -5.49 | 1.21 | 1.34 |
| 41 | AP | 194 | GLU | CA-CB | 5.45 | 1.66 | 1.53 |
| 41 | HB | 194 | GLU | CA-CB | 5.33 | 1.65 | 1.53 |
| 41 | SN | 268 | PRO | CG-CD | -5.13 | 1.33 | 1.50 |
| 41 | NL | 194 | GLU | CA-CB | 5.10 | 1.65 | 1.53 |

All (567) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | BG | 298 | PRO | N-CD-CG | -31.90 | 55.34 | 103.20 |
| 40 | BG | 298 | PRO | CA-CB-CG | -21.99 | 62.23 | 104.00 |
| 41 | QO | 61 | PRO | N-CD-CG | -18.71 | 75.13 | 103.20 |
| 40 | KF | 298 | PRO | CB-CG-CD | -18.04 | 36.15 | 106.50 |
| 40 | KF | 298 | PRO | N-CD-CG | -15.25 | 80.33 | 103.20 |
| 41 | QO | 61 | PRO | CB-CG-CD | 15.12 | 165.47 | 106.50 |
| 41 | QO | 61 | PRO | CA-CB-CG | -14.47 | 76.50 | 104.00 |
| 40 | SF | 298 | PRO | CA-N-CD | -14.19 | 91.64 | 111.50 |
| 41 | TM | 252 | LYS | CD-CE-NZ | 13.36 | 142.44 | 111.70 |
| 40 | KF | 298 | PRO | N-CA-CB | -12.55 | 88.23 | 103.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | QH | 72 | PRO | CA-N-CD | -11.60 | 95.25 | 111.50 |
| 41 | OL | 357 | PRO | CA-N-CD | -11.35 | 95.61 | 111.50 |
| 41 | AM | 421 | PRO | N-CD-CG | -11.15 | 86.48 | 103.20 |
| 40 | TH | 298 | PRO | CA-N-CD | -11.09 | 95.97 | 111.50 |
| 40 | BG | 298 | PRO | CB-CG-CD | -10.33 | 66.20 | 106.50 |
| 41 | SN | 268 | PRO | CA-N-CD | -10.29 | 97.09 | 111.50 |
| 34 | 5Q | 137 | LEU | CA-CB-CG | 10.27 | 138.93 | 115.30 |
| 40 | BG | 298 | PRO | CA-N-CD | -10.24 | 97.17 | 111.50 |
| 41 | JB | 252 | LYS | CD-CE-NZ | 10.08 | 134.89 | 111.70 |
| 22 | 4J | 92 | LYS | CA-CB-CG | 10.07 | 135.55 | 113.40 |
| 41 | NL | 252 | LYS | CD-CE-NZ | 9.97 | 134.64 | 111.70 |
| 41 | GM | 323 | MET | CG-SD-CE | -9.79 | 84.54 | 100.20 |
| 41 | MM | 252 | LYS | CD-CE-NZ | 9.71 | 134.04 | 111.70 |
| 41 | ML | 209 | ASP | CB-CG-OD1 | 9.63 | 126.97 | 118.30 |
| 41 | VO | 252 | LYS | CD-CE-NZ | 9.62 | 133.81 | 111.70 |
| 41 | LL | 362 | LYS | CD-CE-NZ | -9.53 | 89.79 | 111.70 |
| 39 | 6L | 150 | MET | CA-CB-CG | 9.50 | 129.46 | 113.30 |
| 40 | JD | 72 | PRO | CA-N-CD | -9.39 | 98.35 | 111.50 |
| 26 | 4V | 87 | LEU | CA-CB-CG | 9.15 | 136.34 | 115.30 |
| 40 | TE | 273 | ALA | C-N-CD | -9.01 | 100.78 | 120.60 |
| 14 | 3B | 16 | PRO | CA-N-CD | -8.96 | 98.95 | 111.50 |
| 40 | RA | 117 | LEU | CA-CB-CG | 8.90 | 135.76 | 115.30 |
| 40 | QA | 227 | LEU | CB-CG-CD1 | -8.64 | 96.31 | 111.00 |
| 41 | FN | 324 | LYS | CD-CE-NZ | -8.54 | 92.05 | 111.70 |
| 40 | EG | 263 | PRO | CA-N-CD | -8.53 | 99.56 | 111.50 |
| 41 | TM | 323 | MET | CG-SD-CE | -8.53 | 86.55 | 100.20 |
| 41 | TB | 305 | PRO | CA-N-CD | -8.48 | 99.63 | 111.50 |
| 41 | FP | 323 | MET | CA-CB-CG | 8.41 | 127.60 | 113.30 |
| 40 | KF | 298 | PRO | CA-CB-CG | -8.38 | 88.08 | 104.00 |
| 40 | EG | 263 | PRO | N-CD-CG | -8.21 | 90.88 | 103.20 |
| 41 | WB | 324 | LYS | CD-CE-NZ | 8.21 | 130.57 | 111.70 |
| 41 | CB | 246 | LEU | CA-CB-CG | 8.17 | 134.10 | 115.30 |
| 40 | JF | 273 | ALA | C-N-CD | -8.14 | 102.70 | 120.60 |
| 41 | CB | 246 | LEU | CB-CG-CD2 | -8.09 | 97.24 | 111.00 |
| 41 | FN | 171 | PRO | C-N-CA | 8.07 | 141.88 | 121.70 |
| 40 | PA | 286 | LEU | CA-CB-CG | 8.03 | 133.78 | 115.30 |
| 41 | OP | 257 | MET | CA-CB-CG | 8.02 | 126.93 | 113.30 |
| 41 | TP | 246 | LEU | CA-CB-CG | 7.98 | 133.65 | 115.30 |
| 40 | WI | 366 | ASP | CB-CG-OD1 | 7.92 | 125.43 | 118.30 |
| 41 | KB | 324 | LYS | CD-CE-NZ | -7.86 | 93.62 | 111.70 |
| 41 | QO | 7 | LEU | CA-CB-CG | 7.83 | 133.31 | 115.30 |
| 40 | JH | 273 | ALA | C-N-CD | -7.82 | 103.39 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | TO | 246 | LEU | CA-CB-CG | 7.79 | 133.22 | 115.30 |
| 41 | FO | 171 | PRO | C-N-CA | 7.77 | 141.13 | 121.70 |
| 40 | VG | 345 | ASP | CB-CG-OD2 | 7.71 | 125.24 | 118.30 |
| 41 | AM | 421 | PRO | CA-CB-CG | -7.71 | 89.36 | 104.00 |
| 12 | 2N | 255 | LEU | CA-CB-CG | 7.71 | 133.02 | 115.30 |
| 40 | DG | 227 | LEU | CA-CB-CG | 7.64 | 132.87 | 115.30 |
| 40 | WH | 160 | ASP | CB-CG-OD2 | 7.61 | 125.14 | 118.30 |
| 11 | 2I | 119 | LYS | CD-CE-NZ | -7.58 | 94.25 | 111.70 |
| 40 | FE | 286 | LEU | CA-CB-CG | 7.58 | 132.74 | 115.30 |
| 41 | EB | 31 | ASP | CB-CG-OD2 | 7.58 | 125.12 | 118.30 |
| 40 | GG | 274 | PRO | CA-N-CD | -7.55 | 100.93 | 111.50 |
| 41 | SN | 268 | PRO | N-CD-CG | -7.54 | 91.88 | 103.20 |
| 40 | PH | 286 | LEU | CA-CB-CG | 7.52 | 132.60 | 115.30 |
| 41 | UO | 323 | MET | CG-SD-CE | -7.51 | 88.18 | 100.20 |
| 41 | AM | 421 | PRO | CA-N-CD | -7.49 | 101.01 | 111.50 |
| 15 | 3F | 46 | ASP | CB-CG-OD2 | 7.48 | 125.03 | 118.30 |
| 41 | HO | 252 | LYS | CD-CE-NZ | 7.45 | 128.84 | 111.70 |
| 41 | OM | 395 | LEU | CA-CB-CG | 7.44 | 132.42 | 115.30 |
| 40 | NH | 47 | ASP | CB-CG-OD2 | 7.44 | 124.99 | 118.30 |
| 40 | IG | 298 | PRO | CA-N-CD | -7.43 | 101.09 | 111.50 |
| 40 | UA | 273 | ALA | C-N-CD | -7.42 | 104.28 | 120.60 |
| 40 | NE | 437 | ASP | CB-CG-OD2 | 7.41 | 124.97 | 118.30 |
| 41 | RM | 31 | ASP | CB-CG-OD1 | 7.39 | 124.95 | 118.30 |
| 40 | WG | 352 | LYS | CB-CG-CD | -7.37 | 92.43 | 111.60 |
| 40 | BG | 297 | GLU | C-N-CD | 7.37 | 143.87 | 128.40 |
| 40 | QG | 390 | LEU | CA-CB-CG | 7.34 | 132.17 | 115.30 |
| 41 | LB | 395 | LEU | CA-CB-CG | 7.32 | 132.14 | 115.30 |
| 41 | IQ | 44 | LEU | CA-CB-CG | 7.29 | 132.08 | 115.30 |
| 40 | BG | 298 | PRO | N-CA-CB | -7.29 | 94.55 | 103.30 |
| 41 | LB | 171 | PRO | C-N-CA | 7.26 | 139.86 | 121.70 |
| 36 | 5Y | 182 | LEU | CA-CB-CG | 7.22 | 131.91 | 115.30 |
| 2 | 1D | 205 | LEU | CA-CB-CG | 7.21 | 131.88 | 115.30 |
| 40 | IF | 160 | ASP | CB-CG-OD2 | 7.20 | 124.78 | 118.30 |
| 17 | 3O | 185 | LEU | CA-CB-CG | 7.19 | 131.83 | 115.30 |
| 18 | 3U | 318 | LEU | CA-CB-CG | 7.18 | 131.82 | 115.30 |
| 12 | 2Q | 255 | LEU | CA-CB-CG | 7.16 | 131.77 | 115.30 |
| 40 | SG | 76 | ASP | CB-CG-OD1 | 7.15 | 124.73 | 118.30 |
| 41 | EN | 252 | LYS | CD-CE-NZ | 7.14 | 128.13 | 111.70 |
| 12 | 2O | 255 | LEU | CA-CB-CG | 7.13 | 131.70 | 115.30 |
| 12 | 2M | 255 | LEU | CA-CB-CG | 7.12 | 131.68 | 115.30 |
| 40 | CG | 366 | ASP | CB-CG-OD1 | 7.11 | 124.70 | 118.30 |
| 41 | WP | 395 | LEU | CA-CB-CG | 7.10 | 131.64 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 36 | 5X | 189 | LEU | CA-CB-CG | 7.07 | 131.56 | 115.30 |
| 40 | NH | 245 | ASP | CB-CG-OD2 | 7.06 | 124.66 | 118.30 |
| 41 | FM | 323 | MET | CA-CB-CG | 7.06 | 125.30 | 113.30 |
| 41 | FP | 404 | ASP | CB-CG-OD1 | 7.04 | 124.64 | 118.30 |
| 40 | CF | 116 | ASP | CB-CG-OD1 | 7.03 | 124.63 | 118.30 |
| 40 | RG | 437 | ASP | CB-CG-OD2 | 7.03 | 124.63 | 118.30 |
| 22 | 4J | 90 | PRO | N-CA-C | 7.03 | 130.37 | 112.10 |
| 12 | 2R | 255 | LEU | CA-CB-CG | 6.99 | 131.37 | 115.30 |
| 40 | HF | 33 | ASP | CB-CG-OD2 | 6.99 | 124.59 | 118.30 |
| 40 | LE | 26 | LEU | CA-CB-CG | 6.98 | 131.35 | 115.30 |
| 41 | DO | 324 | LYS | CD-CE-NZ | -6.97 | 95.66 | 111.70 |
| 40 | IA | 217 | LEU | CA-CB-CG | 6.97 | 131.34 | 115.30 |
| 38 | 6C | 26 | ASP | CB-CG-OD1 | 6.94 | 124.55 | 118.30 |
| 36 | 5X | 98 | ILE | CG1-CB-CG2 | -6.92 | 96.18 | 111.40 |
| 34 | 5Q | 288 | LEU | CA-CB-CG | 6.92 | 131.21 | 115.30 |
| 41 | NB | 151 | LEU | CB-CG-CD2 | -6.91 | 99.25 | 111.00 |
| 41 | MP | 171 | PRO | C-N-CA | 6.90 | 138.94 | 121.70 |
| 22 | 4I | 35 | LEU | CA-CB-CG | 6.89 | 131.15 | 115.30 |
| 27 | 4Z | 86 | LEU | CA-CB-CG | 6.89 | 131.14 | 115.30 |
| 40 | VA | 273 | ALA | C-N-CD | -6.88 | 105.46 | 120.60 |
| 41 | QN | 31 | ASP | CB-CG-OD1 | 6.88 | 124.49 | 118.30 |
| 41 | NB | 42 | LEU | CA-CB-CG | 6.87 | 131.11 | 115.30 |
| 40 | PG | 286 | LEU | CA-CB-CG | 6.87 | 131.09 | 115.30 |
| 41 | OL | 357 | PRO | N-CD-CG | -6.85 | 92.92 | 103.20 |
| 41 | EB | 117 | LEU | CA-CB-CG | 6.85 | 131.04 | 115.30 |
| 40 | KD | 345 | ASP | CB-CG-OD2 | 6.83 | 124.45 | 118.30 |
| 40 | CF | 256 | GLN | CA-CB-CG | 6.83 | 128.42 | 113.40 |
| 40 | JD | 291 | ILE | CG1-CB-CG2 | -6.82 | 96.39 | 111.40 |
| 41 | FN | 197 | ASP | CB-CG-OD2 | 6.82 | 124.43 | 118.30 |
| 41 | IP | 44 | LEU | CA-CB-CG | 6.81 | 130.97 | 115.30 |
| 4 | 1I | 31 | LEU | CA-CB-CG | 6.79 | 130.93 | 115.30 |
| 15 | 3F | 331 | ASP | CB-CG-OD1 | 6.79 | 124.41 | 118.30 |
| 21 | 4D | 291 | LEU | CA-CB-CG | 6.79 | 130.91 | 115.30 |
| 41 | QN | 252 | LYS | CB-CG-CD | 6.77 | 129.21 | 111.60 |
| 41 | PP | 187 | LEU | CA-CB-CG | 6.77 | 130.86 | 115.30 |
| 41 | QN | 122 | LYS | CD-CE-NZ | -6.77 | 96.14 | 111.70 |
| 40 | RG | 345 | ASP | CB-CG-OD2 | 6.76 | 124.38 | 118.30 |
| 40 | KA | 273 | ALA | C-N-CD | -6.75 | 105.76 | 120.60 |
| 40 | GG | 274 | PRO | CB-CA-C | 6.74 | 128.86 | 112.00 |
| 40 | QH | 72 | PRO | N-CD-CG | -6.72 | 93.13 | 103.20 |
| 40 | WG | 366 | ASP | CB-CG-OD2 | 6.71 | 124.34 | 118.30 |
| 41 | EB | 26 | ASP | CB-CG-OD2 | 6.71 | 124.34 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | AM | 295 | ASP | CB-CG-OD1 | 6.69 | 124.32 | 118.30 |
| 40 | VA | 39 | ASP | CB-CG-OD1 | 6.69 | 124.32 | 118.30 |
| 28 | 5B | 35 | LEU | CB-CG-CD1 | 6.67 | 122.34 | 111.00 |
| 40 | GG | 274 | PRO | CA-CB-CG | -6.67 | 91.32 | 104.00 |
| 40 | RE | 273 | ALA | C-N-CD | -6.67 | 105.93 | 120.60 |
| 40 | SA | 157 | LEU | CA-CB-CG | 6.67 | 130.63 | 115.30 |
| 40 | TH | 298 | PRO | N-CD-CG | -6.65 | 93.23 | 103.20 |
| 40 | AE | 154 | MET | CB-CG-SD | -6.63 | 92.50 | 112.40 |
| 41 | MP | 112 | LEU | CA-CB-CG | 6.63 | 130.55 | 115.30 |
| 41 | GP | 395 | LEU | CA-CB-CG | 6.63 | 130.54 | 115.30 |
| 25 | 4T | 273 | LEU | CB-CG-CD2 | -6.62 | 99.74 | 111.00 |
| 40 | JF | 423 | ASP | CB-CG-OD2 | 6.62 | 124.26 | 118.30 |
| 41 | SN | 391 | ARG | CA-CB-CG | 6.61 | 127.95 | 113.40 |
| 41 | BL | 295 | ASP | CB-CG-OD2 | 6.60 | 124.24 | 118.30 |
| 40 | LD | 155 | GLU | CA-CB-CG | 6.58 | 127.88 | 113.40 |
| 41 | JN | 161 | ASP | CB-CG-OD1 | 6.57 | 124.22 | 118.30 |
| 41 | TO | 252 | LYS | CD-CE-NZ | 6.57 | 126.82 | 111.70 |
| 33 | 5N | 477 | LEU | CA-CB-CG | 6.57 | 130.41 | 115.30 |
| 4 | 1H | 76 | ILE | CG1-CB-CG2 | -6.55 | 96.99 | 111.40 |
| 41 | FP | 395 | LEU | CA-CB-CG | 6.54 | 130.34 | 115.30 |
| 40 | AF | 211 | ASP | CB-CG-OD1 | 6.54 | 124.18 | 118.30 |
| 41 | GM | 7 | LEU | CA-CB-CG | 6.53 | 130.32 | 115.30 |
| 11 | 2J | 90 | LEU | CA-CB-CG | 6.53 | 130.31 | 115.30 |
| 21 | 4D | 291 | LEU | CB-CG-CD2 | 6.53 | 122.09 | 111.00 |
| 16 | 3L | 100 | GLU | CA-CB-CG | 6.51 | 127.72 | 113.40 |
| 41 | UO | 388 | MET | CA-CB-CG | 6.50 | 124.35 | 113.30 |
| 17 | 3O | 305 | ASP | CB-CG-OD2 | 6.49 | 124.14 | 118.30 |
| 41 | TB | 284 | LEU | CA-CB-CG | 6.48 | 130.20 | 115.30 |
| 41 | TM | 252 | LYS | CB-CG-CD | -6.47 | 94.77 | 111.60 |
| 41 | DL | 90 | PHE | N-CA-CB | -6.46 | 98.98 | 110.60 |
| 41 | RL | 324 | LYS | CD-CE-NZ | -6.45 | 96.86 | 111.70 |
| 40 | KH | 430 | ASP | CB-CG-OD1 | 6.44 | 124.10 | 118.30 |
| 41 | ML | 31 | ASP | CB-CG-OD1 | 6.44 | 124.09 | 118.30 |
| 18 | 3T | 107 | LEU | CA-CB-CG | 6.42 | 130.07 | 115.30 |
| 41 | JN | 295 | ASP | CB-CG-OD2 | 6.42 | 124.08 | 118.30 |
| 40 | MD | 274 | PRO | CA-N-CD | -6.42 | 102.52 | 111.50 |
| 41 | GO | 404 | ASP | CB-CG-OD1 | 6.40 | 124.06 | 118.30 |
| 19 | 3Y | 91 | ASP | CB-CG-OD2 | 6.39 | 124.05 | 118.30 |
| 40 | LE | 47 | ASP | CB-CG-OD2 | 6.38 | 124.04 | 118.30 |
| 40 | SI | 400 | LYS | CA-CB-CG | 6.38 | 127.44 | 113.40 |
| 31 | 5I | 313 | VAL | CG1-CB-CG2 | -6.38 | 100.69 | 110.90 |
| 41 | FO | 395 | LEU | CA-CB-CG | 6.36 | 129.93 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | 1X | 337 | MET | CA-CB-CG | 6.36 | 124.11 | 113.30 |
| 41 | LL | 31 | ASP | CB-CG-OD1 | 6.35 | 124.02 | 118.30 |
| 22 | 4J | 482 | LYS | CA-CB-CG | 6.35 | 127.36 | 113.40 |
| 41 | KB | 286 | VAL | CG1-CB-CG2 | -6.34 | 100.75 | 110.90 |
| 41 | FB | 257 | MET | CG-SD-CE | -6.34 | 90.06 | 100.20 |
| 40 | FG | 129 | CYS | CA-CB-SG | 6.33 | 125.39 | 114.00 |
| 41 | WO | 31 | ASP | CB-CG-OD2 | 6.30 | 123.97 | 118.30 |
| 41 | HP | 280 | GLN | CA-CB-CG | 6.30 | 127.27 | 113.40 |
| 40 | QG | 390 | LEU | CB-CG-CD2 | -6.29 | 100.30 | 111.00 |
| 41 | QN | 395 | LEU | CA-CB-CG | 6.29 | 129.77 | 115.30 |
| 40 | LH | 33 | ASP | CB-CG-OD2 | 6.29 | 123.96 | 118.30 |
| 14 | 3B | 113 | ILE | CG1-CB-CG2 | -6.27 | 97.61 | 111.40 |
| 41 | PO | 233 | MET | CB-CG-SD | 6.27 | 131.21 | 112.40 |
| 41 | BN | 295 | ASP | CB-CG-OD2 | 6.26 | 123.93 | 118.30 |
| 41 | UO | 7 | LEU | CA-CB-CG | 6.26 | 129.70 | 115.30 |
| 41 | EB | 395 | LEU | CA-CB-CG | 6.25 | 129.67 | 115.30 |
| 41 | VP | 284 | LEU | CA-CB-CG | 6.24 | 129.66 | 115.30 |
| 40 | PA | 291 | ILE | CG1-CB-CG2 | -6.24 | 97.67 | 111.40 |
| 41 | QM | 7 | LEU | CA-CB-CG | 6.23 | 129.62 | 115.30 |
| 41 | BL | 42 | LEU | CA-CB-CG | 6.23 | 129.62 | 115.30 |
| 41 | UN | 249 | ASP | CB-CG-OD2 | 6.21 | 123.89 | 118.30 |
| 19 | 3Y | 276 | ASP | CB-CG-OD2 | 6.21 | 123.89 | 118.30 |
| 40 | PD | 286 | LEU | CA-CB-CG | 6.21 | 129.59 | 115.30 |
| 41 | AP | 417 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 22 | 4J | 169 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 41 | TP | 84 | ILE | CG1-CB-CG2 | -6.21 | 97.75 | 111.40 |
| 40 | FG | 36 | MET | CA-CB-CG | 6.21 | 123.85 | 113.30 |
| 41 | TN | 7 | LEU | CA-CB-CG | 6.21 | 129.57 | 115.30 |
| 41 | EL | 209 | ASP | CB-CG-OD1 | 6.20 | 123.88 | 118.30 |
| 41 | EL | 130 | LEU | CA-CB-CG | 6.20 | 129.56 | 115.30 |
| 41 | OB | 257 | MET | CA-CB-CG | 6.19 | 123.82 | 113.30 |
| 41 | ON | 31 | ASP | CB-CG-OD2 | 6.19 | 123.87 | 118.30 |
| 21 | 4E | 301 | LEU | CA-CB-CG | 6.18 | 129.52 | 115.30 |
| 40 | RI | 124 | LYS | CD-CE-NZ | 6.18 | 125.91 | 111.70 |
| 41 | UN | 403 | MET | CA-CB-CG | 6.17 | 123.80 | 113.30 |
| 33 | 5N | 427 | LEU | CA-CB-CG | 6.17 | 129.50 | 115.30 |
| 40 | UA | 256 | GLN | CA-CB-CG | 6.17 | 126.97 | 113.40 |
| 41 | GP | 323 | MET | CB-CG-SD | -6.17 | 93.89 | 112.40 |
| 41 | NP | 295 | ASP | CB-CG-OD1 | 6.16 | 123.85 | 118.30 |
| 27 | 4Y | 199 | ASP | CB-CG-OD2 | 6.16 | 123.84 | 118.30 |
| 41 | TN | 284 | LEU | CA-CB-CG | 6.16 | 129.46 | 115.30 |
| 40 | NH | 211 | ASP | CB-CG-OD2 | 6.14 | 123.82 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 40 | SI | 280 | LYS | CA-CB-CG | 6.14 | 126.90 | 113.40 |
| 41 | TO | 7 | LEU | CA-CB-CG | 6.12 | 129.38 | 115.30 |
| 41 | MB | 284 | LEU | CA-CB-CG | 6.12 | 129.37 | 115.30 |
| 7 | 1U | 457 | LEU | CA-CB-CG | 6.11 | 129.35 | 115.30 |
| 16 | 3K | 175 | ASP | CB-CG-OD2 | 6.10 | 123.79 | 118.30 |
| 41 | QO | 246 | LEU | CA-CB-CG | 6.10 | 129.33 | 115.30 |
| 40 | FE | 227 | LEU | CB-CG-CD2 | 6.10 | 121.36 | 111.00 |
| 41 | HQ | 257 | MET | CA-CB-CG | 6.09 | 123.66 | 113.30 |
| 40 | NE | 86 | LEU | CA-CB-CG | 6.09 | 129.30 | 115.30 |
| 41 | QL | 7 | LEU | CA-CB-CG | 6.09 | 129.30 | 115.30 |
| 41 | GO | 41 | ASP | CB-CG-OD2 | 6.08 | 123.77 | 118.30 |
| 41 | TN | 187 | LEU | CA-CB-CG | 6.07 | 129.27 | 115.30 |
| 40 | WG | 306 | ASP | CB-CG-OD1 | 6.07 | 123.77 | 118.30 |
| 41 | GB | 233 | MET | CA-CB-CG | 6.07 | 123.62 | 113.30 |
| 41 | JL | 67 | ASP | CB-CG-OD1 | 6.07 | 123.76 | 118.30 |
| 26 | 4W | 165 | ARG | CA-CB-CG | 6.06 | 126.73 | 113.40 |
| 41 | NB | 192 | LEU | CA-CB-CG | 6.05 | 129.22 | 115.30 |
| 40 | NA | 132 | LEU | CA-CB-CG | 6.05 | 129.22 | 115.30 |
| 27 | 4Z | 236 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 41 | PM | 284 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 41 | UN | 122 | LYS | CA-CB-CG | 6.04 | 126.69 | 113.40 |
| 40 | GG | 274 | PRO | N-CD-CG | -6.03 | 94.16 | 103.20 |
| 41 | WQ | 65 | LEU | CA-CB-CG | 6.03 | 129.17 | 115.30 |
| 41 | GB | 252 | LYS | CD-CE-NZ | 6.01 | 125.53 | 111.70 |
| 22 | 4H | 338 | LEU | CA-CB-CG | 6.01 | 129.12 | 115.30 |
| 40 | RG | 383 | ILE | CG1-CB-CG2 | -6.01 | 98.19 | 111.40 |
| 40 | OF | 306 | ASP | CB-CG-OD2 | 6.00 | 123.70 | 118.30 |
| 41 | EB | 295 | ASP | CB-CG-OD2 | 5.99 | 123.69 | 118.30 |
| 41 | AL | 42 | LEU | CA-CB-CG | 5.98 | 129.06 | 115.30 |
| 41 | UN | 395 | LEU | CA-CB-CG | 5.97 | 129.03 | 115.30 |
| 40 | VI | 276 | ILE | CG1-CB-CG2 | -5.96 | 98.29 | 111.40 |
| 40 | HH | 242 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 41 | OL | 164 | MET | CA-CB-CG | 5.95 | 123.42 | 113.30 |
| 41 | AP | 295 | ASP | CB-CG-OD2 | 5.94 | 123.65 | 118.30 |
| 40 | VJ | 317 | LEU | CA-CB-CG | 5.94 | 128.96 | 115.30 |
| 41 | NN | 284 | LEU | CA-CB-CG | 5.94 | 128.95 | 115.30 |
| 40 | UE | 121 | ARG | CB-CG-CD | 5.94 | 127.03 | 111.60 |
| 40 | ME | 345 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 40 | TH | 69 | ASP | CB-CG-OD2 | 5.93 | 123.64 | 118.30 |
| 40 | SF | 327 | ASP | CB-CG-OD2 | 5.93 | 123.64 | 118.30 |
| 40 | CE | 173 | PRO | CA-N-CD | -5.93 | 103.20 | 111.50 |
| 41 | TM | 293 | MET | CB-CG-SD | -5.93 | 94.62 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | LO | 377 | LEU | CA-CB-CG | 5.92 | 128.91 | 115.30 |
| 41 | GB | 7 | LEU | CA-CB-CG | 5.92 | 128.91 | 115.30 |
| 41 | HP | 252 | LYS | CB-CG-CD | 5.92 | 126.98 | 111.60 |
| 41 | QM | 1 | MET | CA-CB-CG | 5.92 | 123.36 | 113.30 |
| 41 | PM | 363 | MET | CA-CB-CG | 5.91 | 123.35 | 113.30 |
| 41 | FM | 323 | MET | CB-CG-SD | -5.91 | 94.68 | 112.40 |
| 41 | FP | 361 | LEU | CA-CB-CG | 5.91 | 128.88 | 115.30 |
| 40 | HG | 345 | ASP | CB-CG-OD2 | 5.90 | 123.61 | 118.30 |
| 40 | QH | 79 | ARG | CG-CD-NE | 5.90 | 124.20 | 111.80 |
| 40 | ME | 433 | GLU | CA-CB-CG | 5.88 | 126.34 | 113.40 |
| 41 | RM | 395 | LEU | CA-CB-CG | 5.88 | 128.81 | 115.30 |
| 40 | UE | 203 | MET | CA-CB-CG | 5.86 | 123.27 | 113.30 |
| 41 | OP | 26 | ASP | CB-CG-OD1 | 5.86 | 123.58 | 118.30 |
| 40 | WF | 345 | ASP | CB-CG-OD2 | 5.86 | 123.57 | 118.30 |
| 40 | FI | 199 | ASP | CB-CG-OD1 | 5.85 | 123.57 | 118.30 |
| 41 | WB | 415 | MET | CG-SD-CE | -5.84 | 90.86 | 100.20 |
| 28 | 5B | 33 | LEU | CA-CB-CG | 5.84 | 128.73 | 115.30 |
| 4 | 1J | 182 | LEU | CA-CB-CG | 5.83 | 128.72 | 115.30 |
| 41 | LL | 112 | LEU | CA-CB-CG | 5.83 | 128.70 | 115.30 |
| 41 | VB | 161 | ASP | CB-CG-OD2 | 5.81 | 123.53 | 118.30 |
| 41 | AP | 7 | LEU | CA-CB-CG | 5.81 | 128.66 | 115.30 |
| 40 | PE | 412 | MET | CA-CB-CG | 5.81 | 123.18 | 113.30 |
| 41 | UN | 1 | MET | CB-CG-SD | 5.81 | 129.83 | 112.40 |
| 8 | 1W | 337 | MET | CA-CB-CG | 5.81 | 123.17 | 113.30 |
| 41 | OP | 7 | LEU | CA-CB-CG | 5.80 | 128.63 | 115.30 |
| 41 | AM | 203 | ASP | CB-CG-OD1 | 5.79 | 123.51 | 118.30 |
| 41 | TB | 323 | MET | CB-CA-C | -5.78 | 98.83 | 110.40 |
| 21 | 4D | 210 | ASP | CB-CG-OD2 | 5.78 | 123.50 | 118.30 |
| 41 | BN | 327 | ASP | CB-CG-OD1 | 5.78 | 123.50 | 118.30 |
| 41 | QM | 395 | LEU | CA-CB-CG | 5.77 | 128.58 | 115.30 |
| 41 | HQ | 67 | ASP | CB-CG-OD2 | 5.77 | 123.49 | 118.30 |
| 41 | RB | 112 | LEU | CA-CB-CG | 5.76 | 128.56 | 115.30 |
| 12 | 2R | 114 | ASP | CB-CG-OD1 | 5.76 | 123.49 | 118.30 |
| 5 | 1M | 205 | MET | CA-CB-CG | 5.76 | 123.09 | 113.30 |
| 41 | CB | 31 | ASP | CB-CG-OD1 | 5.75 | 123.48 | 118.30 |
| 41 | IN | 112 | LEU | CA-CB-CG | 5.75 | 128.53 | 115.30 |
| 40 | UA | 261 | PRO | CA-N-CD | -5.75 | 103.45 | 111.50 |
| 40 | UA | 397 | MET | CA-CB-CG | 5.75 | 123.07 | 113.30 |
| 22 | 4J | 539 | LYS | CA-CB-CG | 5.74 | 126.04 | 113.40 |
| 41 | VQ | 293 | MET | CA-CB-CG | 5.74 | 123.06 | 113.30 |
| 22 | 4J | 92 | LYS | CB-CG-CD | 5.74 | 126.52 | 111.60 |
| 40 | VJ | 345 | ASP | CB-CG-OD1 | 5.74 | 123.46 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | WF | 98 | ASP | CB-CG-OD1 | 5.73 | 123.46 | 118.30 |
| 40 | WA | 33 | ASP | CB-CG-OD2 | 5.73 | 123.46 | 118.30 |
| 40 | QE | 345 | ASP | CB-CG-OD1 | 5.73 | 123.45 | 118.30 |
| 40 | KG | 218 | ASP | CB-CG-OD1 | 5.72 | 123.45 | 118.30 |
| 41 | OB | 112 | LEU | CA-CB-CG | 5.72 | 128.46 | 115.30 |
| 40 | VG | 120 | ASP | CB-CG-OD1 | 5.72 | 123.44 | 118.30 |
| 40 | EA | 276 | ILE | CG1-CB-CG2 | -5.71 | 98.84 | 111.40 |
| 41 | GP | 323 | MET | CA-CB-CG | 5.71 | 123.01 | 113.30 |
| 41 | UB | 327 | ASP | CB-CG-OD2 | 5.71 | 123.44 | 118.30 |
| 18 | 3T | 313 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 40 | OE | 167 | LEU | CA-CB-CG | 5.71 | 128.42 | 115.30 |
| 41 | PM | 425 | ARG | CB-CG-CD | -5.71 | 96.77 | 111.60 |
| 40 | RI | 124 | LYS | CA-CB-CG | 5.71 | 125.95 | 113.40 |
| 40 | IG | 218 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 40 | KD | 273 | ALA | C-N-CD | -5.69 | 108.09 | 120.60 |
| 40 | SF | 400 | LYS | CA-CB-CG | 5.69 | 125.91 | 113.40 |
| 41 | JN | 112 | LEU | CA-CB-CG | 5.68 | 128.38 | 115.30 |
| 40 | VJ | 217 | LEU | CA-CB-CG | 5.68 | 128.37 | 115.30 |
| 26 | 4W | 120 | LEU | CA-CB-CG | 5.68 | 128.36 | 115.30 |
| 15 | 3E | 67 | LEU | CA-CB-CG | 5.66 | 128.32 | 115.30 |
| 41 | QN | 7 | LEU | CA-CB-CG | 5.66 | 128.32 | 115.30 |
| 41 | TM | 324 | LYS | CD-CE-NZ | -5.66 | 98.68 | 111.70 |
| 40 | BA | 31 | GLN | CA-CB-CG | 5.65 | 125.84 | 113.40 |
| 40 | NE | 33 | ASP | CB-CG-OD2 | 5.65 | 123.38 | 118.30 |
| 40 | BG | 322 | ASP | CB-CG-OD1 | 5.64 | 123.38 | 118.30 |
| 41 | GB | 395 | LEU | CA-CB-CG | 5.64 | 128.28 | 115.30 |
| 41 | IB | 380 | ARG | CB-CG-CD | -5.64 | 96.93 | 111.60 |
| 41 | SM | 395 | LEU | CA-CB-CG | 5.64 | 128.28 | 115.30 |
| 41 | MM | 284 | LEU | CA-CB-CG | 5.63 | 128.26 | 115.30 |
| 40 | OD | 423 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 40 | FH | 357 | TYR | C-N-CA | -5.63 | 107.64 | 121.70 |
| 35 | 5T | 94 | LEU | CA-CB-CG | 5.62 | 128.23 | 115.30 |
| 40 | PD | 306 | ASP | CB-CG-OD2 | 5.62 | 123.36 | 118.30 |
| 41 | OB | 215 | LEU | CA-CB-CG | 5.62 | 128.22 | 115.30 |
| 40 | LE | 227 | LEU | CA-CB-CG | 5.61 | 128.21 | 115.30 |
| 40 | QH | 302 | MET | CB-CG-SD | 5.61 | 129.24 | 112.40 |
| 36 | 5Y | 38 | ASP | CB-CG-OD1 | 5.61 | 123.35 | 118.30 |
| 41 | EN | 284 | LEU | CA-CB-CG | 5.61 | 128.20 | 115.30 |
| 18 | 3T | 237 | ASP | CB-CG-OD1 | 5.61 | 123.35 | 118.30 |
| 40 | AF | 422 | GLU | CA-CB-CG | 5.61 | 125.73 | 113.40 |
| 41 | TO | 395 | LEU | CA-CB-CG | 5.61 | 128.19 | 115.30 |
| 18 | 3T | 405 | LEU | CA-CB-CG | 5.60 | 128.19 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | QL | 300 | MET | CG-SD-CE | -5.60 | 91.24 | 100.20 |
| 41 | AM | 209 | ASP | CB-CG-OD1 | 5.60 | 123.34 | 118.30 |
| 40 | VH | 269 | LEU | CB-CG-CD2 | -5.60 | 101.49 | 111.00 |
| 41 | UM | 26 | ASP | CB-CG-OD2 | 5.59 | 123.33 | 118.30 |
| 10 | 2E | 41 | GLN | C-N-CA | 5.57 | 135.63 | 121.70 |
| 41 | DO | 31 | ASP | CB-CG-OD2 | 5.57 | 123.32 | 118.30 |
| 17 | 3O | 274 | LEU | CA-CB-CG | 5.57 | 128.11 | 115.30 |
| 40 | VA | 218 | ASP | CB-CG-OD1 | 5.57 | 123.31 | 118.30 |
| 33 | 5O | 42 | MET | CA-CB-CG | 5.56 | 122.75 | 113.30 |
| 41 | QL | 395 | LEU | CA-CB-CG | 5.56 | 128.08 | 115.30 |
| 18 | 3U | 317 | LYS | CD-CE-NZ | -5.55 | 98.94 | 111.70 |
| 41 | IP | 41 | ASP | CB-CG-OD1 | 5.55 | 123.29 | 118.30 |
| 41 | TB | 226 | ASN | CB-CA-C | 5.55 | 121.49 | 110.40 |
| 40 | PA | 132 | LEU | CA-CB-CG | 5.54 | 128.05 | 115.30 |
| 41 | VO | 252 | LYS | CA-CB-CG | 5.54 | 125.59 | 113.40 |
| 41 | HP | 112 | LEU | CA-CB-CG | 5.54 | 128.04 | 115.30 |
| 41 | NB | 151 | LEU | CB-CG-CD1 | 5.54 | 120.41 | 111.00 |
| 41 | VB | 44 | LEU | CA-CB-CG | 5.54 | 128.04 | 115.30 |
| 40 | AA | 128 | GLN | CA-CB-CG | 5.53 | 125.56 | 113.40 |
| 9 | 2B | 410 | GLN | CA-CB-CG | 5.51 | 125.53 | 113.40 |
| 41 | TP | 233 | MET | CA-CB-CG | 5.51 | 122.67 | 113.30 |
| 41 | NN | 151 | LEU | CA-CB-CG | 5.51 | 127.96 | 115.30 |
| 9 | 2C | 438 | MET | CA-CB-CG | 5.50 | 122.65 | 113.30 |
| 41 | RL | 217 | LEU | CA-CB-CG | 5.50 | 127.95 | 115.30 |
| 41 | UN | 293 | MET | CA-CB-CG | 5.50 | 122.65 | 113.30 |
| 41 | AL | 7 | LEU | CA-CB-CG | 5.50 | 127.95 | 115.30 |
| 41 | UM | 252 | LYS | CD-CE-NZ | 5.50 | 124.34 | 111.70 |
| 40 | SH | 227 | LEU | CA-CB-CG | 5.50 | 127.94 | 115.30 |
| 40 | PE | 427 | LEU | CA-CB-CG | 5.50 | 127.94 | 115.30 |
| 41 | EB | 284 | LEU | CA-CB-CG | 5.49 | 127.94 | 115.30 |
| 41 | KM | 161 | ASP | CB-CG-OD2 | 5.49 | 123.24 | 118.30 |
| 41 | GB | 39 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 41 | LM | 39 | ASP | CB-CG-OD2 | 5.48 | 123.23 | 118.30 |
| 16 | 3J | 364 | ASP | CB-CG-OD1 | 5.48 | 123.23 | 118.30 |
| 41 | GM | 130 | LEU | CA-CB-CG | 5.48 | 127.90 | 115.30 |
| 40 | RF | 276 | ILE | CG1-CB-CG2 | -5.47 | 99.36 | 111.40 |
| 41 | WQ | 31 | ASP | CB-CG-OD2 | 5.47 | 123.22 | 118.30 |
| 36 | 5X | 130 | LEU | CB-CG-CD2 | -5.47 | 101.70 | 111.00 |
| 40 | IG | 306 | ASP | CB-CG-OD1 | 5.46 | 123.22 | 118.30 |
| 27 | 4Y | 165 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 41 | NB | 295 | ASP | CB-CG-OD2 | 5.44 | 123.20 | 118.30 |
| 41 | DO | 7 | LEU | CA-CB-CG | 5.44 | 127.82 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | VB | 284 | LEU | CA-CB-CG | 5.44 | 127.82 | 115.30 |
| 41 | EO | 395 | LEU | CA-CB-CG | 5.43 | 127.80 | 115.30 |
| 40 | CG | 116 | ASP | CB-CG-OD1 | 5.43 | 123.19 | 118.30 |
| 12 | 2O | 209 | ASP | CB-CG-OD2 | 5.43 | 123.19 | 118.30 |
| 22 | 4K | 471 | ARG | CA-CB-CG | 5.42 | 125.34 | 113.40 |
| 41 | LL | 114 | ASP | CB-CG-OD1 | 5.42 | 123.18 | 118.30 |
| 41 | SN | 293 | MET | CA-CB-CG | 5.42 | 122.52 | 113.30 |
| 41 | HB | 65 | LEU | CA-CB-CG | 5.42 | 127.76 | 115.30 |
| 40 | SE | 383 | ILE | CG1-CB-CG2 | -5.42 | 99.48 | 111.40 |
| 41 | WQ | 112 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 41 | EN | 395 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 41 | PO | 44 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 16 | 3J | 194 | LEU | C-N-CA | 5.41 | 135.22 | 121.70 |
| 40 | QG | 47 | ASP | CB-CG-OD2 | 5.40 | 123.16 | 118.30 |
| 41 | CB | 151 | LEU | CA-CB-CG | 5.40 | 127.72 | 115.30 |
| 41 | SP | 395 | LEU | CA-CB-CG | 5.40 | 127.72 | 115.30 |
| 41 | NN | 58 | LYS | CD-CE-NZ | 5.40 | 124.11 | 111.70 |
| 36 | 5Z | 234 | LEU | CB-CG-CD2 | -5.40 | 101.83 | 111.00 |
| 17 | 3O | 192 | LEU | CA-CB-CG | 5.39 | 127.70 | 115.30 |
| 41 | JO | 415 | MET | CA-CB-CG | 5.39 | 122.47 | 113.30 |
| 41 | AM | 171 | PRO | C-N-CA | 5.39 | 135.17 | 121.70 |
| 41 | PN | 395 | LEU | CA-CB-CG | 5.39 | 127.69 | 115.30 |
| 41 | PB | 324 | LYS | CD-CE-NZ | -5.38 | 99.31 | 111.70 |
| 40 | EG | 26 | LEU | CA-CB-CG | 5.38 | 127.67 | 115.30 |
| 41 | HQ | 233 | MET | CA-CB-CG | 5.38 | 122.44 | 113.30 |
| 41 | LN | 284 | LEU | CA-CB-CG | 5.38 | 127.67 | 115.30 |
| 41 | RN | 171 | PRO | C-N-CA | 5.38 | 135.14 | 121.70 |
| 40 | JE | 423 | ASP | CB-CG-OD2 | 5.37 | 123.13 | 118.30 |
| 41 | OP | 395 | LEU | CA-CB-CG | 5.37 | 127.65 | 115.30 |
| 40 | RE | 157 | LEU | CA-CB-CG | 5.37 | 127.64 | 115.30 |
| 22 | 4J | 251 | LEU | CA-CB-CG | 5.36 | 127.63 | 115.30 |
| 41 | BP | 42 | LEU | CB-CG-CD2 | 5.36 | 120.11 | 111.00 |
| 41 | IM | 353 | VAL | CG1-CB-CG2 | -5.35 | 102.34 | 110.90 |
| 41 | QM | 1 | MET | CB-CG-SD | 5.35 | 128.45 | 112.40 |
| 40 | RA | 302 | MET | CA-CB-CG | 5.35 | 122.40 | 113.30 |
| 40 | PD | 383 | ILE | CG1-CB-CG2 | -5.35 | 99.63 | 111.40 |
| 41 | QL | 299 | MET | CA-CB-CG | 5.35 | 122.39 | 113.30 |
| 5 | 1L | 232 | LEU | CA-CB-CG | 5.35 | 127.60 | 115.30 |
| 41 | OP | 171 | PRO | C-N-CA | 5.34 | 135.06 | 121.70 |
| 26 | 4W | 254 | LEU | CA-CB-CG | 5.34 | 127.58 | 115.30 |
| 41 | AP | 112 | LEU | CA-CB-CG | 5.33 | 127.56 | 115.30 |
| 41 | HQ | 31 | ASP | CB-CG-OD2 | 5.33 | 123.10 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | TN | 20 | PHE | CB-CG-CD1 | 5.33 | 124.53 | 120.80 |
| 41 | VP | 233 | MET | CA-CB-CG | 5.33 | 122.36 | 113.30 |
| 40 | WG | 220 | GLU | OE1-CD-OE2 | -5.33 | 116.91 | 123.30 |
| 41 | DB | 90 | PHE | N-CA-CB | 5.33 | 120.19 | 110.60 |
| 41 | KM | 377 | LEU | CA-CB-CG | 5.32 | 127.54 | 115.30 |
| 22 | 4J | 89 | VAL | CA-CB-CG2 | 5.32 | 118.88 | 110.90 |
| 41 | PM | 7 | LEU | CA-CB-CG | 5.32 | 127.53 | 115.30 |
| 15 | 3F | 351 | LEU | CA-CB-CG | 5.32 | 127.53 | 115.30 |
| 40 | UE | 210 | TYR | CA-CB-CG | 5.31 | 123.49 | 113.40 |
| 41 | GB | 130 | LEU | CA-CB-CG | 5.31 | 127.51 | 115.30 |
| 40 | QG | 227 | LEU | CB-CG-CD2 | 5.30 | 120.01 | 111.00 |
| 40 | SH | 49 | PHE | CB-CG-CD2 | 5.30 | 124.51 | 120.80 |
| 41 | WQ | 8 | GLN | CA-CB-CG | 5.30 | 125.06 | 113.40 |
| 26 | 4V | 330 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 41 | ON | 374 | ILE | CG1-CB-CG2 | -5.29 | 99.75 | 111.40 |
| 41 | GP | 225 | LEU | CA-CB-CG | 5.29 | 127.47 | 115.30 |
| 40 | PD | 317 | LEU | CA-CB-CG | 5.29 | 127.47 | 115.30 |
| 40 | HA | 177 | VAL | CG1-CB-CG2 | -5.28 | 102.45 | 110.90 |
| 41 | OB | 252 | LYS | CA-CB-CG | 5.28 | 125.01 | 113.40 |
| 28 | 5B | 73 | LEU | CA-CB-CG | 5.28 | 127.44 | 115.30 |
| 40 | UA | 132 | LEU | CA-CB-CG | 5.27 | 127.43 | 115.30 |
| 41 | SB | 171 | PRO | C-N-CA | 5.27 | 134.88 | 121.70 |
| 40 | UH | 189 | LEU | CB-CG-CD2 | -5.27 | 102.05 | 111.00 |
| 41 | FB | 395 | LEU | CA-CB-CG | 5.26 | 127.41 | 115.30 |
| 41 | KM | 121 | ARG | CB-CG-CD | 5.26 | 125.29 | 111.60 |
| 41 | OB | 284 | LEU | CA-CB-CG | 5.26 | 127.41 | 115.30 |
| 41 | UB | 249 | ASP | CB-CG-OD1 | 5.26 | 123.04 | 118.30 |
| 40 | WA | 127 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 8 | 1X | 288 | MET | CG-SD-CE | -5.26 | 91.78 | 100.20 |
| 41 | OL | 225 | LEU | CB-CG-CD2 | 5.26 | 119.94 | 111.00 |
| 40 | RH | 152 | LEU | CA-CB-CG | 5.26 | 127.40 | 115.30 |
| 41 | BN | 42 | LEU | CA-CB-CG | 5.26 | 127.39 | 115.30 |
| 41 | DO | 323 | MET | CA-CB-CG | 5.26 | 122.24 | 113.30 |
| 41 | PO | 7 | LEU | CA-CB-CG | 5.25 | 127.38 | 115.30 |
| 41 | FO | 228 | LEU | CA-CB-CG | 5.25 | 127.38 | 115.30 |
| 41 | OP | 65 | LEU | CA-CB-CG | 5.25 | 127.38 | 115.30 |
| 41 | QL | 246 | LEU | CA-CB-CG | 5.25 | 127.37 | 115.30 |
| 41 | IP | 42 | LEU | CA-CB-CG | 5.25 | 127.36 | 115.30 |
| 41 | FN | 114 | ASP | CB-CG-OD2 | 5.24 | 123.02 | 118.30 |
| 41 | KP | 112 | LEU | CA-CB-CG | 5.24 | 127.35 | 115.30 |
| 41 | MM | 395 | LEU | CA-CB-CG | 5.24 | 127.34 | 115.30 |
| 40 | JE | 227 | LEU | CA-CB-CG | 5.23 | 127.34 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | WG | 424 | MET | CB-CG-SD | -5.23 | 96.70 | 112.40 |
| 40 | PE | 9 | VAL | CG1-CB-CG2 | -5.23 | 102.53 | 110.90 |
| 12 | 2R | 186 | LEU | CA-CB-CG | 5.23 | 127.33 | 115.30 |
| 40 | KF | 227 | LEU | CA-CB-CG | 5.23 | 127.32 | 115.30 |
| 40 | AF | 352 | LYS | CD-CE-NZ | 5.22 | 123.71 | 111.70 |
| 40 | FI | 322 | ASP | CB-CG-OD1 | 5.22 | 123.00 | 118.30 |
| 40 | HH | 60 | LYS | CD-CE-NZ | -5.21 | 99.72 | 111.70 |
| 41 | ON | 173 | PRO | CA-N-CD | -5.21 | 104.20 | 111.50 |
| 40 | MD | 274 | PRO | CB-CA-C | 5.20 | 125.00 | 112.00 |
| 22 | 4H | 108 | LEU | CA-CB-CG | 5.20 | 127.25 | 115.30 |
| 41 | LM | 73 | MET | CA-CB-CG | 5.20 | 122.14 | 113.30 |
| 40 | UE | 70 | LEU | CA-CB-CG | 5.20 | 127.26 | 115.30 |
| 41 | IO | 284 | LEU | CA-CB-CG | 5.19 | 127.24 | 115.30 |
| 41 | KM | 112 | LEU | CB-CG-CD1 | -5.19 | 102.17 | 111.00 |
| 41 | LM | 284 | LEU | CA-CB-CG | 5.19 | 127.24 | 115.30 |
| 41 | MB | 331 | LEU | CB-CG-CD1 | -5.19 | 102.17 | 111.00 |
| 41 | PP | 228 | LEU | CA-CB-CG | 5.19 | 127.24 | 115.30 |
| 41 | VO | 284 | LEU | CA-CB-CG | 5.19 | 127.24 | 115.30 |
| 40 | ME | 152 | LEU | CB-CG-CD2 | 5.19 | 119.82 | 111.00 |
| 40 | SG | 132 | LEU | CA-CB-CG | 5.19 | 127.23 | 115.30 |
| 41 | UB | 284 | LEU | CA-CB-CG | 5.19 | 127.23 | 115.30 |
| 24 | 4O | 196 | PHE | CB-CA-C | 5.18 | 120.76 | 110.40 |
| 41 | NL | 252 | LYS | CB-CG-CD | -5.18 | 98.13 | 111.60 |
| 41 | EL | 117 | LEU | CA-CB-CG | 5.18 | 127.21 | 115.30 |
| 22 | 4J | 242 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 10 | 2G | 94 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 41 | UN | 397 | TRP | CA-CB-CG | -5.17 | 103.88 | 113.70 |
| 36 | 5X | 85 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 40 | SA | 26 | LEU | CA-CB-CG | 5.17 | 127.18 | 115.30 |
| 40 | WI | 217 | LEU | CA-CB-CG | 5.17 | 127.18 | 115.30 |
| 40 | OF | 33 | ASP | CB-CG-OD1 | 5.16 | 122.94 | 118.30 |
| 40 | AF | 422 | GLU | N-CA-CB | 5.16 | 119.89 | 110.60 |
| 40 | JD | 263 | PRO | CA-N-CD | -5.16 | 104.28 | 111.50 |
| 41 | NM | 42 | LEU | CA-CB-CG | 5.15 | 127.15 | 115.30 |
| 22 | 4J | 91 | ASP | C-N-CA | 5.15 | 134.57 | 121.70 |
| 41 | UM | 65 | LEU | CA-CB-CG | 5.15 | 127.14 | 115.30 |
| 40 | BF | 69 | ASP | CB-CG-OD1 | 5.14 | 122.93 | 118.30 |
| 41 | IQ | 377 | LEU | CA-CB-CG | 5.14 | 127.12 | 115.30 |
| 41 | OO | 164 | MET | CA-CB-CG | 5.14 | 122.04 | 113.30 |
| 41 | OP | 246 | LEU | CA-CB-CG | 5.14 | 127.12 | 115.30 |
| 40 | BA | 75 | ILE | CG1-CB-CG2 | -5.13 | 100.11 | 111.40 |
| 26 | 4V | 27 | LEU | CA-CB-CG | 5.13 | 127.09 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | HH | 152 | LEU | CA-CB-CG | 5.13 | 127.09 | 115.30 |
| 41 | IO | 252 | LYS | CA-CB-CG | 5.13 | 124.68 | 113.40 |
| 41 | UO | 300 | MET | CG-SD-CE | -5.13 | 91.99 | 100.20 |
| 41 | AP | 65 | LEU | CA-CB-CG | 5.13 | 127.09 | 115.30 |
| 41 | OP | 164 | MET | CA-CB-CG | 5.12 | 122.00 | 113.30 |
| 1 | 1A | 651 | ASP | CB-CG-OD1 | 5.12 | 122.91 | 118.30 |
| 1 | 1A | 480 | MET | CA-CB-CG | 5.11 | 121.99 | 113.30 |
| 10 | 2F | 47 | LEU | CB-CG-CD2 | -5.11 | 102.31 | 111.00 |
| 21 | 4E | 220 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 40 | KG | 242 | LEU | CA-CB-CG | 5.11 | 127.04 | 115.30 |
| 40 | VG | 427 | LEU | CA-CB-CG | 5.11 | 127.04 | 115.30 |
| 40 | RA | 396 | LEU | CA-CB-CG | 5.09 | 127.02 | 115.30 |
| 16 | 3K | 366 | LEU | CA-CB-CG | 5.09 | 127.01 | 115.30 |
| 40 | KD | 433 | GLU | N-CA-CB | 5.09 | 119.76 | 110.60 |
| 40 | MD | 274 | PRO | CA-CB-CG | -5.09 | 94.33 | 104.00 |
| 1 | 1B | 985 | ARG | CB-CG-CD | 5.08 | 124.82 | 111.60 |
| 41 | RB | 383 | GLU | N-CA-CB | 5.08 | 119.75 | 110.60 |
| 40 | QA | 209 | ILE | CB-CA-C | 5.08 | 121.77 | 111.60 |
| 40 | OE | 227 | LEU | CA-CB-CG | 5.08 | 126.99 | 115.30 |
| 41 | GP | 88 | ASP | CB-CG-OD2 | 5.08 | 122.87 | 118.30 |
| 41 | RB | 84 | ILE | CG1-CB-CG2 | -5.08 | 100.23 | 111.40 |
| 40 | TE | 132 | LEU | CA-CB-CG | 5.08 | 126.98 | 115.30 |
| 41 | HM | 147 | MET | CG-SD-CE | 5.08 | 108.32 | 100.20 |
| 41 | VB | 304 | ASP | CB-CG-OD2 | 5.08 | 122.87 | 118.30 |
| 41 | IO | 395 | LEU | CA-CB-CG | 5.07 | 126.97 | 115.30 |
| 41 | TM | 7 | LEU | CA-CB-CG | 5.07 | 126.97 | 115.30 |
| 38 | 6C | 141 | LEU | CA-CB-CG | 5.07 | 126.96 | 115.30 |
| 41 | RM | 330 | MET | CG-SD-CE | 5.07 | 108.31 | 100.20 |
| 10 | 2F | 94 | LEU | CA-CB-CG | 5.07 | 126.95 | 115.30 |
| 40 | NA | 211 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 41 | RN | 225 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 40 | SH | 127 | ASP | CB-CG-OD2 | 5.06 | 122.86 | 118.30 |
| 41 | HQ | 395 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 41 | PO | 284 | LEU | CA-CB-CG | 5.06 | 126.93 | 115.30 |
| 41 | UB | 395 | LEU | CA-CB-CG | 5.05 | 126.93 | 115.30 |
| 41 | FN | 44 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 41 | VO | 377 | LEU | CA-CB-CG | 5.05 | 126.92 | 115.30 |
| 41 | LB | 295 | ASP | CB-CG-OD1 | 5.05 | 122.84 | 118.30 |
| 5 | 1M | 243 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 |
| 41 | WB | 65 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |
| 33 | 5N | 350 | LEU | CB-CG-CD1 | -5.03 | 102.44 | 111.00 |
| 41 | CB | 246 | LEU | CB-CG-CD1 | 5.03 | 119.55 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 41 | KN | 395 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |
| 40 | QA | 2 | ARG | CA-CB-CG | 5.03 | 124.46 | 113.40 |
| 41 | JL | 377 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |
| 40 | FF | 132 | LEU | CA-CB-CG | 5.02 | 126.86 | 115.30 |
| 41 | VB | 391 | ARG | CA-CB-CG | 5.02 | 124.44 | 113.40 |
| 41 | TM | 395 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |
| 27 | 4Z | 97 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |
| 27 | 4Z | 45 | ARG | C-N-CA | 5.01 | 134.22 | 121.70 |
| 40 | RA | 157 | LEU | CA-CB-CG | 5.00 | 126.81 | 115.30 |
| 40 | PD | 313 | MET | CA-CB-CG | 5.00 | 121.80 | 113.30 |
| 40 | SH | 396 | LEU | CA-CB-CG | 5.00 | 126.81 | 115.30 |

There are no chirality outliers.

All (1619) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | 1A | 853 | ASN | Peptide |
| 1 | 1A | 854 | PRO | Peptide |
| 1 | 1A | 985 | ARG | Sidechain |
| 3 | 1F | 239 | LEU | Peptide |
| 5 | 1L | 275 | ARG | Sidechain |
| 5 | 1L | 291 | ARG | Sidechain |
| 5 | 1L | 293 | ARG | Sidechain |
| 5 | 1L | 296 | ARG | Sidechain |
| 5 | 1M | 93 | ASN | Peptide |
| 5 | 1N | 83 | ARG | Peptide |
| 7 | 1S | 243 | GLY | Peptide |
| 7 | 1S | 278 | SER | Peptide |
| 7 | 1S | 458 | LYS | Peptide |
| 7 | 1T | 101 | ARG | Sidechain |
| 7 | 1T | 106 | ARG | Sidechain |
| 7 | 1T | 183 | ARG | Sidechain |
| 7 | 1T | 206 | ARG | Sidechain |
| 7 | 1T | 235 | ARG | Sidechain |
| 7 | 1T | 277 | ARG | Sidechain |
| 7 | 1T | 299 | ARG | Sidechain |
| 7 | 1T | 316 | ARG | Sidechain |
| 7 | 1T | 357 | ARG | Sidechain |
| 7 | 1T | 369 | ARG | Sidechain |
| 7 | 1T | 399 | ARG | Sidechain |
| 7 | 1T | 407 | ARG | Sidechain |
| 7 | 1T | 431 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | 1T | 468 | ARG | Sidechain |
| 7 | 1T | 492 | ARG | Sidechain |
| 7 | 1T | 494 | ARG | Sidechain |
| 7 | 1T | 495 | ARG | Sidechain |
| 7 | 1T | 524 | ARG | Sidechain |
| 7 | 1T | 538 | ARG | Sidechain |
| 7 | 1U | 235 | ARG | Sidechain |
| 7 | 1U | 278 | SER | Peptide |
| 7 | 1U | 373 | PRO | Peptide |
| 8 | 1W | 317 | ASN | Peptide |
| 8 | 1X | 109 | ARG | Sidechain |
| 8 | 1X | 119 | ARG | Sidechain |
| 8 | 1X | 143 | ARG | Sidechain |
| 8 | 1X | 155 | ARG | Sidechain |
| 8 | 1X | 182 | ARG | Sidechain |
| 8 | 1X | 82 | ARG | Sidechain |
| 8 | 1X | 86 | ARG | Sidechain |
| 9 | 2B | 56 | ARG | Sidechain |
| 9 | 2B | 58 | ARG | Sidechain |
| 10 | 2G | 156 | ASN | Peptide |
| 10 | 2G | 158 | GLY | Peptide |
| 11 | 2I | 119 | LYS | Peptide |
| 11 | 2I | 161 | ARG | Sidechain |
| 11 | 2I | 187 | ARG | Sidechain |
| 11 | 2I | 193 | ARG | Sidechain |
| 11 | 2I | 226 | ARG | Sidechain |
| 11 | 2I | 24 | PRO | Peptide |
| 11 | 2K | 193 | ARG | Sidechain |
| 12 | 2N | 103 | LEU | Peptide |
| 12 | 2O | 128 | ARG | Sidechain |
| 12 | 2P | 103 | LEU | Peptide |
| 12 | 2Q | 90 | LYS | Peptide |
| 13 | 2T | 100 | ARG | Sidechain |
| 13 | 2T | 101 | ARG | Sidechain |
| 13 | 2T | 102 | ARG | Sidechain |
| 13 | 2T | 104 | ARG | Sidechain |
| 13 | 2T | 113 | ARG | Sidechain |
| 13 | 2T | 141 | ARG | Sidechain |
| 13 | 2T | 142 | ARG | Sidechain |
| 13 | 2T | 161 | ARG | Sidechain |
| 13 | 2T | 163 | ARG | Sidechain |
| 13 | 2T | 164 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 13 | 2T | 170 | ARG | Sidechain |
| 13 | 2T | 30 | ARG | Sidechain |
| 13 | 2T | 36 | ARG | Sidechain |
| 13 | 2U | 100 | ARG | Sidechain |
| 13 | 2U | 101 | ARG | Sidechain |
| 13 | 2U | 102 | ARG | Sidechain |
| 13 | 2U | 104 | ARG | Sidechain |
| 13 | 2U | 113 | ARG | Sidechain |
| 13 | 2U | 124 | ARG | Sidechain |
| 13 | 2U | 142 | ARG | Sidechain |
| 13 | 2U | 161 | ARG | Sidechain |
| 13 | 2U | 163 | ARG | Sidechain |
| 13 | 2U | 164 | ARG | Sidechain |
| 13 | 2U | 170 | ARG | Sidechain |
| 13 | 2U | 36 | ARG | Sidechain |
| 13 | 2V | 100 | ARG | Sidechain |
| 13 | 2V | 101 | ARG | Sidechain |
| 13 | 2V | 102 | ARG | Sidechain |
| 13 | 2V | 104 | ARG | Sidechain |
| 13 | 2V | 113 | ARG | Sidechain |
| 13 | 2V | 124 | ARG | Sidechain |
| 13 | 2V | 141 | ARG | Sidechain |
| 13 | 2V | 142 | ARG | Sidechain |
| 13 | 2V | 153 | ARG | Sidechain |
| 13 | 2V | 163 | ARG | Sidechain |
| 13 | 2V | 164 | ARG | Sidechain |
| 13 | 2V | 170 | ARG | Sidechain |
| 13 | 2V | 36 | ARG | Sidechain |
| 13 | 2W | 100 | ARG | Sidechain |
| 13 | 2W | 101 | ARG | Sidechain |
| 13 | 2W | 104 | ARG | Sidechain |
| 13 | 2W | 141 | ARG | Sidechain |
| 13 | 2W | 142 | ARG | Sidechain |
| 13 | 2W | 153 | ARG | Sidechain |
| 13 | 2W | 161 | ARG | Sidechain |
| 13 | 2W | 163 | ARG | Sidechain |
| 13 | 2W | 164 | ARG | Sidechain |
| 13 | 2W | 170 | ARG | Sidechain |
| 13 | 2W | 36 | ARG | Sidechain |
| 13 | 2X | 100 | ARG | Sidechain |
| 13 | 2X | 101 | ARG | Sidechain |
| 13 | 2X | 102 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 13 | 2X | 104 | ARG | Sidechain |
| 13 | 2X | 113 | ARG | Sidechain |
| 13 | 2X | 124 | ARG | Sidechain |
| 13 | 2X | 141 | ARG | Sidechain |
| 13 | 2X | 142 | ARG | Sidechain |
| 13 | 2X | 161 | ARG | Sidechain |
| 13 | 2X | 164 | ARG | Sidechain |
| 13 | 2X | 170 | ARG | Sidechain |
| 13 | 2X | 30 | ARG | Sidechain |
| 13 | 2X | 36 | ARG | Sidechain |
| 14 | 3C | 52 | SER | Peptide |
| 15 | 3E | 66 | ARG | Sidechain |
| 17 | 3O | 350 | ARG | Sidechain |
| 17 | 3O | 387 | ARG | Sidechain |
| 17 | 3O | 399 | ARG | Sidechain |
| 17 | 3O | 403 | ARG | Sidechain |
| 17 | 3O | 405 | ARG | Sidechain |
| 17 | 3O | 406 | ARG | Sidechain |
| 17 | 3O | 419 | ARG | Sidechain |
| 17 | 3P | 101 | ARG | Sidechain |
| 17 | 3P | 114 | ARG | Sidechain |
| 17 | 3P | 119 | ARG | Sidechain |
| 17 | 3P | 121 | ARG | Sidechain |
| 17 | 3P | 126 | ARG | Sidechain |
| 17 | 3P | 183 | ARG | Sidechain |
| 17 | 3P | 196 | ARG | Sidechain |
| 17 | 3P | 202 | ARG | Sidechain |
| 17 | 3P | 205 | ARG | Sidechain |
| 17 | 3P | 232 | ARG | Sidechain |
| 17 | 3P | 248 | ARG | Sidechain |
| 17 | 3P | 275 | ARG | Sidechain |
| 17 | 3P | 285 | ARG | Sidechain |
| 17 | 3P | 289 | ARG | Sidechain |
| 17 | 3P | 310 | ARG | Sidechain |
| 17 | 3P | 315 | ARG | Sidechain |
| 17 | 3P | 322 | ARG | Sidechain |
| 17 | 3P | 350 | ARG | Sidechain |
| 17 | 3P | 387 | ARG | Sidechain |
| 17 | 3P | 399 | ARG | Sidechain |
| 17 | 3P | 403 | ARG | Sidechain |
| 17 | 3P | 405 | ARG | Sidechain |
| 17 | 3P | 406 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 17 | 3P | 419 | ARG | Sidechain |
| 17 | 3P | 437 | ARG | Sidechain |
| 17 | 3P | 439 | ARG | Sidechain |
| 17 | 3P | 93 | ARG | Sidechain |
| 17 | 3Q | 387 | ARG | Sidechain |
| 17 | 3Q | 399 | ARG | Sidechain |
| 17 | 3Q | 403 | ARG | Sidechain |
| 17 | 3Q | 406 | ARG | Sidechain |
| 17 | 3Q | 413 | ARG | Sidechain |
| 17 | 3Q | 419 | ARG | Sidechain |
| 17 | 3Q | 437 | ARG | Sidechain |
| 17 | 3Q | 439 | ARG | Sidechain |
| 17 | 3R | 101 | ARG | Sidechain |
| 17 | 3R | 114 | ARG | Sidechain |
| 17 | 3R | 119 | ARG | Sidechain |
| 17 | 3R | 126 | ARG | Sidechain |
| 17 | 3R | 266 | ARG | Sidechain |
| 17 | 3R | 275 | ARG | Sidechain |
| 17 | 3R | 285 | ARG | Sidechain |
| 17 | 3R | 93 | ARG | Sidechain |
| 18 | 3U | 71 | ARG | Sidechain |
| 19 | 3Y | 165 | ARG | Sidechain |
| 19 | 3Y | 173 | ARG | Sidechain |
| 19 | 3Y | 179 | ARG | Sidechain |
| 19 | 3Z | 382 | ARG | Sidechain |
| 20 | 4A | 154 | ARG | Sidechain |
| 20 | 4A | 161 | ARG | Sidechain |
| 20 | 4A | 166 | ARG | Sidechain |
| 20 | 4A | 189 | ARG | Sidechain |
| 20 | 4A | 19 | ARG | Sidechain |
| 20 | 4A | 195 | ARG | Sidechain |
| 20 | 4A | 20 | ARG | Sidechain |
| 20 | 4A | 207 | ARG | Sidechain |
| 20 | 4A | 22 | ARG | Sidechain |
| 20 | 4A | 228 | ARG | Sidechain |
| 20 | 4A | 230 | ARG | Sidechain |
| 20 | 4A | 26 | ARG | Sidechain |
| 20 | 4A | 29 | ARG | Sidechain |
| 20 | 4A | 34 | ARG | Sidechain |
| 20 | 4A | 36 | ARG | Sidechain |
| 20 | 4A | 52 | ARG | Sidechain |
| 20 | 4A | 87 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 20 | 4A | 89 | ARG | Sidechain |
| 20 | 4B | 228 | ARG | Sidechain |
| 20 | 4B | 230 | ARG | Sidechain |
| 20 | 4B | 231 | ARG | Sidechain |
| 20 | 4B | 282 | ARG | Sidechain |
| 20 | 4B | 293 | ARG | Sidechain |
| 20 | 4B | 300 | ARG | Sidechain |
| 20 | 4B | 319 | ARG | Sidechain |
| 20 | 4B | 329 | ARG | Sidechain |
| 21 | 4D | 34 | ARG | Sidechain |
| 21 | 4D | 421 | ARG | Sidechain |
| 21 | 4D | 436 | ARG | Sidechain |
| 21 | 4D | 437 | ARG | Sidechain |
| 21 | 4D | 457 | ARG | Sidechain |
| 21 | 4D | 469 | ARG | Sidechain |
| 21 | 4D | 502 | ARG | Sidechain |
| 21 | 4E | 436 | ARG | Sidechain |
| 21 | 4E | 437 | ARG | Sidechain |
| 21 | 4E | 457 | ARG | Sidechain |
| 21 | 4E | 469 | ARG | Sidechain |
| 21 | 4E | 502 | ARG | Sidechain |
| 21 | 4F | 359 | PHE | Peptide |
| 21 | 4F | 421 | ARG | Sidechain |
| 21 | 4F | 436 | ARG | Sidechain |
| 21 | 4F | 437 | ARG | Sidechain |
| 21 | 4F | 457 | ARG | Sidechain |
| 21 | 4F | 469 | ARG | Sidechain |
| 22 | 4H | 13 | ARG | Sidechain |
| 22 | 4H | 140 | PRO | Peptide |
| 22 | 4H | 31 | ASN | Peptide |
| 22 | 4I | 140 | PRO | Peptide |
| 22 | 4I | 543 | SER | Peptide |
| 22 | 4I | 637 | ARG | Sidechain |
| 22 | 4I | 647 | ARG | Sidechain |
| 22 | 4I | 660 | ARG | Sidechain |
| 22 | 4I | 666 | ARG | Sidechain |
| 22 | 4J | 140 | PRO | Peptide |
| 22 | 4J | 637 | ARG | Sidechain |
| 22 | 4J | 700 | ARG | Sidechain |
| 22 | 4J | 92 | LYS | Peptide |
| 22 | 4K | 637 | ARG | Sidechain |
| 22 | 4K | 647 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 22 | 4K | 660 | ARG | Sidechain |
| 22 | 4K | 666 | ARG | Sidechain |
| 22 | 4K | 700 | ARG | Sidechain |
| 23 | 4M | 177 | ARG | Sidechain |
| 23 | 4M | 180 | ARG | Sidechain |
| 23 | 4M | 193 | ARG | Sidechain |
| 23 | 4M | 195 | ARG | Sidechain |
| 23 | 4M | 234 | ARG | Sidechain |
| 23 | 4M | 30 | ARG | Sidechain |
| 23 | 4N | 177 | ARG | Sidechain |
| 23 | 4N | 180 | ARG | Sidechain |
| 23 | 4N | 193 | ARG | Sidechain |
| 23 | 4N | 195 | ARG | Sidechain |
| 23 | 4N | 58 | ARG | Sidechain |
| 24 | 4O | 177 | ARG | Sidechain |
| 24 | 4O | 193 | ARG | Sidechain |
| 24 | 4O | 195 | ARG | Sidechain |
| 24 | 4O | 234 | ARG | Sidechain |
| 24 | 4O | 259 | ARG | Sidechain |
| 23 | 4P | 177 | ARG | Sidechain |
| 23 | 4P | 180 | ARG | Sidechain |
| 23 | 4P | 193 | ARG | Sidechain |
| 23 | 4P | 195 | ARG | Sidechain |
| 23 | 4Q | 177 | ARG | Sidechain |
| 23 | 4Q | 180 | ARG | Sidechain |
| 23 | 4Q | 193 | ARG | Sidechain |
| 23 | 4Q | 195 | ARG | Sidechain |
| 23 | 4Q | 234 | ARG | Sidechain |
| 23 | 4Q | 259 | ARG | Sidechain |
| 23 | 4R | 177 | ARG | Sidechain |
| 23 | 4R | 180 | ARG | Sidechain |
| 23 | 4R | 193 | ARG | Sidechain |
| 23 | 4R | 234 | ARG | Sidechain |
| 23 | 4R | 259 | ARG | Sidechain |
| 23 | 4R | 30 | ARG | Sidechain |
| 23 | 4R | 46 | ARG | Sidechain |
| 23 | 4R | 58 | ARG | Sidechain |
| 25 | 4T | 289 | VAL | Peptide |
| 25 | 4T | 392 | ARG | Sidechain |
| 25 | 4T | 397 | ARG | Sidechain |
| 25 | 4T | 432 | SER | Peptide |
| 26 | 4V | 30 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 26 | 4V | 31 | GLY | Peptide |
| 26 | 4W | 345 | ILE | Peptide |
| 27 | 4Z | 43 | ASN | Peptide |
| 28 | 5B | 217 | ARG | Sidechain |
| 29 | 5D | 99 | PHE | Peptide |
| 30 | 5G | 57 | ILE | Peptide |
| 31 | 5I | 416 | ASP | Peptide |
| 31 | 5I | 505 | ARG | Sidechain |
| 31 | 5I | 686 | ARG | Sidechain |
| 33 | 5N | 470 | LYS | Peptide |
| 33 | 5O | 137 | ARG | Sidechain |
| 34 | 5R | 332 | ARG | Sidechain |
| 34 | 5R | 337 | ARG | Sidechain |
| 34 | 5R | 349 | ARG | Sidechain |
| 34 | 5R | 380 | ARG | Sidechain |
| 34 | 5R | 386 | ARG | Sidechain |
| 34 | 5R | 397 | ARG | Sidechain |
| 34 | 5R | 407 | ARG | Sidechain |
| 34 | 5R | 415 | ARG | Sidechain |
| 34 | 5R | 421 | ARG | Sidechain |
| 34 | 5R | 431 | ARG | Sidechain |
| 34 | 5R | 439 | ARG | Sidechain |
| 34 | 5R | 440 | ARG | Sidechain |
| 34 | 5R | 448 | ARG | Sidechain |
| 34 | 5R | 458 | ARG | Sidechain |
| 34 | 5R | 462 | ARG | Sidechain |
| 35 | 5U | 26 | ARG | Sidechain |
| 36 | 5W | 109 | THR | Peptide |
| 36 | 5W | 215 | TYR | Peptide |
| 36 | 5X | 215 | TYR | Peptide |
| 38 | 6C | 185 | ARG | Sidechain |
| 38 | 6C | 186 | ARG | Sidechain |
| 38 | 6C | 33 | ASN | Peptide |
| 38 | 6C | 63 | ASP | Peptide |
| 38 | 6C | 67 | VAL | Peptide |
| 38 | 6D | 283 | ARG | Sidechain |
| 39 | 6F | 116 | ARG | Sidechain |
| 39 | 6G | 116 | ARG | Sidechain |
| 39 | 6G | 119 | TYR | Peptide |
| 39 | 6H | 61 | ASN | Peptide |
| 39 | 6L | 116 | ARG | Sidechain |
| 39 | 6L | 119 | TYR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 39 | 6L | 133 | ARG | Sidechain |
| 40 | AA | 273 | ALA | Peptide |
| 41 | AB | 194 | GLU | Peptide |
| 41 | AB | 271 | ALA | Peptide |
| 40 | AE | 273 | ALA | Peptide |
| 40 | AF | 273 | ALA | Peptide |
| 40 | AG | 273 | ALA | Peptide |
| 40 | AH | 273 | ALA | Peptide |
| 41 | AL | 271 | ALA | Peptide |
| 41 | AM | 271 | ALA | Peptide |
| 41 | AN | 271 | ALA | Peptide |
| 41 | AN | 58 | LYS | Peptide |
| 41 | AO | 162 | ARG | Sidechain |
| 41 | AO | 2 | ARG | Sidechain |
| 41 | AO | 213 | ARG | Sidechain |
| 41 | AO | 241 | ARG | Sidechain |
| 41 | AO | 262 | ARG | Sidechain |
| 41 | AO | 276 | ARG | Sidechain |
| 41 | AO | 282 | ARG | Sidechain |
| 41 | AO | 306 | ARG | Sidechain |
| 41 | AO | 309 | ARG | Sidechain |
| 41 | AO | 359 | ARG | Sidechain |
| 41 | AO | 380 | ARG | Sidechain |
| 41 | AO | 390 | ARG | Sidechain |
| 41 | AO | 46 | ARG | Sidechain |
| 41 | AO | 62 | ARG | Sidechain |
| 41 | AO | 77 | ARG | Sidechain |
| 41 | AP | 271 | ALA | Peptide |
| 40 | BA | 273 | ALA | Peptide |
| 41 | BB | 121 | ARG | Sidechain |
| 41 | BB | 156 | ARG | Sidechain |
| 41 | BB | 162 | ARG | Sidechain |
| 41 | BB | 2 | ARG | Sidechain |
| 41 | BB | 213 | ARG | Sidechain |
| 41 | BB | 241 | ARG | Sidechain |
| 41 | BB | 276 | ARG | Sidechain |
| 41 | BB | 282 | ARG | Sidechain |
| 41 | BB | 306 | ARG | Sidechain |
| 41 | BB | 309 | ARG | Sidechain |
| 41 | BB | 318 | ARG | Sidechain |
| 41 | BB | 320 | ARG | Sidechain |
| 41 | BB | 359 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | BB | 380 | ARG | Sidechain |
| 41 | BB | 390 | ARG | Sidechain |
| 41 | BB | 425 | ARG | Sidechain |
| 41 | BB | 46 | ARG | Sidechain |
| 41 | BB | 62 | ARG | Sidechain |
| 41 | BB | 77 | ARG | Sidechain |
| 41 | BB | 86 | ARG | Sidechain |
| 40 | BE | 105 | ARG | Sidechain |
| 40 | BE | 123 | ARG | Sidechain |
| 40 | BE | 156 | ARG | Sidechain |
| 40 | BE | 2 | ARG | Sidechain |
| 40 | BE | 214 | ARG | Sidechain |
| 40 | BE | 215 | ARG | Sidechain |
| 40 | BE | 221 | ARG | Sidechain |
| 40 | BE | 229 | ARG | Sidechain |
| 40 | BE | 243 | ARG | Sidechain |
| 40 | BE | 264 | ARG | Sidechain |
| 40 | BE | 308 | ARG | Sidechain |
| 40 | BE | 320 | ARG | Sidechain |
| 40 | BE | 372 | ARG | Sidechain |
| 40 | BE | 389 | ARG | Sidechain |
| 40 | BE | 401 | ARG | Sidechain |
| 40 | BE | 421 | ARG | Sidechain |
| 40 | BE | 64 | ARG | Sidechain |
| 40 | BE | 79 | ARG | Sidechain |
| 40 | BE | 84 | ARG | Sidechain |
| 40 | BF | 273 | ALA | Peptide |
| 40 | BF | 29 | GLY | Peptide |
| 40 | BG | 273 | ALA | Peptide |
| 40 | BH | 105 | ARG | Sidechain |
| 40 | BH | 121 | ARG | Sidechain |
| 40 | BH | 123 | ARG | Sidechain |
| 40 | BH | 156 | ARG | Sidechain |
| 40 | BH | 214 | ARG | Sidechain |
| 40 | BH | 221 | ARG | Sidechain |
| 40 | BH | 229 | ARG | Sidechain |
| 40 | BH | 243 | ARG | Sidechain |
| 40 | BH | 264 | ARG | Sidechain |
| 40 | BH | 320 | ARG | Sidechain |
| 40 | BH | 339 | ARG | Sidechain |
| 40 | BH | 372 | ARG | Sidechain |
| 40 | BH | 389 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | BH | 401 | ARG | Sidechain |
| 40 | BH | 421 | ARG | Sidechain |
| 40 | BH | 64 | ARG | Sidechain |
| 40 | BH | 79 | ARG | Sidechain |
| 40 | BH | 84 | ARG | Sidechain |
| 40 | BI | 105 | ARG | Sidechain |
| 40 | BI | 121 | ARG | Sidechain |
| 40 | BI | 123 | ARG | Sidechain |
| 40 | BI | 156 | ARG | Sidechain |
| 40 | BI | 214 | ARG | Sidechain |
| 40 | BI | 221 | ARG | Sidechain |
| 40 | BI | 243 | ARG | Sidechain |
| 40 | BI | 264 | ARG | Sidechain |
| 40 | BI | 372 | ARG | Sidechain |
| 40 | BI | 389 | ARG | Sidechain |
| 40 | BI | 401 | ARG | Sidechain |
| 40 | BI | 421 | ARG | Sidechain |
| 40 | BI | 64 | ARG | Sidechain |
| 40 | BI | 79 | ARG | Sidechain |
| 40 | BI | 84 | ARG | Sidechain |
| 41 | BL | 271 | ALA | Peptide |
| 41 | BM | 121 | ARG | Sidechain |
| 41 | BM | 156 | ARG | Sidechain |
| 41 | BM | 162 | ARG | Sidechain |
| 41 | BM | 2 | ARG | Sidechain |
| 41 | BM | 213 | ARG | Sidechain |
| 41 | BM | 241 | ARG | Sidechain |
| 41 | BM | 251 | ARG | Sidechain |
| 41 | BM | 276 | ARG | Sidechain |
| 41 | BM | 282 | ARG | Sidechain |
| 41 | BM | 306 | ARG | Sidechain |
| 41 | BM | 309 | ARG | Sidechain |
| 41 | BM | 318 | ARG | Sidechain |
| 41 | BM | 320 | ARG | Sidechain |
| 41 | BM | 380 | ARG | Sidechain |
| 41 | BM | 390 | ARG | Sidechain |
| 41 | BM | 391 | ARG | Sidechain |
| 41 | BM | 425 | ARG | Sidechain |
| 41 | BM | 46 | ARG | Sidechain |
| 41 | BM | 62 | ARG | Sidechain |
| 41 | BM | 77 | ARG | Sidechain |
| 41 | BN | 107 | THR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | BN | 271 | ALA | Peptide |
| 41 | BN | 274 | THR | Peptide |
| 41 | BN | 278 | SER | Peptide |
| 41 | BO | 121 | ARG | Sidechain |
| 41 | BO | 156 | ARG | Sidechain |
| 41 | BO | 162 | ARG | Sidechain |
| 41 | BO | 2 | ARG | Sidechain |
| 41 | BO | 213 | ARG | Sidechain |
| 41 | BO | 241 | ARG | Sidechain |
| 41 | BO | 276 | ARG | Sidechain |
| 41 | BO | 282 | ARG | Sidechain |
| 41 | BO | 306 | ARG | Sidechain |
| 41 | BO | 309 | ARG | Sidechain |
| 41 | BO | 318 | ARG | Sidechain |
| 41 | BO | 359 | ARG | Sidechain |
| 41 | BO | 380 | ARG | Sidechain |
| 41 | BO | 390 | ARG | Sidechain |
| 41 | BO | 46 | ARG | Sidechain |
| 41 | BO | 62 | ARG | Sidechain |
| 41 | BO | 77 | ARG | Sidechain |
| 41 | BO | 86 | ARG | Sidechain |
| 41 | BP | 121 | ARG | Sidechain |
| 41 | BP | 162 | ARG | Sidechain |
| 41 | BP | 2 | ARG | Sidechain |
| 41 | BP | 213 | ARG | Sidechain |
| 41 | BP | 241 | ARG | Sidechain |
| 41 | BP | 251 | ARG | Sidechain |
| 41 | BP | 262 | ARG | Sidechain |
| 41 | BP | 276 | ARG | Sidechain |
| 41 | BP | 306 | ARG | Sidechain |
| 41 | BP | 309 | ARG | Sidechain |
| 41 | BP | 318 | ARG | Sidechain |
| 41 | BP | 320 | ARG | Sidechain |
| 41 | BP | 380 | ARG | Sidechain |
| 41 | BP | 390 | ARG | Sidechain |
| 41 | BP | 391 | ARG | Sidechain |
| 41 | BP | 425 | ARG | Sidechain |
| 41 | BP | 62 | ARG | Sidechain |
| 41 | BP | 86 | ARG | Sidechain |
| 40 | CA | 105 | ARG | Sidechain |
| 40 | CA | 121 | ARG | Sidechain |
| 40 | CA | 156 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | CA | 2 | ARG | Sidechain |
| 40 | CA | 214 | ARG | Sidechain |
| 40 | CA | 221 | ARG | Sidechain |
| 40 | CA | 229 | ARG | Sidechain |
| 40 | CA | 243 | ARG | Sidechain |
| 40 | CA | 320 | ARG | Sidechain |
| 40 | CA | 339 | ARG | Sidechain |
| 40 | CA | 372 | ARG | Sidechain |
| 40 | CA | 389 | ARG | Sidechain |
| 40 | CA | 401 | ARG | Sidechain |
| 40 | CA | 421 | ARG | Sidechain |
| 40 | CA | 64 | ARG | Sidechain |
| 40 | CA | 84 | ARG | Sidechain |
| 41 | CB | 271 | ALA | Peptide |
| 40 | CE | 273 | ALA | Peptide |
| 40 | CF | 273 | ALA | Peptide |
| 40 | CF | 84 | ARG | Sidechain |
| 40 | CG | 273 | ALA | Peptide |
| 40 | CH | 105 | ARG | Sidechain |
| 40 | CH | 121 | ARG | Sidechain |
| 40 | CH | 123 | ARG | Sidechain |
| 40 | CH | 156 | ARG | Sidechain |
| 40 | CH | 2 | ARG | Sidechain |
| 40 | CH | 214 | ARG | Sidechain |
| 40 | CH | 229 | ARG | Sidechain |
| 40 | CH | 243 | ARG | Sidechain |
| 40 | CH | 264 | ARG | Sidechain |
| 40 | CH | 320 | ARG | Sidechain |
| 40 | CH | 339 | ARG | Sidechain |
| 40 | CH | 372 | ARG | Sidechain |
| 40 | CH | 389 | ARG | Sidechain |
| 40 | CH | 401 | ARG | Sidechain |
| 40 | CH | 64 | ARG | Sidechain |
| 40 | CH | 84 | ARG | Sidechain |
| 40 | CI | 110 | ILE | Peptide |
| 40 | CI | 273 | ALA | Peptide |
| 41 | CL | 121 | ARG | Sidechain |
| 41 | CL | 156 | ARG | Sidechain |
| 41 | CL | 162 | ARG | Sidechain |
| 41 | CL | 2 | ARG | Sidechain |
| 41 | CL | 241 | ARG | Sidechain |
| 41 | CL | 251 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | CL | 262 | ARG | Sidechain |
| 41 | CL | 276 | ARG | Sidechain |
| 41 | CL | 282 | ARG | Sidechain |
| 41 | CL | 306 | ARG | Sidechain |
| 41 | CL | 309 | ARG | Sidechain |
| 41 | CL | 318 | ARG | Sidechain |
| 41 | CL | 320 | ARG | Sidechain |
| 41 | CL | 359 | ARG | Sidechain |
| 41 | CL | 390 | ARG | Sidechain |
| 41 | CL | 391 | ARG | Sidechain |
| 41 | CL | 425 | ARG | Sidechain |
| 41 | CL | 77 | ARG | Sidechain |
| 41 | CL | 86 | ARG | Sidechain |
| 41 | CM | 121 | ARG | Sidechain |
| 41 | CM | 162 | ARG | Sidechain |
| 41 | CM | 2 | ARG | Sidechain |
| 41 | CM | 213 | ARG | Sidechain |
| 41 | CM | 241 | ARG | Sidechain |
| 41 | CM | 262 | ARG | Sidechain |
| 41 | CM | 282 | ARG | Sidechain |
| 41 | CM | 306 | ARG | Sidechain |
| 41 | CM | 309 | ARG | Sidechain |
| 41 | CM | 318 | ARG | Sidechain |
| 41 | CM | 320 | ARG | Sidechain |
| 41 | CM | 359 | ARG | Sidechain |
| 41 | CM | 380 | ARG | Sidechain |
| 41 | CM | 390 | ARG | Sidechain |
| 41 | CM | 391 | ARG | Sidechain |
| 41 | CM | 425 | ARG | Sidechain |
| 41 | CM | 46 | ARG | Sidechain |
| 41 | CM | 77 | ARG | Sidechain |
| 41 | CM | 86 | ARG | Sidechain |
| 41 | CN | 156 | ARG | Sidechain |
| 41 | CN | 162 | ARG | Sidechain |
| 41 | CN | 2 | ARG | Sidechain |
| 41 | CN | 213 | ARG | Sidechain |
| 41 | CN | 241 | ARG | Sidechain |
| 41 | CN | 251 | ARG | Sidechain |
| 41 | CN | 262 | ARG | Sidechain |
| 41 | CN | 276 | ARG | Sidechain |
| 41 | CN | 282 | ARG | Sidechain |
| 41 | CN | 306 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | CN | 318 | ARG | Sidechain |
| 41 | CN | 320 | ARG | Sidechain |
| 41 | CN | 359 | ARG | Sidechain |
| 41 | CN | 380 | ARG | Sidechain |
| 41 | CN | 390 | ARG | Sidechain |
| 41 | CN | 391 | ARG | Sidechain |
| 41 | CN | 425 | ARG | Sidechain |
| 41 | CN | 77 | ARG | Sidechain |
| 41 | CN | 86 | ARG | Sidechain |
| 41 | CO | 121 | ARG | Sidechain |
| 41 | CO | 156 | ARG | Sidechain |
| 41 | CO | 162 | ARG | Sidechain |
| 41 | CO | 2 | ARG | Sidechain |
| 41 | CO | 213 | ARG | Sidechain |
| 41 | CO | 241 | ARG | Sidechain |
| 41 | CO | 251 | ARG | Sidechain |
| 41 | CO | 276 | ARG | Sidechain |
| 41 | CO | 282 | ARG | Sidechain |
| 41 | CO | 306 | ARG | Sidechain |
| 41 | CO | 309 | ARG | Sidechain |
| 41 | CO | 320 | ARG | Sidechain |
| 41 | CO | 359 | ARG | Sidechain |
| 41 | CO | 380 | ARG | Sidechain |
| 41 | CO | 390 | ARG | Sidechain |
| 41 | CO | 391 | ARG | Sidechain |
| 41 | CO | 425 | ARG | Sidechain |
| 41 | CO | 46 | ARG | Sidechain |
| 41 | CO | 62 | ARG | Sidechain |
| 41 | CO | 86 | ARG | Sidechain |
| 41 | CP | 121 | ARG | Sidechain |
| 41 | CP | 156 | ARG | Sidechain |
| 41 | CP | 162 | ARG | Sidechain |
| 41 | CP | 2 | ARG | Sidechain |
| 41 | CP | 213 | ARG | Sidechain |
| 41 | CP | 251 | ARG | Sidechain |
| 41 | CP | 262 | ARG | Sidechain |
| 41 | CP | 276 | ARG | Sidechain |
| 41 | CP | 282 | ARG | Sidechain |
| 41 | CP | 306 | ARG | Sidechain |
| 41 | CP | 309 | ARG | Sidechain |
| 41 | CP | 318 | ARG | Sidechain |
| 41 | CP | 320 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | CP | 359 | ARG | Sidechain |
| 41 | CP | 380 | ARG | Sidechain |
| 41 | CP | 391 | ARG | Sidechain |
| 41 | CP | 425 | ARG | Sidechain |
| 41 | CP | 62 | ARG | Sidechain |
| 41 | CP | 77 | ARG | Sidechain |
| 40 | DA | 105 | ARG | Sidechain |
| 40 | DA | 123 | ARG | Sidechain |
| 40 | DA | 156 | ARG | Sidechain |
| 40 | DA | 2 | ARG | Sidechain |
| 40 | DA | 214 | ARG | Sidechain |
| 40 | DA | 215 | ARG | Sidechain |
| 40 | DA | 221 | ARG | Sidechain |
| 40 | DA | 229 | ARG | Sidechain |
| 40 | DA | 243 | ARG | Sidechain |
| 40 | DA | 264 | ARG | Sidechain |
| 40 | DA | 320 | ARG | Sidechain |
| 40 | DA | 339 | ARG | Sidechain |
| 40 | DA | 372 | ARG | Sidechain |
| 40 | DA | 389 | ARG | Sidechain |
| 40 | DA | 421 | ARG | Sidechain |
| 40 | DA | 64 | ARG | Sidechain |
| 40 | DA | 84 | ARG | Sidechain |
| 41 | DB | 121 | ARG | Sidechain |
| 41 | DB | 156 | ARG | Sidechain |
| 41 | DB | 162 | ARG | Sidechain |
| 41 | DB | 213 | ARG | Sidechain |
| 41 | DB | 262 | ARG | Sidechain |
| 41 | DB | 276 | ARG | Sidechain |
| 41 | DB | 282 | ARG | Sidechain |
| 41 | DB | 306 | ARG | Sidechain |
| 41 | DB | 309 | ARG | Sidechain |
| 41 | DB | 318 | ARG | Sidechain |
| 41 | DB | 359 | ARG | Sidechain |
| 41 | DB | 380 | ARG | Sidechain |
| 41 | DB | 390 | ARG | Sidechain |
| 41 | DB | 391 | ARG | Sidechain |
| 41 | DB | 46 | ARG | Sidechain |
| 41 | DB | 62 | ARG | Sidechain |
| 41 | DB | 77 | ARG | Sidechain |
| 41 | DB | 86 | ARG | Sidechain |
| 40 | DE | 121 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | DE | 123 | ARG | Sidechain |
| 40 | DE | 156 | ARG | Sidechain |
| 40 | DE | 2 | ARG | Sidechain |
| 40 | DE | 214 | ARG | Sidechain |
| 40 | DE | 215 | ARG | Sidechain |
| 40 | DE | 221 | ARG | Sidechain |
| 40 | DE | 229 | ARG | Sidechain |
| 40 | DE | 243 | ARG | Sidechain |
| 40 | DE | 264 | ARG | Sidechain |
| 40 | DE | 308 | ARG | Sidechain |
| 40 | DE | 339 | ARG | Sidechain |
| 40 | DE | 372 | ARG | Sidechain |
| 40 | DE | 389 | ARG | Sidechain |
| 40 | DE | 421 | ARG | Sidechain |
| 40 | DE | 64 | ARG | Sidechain |
| 40 | DE | 79 | ARG | Sidechain |
| 40 | DE | 84 | ARG | Sidechain |
| 40 | DF | 105 | ARG | Sidechain |
| 40 | DF | 121 | ARG | Sidechain |
| 40 | DF | 2 | ARG | Sidechain |
| 40 | DF | 214 | ARG | Sidechain |
| 40 | DF | 215 | ARG | Sidechain |
| 40 | DF | 221 | ARG | Sidechain |
| 40 | DF | 229 | ARG | Sidechain |
| 40 | DF | 243 | ARG | Sidechain |
| 40 | DF | 264 | ARG | Sidechain |
| 40 | DF | 320 | ARG | Sidechain |
| 40 | DF | 339 | ARG | Sidechain |
| 40 | DF | 389 | ARG | Sidechain |
| 40 | DF | 401 | ARG | Sidechain |
| 40 | DF | 421 | ARG | Sidechain |
| 40 | DF | 64 | ARG | Sidechain |
| 40 | DF | 79 | ARG | Sidechain |
| 40 | DF | 84 | ARG | Sidechain |
| 40 | DH | 121 | ARG | Sidechain |
| 40 | DH | 123 | ARG | Sidechain |
| 40 | DH | 156 | ARG | Sidechain |
| 40 | DH | 2 | ARG | Sidechain |
| 40 | DH | 214 | ARG | Sidechain |
| 40 | DH | 215 | ARG | Sidechain |
| 40 | DH | 229 | ARG | Sidechain |
| 40 | DH | 243 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | DH | 264 | ARG | Sidechain |
| 40 | DH | 339 | ARG | Sidechain |
| 40 | DH | 389 | ARG | Sidechain |
| 40 | DH | 421 | ARG | Sidechain |
| 40 | DH | 64 | ARG | Sidechain |
| 40 | DH | 79 | ARG | Sidechain |
| 40 | DH | 84 | ARG | Sidechain |
| 40 | DI | 121 | ARG | Sidechain |
| 40 | DI | 123 | ARG | Sidechain |
| 40 | DI | 156 | ARG | Sidechain |
| 40 | DI | 2 | ARG | Sidechain |
| 40 | DI | 214 | ARG | Sidechain |
| 40 | DI | 215 | ARG | Sidechain |
| 40 | DI | 221 | ARG | Sidechain |
| 40 | DI | 229 | ARG | Sidechain |
| 40 | DI | 243 | ARG | Sidechain |
| 40 | DI | 264 | ARG | Sidechain |
| 40 | DI | 320 | ARG | Sidechain |
| 40 | DI | 339 | ARG | Sidechain |
| 40 | DI | 372 | ARG | Sidechain |
| 40 | DI | 389 | ARG | Sidechain |
| 40 | DI | 401 | ARG | Sidechain |
| 40 | DI | 421 | ARG | Sidechain |
| 40 | DI | 64 | ARG | Sidechain |
| 40 | DI | 79 | ARG | Sidechain |
| 40 | DI | 84 | ARG | Sidechain |
| 41 | DL | 121 | ARG | Sidechain |
| 41 | DL | 156 | ARG | Sidechain |
| 41 | DL | 2 | ARG | Sidechain |
| 41 | DL | 213 | ARG | Sidechain |
| 41 | DL | 251 | ARG | Sidechain |
| 41 | DL | 262 | ARG | Sidechain |
| 41 | DL | 276 | ARG | Sidechain |
| 41 | DL | 282 | ARG | Sidechain |
| 41 | DL | 306 | ARG | Sidechain |
| 41 | DL | 318 | ARG | Sidechain |
| 41 | DL | 359 | ARG | Sidechain |
| 41 | DL | 380 | ARG | Sidechain |
| 41 | DL | 390 | ARG | Sidechain |
| 41 | DL | 391 | ARG | Sidechain |
| 41 | DL | 425 | ARG | Sidechain |
| 41 | DL | 77 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | DM | 121 | ARG | Sidechain |
| 41 | DM | 156 | ARG | Sidechain |
| 41 | DM | 162 | ARG | Sidechain |
| 41 | DM | 2 | ARG | Sidechain |
| 41 | DM | 213 | ARG | Sidechain |
| 41 | DM | 241 | ARG | Sidechain |
| 41 | DM | 251 | ARG | Sidechain |
| 41 | DM | 276 | ARG | Sidechain |
| 41 | DM | 282 | ARG | Sidechain |
| 41 | DM | 306 | ARG | Sidechain |
| 41 | DM | 309 | ARG | Sidechain |
| 41 | DM | 318 | ARG | Sidechain |
| 41 | DM | 320 | ARG | Sidechain |
| 41 | DM | 359 | ARG | Sidechain |
| 41 | DM | 380 | ARG | Sidechain |
| 41 | DM | 390 | ARG | Sidechain |
| 41 | DM | 391 | ARG | Sidechain |
| 41 | DM | 425 | ARG | Sidechain |
| 41 | DM | 46 | ARG | Sidechain |
| 41 | DM | 77 | ARG | Sidechain |
| 41 | DN | 121 | ARG | Sidechain |
| 41 | DN | 156 | ARG | Sidechain |
| 41 | DN | 162 | ARG | Sidechain |
| 41 | DN | 2 | ARG | Sidechain |
| 41 | DN | 213 | ARG | Sidechain |
| 41 | DN | 241 | ARG | Sidechain |
| 41 | DN | 251 | ARG | Sidechain |
| 41 | DN | 262 | ARG | Sidechain |
| 41 | DN | 282 | ARG | Sidechain |
| 41 | DN | 306 | ARG | Sidechain |
| 41 | DN | 309 | ARG | Sidechain |
| 41 | DN | 320 | ARG | Sidechain |
| 41 | DN | 380 | ARG | Sidechain |
| 41 | DN | 390 | ARG | Sidechain |
| 41 | DN | 391 | ARG | Sidechain |
| 41 | DN | 425 | ARG | Sidechain |
| 41 | DN | 46 | ARG | Sidechain |
| 41 | DN | 62 | ARG | Sidechain |
| 41 | DO | 271 | ALA | Peptide |
| 41 | DO | 320 | ARG | Peptide |
| 41 | DO | 425 | ARG | Sidechain |
| 41 | DP | 121 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | DP | 156 | ARG | Sidechain |
| 41 | DP | 162 | ARG | Sidechain |
| 41 | DP | 2 | ARG | Sidechain |
| 41 | DP | 213 | ARG | Sidechain |
| 41 | DP | 241 | ARG | Sidechain |
| 41 | DP | 251 | ARG | Sidechain |
| 41 | DP | 262 | ARG | Sidechain |
| 41 | DP | 276 | ARG | Sidechain |
| 41 | DP | 282 | ARG | Sidechain |
| 41 | DP | 306 | ARG | Sidechain |
| 41 | DP | 309 | ARG | Sidechain |
| 41 | DP | 318 | ARG | Sidechain |
| 41 | DP | 320 | ARG | Sidechain |
| 41 | DP | 359 | ARG | Sidechain |
| 41 | DP | 380 | ARG | Sidechain |
| 41 | DP | 390 | ARG | Sidechain |
| 41 | DP | 391 | ARG | Sidechain |
| 41 | DP | 425 | ARG | Sidechain |
| 41 | DP | 46 | ARG | Sidechain |
| 41 | DP | 62 | ARG | Sidechain |
| 41 | DP | 77 | ARG | Sidechain |
| 41 | DP | 86 | ARG | Sidechain |
| 40 | EA | 273 | ALA | Peptide |
| 41 | EB | 271 | ALA | Peptide |
| 41 | EB | 7 | LEU | Peptide |
| 40 | EE | 273 | ALA | Peptide |
| 40 | EE | 276 | ILE | Peptide |
| 40 | EF | 273 | ALA | Peptide |
| 40 | EF | 326 | LYS | Peptide |
| 40 | EG | 273 | ALA | Peptide |
| 40 | EG | 326 | LYS | Peptide |
| 40 | EH | 105 | ARG | Sidechain |
| 40 | EH | 121 | ARG | Sidechain |
| 40 | EH | 123 | ARG | Sidechain |
| 40 | EH | 156 | ARG | Sidechain |
| 40 | EH | 2 | ARG | Sidechain |
| 40 | EH | 229 | ARG | Sidechain |
| 40 | EH | 243 | ARG | Sidechain |
| 40 | EH | 320 | ARG | Sidechain |
| 40 | EH | 389 | ARG | Sidechain |
| 40 | EH | 401 | ARG | Sidechain |
| 40 | EH | 421 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | EH | 84 | ARG | Sidechain |
| 40 | EI | 105 | ARG | Sidechain |
| 40 | EI | 121 | ARG | Sidechain |
| 40 | EI | 123 | ARG | Sidechain |
| 40 | EI | 156 | ARG | Sidechain |
| 40 | EI | 2 | ARG | Sidechain |
| 40 | EI | 214 | ARG | Sidechain |
| 40 | EI | 215 | ARG | Sidechain |
| 40 | EI | 221 | ARG | Sidechain |
| 40 | EI | 229 | ARG | Sidechain |
| 40 | EI | 243 | ARG | Sidechain |
| 40 | EI | 264 | ARG | Sidechain |
| 40 | EI | 308 | ARG | Sidechain |
| 40 | EI | 320 | ARG | Sidechain |
| 40 | EI | 339 | ARG | Sidechain |
| 40 | EI | 401 | ARG | Sidechain |
| 40 | EI | 421 | ARG | Sidechain |
| 40 | EI | 64 | ARG | Sidechain |
| 40 | EI | 79 | ARG | Sidechain |
| 40 | EI | 84 | ARG | Sidechain |
| 41 | EL | 271 | ALA | Peptide |
| 41 | EL | 359 | ARG | Sidechain |
| 41 | EM | 121 | ARG | Sidechain |
| 41 | EM | 156 | ARG | Sidechain |
| 41 | EM | 2 | ARG | Sidechain |
| 41 | EM | 213 | ARG | Sidechain |
| 41 | EM | 241 | ARG | Sidechain |
| 41 | EM | 251 | ARG | Sidechain |
| 41 | EM | 262 | ARG | Sidechain |
| 41 | EM | 276 | ARG | Sidechain |
| 41 | EM | 318 | ARG | Sidechain |
| 41 | EM | 320 | ARG | Sidechain |
| 41 | EM | 359 | ARG | Sidechain |
| 41 | EM | 390 | ARG | Sidechain |
| 41 | EM | 425 | ARG | Sidechain |
| 41 | EM | 46 | ARG | Sidechain |
| 41 | EM | 62 | ARG | Sidechain |
| 41 | EM | 77 | ARG | Sidechain |
| 41 | EM | 86 | ARG | Sidechain |
| 41 | EN | 271 | ALA | Peptide |
| 41 | EO | 271 | ALA | Peptide |
| 41 | EO | 7 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | EP | 156 | ARG | Sidechain |
| 41 | EP | 162 | ARG | Sidechain |
| 41 | EP | 2 | ARG | Sidechain |
| 41 | EP | 213 | ARG | Sidechain |
| 41 | EP | 241 | ARG | Sidechain |
| 41 | EP | 251 | ARG | Sidechain |
| 41 | EP | 276 | ARG | Sidechain |
| 41 | EP | 282 | ARG | Sidechain |
| 41 | EP | 306 | ARG | Sidechain |
| 41 | EP | 318 | ARG | Sidechain |
| 41 | EP | 320 | ARG | Sidechain |
| 41 | EP | 359 | ARG | Sidechain |
| 41 | EP | 425 | ARG | Sidechain |
| 41 | EP | 46 | ARG | Sidechain |
| 41 | EP | 62 | ARG | Sidechain |
| 41 | EP | 77 | ARG | Sidechain |
| 41 | EP | 86 | ARG | Sidechain |
| 40 | FA | 105 | ARG | Sidechain |
| 40 | FA | 121 | ARG | Sidechain |
| 40 | FA | 123 | ARG | Sidechain |
| 40 | FA | 156 | ARG | Sidechain |
| 40 | FA | 2 | ARG | Sidechain |
| 40 | FA | 214 | ARG | Sidechain |
| 40 | FA | 215 | ARG | Sidechain |
| 40 | FA | 221 | ARG | Sidechain |
| 40 | FA | 229 | ARG | Sidechain |
| 40 | FA | 243 | ARG | Sidechain |
| 40 | FA | 264 | ARG | Sidechain |
| 40 | FA | 308 | ARG | Sidechain |
| 40 | FA | 320 | ARG | Sidechain |
| 40 | FA | 339 | ARG | Sidechain |
| 40 | FA | 372 | ARG | Sidechain |
| 40 | FA | 389 | ARG | Sidechain |
| 40 | FA | 401 | ARG | Sidechain |
| 40 | FA | 421 | ARG | Sidechain |
| 40 | FA | 84 | ARG | Sidechain |
| 41 | FB | 271 | ALA | Peptide |
| 41 | FB | 283 | ALA | Peptide |
| 41 | FB | 323 | MET | Peptide |
| 40 | FF | 273 | ALA | Peptide |
| 40 | FG | 128 | GLN | Peptide |
| 40 | FG | 273 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | FG | 58 | ALA | Peptide |
| 40 | FI | 273 | ALA | Peptide |
| 41 | FM | 107 | THR | Peptide |
| 41 | FM | 271 | ALA | Peptide |
| 41 | FM | 323 | MET | Peptide |
| 41 | FN | 271 | ALA | Peptide |
| 41 | FO | 271 | ALA | Peptide |
| 41 | FP | 225 | LEU | Peptide |
| 41 | FP | 226 | ASN | Peptide |
| 41 | FP | 271 | ALA | Peptide |
| 41 | GB | 271 | ALA | Peptide |
| 40 | GE | 105 | ARG | Sidechain |
| 40 | GE | 121 | ARG | Sidechain |
| 40 | GE | 123 | ARG | Sidechain |
| 40 | GE | 214 | ARG | Sidechain |
| 40 | GE | 215 | ARG | Sidechain |
| 40 | GE | 229 | ARG | Sidechain |
| 40 | GE | 243 | ARG | Sidechain |
| 40 | GE | 264 | ARG | Sidechain |
| 40 | GE | 320 | ARG | Sidechain |
| 40 | GE | 339 | ARG | Sidechain |
| 40 | GE | 372 | ARG | Sidechain |
| 40 | GE | 421 | ARG | Sidechain |
| 40 | GE | 79 | ARG | Sidechain |
| 40 | GE | 84 | ARG | Sidechain |
| 40 | GF | 273 | ALA | Peptide |
| 40 | GH | 105 | ARG | Sidechain |
| 40 | GH | 121 | ARG | Sidechain |
| 40 | GH | 123 | ARG | Sidechain |
| 40 | GH | 156 | ARG | Sidechain |
| 40 | GH | 2 | ARG | Sidechain |
| 40 | GH | 221 | ARG | Sidechain |
| 40 | GH | 229 | ARG | Sidechain |
| 40 | GH | 243 | ARG | Sidechain |
| 40 | GH | 308 | ARG | Sidechain |
| 40 | GH | 339 | ARG | Sidechain |
| 40 | GH | 372 | ARG | Sidechain |
| 40 | GH | 389 | ARG | Sidechain |
| 40 | GH | 401 | ARG | Sidechain |
| 40 | GH | 421 | ARG | Sidechain |
| 40 | GH | 64 | ARG | Sidechain |
| 40 | GH | 79 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | GI | 105 | ARG | Sidechain |
| 40 | GI | 121 | ARG | Sidechain |
| 40 | GI | 123 | ARG | Sidechain |
| 40 | GI | 156 | ARG | Sidechain |
| 40 | GI | 2 | ARG | Sidechain |
| 40 | GI | 214 | ARG | Sidechain |
| 40 | GI | 221 | ARG | Sidechain |
| 40 | GI | 243 | ARG | Sidechain |
| 40 | GI | 264 | ARG | Sidechain |
| 40 | GI | 308 | ARG | Sidechain |
| 40 | GI | 320 | ARG | Sidechain |
| 40 | GI | 339 | ARG | Sidechain |
| 40 | GI | 372 | ARG | Sidechain |
| 40 | GI | 389 | ARG | Sidechain |
| 40 | GI | 401 | ARG | Sidechain |
| 40 | GI | 421 | ARG | Sidechain |
| 40 | GI | 64 | ARG | Sidechain |
| 40 | GI | 79 | ARG | Sidechain |
| 40 | GI | 84 | ARG | Sidechain |
| 41 | GM | 107 | THR | Peptide |
| 41 | GM | 271 | ALA | Peptide |
| 41 | GM | 323 | MET | Peptide |
| 41 | GN | 156 | ARG | Sidechain |
| 41 | GN | 2 | ARG | Sidechain |
| 41 | GN | 213 | ARG | Sidechain |
| 41 | GN | 241 | ARG | Sidechain |
| 41 | GN | 262 | ARG | Sidechain |
| 41 | GN | 276 | ARG | Sidechain |
| 41 | GN | 282 | ARG | Sidechain |
| 41 | GN | 306 | ARG | Sidechain |
| 41 | GN | 318 | ARG | Sidechain |
| 41 | GN | 320 | ARG | Sidechain |
| 41 | GN | 359 | ARG | Sidechain |
| 41 | GN | 380 | ARG | Sidechain |
| 41 | GN | 390 | ARG | Sidechain |
| 41 | GN | 391 | ARG | Sidechain |
| 41 | GN | 425 | ARG | Sidechain |
| 41 | GN | 46 | ARG | Sidechain |
| 41 | GN | 62 | ARG | Sidechain |
| 41 | GN | 77 | ARG | Sidechain |
| 41 | GN | 86 | ARG | Sidechain |
| 41 | GP | 226 | ASN | Mainchain,Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | GP | 271 | ALA | Peptide |
| 41 | GP | 323 | MET | Peptide |
| 40 | HA | 273 | ALA | Peptide |
| 40 | HA | 326 | LYS | Peptide |
| 41 | HB | 271 | ALA | Peptide |
| 40 | HE | 105 | ARG | Sidechain |
| 40 | HE | 121 | ARG | Sidechain |
| 40 | HE | 156 | ARG | Sidechain |
| 40 | HE | 2 | ARG | Sidechain |
| 40 | HE | 214 | ARG | Sidechain |
| 40 | HE | 215 | ARG | Sidechain |
| 40 | HE | 221 | ARG | Sidechain |
| 40 | HE | 229 | ARG | Sidechain |
| 40 | HE | 243 | ARG | Sidechain |
| 40 | HE | 264 | ARG | Sidechain |
| 40 | HE | 308 | ARG | Sidechain |
| 40 | HE | 320 | ARG | Sidechain |
| 40 | HE | 339 | ARG | Sidechain |
| 40 | HE | 372 | ARG | Sidechain |
| 40 | HE | 389 | ARG | Sidechain |
| 40 | HE | 401 | ARG | Sidechain |
| 40 | HE | 421 | ARG | Sidechain |
| 40 | HE | 64 | ARG | Sidechain |
| 40 | HE | 79 | ARG | Sidechain |
| 40 | HE | 84 | ARG | Sidechain |
| 40 | HF | 273 | ALA | Peptide |
| 40 | HG | 273 | ALA | Peptide |
| 40 | HG | 326 | LYS | Peptide |
| 40 | HH | 273 | ALA | Peptide |
| 40 | HI | 273 | ALA | Peptide |
| 41 | HM | 107 | THR | Peptide |
| 41 | HM | 271 | ALA | Peptide |
| 41 | HN | 121 | ARG | Sidechain |
| 41 | HN | 156 | ARG | Sidechain |
| 41 | HN | 162 | ARG | Sidechain |
| 41 | HN | 2 | ARG | Sidechain |
| 41 | HN | 213 | ARG | Sidechain |
| 41 | HN | 251 | ARG | Sidechain |
| 41 | HN | 262 | ARG | Sidechain |
| 41 | HN | 276 | ARG | Sidechain |
| 41 | HN | 282 | ARG | Sidechain |
| 41 | HN | 309 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | HN | 318 | ARG | Sidechain |
| 41 | HN | 320 | ARG | Sidechain |
| 41 | HN | 359 | ARG | Sidechain |
| 41 | HN | 390 | ARG | Sidechain |
| 41 | HN | 391 | ARG | Sidechain |
| 41 | HN | 425 | ARG | Sidechain |
| 41 | HN | 46 | ARG | Sidechain |
| 41 | HN | 62 | ARG | Sidechain |
| 41 | HN | 77 | ARG | Sidechain |
| 41 | HN | 86 | ARG | Sidechain |
| 41 | HO | 271 | ALA | Peptide |
| 41 | HP | 107 | THR | Peptide |
| 41 | HP | 271 | ALA | Peptide |
| 41 | HQ | 271 | ALA | Peptide |
| 40 | IA | 273 | ALA | Peptide |
| 40 | IA | 326 | LYS | Peptide |
| 41 | IB | 271 | ALA | Peptide |
| 40 | IE | 273 | ALA | Peptide |
| 40 | IF | 34 | GLY | Peptide |
| 40 | IG | 273 | ALA | Peptide |
| 40 | IG | 64 | ARG | Sidechain |
| 40 | IH | 273 | ALA | Peptide |
| 40 | II | 273 | ALA | Peptide |
| 41 | IM | 107 | THR | Peptide |
| 41 | IM | 271 | ALA | Peptide |
| 41 | IM | 48 | ASN | Peptide |
| 41 | IN | 107 | THR | Peptide |
| 41 | IN | 271 | ALA | Peptide |
| 41 | IO | 271 | ALA | Peptide |
| 41 | IP | 271 | ALA | Peptide |
| 41 | IQ | 271 | ALA | Peptide |
| 40 | JA | 273 | ALA | Peptide |
| 41 | JB | 271 | ALA | Peptide |
| 40 | JD | 273 | ALA | Peptide |
| 40 | JE | 273 | ALA | Peptide |
| 40 | JF | 273 | ALA | Peptide |
| 40 | JG | 15 | GLN | Peptide |
| 40 | JG | 228 | ASN | Peptide |
| 40 | JG | 273 | ALA | Peptide |
| 40 | JH | 273 | ALA | Peptide |
| 41 | JL | 225 | LEU | Peptide |
| 41 | JL | 271 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | JM | 121 | ARG | Sidechain |
| 41 | JM | 156 | ARG | Sidechain |
| 41 | JM | 162 | ARG | Sidechain |
| 41 | JM | 2 | ARG | Sidechain |
| 41 | JM | 213 | ARG | Sidechain |
| 41 | JM | 262 | ARG | Sidechain |
| 41 | JM | 276 | ARG | Sidechain |
| 41 | JM | 282 | ARG | Sidechain |
| 41 | JM | 306 | ARG | Sidechain |
| 41 | JM | 309 | ARG | Sidechain |
| 41 | JM | 320 | ARG | Sidechain |
| 41 | JM | 359 | ARG | Sidechain |
| 41 | JM | 380 | ARG | Sidechain |
| 41 | JM | 46 | ARG | Sidechain |
| 41 | JM | 62 | ARG | Sidechain |
| 41 | JM | 77 | ARG | Sidechain |
| 41 | JM | 86 | ARG | Sidechain |
| 41 | JO | 271 | ALA | Peptide |
| 41 | JO | 380 | ARG | Sidechain |
| 40 | KA | 228 | ASN | Peptide |
| 40 | KA | 273 | ALA | Peptide |
| 40 | KA | 302 | MET | Peptide |
| 41 | KB | 271 | ALA | Peptide |
| 40 | KD | 273 | ALA | Peptide |
| 40 | KE | 273 | ALA | Peptide |
| 40 | KF | 228 | ASN | Peptide |
| 40 | KF | 273 | ALA | Peptide |
| 40 | KG | 273 | ALA | Peptide |
| 40 | KH | 273 | ALA | Peptide |
| 40 | KH | 400 | LYS | Peptide |
| 41 | KL | 162 | ARG | Sidechain |
| 41 | KL | 213 | ARG | Sidechain |
| 41 | KL | 251 | ARG | Sidechain |
| 41 | KL | 262 | ARG | Sidechain |
| 41 | KL | 276 | ARG | Sidechain |
| 41 | KL | 282 | ARG | Sidechain |
| 41 | KL | 309 | ARG | Sidechain |
| 41 | KL | 320 | ARG | Sidechain |
| 41 | KL | 380 | ARG | Sidechain |
| 41 | KL | 390 | ARG | Sidechain |
| 41 | KL | 391 | ARG | Sidechain |
| 41 | KL | 425 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | KL | 46 | ARG | Sidechain |
| 41 | KL | 62 | ARG | Sidechain |
| 41 | KL | 77 | ARG | Sidechain |
| 41 | KL | 86 | ARG | Sidechain |
| 41 | KM | 121 | ARG | Sidechain |
| 41 | KM | 178 | THR | Peptide |
| 41 | KM | 271 | ALA | Peptide |
| 41 | KN | 271 | ALA | Peptide |
| 41 | KN | 422 | VAL | Peptide |
| 41 | KO | 271 | ALA | Peptide |
| 41 | KP | 271 | ALA | Peptide |
| 40 | LA | 273 | ALA | Peptide |
| 41 | LB | 271 | ALA | Peptide |
| 40 | LD | 273 | ALA | Peptide |
| 40 | LE | 15 | GLN | Peptide |
| 40 | LE | 228 | ASN | Peptide |
| 40 | LE | 273 | ALA | Peptide |
| 40 | LE | 64 | ARG | Sidechain |
| 40 | LF | 121 | ARG | Sidechain |
| 40 | LF | 123 | ARG | Sidechain |
| 40 | LF | 156 | ARG | Sidechain |
| 40 | LF | 2 | ARG | Sidechain |
| 40 | LF | 214 | ARG | Sidechain |
| 40 | LF | 215 | ARG | Sidechain |
| 40 | LF | 229 | ARG | Sidechain |
| 40 | LF | 243 | ARG | Sidechain |
| 40 | LF | 308 | ARG | Sidechain |
| 40 | LF | 320 | ARG | Sidechain |
| 40 | LF | 339 | ARG | Sidechain |
| 40 | LF | 372 | ARG | Sidechain |
| 40 | LF | 421 | ARG | Sidechain |
| 40 | LF | 64 | ARG | Sidechain |
| 40 | LF | 79 | ARG | Sidechain |
| 40 | LF | 84 | ARG | Sidechain |
| 40 | LG | 105 | ARG | Sidechain |
| 40 | LG | 121 | ARG | Sidechain |
| 40 | LG | 123 | ARG | Sidechain |
| 40 | LG | 156 | ARG | Sidechain |
| 40 | LG | 214 | ARG | Sidechain |
| 40 | LG | 221 | ARG | Sidechain |
| 40 | LG | 229 | ARG | Sidechain |
| 40 | LG | 243 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | LG | 264 | ARG | Sidechain |
| 40 | LG | 308 | ARG | Sidechain |
| 40 | LG | 320 | ARG | Sidechain |
| 40 | LG | 339 | ARG | Sidechain |
| 40 | LG | 372 | ARG | Sidechain |
| 40 | LG | 389 | ARG | Sidechain |
| 40 | LG | 401 | ARG | Sidechain |
| 40 | LG | 421 | ARG | Sidechain |
| 40 | LG | 79 | ARG | Sidechain |
| 40 | LG | 84 | ARG | Sidechain |
| 40 | LH | 273 | ALA | Peptide |
| 41 | LL | 271 | ALA | Peptide |
| 41 | LM | 271 | ALA | Peptide |
| 41 | LN | 271 | ALA | Peptide |
| 41 | LO | 271 | ALA | Peptide |
| 41 | LP | 213 | ARG | Sidechain |
| 41 | LP | 271 | ALA | Peptide |
| 40 | MA | 105 | ARG | Sidechain |
| 40 | MA | 123 | ARG | Sidechain |
| 40 | MA | 2 | ARG | Sidechain |
| 40 | MA | 214 | ARG | Sidechain |
| 40 | MA | 215 | ARG | Sidechain |
| 40 | MA | 221 | ARG | Sidechain |
| 40 | MA | 229 | ARG | Sidechain |
| 40 | MA | 243 | ARG | Sidechain |
| 40 | MA | 320 | ARG | Sidechain |
| 40 | MA | 401 | ARG | Sidechain |
| 40 | MA | 421 | ARG | Sidechain |
| 40 | MA | 79 | ARG | Sidechain |
| 40 | MA | 84 | ARG | Sidechain |
| 41 | MB | 271 | ALA | Peptide |
| 40 | ME | 228 | ASN | Peptide |
| 40 | ME | 273 | ALA | Peptide |
| 40 | MF | 105 | ARG | Sidechain |
| 40 | MF | 121 | ARG | Sidechain |
| 40 | MF | 123 | ARG | Sidechain |
| 40 | MF | 2 | ARG | Sidechain |
| 40 | MF | 215 | ARG | Sidechain |
| 40 | MF | 221 | ARG | Sidechain |
| 40 | MF | 229 | ARG | Sidechain |
| 40 | MF | 243 | ARG | Sidechain |
| 40 | MF | 264 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | MF | 320 | ARG | Sidechain |
| 40 | MF | 339 | ARG | Sidechain |
| 40 | MF | 372 | ARG | Sidechain |
| 40 | MF | 389 | ARG | Sidechain |
| 40 | MF | 64 | ARG | Sidechain |
| 40 | MF | 79 | ARG | Sidechain |
| 40 | MF | 84 | ARG | Sidechain |
| 40 | MG | 105 | ARG | Sidechain |
| 40 | MG | 121 | ARG | Sidechain |
| 40 | MG | 123 | ARG | Sidechain |
| 40 | MG | 214 | ARG | Sidechain |
| 40 | MG | 215 | ARG | Sidechain |
| 40 | MG | 221 | ARG | Sidechain |
| 40 | MG | 229 | ARG | Sidechain |
| 40 | MG | 243 | ARG | Sidechain |
| 40 | MG | 264 | ARG | Sidechain |
| 40 | MG | 320 | ARG | Sidechain |
| 40 | MG | 401 | ARG | Sidechain |
| 40 | MG | 421 | ARG | Sidechain |
| 40 | MG | 64 | ARG | Sidechain |
| 40 | MG | 79 | ARG | Sidechain |
| 40 | MG | 84 | ARG | Sidechain |
| 40 | MH | 105 | ARG | Sidechain |
| 40 | MH | 121 | ARG | Sidechain |
| 40 | MH | 123 | ARG | Sidechain |
| 40 | MH | 156 | ARG | Sidechain |
| 40 | MH | 2 | ARG | Sidechain |
| 40 | MH | 214 | ARG | Sidechain |
| 40 | MH | 221 | ARG | Sidechain |
| 40 | MH | 229 | ARG | Sidechain |
| 40 | MH | 243 | ARG | Sidechain |
| 40 | MH | 264 | ARG | Sidechain |
| 40 | MH | 320 | ARG | Sidechain |
| 40 | MH | 339 | ARG | Sidechain |
| 40 | MH | 372 | ARG | Sidechain |
| 40 | MH | 389 | ARG | Sidechain |
| 40 | MH | 401 | ARG | Sidechain |
| 40 | MH | 421 | ARG | Sidechain |
| 40 | MH | 79 | ARG | Sidechain |
| 40 | MH | 84 | ARG | Sidechain |
| 41 | ML | 271 | ALA | Peptide |
| 41 | MM | 125 | GLU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | MM | 271 | ALA | Peptide |
| 41 | MN | 271 | ALA | Peptide |
| 41 | MN | 359 | ARG | Sidechain |
| 41 | MO | 156 | ARG | Sidechain |
| 41 | MO | 162 | ARG | Sidechain |
| 41 | MO | 2 | ARG | Sidechain |
| 41 | MO | 241 | ARG | Sidechain |
| 41 | MO | 262 | ARG | Sidechain |
| 41 | MO | 276 | ARG | Sidechain |
| 41 | MO | 282 | ARG | Sidechain |
| 41 | MO | 306 | ARG | Sidechain |
| 41 | MO | 320 | ARG | Sidechain |
| 41 | MO | 359 | ARG | Sidechain |
| 41 | MO | 390 | ARG | Sidechain |
| 41 | MO | 391 | ARG | Sidechain |
| 41 | MO | 425 | ARG | Sidechain |
| 41 | MO | 46 | ARG | Sidechain |
| 41 | MO | 62 | ARG | Sidechain |
| 41 | MO | 77 | ARG | Sidechain |
| 41 | MP | 125 | GLU | Peptide |
| 41 | MP | 271 | ALA | Peptide |
| 40 | NA | 228 | ASN | Peptide |
| 40 | NA | 273 | ALA | Peptide |
| 41 | NB | 271 | ALA | Peptide |
| 41 | NB | 323 | MET | Peptide |
| 40 | ND | 105 | ARG | Sidechain |
| 40 | ND | 121 | ARG | Sidechain |
| 40 | ND | 156 | ARG | Sidechain |
| 40 | ND | 214 | ARG | Sidechain |
| 40 | ND | 215 | ARG | Sidechain |
| 40 | ND | 221 | ARG | Sidechain |
| 40 | ND | 229 | ARG | Sidechain |
| 40 | ND | 243 | ARG | Sidechain |
| 40 | ND | 264 | ARG | Sidechain |
| 40 | ND | 308 | ARG | Sidechain |
| 40 | ND | 320 | ARG | Sidechain |
| 40 | ND | 339 | ARG | Sidechain |
| 40 | ND | 372 | ARG | Sidechain |
| 40 | ND | 389 | ARG | Sidechain |
| 40 | ND | 401 | ARG | Sidechain |
| 40 | ND | 421 | ARG | Sidechain |
| 40 | ND | 79 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | ND | 84 | ARG | Sidechain |
| 40 | NE | 121 | ARG | Sidechain |
| 40 | NE | 273 | ALA | Peptide |
| 40 | NF | 273 | ALA | Peptide |
| 40 | NG | 273 | ALA | Peptide |
| 40 | NG | 339 | ARG | Sidechain |
| 40 | NH | 273 | ALA | Peptide |
| 41 | NL | 107 | THR | Peptide |
| 41 | NL | 21 | TRP | Peptide |
| 41 | NL | 271 | ALA | Peptide |
| 41 | NL | 46 | ARG | Sidechain |
| 41 | NM | 271 | ALA | Peptide |
| 41 | NN | 226 | ASN | Peptide |
| 41 | NN | 271 | ALA | Peptide |
| 41 | NO | 107 | THR | Peptide |
| 41 | NO | 271 | ALA | Peptide |
| 41 | NP | 107 | THR | Peptide |
| 41 | NP | 271 | ALA | Peptide |
| 40 | OA | 259 | LEU | Peptide |
| 40 | OA | 273 | ALA | Peptide |
| 40 | OA | 279 | GLU | Peptide |
| 41 | OB | 107 | THR | Peptide |
| 41 | OB | 271 | ALA | Peptide |
| 41 | OB | 276 | ARG | Sidechain |
| 40 | OD | 273 | ALA | Peptide |
| 40 | OD | 324 | VAL | Peptide |
| 40 | OD | 326 | LYS | Peptide |
| 40 | OD | 79 | ARG | Sidechain |
| 40 | OE | 2 | ARG | Sidechain |
| 40 | OE | 273 | ALA | Peptide |
| 40 | OF | 273 | ALA | Peptide |
| 40 | OG | 273 | ALA | Peptide |
| 40 | OH | 105 | ARG | Sidechain |
| 40 | OH | 121 | ARG | Sidechain |
| 40 | OH | 123 | ARG | Sidechain |
| 40 | OH | 156 | ARG | Sidechain |
| 40 | OH | 2 | ARG | Sidechain |
| 40 | OH | 215 | ARG | Sidechain |
| 40 | OH | 221 | ARG | Sidechain |
| 40 | OH | 243 | ARG | Sidechain |
| 40 | OH | 308 | ARG | Sidechain |
| 40 | OH | 320 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | OH | 339 | ARG | Sidechain |
| 40 | OH | 372 | ARG | Sidechain |
| 40 | OH | 389 | ARG | Sidechain |
| 40 | OH | 401 | ARG | Sidechain |
| 40 | OH | 421 | ARG | Sidechain |
| 40 | OH | 64 | ARG | Sidechain |
| 40 | OH | 79 | ARG | Sidechain |
| 40 | OH | 84 | ARG | Sidechain |
| 41 | OL | 107 | THR | Peptide |
| 41 | OL | 271 | ALA | Peptide |
| 41 | OM | 245 | GLN | Peptide |
| 41 | OM | 271 | ALA | Peptide |
| 41 | ON | 271 | ALA | Peptide |
| 41 | OO | 271 | ALA | Peptide |
| 41 | OP | 271 | ALA | Peptide |
| 41 | OP | 380 | ARG | Sidechain |
| 41 | OP | 391 | ARG | Sidechain |
| 40 | PA | 273 | ALA | Peptide |
| 41 | PB | 271 | ALA | Peptide |
| 40 | PD | 273 | ALA | Peptide |
| 40 | PE | 273 | ALA | Peptide |
| 40 | PE | 279 | GLU | Peptide |
| 40 | PE | 412 | MET | Peptide |
| 40 | PF | 273 | ALA | Peptide |
| 40 | PG | 273 | ALA | Peptide |
| 40 | PH | 273 | ALA | Peptide |
| 41 | PL | 271 | ALA | Peptide |
| 41 | PM | 271 | ALA | Peptide |
| 41 | PN | 271 | ALA | Peptide |
| 41 | PN | 283 | ALA | Peptide |
| 41 | PO | 271 | ALA | Peptide |
| 41 | PP | 271 | ALA | Peptide |
| 40 | QA | 273 | ALA | Peptide |
| 41 | QB | 121 | ARG | Sidechain |
| 41 | QB | 156 | ARG | Sidechain |
| 41 | QB | 162 | ARG | Sidechain |
| 41 | QB | 213 | ARG | Sidechain |
| 41 | QB | 241 | ARG | Sidechain |
| 41 | QB | 251 | ARG | Sidechain |
| 41 | QB | 262 | ARG | Sidechain |
| 41 | QB | 276 | ARG | Sidechain |
| 41 | QB | 282 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | QB | 309 | ARG | Sidechain |
| 41 | QB | 320 | ARG | Sidechain |
| 41 | QB | 359 | ARG | Sidechain |
| 41 | QB | 380 | ARG | Sidechain |
| 41 | QB | 390 | ARG | Sidechain |
| 41 | QB | 391 | ARG | Sidechain |
| 41 | QB | 425 | ARG | Sidechain |
| 41 | QB | 46 | ARG | Sidechain |
| 41 | QB | 77 | ARG | Sidechain |
| 41 | QB | 86 | ARG | Sidechain |
| 40 | QE | 228 | ASN | Peptide |
| 40 | QE | 273 | ALA | Peptide |
| 40 | QF | 273 | ALA | Peptide |
| 40 | QG | 214 | ARG | Sidechain |
| 40 | QG | 273 | ALA | Peptide |
| 40 | QG | 89 | PRO | Peptide |
| 40 | QH | 273 | ALA | Peptide |
| 41 | QL | 271 | ALA | Peptide |
| 41 | QO | 271 | ALA | Peptide |
| 41 | QP | 121 | ARG | Sidechain |
| 41 | QP | 156 | ARG | Sidechain |
| 41 | QP | 162 | ARG | Sidechain |
| 41 | QP | 2 | ARG | Sidechain |
| 41 | QP | 213 | ARG | Sidechain |
| 41 | QP | 276 | ARG | Sidechain |
| 41 | QP | 282 | ARG | Sidechain |
| 41 | QP | 306 | ARG | Sidechain |
| 41 | QP | 309 | ARG | Sidechain |
| 41 | QP | 320 | ARG | Sidechain |
| 41 | QP | 359 | ARG | Sidechain |
| 41 | QP | 380 | ARG | Sidechain |
| 41 | QP | 391 | ARG | Sidechain |
| 41 | QP | 425 | ARG | Sidechain |
| 41 | QP | 46 | ARG | Sidechain |
| 41 | QP | 62 | ARG | Sidechain |
| 41 | QP | 77 | ARG | Sidechain |
| 41 | QP | 86 | ARG | Sidechain |
| 40 | RA | 273 | ALA | Peptide |
| 41 | RB | 107 | THR | Peptide |
| 41 | RB | 21 | TRP | Peptide |
| 41 | RB | 271 | ALA | Peptide |
| 41 | RB | 323 | MET | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | RE | 273 | ALA | Peptide |
| 40 | RF | 273 | ALA | Peptide |
| 40 | RG | 2 | ARG | Sidechain |
| 40 | RG | 273 | ALA | Peptide |
| 40 | RH | 273 | ALA | Peptide |
| 40 | RI | 121 | ARG | Sidechain |
| 40 | RI | 273 | ALA | Peptide |
| 40 | RI | 276 | ILE | Peptide |
| 41 | RL | 271 | ALA | Peptide |
| 41 | RM | 271 | ALA | Peptide |
| 41 | RM | 422 | VAL | Peptide |
| 41 | RO | 107 | THR | Peptide |
| 41 | RO | 271 | ALA | Peptide |
| 41 | RP | 271 | ALA | Peptide |
| 40 | SA | 221 | ARG | Peptide |
| 40 | SA | 228 | ASN | Peptide |
| 40 | SA | 273 | ALA | Peptide |
| 40 | SA | 276 | ILE | Peptide |
| 40 | SA | 326 | LYS | Peptide |
| 41 | SB | 271 | ALA | Peptide |
| 41 | SB | 390 | ARG | Sidechain |
| 41 | SB | 391 | ARG | Sidechain |
| 40 | SE | 273 | ALA | Peptide |
| 40 | SE | 276 | ILE | Peptide |
| 40 | SF | 273 | ALA | Peptide |
| 40 | SG | 273 | ALA | Peptide |
| 40 | SH | 273 | ALA | Peptide |
| 40 | SH | 276 | ILE | Peptide |
| 40 | SI | 228 | ASN | Peptide |
| 40 | SI | 273 | ALA | Peptide |
| 41 | SL | 226 | ASN | Peptide |
| 41 | SL | 271 | ALA | Peptide |
| 41 | SM | 271 | ALA | Peptide |
| 41 | SN | 271 | ALA | Peptide |
| 41 | SN | 425 | ARG | Sidechain |
| 41 | SO | 121 | ARG | Sidechain |
| 41 | SO | 156 | ARG | Sidechain |
| 41 | SO | 162 | ARG | Sidechain |
| 41 | SO | 2 | ARG | Sidechain |
| 41 | SO | 213 | ARG | Sidechain |
| 41 | SO | 241 | ARG | Sidechain |
| 41 | SO | 251 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | SO | 262 | ARG | Sidechain |
| 41 | SO | 276 | ARG | Sidechain |
| 41 | SO | 282 | ARG | Sidechain |
| 41 | SO | 306 | ARG | Sidechain |
| 41 | SO | 309 | ARG | Sidechain |
| 41 | SO | 320 | ARG | Sidechain |
| 41 | SO | 359 | ARG | Sidechain |
| 41 | SO | 380 | ARG | Sidechain |
| 41 | SO | 391 | ARG | Sidechain |
| 41 | SO | 425 | ARG | Sidechain |
| 41 | SO | 46 | ARG | Sidechain |
| 41 | SO | 62 | ARG | Sidechain |
| 41 | SO | 77 | ARG | Sidechain |
| 41 | SP | 225 | LEU | Peptide |
| 41 | SP | 265 | PHE | Peptide |
| 41 | SP | 271 | ALA | Peptide |
| 40 | TA | 273 | ALA | Peptide |
| 41 | TB | 271 | ALA | Peptide |
| 40 | TE | 273 | ALA | Peptide |
| 40 | TF | 15 | GLN | Peptide |
| 40 | TF | 228 | ASN | Peptide |
| 40 | TF | 273 | ALA | Peptide |
| 40 | TG | 273 | ALA | Peptide |
| 40 | TH | 273 | ALA | Peptide |
| 40 | TI | 221 | ARG | Peptide |
| 40 | TI | 273 | ALA | Peptide |
| 41 | TL | 271 | ALA | Peptide |
| 41 | TM | 252 | LYS | Peptide |
| 41 | TM | 271 | ALA | Peptide |
| 41 | TN | 271 | ALA | Peptide |
| 41 | TO | 171 | PRO | Peptide |
| 41 | TO | 271 | ALA | Peptide |
| 41 | TO | 276 | ARG | Sidechain |
| 41 | TP | 271 | ALA | Peptide |
| 40 | UA | 228 | ASN | Peptide |
| 40 | UA | 273 | ALA | Peptide |
| 41 | UB | 271 | ALA | Peptide |
| 41 | UB | 299 | MET | Peptide |
| 40 | UE | 121 | ARG | Sidechain |
| 40 | UE | 273 | ALA | Peptide |
| 40 | UF | 121 | ARG | Sidechain |
| 40 | UF | 156 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 40 | UF | 2 | ARG | Sidechain |
| 40 | UF | 214 | ARG | Sidechain |
| 40 | UF | 215 | ARG | Sidechain |
| 40 | UF | 221 | ARG | Sidechain |
| 40 | UF | 229 | ARG | Sidechain |
| 40 | UF | 264 | ARG | Sidechain |
| 40 | UF | 308 | ARG | Sidechain |
| 40 | UF | 320 | ARG | Sidechain |
| 40 | UF | 339 | ARG | Sidechain |
| 40 | UF | 372 | ARG | Sidechain |
| 40 | UF | 389 | ARG | Sidechain |
| 40 | UF | 401 | ARG | Sidechain |
| 40 | UF | 421 | ARG | Sidechain |
| 40 | UF | 64 | ARG | Sidechain |
| 40 | UF | 84 | ARG | Sidechain |
| 40 | UG | 273 | ALA | Peptide |
| 40 | UH | 273 | ALA | Peptide |
| 40 | UI | 105 | ARG | Sidechain |
| 40 | UI | 121 | ARG | Sidechain |
| 40 | UI | 123 | ARG | Sidechain |
| 40 | UI | 156 | ARG | Sidechain |
| 40 | UI | 2 | ARG | Sidechain |
| 40 | UI | 214 | ARG | Sidechain |
| 40 | UI | 221 | ARG | Sidechain |
| 40 | UI | 229 | ARG | Sidechain |
| 40 | UI | 243 | ARG | Sidechain |
| 40 | UI | 308 | ARG | Sidechain |
| 40 | UI | 320 | ARG | Sidechain |
| 40 | UI | 339 | ARG | Sidechain |
| 40 | UI | 372 | ARG | Sidechain |
| 40 | UI | 421 | ARG | Sidechain |
| 40 | UI | 64 | ARG | Sidechain |
| 40 | UI | 79 | ARG | Sidechain |
| 40 | UI | 84 | ARG | Sidechain |
| 41 | UM | 252 | LYS | Peptide |
| 41 | UM | 271 | ALA | Peptide |
| 41 | UN | 121 | ARG | Sidechain |
| 41 | UN | 271 | ALA | Peptide |
| 41 | UO | 271 | ALA | Peptide |
| 41 | UP | 156 | ARG | Sidechain |
| 41 | UP | 162 | ARG | Sidechain |
| 41 | UP | 2 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | UP | 213 | ARG | Sidechain |
| 41 | UP | 241 | ARG | Sidechain |
| 41 | UP | 262 | ARG | Sidechain |
| 41 | UP | 282 | ARG | Sidechain |
| 41 | UP | 306 | ARG | Sidechain |
| 41 | UP | 309 | ARG | Sidechain |
| 41 | UP | 318 | ARG | Sidechain |
| 41 | UP | 320 | ARG | Sidechain |
| 41 | UP | 359 | ARG | Sidechain |
| 41 | UP | 380 | ARG | Sidechain |
| 41 | UP | 390 | ARG | Sidechain |
| 41 | UP | 391 | ARG | Sidechain |
| 41 | UP | 425 | ARG | Sidechain |
| 41 | UP | 46 | ARG | Sidechain |
| 41 | UP | 77 | ARG | Sidechain |
| 40 | VA | 273 | ALA | Peptide |
| 41 | VB | 271 | ALA | Peptide |
| 40 | VF | 273 | ALA | Peptide |
| 40 | VG | 273 | ALA | Peptide |
| 40 | VH | 273 | ALA | Peptide |
| 40 | VH | 326 | LYS | Peptide |
| 40 | VI | 273 | ALA | Peptide |
| 40 | VI | 326 | LYS | Peptide |
| 40 | VJ | 273 | ALA | Peptide |
| 41 | VN | 271 | ALA | Peptide |
| 41 | VO | 252 | LYS | Peptide |
| 41 | VO | 271 | ALA | Peptide |
| 41 | VP | 271 | ALA | Peptide |
| 41 | VQ | 271 | ALA | Peptide |
| 41 | VQ | 283 | ALA | Peptide |
| 40 | WA | 273 | ALA | Peptide |
| 41 | WB | 271 | ALA | Peptide |
| 40 | WE | 273 | ALA | Peptide |
| 40 | WE | 326 | LYS | Peptide |
| 40 | WF | 273 | ALA | Peptide |
| 40 | WG | 273 | ALA | Peptide |
| 40 | WH | 215 | ARG | Sidechain |
| 40 | WH | 273 | ALA | Peptide |
| 40 | WI | 273 | ALA | Peptide |
| 41 | WM | 156 | ARG | Sidechain |
| 41 | WM | 162 | ARG | Sidechain |
| 41 | WM | 2 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 41 | WM | 213 | ARG | Sidechain |
| 41 | WM | 241 | ARG | Sidechain |
| 41 | WM | 251 | ARG | Sidechain |
| 41 | WM | 262 | ARG | Sidechain |
| 41 | WM | 276 | ARG | Sidechain |
| 41 | WM | 282 | ARG | Sidechain |
| 41 | WM | 306 | ARG | Sidechain |
| 41 | WM | 309 | ARG | Sidechain |
| 41 | WM | 359 | ARG | Sidechain |
| 41 | WM | 380 | ARG | Sidechain |
| 41 | WM | 390 | ARG | Sidechain |
| 41 | WM | 391 | ARG | Sidechain |
| 41 | WM | 425 | ARG | Sidechain |
| 41 | WM | 46 | ARG | Sidechain |
| 41 | WM | 62 | ARG | Sidechain |
| 41 | WM | 86 | ARG | Sidechain |
| 41 | WN | 156 | ARG | Sidechain |
| 41 | WN | 162 | ARG | Sidechain |
| 41 | WN | 213 | ARG | Sidechain |
| 41 | WN | 241 | ARG | Sidechain |
| 41 | WN | 251 | ARG | Sidechain |
| 41 | WN | 262 | ARG | Sidechain |
| 41 | WN | 276 | ARG | Sidechain |
| 41 | WN | 306 | ARG | Sidechain |
| 41 | WN | 309 | ARG | Sidechain |
| 41 | WN | 318 | ARG | Sidechain |
| 41 | WN | 320 | ARG | Sidechain |
| 41 | WN | 359 | ARG | Sidechain |
| 41 | WN | 380 | ARG | Sidechain |
| 41 | WN | 390 | ARG | Sidechain |
| 41 | WN | 391 | ARG | Sidechain |
| 41 | WN | 425 | ARG | Sidechain |
| 41 | WN | 62 | ARG | Sidechain |
| 41 | WN | 77 | ARG | Sidechain |
| 41 | WN | 86 | ARG | Sidechain |
| 41 | WO | 271 | ALA | Peptide |
| 41 | WP | 271 | ALA | Peptide |
| 41 | WQ | 271 | ALA | Peptide |

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 1A | 4498 | 0 | 4639 | 0 | 0 |
| 1 | 1B | 1135 | 0 | 1145 | 0 | 0 |
| 2 | 1C | 1699 | 0 | 1707 | 3 | 0 |
| 2 | 1D | 1699 | 0 | 1707 | 5 | 0 |
| 3 | 1F | 1375 | 0 | 1352 | 0 | 0 |
| 3 | 1G | 1375 | 0 | 1352 | 0 | 0 |
| 4 | 1H | 1633 | 0 | 1697 | 9 | 0 |
| 4 | 1I | 727 | 0 | 760 | 2 | 0 |
| 4 | 1J | 973 | 0 | 1000 | 2 | 0 |
| 5 | 1L | 1306 | 0 | 1320 | 0 | 0 |
| 5 | 1M | 2086 | 0 | 2111 | 5 | 0 |
| 5 | 1N | 865 | 0 | 883 | 5 | 0 |
| 6 | 1P | 704 | 0 | 693 | 3 | 0 |
| 6 | 1Q | 675 | 0 | 665 | 1 | 0 |
| 7 | 1S | 4712 | 0 | 4688 | 43 | 0 |
| 7 | 1T | 4712 | 0 | 4688 | 175 | 0 |
| 7 | 1U | 4712 | 0 | 4688 | 99 | 0 |
| 8 | 1W | 2722 | 0 | 2757 | 50 | 0 |
| 8 | 1X | 2293 | 0 | 2341 | 75 | 0 |
| 8 | 1Y | 1331 | 0 | 1385 | 30 | 0 |
| 8 | 1Z | 1680 | 0 | 1702 | 25 | 0 |
| 9 | 2B | 3205 | 0 | 3280 | 68 | 0 |
| 9 | 2C | 665 | 0 | 684 | 12 | 0 |
| 10 | 2E | 930 | 0 | 884 | 28 | 0 |
| 10 | 2F | 930 | 0 | 883 | 32 | 0 |
| 10 | 2G | 930 | 0 | 884 | 19 | 0 |
| 11 | 2I | 2024 | 0 | 2087 | 81 | 0 |
| 11 | 2J | 2027 | 0 | 2094 | 53 | 0 |
| 11 | 2K | 1947 | 0 | 2005 | 54 | 0 |
| 12 | 2M | 1767 | 0 | 1775 | 26 | 0 |
| 12 | 2N | 1767 | 0 | 1775 | 23 | 0 |
| 12 | 2O | 1767 | 0 | 1775 | 36 | 0 |
| 12 | 2P | 1767 | 0 | 1775 | 22 | 0 |
| 12 | 2Q | 1767 | 0 | 1775 | 23 | 0 |
| 12 | 2R | 1767 | 0 | 1775 | 34 | 0 |
| 13 | 2T | 1540 | 0 | 1570 | 57 | 0 |
| 13 | 2U | 1540 | 0 | 1570 | 54 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 13 | 2V | 1540 | 0 | 1570 | 66 | 0 |
| 13 | 2W | 1540 | 0 | 1570 | 56 | 0 |
| 13 | 2X | 1540 | 0 | 1570 | 67 | 0 |
| 14 | 3A | 924 | 0 | 929 | 26 | 0 |
| 14 | 3B | 924 | 0 | 929 | 22 | 0 |
| 14 | 3C | 924 | 0 | 929 | 25 | 0 |
| 15 | 3E | 3216 | 0 | 3264 | 34 | 0 |
| 15 | 3F | 3241 | 0 | 3293 | 55 | 0 |
| 15 | 3G | 1096 | 0 | 1133 | 17 | 0 |
| 15 | 3H | 2451 | 0 | 2472 | 31 | 0 |
| 16 | 3J | 3234 | 0 | 3253 | 56 | 0 |
| 16 | 3K | 2559 | 0 | 2580 | 37 | 0 |
| 16 | 3L | 3234 | 0 | 3253 | 69 | 0 |
| 16 | 3M | 939 | 0 | 921 | 19 | 0 |
| 17 | 3O | 3180 | 0 | 3164 | 59 | 0 |
| 17 | 3P | 3180 | 0 | 3164 | 87 | 0 |
| 17 | 3Q | 1058 | 0 | 1084 | 34 | 0 |
| 17 | 3R | 2149 | 0 | 2100 | 153 | 0 |
| 18 | 3T | 3284 | 0 | 3219 | 57 | 0 |
| 18 | 3U | 3289 | 0 | 3224 | 59 | 0 |
| 18 | 3V | 1405 | 0 | 1305 | 23 | 0 |
| 18 | 3W | 2121 | 0 | 2172 | 28 | 0 |
| 19 | 3Y | 2977 | 0 | 2950 | 40 | 0 |
| 19 | 3Z | 194 | 0 | 178 | 6 | 0 |
| 20 | 4A | 1485 | 0 | 1469 | 69 | 0 |
| 20 | 4B | 943 | 0 | 892 | 34 | 0 |
| 21 | 4D | 3844 | 0 | 3793 | 110 | 0 |
| 21 | 4E | 3844 | 0 | 3793 | 100 | 0 |
| 21 | 4F | 3844 | 0 | 3793 | 111 | 0 |
| 22 | 4H | 2895 | 0 | 2829 | 59 | 0 |
| 22 | 4I | 5027 | 0 | 4986 | 124 | 0 |
| 22 | 4J | 5055 | 0 | 5016 | 159 | 0 |
| 22 | 4K | 1983 | 0 | 2007 | 81 | 0 |
| 23 | 4M | 1330 | 0 | 1263 | 112 | 0 |
| 23 | 4N | 1320 | 0 | 1243 | 118 | 0 |
| 23 | 4P | 705 | 0 | 667 | 87 | 0 |
| 23 | 4Q | 1070 | 0 | 980 | 84 | 0 |
| 23 | 4R | 1319 | 0 | 1254 | 121 | 0 |
| 24 | 4O | 702 | 0 | 660 | 51 | 0 |
| 25 | 4T | 1320 | 0 | 1261 | 36 | 0 |
| 26 | 4V | 2946 | 0 | 2926 | 65 | 0 |
| 26 | 4W | 2946 | 0 | 2926 | 75 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 27 | 4Y | 2145 | 0 | 2100 | 34 | 0 |
| 27 | 4Z | 2160 | 0 | 2105 | 40 | 0 |
| 28 | 5B | 1625 | 0 | 1551 | 33 | 0 |
| 29 | 5D | 697 | 0 | 655 | 14 | 0 |
| 29 | 5E | 280 | 0 | 265 | 7 | 0 |
| 30 | 5G | 708 | 0 | 640 | 20 | 0 |
| 31 | 5I | 3576 | 0 | 3546 | 81 | 0 |
| 31 | 5J | 898 | 0 | 877 | 27 | 0 |
| 32 | 5L | 736 | 0 | 697 | 13 | 0 |
| 33 | 5N | 2883 | 0 | 2948 | 36 | 0 |
| 33 | 5O | 1277 | 0 | 1295 | 23 | 0 |
| 34 | 5Q | 2216 | 0 | 2238 | 57 | 0 |
| 34 | 5R | 1671 | 0 | 1683 | 83 | 0 |
| 35 | 5T | 1118 | 0 | 1046 | 31 | 0 |
| 35 | 5U | 223 | 0 | 199 | 2 | 0 |
| 36 | 5W | 1868 | 0 | 1868 | 50 | 0 |
| 36 | 5X | 1868 | 0 | 1868 | 41 | 0 |
| 36 | 5Y | 1487 | 0 | 1504 | 38 | 0 |
| 36 | 5Z | 488 | 0 | 474 | 6 | 0 |
| 37 | 6A | 992 | 0 | 965 | 33 | 0 |
| 38 | 6C | 1698 | 0 | 1638 | 67 | 0 |
| 38 | 6D | 495 | 0 | 500 | 12 | 0 |
| 39 | 6F | 1264 | 0 | 1236 | 17 | 0 |
| 39 | 6G | 1264 | 0 | 1236 | 14 | 0 |
| 39 | 6H | 1134 | 0 | 1103 | 16 | 0 |
| 39 | 6I | 1264 | 0 | 1236 | 22 | 0 |
| 39 | 6J | 1264 | 0 | 1236 | 15 | 0 |
| 39 | 6K | 1264 | 0 | 1236 | 18 | 0 |
| 39 | 6L | 1095 | 0 | 1090 | 19 | 0 |
| 40 | AA | 3442 | 0 | 3348 | 79 | 0 |
| 40 | AE | 3442 | 0 | 3348 | 66 | 0 |
| 40 | AF | 3442 | 0 | 3348 | 59 | 0 |
| 40 | AG | 3442 | 0 | 3348 | 105 | 0 |
| 40 | AH | 3442 | 0 | 3349 | 60 | 0 |
| 40 | BA | 3442 | 0 | 3348 | 70 | 0 |
| 40 | BE | 3442 | 0 | 3349 | 140 | 0 |
| 40 | BF | 3398 | 0 | 3304 | 88 | 0 |
| 40 | BG | 3392 | 0 | 3299 | 85 | 0 |
| 40 | BH | 3442 | 0 | 3349 | 134 | 0 |
| 40 | BI | 2932 | 0 | 2845 | 139 | 0 |
| 40 | CA | 3442 | 0 | 3349 | 170 | 0 |
| 40 | CE | 3438 | 0 | 3338 | 96 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 40 | CF | 3442 | 0 | 3349 | 77 | 0 |
| 40 | CG | 3442 | 0 | 3349 | 75 | 0 |
| 40 | CH | 3442 | 0 | 3349 | 168 | 0 |
| 40 | CI | 3442 | 0 | 3347 | 79 | 0 |
| 40 | DA | 3390 | 0 | 3300 | 262 | 0 |
| 40 | DE | 3410 | 0 | 3311 | 211 | 0 |
| 40 | DF | 3390 | 0 | 3300 | 211 | 0 |
| 40 | DG | 3398 | 0 | 3304 | 91 | 0 |
| 40 | DH | 3398 | 0 | 3304 | 215 | 0 |
| 40 | DI | 3390 | 0 | 3300 | 225 | 0 |
| 40 | EA | 3406 | 0 | 3308 | 96 | 0 |
| 40 | EE | 3415 | 0 | 3321 | 86 | 0 |
| 40 | EF | 3415 | 0 | 3321 | 99 | 0 |
| 40 | EG | 3406 | 0 | 3308 | 81 | 0 |
| 40 | EH | 3398 | 0 | 3304 | 178 | 0 |
| 40 | EI | 3406 | 0 | 3308 | 221 | 0 |
| 40 | FA | 3406 | 0 | 3308 | 214 | 0 |
| 40 | FE | 3406 | 0 | 3308 | 68 | 0 |
| 40 | FF | 3406 | 0 | 3308 | 65 | 0 |
| 40 | FG | 3398 | 0 | 3304 | 66 | 0 |
| 40 | FH | 3406 | 0 | 3308 | 71 | 0 |
| 40 | FI | 3402 | 0 | 3297 | 72 | 0 |
| 40 | GA | 3406 | 0 | 3308 | 105 | 0 |
| 40 | GE | 3406 | 0 | 3308 | 201 | 0 |
| 40 | GF | 3398 | 0 | 3302 | 83 | 0 |
| 40 | GG | 3398 | 0 | 3304 | 87 | 0 |
| 40 | GH | 3398 | 0 | 3304 | 160 | 0 |
| 40 | GI | 3406 | 0 | 3308 | 188 | 0 |
| 40 | HA | 3410 | 0 | 3311 | 76 | 0 |
| 40 | HE | 3398 | 0 | 3304 | 194 | 0 |
| 40 | HF | 3392 | 0 | 3299 | 77 | 0 |
| 40 | HG | 3402 | 0 | 3304 | 62 | 0 |
| 40 | HH | 3406 | 0 | 3308 | 71 | 0 |
| 40 | HI | 3415 | 0 | 3321 | 95 | 0 |
| 40 | IA | 3406 | 0 | 3308 | 78 | 0 |
| 40 | IE | 3286 | 0 | 3197 | 70 | 0 |
| 40 | IF | 3406 | 0 | 3308 | 81 | 0 |
| 40 | IG | 3398 | 0 | 3304 | 79 | 0 |
| 40 | IH | 3406 | 0 | 3308 | 90 | 0 |
| 40 | II | 3406 | 0 | 3308 | 104 | 0 |
| 40 | JA | 3406 | 0 | 3308 | 76 | 0 |
| 40 | JD | 3406 | 0 | 3308 | 82 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 40 | JE | 3406 | 0 | 3307 | 90 | 0 |
| 40 | JF | 3398 | 0 | 3304 | 64 | 0 |
| 40 | JG | 3442 | 0 | 3349 | 65 | 0 |
| 40 | JH | 3398 | 0 | 3304 | 76 | 0 |
| 40 | KA | 3406 | 0 | 3308 | 69 | 0 |
| 40 | KD | 3398 | 0 | 3304 | 68 | 0 |
| 40 | KE | 3402 | 0 | 3306 | 83 | 0 |
| 40 | KF | 3406 | 0 | 3308 | 72 | 0 |
| 40 | KG | 3442 | 0 | 3349 | 80 | 0 |
| 40 | KH | 3442 | 0 | 3349 | 84 | 0 |
| 40 | LA | 3442 | 0 | 3349 | 74 | 0 |
| 40 | LD | 3398 | 0 | 3304 | 66 | 0 |
| 40 | LE | 3442 | 0 | 3349 | 60 | 0 |
| 40 | LF | 3398 | 0 | 3304 | 130 | 0 |
| 40 | LG | 3406 | 0 | 3308 | 168 | 0 |
| 40 | LH | 3406 | 0 | 3308 | 69 | 0 |
| 40 | MA | 3392 | 0 | 3299 | 116 | 0 |
| 40 | MD | 3406 | 0 | 3307 | 57 | 0 |
| 40 | ME | 3406 | 0 | 3308 | 59 | 0 |
| 40 | MF | 3398 | 0 | 3304 | 157 | 0 |
| 40 | MG | 3398 | 0 | 3304 | 159 | 0 |
| 40 | MH | 3398 | 0 | 3304 | 138 | 0 |
| 40 | NA | 3392 | 0 | 3299 | 89 | 0 |
| 40 | ND | 3398 | 0 | 3304 | 155 | 0 |
| 40 | NE | 3402 | 0 | 3304 | 81 | 0 |
| 40 | NF | 3398 | 0 | 3304 | 80 | 0 |
| 40 | NG | 3392 | 0 | 3299 | 74 | 0 |
| 40 | NH | 3398 | 0 | 3304 | 82 | 0 |
| 40 | OA | 3422 | 0 | 3328 | 78 | 0 |
| 40 | OD | 3406 | 0 | 3308 | 100 | 0 |
| 40 | OE | 3406 | 0 | 3308 | 72 | 0 |
| 40 | OF | 3419 | 0 | 3324 | 85 | 0 |
| 40 | OG | 3415 | 0 | 3313 | 88 | 0 |
| 40 | OH | 3419 | 0 | 3324 | 211 | 0 |
| 40 | PA | 3392 | 0 | 3299 | 90 | 0 |
| 40 | PD | 3196 | 0 | 3120 | 76 | 0 |
| 40 | PE | 3398 | 0 | 3304 | 73 | 0 |
| 40 | PF | 3398 | 0 | 3304 | 84 | 0 |
| 40 | PG | 3384 | 0 | 3295 | 82 | 0 |
| 40 | PH | 3384 | 0 | 3295 | 89 | 0 |
| 40 | QA | 3392 | 0 | 3299 | 88 | 0 |
| 40 | QE | 3384 | 0 | 3295 | 116 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 40 | QF | 3384 | 0 | 3295 | 79 | 0 |
| 40 | QG | 3390 | 0 | 3300 | 98 | 0 |
| 40 | QH | 3398 | 0 | 3304 | 62 | 0 |
| 40 | RA | 3390 | 0 | 3300 | 87 | 0 |
| 40 | RE | 3384 | 0 | 3295 | 92 | 0 |
| 40 | RF | 3384 | 0 | 3295 | 83 | 0 |
| 40 | RG | 3390 | 0 | 3300 | 98 | 0 |
| 40 | RH | 3384 | 0 | 3295 | 76 | 0 |
| 40 | RI | 2962 | 0 | 2876 | 76 | 0 |
| 40 | SA | 3390 | 0 | 3300 | 105 | 0 |
| 40 | SE | 3406 | 0 | 3308 | 94 | 0 |
| 40 | SF | 3390 | 0 | 3300 | 103 | 0 |
| 40 | SG | 3406 | 0 | 3308 | 105 | 0 |
| 40 | SH | 3398 | 0 | 3304 | 111 | 0 |
| 40 | SI | 3398 | 0 | 3304 | 78 | 0 |
| 40 | TA | 3390 | 0 | 3300 | 80 | 0 |
| 40 | TE | 3392 | 0 | 3299 | 79 | 0 |
| 40 | TF | 3392 | 0 | 3298 | 74 | 0 |
| 40 | TG | 3406 | 0 | 3308 | 90 | 0 |
| 40 | TH | 3398 | 0 | 3304 | 90 | 0 |
| 40 | TI | 3398 | 0 | 3304 | 79 | 0 |
| 40 | UA | 3398 | 0 | 3304 | 76 | 0 |
| 40 | UE | 3406 | 0 | 3308 | 86 | 0 |
| 40 | UF | 3406 | 0 | 3308 | 215 | 0 |
| 40 | UG | 3406 | 0 | 3308 | 85 | 0 |
| 40 | UH | 3398 | 0 | 3304 | 89 | 0 |
| 40 | UI | 3398 | 0 | 3304 | 205 | 0 |
| 40 | VA | 3442 | 0 | 3349 | 85 | 0 |
| 40 | VF | 3442 | 0 | 3349 | 84 | 0 |
| 40 | VG | 3398 | 0 | 3304 | 83 | 0 |
| 40 | VH | 3406 | 0 | 3308 | 65 | 0 |
| 40 | VI | 3442 | 0 | 3349 | 77 | 0 |
| 40 | VJ | 3398 | 0 | 3304 | 87 | 0 |
| 40 | WA | 3442 | 0 | 3349 | 90 | 0 |
| 40 | WE | 3442 | 0 | 3349 | 76 | 0 |
| 40 | WF | 3398 | 0 | 3304 | 98 | 0 |
| 40 | WG | 3390 | 0 | 3300 | 100 | 0 |
| 40 | WH | 3442 | 0 | 3349 | 79 | 0 |
| 40 | WI | 3398 | 0 | 3304 | 73 | 0 |
| 41 | AB | 3341 | 0 | 3241 | 73 | 0 |
| 41 | AL | 3341 | 0 | 3241 | 63 | 0 |
| 41 | AM | 3341 | 0 | 3241 | 62 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | AN | 3341 | 0 | 3240 | 67 | 0 |
| 41 | AO | 3341 | 0 | 3241 | 109 | 0 |
| 41 | AP | 3341 | 0 | 3241 | 54 | 0 |
| 41 | BB | 3341 | 0 | 3241 | 115 | 0 |
| 41 | BL | 3341 | 0 | 3239 | 74 | 0 |
| 41 | BM | 3341 | 0 | 3241 | 145 | 0 |
| 41 | BN | 3341 | 0 | 3239 | 94 | 0 |
| 41 | BO | 3341 | 0 | 3241 | 127 | 0 |
| 41 | BP | 3341 | 0 | 3241 | 159 | 0 |
| 41 | CB | 3341 | 0 | 3241 | 94 | 0 |
| 41 | CL | 3341 | 0 | 3241 | 166 | 0 |
| 41 | CM | 3341 | 0 | 3241 | 161 | 0 |
| 41 | CN | 3341 | 0 | 3241 | 195 | 0 |
| 41 | CO | 3341 | 0 | 3241 | 175 | 0 |
| 41 | CP | 3341 | 0 | 3241 | 166 | 0 |
| 41 | DB | 3341 | 0 | 3241 | 187 | 0 |
| 41 | DL | 3341 | 0 | 3241 | 221 | 0 |
| 41 | DM | 3341 | 0 | 3241 | 227 | 0 |
| 41 | DN | 3341 | 0 | 3241 | 245 | 0 |
| 41 | DO | 3341 | 0 | 3241 | 80 | 0 |
| 41 | DP | 3337 | 0 | 3237 | 205 | 0 |
| 41 | EB | 3341 | 0 | 3239 | 78 | 0 |
| 41 | EL | 2826 | 0 | 2764 | 67 | 0 |
| 41 | EM | 3341 | 0 | 3241 | 209 | 0 |
| 41 | EN | 3341 | 0 | 3239 | 76 | 0 |
| 41 | EO | 3341 | 0 | 3241 | 68 | 0 |
| 41 | EP | 3341 | 0 | 3241 | 179 | 0 |
| 41 | FB | 3341 | 0 | 3239 | 74 | 0 |
| 41 | FM | 3341 | 0 | 3239 | 91 | 0 |
| 41 | FN | 3341 | 0 | 3239 | 74 | 0 |
| 41 | FO | 3341 | 0 | 3240 | 81 | 0 |
| 41 | FP | 3341 | 0 | 3241 | 84 | 0 |
| 41 | GB | 3341 | 0 | 3240 | 68 | 0 |
| 41 | GM | 3341 | 0 | 3239 | 97 | 0 |
| 41 | GN | 3341 | 0 | 3241 | 176 | 0 |
| 41 | GO | 3335 | 0 | 3230 | 73 | 0 |
| 41 | GP | 3341 | 0 | 3239 | 93 | 0 |
| 41 | HB | 3341 | 0 | 3240 | 61 | 0 |
| 41 | HM | 3341 | 0 | 3240 | 89 | 0 |
| 41 | HN | 3341 | 0 | 3241 | 152 | 0 |
| 41 | HO | 3341 | 0 | 3240 | 82 | 0 |
| 41 | HP | 3341 | 0 | 3239 | 56 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | HQ | 3341 | 0 | 3241 | 72 | 0 |
| 41 | IB | 3341 | 0 | 3241 | 67 | 0 |
| 41 | IM | 3341 | 0 | 3241 | 81 | 0 |
| 41 | IN | 3341 | 0 | 3239 | 84 | 0 |
| 41 | IO | 3341 | 0 | 3239 | 69 | 0 |
| 41 | IP | 3341 | 0 | 3241 | 86 | 0 |
| 41 | IQ | 3341 | 0 | 3241 | 76 | 0 |
| 41 | JB | 3341 | 0 | 3240 | 87 | 0 |
| 41 | JL | 3341 | 0 | 3239 | 78 | 0 |
| 41 | JM | 3341 | 0 | 3241 | 188 | 0 |
| 41 | JN | 3341 | 0 | 3239 | 79 | 0 |
| 41 | JO | 3341 | 0 | 3240 | 61 | 0 |
| 41 | KB | 3341 | 0 | 3238 | 71 | 0 |
| 41 | KL | 3341 | 0 | 3241 | 143 | 0 |
| 41 | KM | 3341 | 0 | 3240 | 59 | 0 |
| 41 | KN | 3341 | 0 | 3239 | 71 | 0 |
| 41 | KO | 3341 | 0 | 3239 | 89 | 0 |
| 41 | KP | 3007 | 0 | 2916 | 57 | 0 |
| 41 | LB | 3341 | 0 | 3239 | 74 | 0 |
| 41 | LL | 3341 | 0 | 3239 | 65 | 0 |
| 41 | LM | 3341 | 0 | 3239 | 55 | 0 |
| 41 | LN | 3341 | 0 | 3239 | 80 | 0 |
| 41 | LO | 3341 | 0 | 3239 | 81 | 0 |
| 41 | LP | 3341 | 0 | 3241 | 55 | 0 |
| 41 | MB | 3341 | 0 | 3239 | 77 | 0 |
| 41 | ML | 3341 | 0 | 3239 | 73 | 0 |
| 41 | MM | 3341 | 0 | 3240 | 55 | 0 |
| 41 | MN | 3341 | 0 | 3239 | 81 | 0 |
| 41 | MO | 3341 | 0 | 3241 | 125 | 0 |
| 41 | MP | 3341 | 0 | 3241 | 75 | 0 |
| 41 | NB | 3341 | 0 | 3239 | 83 | 0 |
| 41 | NL | 3341 | 0 | 3240 | 82 | 0 |
| 41 | NM | 3341 | 0 | 3239 | 77 | 0 |
| 41 | NN | 3341 | 0 | 3240 | 85 | 0 |
| 41 | NO | 3341 | 0 | 3239 | 64 | 0 |
| 41 | NP | 3264 | 0 | 3165 | 84 | 0 |
| 41 | OB | 3341 | 0 | 3239 | 93 | 0 |
| 41 | OL | 3341 | 0 | 3239 | 88 | 0 |
| 41 | OM | 3341 | 0 | 3238 | 81 | 0 |
| 41 | ON | 3341 | 0 | 3239 | 95 | 0 |
| 41 | OO | 3341 | 0 | 3239 | 104 | 0 |
| 41 | OP | 3341 | 0 | 3241 | 77 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | PB | 3341 | 0 | 3239 | 111 | 0 |
| 41 | PL | 3341 | 0 | 3241 | 87 | 0 |
| 41 | PM | 3341 | 0 | 3239 | 88 | 0 |
| 41 | PN | 3341 | 0 | 3239 | 68 | 0 |
| 41 | PO | 3341 | 0 | 3240 | 76 | 0 |
| 41 | PP | 3341 | 0 | 3241 | 84 | 0 |
| 41 | QB | 3341 | 0 | 3241 | 260 | 0 |
| 41 | QL | 3341 | 0 | 3240 | 74 | 0 |
| 41 | QM | 3341 | 0 | 3241 | 91 | 0 |
| 41 | QN | 3341 | 0 | 3239 | 85 | 0 |
| 41 | QO | 3341 | 0 | 3239 | 69 | 0 |
| 41 | QP | 3327 | 0 | 3220 | 270 | 0 |
| 41 | RB | 3341 | 0 | 3241 | 79 | 0 |
| 41 | RL | 3341 | 0 | 3241 | 71 | 0 |
| 41 | RM | 3341 | 0 | 3241 | 88 | 0 |
| 41 | RN | 3341 | 0 | 3238 | 89 | 0 |
| 41 | RO | 3341 | 0 | 3239 | 96 | 0 |
| 41 | RP | 3341 | 0 | 3240 | 90 | 0 |
| 41 | SB | 3341 | 0 | 3241 | 86 | 0 |
| 41 | SL | 2964 | 0 | 2892 | 79 | 0 |
| 41 | SM | 3341 | 0 | 3240 | 82 | 0 |
| 41 | SN | 3341 | 0 | 3240 | 71 | 0 |
| 41 | SO | 3341 | 0 | 3241 | 253 | 0 |
| 41 | SP | 3341 | 0 | 3239 | 91 | 0 |
| 41 | TB | 3341 | 0 | 3240 | 79 | 0 |
| 41 | TL | 3019 | 0 | 2950 | 60 | 0 |
| 41 | TM | 3341 | 0 | 3240 | 88 | 0 |
| 41 | TN | 3341 | 0 | 3239 | 82 | 0 |
| 41 | TO | 3341 | 0 | 3239 | 97 | 0 |
| 41 | TP | 3341 | 0 | 3241 | 93 | 0 |
| 41 | UB | 3341 | 0 | 3239 | 83 | 0 |
| 41 | UM | 3341 | 0 | 3240 | 88 | 0 |
| 41 | UN | 3341 | 0 | 3241 | 104 | 0 |
| 41 | UO | 3341 | 0 | 3240 | 87 | 0 |
| 41 | UP | 3341 | 0 | 3241 | 203 | 0 |
| 41 | VB | 3341 | 0 | 3239 | 88 | 0 |
| 41 | VN | 3341 | 0 | 3239 | 76 | 0 |
| 41 | VO | 3341 | 0 | 3240 | 90 | 0 |
| 41 | VP | 3341 | 0 | 3239 | 86 | 0 |
| 41 | VQ | 3341 | 0 | 3239 | 78 | 0 |
| 41 | WB | 3341 | 0 | 3241 | 87 | 0 |
| 41 | WM | 3341 | 0 | 3241 | 167 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 41 | WN | 3341 | 0 | 3241 | 164 | 0 |
| 41 | WO | 3341 | 0 | 3239 | 82 | 0 |
| 41 | WP | 3341 | 0 | 3241 | 73 | 0 |
| 41 | WQ | 3285 | 0 | 3188 | 60 | 0 |
| 42 | AA | 32 | 0 | 12 | 1 | 0 |
| 42 | AE | 32 | 0 | 12 | 2 | 0 |
| 42 | AF | 32 | 0 | 12 | 0 | 0 |
| 42 | AG | 32 | 0 | 12 | 3 | 0 |
| 42 | AH | 32 | 0 | 12 | 2 | 0 |
| 42 | BA | 32 | 0 | 12 | 0 | 0 |
| 42 | BF | 32 | 0 | 11 | 2 | 0 |
| 42 | BG | 32 | 0 | 12 | 2 | 0 |
| 42 | BH | 32 | 0 | 12 | 1 | 0 |
| 42 | BI | 32 | 0 | 12 | 1 | 0 |
| 42 | BL | 32 | 0 | 12 | 1 | 0 |
| 42 | CA | 32 | 0 | 12 | 1 | 0 |
| 42 | CE | 32 | 0 | 11 | 5 | 0 |
| 42 | CF | 32 | 0 | 11 | 2 | 0 |
| 42 | CG | 32 | 0 | 11 | 3 | 0 |
| 42 | CH | 32 | 0 | 12 | 1 | 0 |
| 42 | CI | 32 | 0 | 12 | 4 | 0 |
| 42 | DA | 32 | 0 | 12 | 7 | 0 |
| 42 | DE | 32 | 0 | 12 | 6 | 0 |
| 42 | DF | 32 | 0 | 12 | 4 | 0 |
| 42 | DG | 32 | 0 | 11 | 4 | 0 |
| 42 | DH | 32 | 0 | 12 | 2 | 0 |
| 42 | DI | 32 | 0 | 12 | 8 | 0 |
| 42 | EA | 32 | 0 | 11 | 5 | 0 |
| 42 | EF | 32 | 0 | 11 | 2 | 0 |
| 42 | EG | 32 | 0 | 11 | 1 | 0 |
| 42 | EH | 32 | 0 | 12 | 1 | 0 |
| 42 | EI | 32 | 0 | 12 | 0 | 0 |
| 42 | EL | 32 | 0 | 11 | 2 | 0 |
| 42 | FB | 32 | 0 | 11 | 3 | 0 |
| 42 | FE | 32 | 0 | 11 | 1 | 0 |
| 42 | FI | 32 | 0 | 11 | 2 | 0 |
| 42 | FM | 32 | 0 | 11 | 3 | 0 |
| 42 | FN | 32 | 0 | 12 | 2 | 0 |
| 42 | FO | 32 | 0 | 11 | 1 | 0 |
| 42 | GA | 32 | 0 | 10 | 4 | 0 |
| 42 | GB | 32 | 0 | 11 | 3 | 0 |
| 42 | GE | 32 | 0 | 12 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 42 | GF | 32 | 0 | 10 | 1 | 0 |
| 42 | GH | 32 | 0 | 12 | 2 | 0 |
| 42 | GP | 32 | 0 | 12 | 3 | 0 |
| 42 | HA | 32 | 0 | 11 | 4 | 0 |
| 42 | HB | 32 | 0 | 12 | 1 | 0 |
| 42 | HE | 32 | 0 | 12 | 0 | 0 |
| 42 | HH | 32 | 0 | 11 | 2 | 0 |
| 42 | HM | 32 | 0 | 11 | 2 | 0 |
| 42 | HP | 32 | 0 | 11 | 2 | 0 |
| 42 | IA | 32 | 0 | 11 | 2 | 0 |
| 42 | IE | 32 | 0 | 11 | 3 | 0 |
| 42 | IF | 32 | 0 | 11 | 2 | 0 |
| 42 | IG | 32 | 0 | 11 | 4 | 0 |
| 42 | IH | 32 | 0 | 11 | 3 | 0 |
| 42 | II | 32 | 0 | 11 | 3 | 0 |
| 42 | JA | 32 | 0 | 11 | 4 | 0 |
| 42 | JB | 32 | 0 | 11 | 3 | 0 |
| 42 | JD | 32 | 0 | 10 | 0 | 0 |
| 42 | JE | 32 | 0 | 11 | 3 | 0 |
| 42 | JF | 32 | 0 | 11 | 2 | 0 |
| 42 | JO | 32 | 0 | 11 | 5 | 0 |
| 42 | KB | 32 | 0 | 11 | 3 | 0 |
| 42 | KD | 32 | 0 | 11 | 3 | 0 |
| 42 | KE | 32 | 0 | 11 | 3 | 0 |
| 42 | KM | 32 | 0 | 10 | 2 | 0 |
| 42 | KN | 32 | 0 | 10 | 3 | 0 |
| 42 | KO | 32 | 0 | 10 | 2 | 0 |
| 42 | LA | 32 | 0 | 11 | 4 | 0 |
| 42 | LB | 32 | 0 | 12 | 3 | 0 |
| 42 | LD | 32 | 0 | 11 | 2 | 0 |
| 42 | LL | 32 | 0 | 11 | 3 | 0 |
| 42 | LM | 32 | 0 | 12 | 5 | 0 |
| 42 | LO | 32 | 0 | 11 | 4 | 0 |
| 42 | MB | 32 | 0 | 12 | 9 | 0 |
| 42 | MD | 32 | 0 | 11 | 2 | 0 |
| 42 | MH | 32 | 0 | 12 | 1 | 0 |
| 42 | ML | 32 | 0 | 11 | 2 | 0 |
| 42 | MM | 32 | 0 | 12 | 8 | 0 |
| 42 | MN | 32 | 0 | 12 | 9 | 0 |
| 42 | ND | 32 | 0 | 12 | 1 | 0 |
| 42 | NE | 32 | 0 | 11 | 3 | 0 |
| 42 | NG | 32 | 0 | 11 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 42 | NM | 32 | 0 | 11 | 4 | 0 |
| 42 | NN | 32 | 0 | 10 | 4 | 0 |
| 42 | NO | 32 | 0 | 11 | 3 | 0 |
| 42 | OB | 32 | 0 | 11 | 4 | 0 |
| 42 | OD | 32 | 0 | 11 | 5 | 0 |
| 42 | OL | 32 | 0 | 11 | 2 | 0 |
| 42 | OM | 32 | 0 | 10 | 2 | 0 |
| 42 | ON | 32 | 0 | 11 | 2 | 0 |
| 42 | OO | 32 | 0 | 12 | 3 | 0 |
| 42 | PB | 32 | 0 | 11 | 0 | 0 |
| 42 | PD | 32 | 0 | 11 | 0 | 0 |
| 42 | PE | 32 | 0 | 11 | 2 | 0 |
| 42 | PM | 32 | 0 | 11 | 0 | 0 |
| 42 | PN | 32 | 0 | 12 | 2 | 0 |
| 42 | PO | 32 | 0 | 11 | 2 | 0 |
| 42 | QF | 32 | 0 | 11 | 2 | 0 |
| 42 | QG | 32 | 0 | 11 | 2 | 0 |
| 42 | QL | 32 | 0 | 10 | 2 | 0 |
| 42 | QN | 32 | 0 | 11 | 2 | 0 |
| 42 | QO | 32 | 0 | 11 | 1 | 0 |
| 42 | RE | 32 | 0 | 11 | 0 | 0 |
| 42 | RF | 32 | 0 | 11 | 4 | 0 |
| 42 | RG | 32 | 0 | 11 | 3 | 0 |
| 42 | RN | 32 | 0 | 11 | 0 | 0 |
| 42 | RO | 32 | 0 | 11 | 1 | 0 |
| 42 | RP | 32 | 0 | 11 | 4 | 0 |
| 42 | SG | 32 | 0 | 11 | 0 | 0 |
| 42 | SH | 32 | 0 | 10 | 3 | 0 |
| 42 | SL | 32 | 0 | 10 | 1 | 0 |
| 42 | SM | 32 | 0 | 11 | 2 | 0 |
| 42 | SN | 32 | 0 | 10 | 3 | 0 |
| 42 | SP | 32 | 0 | 10 | 1 | 0 |
| 42 | TF | 32 | 0 | 9 | 0 | 0 |
| 42 | TG | 32 | 0 | 10 | 5 | 0 |
| 42 | TH | 32 | 0 | 11 | 2 | 0 |
| 42 | TI | 32 | 0 | 10 | 4 | 0 |
| 42 | TL | 32 | 0 | 10 | 3 | 0 |
| 42 | TN | 32 | 0 | 10 | 1 | 0 |
| 42 | UA | 32 | 0 | 10 | 2 | 0 |
| 42 | UB | 32 | 0 | 11 | 3 | 0 |
| 42 | UE | 32 | 0 | 11 | 3 | 0 |
| 42 | UI | 32 | 0 | 12 | 5 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 42 | UM | 32 | 0 | 12 | 1 | 0 |
| 42 | UO | 32 | 0 | 11 | 3 | 0 |
| 42 | VA | 32 | 0 | 11 | 3 | 0 |
| 42 | VB | 32 | 0 | 11 | 4 | 0 |
| 42 | VF | 32 | 0 | 11 | 1 | 0 |
| 42 | VN | 32 | 0 | 11 | 2 | 0 |
| 42 | VP | 32 | 0 | 11 | 1 | 0 |
| 42 | VQ | 32 | 0 | 11 | 1 | 0 |
| 42 | WA | 32 | 0 | 11 | 3 | 0 |
| 42 | WE | 32 | 0 | 11 | 4 | 0 |
| 42 | WF | 32 | 0 | 11 | 2 | 0 |
| 42 | WG | 32 | 0 | 11 | 5 | 0 |
| 42 | WI | 32 | 0 | 11 | 4 | 0 |
| 42 | WO | 32 | 0 | 10 | 1 | 0 |
| 43 | AB | 28 | 0 | 11 | 1 | 0 |
| 43 | AL | 28 | 0 | 11 | 0 | 0 |
| 43 | AM | 28 | 0 | 11 | 1 | 0 |
| 43 | AN | 28 | 0 | 11 | 1 | 0 |
| 43 | AO | 28 | 0 | 12 | 0 | 0 |
| 43 | AP | 28 | 0 | 12 | 0 | 0 |
| 43 | BB | 28 | 0 | 12 | 3 | 0 |
| 43 | BL | 28 | 0 | 11 | 2 | 0 |
| 43 | BM | 28 | 0 | 12 | 2 | 0 |
| 43 | BN | 28 | 0 | 11 | 1 | 0 |
| 43 | BO | 28 | 0 | 12 | 0 | 0 |
| 43 | BP | 28 | 0 | 12 | 1 | 0 |
| 43 | CB | 28 | 0 | 11 | 1 | 0 |
| 43 | CL | 28 | 0 | 12 | 1 | 0 |
| 43 | CM | 28 | 0 | 12 | 2 | 0 |
| 43 | CN | 28 | 0 | 12 | 4 | 0 |
| 43 | CO | 28 | 0 | 12 | 5 | 0 |
| 43 | CP | 28 | 0 | 12 | 4 | 0 |
| 43 | DB | 28 | 0 | 12 | 4 | 0 |
| 43 | DL | 28 | 0 | 12 | 3 | 0 |
| 43 | DM | 28 | 0 | 12 | 2 | 0 |
| 43 | DN | 28 | 0 | 12 | 3 | 0 |
| 43 | DO | 28 | 0 | 11 | 1 | 0 |
| 43 | DP | 28 | 0 | 12 | 5 | 0 |
| 43 | EB | 28 | 0 | 11 | 1 | 0 |
| 43 | EL | 28 | 0 | 11 | 0 | 0 |
| 43 | EM | 28 | 0 | 12 | 4 | 0 |
| 43 | EN | 28 | 0 | 11 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 43 | EO | 28 | 0 | 11 | 0 | 0 |
| 43 | EP | 28 | 0 | 12 | 5 | 0 |
| 43 | FB | 28 | 0 | 11 | 0 | 0 |
| 43 | FM | 28 | 0 | 11 | 0 | 0 |
| 43 | FN | 28 | 0 | 11 | 0 | 0 |
| 43 | FO | 28 | 0 | 11 | 2 | 0 |
| 43 | FP | 28 | 0 | 11 | 3 | 0 |
| 43 | GB | 28 | 0 | 11 | 1 | 0 |
| 43 | GM | 28 | 0 | 11 | 2 | 0 |
| 43 | GN | 28 | 0 | 12 | 2 | 0 |
| 43 | GO | 28 | 0 | 11 | 0 | 0 |
| 43 | GP | 28 | 0 | 11 | 2 | 0 |
| 43 | HB | 28 | 0 | 11 | 0 | 0 |
| 43 | HM | 28 | 0 | 11 | 1 | 0 |
| 43 | HN | 28 | 0 | 12 | 2 | 0 |
| 43 | HO | 28 | 0 | 11 | 1 | 0 |
| 43 | HP | 28 | 0 | 11 | 0 | 0 |
| 43 | HQ | 28 | 0 | 11 | 0 | 0 |
| 43 | IB | 28 | 0 | 11 | 0 | 0 |
| 43 | IM | 28 | 0 | 11 | 0 | 0 |
| 43 | IN | 28 | 0 | 11 | 0 | 0 |
| 43 | IO | 28 | 0 | 11 | 1 | 0 |
| 43 | IP | 28 | 0 | 11 | 0 | 0 |
| 43 | IQ | 28 | 0 | 11 | 0 | 0 |
| 43 | JB | 28 | 0 | 11 | 2 | 0 |
| 43 | JL | 28 | 0 | 11 | 1 | 0 |
| 43 | JM | 28 | 0 | 12 | 6 | 0 |
| 43 | JN | 28 | 0 | 11 | 1 | 0 |
| 43 | JO | 28 | 0 | 11 | 1 | 0 |
| 43 | KB | 28 | 0 | 10 | 0 | 0 |
| 43 | KL | 28 | 0 | 12 | 2 | 0 |
| 43 | KM | 28 | 0 | 11 | 1 | 0 |
| 43 | KN | 28 | 0 | 11 | 3 | 0 |
| 43 | KO | 28 | 0 | 11 | 0 | 0 |
| 43 | KP | 28 | 0 | 11 | 2 | 0 |
| 43 | LB | 28 | 0 | 11 | 2 | 0 |
| 43 | LL | 28 | 0 | 11 | 0 | 0 |
| 43 | LM | 28 | 0 | 11 | 1 | 0 |
| 43 | LN | 28 | 0 | 11 | 1 | 0 |
| 43 | LO | 28 | 0 | 11 | 2 | 0 |
| 43 | LP | 28 | 0 | 11 | 1 | 0 |
| 43 | MB | 28 | 0 | 11 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 43 | ML | 28 | 0 | 11 | 2 | 0 |
| 43 | MM | 28 | 0 | 11 | 1 | 0 |
| 43 | MN | 28 | 0 | 11 | 2 | 0 |
| 43 | MO | 28 | 0 | 12 | 1 | 0 |
| 43 | MP | 28 | 0 | 11 | 1 | 0 |
| 43 | NB | 28 | 0 | 11 | 0 | 0 |
| 43 | NL | 28 | 0 | 11 | 0 | 0 |
| 43 | NM | 28 | 0 | 11 | 2 | 0 |
| 43 | NN | 28 | 0 | 11 | 2 | 0 |
| 43 | NO | 28 | 0 | 11 | 1 | 0 |
| 43 | NP | 28 | 0 | 11 | 0 | 0 |
| 43 | OB | 28 | 0 | 11 | 1 | 0 |
| 43 | OL | 28 | 0 | 11 | 2 | 0 |
| 43 | OM | 28 | 0 | 11 | 0 | 0 |
| 43 | ON | 28 | 0 | 11 | 1 | 0 |
| 43 | OO | 28 | 0 | 11 | 0 | 0 |
| 43 | OP | 28 | 0 | 11 | 0 | 0 |
| 43 | PB | 28 | 0 | 11 | 2 | 0 |
| 43 | PL | 28 | 0 | 11 | 4 | 0 |
| 43 | PM | 28 | 0 | 11 | 0 | 0 |
| 43 | PN | 28 | 0 | 11 | 1 | 0 |
| 43 | PO | 28 | 0 | 11 | 0 | 0 |
| 43 | PP | 28 | 0 | 11 | 3 | 0 |
| 43 | QB | 28 | 0 | 12 | 5 | 0 |
| 43 | QL | 28 | 0 | 11 | 0 | 0 |
| 43 | QM | 28 | 0 | 11 | 2 | 0 |
| 43 | QN | 28 | 0 | 11 | 1 | 0 |
| 43 | QO | 28 | 0 | 11 | 1 | 0 |
| 43 | QP | 28 | 0 | 12 | 6 | 0 |
| 43 | RB | 28 | 0 | 11 | 0 | 0 |
| 43 | RL | 28 | 0 | 11 | 1 | 0 |
| 43 | RM | 28 | 0 | 11 | 1 | 0 |
| 43 | RN | 28 | 0 | 11 | 1 | 0 |
| 43 | RO | 28 | 0 | 11 | 1 | 0 |
| 43 | RP | 28 | 0 | 11 | 2 | 0 |
| 43 | SB | 28 | 0 | 11 | 1 | 0 |
| 43 | SL | 28 | 0 | 11 | 2 | 0 |
| 43 | SM | 28 | 0 | 11 | 0 | 0 |
| 43 | SN | 28 | 0 | 11 | 1 | 0 |
| 43 | SO | 28 | 0 | 12 | 3 | 0 |
| 43 | SP | 28 | 0 | 11 | 1 | 0 |
| 43 | TB | 28 | 0 | 11 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 43 | TL | 28 | 0 | 11 | 0 | 0 |
| 43 | TM | 28 | 0 | 11 | 0 | 0 |
| 43 | TN | 28 | 0 | 11 | 2 | 0 |
| 43 | TO | 28 | 0 | 11 | 1 | 0 |
| 43 | TP | 28 | 0 | 11 | 1 | 0 |
| 43 | UB | 28 | 0 | 11 | 1 | 0 |
| 43 | UM | 28 | 0 | 11 | 1 | 0 |
| 43 | UN | 28 | 0 | 11 | 1 | 0 |
| 43 | UO | 28 | 0 | 11 | 2 | 0 |
| 43 | UP | 28 | 0 | 12 | 2 | 0 |
| 43 | VB | 28 | 0 | 11 | 1 | 0 |
| 43 | VN | 28 | 0 | 11 | 0 | 0 |
| 43 | VO | 28 | 0 | 11 | 1 | 0 |
| 43 | VP | 28 | 0 | 11 | 1 | 0 |
| 43 | VQ | 28 | 0 | 11 | 1 | 0 |
| 43 | WB | 28 | 0 | 11 | 1 | 0 |
| 43 | WM | 28 | 0 | 12 | 1 | 0 |
| 43 | WN | 28 | 0 | 12 | 1 | 0 |
| 43 | WO | 28 | 0 | 11 | 2 | 0 |
| 43 | WP | 28 | 0 | 11 | 1 | 0 |
| 43 | WQ | 28 | 0 | 11 | 1 | 0 |
| All | All | 1114625 | 0 | 1082601 | 28457 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (28457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4M:92:PRO:HG2 | 40:AG:89:PRO:CG | 1.36 | 1.53 |
| 40:KF:298:PRO:N | 40:KF:298:PRO:CG | 1.71 | 1.46 |
| 11:2I:167:LYS:HZ3 | 11:2I:167:LYS:CB | 1.09 | 1.44 |
| 11:2I:83:PRO:CB | 11:2I:83:PRO:CG | 1.89 | 1.43 |
| 41:QB:104:GLY:HA2 | 41:QB:109:GLY:CA | 1.51 | 1.39 |
| 20:4A:149:ARG:NH1 | 20:4A:150:SER:H | 1.26 | 1.32 |
| 41:QB:104:GLY:CA | 41:QB:109:GLY:HA3 | 1.62 | 1.29 |
| 41:DN:104:GLY:CA | 41:DN:109:GLY:HA3 | 1.66 | 1.26 |
| 40:GE:204:VAL:CG2 | 40:GE:302:MET:HE3 | 1.65 | 1.26 |
| 23:4M:92:PRO:CG | 40:AG:89:PRO:HG2 | 1.67 | 1.22 |
| 41:QP:313:VAL:HA | 41:QP:369:GLY:CA | 1.69 | 1.21 |
| 11:2I:167:LYS:NZ | 11:2I:167:LYS:HB2 | 1.05 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DM:174:LYS:HE3 | 41:DM:175:VAL:HG22 | 1.25 | 1.19 |
| 23:4M:92:PRO:HG2 | 40:AG:89:PRO:CB | 1.71 | 1.17 |
| 40:EI:210:TYR:HE1 | 41:EP:324:LYS:HA | 1.05 | 1.17 |
| 41:JL:222:TYR:O | 41:JL:226:ASN:HB2 | 1.45 | 1.16 |
| 23:4N:260:THR:HG22 | 40:EF:219:ILE:HD11 | 1.18 | 1.15 |
| 11:2I:162:ASN:O | 11:2I:165:VAL:HG23 | 1.46 | 1.15 |
| 23:4P:260:THR:HG22 | 40:EA:219:ILE:HD11 | 1.27 | 1.12 |
| 41:DN:104:GLY:HA2 | 41:DN:109:GLY:CA | 1.78 | 1.12 |
| 40:KF:298:PRO:CD | 40:KF:298:PRO:HG3 | 1.65 | 1.12 |
| 41:CM:104:GLY:HA2 | 41:CM:109:GLY:HA3 | 1.19 | 1.11 |
| 40:DE:106:GLY:HA3 | 40:DE:148:GLY:HA3 | 1.16 | 1.11 |
| 41:DM:174:LYS:CE | 41:DM:175:VAL:HG22 | 1.80 | 1.10 |
| 40:KF:298:PRO:CD | 40:KF:298:PRO:HG2 | 1.65 | 1.10 |
| 41:QP:313:VAL:CA | 41:QP:369:GLY:HA3 | 1.80 | 1.10 |
| 41:QP:266:PHE:HB3 | 41:QP:370:ASN:HA | 1.31 | 1.10 |
| 40:DE:350:GLY:HA2 | 41:DM:179:VAL:HB | 1.32 | 1.09 |
| 41:QP:272:PRO:HG3 | 41:QP:364:SER:HB2 | 1.34 | 1.08 |
| 34:5Q:158:ARG:HH12 | 34:5R:490:ILE:HG12 | 1.18 | 1.08 |
| 40:KF:298:PRO:CG | 40:KF:298:PRO:HD3 | 1.59 | 1.08 |
| 23:4P:260:THR:HG22 | 40:EA:219:ILE:CD1 | 1.85 | 1.07 |
| 40:HE:106:GLY:HA3 | 40:HE:148:GLY:HA3 | 1.27 | 1.07 |
| 15:3F:194:ASN:ND2 | 17:3R:168:ILE:HD13 | 1.68 | 1.07 |
| 34:5Q:161:CYS:SG | 34:5R:487:ILE:CD1 | 2.43 | 1.07 |
| 20:4A:149:ARG:CZ | 20:4A:150:SER:H | 1.65 | 1.07 |
| 41:CN:104:GLY:HA2 | 41:CN:109:GLY:HA3 | 1.38 | 1.06 |
| 41:RP:222:TYR:O | 41:RP:226:ASN:HB2 | 1.53 | 1.06 |
| 40:BI:16:ILE:HD11 | 40:BI:231:ILE:HB | 1.37 | 1.06 |
| 35:5T:98:TYR:O | 35:5T:102:TYR:HB2 | 1.53 | 1.05 |
| 41:QP:105:HIS:HA | 41:QP:109:GLY:CA | 1.86 | 1.05 |
| 40:KF:298:PRO:CG | 40:KF:298:PRO:HD2 | 1.59 | 1.04 |
| 40:DE:106:GLY:HA3 | 40:DE:148:GLY:CA | 1.88 | 1.04 |
| 41:QP:105:HIS:CA | 41:QP:109:GLY:HA3 | 1.87 | 1.04 |
| 34:5Q:161:CYS:SG | 34:5R:487:ILE:HD13 | 1.98 | 1.03 |
| 20:4A:149:ARG:NH1 | 20:4A:150:SER:N | 2.05 | 1.03 |
| 23:4N:260:THR:HG22 | 40:EF:219:ILE:CD1 | 1.89 | 1.03 |
| 21:4F:411:LYS:NZ | 21:4F:412:MET:HG3 | 1.73 | 1.03 |
| 41:DL:226:ASN:HB3 | 43:DL:501:GDP:HN1 | 1.24 | 1.02 |
| 23:4R:236:TYR:HA | 23:4R:267:ASP:HA | 1.38 | 1.02 |
| 40:DE:12:ALA:HA | 40:DE:15:GLN:HG3 | 1.42 | 1.02 |
| 40:EI:274:PRO:HG2 | 40:EI:373:ALA:HA | 1.40 | 1.01 |
| 40:MH:273:ALA:HB2 | 40:MH:374:VAL:HG12 | 1.40 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UP:87:PRO:HD3 | 41:VQ:281:TYR:HD2 | 1.25 | 1.01 |
| 7:1T:278:SER:HB3 | 7:1T:279:PRO:HD2 | 1.41 | 1.00 |
| 40:GE:204:VAL:CG2 | 40:GE:302:MET:CE | 2.39 | 1.00 |
| 40:WA:96:LYS:HZ1 | 41:WN:1:MET:HG2 | 1.26 | 1.00 |
| 23:4M:198:PHE:HB3 | 40:DG:221:ARG:HG3 | 1.43 | 1.00 |
| 41:UB:253:LEU:O | 41:UB:257:MET:HB2 | 1.60 | 1.00 |
| 41:CO:104:GLY:HA2 | 41:CO:109:GLY:HA3 | 1.44 | 1.00 |
| 40:GI:273:ALA:HB1 | 40:GI:274:PRO:HD2 | 1.41 | 1.00 |
| 41:SO:55:THR:H | 41:TO:283:ALA:HA | 1.25 | 1.00 |
| 41:QN:253:LEU:O | 41:QN:257:MET:HB2 | 1.62 | 0.99 |
| 23:4P:259:ARG:HH21 | 40:EA:365:GLY:HA2 | 1.27 | 0.99 |
| 40:EI:210:TYR:CE1 | 41:EP:324:LYS:HA | 1.97 | 0.99 |
| 41:BP:100:ASN:HB3 | 41:BP:103:LYS:HB2 | 1.43 | 0.98 |
| 41:UM:253:LEU:O | 41:UM:257:MET:HB2 | 1.63 | 0.98 |
| 21:4D:529:LEU:HA | 21:4D:533:ASN:HB2 | 1.45 | 0.98 |
| 23:4M:92:PRO:CG | 40:AG:89:PRO:CG | 2.31 | 0.98 |
| 17:3R:232:ARG:HH21 | 17:3R:328:LEU:HA | 1.28 | 0.98 |
| 40:GG:276:ILE:HG21 | 40:GG:281:ALA:HB2 | 1.45 | 0.98 |
| 40:KF:298:PRO:N | 40:KF:298:PRO:HG2 | 1.72 | 0.98 |
| 40:GH:97:GLU:HG2 | 41:GO:131:GLN:HE21 | 1.29 | 0.97 |
| 20:4A:149:ARG:HH12 | 20:4A:150:SER:HB3 | 1.27 | 0.97 |
| 13:2V:115:LYS:HD2 | 40:AH:264:ARG:HE | 1.30 | 0.97 |
| 11:2I:167:LYS:HB2 | 11:2I:167:LYS:HZ2 | 1.19 | 0.97 |
| 23:4N:19:ILE:H | 23:4N:19:ILE:CD1 | 1.75 | 0.97 |
| 40:OH:88:HIS:HB3 | 40:OH:91:GLN:HB3 | 1.45 | 0.97 |
| 41:QP:101:TRP:H | 41:QP:184:ASN:HB3 | 1.28 | 0.96 |
| 41:DB:308:GLY:HA3 | 41:DB:373:ALA:HB2 | 1.44 | 0.96 |
| 40:DE:228:ASN:HB3 | 42:DE:501:GTP:HN21 | 1.29 | 0.96 |
| 11:2I:167:LYS:HZ3 | 11:2I:167:LYS:HB3 | 1.28 | 0.96 |
| 20:4A:149:ARG:CZ | 20:4A:150:SER:N | 2.28 | 0.96 |
| 17:3R:218:GLU:HB3 | 17:3R:343:VAL:HG22 | 1.48 | 0.95 |
| 40:MH:101:ASN:HD22 | 41:MO:256:ASN:HD21 | 1.11 | 0.95 |
| 8:1X:134:GLU:OE1 | 8:1X:134:GLU:HA | 1.62 | 0.95 |
| 41:CM:165:ASN:HA | 41:CM:198:GLU:HB3 | 1.44 | 0.95 |
| 23:4N:37:TYR:CE2 | 23:4N:41:THR:HG21 | 2.01 | 0.95 |
| 40:BE:222:PRO:HD2 | 41:BL:324:LYS:HE2 | 1.49 | 0.95 |
| 40:FA:273:ALA:HB1 | 40:FA:274:PRO:HD2 | 1.45 | 0.95 |
| 40:ND:273:ALA:HB1 | 40:ND:274:PRO:HD2 | 1.48 | 0.95 |
| 22:4J:92:LYS:H | 41:BN:279:GLN:H | 1.15 | 0.94 |
| 40:CH:350:GLY:HA2 | 41:CP:179:VAL:HG23 | 1.48 | 0.94 |
| 41:TO:222:TYR:O | 41:TO:226:ASN:HB2 | 1.66 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:2K:221:ILE:HG22 | 11:2K:222:PRO:HD3 | 1.45 | 0.94 |
| 40:GE:204:VAL:HG23 | 40:GE:302:MET:HE3 | 1.47 | 0.94 |
| 40:LG:273:ALA:HB1 | 40:LG:274:PRO:HD2 | 1.50 | 0.94 |
| 40:DH:11:GLN:HB2 | 40:DH:74:VAL:HG21 | 1.49 | 0.94 |
| 40:DI:222:PRO:HD2 | 41:DP:324:LYS:HG3 | 1.47 | 0.93 |
| 40:OF:254:GLU:O | 40:OF:258:ASN:HB2 | 1.66 | 0.93 |
| 40:MG:258:ASN:HB2 | 40:MG:352:LYS:HE3 | 1.48 | 0.93 |
| 21:4F:411:LYS:HZ3 | 21:4F:412:MET:HG3 | 1.26 | 0.93 |
| 34:5Q:158:ARG:NH1 | 34:5R:490:ILE:HG12 | 1.82 | 0.93 |
| 34:5Q:161:CYS:SG | 34:5R:487:ILE:HD11 | 2.09 | 0.93 |
| 41:QP:66:VAL:HG13 | 41:QP:91:VAL:HG21 | 1.51 | 0.93 |
| 41:SO:97:ALA:HA | 41:SO:103:LYS:HB2 | 1.49 | 0.93 |
| 40:AH:191:THR:O | 40:AH:195:LEU:HB2 | 1.69 | 0.92 |
| 40:CG:254:GLU:HG2 | 41:CO:98:GLY:HA2 | 1.50 | 0.92 |
| 40:MG:273:ALA:HB1 | 40:MG:274:PRO:HD2 | 1.52 | 0.92 |
| 41:DL:68:LEU:HB2 | 41:DL:143:THR:HG23 | 1.51 | 0.91 |
| 40:DE:310:GLY:HA3 | 40:DE:382:ALA:HB2 | 1.52 | 0.91 |
| 41:DM:174:LYS:HE3 | 41:DM:175:VAL:CG2 | 2.00 | 0.91 |
| 41:KO:222:TYR:O | 41:KO:226:ASN:HB2 | 1.71 | 0.91 |
| 41:QP:311:LEU:HB3 | 41:QP:370:ASN:HB3 | 1.50 | 0.91 |
| 41:QP:86:ARG:HB3 | 41:RP:281:TYR:CE2 | 2.05 | 0.91 |
| 40:UI:16:ILE:HD11 | 40:UI:138:PHE:HB3 | 1.51 | 0.91 |
| 23:4M:250:VAL:HG13 | 23:4M:253:TYR:HB2 | 1.52 | 0.91 |
| 41:TP:222:TYR:O | 41:TP:226:ASN:HB2 | 1.71 | 0.91 |
| 41:CN:24:ILE:HG22 | 41:CN:234:SER:HB2 | 1.50 | 0.90 |
| 41:WM:13:GLY:HA2 | 41:WM:136:THR:HB | 1.50 | 0.90 |
| 11:2I:167:LYS:CB | 11:2I:167:LYS:NZ | 1.88 | 0.90 |
| 23:4M:92:PRO:HG2 | 40:AG:89:PRO:HG2 | 0.91 | 0.90 |
| 40:UF:106:GLY:HA3 | 40:UF:148:GLY:HA3 | 1.53 | 0.90 |
| 22:4J:272:ARG:NH1 | 41:DN:277:GLY:HA2 | 1.86 | 0.90 |
| 40:DH:20:CYS:HA | 40:DH:232:SER:HB2 | 1.53 | 0.90 |
| 40:EI:250:VAL:HG23 | 40:EI:254:GLU:HB2 | 1.52 | 0.90 |
| 40:EF:397:MET:HG2 | 41:EM:345:ILE:HG22 | 1.54 | 0.90 |
| 8:1X:127:GLN:HA | 8:1X:130:LYS:HE2 | 1.53 | 0.90 |
| 41:CN:165:ASN:HB3 | 41:CN:198:GLU:HB2 | 1.54 | 0.90 |
| 40:KF:298:PRO:CG | 40:KF:298:PRO:CD | 0.90 | 0.90 |
| 41:SO:61:PRO:HG3 | 41:SO:84:ILE:HG22 | 1.53 | 0.90 |
| 41:TP:58:LYS:HZ3 | 41:UP:280:GLN:HB2 | 1.36 | 0.90 |
| 41:CN:86:ARG:HB3 | 41:CN:89:ASN:HB2 | 1.53 | 0.90 |
| 41:EM:14:ASN:HB3 | 41:EM:76:VAL:HG21 | 1.51 | 0.89 |
| 7:1T:522:THR:HA | 7:1T:547:SER:HB2 | 1.54 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SP:222:TYR:O | 41:SP:226:ASN:HB3 | 1.71 | 0.89 |
| 41:DM:104:GLY:HA3 | 41:DM:146:GLY:HA3 | 1.54 | 0.89 |
| 41:OM:165:ASN:HA | 41:OM:198:GLU:O | 1.73 | 0.89 |
| 23:4N:260:THR:CG2 | 40:EF:219:ILE:HD11 | 2.03 | 0.89 |
| 41:LP:287:PRO:O | 41:LP:291:GLN:HB2 | 1.73 | 0.89 |
| 41:BB:358:PRO:HG3 | 41:BB:364:SER:HB3 | 1.51 | 0.89 |
| 40:TI:104:ALA:O | 40:TI:108:TYR:HB2 | 1.73 | 0.89 |
| 40:VF:255:PHE:O | 40:VF:259:LEU:HB2 | 1.72 | 0.89 |
| 41:QP:313:VAL:HA | 41:QP:369:GLY:HA3 | 0.90 | 0.89 |
| 41:AB:191:GLN:O | 41:AB:195:ASN:HB2 | 1.73 | 0.89 |
| 40:KH:224:TYR:O | 40:KH:228:ASN:HB2 | 1.72 | 0.89 |
| 20:4A:149:ARG:HH12 | 20:4A:150:SER:CB | 1.84 | 0.88 |
| 40:DA:71:GLU:HB3 | 40:DA:98:ASP:HB2 | 1.54 | 0.88 |
| 41:OL:132:GLY:HA2 | 41:OL:163:ILE:O | 1.72 | 0.88 |
| 23:4N:250:VAL:HG13 | 23:4N:253:TYR:HB2 | 1.55 | 0.88 |
| 23:4P:250:VAL:HG13 | 23:4P:253:TYR:HB2 | 1.55 | 0.88 |
| 41:DB:51:TYR:HB3 | 41:DB:59:TYR:HB3 | 1.54 | 0.88 |
| 41:DL:49:VAL:HG21 | 41:DL:241:ARG:HG2 | 1.54 | 0.88 |
| 40:KF:298:PRO:CG | 40:KF:298:PRO:CB | 2.50 | 0.88 |
| 22:4J:91:ASP:HA | 41:BN:278:SER:HA | 1.54 | 0.88 |
| 23:4P:236:TYR:HA | 23:4P:267:ASP:HB3 | 1.55 | 0.88 |
| 41:ON:132:GLY:HA2 | 41:ON:163:ILE:O | 1.74 | 0.88 |
| 23:4M:92:PRO:CG | 40:AG:89:PRO:CB | 2.51 | 0.88 |
| 23:4N:236:TYR:HA | 23:4N:267:ASP:HB3 | 1.55 | 0.88 |
| 40:BI:273:ALA:HB1 | 40:BI:274:PRO:HD2 | 1.55 | 0.88 |
| 41:DO:10:GLY:O | 41:DO:14:ASN:HB2 | 1.74 | 0.88 |
| 40:GE:204:VAL:HG21 | 40:GE:302:MET:HE3 | 1.52 | 0.88 |
| 34:5Q:158:ARG:HH12 | 34:5R:490:ILE:CG1 | 1.87 | 0.88 |
| 34:5Q:167:GLU:HG2 | 34:5R:491:LEU:HD22 | 1.53 | 0.88 |
| 40:EH:222:PRO:HD2 | 41:EO:324:LYS:HG3 | 1.52 | 0.88 |
| 40:GE:204:VAL:HG21 | 40:GE:302:MET:CE | 2.00 | 0.88 |
| 40:MH:214:ARG:HH22 | 41:MO:324:LYS:HG3 | 1.35 | 0.88 |
| 41:RN:222:TYR:O | 41:RN:226:ASN:HB2 | 1.73 | 0.88 |
| 41:NP:191:GLN:O | 41:NP:195:ASN:HB2 | 1.74 | 0.88 |
| 41:UP:104:GLY:HA3 | 41:UP:146:GLY:HA3 | 1.56 | 0.88 |
| 41:CM:104:GLY:CA | 41:CM:109:GLY:HA3 | 2.03 | 0.87 |
| 40:EH:273:ALA:HB1 | 40:EH:274:PRO:HD2 | 1.54 | 0.87 |
| 40:OH:274:PRO:HG3 | 40:OH:373:ALA:HA | 1.53 | 0.87 |
| 40:FA:16:ILE:HG12 | 40:FA:228:ASN:HB3 | 1.57 | 0.87 |
| 40:GE:261:PRO:HD2 | 40:GE:265:ILE:HG13 | 1.56 | 0.87 |
| 41:UM:325:GLU:O | 41:UM:329:GLN:HB2 | 1.74 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SH:221:ARG:HH22 | 41:SO:325:GLU:HB2 | 1.40 | 0.87 |
| 11:2I:119:LYS:HZ1 | 40:LG:409:GLY:HA2 | 1.40 | 0.87 |
| 22:4J:91:ASP:H | 41:BN:281:TYR:H | 1.19 | 0.87 |
| 41:DP:226:ASN:ND2 | 43:DP:501:GDP:HN1 | 1.73 | 0.87 |
| 41:QP:105:HIS:HA | 41:QP:109:GLY:HA3 | 0.92 | 0.87 |
| 40:CA:346:TRP:HB3 | 41:CB:391:ARG:HD3 | 1.56 | 0.86 |
| 40:CF:75:ILE:HG23 | 40:CF:92:LEU:HD12 | 1.56 | 0.86 |
| 40:DI:273:ALA:HB3 | 40:DI:274:PRO:HD3 | 1.57 | 0.86 |
| 40:DA:268:PRO:HA | 40:DA:379:ASN:HA | 1.57 | 0.86 |
| 41:DN:104:GLY:HA2 | 41:DN:109:GLY:HA3 | 0.92 | 0.86 |
| 41:EP:2:ARG:HB2 | 41:EP:131:GLN:HB2 | 1.58 | 0.86 |
| 41:DM:101:TRP:HB2 | 41:DM:184:ASN:HA | 1.58 | 0.86 |
| 41:DN:51:TYR:HB3 | 41:DN:59:TYR:HB3 | 1.58 | 0.86 |
| 40:FA:106:GLY:HA3 | 40:FA:148:GLY:HA3 | 1.58 | 0.86 |
| 40:UA:16:ILE:HD13 | 40:UA:228:ASN:HD22 | 1.39 | 0.86 |
| 40:DH:126:ALA:HA | 40:DH:132:LEU:HD21 | 1.57 | 0.86 |
| 41:IO:332:ASN:O | 41:IO:336:LYS:HB2 | 1.75 | 0.86 |
| 40:PG:254:GLU:O | 40:PG:258:ASN:HB2 | 1.76 | 0.86 |
| 41:DL:25:SER:HB2 | 41:DL:30:ILE:HG12 | 1.57 | 0.85 |
| 41:CM:61:PRO:HD3 | 41:CM:84:ILE:HG12 | 1.56 | 0.85 |
| 34:5R:375:LYS:HA | 34:5R:378:GLU:HB3 | 1.56 | 0.85 |
| 41:WN:296:ALA:HB1 | 41:WN:305:PRO:HD2 | 1.57 | 0.85 |
| 23:4N:19:ILE:H | 23:4N:19:ILE:HD13 | 1.41 | 0.85 |
| 23:4Q:173:SER:HB2 | 23:4Q:181:LYS:HA | 1.56 | 0.85 |
| 40:CA:88:HIS:HB3 | 40:CA:91:GLN:HB2 | 1.58 | 0.85 |
| 40:DI:20:CYS:HA | 40:DI:232:SER:HB2 | 1.58 | 0.85 |
| 40:DI:75:ILE:HG23 | 40:DI:92:LEU:HD23 | 1.58 | 0.85 |
| 40:DF:250:VAL:HG23 | 40:DF:254:GLU:HB2 | 1.58 | 0.85 |
| 41:QP:64:VAL:HA | 41:QP:89:ASN:HD21 | 1.39 | 0.85 |
| 41:WN:2:ARG:HB3 | 41:WN:131:GLN:HB2 | 1.58 | 0.85 |
| 41:CP:60:VAL:HG11 | 41:DP:281:TYR:HA | 1.58 | 0.85 |
| 26:4V:342:LEU:O | 26:4V:346:PHE:HB2 | 1.75 | 0.85 |
| 34:5Q:167:GLU:CG | 34:5R:491:LEU:HD22 | 2.07 | 0.85 |
| 41:QB:207:LEU:HD21 | 41:QB:229:VAL:HG13 | 1.59 | 0.85 |
| 40:UF:100:ALA:HA | 41:UM:252:LYS:HB3 | 1.58 | 0.85 |
| 21:4F:222:LYS:HD2 | 40:BE:41:THR:HG23 | 1.59 | 0.85 |
| 26:4W:96:ALA:O | 26:4W:161:MET:HB2 | 1.77 | 0.85 |
| 40:DH:228:ASN:HB3 | 42:DH:501:GTP:N2 | 1.92 | 0.85 |
| 40:CH:180:ALA:HA | 41:CO:256:ASN:HD21 | 1.42 | 0.84 |
| 40:DH:326:LYS:HE2 | 41:DP:220:PRO:HB2 | 1.59 | 0.84 |
| 41:OO:132:GLY:HA2 | 41:OO:163:ILE:O | 1.77 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TP:27:GLU:HA | 41:TP:359:ARG:HH12 | 1.42 | 0.84 |
| 40:MF:326:LYS:HE3 | 40:MF:330:ALA:HB2 | 1.59 | 0.84 |
| 41:QB:54:ALA:HA | 41:RB:283:ALA:HA | 1.59 | 0.84 |
| 40:BH:40:LYS:HE3 | 40:BH:42:ILE:HD11 | 1.59 | 0.84 |
| 40:MD:191:THR:O | 40:MD:195:LEU:HB2 | 1.77 | 0.84 |
| 40:OH:20:CYS:HA | 40:OH:232:SER:HB2 | 1.58 | 0.84 |
| 40:UF:222:PRO:HD2 | 41:UM:324:LYS:HB2 | 1.57 | 0.84 |
| 23:4N:19:ILE:HD13 | 23:4N:19:ILE:N | 1.93 | 0.84 |
| 40:UI:71:GLU:HG2 | 40:UI:72:PRO:HD2 | 1.58 | 0.84 |
| 22:4I:282:ARG:HH12 | 41:CO:80:PRO:HD3 | 1.42 | 0.84 |
| 40:DA:278:ALA:HA | 40:DA:368:ALA:HB2 | 1.59 | 0.84 |
| 11:2K:221:ILE:HG22 | 11:2K:222:PRO:CD | 2.07 | 0.84 |
| 8:1Y:101:ILE:HD12 | 11:2J:250:ILE:HA | 1.60 | 0.83 |
| 40:GA:210:TYR:CE1 | 41:GN:324:LYS:HA | 2.12 | 0.83 |
| 40:DH:3:GLU:HA | 40:DH:51:THR:HA | 1.60 | 0.83 |
| 40:FA:219:ILE:HB | 40:FA:222:PRO:HD3 | 1.58 | 0.83 |
| 40:GE:273:ALA:HB3 | 40:GE:274:PRO:HD3 | 1.60 | 0.83 |
| 40:NA:199:ASP:HB3 | 40:NA:256:GLN:HE22 | 1.43 | 0.83 |
| 41:UO:384:GLN:O | 41:UO:388:MET:HB2 | 1.77 | 0.83 |
| 23:4N:253:TYR:CE2 | 40:EF:220:GLU:OE2 | 2.32 | 0.83 |
| 40:DA:228:ASN:HB3 | 42:DA:501:GTP:N2 | 1.94 | 0.83 |
| 40:GI:100:ALA:HA | 41:GP:252:LYS:HB3 | 1.59 | 0.83 |
| 41:EM:420:ASN:HA | 41:EM:423:VAL:HG22 | 1.60 | 0.83 |
| 40:ND:60:LYS:HD3 | 40:OD:282:TYR:HB3 | 1.61 | 0.83 |
| 41:DN:290:THR:HG21 | 41:DN:329:GLN:HB3 | 1.61 | 0.83 |
| 40:GH:325:PRO:HB2 | 41:GP:222:TYR:CE2 | 2.13 | 0.83 |
| 40:UF:352:LYS:HG2 | 41:UN:179:VAL:HG23 | 1.59 | 0.83 |
| 41:BO:173:PRO:HD2 | 41:BO:205:GLU:HG2 | 1.61 | 0.83 |
| 40:MF:278:ALA:H | 40:MF:368:ALA:HB2 | 1.44 | 0.83 |
| 26:4W:90:LYS:HG3 | 26:4W:166:ASP:HB3 | 1.61 | 0.83 |
| 34:5Q:164:LEU:HD23 | 34:5R:487:ILE:HD11 | 1.60 | 0.83 |
| 41:CL:61:PRO:HD3 | 41:CL:84:ILE:HG13 | 1.60 | 0.83 |
| 40:TA:222:PRO:HG2 | 41:TN:324:LYS:HE3 | 1.59 | 0.83 |
| 11:2I:155:PRO:HG2 | 11:2I:158:ILE:HG13 | 1.60 | 0.83 |
| 22:4I:252:HIS:HB2 | 22:4I:261:GLU:O | 1.78 | 0.83 |
| 34:5R:396:THR:HB | 40:GH:369:LYS:HD3 | 1.59 | 0.83 |
| 40:CH:391:ASP:HB3 | 40:CH:421:ARG:CZ | 2.09 | 0.83 |
| 40:KD:228:ASN:HD21 | 42:KD:501:GTP:HN1 | 1.25 | 0.83 |
| 41:DL:86:ARG:HA | 41:EL:281:TYR:HD2 | 1.44 | 0.83 |
| 41:PP:86:ARG:HD3 | 41:QP:281:TYR:HB3 | 1.60 | 0.83 |
| 23:4N:34:GLY:O | 23:4N:35:GLN:HB2 | 1.79 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4R:257:PHE:HB3 | 40:EI:221:ARG:HD2 | 1.61 | 0.82 |
| 41:BM:202:ILE:HD12 | 41:BM:229:VAL:HG13 | 1.60 | 0.82 |
| 41:BO:358:PRO:HG3 | 41:BO:364:SER:HB3 | 1.61 | 0.82 |
| 23:4R:57:HIS:HA | 41:BP:41:ASP:HB3 | 1.61 | 0.82 |
| 40:JE:51:THR:HG21 | 40:JE:243:ARG:HG2 | 1.61 | 0.82 |
| 40:LG:247:ALA:HB1 | 41:LO:222:TYR:HD2 | 1.43 | 0.82 |
| 40:UH:228:ASN:HD21 | 42:UO:501:GTP:HN1 | 1.27 | 0.82 |
| 17:3R:196:ARG:HA | 17:3R:199:LEU:HD12 | 1.59 | 0.82 |
| 40:RF:228:ASN:HD21 | 42:RF:501:GTP:HN1 | 1.26 | 0.82 |
| 23:4P:251:PRO:HD2 | 23:4P:268:ALA:HB1 | 1.61 | 0.82 |
| 40:RE:288:VAL:HG11 | 40:RE:327:ASP:HB3 | 1.60 | 0.82 |
| 23:4N:251:PRO:HD2 | 23:4N:268:ALA:HB1 | 1.61 | 0.82 |
| 36:5W:247:LEU:HD12 | 40:LG:430:ASP:HB3 | 1.62 | 0.82 |
| 41:BP:42:LEU:HG | 41:BP:45:GLU:HB2 | 1.62 | 0.82 |
| 21:4F:407:LYS:HZ3 | 21:4F:410:ILE:HD12 | 1.44 | 0.82 |
| 41:UP:87:PRO:HD3 | 41:VQ:281:TYR:CD2 | 2.14 | 0.82 |
| 17:3O:410:GLU:HG2 | 17:3R:264:ALA:HB2 | 1.61 | 0.81 |
| 41:AO:358:PRO:HG3 | 41:AO:364:SER:HB3 | 1.61 | 0.81 |
| 40:GI:223:THR:HG23 | 41:GP:322:SER:HA | 1.62 | 0.81 |
| 21:4D:475:PRO:HD2 | 21:4D:483:ILE:HG21 | 1.60 | 0.81 |
| 40:BG:326:LYS:HZ2 | 41:BO:225:LEU:HD21 | 1.43 | 0.81 |
| 41:GN:70:PRO:HG3 | 41:GN:92:PHE:HB3 | 1.61 | 0.81 |
| 41:KL:31:ASP:HB2 | 41:KL:32:PRO:HD2 | 1.62 | 0.81 |
| 40:OH:178:SER:HB2 | 41:OO:347:ASN:HB2 | 1.62 | 0.81 |
| 40:UH:326:LYS:HE3 | 41:UP:208:TYR:HB2 | 1.61 | 0.81 |
| 41:CM:60:VAL:HG11 | 41:DM:281:TYR:HB3 | 1.62 | 0.81 |
| 41:DL:164:MET:HB3 | 41:DL:197:ASP:H | 1.45 | 0.81 |
| 40:HE:306:ASP:HB3 | 40:HE:309:HIS:HB2 | 1.62 | 0.81 |
| 41:WN:273:LEU:H | 41:WN:292:GLN:HE22 | 1.26 | 0.81 |
| 17:3R:232:ARG:HG3 | 17:3R:328:LEU:HD12 | 1.61 | 0.81 |
| 41:ON:275:SER:O | 41:ON:279:GLN:HB2 | 1.81 | 0.81 |
| 24:4O:173:SER:HB2 | 24:4O:181:LYS:HG3 | 1.62 | 0.81 |
| 23:4P:173:SER:HB2 | 23:4P:181:LYS:HA | 1.61 | 0.81 |
| 40:CH:88:HIS:HB3 | 40:CH:91:GLN:HB2 | 1.63 | 0.81 |
| 40:GE:217:LEU:HA | 40:GE:277:SER:HB2 | 1.62 | 0.81 |
| 41:CO:311:LEU:HD11 | 41:CO:372:THR:HG23 | 1.62 | 0.81 |
| 40:DE:238:ILE:HD12 | 40:DE:377:LEU:HD11 | 1.61 | 0.81 |
| 41:SL:16:ILE:HG13 | 41:SL:226:ASN:HD22 | 1.44 | 0.81 |
| 23:4P:260:THR:CG2 | 40:EA:219:ILE:HD11 | 2.10 | 0.81 |
| 40:CE:228:ASN:HD21 | 42:CE:501:GTP:HN1 | 1.29 | 0.81 |
| 40:DI:319:TYR:HB3 | 40:DI:323:VAL:HG21 | 1.63 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CO:3:GLU:HG3 | 41:CO:127:CYS:HB3 | 1.63 | 0.81 |
| 40:DE:106:GLY:CA | 40:DE:148:GLY:HA3 | 2.07 | 0.81 |
| 41:JM:170:VAL:HG11 | 41:JM:377:LEU:HD21 | 1.62 | 0.81 |
| 23:4R:235:THR:HG21 | 23:4R:242:LEU:HG | 1.61 | 0.80 |
| 40:DE:209:ILE:HA | 40:DE:212:ILE:HG12 | 1.63 | 0.80 |
| 41:SN:222:TYR:O | 41:SN:226:ASN:HB2 | 1.81 | 0.80 |
| 40:WF:228:ASN:HD21 | 42:WF:501:GTP:HN1 | 1.29 | 0.80 |
| 40:CH:71:GLU:HB3 | 40:CH:98:ASP:HA | 1.63 | 0.80 |
| 41:RL:6:HIS:CE1 | 41:RL:8:GLN:HG2 | 2.15 | 0.80 |
| 40:BI:219:ILE:HB | 40:BI:222:PRO:HD3 | 1.62 | 0.80 |
| 13:2X:22:LEU:HD11 | 13:2X:47:LEU:HD21 | 1.63 | 0.80 |
| 40:DH:219:ILE:C | 40:DH:221:ARG:H | 1.82 | 0.80 |
| 40:GE:352:LYS:HD2 | 41:GM:178:THR:HA | 1.64 | 0.80 |
| 40:HE:326:LYS:HE3 | 41:HM:208:TYR:HB2 | 1.61 | 0.80 |
| 40:LG:247:ALA:HB1 | 41:LO:222:TYR:CD2 | 2.15 | 0.80 |
| 40:ME:429:LYS:O | 40:ME:433:GLU:HB2 | 1.82 | 0.80 |
| 41:MO:313:VAL:HB | 41:MO:349:VAL:HG22 | 1.63 | 0.80 |
| 41:QP:216:LYS:HB2 | 41:QP:275:SER:HB2 | 1.63 | 0.80 |
| 40:BF:228:ASN:HD21 | 42:BF:501:GTP:HN1 | 1.30 | 0.80 |
| 40:CA:254:GLU:HG2 | 41:CB:98:GLY:HA2 | 1.63 | 0.80 |
| 40:MA:273:ALA:HB3 | 40:MA:274:PRO:HD3 | 1.62 | 0.80 |
| 23:4N:259:ARG:HH21 | 40:EF:365:GLY:HA2 | 1.47 | 0.80 |
| 40:SG:270:ALA:HA | 40:SG:376:MET:O | 1.81 | 0.80 |
| 40:DI:344:VAL:HG23 | 40:DI:347:CYS:HB2 | 1.63 | 0.80 |
| 41:DL:358:PRO:HG2 | 41:DL:361:LEU:HB2 | 1.62 | 0.80 |
| 41:HN:87:PRO:HD3 | 41:IN:281:TYR:CE2 | 2.16 | 0.80 |
| 41:NN:16:ILE:HD13 | 41:NN:226:ASN:HD22 | 1.45 | 0.80 |
| 41:SP:45:GLU:HG3 | 41:SP:46:ARG:HG2 | 1.63 | 0.80 |
| 40:UI:328:VAL:HG11 | 40:UI:353:VAL:HG13 | 1.64 | 0.80 |
| 40:DE:25:CYS:HA | 40:DE:30:ILE:HG23 | 1.64 | 0.79 |
| 40:DF:258:ASN:HB3 | 41:DN:179:VAL:HG13 | 1.64 | 0.79 |
| 40:GE:241:SER:HB3 | 40:GE:249:ASN:HB2 | 1.62 | 0.79 |
| 41:HN:87:PRO:HD3 | 41:IN:281:TYR:CD2 | 2.16 | 0.79 |
| 40:EH:204:VAL:HG13 | 40:EH:302:MET:HB3 | 1.63 | 0.79 |
| 40:GE:246:GLY:HA3 | 40:GE:357:TYR:HB2 | 1.63 | 0.79 |
| 40:HE:51:THR:HG21 | 40:HE:243:ARG:HA | 1.63 | 0.79 |
| 40:SI:152:LEU:HG | 40:SI:156:ARG:HH22 | 1.47 | 0.79 |
| 11:2I:119:LYS:HZ1 | 40:LG:409:GLY:CA | 1.95 | 0.79 |
| 40:BE:101:ASN:HA | 40:BE:144:GLY:H | 1.47 | 0.79 |
| 40:CF:181:VAL:HG22 | 41:CM:256:ASN:HB3 | 1.64 | 0.79 |
| 23:4M:91:ILE:CD1 | 40:AG:79:ARG:HD3 | 2.12 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:5Z:234:LEU:HD21 | 40:LD:392:HIS:HB2 | 1.65 | 0.79 |
| 41:DN:252:LYS:HG3 | 41:DN:256:ASN:HD21 | 1.48 | 0.79 |
| 41:FP:207:LEU:HB3 | 41:FP:225:LEU:HD22 | 1.63 | 0.79 |
| 40:IG:228:ASN:HD21 | 42:IG:501:GTP:HN1 | 1.29 | 0.79 |
| 41:HN:68:LEU:HB2 | 41:HN:143:THR:HG22 | 1.64 | 0.79 |
| 40:VF:318:LEU:O | 40:VF:374:VAL:HA | 1.83 | 0.79 |
| 40:DA:258:ASN:HD21 | 41:DB:179:VAL:H | 1.28 | 0.79 |
| 40:DE:205:ASP:HB3 | 40:DE:303:VAL:HA | 1.65 | 0.79 |
| 40:UF:71:GLU:HB3 | 40:UF:98:ASP:HA | 1.64 | 0.79 |
| 40:OH:269:LEU:HD22 | 40:OH:303:VAL:HG21 | 1.63 | 0.79 |
| 23:4N:33:MET:HG2 | 41:CM:320:ARG:HH12 | 1.47 | 0.79 |
| 40:CG:71:GLU:HB3 | 40:CG:98:ASP:HB3 | 1.65 | 0.79 |
| 40:DE:137:ILE:HB | 40:DE:168:GLU:HG2 | 1.65 | 0.79 |
| 41:QP:186:THR:HG21 | 41:QP:385:PHE:HB2 | 1.63 | 0.79 |
| 41:UP:97:ALA:HA | 41:UP:103:LYS:HD2 | 1.65 | 0.79 |
| 40:WI:51:THR:HG21 | 40:WI:243:ARG:HG2 | 1.64 | 0.79 |
| 23:4R:240:LEU:HA | 23:4R:266:HIS:HA | 1.64 | 0.79 |
| 40:CA:440:GLU:HB2 | 41:CB:390:ARG:HD2 | 1.65 | 0.79 |
| 40:DA:258:ASN:OD1 | 41:DB:179:VAL:HB | 1.83 | 0.79 |
| 40:DE:51:THR:HG21 | 40:DE:243:ARG:HA | 1.64 | 0.79 |
| 41:EP:132:GLY:HA2 | 41:EP:162:ARG:HB3 | 1.65 | 0.79 |
| 40:GI:228:ASN:HD22 | 42:GP:501:GTP:HN21 | 1.30 | 0.79 |
| 41:UP:240:LEU:HD21 | 41:UP:249:ASP:HB2 | 1.65 | 0.79 |
| 21:4F:443:PHE:HB2 | 21:4F:448:MET:HB2 | 1.65 | 0.78 |
| 41:DM:104:GLY:CA | 41:DM:146:GLY:HA3 | 2.13 | 0.78 |
| 41:EP:231:ALA:HB3 | 41:EP:270:PHE:HZ | 1.48 | 0.78 |
| 40:GH:2:ARG:HH22 | 40:GH:50:ASN:HB3 | 1.47 | 0.78 |
| 41:SO:417:ASP:O | 41:SO:421:PRO:HD2 | 1.83 | 0.78 |
| 11:2I:162:ASN:O | 11:2I:165:VAL:CG2 | 2.29 | 0.78 |
| 21:4E:497:GLU:HA | 21:4E:502:ARG:HA | 1.65 | 0.78 |
| 41:BP:46:ARG:HB2 | 41:BP:241:ARG:HA | 1.65 | 0.78 |
| 40:DI:72:PRO:HD2 | 41:DP:2:ARG:NH2 | 1.99 | 0.78 |
| 40:GI:11:GLN:HA | 40:GI:74:VAL:HG11 | 1.65 | 0.78 |
| 41:HQ:2:ARG:HG2 | 41:HQ:131:GLN:HE22 | 1.48 | 0.78 |
| 34:5R:434:GLN:HA | 34:5R:437:PHE:HB3 | 1.65 | 0.78 |
| 36:5W:118:TYR:HA | 36:5W:121:MET:HB2 | 1.64 | 0.78 |
| 40:BI:171:ILE:HG23 | 40:BI:206:ASN:HD21 | 1.46 | 0.78 |
| 41:CO:124:ALA:HA | 41:CO:130:LEU:HD21 | 1.65 | 0.78 |
| 40:FG:31:GLN:HE21 | 40:FG:37:PRO:HG3 | 1.47 | 0.78 |
| 40:RF:64:ARG:HA | 40:RF:125:LEU:HD11 | 1.66 | 0.78 |
| 40:SI:11:GLN:HE22 | 41:SP:246:LEU:H | 1.30 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:5U:26:ARG:HH12 | 41:IQ:44:LEU:HB3 | 1.47 | 0.78 |
| 41:BM:163:ILE:HG23 | 41:BM:197:ASP:HB3 | 1.65 | 0.78 |
| 40:CA:406:TRP:HE1 | 41:CN:258:VAL:HG13 | 1.48 | 0.78 |
| 41:DL:7:LEU:HB3 | 41:DL:135:LEU:HD13 | 1.65 | 0.78 |
| 40:JE:352:LYS:HD2 | 41:JM:179:VAL:HG13 | 1.65 | 0.78 |
| 40:DF:349:THR:HG21 | 41:DN:182:PRO:HD2 | 1.66 | 0.78 |
| 41:DM:174:LYS:HE2 | 41:DM:175:VAL:HG22 | 1.66 | 0.78 |
| 41:QB:104:GLY:HA2 | 41:QB:109:GLY:HA3 | 0.79 | 0.78 |
| 41:DL:263:LEU:HD11 | 41:DL:425:ARG:HG3 | 1.65 | 0.78 |
| 41:DM:103:LYS:HB3 | 41:DM:108:GLU:HB2 | 1.65 | 0.78 |
| 40:MH:177:VAL:HG21 | 41:MO:327:ASP:HB3 | 1.63 | 0.78 |
| 41:SO:89:ASN:HA | 41:SO:119:VAL:HG11 | 1.66 | 0.78 |
| 40:DF:11:GLN:HB2 | 40:DF:74:VAL:HG21 | 1.65 | 0.78 |
| 41:DP:5:VAL:HG23 | 41:DP:130:LEU:HD11 | 1.64 | 0.78 |
| 40:GH:352:LYS:HG2 | 41:GP:178:THR:HA | 1.65 | 0.78 |
| 40:LE:15:GLN:NE2 | 42:LL:501:GTP:O6 | 2.16 | 0.78 |
| 41:TL:222:TYR:O | 41:TL:226:ASN:HB2 | 1.84 | 0.78 |
| 22:4H:6:LEU:HD21 | 41:ML:360:GLY:HA3 | 1.66 | 0.78 |
| 24:4O:173:SER:HB2 | 24:4O:181:LYS:HA | 1.66 | 0.78 |
| 23:4R:110:ASN:HD21 | 40:BI:279:GLU:HB3 | 1.48 | 0.78 |
| 40:FA:310:GLY:HA3 | 40:FA:382:ALA:HB2 | 1.65 | 0.78 |
| 41:OP:207:LEU:HB3 | 41:OP:225:LEU:HD22 | 1.66 | 0.78 |
| 23:4N:189:GLY:HA2 | 41:CM:46:ARG:HH12 | 1.49 | 0.77 |
| 40:DI:258:ASN:HB3 | 40:DI:352:LYS:HG3 | 1.66 | 0.77 |
| 40:VG:90:GLU:HG2 | 40:WF:280:LYS:HE3 | 1.67 | 0.77 |
| 23:4N:19:ILE:CD1 | 23:4N:19:ILE:N | 2.45 | 0.77 |
| 41:CM:268:PRO:HG2 | 41:CM:300:MET:HB2 | 1.65 | 0.77 |
| 40:JF:224:TYR:CD2 | 41:JM:323:MET:HG3 | 2.19 | 0.77 |
| 40:QE:66:VAL:HA | 40:QE:91:GLN:HE22 | 1.49 | 0.77 |
| 23:4M:198:PHE:HB3 | 40:DG:221:ARG:CG | 2.13 | 0.77 |
| 40:MA:438:SER:HB3 | 41:MB:391:ARG:HH22 | 1.50 | 0.77 |
| 41:NN:6:HIS:O | 41:NN:63:ALA:HA | 1.82 | 0.77 |
| 10:2G:97:GLN:O | 10:2G:101:GLN:HB2 | 1.85 | 0.77 |
| 41:EP:231:ALA:HB3 | 41:EP:270:PHE:CZ | 2.20 | 0.77 |
| 41:QB:313:VAL:HA | 41:QB:369:GLY:HA2 | 1.67 | 0.77 |
| 40:SA:11:GLN:HG2 | 40:SA:15:GLN:HE22 | 1.49 | 0.77 |
| 40:TE:51:THR:HG21 | 40:TE:243:ARG:HG2 | 1.65 | 0.77 |
| 40:UF:3:GLU:HG3 | 40:UF:129:CYS:HB2 | 1.66 | 0.77 |
| 8:1W:256:ARG:HH21 | 40:UI:56:THR:HB | 1.49 | 0.77 |
| 40:GE:323:VAL:HG22 | 40:GE:328:VAL:HG22 | 1.67 | 0.77 |
| 40:II:51:THR:HG21 | 40:II:243:ARG:HG2 | 1.66 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RH:320:ARG:O | 40:RH:372:ARG:HA | 1.84 | 0.77 |
| 37:6A:77:GLY:O | 37:6A:81:LYS:HB2 | 1.84 | 0.77 |
| 41:BM:87:PRO:HD3 | 41:CM:281:TYR:HD1 | 1.49 | 0.77 |
| 40:EI:3:GLU:HG3 | 40:EI:129:CYS:HB3 | 1.66 | 0.77 |
| 40:UF:346:TRP:HB3 | 41:UN:391:ARG:HD3 | 1.67 | 0.77 |
| 40:GE:204:VAL:HG23 | 40:GE:302:MET:CE | 2.10 | 0.77 |
| 40:DI:269:LEU:HD11 | 40:DI:383:ILE:HD13 | 1.66 | 0.77 |
| 40:OA:228:ASN:HD21 | 42:ON:501:GTP:HN1 | 1.32 | 0.77 |
| 23:4R:104:ILE:HG13 | 23:4R:112:VAL:HG13 | 1.65 | 0.77 |
| 41:BO:120:VAL:HG21 | 41:BO:155:ILE:HD11 | 1.67 | 0.77 |
| 40:LF:212:ILE:HD11 | 40:LF:300:ASN:HA | 1.66 | 0.77 |
| 41:PP:54:ALA:HA | 41:QP:283:ALA:HB2 | 1.65 | 0.77 |
| 40:RA:117:LEU:HD23 | 40:RA:121:ARG:HH22 | 1.48 | 0.77 |
| 41:VB:246:LEU:H | 40:VH:11:GLN:HE22 | 1.33 | 0.77 |
| 41:VN:235:GLY:HA3 | 41:VN:366:THR:HG21 | 1.67 | 0.77 |
| 40:BI:51:THR:HG21 | 40:BI:243:ARG:HA | 1.67 | 0.76 |
| 41:LN:253:LEU:O | 41:LN:257:MET:HB2 | 1.84 | 0.76 |
| 40:MG:254:GLU:HG2 | 41:MO:98:GLY:HA2 | 1.67 | 0.76 |
| 41:QB:104:GLY:HA2 | 41:QB:109:GLY:HA2 | 1.66 | 0.76 |
| 41:WO:341:PHE:HB3 | 41:WO:348:ASN:HD21 | 1.50 | 0.76 |
| 41:UM:165:ASN:HD21 | 41:UM:250:LEU:HD13 | 1.49 | 0.76 |
| 41:WM:2:ARG:HB3 | 41:WM:131:GLN:HB2 | 1.66 | 0.76 |
| 40:CA:8:HIS:HA | 40:CA:138:PHE:HB2 | 1.68 | 0.76 |
| 40:CH:106:GLY:HA3 | 40:CH:148:GLY:HA3 | 1.67 | 0.76 |
| 40:DA:228:ASN:HB3 | 42:DA:501:GTP:HN21 | 1.47 | 0.76 |
| 40:JH:228:ASN:HD21 | 42:JO:501:GTP:HN1 | 1.31 | 0.76 |
| 41:MO:275:SER:HB3 | 41:MO:278:SER:HB2 | 1.67 | 0.76 |
| 34:5Q:158:ARG:NH1 | 34:5R:490:ILE:CG1 | 2.46 | 0.76 |
| 40:BE:273:ALA:HB3 | 40:BE:274:PRO:HD3 | 1.67 | 0.76 |
| 40:CF:228:ASN:HD21 | 42:CF:501:GTP:HN1 | 1.32 | 0.76 |
| 41:DL:86:ARG:HA | 41:EL:281:TYR:CD2 | 2.20 | 0.76 |
| 21:4D:434:LYS:HZ3 | 21:4D:435:GLY:H | 1.32 | 0.76 |
| 41:AN:178:THR:HB | 41:AN:181:GLU:HG3 | 1.68 | 0.76 |
| 40:DF:222:PRO:HD2 | 41:DM:324:LYS:HE3 | 1.66 | 0.76 |
| 40:FA:325:PRO:HB2 | 41:FB:222:TYR:CZ | 2.19 | 0.76 |
| 40:HE:173:PRO:HB2 | 40:HE:390:LEU:HD21 | 1.68 | 0.76 |
| 41:QM:10:GLY:O | 41:QM:14:ASN:HB2 | 1.86 | 0.76 |
| 41:SO:237:THR:HB | 41:SO:240:LEU:HD11 | 1.68 | 0.76 |
| 41:WM:66:VAL:HG21 | 41:WM:116:VAL:HG13 | 1.66 | 0.76 |
| 40:MD:273:ALA:HB1 | 40:MD:274:PRO:HD2 | 1.67 | 0.76 |
| 40:UF:273:ALA:HB2 | 40:UF:374:VAL:HG12 | 1.66 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EA:51:THR:HG21 | 40:EA:243:ARG:HG2 | 1.68 | 0.76 |
| 40:OH:3:GLU:HG3 | 40:OH:129:CYS:HB2 | 1.67 | 0.76 |
| 41:PO:210:ILE:HD11 | 41:PO:298:ASN:HA | 1.68 | 0.76 |
| 41:CO:86:ARG:HB3 | 41:CO:89:ASN:HB2 | 1.66 | 0.76 |
| 41:DB:61:PRO:HG2 | 41:DB:84:ILE:HG23 | 1.66 | 0.76 |
| 40:PE:228:ASN:HD21 | 42:PE:501:GTP:HN1 | 1.34 | 0.76 |
| 40:RI:211:ASP:O | 40:RI:215:ARG:HB2 | 1.86 | 0.76 |
| 22:4K:435:ARG:HA | 22:4K:454:ILE:O | 1.86 | 0.76 |
| 41:BN:215:LEU:HD12 | 41:BN:275:SER:HB3 | 1.68 | 0.76 |
| 40:DF:324:VAL:HG13 | 40:DF:327:ASP:HB2 | 1.68 | 0.76 |
| 40:GH:278:ALA:HA | 40:GH:368:ALA:HB2 | 1.67 | 0.76 |
| 41:JB:375:GLN:HE21 | 41:JB:379:LYS:HG3 | 1.49 | 0.76 |
| 40:MF:335:ILE:HG23 | 40:MF:341:ILE:HD13 | 1.67 | 0.76 |
| 40:ND:274:PRO:HB3 | 40:ND:370:VAL:HG11 | 1.68 | 0.76 |
| 40:TG:14:VAL:HG23 | 40:TG:67:PHE:HD2 | 1.51 | 0.76 |
| 40:UF:106:GLY:HA3 | 40:UF:148:GLY:CA | 2.14 | 0.76 |
| 20:4A:227:GLU:HB2 | 20:4A:231:ARG:HH21 | 1.51 | 0.76 |
| 40:AF:259:LEU:HD21 | 40:AF:316:CYS:HB2 | 1.68 | 0.76 |
| 41:BO:258:VAL:HG22 | 41:BO:266:PHE:HZ | 1.51 | 0.76 |
| 40:CH:391:ASP:HB3 | 40:CH:421:ARG:NH2 | 2.01 | 0.76 |
| 41:EM:193:VAL:HG21 | 41:EM:418:LEU:HD11 | 1.66 | 0.76 |
| 41:FO:54:ALA:HA | 41:GO:283:ALA:HB2 | 1.66 | 0.76 |
| 40:OF:258:ASN:HD21 | 40:OF:352:LYS:HG3 | 1.50 | 0.76 |
| 40:OG:31:GLN:HE22 | 40:OG:37:PRO:HG3 | 1.51 | 0.76 |
| 40:EI:11:GLN:HA | 40:EI:74:VAL:HG21 | 1.66 | 0.75 |
| 41:CP:61:PRO:HD3 | 41:CP:84:ILE:HG12 | 1.67 | 0.75 |
| 40:EH:307:PRO:HB2 | 40:EH:312:TYR:HE2 | 1.50 | 0.75 |
| 40:FI:228:ASN:HD21 | 42:FI:501:GTP:HN1 | 1.31 | 0.75 |
| 41:JM:20:PHE:HA | 41:JM:230:SER:HB3 | 1.68 | 0.75 |
| 41:NL:6:HIS:O | 41:NL:63:ALA:HA | 1.86 | 0.75 |
| 41:QP:395:LEU:HA | 41:QP:398:TYR:HB2 | 1.67 | 0.75 |
| 40:TF:311:LYS:HG2 | 40:TF:342:GLN:HE22 | 1.50 | 0.75 |
| 40:FA:188:ILE:HG13 | 40:FA:394:PHE:HB2 | 1.67 | 0.75 |
| 40:MH:273:ALA:HB3 | 40:MH:274:PRO:HD3 | 1.68 | 0.75 |
| 41:MO:417:ASP:O | 41:MO:421:PRO:HD2 | 1.85 | 0.75 |
| 22:4H:282:ARG:HH22 | 41:CL:80:PRO:HG3 | 1.49 | 0.75 |
| 36:5Y:118:TYR:HA | 36:5Y:121:MET:HB2 | 1.68 | 0.75 |
| 40:DF:350:GLY:HA2 | 41:DN:179:VAL:HB | 1.67 | 0.75 |
| 41:EP:226:ASN:HA | 43:EP:501:GDP:HN21 | 1.52 | 0.75 |
| 40:GI:167:LEU:HD23 | 40:GI:202:PHE:HE2 | 1.51 | 0.75 |
| 40:MG:273:ALA:HB2 | 40:MG:374:VAL:HG22 | 1.69 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4J:92:LYS:N | 41:BN:279:GLN:H | 1.84 | 0.75 |
| 41:DL:5:VAL:HG22 | 41:DL:130:LEU:HD11 | 1.68 | 0.75 |
| 41:GN:375:GLN:HB3 | 41:GN:422:VAL:HG11 | 1.67 | 0.75 |
| 41:TP:163:ILE:HG13 | 41:TP:251:ARG:HB2 | 1.68 | 0.75 |
| 40:UI:262:TYR:H | 40:UI:265:ILE:HD11 | 1.51 | 0.75 |
| 41:CO:104:GLY:CA | 41:CO:109:GLY:HA3 | 2.16 | 0.75 |
| 41:DL:11:GLN:HA | 41:DL:72:THR:HG21 | 1.67 | 0.75 |
| 40:FF:177:VAL:HA | 41:FM:331:LEU:HD21 | 1.67 | 0.75 |
| 41:QP:236:VAL:HG13 | 41:QP:250:LEU:HD11 | 1.68 | 0.75 |
| 40:SG:278:ALA:H | 40:SG:368:ALA:HB2 | 1.51 | 0.75 |
| 7:1T:335:VAL:HG21 | 7:1T:605:VAL:HB | 1.67 | 0.75 |
| 14:3C:10:TYR:HE1 | 41:MO:297:LYS:HA | 1.52 | 0.75 |
| 40:DF:320:ARG:HG2 | 40:DF:356:ASN:HB3 | 1.68 | 0.75 |
| 40:IG:121:ARG:HH21 | 40:IG:124:LYS:HD3 | 1.50 | 0.75 |
| 40:MA:71:GLU:HG2 | 40:MA:72:PRO:HD2 | 1.68 | 0.75 |
| 40:MG:352:LYS:HD3 | 41:MO:178:THR:HA | 1.68 | 0.75 |
| 40:QG:228:ASN:HD21 | 42:QG:501:GTP:HN1 | 1.33 | 0.75 |
| 41:QP:112:LEU:HD22 | 41:QP:147:MET:HB3 | 1.67 | 0.75 |
| 40:WF:222:PRO:HG2 | 41:WM:324:LYS:HD3 | 1.69 | 0.75 |
| 22:4H:38:GLU:HB3 | 41:AL:276:ARG:HH12 | 1.50 | 0.75 |
| 40:DH:273:ALA:HB3 | 40:DH:274:PRO:HD3 | 1.67 | 0.75 |
| 41:DP:293:MET:HG3 | 41:DP:367:PHE:HB2 | 1.68 | 0.75 |
| 41:NL:174:LYS:HD2 | 41:NL:175:VAL:HG13 | 1.67 | 0.75 |
| 41:QB:7:LEU:HB2 | 41:QB:135:LEU:HB2 | 1.68 | 0.75 |
| 41:SN:289:LEU:O | 41:SN:293:MET:HB2 | 1.86 | 0.75 |
| 41:UP:258:VAL:HG22 | 41:UP:266:PHE:HZ | 1.51 | 0.75 |
| 21:4D:472:VAL:HG11 | 21:4D:498:VAL:HB | 1.69 | 0.75 |
| 26:4W:165:ARG:NH1 | 26:4W:166:ASP:OD1 | 2.20 | 0.75 |
| 40:CE:326:LYS:NZ | 41:CM:208:TYR:HB2 | 2.01 | 0.75 |
| 40:DI:268:PRO:HA | 40:DI:379:ASN:HA | 1.69 | 0.75 |
| 40:NH:237:SER:HG | 40:NH:375:CYS:HG | 1.31 | 0.75 |
| 41:QB:101:TRP:H | 41:QB:184:ASN:HD21 | 1.35 | 0.75 |
| 7:1T:211:ILE:HD13 | 7:1T:222:LEU:HB3 | 1.67 | 0.74 |
| 17:3P:177:VAL:HA | 17:3P:180:LYS:HD2 | 1.68 | 0.74 |
| 41:GM:253:LEU:O | 41:GM:257:MET:HB2 | 1.86 | 0.74 |
| 40:PE:254:GLU:O | 40:PE:258:ASN:HB2 | 1.87 | 0.74 |
| 2:1D:10:ARG:HE | 40:GH:401:ARG:H | 1.35 | 0.74 |
| 40:CA:328:VAL:HG11 | 40:CA:353:VAL:HG11 | 1.68 | 0.74 |
| 40:DH:228:ASN:HB3 | 42:DH:501:GTP:HN21 | 1.52 | 0.74 |
| 40:ME:16:ILE:HG13 | 40:ME:228:ASN:HD22 | 1.52 | 0.74 |
| 40:MH:225:THR:HA | 40:MH:228:ASN:HD21 | 1.51 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NF:222:PRO:O | 41:NM:324:LYS:NZ | 2.20 | 0.74 |
| 40:OH:301:GLN:HG2 | 40:OH:307:PRO:HG3 | 1.67 | 0.74 |
| 41:PM:253:LEU:O | 41:PM:257:MET:HB2 | 1.87 | 0.74 |
| 40:BE:222:PRO:HD2 | 41:BL:324:LYS:CE | 2.16 | 0.74 |
| 40:CA:278:ALA:H | 40:CA:368:ALA:HB2 | 1.52 | 0.74 |
| 41:DL:186:THR:HG22 | 41:DL:411:ALA:HB1 | 1.69 | 0.74 |
| 41:DL:226:ASN:HB3 | 43:DL:501:GDP:N1 | 2.01 | 0.74 |
| 40:EI:273:ALA:HB3 | 40:EI:274:PRO:HD3 | 1.69 | 0.74 |
| 41:EP:3:GLU:H | 41:EP:131:GLN:H | 1.34 | 0.74 |
| 40:QE:291:ILE:HG12 | 40:QE:374:VAL:HG12 | 1.67 | 0.74 |
| 7:1S:458:LYS:HE2 | 40:WG:279:GLU:HA | 1.69 | 0.74 |
| 7:1T:43:LEU:HD21 | 7:1T:610:ALA:HB2 | 1.69 | 0.74 |
| 40:DE:216:ASN:HB3 | 40:DE:275:VAL:HB | 1.68 | 0.74 |
| 41:DM:417:ASP:O | 41:DM:421:PRO:HD2 | 1.86 | 0.74 |
| 41:EP:216:LYS:HB2 | 41:EP:275:SER:HB2 | 1.69 | 0.74 |
| 40:FA:23:LEU:HD21 | 40:FA:236:SER:HB2 | 1.69 | 0.74 |
| 40:GF:352:LYS:HZ2 | 41:GN:178:THR:C | 1.91 | 0.74 |
| 41:HN:248:ALA:HA | 41:HN:252:LYS:HD3 | 1.68 | 0.74 |
| 40:VI:174:ALA:HB3 | 40:VI:178:SER:H | 1.52 | 0.74 |
| 41:VP:49:VAL:HG11 | 41:VP:241:ARG:HG2 | 1.69 | 0.74 |
| 41:AB:248:ALA:HA | 41:AB:252:LYS:HG2 | 1.70 | 0.74 |
| 40:DE:210:TYR:CE1 | 41:DL:324:LYS:HB3 | 2.23 | 0.74 |
| 41:QP:66:VAL:HA | 41:QP:91:VAL:HG22 | 1.70 | 0.74 |
| 40:DF:1:GLN:HG2 | 40:DF:2:ARG:H | 1.53 | 0.74 |
| 41:JM:323:MET:SD | 41:JM:353:VAL:HG11 | 2.28 | 0.74 |
| 40:MH:3:GLU:HA | 40:MH:51:THR:HA | 1.69 | 0.74 |
| 40:SF:276:ILE:HG23 | 40:SF:280:LYS:HG3 | 1.69 | 0.74 |
| 23:4M:92:PRO:HB2 | 40:AG:89:PRO:HB3 | 1.69 | 0.74 |
| 38:6C:37:ASN:ND2 | 41:VO:209:ASP:OD1 | 2.21 | 0.74 |
| 41:CN:113:VAL:HA | 41:CN:116:VAL:HG12 | 1.69 | 0.74 |
| 40:EI:191:THR:HB | 40:EI:387:TRP:HZ3 | 1.53 | 0.74 |
| 40:LE:174:ALA:HB3 | 40:LE:178:SER:H | 1.53 | 0.74 |
| 41:BB:44:LEU:HD23 | 41:BB:47:ILE:HD13 | 1.68 | 0.74 |
| 40:NE:298:PRO:HA | 40:NE:301:GLN:HE22 | 1.49 | 0.74 |
| 15:3F:194:ASN:ND2 | 17:3R:168:ILE:CD1 | 2.50 | 0.74 |
| 40:AG:256:GLN:HB3 | 41:AO:397:TRP:CZ2 | 2.23 | 0.74 |
| 41:AL:7:LEU:O | 41:AL:135:LEU:HA | 1.88 | 0.74 |
| 40:CG:262:TYR:HB2 | 40:CG:265:ILE:HG12 | 1.70 | 0.74 |
| 40:DH:213:CYS:HB3 | 40:DH:219:ILE:HD11 | 1.69 | 0.74 |
| 41:DN:131:GLN:HE22 | 41:DN:249:ASP:HB2 | 1.52 | 0.74 |
| 40:GF:133:GLN:HE22 | 40:GF:252:LEU:HB2 | 1.52 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GN:132:GLY:HA3 | 41:GN:163:ILE:HG22 | 1.69 | 0.74 |
| 41:VB:7:LEU:O | 41:VB:135:LEU:HA | 1.87 | 0.74 |
| 7:1T:161:ALA:HA | 7:1T:178:GLY:HA3 | 1.68 | 0.74 |
| 40:BF:224:TYR:CD2 | 41:BM:323:MET:HG3 | 2.22 | 0.74 |
| 41:UB:237:THR:HG22 | 41:UB:250:LEU:HD21 | 1.70 | 0.74 |
| 41:VN:87:PRO:HD3 | 41:WM:281:TYR:HD2 | 1.52 | 0.74 |
| 13:2W:62:PRO:HD3 | 13:2W:69:LEU:HD23 | 1.70 | 0.73 |
| 21:4E:440:LEU:HD13 | 21:4E:451:ILE:HD13 | 1.69 | 0.73 |
| 41:CO:61:PRO:HG2 | 41:CO:84:ILE:HG23 | 1.70 | 0.73 |
| 40:DA:142:GLY:HA2 | 40:DA:183:GLU:HG3 | 1.68 | 0.73 |
| 40:DI:210:TYR:HB2 | 41:DP:324:LYS:NZ | 2.03 | 0.73 |
| 41:EP:258:VAL:HG22 | 41:EP:266:PHE:HZ | 1.53 | 0.73 |
| 40:LG:273:ALA:HB2 | 40:LG:374:VAL:HG12 | 1.68 | 0.73 |
| 41:MM:292:GLN:HG2 | 41:MM:298:ASN:HD21 | 1.53 | 0.73 |
| 40:RH:231:ILE:HA | 40:RH:234:ILE:HD12 | 1.69 | 0.73 |
| 41:UO:388:MET:SD | 41:UO:391:ARG:NH2 | 2.61 | 0.73 |
| 41:UP:206:ALA:HB2 | 41:UP:302:ALA:H | 1.53 | 0.73 |
| 22:4I:528:TYR:HB2 | 40:EG:39:ASP:HB2 | 1.68 | 0.73 |
| 40:GE:274:PRO:HB2 | 40:GE:370:VAL:HG11 | 1.69 | 0.73 |
| 41:HP:271:ALA:HB1 | 41:HP:292:GLN:HG2 | 1.69 | 0.73 |
| 40:PA:132:LEU:HG | 40:PA:164:LYS:HG2 | 1.69 | 0.73 |
| 7:1T:424:ALA:HB3 | 7:1T:433:ILE:HG23 | 1.70 | 0.73 |
| 8:1X:140:VAL:O | 8:1X:144:LYS:HG3 | 1.87 | 0.73 |
| 22:4I:284:LEU:HD11 | 22:4I:346:VAL:HG23 | 1.69 | 0.73 |
| 41:BM:385:PHE:HZ | 41:BM:408:PHE:HB3 | 1.53 | 0.73 |
| 40:CG:262:TYR:HE1 | 41:CO:393:ALA:HA | 1.54 | 0.73 |
| 41:DB:104:GLY:HA3 | 41:DB:146:GLY:HA3 | 1.68 | 0.73 |
| 41:DL:19:LYS:HB3 | 41:DL:226:ASN:HD21 | 1.53 | 0.73 |
| 40:KG:62:VAL:HG11 | 40:LG:283:HIS:HB3 | 1.70 | 0.73 |
| 40:LG:27:GLU:HG2 | 40:LG:361:THR:HG21 | 1.68 | 0.73 |
| 41:OO:207:LEU:HB3 | 41:OO:225:LEU:HD11 | 1.70 | 0.73 |
| 40:TE:254:GLU:OE1 | 41:TM:99:ASN:ND2 | 2.21 | 0.73 |
| 41:TP:58:LYS:NZ | 41:UP:280:GLN:HB2 | 2.03 | 0.73 |
| 41:UN:100:ASN:HB3 | 41:UN:103:LYS:HB2 | 1.69 | 0.73 |
| 40:WA:221:ARG:HH12 | 41:WN:325:GLU:HB2 | 1.52 | 0.73 |
| 41:BB:86:ARG:HB2 | 41:BB:89:ASN:HB2 | 1.70 | 0.73 |
| 40:BE:274:PRO:HB2 | 40:BE:370:VAL:HG21 | 1.70 | 0.73 |
| 40:GH:11:GLN:HA | 40:GH:74:VAL:HG11 | 1.71 | 0.73 |
| 42:MB:502:GTP:N2 | 40:MG:228:ASN:HB3 | 2.02 | 0.73 |
| 41:ON:202:ILE:HG12 | 41:ON:268:PRO:HG3 | 1.70 | 0.73 |
| 40:QG:139:HIS:O | 40:QG:170:SER:HA | 1.87 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QO:10:GLY:O | 41:QO:14:ASN:HB2 | 1.89 | 0.73 |
| 41:QP:3:GLU:HB2 | 41:QP:130:LEU:HA | 1.70 | 0.73 |
| 40:SH:174:ALA:HB3 | 40:SH:178:SER:H | 1.54 | 0.73 |
| 10:2E:157:ARG:HH22 | 41:VN:51:TYR:HB3 | 1.54 | 0.73 |
| 21:4D:418:LYS:HB2 | 21:4D:444:LEU:HD12 | 1.71 | 0.73 |
| 38:6C:123:PHE:HB2 | 40:UG:119:LEU:HD11 | 1.68 | 0.73 |
| 40:AH:101:ASN:HD22 | 41:AO:256:ASN:HD21 | 1.35 | 0.73 |
| 40:CH:172:TYR:HB2 | 40:CH:203:MET:HG2 | 1.69 | 0.73 |
| 41:EO:178:THR:HB | 41:EO:181:GLU:HB2 | 1.71 | 0.73 |
| 40:GI:88:HIS:HB2 | 40:HI:283:HIS:HB3 | 1.70 | 0.73 |
| 41:QB:136:THR:HG22 | 41:QB:167:PHE:HB2 | 1.69 | 0.73 |
| 41:QO:135:LEU:HG | 41:QO:137:HIS:HD2 | 1.52 | 0.73 |
| 40:UI:222:PRO:HD2 | 41:UP:324:LYS:HE3 | 1.70 | 0.73 |
| 40:WG:104:ALA:HB2 | 40:WG:412:MET:HG2 | 1.70 | 0.73 |
| 13:2X:13:ILE:HG13 | 13:2X:25:TRP:HZ2 | 1.53 | 0.73 |
| 23:4M:110:ASN:HA | 23:4M:113:TRP:CE3 | 2.22 | 0.73 |
| 37:6A:111:HIS:HB3 | 40:TH:245:ASP:HB2 | 1.69 | 0.73 |
| 40:AH:42:ILE:HG23 | 40:AH:44:GLY:H | 1.54 | 0.73 |
| 40:HA:228:ASN:HD21 | 42:HA:501:GTP:HN1 | 1.37 | 0.73 |
| 40:HI:51:THR:HG21 | 40:HI:243:ARG:HG2 | 1.70 | 0.73 |
| 15:3F:194:ASN:HD21 | 17:3R:168:ILE:HD13 | 1.52 | 0.73 |
| 21:4F:411:LYS:HZ3 | 21:4F:412:MET:CG | 2.01 | 0.73 |
| 41:JB:182:PRO:HG3 | 41:JB:384:GLN:HG3 | 1.69 | 0.73 |
| 41:TO:187:LEU:O | 41:TO:191:GLN:NE2 | 2.21 | 0.73 |
| 40:VG:326:LYS:HZ3 | 41:VO:208:TYR:HB2 | 1.53 | 0.73 |
| 40:PA:133:GLN:HG3 | 40:PA:252:LEU:HB2 | 1.70 | 0.73 |
| 40:RE:326:LYS:HE3 | 41:RM:212:PHE:HE1 | 1.54 | 0.73 |
| 40:WE:350:GLY:HA2 | 41:WM:179:VAL:HG13 | 1.71 | 0.73 |
| 14:3C:85:THR:HG21 | 36:5W:245:PRO:HB2 | 1.70 | 0.73 |
| 23:4M:236:TYR:HA | 23:4M:267:ASP:HB3 | 1.70 | 0.73 |
| 26:4V:72:GLN:NE2 | 26:4V:277:MET:O | 2.21 | 0.73 |
| 40:BG:228:ASN:HD21 | 42:BG:501:GTP:HN1 | 1.34 | 0.73 |
| 40:IA:210:TYR:HD2 | 41:IN:324:LYS:HE3 | 1.52 | 0.73 |
| 40:KH:101:ASN:HD22 | 41:KO:256:ASN:HD21 | 1.36 | 0.73 |
| 40:NF:438:SER:HA | 41:NN:391:ARG:HH22 | 1.53 | 0.73 |
| 41:QN:7:LEU:O | 41:QN:135:LEU:HA | 1.89 | 0.73 |
| 41:UP:268:PRO:HG2 | 41:UP:300:MET:HB2 | 1.69 | 0.73 |
| 40:EE:256:GLN:HE22 | 41:EM:397:TRP:HE1 | 1.35 | 0.73 |
| 40:FH:222:PRO:HD2 | 41:FO:324:LYS:HE3 | 1.71 | 0.73 |
| 40:HF:326:LYS:NZ | 41:HN:208:TYR:HB2 | 2.04 | 0.73 |
| 40:JH:128:GLN:HE22 | 40:KH:285:GLN:HE21 | 1.35 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SI:54:SER:O | 40:SI:61:HIS:HA | 1.88 | 0.73 |
| 41:SL:86:ARG:HH21 | 41:SL:88:ASP:HB3 | 1.53 | 0.73 |
| 41:TO:135:LEU:HD21 | 41:TO:166:THR:HG22 | 1.71 | 0.73 |
| 34:5R:332:ARG:HH21 | 40:FI:58:ALA:HA | 1.53 | 0.72 |
| 40:CA:335:ILE:HG13 | 40:CA:338:LYS:HD2 | 1.70 | 0.72 |
| 41:CM:55:THR:HG21 | 41:DM:284:LEU:HG | 1.70 | 0.72 |
| 41:CN:311:LEU:HD11 | 41:CN:372:THR:HG23 | 1.71 | 0.72 |
| 40:HE:200:CYS:HB2 | 40:HE:256:GLN:HE22 | 1.53 | 0.72 |
| 40:IF:326:LYS:HD2 | 41:IN:208:TYR:HD1 | 1.54 | 0.72 |
| 40:OH:222:PRO:HD2 | 41:OO:324:LYS:NZ | 2.03 | 0.72 |
| 41:PO:8:GLN:HE22 | 41:PO:136:THR:H | 1.37 | 0.72 |
| 40:QE:56:THR:HA | 40:RE:285:GLN:HG2 | 1.70 | 0.72 |
| 40:UF:344:VAL:HG23 | 40:UF:347:CYS:HB2 | 1.71 | 0.72 |
| 8:1X:103:SER:HB2 | 8:1X:107:PHE:HB2 | 1.71 | 0.72 |
| 13:2X:17:ILE:HD12 | 41:WM:125:GLU:HB3 | 1.69 | 0.72 |
| 18:3T:306:ARG:HH12 | 25:4T:398:THR:HB | 1.54 | 0.72 |
| 41:AB:256:ASN:HD22 | 40:AG:181:VAL:HG22 | 1.54 | 0.72 |
| 41:FN:54:ALA:HA | 41:GN:283:ALA:HB2 | 1.72 | 0.72 |
| 40:MH:250:VAL:HG23 | 40:MH:254:GLU:HB2 | 1.71 | 0.72 |
| 40:OE:237:SER:OG | 40:OE:375:CYS:SG | 2.47 | 0.72 |
| 41:QP:417:ASP:O | 41:QP:421:PRO:HD2 | 1.89 | 0.72 |
| 40:WH:104:ALA:HB2 | 40:WH:412:MET:HG2 | 1.70 | 0.72 |
| 12:2M:78:ARG:NH2 | 13:2T:72:LYS:HB2 | 2.03 | 0.72 |
| 16:3L:96:LYS:O | 16:3L:100:GLU:HB2 | 1.90 | 0.72 |
| 17:3R:222:GLU:HA | 17:3R:339:GLN:HG3 | 1.69 | 0.72 |
| 27:4Z:234:LEU:HD11 | 27:4Z:245:GLU:HG2 | 1.72 | 0.72 |
| 40:AF:274:PRO:HG3 | 40:AF:286:LEU:HD12 | 1.72 | 0.72 |
| 40:DE:332:ILE:HA | 40:DE:335:ILE:HD13 | 1.70 | 0.72 |
| 41:JB:166:THR:HG23 | 41:JB:199:THR:HG23 | 1.72 | 0.72 |
| 40:LG:51:THR:HG21 | 40:LG:243:ARG:HG2 | 1.71 | 0.72 |
| 40:MG:258:ASN:HB2 | 40:MG:352:LYS:CE | 2.19 | 0.72 |
| 40:PA:214:ARG:HD3 | 41:PN:324:LYS:HE2 | 1.69 | 0.72 |
| 40:QG:209:ILE:HG13 | 40:QG:227:LEU:HD22 | 1.70 | 0.72 |
| 40:QG:273:ALA:HB1 | 40:QG:291:ILE:HB | 1.70 | 0.72 |
| 40:VG:228:ASN:HD21 | 42:VN:501:GTP:HN1 | 1.36 | 0.72 |
| 40:DF:157:LEU:HB3 | 40:DF:166:LYS:HD3 | 1.72 | 0.72 |
| 41:DL:258:VAL:HG22 | 41:DL:266:PHE:HZ | 1.54 | 0.72 |
| 41:EM:167:PHE:HZ | 41:EM:236:VAL:HG11 | 1.54 | 0.72 |
| 40:GA:210:TYR:HE1 | 41:GN:324:LYS:HA | 1.54 | 0.72 |
| 40:GA:320:ARG:HH21 | 40:GA:360:PRO:HA | 1.52 | 0.72 |
| 40:NF:100:ALA:HA | 41:NM:252:LYS:HD2 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PN:100:ASN:HB3 | 41:PN:103:LYS:HG2 | 1.70 | 0.72 |
| 40:UG:376:MET:SD | 40:UG:378:SER:OG | 2.47 | 0.72 |
| 8:1X:134:GLU:OE1 | 8:1X:134:GLU:CA | 2.35 | 0.72 |
| 12:2N:154:LYS:HD3 | 12:2N:192:GLN:HB3 | 1.70 | 0.72 |
| 22:4J:89:VAL:H | 41:BN:280:GLN:HA | 1.54 | 0.72 |
| 40:DF:406:TRP:HZ2 | 41:DM:258:VAL:HB | 1.53 | 0.72 |
| 41:DM:113:VAL:HG23 | 41:DM:151:LEU:HD22 | 1.71 | 0.72 |
| 41:EL:7:LEU:O | 41:EL:135:LEU:HA | 1.89 | 0.72 |
| 40:IF:228:ASN:HD21 | 42:IF:501:GTP:HN1 | 1.36 | 0.72 |
| 40:MH:187:SER:HB2 | 40:MH:390:LEU:HD21 | 1.72 | 0.72 |
| 41:PB:267:MET:HB2 | 41:PB:374:ILE:HD11 | 1.72 | 0.72 |
| 40:RF:20:CYS:HA | 40:RF:232:SER:HB2 | 1.71 | 0.72 |
| 40:VA:133:GLN:NE2 | 40:VA:251:ASP:OD2 | 2.23 | 0.72 |
| 7:1T:537:ILE:HG22 | 8:1Y:147:MET:HG2 | 1.70 | 0.72 |
| 7:1U:551:MET:HG2 | 7:1U:562:THR:HG22 | 1.72 | 0.72 |
| 13:2V:95:ASP:HB3 | 13:2V:146:THR:HB | 1.71 | 0.72 |
| 15:3H:82:GLU:HB2 | 17:3P:275:ARG:HH21 | 1.53 | 0.72 |
| 23:4R:107:LYS:HG2 | 23:4R:111:GLN:HB3 | 1.72 | 0.72 |
| 41:CM:132:GLY:HA2 | 41:CM:162:ARG:HG3 | 1.70 | 0.72 |
| 41:DO:7:LEU:O | 41:DO:135:LEU:HA | 1.90 | 0.72 |
| 41:JN:122:LYS:HD3 | 41:KN:291:GLN:HE22 | 1.52 | 0.72 |
| 41:LO:217:LEU:HD23 | 41:LO:276:ARG:HH12 | 1.55 | 0.72 |
| 40:RI:318:LEU:HB2 | 40:RI:375:CYS:HB3 | 1.70 | 0.72 |
| 40:TI:224:TYR:O | 40:TI:228:ASN:HB2 | 1.90 | 0.72 |
| 41:TO:7:LEU:O | 41:TO:135:LEU:HA | 1.89 | 0.72 |
| 23:4N:240:LEU:HD22 | 23:4N:266:HIS:HB3 | 1.71 | 0.72 |
| 23:4R:173:SER:HB2 | 23:4R:181:LYS:HA | 1.71 | 0.72 |
| 41:CM:2:ARG:HB3 | 41:CM:131:GLN:HB2 | 1.71 | 0.72 |
| 40:EI:74:VAL:HG13 | 40:EI:75:ILE:HG12 | 1.71 | 0.72 |
| 41:EN:330:MET:O | 41:EN:334:GLN:NE2 | 2.23 | 0.72 |
| 41:KO:208:TYR:O | 41:KO:212:PHE:HB3 | 1.89 | 0.72 |
| 41:SP:222:TYR:O | 41:SP:226:ASN:CB | 2.38 | 0.72 |
| 40:WA:228:ASN:HD21 | 42:WA:501:GTP:HN1 | 1.37 | 0.72 |
| 13:2V:115:LYS:HG2 | 13:2V:118:ILE:HG22 | 1.70 | 0.72 |
| 28:5B:156:TYR:O | 28:5B:160:TYR:HB2 | 1.90 | 0.72 |
| 31:5J:782:ARG:NH2 | 41:HM:70:PRO:O | 2.22 | 0.72 |
| 38:6C:122:PRO:HB2 | 40:VH:308:ARG:HH12 | 1.54 | 0.72 |
| 40:DI:259:LEU:HD22 | 40:DI:316:CYS:HB3 | 1.70 | 0.72 |
| 41:GB:282:ARG:NH1 | 41:GB:288:GLU:OE1 | 2.23 | 0.72 |
| 40:PD:318:LEU:O | 40:PD:374:VAL:HA | 1.90 | 0.72 |
| 40:VA:228:ASN:HD21 | 42:VA:501:GTP:HN1 | 1.34 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:1Y:104:PRO:HG3 | 11:2J:253:ALA:HB3 | 1.70 | 0.72 |
| 17:3O:360:LYS:HB3 | 17:3R:107:TYR:OH | 1.90 | 0.72 |
| 23:4N:263:HIS:HA | 23:4N:266:HIS:NE2 | 2.05 | 0.72 |
| 23:4P:240:LEU:HD22 | 23:4P:266:HIS:HB3 | 1.71 | 0.72 |
| 23:4P:263:HIS:HA | 23:4P:266:HIS:NE2 | 2.05 | 0.72 |
| 27:4Z:69:LYS:HD3 | 27:4Z:126:THR:HB | 1.70 | 0.72 |
| 41:DM:272:PRO:HG3 | 41:DM:364:SER:HB2 | 1.71 | 0.72 |
| 40:EH:180:ALA:HB3 | 40:EH:183:GLU:HG3 | 1.72 | 0.72 |
| 40:EI:105:ARG:HG2 | 40:EI:410:GLU:HG3 | 1.70 | 0.72 |
| 41:FP:7:LEU:O | 41:FP:135:LEU:HA | 1.89 | 0.72 |
| 41:HB:10:GLY:O | 41:HB:14:ASN:HB2 | 1.89 | 0.72 |
| 41:HN:86:ARG:HA | 41:IN:281:TYR:CD2 | 2.25 | 0.72 |
| 41:LN:51:TYR:HB3 | 41:LN:59:TYR:HB3 | 1.72 | 0.72 |
| 40:TF:174:ALA:HB3 | 40:TF:178:SER:H | 1.55 | 0.72 |
| 41:EM:200:TYR:HE2 | 41:EM:236:VAL:HG21 | 1.55 | 0.72 |
| 40:GH:71:GLU:HG2 | 40:GH:72:PRO:HD2 | 1.72 | 0.72 |
| 40:II:228:ASN:HD21 | 42:II:501:GTP:HN1 | 1.35 | 0.72 |
| 40:LA:177:VAL:HG23 | 41:LN:331:LEU:HB2 | 1.72 | 0.72 |
| 40:UF:287:SER:HA | 40:UF:372:ARG:HH22 | 1.54 | 0.72 |
| 22:4J:89:VAL:O | 41:BN:281:TYR:N | 2.22 | 0.71 |
| 41:DM:268:PRO:HG2 | 41:DM:300:MET:HB2 | 1.70 | 0.71 |
| 40:IE:240:ALA:HA | 40:IE:243:ARG:HE | 1.55 | 0.71 |
| 40:MF:20:CYS:HA | 40:MF:232:SER:HB2 | 1.70 | 0.71 |
| 41:QO:7:LEU:O | 41:QO:135:LEU:HA | 1.90 | 0.71 |
| 40:SH:16:ILE:HG12 | 40:SH:231:ILE:HD11 | 1.69 | 0.71 |
| 13:2V:61:CYS:HB3 | 13:2V:62:PRO:HD3 | 1.72 | 0.71 |
| 13:2V:92:GLN:HG3 | 13:2V:102:ARG:HG3 | 1.71 | 0.71 |
| 23:4R:56:ALA:HB3 | 41:BP:40:SER:HA | 1.72 | 0.71 |
| 40:CA:106:GLY:HA3 | 40:CA:148:GLY:HA3 | 1.72 | 0.71 |
| 41:DB:60:VAL:HG11 | 41:EB:281:TYR:HB3 | 1.71 | 0.71 |
| 41:DN:385:PHE:CE2 | 41:DN:389:PHE:HB2 | 2.25 | 0.71 |
| 41:EP:14:ASN:HB3 | 41:EP:76:VAL:HG21 | 1.71 | 0.71 |
| 40:JG:11:GLN:HG2 | 40:JG:74:VAL:HG21 | 1.72 | 0.71 |
| 40:RH:88:HIS:HB3 | 40:RH:91:GLN:HB2 | 1.72 | 0.71 |
| 41:SO:242:PHE:HB3 | 41:SO:356:ILE:HG13 | 1.71 | 0.71 |
| 8:1Y:201:CYS:SG | 40:VF:371:GLN:NE2 | 2.62 | 0.71 |
| 13:2X:94:LEU:HB2 | 13:2X:152:LEU:HD11 | 1.72 | 0.71 |
| 24:4O:199:GLY:H | 40:DE:221:ARG:HG3 | 1.56 | 0.71 |
| 40:BF:238:ILE:HG23 | 40:BF:255:PHE:HE2 | 1.54 | 0.71 |
| 41:GN:61:PRO:HG3 | 41:GN:84:ILE:HG23 | 1.71 | 0.71 |
| 40:JA:123:ARG:NH1 | 40:JA:161:TYR:OH | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JH:222:PRO:HD2 | 41:JO:324:LYS:HE2 | 1.72 | 0.71 |
| 41:JM:185:ALA:HB3 | 41:JM:381:ILE:HD11 | 1.72 | 0.71 |
| 41:KL:258:VAL:HG22 | 41:KL:266:PHE:HZ | 1.55 | 0.71 |
| 40:LH:56:THR:HG22 | 40:MH:285:GLN:HG2 | 1.72 | 0.71 |
| 40:LH:228:ASN:HD21 | 42:LO:501:GTP:HN1 | 1.38 | 0.71 |
| 42:OB:502:GTP:HN1 | 40:OG:228:ASN:HD21 | 1.36 | 0.71 |
| 41:QP:86:ARG:HB3 | 41:RP:281:TYR:HE2 | 1.52 | 0.71 |
| 13:2X:69:LEU:HD21 | 13:2X:153:ARG:HA | 1.71 | 0.71 |
| 40:CG:75:ILE:HG23 | 40:CG:92:LEU:HD12 | 1.71 | 0.71 |
| 40:EH:250:VAL:HG12 | 40:EH:254:GLU:HG2 | 1.71 | 0.71 |
| 40:JG:6:SER:O | 40:JG:65:ALA:HA | 1.91 | 0.71 |
| 41:JM:222:TYR:HA | 41:JM:225:LEU:HD12 | 1.71 | 0.71 |
| 40:LH:177:VAL:O | 41:LO:347:ASN:ND2 | 2.22 | 0.71 |
| 41:OP:8:GLN:HE21 | 41:OP:14:ASN:HD22 | 1.37 | 0.71 |
| 41:UM:45:GLU:HG2 | 41:UM:46:ARG:HG2 | 1.72 | 0.71 |
| 13:2T:62:PRO:HD3 | 13:2T:69:LEU:HD23 | 1.72 | 0.71 |
| 23:4P:259:ARG:NH2 | 40:EA:365:GLY:HA2 | 2.04 | 0.71 |
| 26:4W:246:LYS:HZ2 | 26:4W:353:ASN:HB3 | 1.55 | 0.71 |
| 27:4Z:238:THR:HG23 | 27:4Z:240:PHE:H | 1.54 | 0.71 |
| 41:HN:60:VAL:HG11 | 41:HN:86:ARG:HG3 | 1.71 | 0.71 |
| 40:IE:209:ILE:HG21 | 40:IE:227:LEU:HA | 1.72 | 0.71 |
| 40:MD:27:GLU:OE1 | 40:MD:243:ARG:NH1 | 2.23 | 0.71 |
| 40:UI:274:PRO:HB2 | 40:UI:370:VAL:HG11 | 1.72 | 0.71 |
| 8:1Y:99:SER:HB2 | 8:1Y:101:ILE:HG12 | 1.73 | 0.71 |
| 38:6C:22:VAL:HG12 | 40:VG:298:PRO:HD3 | 1.72 | 0.71 |
| 40:CF:262:TYR:HB2 | 40:CF:265:ILE:HG12 | 1.72 | 0.71 |
| 40:DE:210:TYR:CD1 | 41:DL:324:LYS:HB3 | 2.25 | 0.71 |
| 40:EF:11:GLN:HG3 | 40:EF:74:VAL:HG21 | 1.73 | 0.71 |
| 40:KE:11:GLN:HG3 | 40:KE:74:VAL:HG11 | 1.72 | 0.71 |
| 41:KN:7:LEU:O | 41:KN:135:LEU:HA | 1.91 | 0.71 |
| 41:QO:271:ALA:HB1 | 41:QO:292:GLN:HG3 | 1.73 | 0.71 |
| 40:SF:109:THR:HG23 | 40:SF:110:ILE:HD12 | 1.71 | 0.71 |
| 40:UH:90:GLU:O | 40:UH:121:ARG:NH1 | 2.23 | 0.71 |
| 40:WH:228:ASN:HD21 | 42:WO:501:GTP:HN1 | 1.38 | 0.71 |
| 17:3P:361:MET:HE1 | 17:3P:458:ASP:HB3 | 1.73 | 0.71 |
| 40:CF:254:GLU:HB3 | 41:CN:98:GLY:CA | 2.21 | 0.71 |
| 40:HE:212:ILE:HD11 | 40:HE:300:ASN:HA | 1.73 | 0.71 |
| 41:HN:69:GLU:HB3 | 41:HN:96:GLY:HA2 | 1.73 | 0.71 |
| 40:IE:228:ASN:HD21 | 42:IE:501:GTP:HN1 | 1.39 | 0.71 |
| 40:II:315:CYS:HA | 40:II:377:LEU:O | 1.91 | 0.71 |
| 41:NP:42:LEU:HD13 | 41:NP:356:ILE:HD13 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PL:136:THR:HG22 | 41:PL:167:PHE:HB2 | 1.72 | 0.71 |
| 40:SH:11:GLN:HE22 | 41:SO:247:ASN:HB2 | 1.56 | 0.71 |
| 40:UE:228:ASN:HD21 | 42:UE:501:GTP:HN1 | 1.39 | 0.71 |
| 41:UM:222:TYR:O | 41:UM:226:ASN:ND2 | 2.23 | 0.71 |
| 41:UN:209:ASP:O | 41:UN:213:ARG:HB2 | 1.88 | 0.71 |
| 8:1X:174:LEU:HD21 | 41:UB:83:GLN:HG3 | 1.73 | 0.71 |
| 11:2J:161:ARG:HH12 | 40:MF:401:ARG:HG2 | 1.56 | 0.71 |
| 25:4T:401:PRO:HB3 | 40:LA:371:GLN:HG3 | 1.73 | 0.71 |
| 41:CN:170:VAL:HG11 | 41:CN:377:LEU:HD21 | 1.73 | 0.71 |
| 40:DE:350:GLY:CA | 41:DM:179:VAL:HB | 2.16 | 0.71 |
| 40:EI:210:TYR:HE1 | 41:EP:324:LYS:CA | 1.96 | 0.71 |
| 41:GP:282:ARG:HD3 | 41:GP:283:ALA:H | 1.56 | 0.71 |
| 40:HF:154:MET:HG3 | 40:HF:194:THR:HG23 | 1.73 | 0.71 |
| 40:KD:292:THR:HG21 | 40:KD:331:ALA:HB1 | 1.72 | 0.71 |
| 7:1U:65:ASN:HD22 | 7:1U:85:THR:HA | 1.55 | 0.71 |
| 34:5R:362:ARG:HA | 34:5R:365:GLU:HG2 | 1.73 | 0.71 |
| 40:CA:49:PHE:HE2 | 40:CA:55:GLU:HB2 | 1.55 | 0.71 |
| 41:FB:174:LYS:HD2 | 41:FB:175:VAL:HG13 | 1.72 | 0.71 |
| 40:GE:139:HIS:H | 40:GE:139:HIS:CD2 | 2.09 | 0.71 |
| 41:KB:173:PRO:HB3 | 41:KB:380:ARG:HD3 | 1.72 | 0.71 |
| 40:OH:220:GLU:C | 41:OO:324:LYS:HZ2 | 1.93 | 0.71 |
| 40:RI:90:GLU:O | 40:RI:121:ARG:NH1 | 2.22 | 0.71 |
| 41:UB:248:ALA:HA | 41:UB:252:LYS:HD3 | 1.71 | 0.71 |
| 41:VN:108:GLU:HA | 41:VN:111:GLU:HG2 | 1.72 | 0.71 |
| 13:2V:74:PRO:HD2 | 13:2V:169:ASP:HA | 1.73 | 0.71 |
| 36:5Y:119:ILE:HD11 | 40:KH:400:LYS:HD2 | 1.71 | 0.71 |
| 41:CO:64:VAL:HG21 | 41:CO:120:VAL:HG22 | 1.73 | 0.71 |
| 41:DP:104:GLY:HA2 | 41:DP:109:GLY:HA3 | 1.73 | 0.71 |
| 41:HM:317:PHE:HB2 | 41:HM:353:VAL:HG12 | 1.72 | 0.71 |
| 42:KB:502:GTP:HN1 | 40:KG:228:ASN:HD21 | 1.39 | 0.71 |
| 40:OH:273:ALA:HB3 | 40:OH:374:VAL:HG13 | 1.72 | 0.71 |
| 41:SO:385:PHE:HZ | 41:SO:408:PHE:HB3 | 1.56 | 0.71 |
| 40:UF:183:GLU:HB3 | 40:UF:184:PRO:HD3 | 1.72 | 0.71 |
| 40:UI:211:ASP:HA | 40:UI:214:ARG:HD3 | 1.72 | 0.71 |
| 7:1U:174:PHE:HB2 | 7:1U:185:TRP:HB2 | 1.72 | 0.70 |
| 35:5T:94:LEU:HB2 | 41:JL:356:ILE:HD12 | 1.73 | 0.70 |
| 40:AG:352:LYS:HD2 | 41:AO:179:VAL:N | 2.05 | 0.70 |
| 40:EH:76:ASP:HA | 40:EH:79:ARG:HE | 1.55 | 0.70 |
| 40:GG:102:ASN:HD22 | 40:GG:105:ARG:HD3 | 1.56 | 0.70 |
| 40:ND:335:ILE:HG23 | 40:ND:341:ILE:HD13 | 1.71 | 0.70 |
| 40:SF:228:ASN:HD21 | 42:SM:501:GTP:HN1 | 1.39 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:4W:330:ASP:HB3 | 26:4W:333:ILE:HG12 | 1.73 | 0.70 |
| 41:BM:210:ILE:HD11 | 41:BM:300:MET:HA | 1.72 | 0.70 |
| 40:EE:346:TRP:CZ3 | 41:EM:393:ALA:HB3 | 2.26 | 0.70 |
| 41:EP:11:GLN:HA | 41:EP:72:THR:HG21 | 1.73 | 0.70 |
| 40:MA:224:TYR:HB3 | 42:MN:501:GTP:N1 | 2.06 | 0.70 |
| 41:TM:331:LEU:HD23 | 41:TM:335:ASN:HD21 | 1.56 | 0.70 |
| 41:VO:66:VAL:HG22 | 41:VO:91:VAL:HB | 1.72 | 0.70 |
| 41:WB:341:PHE:HB3 | 41:WB:348:ASN:HD21 | 1.56 | 0.70 |
| 40:WG:228:ASN:HD21 | 42:WG:501:GTP:HN1 | 1.39 | 0.70 |
| 40:FG:124:LYS:NZ | 40:GG:297:GLU:OE2 | 2.22 | 0.70 |
| 41:GO:113:VAL:HA | 41:GO:116:VAL:HG12 | 1.74 | 0.70 |
| 40:WF:316:CYS:HA | 40:WF:352:LYS:HB2 | 1.73 | 0.70 |
| 41:WQ:107:THR:O | 41:WQ:110:ALA:N | 2.24 | 0.70 |
| 33:5N:220:VAL:HA | 33:5N:223:ILE:HG12 | 1.73 | 0.70 |
| 41:BN:272:PRO:HG3 | 41:BN:364:SER:HA | 1.72 | 0.70 |
| 41:LN:191:GLN:O | 41:LN:195:ASN:HB2 | 1.91 | 0.70 |
| 41:MO:248:ALA:HB3 | 41:MO:352:ALA:HB2 | 1.74 | 0.70 |
| 41:RB:23:VAL:HG13 | 41:RB:359:ARG:HH12 | 1.55 | 0.70 |
| 41:SL:253:LEU:O | 41:SL:257:MET:HB2 | 1.92 | 0.70 |
| 7:1T:350:THR:HG21 | 7:1T:611:ILE:HG12 | 1.72 | 0.70 |
| 23:4M:242:LEU:HA | 40:DG:84:ARG:HH22 | 1.56 | 0.70 |
| 41:EP:163:ILE:HD11 | 41:EP:251:ARG:HG2 | 1.73 | 0.70 |
| 40:LF:259:LEU:HD21 | 40:LF:377:LEU:HB2 | 1.74 | 0.70 |
| 40:ME:274:PRO:HG3 | 40:ME:286:LEU:HD12 | 1.73 | 0.70 |
| 40:OE:228:ASN:HD21 | 42:OL:501:GTP:HN1 | 1.38 | 0.70 |
| 40:OE:316:CYS:HA | 40:OE:352:LYS:HB2 | 1.74 | 0.70 |
| 40:PA:128:GLN:NE2 | 40:QA:290:GLU:OE1 | 2.25 | 0.70 |
| 41:PB:165:ASN:ND2 | 41:PB:198:GLU:OE1 | 2.25 | 0.70 |
| 40:PE:408:VAL:HA | 40:PE:412:MET:HB2 | 1.74 | 0.70 |
| 41:WM:210:ILE:HG12 | 41:WM:213:ARG:HH21 | 1.56 | 0.70 |
| 23:4M:29:LEU:HD13 | 23:4M:44:LEU:HD11 | 1.74 | 0.70 |
| 40:BI:101:ASN:HA | 40:BI:144:GLY:H | 1.56 | 0.70 |
| 40:FH:53:PHE:HB3 | 40:FH:61:HIS:HB3 | 1.73 | 0.70 |
| 41:NB:215:LEU:HB3 | 41:NB:217:LEU:HD23 | 1.74 | 0.70 |
| 40:VI:141:PHE:HB2 | 40:VI:173:PRO:HD3 | 1.72 | 0.70 |
| 15:3E:255:ARG:HH12 | 16:3J:237:VAL:HG21 | 1.55 | 0.70 |
| 23:4P:260:THR:CG2 | 40:EA:219:ILE:CD1 | 2.67 | 0.70 |
| 41:EL:127:CYS:SG | 41:EL:128:ASP:N | 2.64 | 0.70 |
| 40:GI:282:TYR:O | 40:GI:284:GLU:N | 2.24 | 0.70 |
| 40:HG:376:MET:SD | 40:HG:378:SER:OG | 2.49 | 0.70 |
| 40:HI:218:ASP:OD2 | 40:HI:280:LYS:NZ | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JN:10:GLY:O | 41:JN:14:ASN:HB2 | 1.92 | 0.70 |
| 41:LB:16:ILE:HA | 41:LB:226:ASN:HB3 | 1.72 | 0.70 |
| 41:NP:159:TYR:HB3 | 41:NP:162:ARG:HD3 | 1.73 | 0.70 |
| 40:PE:68:VAL:HG12 | 40:PE:93:ILE:HB | 1.72 | 0.70 |
| 40:SH:221:ARG:NH2 | 41:SO:325:GLU:HB2 | 2.05 | 0.70 |
| 41:SO:271:ALA:HB3 | 41:SO:272:PRO:HD3 | 1.73 | 0.70 |
| 40:UF:328:VAL:HG21 | 40:UF:355:ILE:HD11 | 1.73 | 0.70 |
| 40:DH:213:CYS:CB | 40:DH:222:PRO:HB3 | 2.22 | 0.70 |
| 41:DL:313:VAL:HA | 41:DL:369:GLY:HA2 | 1.73 | 0.70 |
| 41:EP:100:ASN:HB3 | 41:EP:103:LYS:HB2 | 1.73 | 0.70 |
| 41:JL:121:ARG:HH22 | 41:JL:158:GLU:HG3 | 1.56 | 0.70 |
| 40:LD:102:ASN:HB3 | 40:LD:105:ARG:HB2 | 1.73 | 0.70 |
| 40:MG:352:LYS:NZ | 41:MO:179:VAL:HG23 | 2.06 | 0.70 |
| 40:OG:71:GLU:HB3 | 40:OG:98:ASP:HB3 | 1.74 | 0.70 |
| 41:PM:191:GLN:O | 41:PM:195:ASN:CB | 2.40 | 0.70 |
| 41:QB:8:GLN:HG2 | 41:QB:65:LEU:HB3 | 1.73 | 0.70 |
| 40:RH:73:THR:HG22 | 41:RO:46:ARG:HE | 1.57 | 0.70 |
| 13:2U:48:GLU:HG2 | 13:2U:161:ARG:HG2 | 1.73 | 0.70 |
| 41:BM:248:ALA:HA | 41:BM:252:LYS:HD3 | 1.73 | 0.70 |
| 41:GO:309:ARG:H | 41:GO:372:THR:HG1 | 1.38 | 0.70 |
| 41:TL:318:ARG:HG2 | 41:TL:357:PRO:HA | 1.72 | 0.70 |
| 41:UO:271:ALA:HB1 | 41:UO:292:GLN:HG2 | 1.72 | 0.70 |
| 11:2K:247:HIS:CE1 | 11:2K:249:ILE:HB | 2.27 | 0.70 |
| 12:2P:154:LYS:HE2 | 41:AL:413:SER:HB2 | 1.72 | 0.70 |
| 17:3R:190:ALA:HB3 | 17:3R:191:PRO:HD3 | 1.74 | 0.70 |
| 18:3T:168:VAL:HG12 | 18:3U:51:TYR:HB2 | 1.73 | 0.70 |
| 22:4H:24:GLN:HE22 | 40:MD:50:ASN:HB2 | 1.57 | 0.70 |
| 40:DE:5:ILE:HD12 | 40:DE:125:LEU:HB3 | 1.74 | 0.70 |
| 40:EG:11:GLN:HG3 | 40:EG:74:VAL:HG21 | 1.73 | 0.70 |
| 41:EM:30:ILE:HG23 | 41:EM:34:GLY:HA2 | 1.73 | 0.70 |
| 41:GB:173:PRO:HB3 | 41:GB:380:ARG:HD3 | 1.74 | 0.70 |
| 41:HN:163:ILE:HG12 | 41:HN:251:ARG:HE | 1.55 | 0.70 |
| 41:IM:10:GLY:O | 41:IM:14:ASN:HB2 | 1.92 | 0.70 |
| 41:LN:318:ARG:HD2 | 41:LN:358:PRO:HD3 | 1.74 | 0.70 |
| 41:MP:135:LEU:HB3 | 41:MP:166:THR:HG22 | 1.73 | 0.70 |
| 41:OB:296:ALA:HA | 41:OB:299:MET:HG2 | 1.74 | 0.70 |
| 40:VF:228:ASN:HD21 | 42:VF:501:GTP:HN1 | 1.38 | 0.70 |
| 20:4A:149:ARG:NH2 | 20:4A:150:SER:HA | 2.06 | 0.69 |
| 23:4Q:29:LEU:HD13 | 23:4Q:44:LEU:HD11 | 1.74 | 0.69 |
| 34:5Q:212:LYS:HB3 | 41:GN:276:ARG:HG3 | 1.73 | 0.69 |
| 40:CH:384:ALA:HA | 40:CH:387:TRP:HD1 | 1.57 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CP:64:VAL:HG21 | 41:CP:120:VAL:HG22 | 1.74 | 0.69 |
| 41:DN:392:LYS:HA | 41:DN:395:LEU:HD21 | 1.73 | 0.69 |
| 40:MG:273:ALA:CB | 40:MG:274:PRO:HD2 | 2.22 | 0.69 |
| 40:PH:217:LEU:HD12 | 40:PH:277:SER:HB3 | 1.74 | 0.69 |
| 41:SO:313:VAL:HG22 | 41:SO:367:PHE:HE1 | 1.57 | 0.69 |
| 40:UE:207:GLU:HA | 40:UE:210:TYR:HD2 | 1.57 | 0.69 |
| 40:UH:329:ASN:HB2 | 41:UP:175:VAL:HG21 | 1.72 | 0.69 |
| 40:WH:213:CYS:HA | 40:WH:217:LEU:HB2 | 1.74 | 0.69 |
| 21:4F:411:LYS:NZ | 21:4F:412:MET:CG | 2.53 | 0.69 |
| 36:5W:26:ILE:HG13 | 36:5W:28:PRO:HD2 | 1.73 | 0.69 |
| 40:BE:391:ASP:HB3 | 40:BE:421:ARG:HH11 | 1.57 | 0.69 |
| 40:CA:241:SER:HB3 | 40:CA:249:ASN:HB3 | 1.72 | 0.69 |
| 40:HI:371:GLN:HG2 | 40:HI:372:ARG:HD2 | 1.73 | 0.69 |
| 40:IA:259:LEU:O | 40:IA:379:ASN:ND2 | 2.25 | 0.69 |
| 41:JB:7:LEU:O | 41:JB:135:LEU:HA | 1.92 | 0.69 |
| 41:KO:6:HIS:O | 41:KO:63:ALA:HA | 1.92 | 0.69 |
| 41:MB:252:LYS:HB2 | 40:MG:100:ALA:HA | 1.72 | 0.69 |
| 40:PE:88:HIS:HB3 | 40:PE:91:GLN:HB2 | 1.73 | 0.69 |
| 40:SH:319:TYR:HB3 | 40:SH:323:VAL:HG21 | 1.74 | 0.69 |
| 40:TF:220:GLU:HG2 | 40:TF:221:ARG:HD2 | 1.74 | 0.69 |
| 40:WA:181:VAL:HG12 | 41:WN:347:ASN:O | 1.92 | 0.69 |
| 13:2X:48:GLU:HG2 | 13:2X:161:ARG:HG2 | 1.73 | 0.69 |
| 23:4M:91:ILE:HD11 | 40:AG:79:ARG:HD3 | 1.72 | 0.69 |
| 40:DH:76:ASP:O | 40:DH:79:ARG:HG2 | 1.92 | 0.69 |
| 41:DM:86:ARG:HG3 | 41:DM:89:ASN:HB2 | 1.74 | 0.69 |
| 41:GN:61:PRO:HD3 | 41:GN:84:ILE:HG12 | 1.75 | 0.69 |
| 40:KE:88:HIS:HB3 | 40:KE:91:GLN:HG3 | 1.74 | 0.69 |
| 41:KO:156:ARG:NH1 | 41:KO:195:ASN:O | 2.25 | 0.69 |
| 40:PE:209:ILE:HG23 | 40:PE:227:LEU:HD22 | 1.74 | 0.69 |
| 41:PL:238:THR:HG22 | 41:PL:318:ARG:HH21 | 1.57 | 0.69 |
| 41:QP:186:THR:HG22 | 41:QP:381:ILE:HG23 | 1.74 | 0.69 |
| 40:VJ:228:ASN:HD21 | 42:VQ:501:GTP:HN1 | 1.40 | 0.69 |
| 41:VP:62:ARG:NH1 | 41:VP:127:CYS:SG | 2.65 | 0.69 |
| 8:1Y:101:ILE:HD12 | 11:2J:250:ILE:O | 1.92 | 0.69 |
| 9:2B:270:LEU:O | 9:2B:274:HIS:ND1 | 2.25 | 0.69 |
| 40:DA:400:LYS:HD3 | 41:DN:344:TRP:HB2 | 1.74 | 0.69 |
| 40:DF:259:LEU:HD11 | 40:DF:377:LEU:HB2 | 1.74 | 0.69 |
| 40:DI:228:ASN:HB3 | 42:DI:501:GTP:HN21 | 1.57 | 0.69 |
| 41:EP:313:VAL:HB | 41:EP:349:VAL:HG22 | 1.74 | 0.69 |
| 40:HE:88:HIS:NE2 | 40:IE:284:GLU:OE1 | 2.24 | 0.69 |
| 41:MB:347:ASN:HD22 | 40:MG:178:SER:HB3 | 1.56 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:TI:362:VAL:HB | 40:TI:369:LYS:HB3 | 1.75 | 0.69 |
| 40:UF:261:PRO:HA | 41:UN:394:PHE:CE1 | 2.27 | 0.69 |
| 40:BE:105:ARG:HG2 | 40:BE:410:GLU:HG3 | 1.73 | 0.69 |
| 41:BM:175:VAL:HG13 | 41:BM:205:GLU:HB3 | 1.74 | 0.69 |
| 40:II:177:VAL:O | 41:IP:347:ASN:ND2 | 2.25 | 0.69 |
| 41:IQ:290:THR:HA | 41:IQ:293:MET:HG3 | 1.74 | 0.69 |
| 40:JD:165:SER:HB2 | 40:JD:256:GLN:HE22 | 1.58 | 0.69 |
| 41:RB:248:ALA:HA | 41:RB:252:LYS:HD3 | 1.74 | 0.69 |
| 41:RL:341:PHE:HB3 | 41:RL:348:ASN:HD21 | 1.55 | 0.69 |
| 7:1U:569:VAL:HG23 | 7:1U:586:HIS:CE1 | 2.27 | 0.69 |
| 13:2U:61:CYS:HB3 | 13:2U:62:PRO:HD3 | 1.74 | 0.69 |
| 41:DO:222:TYR:O | 41:DO:226:ASN:ND2 | 2.26 | 0.69 |
| 41:FM:100:ASN:HB3 | 41:FM:103:LYS:HB2 | 1.73 | 0.69 |
| 40:GE:132:LEU:HB2 | 40:GE:164:LYS:HD3 | 1.75 | 0.69 |
| 40:GE:205:ASP:HB3 | 40:GE:303:VAL:HA | 1.73 | 0.69 |
| 41:GM:325:GLU:O | 41:GM:329:GLN:NE2 | 2.25 | 0.69 |
| 41:LO:54:ALA:HB3 | 41:LO:58:LYS:HB2 | 1.75 | 0.69 |
| 40:OD:213:CYS:HB3 | 40:OD:219:ILE:HB | 1.75 | 0.69 |
| 41:RM:100:ASN:HB3 | 41:RM:103:LYS:HB2 | 1.73 | 0.69 |
| 41:UB:252:LYS:HE3 | 41:UB:350:LYS:HZ1 | 1.55 | 0.69 |
| 41:VQ:324:LYS:O | 41:VQ:328:GLU:HB2 | 1.93 | 0.69 |
| 40:EF:259:LEU:O | 40:EF:379:ASN:ND2 | 2.26 | 0.69 |
| 40:GA:318:LEU:O | 40:GA:374:VAL:HA | 1.92 | 0.69 |
| 41:IN:7:LEU:HD22 | 41:IN:151:LEU:HD21 | 1.74 | 0.69 |
| 41:MB:173:PRO:HB3 | 41:MB:380:ARG:HD2 | 1.75 | 0.69 |
| 40:NH:180:ALA:HB3 | 40:NH:183:GLU:HG3 | 1.75 | 0.69 |
| 41:OP:178:THR:HB | 41:OP:181:GLU:HB2 | 1.75 | 0.69 |
| 40:PH:228:ASN:HD21 | 42:PO:501:GTP:HN1 | 1.39 | 0.69 |
| 40:QF:100:ALA:HA | 41:QM:252:LYS:HE2 | 1.75 | 0.69 |
| 41:QP:86:ARG:HG3 | 41:QP:89:ASN:H | 1.56 | 0.69 |
| 41:QP:170:VAL:HG22 | 41:QP:171:PRO:HD2 | 1.73 | 0.69 |
| 40:WF:316:CYS:HB3 | 40:WF:377:LEU:HB2 | 1.75 | 0.69 |
| 12:2N:212:ASP:HB2 | 13:2T:37:ILE:HD11 | 1.74 | 0.69 |
| 23:4R:100:GLN:HA | 23:4R:103:PHE:HE2 | 1.58 | 0.69 |
| 41:BL:317:PHE:HB2 | 41:BL:353:VAL:HG12 | 1.74 | 0.69 |
| 40:CA:273:ALA:HB3 | 40:CA:274:PRO:HD3 | 1.74 | 0.69 |
| 40:DE:213:CYS:SG | 40:DE:214:ARG:N | 2.65 | 0.69 |
| 40:DH:213:CYS:HB2 | 40:DH:222:PRO:HB3 | 1.75 | 0.69 |
| 40:DI:223:THR:HA | 41:DP:323:MET:SD | 2.33 | 0.69 |
| 41:EM:54:ALA:HB3 | 41:EM:58:LYS:HB3 | 1.74 | 0.69 |
| 40:FG:239:THR:O | 40:FG:243:ARG:NH1 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 42:GB:502:GTP:HN1 | 40:GG:228:ASN:HD21 | 1.41 | 0.69 |
| 41:HN:310:TYR:HA | 41:HN:371:SER:HA | 1.75 | 0.69 |
| 40:IA:177:VAL:HG11 | 41:IN:327:ASP:HB3 | 1.74 | 0.69 |
| 40:PD:203:MET:HG3 | 40:PD:303:VAL:HG21 | 1.73 | 0.69 |
| 40:PF:26:LEU:HD21 | 40:PF:363:VAL:HG12 | 1.75 | 0.69 |
| 41:PN:179:VAL:HG13 | 41:PN:180:VAL:HG13 | 1.75 | 0.69 |
| 41:PP:149:THR:HB | 41:PP:191:GLN:HG2 | 1.74 | 0.69 |
| 40:RI:6:SER:O | 40:RI:65:ALA:HA | 1.92 | 0.69 |
| 41:RO:272:PRO:HG3 | 41:RO:364:SER:HB2 | 1.74 | 0.69 |
| 41:TO:274:THR:HG23 | 41:TO:282:ARG:HH21 | 1.56 | 0.69 |
| 40:UH:58:ALA:HB3 | 40:UH:60:LYS:HE2 | 1.74 | 0.69 |
| 41:WM:70:PRO:HD3 | 41:WM:94:GLN:HA | 1.72 | 0.69 |
| 41:WN:248:ALA:HA | 41:WN:252:LYS:HE3 | 1.74 | 0.69 |
| 8:1W:346:MET:HB3 | 41:VP:276:ARG:HH22 | 1.58 | 0.69 |
| 13:2W:17:ILE:HD12 | 41:WN:125:GLU:HB3 | 1.74 | 0.69 |
| 40:CG:228:ASN:HD21 | 42:CG:501:GTP:HN1 | 1.41 | 0.69 |
| 40:DI:222:PRO:CD | 41:DP:324:LYS:HG3 | 2.20 | 0.69 |
| 41:FM:12:CYS:HG | 41:FM:138:SER:HG | 1.37 | 0.69 |
| 41:NO:28:HIS:HE2 | 41:NO:241:ARG:HD3 | 1.58 | 0.69 |
| 40:RI:271:THR:HG22 | 40:RI:301:GLN:HA | 1.74 | 0.69 |
| 40:TH:180:ALA:HB3 | 40:TH:183:GLU:HG3 | 1.75 | 0.69 |
| 41:UN:14:ASN:HD22 | 41:UN:72:THR:HG22 | 1.57 | 0.69 |
| 22:4J:652:VAL:HA | 22:4J:689:ASN:HA | 1.75 | 0.69 |
| 23:4R:86:LEU:HD22 | 23:4R:117:LEU:HD13 | 1.75 | 0.69 |
| 40:AF:280:LYS:HB3 | 40:MF:88:HIS:HE1 | 1.57 | 0.69 |
| 40:AF:298:PRO:HG2 | 40:AF:308:ARG:HE | 1.58 | 0.69 |
| 40:ND:88:HIS:CE1 | 40:ND:90:GLU:HB2 | 2.28 | 0.69 |
| 40:NF:207:GLU:HG3 | 40:NF:304:LYS:HG3 | 1.74 | 0.69 |
| 40:NF:274:PRO:HG2 | 40:NF:370:VAL:HG11 | 1.75 | 0.69 |
| 41:QL:375:GLN:HE21 | 41:QL:379:LYS:HB3 | 1.58 | 0.69 |
| 41:SL:86:ARG:HD2 | 41:TL:282:ARG:HH22 | 1.58 | 0.69 |
| 41:TB:179:VAL:HG23 | 41:TB:180:VAL:HG13 | 1.75 | 0.69 |
| 40:TF:16:ILE:HG13 | 40:TF:228:ASN:HD22 | 1.58 | 0.69 |
| 41:TP:372:THR:O | 41:TP:375:GLN:NE2 | 2.25 | 0.69 |
| 21:4D:473:VAL:HB | 21:4D:482:PRO:HB2 | 1.75 | 0.68 |
| 22:4K:619:VAL:HG21 | 22:4K:680:LYS:HG3 | 1.75 | 0.68 |
| 41:AO:178:THR:HB | 41:AO:181:GLU:HG3 | 1.75 | 0.68 |
| 41:DB:42:LEU:HD12 | 41:DB:43:GLN:HG2 | 1.74 | 0.68 |
| 41:DP:42:LEU:HD13 | 41:DP:356:ILE:HG12 | 1.76 | 0.68 |
| 40:EI:239:THR:HA | 40:EI:242:LEU:HG | 1.76 | 0.68 |
| 40:MD:276:ILE:HG13 | 40:MD:281:ALA:HB2 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PM:113:VAL:HG11 | 41:PM:150:LEU:HD22 | 1.75 | 0.68 |
| 41:QB:327:ASP:HB3 | 40:QG:177:VAL:HG21 | 1.74 | 0.68 |
| 40:RH:195:LEU:HD21 | 40:RH:264:ARG:HG3 | 1.75 | 0.68 |
| 40:SH:180:ALA:HB3 | 40:SH:183:GLU:HG3 | 1.75 | 0.68 |
| 41:WO:107:THR:O | 41:WO:110:ALA:N | 2.25 | 0.68 |
| 40:BE:298:PRO:HB3 | 40:BE:307:PRO:HD2 | 1.75 | 0.68 |
| 40:GG:217:LEU:HA | 40:GG:277:SER:HB2 | 1.75 | 0.68 |
| 41:LM:421:PRO:HA | 41:LM:424:THR:HG22 | 1.75 | 0.68 |
| 40:RG:228:ASN:HD21 | 42:RG:501:GTP:HN1 | 1.39 | 0.68 |
| 41:SO:404:ASP:HB2 | 41:SO:406:MET:HG2 | 1.75 | 0.68 |
| 40:TA:90:GLU:HB3 | 40:TA:121:ARG:HH12 | 1.57 | 0.68 |
| 40:TG:326:LYS:HZ1 | 41:TO:219:THR:HA | 1.56 | 0.68 |
| 17:3O:211:VAL:HG11 | 17:3R:99:TRP:HB2 | 1.75 | 0.68 |
| 21:4E:233:LYS:NZ | 40:BH:58:ALA:HB1 | 2.08 | 0.68 |
| 34:5Q:292:LEU:HD21 | 40:GE:279:GLU:N | 2.09 | 0.68 |
| 40:LD:207:GLU:HG3 | 40:LD:304:LYS:HD3 | 1.75 | 0.68 |
| 40:MF:273:ALA:HB3 | 40:MF:274:PRO:HD3 | 1.75 | 0.68 |
| 40:OD:122:ILE:HG21 | 40:OD:157:LEU:HD11 | 1.74 | 0.68 |
| 40:PA:178:SER:HB2 | 41:PN:347:ASN:HB2 | 1.75 | 0.68 |
| 41:PM:179:VAL:HG23 | 41:PM:180:VAL:HG13 | 1.75 | 0.68 |
| 40:QG:288:VAL:HA | 40:QG:291:ILE:HG12 | 1.73 | 0.68 |
| 40:TF:203:MET:HG3 | 40:TF:303:VAL:HG21 | 1.75 | 0.68 |
| 8:1X:127:GLN:HA | 8:1X:130:LYS:CE | 2.24 | 0.68 |
| 27:4Y:91:SER:O | 27:4Y:115:ALA:HA | 1.93 | 0.68 |
| 40:AA:280:LYS:HB3 | 40:MA:88:HIS:HE1 | 1.58 | 0.68 |
| 41:BO:170:VAL:HG11 | 41:BO:377:LEU:HD21 | 1.74 | 0.68 |
| 40:CE:167:LEU:HD22 | 40:CE:200:CYS:HB3 | 1.75 | 0.68 |
| 41:CN:141:GLY:HA3 | 43:CN:501:GDP:O1A | 1.93 | 0.68 |
| 40:DA:350:GLY:HA2 | 41:DB:179:VAL:HG22 | 1.74 | 0.68 |
| 40:JA:70:LEU:HD23 | 40:JA:114:LEU:HD12 | 1.75 | 0.68 |
| 41:NL:334:GLN:HE21 | 41:NL:349:VAL:HG23 | 1.58 | 0.68 |
| 40:QF:224:TYR:O | 40:QF:228:ASN:ND2 | 2.26 | 0.68 |
| 41:UP:198:GLU:HA | 41:UP:266:PHE:HE2 | 1.59 | 0.68 |
| 13:2T:54:VAL:HG13 | 13:2T:158:ALA:HB3 | 1.74 | 0.68 |
| 23:4Q:35:GLN:HB2 | 23:4Q:40:THR:HG23 | 1.75 | 0.68 |
| 36:5W:66:LEU:HD13 | 40:OF:221:ARG:HE | 1.59 | 0.68 |
| 40:CH:273:ALA:HB3 | 40:CH:274:PRO:HD3 | 1.76 | 0.68 |
| 41:EM:61:PRO:HG2 | 41:EM:84:ILE:HG23 | 1.75 | 0.68 |
| 41:EN:156:ARG:NH1 | 41:EN:195:ASN:O | 2.26 | 0.68 |
| 41:FB:170:VAL:HG11 | 41:FB:377:LEU:HD23 | 1.73 | 0.68 |
| 40:GI:200:CYS:H | 40:GI:266:HIS:HB2 | 1.58 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HG:204:VAL:HG13 | 40:HG:302:MET:HB3 | 1.76 | 0.68 |
| 41:QB:395:LEU:HA | 41:QB:398:TYR:HB2 | 1.76 | 0.68 |
| 41:QP:309:ARG:HB3 | 41:QP:342:VAL:HG22 | 1.75 | 0.68 |
| 18:3V:218:LYS:HE3 | 18:3V:257:TRP:HE1 | 1.59 | 0.68 |
| 41:BP:425:ARG:HH11 | 41:BP:425:ARG:HB3 | 1.59 | 0.68 |
| 40:DE:265:ILE:HD13 | 40:DE:431:TYR:HE1 | 1.59 | 0.68 |
| 41:DM:374:ILE:HG22 | 41:DM:422:VAL:HG21 | 1.76 | 0.68 |
| 41:DP:16:ILE:HG21 | 41:DP:136:THR:HG21 | 1.75 | 0.68 |
| 40:OH:174:ALA:HB3 | 40:OH:177:VAL:HG22 | 1.74 | 0.68 |
| 40:QG:272:TYR:O | 40:QG:300:ASN:ND2 | 2.27 | 0.68 |
| 41:QP:115:SER:O | 41:QP:118:ASP:HB3 | 1.94 | 0.68 |
| 41:QP:244:GLY:HA3 | 41:QP:354:CYS:HA | 1.76 | 0.68 |
| 40:SH:298:PRO:HB3 | 40:SH:307:PRO:HD2 | 1.76 | 0.68 |
| 41:SO:99:ASN:HA | 41:SO:142:GLY:H | 1.58 | 0.68 |
| 17:3P:267:ILE:HG23 | 17:3Q:402:GLU:HG3 | 1.74 | 0.68 |
| 22:4J:660:ARG:HH22 | 41:EM:37:HIS:C | 1.97 | 0.68 |
| 22:4J:660:ARG:HH22 | 41:EM:38:GLY:N | 1.92 | 0.68 |
| 26:4V:96:ALA:HB3 | 26:4V:161:MET:HB2 | 1.74 | 0.68 |
| 28:5B:115:LEU:HD11 | 32:5L:66:LEU:HD23 | 1.76 | 0.68 |
| 36:5X:102:ASN:OD1 | 41:OL:276:ARG:NH2 | 2.27 | 0.68 |
| 40:BI:188:ILE:HD12 | 40:BI:424:MET:HG3 | 1.76 | 0.68 |
| 40:GG:90:GLU:O | 40:GG:121:ARG:NH1 | 2.26 | 0.68 |
| 40:GI:240:ALA:HA | 40:GI:243:ARG:HD2 | 1.74 | 0.68 |
| 40:JD:7:VAL:HB | 40:JD:137:ILE:HG22 | 1.75 | 0.68 |
| 41:KB:6:HIS:O | 41:KB:63:ALA:HA | 1.93 | 0.68 |
| 40:KE:393:LYS:HB3 | 41:KL:346:PRO:HG3 | 1.74 | 0.68 |
| 41:OP:165:ASN:HA | 41:OP:198:GLU:O | 1.94 | 0.68 |
| 41:WB:49:VAL:HG11 | 41:WB:241:ARG:HG2 | 1.75 | 0.68 |
| 7:1T:46:THR:HG21 | 7:1T:59:PHE:HB3 | 1.75 | 0.68 |
| 22:4J:92:LYS:HE3 | 41:BN:280:GLN:HB2 | 1.75 | 0.68 |
| 23:4P:235:THR:OG1 | 23:4P:240:LEU:HA | 1.94 | 0.68 |
| 40:CE:237:SER:HG | 40:CE:375:CYS:HG | 1.41 | 0.68 |
| 40:GI:63:PRO:HD3 | 40:GI:86:LEU:HG | 1.76 | 0.68 |
| 40:HH:181:VAL:HG12 | 41:HO:256:ASN:HD22 | 1.59 | 0.68 |
| 40:II:362:VAL:HB | 40:II:369:LYS:HB3 | 1.75 | 0.68 |
| 41:LN:178:THR:HB | 41:LN:181:GLU:HG3 | 1.76 | 0.68 |
| 40:NE:254:GLU:HG2 | 41:NM:98:GLY:HA2 | 1.76 | 0.68 |
| 41:OL:4:ILE:HA | 41:OL:132:GLY:O | 1.94 | 0.68 |
| 41:OM:86:ARG:NH1 | 41:OM:123:GLU:OE2 | 2.27 | 0.68 |
| 41:VN:121:ARG:NH1 | 41:VN:158:GLU:OE2 | 2.27 | 0.68 |
| 16:3J:60:ASN:ND2 | 16:3K:341:GLU:OE1 | 2.24 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4N:235:THR:OG1 | 23:4N:240:LEU:HA | 1.94 | 0.68 |
| 38:6C:152:TYR:HB3 | 40:UH:90:GLU:HB3 | 1.75 | 0.68 |
| 41:DB:117:LEU:HD21 | 41:DB:154:LYS:HB3 | 1.76 | 0.68 |
| 40:DF:217:LEU:HD21 | 40:DF:367:LEU:HG | 1.74 | 0.68 |
| 41:DM:135:LEU:HD13 | 41:DM:152:ILE:HG12 | 1.75 | 0.68 |
| 41:QP:5:VAL:HG11 | 41:QP:123:GLU:HG3 | 1.75 | 0.68 |
| 40:VA:180:ALA:HB3 | 40:VA:183:GLU:HB2 | 1.76 | 0.68 |
| 40:VI:212:ILE:HD11 | 40:VI:300:ASN:HA | 1.76 | 0.68 |
| 7:1T:278:SER:HB3 | 7:1T:279:PRO:CD | 2.22 | 0.68 |
| 18:3U:388:LEU:HB3 | 18:3U:392:ARG:HH12 | 1.58 | 0.68 |
| 23:4M:108:ASN:HA | 40:BG:219:ILE:HD13 | 1.76 | 0.68 |
| 40:CI:218:ASP:OD2 | 40:CI:280:LYS:NZ | 2.27 | 0.68 |
| 40:IE:73:THR:HA | 40:IE:76:ASP:HB2 | 1.75 | 0.68 |
| 40:LF:104:ALA:HB1 | 40:LF:410:GLU:CG | 2.24 | 0.68 |
| 41:PB:207:LEU:HB3 | 41:PB:225:LEU:HD22 | 1.76 | 0.68 |
| 41:SP:40:SER:H | 41:SP:43:GLN:HE22 | 1.42 | 0.68 |
| 41:UB:99:ASN:HD22 | 41:UB:178:THR:HB | 1.59 | 0.68 |
| 26:4W:193:ARG:HG2 | 26:4W:203:ASN:HB2 | 1.74 | 0.67 |
| 40:DE:390:LEU:HD23 | 40:DE:393:LYS:HD2 | 1.74 | 0.67 |
| 41:DN:136:THR:HG22 | 41:DN:167:PHE:HB2 | 1.76 | 0.67 |
| 41:DP:189:VAL:HG11 | 41:DP:415:MET:HG3 | 1.76 | 0.67 |
| 40:EI:313:MET:HA | 40:EI:344:VAL:HG22 | 1.76 | 0.67 |
| 40:MF:222:PRO:HD2 | 41:MM:324:LYS:HD2 | 1.76 | 0.67 |
| 41:RB:253:LEU:O | 41:RB:257:MET:HB2 | 1.94 | 0.67 |
| 40:SF:98:ASP:O | 41:SM:251:ARG:NH2 | 2.27 | 0.67 |
| 40:UF:3:GLU:HA | 40:UF:51:THR:HA | 1.77 | 0.67 |
| 4:1H:69:LYS:HE3 | 40:HA:308:ARG:HH12 | 1.56 | 0.67 |
| 22:4H:269:ASN:OD1 | 41:DL:219:THR:N | 2.27 | 0.67 |
| 23:4Q:193:ARG:HA | 23:4Q:196:PHE:CZ | 2.29 | 0.67 |
| 27:4Z:32:LYS:HB3 | 27:4Z:38:LEU:HB3 | 1.76 | 0.67 |
| 34:5R:315:GLN:HA | 34:5R:318:LEU:HD12 | 1.76 | 0.67 |
| 38:6C:157:ILE:HG23 | 38:6C:158:THR:HG23 | 1.76 | 0.67 |
| 40:AG:280:LYS:HG3 | 40:MG:89:PRO:HG2 | 1.76 | 0.67 |
| 41:BP:47:ILE:HG23 | 41:BP:51:TYR:HB2 | 1.76 | 0.67 |
| 41:CM:248:ALA:HA | 41:CM:252:LYS:HE3 | 1.76 | 0.67 |
| 41:CN:271:ALA:HB3 | 41:CN:272:PRO:HD3 | 1.77 | 0.67 |
| 40:DI:269:LEU:HD21 | 40:DI:383:ILE:HB | 1.76 | 0.67 |
| 41:EB:178:THR:HB | 41:EB:181:GLU:HG3 | 1.77 | 0.67 |
| 40:MA:269:LEU:HD21 | 40:MA:380:THR:HG22 | 1.76 | 0.67 |
| 40:OF:254:GLU:O | 40:OF:258:ASN:CB | 2.42 | 0.67 |
| 40:OH:219:ILE:HG12 | 40:OH:222:PRO:HD3 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QG:211:ASP:OD1 | 40:QG:214:ARG:NH2 | 2.26 | 0.67 |
| 41:RM:192:LEU:HD21 | 41:RM:199:THR:HG21 | 1.77 | 0.67 |
| 41:SM:22:GLU:HG2 | 41:SM:81:PHE:HB2 | 1.76 | 0.67 |
| 41:VN:27:GLU:HG2 | 41:VN:359:ARG:HH12 | 1.59 | 0.67 |
| 7:1U:53:LYS:HG3 | 7:1U:54:THR:HG23 | 1.76 | 0.67 |
| 17:3O:402:GLU:HG3 | 17:3R:267:ILE:HG23 | 1.76 | 0.67 |
| 23:4R:110:ASN:HA | 23:4R:113:TRP:CE3 | 2.29 | 0.67 |
| 31:5J:769:PRO:HD2 | 31:5J:772:ARG:HG2 | 1.76 | 0.67 |
| 41:BB:100:ASN:HB3 | 41:BB:103:LYS:HB2 | 1.76 | 0.67 |
| 41:CL:7:LEU:HB3 | 41:CL:135:LEU:HD13 | 1.74 | 0.67 |
| 40:DI:269:LEU:HD23 | 40:DI:380:THR:HG23 | 1.75 | 0.67 |
| 41:EP:417:ASP:O | 41:EP:421:PRO:HD2 | 1.94 | 0.67 |
| 40:GI:221:ARG:HA | 41:GP:324:LYS:HZ3 | 1.57 | 0.67 |
| 40:IA:228:ASN:HD21 | 42:IA:501:GTP:HN1 | 1.40 | 0.67 |
| 40:MH:256:GLN:HB3 | 41:MP:397:TRP:CH2 | 2.30 | 0.67 |
| 40:QA:386:ALA:HA | 40:QA:389:ARG:HH21 | 1.59 | 0.67 |
| 41:UN:222:TYR:O | 41:UN:226:ASN:ND2 | 2.28 | 0.67 |
| 13:2V:39:ASP:HB3 | 13:2V:42:ILE:HG22 | 1.76 | 0.67 |
| 20:4B:293:ARG:HE | 40:MH:279:GLU:HA | 1.59 | 0.67 |
| 40:AF:177:VAL:HB | 41:AM:327:ASP:HB3 | 1.77 | 0.67 |
| 41:DN:11:GLN:HA | 41:DN:72:THR:HG21 | 1.76 | 0.67 |
| 40:GH:54:SER:HB3 | 40:GH:62:VAL:HG13 | 1.76 | 0.67 |
| 40:GH:273:ALA:HB3 | 40:GH:274:PRO:HD3 | 1.77 | 0.67 |
| 40:II:7:VAL:HB | 40:II:137:ILE:HG12 | 1.74 | 0.67 |
| 40:LF:326:LYS:HE3 | 41:LN:208:TYR:HB2 | 1.76 | 0.67 |
| 41:QP:137:HIS:HE1 | 41:QP:166:THR:HB | 1.59 | 0.67 |
| 41:SO:420:ASN:O | 41:SO:423:VAL:N | 2.25 | 0.67 |
| 22:4J:366:THR:HG23 | 22:4J:367:LYS:HD2 | 1.77 | 0.67 |
| 41:BP:42:LEU:HG | 41:BP:42:LEU:O | 1.95 | 0.67 |
| 41:CM:5:VAL:HG22 | 41:CM:62:ARG:HD2 | 1.75 | 0.67 |
| 40:DF:326:LYS:HE3 | 41:DN:220:PRO:HB2 | 1.76 | 0.67 |
| 40:FA:137:ILE:HB | 40:FA:168:GLU:HG2 | 1.75 | 0.67 |
| 40:FH:174:ALA:HB3 | 40:FH:178:SER:H | 1.57 | 0.67 |
| 40:GA:274:PRO:HG3 | 40:GA:286:LEU:HD12 | 1.77 | 0.67 |
| 40:GI:221:ARG:HA | 41:GP:324:LYS:NZ | 2.09 | 0.67 |
| 40:IH:177:VAL:HA | 41:IO:331:LEU:HD21 | 1.76 | 0.67 |
| 40:JH:220:GLU:O | 41:JO:324:LYS:NZ | 2.24 | 0.67 |
| 41:KL:257:MET:HG3 | 41:KL:314:ALA:HB2 | 1.76 | 0.67 |
| 40:LG:274:PRO:HB3 | 40:LG:370:VAL:HG11 | 1.76 | 0.67 |
| 40:ME:429:LYS:O | 40:ME:433:GLU:CB | 2.42 | 0.67 |
| 40:MG:188:ILE:HD13 | 40:MG:424:MET:HG3 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OP:319:GLY:HA2 | 41:OP:357:PRO:HG3 | 1.77 | 0.67 |
| 41:SO:309:ARG:HA | 41:SO:340:TYR:HA | 1.75 | 0.67 |
| 40:UI:88:HIS:HE1 | 40:VJ:280:LYS:HB2 | 1.58 | 0.67 |
| 40:VG:121:ARG:HE | 40:VG:124:LYS:HD2 | 1.59 | 0.67 |
| 41:WB:86:ARG:NH2 | 41:WB:123:GLU:OE2 | 2.28 | 0.67 |
| 15:3F:270:GLU:OE2 | 16:3L:73:ARG:NH1 | 2.25 | 0.67 |
| 41:DL:70:PRO:HD3 | 41:DL:94:GLN:HA | 1.76 | 0.67 |
| 40:EH:56:THR:HB | 40:EH:60:LYS:HB3 | 1.75 | 0.67 |
| 40:FH:273:ALA:HB2 | 40:FH:374:VAL:H | 1.57 | 0.67 |
| 40:GF:352:LYS:HZ2 | 41:GN:179:VAL:N | 1.92 | 0.67 |
| 41:JM:285:THR:H | 41:JM:288:GLU:HG2 | 1.60 | 0.67 |
| 41:LB:8:GLN:HE21 | 41:LB:65:LEU:HD22 | 1.59 | 0.67 |
| 40:ME:27:GLU:OE2 | 40:ME:243:ARG:NH1 | 2.26 | 0.67 |
| 40:MH:221:ARG:HG2 | 41:MO:325:GLU:HG3 | 1.76 | 0.67 |
| 40:NF:204:VAL:HG11 | 40:NF:231:ILE:HD11 | 1.75 | 0.67 |
| 40:OE:134:GLY:HA3 | 40:OE:165:SER:O | 1.95 | 0.67 |
| 41:PO:139:LEU:HD12 | 41:PO:170:VAL:HG12 | 1.77 | 0.67 |
| 40:RF:320:ARG:O | 40:RF:372:ARG:HA | 1.94 | 0.67 |
| 40:TG:53:PHE:HB3 | 40:TG:61:HIS:HB3 | 1.76 | 0.67 |
| 40:TH:213:CYS:HA | 40:TH:217:LEU:HD23 | 1.77 | 0.67 |
| 41:TL:317:PHE:HB2 | 41:TL:353:VAL:HG12 | 1.76 | 0.67 |
| 41:AM:421:PRO:HA | 41:AM:424:THR:HG22 | 1.77 | 0.67 |
| 40:BE:103:TYR:HB3 | 40:BE:407:TYR:HE2 | 1.59 | 0.67 |
| 41:DB:42:LEU:HD13 | 41:DB:356:ILE:HG12 | 1.76 | 0.67 |
| 41:FB:62:ARG:NH1 | 41:FB:127:CYS:SG | 2.68 | 0.67 |
| 40:GF:278:ALA:H | 40:GF:368:ALA:HB2 | 1.60 | 0.67 |
| 40:GI:225:THR:HA | 40:GI:228:ASN:HD21 | 1.59 | 0.67 |
| 40:HA:318:LEU:HB2 | 40:HA:375:CYS:HB3 | 1.76 | 0.67 |
| 41:IM:421:PRO:HA | 41:IM:424:THR:HG22 | 1.77 | 0.67 |
| 40:ND:105:ARG:HG2 | 40:ND:110:ILE:HG13 | 1.77 | 0.67 |
| 41:OP:134:GLN:NE2 | 41:OP:233:MET:SD | 2.67 | 0.67 |
| 40:PD:26:LEU:HD11 | 40:PD:363:VAL:HG22 | 1.77 | 0.67 |
| 40:RF:76:ASP:OD2 | 41:RM:46:ARG:NH2 | 2.27 | 0.67 |
| 16:3L:26:THR:OG1 | 16:3L:30:ARG:NH1 | 2.28 | 0.67 |
| 18:3U:394:LYS:NZ | 18:3V:80:GLU:OE2 | 2.25 | 0.67 |
| 22:4J:91:ASP:N | 41:BN:281:TYR:H | 1.93 | 0.67 |
| 23:4N:249:TYR:CE1 | 41:DM:53:GLU:HG2 | 2.29 | 0.67 |
| 41:BL:293:MET:HE1 | 41:BL:365:ALA:HB3 | 1.75 | 0.67 |
| 41:CM:394:PHE:HB3 | 41:CM:397:TRP:HZ3 | 1.60 | 0.67 |
| 41:CO:61:PRO:HD3 | 41:CO:84:ILE:HG12 | 1.75 | 0.67 |
| 41:CP:66:VAL:HG12 | 41:CP:91:VAL:HB | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DF:269:LEU:HD11 | 40:DF:383:ILE:HB | 1.75 | 0.67 |
| 41:DP:193:VAL:HA | 41:DP:264:HIS:HE1 | 1.59 | 0.67 |
| 40:EG:101:ASN:HB3 | 40:EG:182:VAL:HG11 | 1.76 | 0.67 |
| 40:EI:188:ILE:HG23 | 40:EI:424:MET:HG2 | 1.76 | 0.67 |
| 40:FF:104:ALA:O | 40:FF:108:TYR:HB2 | 1.94 | 0.67 |
| 41:GP:242:PHE:HB3 | 41:GP:356:ILE:HD13 | 1.76 | 0.67 |
| 41:IB:1:MET:SD | 41:IB:48:ASN:ND2 | 2.68 | 0.67 |
| 40:LG:275:VAL:HA | 40:LG:367:LEU:HD21 | 1.76 | 0.67 |
| 41:LM:100:ASN:HB3 | 41:LM:103:LYS:HB2 | 1.77 | 0.67 |
| 40:PA:129:CYS:SG | 40:PA:130:THR:N | 2.68 | 0.67 |
| 40:PG:75:ILE:HG23 | 40:PG:92:LEU:HD12 | 1.77 | 0.67 |
| 41:QB:232:THR:HG21 | 41:QB:268:PRO:HB2 | 1.77 | 0.67 |
| 41:QB:271:ALA:H | 41:QB:272:PRO:HD2 | 1.59 | 0.67 |
| 40:RF:73:THR:HG22 | 41:RM:46:ARG:HE | 1.60 | 0.67 |
| 41:SB:242:PHE:HB3 | 41:SB:356:ILE:HD13 | 1.76 | 0.67 |
| 40:TH:206:ASN:ND2 | 42:TH:501:GTP:O2' | 2.28 | 0.67 |
| 40:UF:254:GLU:HG2 | 41:UN:98:GLY:HA2 | 1.75 | 0.67 |
| 41:WB:248:ALA:HA | 41:WB:252:LYS:HE3 | 1.77 | 0.67 |
| 16:3K:154:LYS:HB3 | 16:3K:243:ILE:HG12 | 1.77 | 0.67 |
| 41:AL:45:GLU:HG2 | 41:AL:46:ARG:HG2 | 1.77 | 0.67 |
| 41:BO:46:ARG:HB2 | 41:BO:241:ARG:HA | 1.75 | 0.67 |
| 41:CB:46:ARG:HH21 | 40:CG:72:PRO:HB2 | 1.59 | 0.67 |
| 41:DM:207:LEU:HB3 | 41:DM:225:LEU:HD22 | 1.76 | 0.67 |
| 40:EI:109:THR:OG1 | 40:EI:110:ILE:N | 2.27 | 0.67 |
| 41:IO:252:LYS:HA | 41:IO:255:VAL:HG12 | 1.76 | 0.67 |
| 41:OL:325:GLU:HA | 41:OL:328:GLU:HG2 | 1.76 | 0.67 |
| 41:PM:191:GLN:O | 41:PM:195:ASN:HB2 | 1.95 | 0.67 |
| 40:UA:332:ILE:HD12 | 40:UA:351:PHE:HB3 | 1.76 | 0.67 |
| 40:UI:184:PRO:HA | 40:UI:390:LEU:HD11 | 1.77 | 0.67 |
| 41:VO:396:HIS:HA | 41:VO:399:THR:HG22 | 1.77 | 0.67 |
| 40:WA:221:ARG:NH1 | 41:WN:325:GLU:HB2 | 2.10 | 0.67 |
| 13:2X:61:CYS:HB3 | 13:2X:69:LEU:HD22 | 1.77 | 0.67 |
| 17:3O:124:THR:HG23 | 17:3P:382:ILE:HD11 | 1.76 | 0.67 |
| 38:6C:68:ARG:HH22 | 40:UA:116:ASP:HA | 1.59 | 0.67 |
| 41:CB:350:LYS:HZ3 | 40:CG:180:ALA:HA | 1.59 | 0.67 |
| 41:DB:12:CYS:HB2 | 43:DB:501:GDP:C8 | 2.30 | 0.67 |
| 40:EE:228:ASN:HD21 | 42:EL:501:GTP:HN1 | 1.43 | 0.67 |
| 41:FM:179:VAL:HG23 | 41:FM:180:VAL:HG13 | 1.76 | 0.67 |
| 41:FN:222:TYR:O | 41:FN:226:ASN:HB2 | 1.93 | 0.67 |
| 41:IB:317:PHE:HB2 | 41:IB:353:VAL:HG12 | 1.76 | 0.67 |
| 41:IP:407:GLU:HA | 41:IP:410:GLU:HB2 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JH:100:ALA:HA | 41:JO:252:LYS:HE2 | 1.77 | 0.67 |
| 41:NO:341:PHE:HB3 | 41:NO:348:ASN:HD21 | 1.60 | 0.67 |
| 41:PB:46:ARG:NH1 | 40:PG:73:THR:OG1 | 2.27 | 0.67 |
| 40:SF:371:GLN:HG2 | 40:SF:372:ARG:HD2 | 1.75 | 0.67 |
| 40:SF:406:TRP:HZ3 | 41:SM:255:VAL:HA | 1.59 | 0.67 |
| 40:TG:121:ARG:HH11 | 40:TG:124:LYS:HE2 | 1.60 | 0.67 |
| 41:VN:107:THR:O | 41:VN:110:ALA:N | 2.28 | 0.67 |
| 40:WI:212:ILE:HD11 | 40:WI:300:ASN:HA | 1.76 | 0.67 |
| 4:1I:76:ILE:HG23 | 40:HI:342:GLN:HB2 | 1.75 | 0.66 |
| 7:1T:326:LEU:HD21 | 7:1T:329:THR:HB | 1.75 | 0.66 |
| 21:4D:222:LYS:HA | 40:BA:43:GLY:HA2 | 1.77 | 0.66 |
| 40:BH:104:ALA:HA | 40:BH:108:TYR:HD2 | 1.60 | 0.66 |
| 41:BP:268:PRO:HG2 | 41:BP:300:MET:HB2 | 1.75 | 0.66 |
| 41:CB:132:GLY:HA3 | 41:CB:163:ILE:O | 1.94 | 0.66 |
| 40:CI:180:ALA:HB1 | 41:CP:256:ASN:HD21 | 1.59 | 0.66 |
| 41:CL:192:LEU:HD12 | 41:CL:196:THR:HB | 1.77 | 0.66 |
| 40:FI:56:THR:HA | 40:GI:285:GLN:HB3 | 1.76 | 0.66 |
| 41:IQ:19:LYS:HE3 | 41:IQ:223:GLY:HA2 | 1.76 | 0.66 |
| 40:JE:133:GLN:HE21 | 40:JE:252:LEU:HB2 | 1.60 | 0.66 |
| 40:NE:271:THR:HG22 | 40:NE:301:GLN:HA | 1.77 | 0.66 |
| 41:OO:282:ARG:HE | 41:OO:283:ALA:H | 1.40 | 0.66 |
| 41:PM:2:ARG:HH12 | 41:PM:46:ARG:HE | 1.41 | 0.66 |
| 41:RM:191:GLN:NE2 | 41:RM:195:ASN:OD1 | 2.29 | 0.66 |
| 40:WI:228:ASN:HD21 | 42:WI:501:GTP:HN1 | 1.43 | 0.66 |
| 20:4A:149:ARG:NH1 | 20:4A:150:SER:HB3 | 2.07 | 0.66 |
| 23:4M:192:PRO:HG3 | 41:CB:44:LEU:HD21 | 1.77 | 0.66 |
| 23:4R:110:ASN:ND2 | 40:BI:279:GLU:HB3 | 2.10 | 0.66 |
| 37:6A:42:LEU:HD11 | 37:6A:70:LEU:HG | 1.75 | 0.66 |
| 38:6C:89:GLU:HB2 | 41:VB:307:HIS:HE1 | 1.61 | 0.66 |
| 40:CI:123:ARG:NH2 | 40:CI:160:ASP:OD2 | 2.27 | 0.66 |
| 41:CL:290:THR:HA | 41:CL:293:MET:HG2 | 1.75 | 0.66 |
| 41:CM:139:LEU:HD21 | 41:CM:192:LEU:HD11 | 1.78 | 0.66 |
| 41:CN:271:ALA:HB1 | 41:CN:289:LEU:HD13 | 1.77 | 0.66 |
| 41:DP:104:GLY:HA2 | 41:DP:109:GLY:CA | 2.25 | 0.66 |
| 40:FG:326:LYS:NZ | 41:FO:208:TYR:O | 2.28 | 0.66 |
| 40:GI:175:PRO:HA | 40:GI:389:ARG:HD3 | 1.77 | 0.66 |
| 40:HI:224:TYR:HA | 40:HI:227:LEU:HB2 | 1.76 | 0.66 |
| 40:IA:258:ASN:HD22 | 40:IA:352:LYS:HD2 | 1.60 | 0.66 |
| 41:MN:100:ASN:HB3 | 41:MN:103:LYS:HB2 | 1.78 | 0.66 |
| 4:1H:160:ASP:OD2 | 41:HO:306:ARG:NH1 | 2.28 | 0.66 |
| 22:4I:658:ILE:HG13 | 22:4I:688:ILE:HD12 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:5J:777:ALA:HB3 | 31:5J:812:ARG:HH22 | 1.58 | 0.66 |
| 41:DM:248:ALA:HB1 | 41:DM:252:LYS:HG2 | 1.77 | 0.66 |
| 40:EH:286:LEU:HD13 | 40:EH:370:VAL:HG23 | 1.76 | 0.66 |
| 41:FM:323:MET:HB2 | 41:FM:326:VAL:HG22 | 1.77 | 0.66 |
| 40:HE:326:LYS:HG2 | 41:HM:220:PRO:HG2 | 1.75 | 0.66 |
| 40:HF:70:LEU:HD12 | 40:HF:99:ALA:HB2 | 1.76 | 0.66 |
| 41:JN:316:VAL:HG12 | 41:JN:352:ALA:HB3 | 1.76 | 0.66 |
| 41:MB:324:LYS:HB3 | 40:MG:222:PRO:HD2 | 1.76 | 0.66 |
| 40:OF:316:CYS:HA | 40:OF:352:LYS:HB2 | 1.76 | 0.66 |
| 40:OH:12:ALA:HB3 | 40:OH:140:SER:HB2 | 1.77 | 0.66 |
| 41:ON:100:ASN:HB3 | 41:ON:103:LYS:HB3 | 1.77 | 0.66 |
| 40:QA:73:THR:OG1 | 41:QN:46:ARG:NH1 | 2.27 | 0.66 |
| 41:QN:120:VAL:HG11 | 41:QN:155:ILE:HD13 | 1.75 | 0.66 |
| 41:QP:152:ILE:HG22 | 41:QP:156:ARG:HH12 | 1.58 | 0.66 |
| 40:SA:75:ILE:HG23 | 40:SA:92:LEU:HD12 | 1.77 | 0.66 |
| 41:SO:374:ILE:HG22 | 41:SO:422:VAL:HG21 | 1.77 | 0.66 |
| 42:VB:502:GTP:HN1 | 40:VH:228:ASN:HD21 | 1.44 | 0.66 |
| 41:WP:318:ARG:HE | 41:WP:358:PRO:HD3 | 1.59 | 0.66 |
| 4:1H:79:SER:OG | 40:HA:342:GLN:NE2 | 2.27 | 0.66 |
| 11:2K:108:THR:O | 11:2K:112:ASN:ND2 | 2.27 | 0.66 |
| 12:2M:78:ARG:CZ | 13:2T:72:LYS:HB2 | 2.25 | 0.66 |
| 16:3L:258:ARG:HD3 | 16:3L:397:LEU:HD22 | 1.77 | 0.66 |
| 40:BA:180:ALA:O | 41:BN:347:ASN:ND2 | 2.28 | 0.66 |
| 41:BB:341:PHE:HB3 | 41:BB:348:ASN:HD21 | 1.59 | 0.66 |
| 41:CP:274:THR:HB | 41:CP:282:ARG:HD2 | 1.77 | 0.66 |
| 40:DH:188:ILE:HD11 | 40:DH:390:LEU:HB3 | 1.78 | 0.66 |
| 41:FB:314:ALA:HB3 | 41:FB:368:ILE:HB | 1.76 | 0.66 |
| 40:IH:177:VAL:O | 41:IO:347:ASN:ND2 | 2.29 | 0.66 |
| 40:LG:439:VAL:O | 40:LG:440:GLU:C | 2.33 | 0.66 |
| 40:OG:53:PHE:HB3 | 40:OG:61:HIS:HB3 | 1.78 | 0.66 |
| 41:OO:171:PRO:O | 41:OO:380:ARG:NH2 | 2.27 | 0.66 |
| 41:RB:313:VAL:O | 41:RB:349:VAL:HA | 1.94 | 0.66 |
| 41:RP:62:ARG:NH2 | 41:RP:127:CYS:SG | 2.69 | 0.66 |
| 40:SE:98:ASP:O | 40:SE:105:ARG:NH1 | 2.28 | 0.66 |
| 41:SL:237:THR:HG22 | 41:SL:250:LEU:HD21 | 1.76 | 0.66 |
| 40:TF:26:LEU:HD21 | 40:TF:363:VAL:HG22 | 1.77 | 0.66 |
| 41:TN:113:VAL:HG11 | 41:TN:150:LEU:HD22 | 1.78 | 0.66 |
| 40:UH:177:VAL:HG23 | 41:UO:331:LEU:HB2 | 1.77 | 0.66 |
| 40:VF:73:THR:HA | 40:VF:76:ASP:HB2 | 1.76 | 0.66 |
| 7:1U:602:ILE:HB | 7:1U:614:TRP:HB2 | 1.78 | 0.66 |
| 16:3L:132:PRO:HD3 | 16:3M:14:LEU:HD21 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:4A:168:LEU:HG | 40:ME:279:GLU:HG2 | 1.77 | 0.66 |
| 41:CN:104:GLY:CA | 41:CN:109:GLY:HA3 | 2.21 | 0.66 |
| 40:DA:137:ILE:HG12 | 40:DA:168:GLU:HG2 | 1.78 | 0.66 |
| 40:DG:76:ASP:HA | 40:DG:79:ARG:HD2 | 1.76 | 0.66 |
| 41:DP:74:ASP:HA | 41:DP:77:ARG:HH11 | 1.58 | 0.66 |
| 41:EM:378:PHE:HA | 41:EM:381:ILE:HG12 | 1.76 | 0.66 |
| 41:EO:341:PHE:HB3 | 41:EO:348:ASN:HD21 | 1.60 | 0.66 |
| 40:JH:34:GLY:HA3 | 40:JH:60:LYS:HD2 | 1.78 | 0.66 |
| 40:LE:177:VAL:O | 41:LL:347:ASN:ND2 | 2.29 | 0.66 |
| 40:MA:181:VAL:HG13 | 41:MN:348:ASN:HA | 1.78 | 0.66 |
| 40:OA:79:ARG:HB3 | 40:OA:92:LEU:HD11 | 1.78 | 0.66 |
| 40:OA:97:GLU:OE2 | 41:ON:251:ARG:NH1 | 2.29 | 0.66 |
| 40:OD:213:CYS:HA | 40:OD:217:LEU:HB2 | 1.77 | 0.66 |
| 41:OP:354:CYS:SG | 41:OP:355:ASP:N | 2.69 | 0.66 |
| 41:QB:325:GLU:HG2 | 40:QG:221:ARG:HH11 | 1.60 | 0.66 |
| 40:UF:17:GLY:HA2 | 40:UF:20:CYS:HB2 | 1.77 | 0.66 |
| 40:WH:68:VAL:HG22 | 40:WH:93:ILE:HB | 1.78 | 0.66 |
| 9:2B:204:GLU:HG3 | 9:2B:208:ARG:HH22 | 1.60 | 0.66 |
| 15:3E:67:LEU:HB3 | 15:3E:71:ARG:HH12 | 1.59 | 0.66 |
| 17:3Q:470:GLN:HA | 17:3Q:474:MET:HB2 | 1.77 | 0.66 |
| 17:3R:236:HIS:HD2 | 17:3R:325:ILE:HG13 | 1.60 | 0.66 |
| 22:4K:677:LEU:HA | 22:4K:680:LYS:HB2 | 1.77 | 0.66 |
| 23:4N:260:THR:CG2 | 40:EF:219:ILE:CD1 | 2.69 | 0.66 |
| 40:AA:180:ALA:HB3 | 40:AA:183:GLU:HG3 | 1.78 | 0.66 |
| 41:BM:245:GLN:O | 41:BM:246:LEU:C | 2.34 | 0.66 |
| 40:CH:87:PHE:HB3 | 40:CH:92:LEU:HD11 | 1.78 | 0.66 |
| 40:DH:9:VAL:HG13 | 40:DH:68:VAL:HG13 | 1.78 | 0.66 |
| 41:DM:417:ASP:O | 41:DM:420:ASN:N | 2.28 | 0.66 |
| 40:FA:30:ILE:HG22 | 40:FA:34:GLY:HA2 | 1.78 | 0.66 |
| 40:MD:274:PRO:HG3 | 40:MD:286:LEU:HD22 | 1.77 | 0.66 |
| 41:NB:189:VAL:HA | 41:NB:192:LEU:HB2 | 1.78 | 0.66 |
| 40:NF:72:PRO:HB2 | 41:NM:46:ARG:HH22 | 1.59 | 0.66 |
| 41:NM:103:LYS:HG2 | 41:NM:107:THR:HG21 | 1.78 | 0.66 |
| 40:OH:177:VAL:HG13 | 40:OH:207:GLU:HG2 | 1.78 | 0.66 |
| 41:PP:204:ASN:ND2 | 43:PP:501:GDP:O2' | 2.28 | 0.66 |
| 40:QF:288:VAL:HG11 | 40:QF:327:ASP:HB3 | 1.76 | 0.66 |
| 40:SH:219:ILE:HG22 | 40:SH:221:ARG:H | 1.60 | 0.66 |
| 41:TO:49:VAL:HG11 | 41:TO:241:ARG:HG2 | 1.75 | 0.66 |
| 40:WA:413:GLU:HG3 | 40:WA:415:GLY:H | 1.60 | 0.66 |
| 9:2B:202:LYS:HA | 9:2B:205:LYS:HE2 | 1.77 | 0.66 |
| 12:2R:120:THR:HG22 | 12:2R:122:PRO:HD2 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 38:6C:141:LEU:HD22 | 41:VP:294:PHE:HB3 | 1.77 | 0.66 |
| 41:CN:202:ILE:HG23 | 41:CN:268:PRO:HG3 | 1.77 | 0.66 |
| 41:DB:20:PHE:HA | 41:DB:230:SER:HB2 | 1.78 | 0.66 |
| 40:EE:213:CYS:HA | 40:EE:217:LEU:HB2 | 1.78 | 0.66 |
| 41:EM:313:VAL:HB | 41:EM:349:VAL:HG13 | 1.76 | 0.66 |
| 41:EP:20:PHE:HA | 41:EP:230:SER:HB3 | 1.78 | 0.66 |
| 40:FG:319:TYR:HB3 | 40:FG:323:VAL:HG21 | 1.78 | 0.66 |
| 40:GA:102:ASN:HD21 | 40:GA:410:GLU:HG2 | 1.59 | 0.66 |
| 40:HF:239:THR:O | 40:HF:243:ARG:NH1 | 2.28 | 0.66 |
| 41:IQ:174:LYS:HG2 | 41:IQ:205:GLU:HB3 | 1.77 | 0.66 |
| 41:IQ:178:THR:HB | 41:IQ:181:GLU:HG3 | 1.78 | 0.66 |
| 40:KE:397:MET:HG3 | 40:KE:402:ALA:HB3 | 1.78 | 0.66 |
| 40:LF:326:LYS:HE2 | 41:LN:225:LEU:HD11 | 1.78 | 0.66 |
| 40:LG:136:LEU:HB3 | 40:LG:169:PHE:HE1 | 1.61 | 0.66 |
| 40:ND:102:ASN:HB3 | 40:ND:105:ARG:HB2 | 1.77 | 0.66 |
| 41:NL:316:VAL:HG12 | 41:NL:352:ALA:HB3 | 1.78 | 0.66 |
| 40:PH:102:ASN:HB3 | 40:PH:105:ARG:HB3 | 1.78 | 0.66 |
| 41:PO:136:THR:HG22 | 41:PO:167:PHE:HB2 | 1.77 | 0.66 |
| 41:TL:292:GLN:O | 41:TL:298:ASN:ND2 | 2.29 | 0.66 |
| 40:WE:228:ASN:HD21 | 42:WE:501:GTP:HN1 | 1.42 | 0.66 |
| 22:4J:91:ASP:HB3 | 41:BN:281:TYR:HB2 | 1.78 | 0.66 |
| 23:4N:33:MET:CG | 41:CM:320:ARG:HH22 | 2.08 | 0.66 |
| 25:4T:274:LEU:HA | 41:IN:1:MET:HG2 | 1.78 | 0.66 |
| 41:BN:237:THR:HG22 | 41:BN:250:LEU:HD21 | 1.77 | 0.66 |
| 40:CA:63:PRO:HD3 | 40:CA:86:LEU:HG | 1.77 | 0.66 |
| 40:DA:165:SER:HB3 | 40:DA:256:GLN:HE22 | 1.60 | 0.66 |
| 40:FA:263:PRO:HB3 | 41:FB:396:HIS:CD2 | 2.30 | 0.66 |
| 41:FB:248:ALA:HA | 41:FB:252:LYS:HD2 | 1.78 | 0.66 |
| 40:GE:137:ILE:HB | 40:GE:168:GLU:HG2 | 1.77 | 0.66 |
| 40:GF:271:THR:HG22 | 40:GF:301:GLN:HA | 1.77 | 0.66 |
| 40:GG:326:LYS:NZ | 41:GO:204:ASN:O | 2.29 | 0.66 |
| 41:GP:316:VAL:HG12 | 41:GP:352:ALA:HB3 | 1.78 | 0.66 |
| 40:KE:101:ASN:HD22 | 40:KE:143:GLY:HA2 | 1.60 | 0.66 |
| 40:LE:236:SER:O | 40:LE:243:ARG:NH2 | 2.29 | 0.66 |
| 40:PD:252:LEU:HA | 40:PD:255:PHE:HD2 | 1.60 | 0.66 |
| 41:RN:334:GLN:HA | 41:RN:341:PHE:HE2 | 1.61 | 0.66 |
| 41:TO:8:GLN:NE2 | 41:TO:14:ASN:O | 2.29 | 0.66 |
| 41:TP:61:PRO:HD3 | 41:TP:84:ILE:HG22 | 1.76 | 0.66 |
| 41:UP:12:CYS:HB3 | 41:UP:138:SER:HB3 | 1.76 | 0.66 |
| 40:VJ:174:ALA:HB3 | 40:VJ:178:SER:H | 1.60 | 0.66 |
| 40:WG:206:ASN:ND2 | 42:WG:501:GTP:O2' | 2.29 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WM:263:LEU:HG | 41:WM:425:ARG:HH22 | 1.61 | 0.66 |
| 9:2C:438:MET:SD | 9:2C:442:LYS:NZ | 2.69 | 0.66 |
| 10:2F:39:GLN:NE2 | 41:MB:389:PHE:O | 2.26 | 0.66 |
| 11:2K:87:PRO:HD3 | 40:LH:264:ARG:HD3 | 1.78 | 0.66 |
| 22:4I:553:LYS:HA | 22:4I:556:GLU:HB2 | 1.78 | 0.66 |
| 40:BF:98:ASP:O | 40:BF:105:ARG:NH1 | 2.29 | 0.66 |
| 40:BI:285:GLN:HG3 | 40:BI:287:SER:HB3 | 1.77 | 0.66 |
| 41:CB:421:PRO:HA | 41:CB:424:THR:HG22 | 1.78 | 0.66 |
| 40:CH:20:CYS:HA | 40:CH:232:SER:HB2 | 1.77 | 0.66 |
| 41:HB:235:GLY:HA3 | 41:HB:366:THR:HG21 | 1.77 | 0.66 |
| 41:HP:260:PHE:HE2 | 41:HP:425:ARG:HE | 1.44 | 0.66 |
| 40:LD:228:ASN:HD21 | 42:LD:501:GTP:HN1 | 1.44 | 0.66 |
| 40:MF:99:ALA:HA | 40:MF:110:ILE:HD11 | 1.77 | 0.66 |
| 41:NP:179:VAL:HG23 | 41:NP:180:VAL:HG13 | 1.76 | 0.66 |
| 40:OA:26:LEU:HD21 | 40:OA:363:VAL:HG12 | 1.78 | 0.66 |
| 41:OB:273:LEU:O | 41:OB:292:GLN:NE2 | 2.29 | 0.66 |
| 40:PD:133:GLN:NE2 | 40:PD:251:ASP:OD1 | 2.27 | 0.66 |
| 40:QA:260:VAL:HB | 41:QB:397:TRP:HZ2 | 1.61 | 0.66 |
| 40:RG:277:SER:H | 40:RG:280:LYS:HB3 | 1.61 | 0.66 |
| 41:RN:163:ILE:HD13 | 41:RN:251:ARG:HG2 | 1.77 | 0.66 |
| 40:TI:370:VAL:HG12 | 40:TI:372:ARG:H | 1.61 | 0.66 |
| 40:WA:221:ARG:NH1 | 41:WN:322:SER:HB2 | 2.10 | 0.66 |
| 12:2M:47:MET:HG3 | 41:AB:336:LYS:HG3 | 1.77 | 0.66 |
| 15:3G:275:ARG:NH1 | 15:3G:276:ASP:OD1 | 2.29 | 0.66 |
| 22:4J:275:MET:HG3 | 41:CN:77:ARG:HD2 | 1.78 | 0.66 |
| 34:5Q:164:LEU:CD2 | 34:5R:487:ILE:HD11 | 2.25 | 0.66 |
| 40:BG:258:ASN:HD21 | 40:BG:352:LYS:HE3 | 1.59 | 0.66 |
| 41:CM:20:PHE:HA | 41:CM:230:SER:HB3 | 1.78 | 0.66 |
| 40:EA:240:ALA:HB1 | 40:EA:356:ASN:HD22 | 1.60 | 0.66 |
| 40:EH:247:ALA:O | 40:EH:248:LEU:C | 2.34 | 0.66 |
| 40:FI:210:TYR:HE1 | 41:FP:324:LYS:HA | 1.61 | 0.66 |
| 41:GN:385:PHE:HZ | 41:GN:408:PHE:HB3 | 1.61 | 0.66 |
| 40:IH:66:VAL:HA | 40:IH:91:GLN:HE21 | 1.61 | 0.66 |
| 41:MM:174:LYS:HD2 | 41:MM:175:VAL:HG13 | 1.78 | 0.66 |
| 41:OL:385:PHE:O | 41:OL:389:PHE:HB2 | 1.96 | 0.66 |
| 41:RP:292:GLN:O | 41:RP:298:ASN:ND2 | 2.29 | 0.66 |
| 41:TP:178:THR:HB | 41:TP:181:GLU:HB2 | 1.78 | 0.66 |
| 7:1T:109:LEU:HD21 | 40:VF:42:ILE:HA | 1.77 | 0.65 |
| 9:2B:344:ASP:HA | 9:2B:347:ILE:HG12 | 1.78 | 0.65 |
| 17:3O:213:ASP:HA | 17:3R:96:PRO:HG3 | 1.78 | 0.65 |
| 39:6J:138:GLY:HA2 | 39:6J:141:SER:HB2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BH:386:ALA:HA | 40:BH:389:ARG:HD2 | 1.78 | 0.65 |
| 40:CE:286:LEU:HD21 | 40:CE:370:VAL:HG13 | 1.78 | 0.65 |
| 40:DH:28:HIS:HE1 | 40:DH:243:ARG:HD2 | 1.61 | 0.65 |
| 41:FB:392:LYS:NZ | 41:FB:405:GLU:OE2 | 2.29 | 0.65 |
| 40:IH:180:ALA:HB3 | 40:IH:183:GLU:HB2 | 1.77 | 0.65 |
| 41:IO:191:GLN:O | 41:IO:195:ASN:ND2 | 2.29 | 0.65 |
| 41:JN:252:LYS:HA | 41:JN:255:VAL:HG12 | 1.78 | 0.65 |
| 40:ME:115:ILE:HG12 | 40:ME:152:LEU:HD22 | 1.78 | 0.65 |
| 41:QM:165:ASN:ND2 | 41:QM:200:TYR:OH | 2.29 | 0.65 |
| 41:TN:19:LYS:NZ | 41:TN:223:GLY:O | 2.29 | 0.65 |
| 40:UA:98:ASP:O | 40:UA:105:ARG:NH1 | 2.29 | 0.65 |
| 40:UH:371:GLN:HG3 | 40:UH:372:ARG:HD2 | 1.78 | 0.65 |
| 40:UI:394:PHE:HZ | 40:UI:417:PHE:HB3 | 1.61 | 0.65 |
| 41:WM:311:LEU:HD22 | 41:WM:342:VAL:HG21 | 1.76 | 0.65 |
| 23:4Q:259:ARG:CZ | 40:EH:365:GLY:HA3 | 2.26 | 0.65 |
| 40:AA:177:VAL:O | 41:AN:347:ASN:ND2 | 2.30 | 0.65 |
| 41:BB:70:PRO:HG3 | 41:BB:94:GLN:HG3 | 1.78 | 0.65 |
| 40:CF:260:VAL:HB | 41:CN:397:TRP:HH2 | 1.61 | 0.65 |
| 41:EL:165:ASN:HD21 | 41:EL:250:LEU:HD11 | 1.59 | 0.65 |
| 41:EM:87:PRO:HD3 | 41:FM:281:TYR:CD2 | 2.31 | 0.65 |
| 41:EM:178:THR:O | 41:EM:181:GLU:N | 2.29 | 0.65 |
| 40:FE:228:ASN:HD21 | 42:FE:501:GTP:HN1 | 1.42 | 0.65 |
| 41:GP:317:PHE:HB2 | 41:GP:353:VAL:HG12 | 1.78 | 0.65 |
| 41:HP:292:GLN:O | 41:HP:298:ASN:ND2 | 2.29 | 0.65 |
| 41:JM:165:ASN:HB3 | 41:JM:200:TYR:HE2 | 1.61 | 0.65 |
| 41:NB:163:ILE:HD11 | 41:NB:250:LEU:HB3 | 1.78 | 0.65 |
| 40:NG:333:ALA:HB2 | 41:NO:174:LYS:HZ1 | 1.61 | 0.65 |
| 41:PN:49:VAL:HG21 | 41:PN:241:ARG:HG2 | 1.78 | 0.65 |
| 41:RB:324:LYS:HG2 | 40:RG:222:PRO:HD2 | 1.77 | 0.65 |
| 41:RM:62:ARG:NH1 | 41:RM:127:CYS:SG | 2.69 | 0.65 |
| 41:SB:127:CYS:SG | 41:SB:128:ASP:N | 2.70 | 0.65 |
| 40:SE:16:ILE:O | 40:SE:20:CYS:HB2 | 1.96 | 0.65 |
| 41:SL:328:GLU:OE1 | 41:SL:332:ASN:ND2 | 2.29 | 0.65 |
| 41:TM:125:GLU:OE1 | 41:UM:336:LYS:NZ | 2.26 | 0.65 |
| 7:1U:508:VAL:HG23 | 7:1U:519:THR:HG22 | 1.79 | 0.65 |
| 11:2J:113:VAL:HG11 | 40:LF:404:VAL:HG13 | 1.78 | 0.65 |
| 41:DB:271:ALA:HB2 | 41:DB:293:MET:HG3 | 1.78 | 0.65 |
| 40:DE:228:ASN:HB3 | 42:DE:501:GTP:N2 | 2.07 | 0.65 |
| 40:DF:223:THR:HA | 41:DM:323:MET:HG2 | 1.78 | 0.65 |
| 40:EG:217:LEU:HD21 | 40:EG:367:LEU:HD23 | 1.78 | 0.65 |
| 40:IE:213:CYS:HA | 40:IE:217:LEU:HB2 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IH:101:ASN:HB2 | 41:IO:252:LYS:HD2 | 1.79 | 0.65 |
| 40:JA:11:GLN:NE2 | 41:JN:247:ASN:OD1 | 2.28 | 0.65 |
| 41:JB:253:LEU:O | 41:JB:257:MET:HB2 | 1.96 | 0.65 |
| 41:QN:50:TYR:HE1 | 41:QN:241:ARG:HD3 | 1.61 | 0.65 |
| 41:RL:58:LYS:NZ | 41:SL:280:GLN:OE1 | 2.30 | 0.65 |
| 40:SA:51:THR:HG21 | 40:SA:243:ARG:HB3 | 1.77 | 0.65 |
| 41:UB:285:THR:HG23 | 41:UB:287:PRO:HD2 | 1.78 | 0.65 |
| 40:UH:53:PHE:HB3 | 40:UH:61:HIS:HB3 | 1.77 | 0.65 |
| 40:UH:207:GLU:OE1 | 40:UH:304:LYS:NZ | 2.30 | 0.65 |
| 40:WF:326:LYS:HG3 | 41:WN:220:PRO:HB2 | 1.78 | 0.65 |
| 23:4N:19:ILE:H | 23:4N:19:ILE:HD12 | 1.58 | 0.65 |
| 35:5T:163:TYR:HE2 | 40:KE:81:GLY:HA3 | 1.62 | 0.65 |
| 40:CA:10:GLY:HA2 | 40:CA:145:THR:HG22 | 1.78 | 0.65 |
| 41:DB:131:GLN:HG3 | 41:DB:163:ILE:HD12 | 1.78 | 0.65 |
| 41:EP:272:PRO:HG3 | 41:EP:364:SER:HB2 | 1.78 | 0.65 |
| 41:FM:62:ARG:NH2 | 41:FM:123:GLU:O | 2.30 | 0.65 |
| 40:HE:88:HIS:CD2 | 40:IE:283:HIS:HB2 | 2.32 | 0.65 |
| 40:LG:31:GLN:HG2 | 40:LG:37:PRO:HD3 | 1.78 | 0.65 |
| 40:NE:188:ILE:HD12 | 40:NE:424:MET:HG3 | 1.78 | 0.65 |
| 40:PE:76:ASP:HA | 40:PE:79:ARG:HG2 | 1.78 | 0.65 |
| 41:PL:7:LEU:O | 41:PL:135:LEU:HA | 1.96 | 0.65 |
| 41:QB:256:ASN:CG | 41:QB:350:LYS:HZ2 | 2.00 | 0.65 |
| 41:QL:200:TYR:HB3 | 41:QL:268:PRO:HD3 | 1.77 | 0.65 |
| 41:QM:232:THR:HG22 | 41:QM:270:PHE:HB2 | 1.78 | 0.65 |
| 40:SE:57:GLY:O | 40:SE:60:LYS:NZ | 2.30 | 0.65 |
| 40:UI:119:LEU:HA | 40:UI:122:ILE:HD13 | 1.78 | 0.65 |
| 40:VA:154:MET:HG3 | 40:VA:194:THR:HG22 | 1.77 | 0.65 |
| 41:VB:253:LEU:O | 41:VB:257:MET:HB2 | 1.97 | 0.65 |
| 7:1S:554:THR:HG23 | 7:1S:557:GLY:H | 1.60 | 0.65 |
| 9:2C:443:PHE:O | 9:2C:447:GLN:NE2 | 2.29 | 0.65 |
| 18:3U:394:LYS:HE3 | 18:3V:77:GLN:HE21 | 1.61 | 0.65 |
| 21:4E:409:VAL:HG21 | 40:DH:57:GLY:HA3 | 1.79 | 0.65 |
| 27:4Z:107:LEU:HD23 | 27:4Z:110:PRO:HG2 | 1.79 | 0.65 |
| 40:CA:20:CYS:HA | 40:CA:232:SER:HB2 | 1.79 | 0.65 |
| 41:DM:186:THR:HG21 | 41:DM:385:PHE:HB2 | 1.78 | 0.65 |
| 41:FB:156:ARG:NH1 | 41:FB:195:ASN:O | 2.29 | 0.65 |
| 41:FO:4:ILE:HB | 41:FO:50:TYR:HE2 | 1.61 | 0.65 |
| 41:GM:7:LEU:O | 41:GM:135:LEU:HA | 1.97 | 0.65 |
| 40:HE:394:PHE:HA | 40:HE:397:MET:HE2 | 1.79 | 0.65 |
| 40:HH:228:ASN:HD21 | 42:HH:501:GTP:HN1 | 1.43 | 0.65 |
| 41:MP:86:ARG:HG3 | 41:MP:88:ASP:H | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:NL:317:PHE:HB2 | 41:NL:353:VAL:HG22 | 1.76 | 0.65 |
| 40:RE:98:ASP:O | 41:RL:251:ARG:NH2 | 2.29 | 0.65 |
| 41:RL:63:ALA:O | 41:RL:89:ASN:ND2 | 2.29 | 0.65 |
| 41:TO:54:ALA:HB3 | 41:TO:58:LYS:HB3 | 1.78 | 0.65 |
| 8:1Y:101:ILE:HD12 | 11:2J:250:ILE:CA | 2.27 | 0.65 |
| 17:3R:160:ILE:HG22 | 17:3R:258:LEU:HD22 | 1.78 | 0.65 |
| 22:4I:85:LEU:HD13 | 22:4I:102:TYR:HE2 | 1.60 | 0.65 |
| 23:4P:238:HIS:O | 23:4P:240:LEU:HG | 1.97 | 0.65 |
| 23:4R:107:LYS:HZ1 | 23:4R:115:GLU:HB2 | 1.60 | 0.65 |
| 23:4R:113:TRP:HA | 23:4R:116:ALA:HB3 | 1.79 | 0.65 |
| 31:5J:782:ARG:HG3 | 31:5J:784:SER:H | 1.61 | 0.65 |
| 41:AB:317:PHE:HB2 | 41:AB:353:VAL:HG12 | 1.79 | 0.65 |
| 40:AG:134:GLY:HA2 | 40:AG:164:LYS:HG3 | 1.79 | 0.65 |
| 40:BH:88:HIS:CE1 | 40:BH:90:GLU:HB2 | 2.31 | 0.65 |
| 41:CL:269:GLY:HA3 | 41:CL:367:PHE:HB3 | 1.77 | 0.65 |
| 41:DL:286:VAL:HB | 41:DL:287:PRO:HD3 | 1.79 | 0.65 |
| 41:GN:311:LEU:HD23 | 41:GN:344:TRP:HZ2 | 1.61 | 0.65 |
| 40:IG:175:PRO:HB2 | 40:IG:389:ARG:HH22 | 1.62 | 0.65 |
| 41:JL:99:ASN:HD21 | 41:JL:178:THR:HG23 | 1.61 | 0.65 |
| 41:KB:286:VAL:HG23 | 41:KB:287:PRO:HD3 | 1.76 | 0.65 |
| 40:OE:2:ARG:HB3 | 40:OE:133:GLN:HE22 | 1.62 | 0.65 |
| 41:OP:5:VAL:HG23 | 41:OP:62:ARG:HD3 | 1.78 | 0.65 |
| 40:PF:254:GLU:OE1 | 41:PN:99:ASN:ND2 | 2.26 | 0.65 |
| 41:PP:412:GLU:O | 41:PP:416:ASN:ND2 | 2.29 | 0.65 |
| 40:QE:65:ALA:O | 40:QE:91:GLN:NE2 | 2.29 | 0.65 |
| 40:QF:406:TRP:HH2 | 41:QM:258:VAL:HB | 1.61 | 0.65 |
| 41:QP:66:VAL:HG13 | 41:QP:91:VAL:CG2 | 2.26 | 0.65 |
| 40:UF:222:PRO:HD2 | 41:UM:324:LYS:CB | 2.25 | 0.65 |
| 40:UG:319:TYR:HB2 | 40:UG:355:ILE:HG22 | 1.77 | 0.65 |
| 40:UI:25:CYS:O | 40:UI:26:LEU:C | 2.35 | 0.65 |
| 41:VP:267:MET:HB2 | 41:VP:374:ILE:HD11 | 1.78 | 0.65 |
| 7:1T:530:GLU:HB2 | 7:1T:537:ILE:HD11 | 1.79 | 0.65 |
| 7:1U:49:ILE:HB | 7:1U:58:ASN:HB2 | 1.77 | 0.65 |
| 12:2M:120:THR:HG22 | 12:2M:122:PRO:HD2 | 1.79 | 0.65 |
| 15:3F:105:LEU:HD21 | 15:3F:146:VAL:HG23 | 1.79 | 0.65 |
| 21:4D:474:LYS:H | 21:4D:483:ILE:HG23 | 1.61 | 0.65 |
| 21:4E:485:TYR:CZ | 21:4E:496:ILE:HA | 2.32 | 0.65 |
| 23:4N:238:HIS:O | 23:4N:240:LEU:HG | 1.97 | 0.65 |
| 23:4N:263:HIS:HA | 23:4N:266:HIS:CE1 | 2.32 | 0.65 |
| 23:4P:263:HIS:HA | 23:4P:266:HIS:CE1 | 2.32 | 0.65 |
| 25:4T:310:THR:HG22 | 41:JM:279:GLN:HG2 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AA:174:ALA:HB3 | 40:AA:178:SER:H | 1.62 | 0.65 |
| 40:AG:326:LYS:HD3 | 41:AO:220:PRO:HD2 | 1.78 | 0.65 |
| 40:DA:100:ALA:HA | 41:DN:252:LYS:HZ1 | 1.60 | 0.65 |
| 40:EF:228:ASN:HD21 | 42:EF:501:GTP:HN1 | 1.42 | 0.65 |
| 40:GA:224:TYR:HE1 | 42:GA:501:GTP:H2' | 1.62 | 0.65 |
| 40:GF:191:THR:HA | 40:GF:194:THR:HG22 | 1.78 | 0.65 |
| 40:GH:325:PRO:HB2 | 41:GP:222:TYR:HE2 | 1.60 | 0.65 |
| 40:HG:298:PRO:HB3 | 40:HG:307:PRO:HD2 | 1.79 | 0.65 |
| 40:II:274:PRO:HD2 | 40:II:291:ILE:HG22 | 1.79 | 0.65 |
| 41:JN:222:TYR:O | 41:JN:226:ASN:ND2 | 2.30 | 0.65 |
| 41:KB:253:LEU:O | 41:KB:257:MET:HB2 | 1.97 | 0.65 |
| 41:LO:318:ARG:HG2 | 41:LO:357:PRO:HA | 1.78 | 0.65 |
| 40:MF:244:PHE:HB2 | 40:MF:356:ASN:HD21 | 1.62 | 0.65 |
| 40:PA:332:ILE:HA | 40:PA:335:ILE:HG22 | 1.79 | 0.65 |
| 41:PL:40:SER:HB2 | 41:PL:43:GLN:HG3 | 1.78 | 0.65 |
| 41:PN:73:MET:HA | 41:PN:76:VAL:HG12 | 1.78 | 0.65 |
| 41:QB:259:PRO:HA | 40:QG:403:PHE:CE1 | 2.31 | 0.65 |
| 40:QE:75:ILE:HG23 | 40:QE:92:LEU:HD12 | 1.79 | 0.65 |
| 41:QN:24:ILE:HA | 41:QN:27:GLU:HG2 | 1.77 | 0.65 |
| 40:SG:286:LEU:HB2 | 40:SG:372:ARG:HH21 | 1.62 | 0.65 |
| 40:SI:285:GLN:O | 40:SI:372:ARG:NH2 | 2.30 | 0.65 |
| 40:TA:101:ASN:OD1 | 41:TN:252:LYS:NZ | 2.30 | 0.65 |
| 40:UA:215:ARG:HH12 | 40:UA:299:ALA:HB1 | 1.61 | 0.65 |
| 40:UH:90:GLU:OE2 | 40:UH:124:LYS:NZ | 2.24 | 0.65 |
| 41:WB:207:LEU:HB3 | 41:WB:225:LEU:HD22 | 1.78 | 0.65 |
| 12:2M:119:MET:SD | 12:2M:161:ASN:ND2 | 2.70 | 0.65 |
| 20:4A:167:GLN:HE22 | 40:ME:369:LYS:HG2 | 1.62 | 0.65 |
| 23:4Q:243:LEU:HD13 | 40:DH:79:ARG:HG3 | 1.77 | 0.65 |
| 26:4W:84:ALA:O | 26:4W:88:GLY:HA3 | 1.97 | 0.65 |
| 40:CH:235:VAL:HA | 40:CH:238:ILE:HG22 | 1.79 | 0.65 |
| 40:EG:326:LYS:NZ | 41:EO:204:ASN:O | 2.29 | 0.65 |
| 40:EH:71:GLU:HG2 | 40:EH:74:VAL:HG12 | 1.77 | 0.65 |
| 40:EI:363:VAL:O | 40:EI:365:GLY:N | 2.30 | 0.65 |
| 40:GF:314:ALA:HB1 | 41:GN:179:VAL:HG11 | 1.77 | 0.65 |
| 40:GH:3:GLU:HG3 | 40:GH:129:CYS:HB3 | 1.79 | 0.65 |
| 40:GH:51:THR:HG21 | 40:GH:243:ARG:HB3 | 1.79 | 0.65 |
| 40:GH:406:TRP:HE1 | 41:GO:258:VAL:HB | 1.60 | 0.65 |
| 41:IB:274:THR:HG22 | 41:IB:282:ARG:HE | 1.61 | 0.65 |
| 40:IG:212:ILE:HD11 | 40:IG:275:VAL:HG21 | 1.78 | 0.65 |
| 40:MF:259:LEU:HD21 | 40:MF:377:LEU:HB2 | 1.78 | 0.65 |
| 40:NE:286:LEU:HD13 | 40:NE:370:VAL:HG13 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OO:6:HIS:O | 41:OO:63:ALA:HA | 1.96 | 0.65 |
| 41:RO:166:THR:O | 41:RO:199:THR:HA | 1.97 | 0.65 |
| 40:SI:180:ALA:HB3 | 40:SI:183:GLU:HG3 | 1.79 | 0.65 |
| 40:TG:75:ILE:HG22 | 40:TG:79:ARG:HD2 | 1.79 | 0.65 |
| 41:TL:100:ASN:HB3 | 41:TL:103:LYS:HB2 | 1.79 | 0.65 |
| 40:UF:258:ASN:O | 41:UN:179:VAL:HG21 | 1.97 | 0.65 |
| 40:UG:298:PRO:HB3 | 40:UG:307:PRO:HD2 | 1.79 | 0.65 |
| 40:WF:212:ILE:HD11 | 40:WF:300:ASN:HA | 1.78 | 0.65 |
| 8:1X:140:VAL:HG12 | 8:1X:141:THR:N | 2.12 | 0.65 |
| 13:2X:178:PRO:HG2 | 13:2X:181:PHE:HB2 | 1.79 | 0.65 |
| 24:4O:243:LEU:HD12 | 40:DE:84:ARG:HG3 | 1.77 | 0.65 |
| 23:4R:196:PHE:HE1 | 41:DP:283:ALA:HB1 | 1.60 | 0.65 |
| 26:4W:65:LYS:NZ | 26:4W:72:GLN:OE1 | 2.30 | 0.65 |
| 40:BF:298:PRO:HB3 | 40:BF:307:PRO:HD2 | 1.78 | 0.65 |
| 40:DI:338:LYS:HB3 | 40:DI:341:ILE:HG13 | 1.77 | 0.65 |
| 41:DO:242:PHE:HB3 | 41:DO:356:ILE:HD13 | 1.79 | 0.65 |
| 41:EM:270:PHE:HB3 | 41:EM:273:LEU:HD21 | 1.79 | 0.65 |
| 41:HB:237:THR:HG22 | 41:HB:250:LEU:HD21 | 1.79 | 0.65 |
| 41:KO:248:ALA:HA | 41:KO:252:LYS:HD3 | 1.79 | 0.65 |
| 41:KO:295:ASP:OD2 | 41:KO:297:LYS:NZ | 2.29 | 0.65 |
| 40:OA:210:TYR:HD1 | 41:ON:324:LYS:HZ3 | 1.45 | 0.65 |
| 41:OP:286:VAL:HG21 | 41:OP:325:GLU:HG3 | 1.79 | 0.65 |
| 41:PN:309:ARG:H | 41:PN:372:THR:HG1 | 1.44 | 0.65 |
| 40:RI:222:PRO:HD2 | 41:RP:324:LYS:HB2 | 1.78 | 0.65 |
| 41:SB:21:TRP:HA | 41:SB:24:ILE:HG12 | 1.78 | 0.65 |
| 40:SE:318:LEU:O | 40:SE:374:VAL:HA | 1.96 | 0.65 |
| 40:SI:274:PRO:HG3 | 40:SI:286:LEU:HD13 | 1.79 | 0.65 |
| 41:SO:12:CYS:HB2 | 43:SO:501:GDP:O4' | 1.97 | 0.65 |
| 41:SO:270:PHE:HB3 | 41:SO:273:LEU:HD21 | 1.78 | 0.65 |
| 40:UI:88:HIS:HA | 40:VJ:283:HIS:ND1 | 2.12 | 0.65 |
| 40:UI:224:TYR:HA | 40:UI:227:LEU:HD12 | 1.79 | 0.65 |
| 8:1W:349:GLU:OE2 | 41:VP:276:ARG:NH1 | 2.30 | 0.65 |
| 16:3J:177:ARG:NH1 | 18:3T:139:GLU:OE2 | 2.29 | 0.65 |
| 34:5R:463:GLU:HA | 34:5R:466:LYS:HD2 | 1.79 | 0.65 |
| 38:6C:48:PRO:HB3 | 41:VO:333:VAL:CG2 | 2.27 | 0.65 |
| 39:6I:128:SER:HA | 40:OA:84:ARG:HH22 | 1.61 | 0.65 |
| 40:CH:433:GLU:HA | 40:CH:436:MET:HG2 | 1.79 | 0.65 |
| 40:DH:250:VAL:HG23 | 40:DH:254:GLU:HB2 | 1.78 | 0.65 |
| 40:DI:139:HIS:CD2 | 40:DI:139:HIS:H | 2.13 | 0.65 |
| 40:EH:205:ASP:H | 40:EH:303:VAL:HG22 | 1.61 | 0.65 |
| 40:FA:406:TRP:HE1 | 41:FN:258:VAL:HG23 | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GB:252:LYS:NZ | 40:GG:101:ASN:OD1 | 2.29 | 0.65 |
| 40:GE:204:VAL:HG21 | 40:GE:302:MET:HE1 | 1.77 | 0.65 |
| 40:GH:70:LEU:HD12 | 40:GH:99:ALA:HB2 | 1.79 | 0.65 |
| 40:IG:9:VAL:HG23 | 40:IG:139:HIS:HB3 | 1.78 | 0.65 |
| 40:IG:260:VAL:HG13 | 41:IO:397:TRP:HH2 | 1.62 | 0.65 |
| 41:JO:412:GLU:O | 41:JO:416:ASN:ND2 | 2.30 | 0.65 |
| 40:ME:228:ASN:HB3 | 40:ME:231:ILE:HD12 | 1.79 | 0.65 |
| 41:NO:178:THR:HB | 41:NO:181:GLU:HG3 | 1.79 | 0.65 |
| 41:PL:136:THR:HA | 41:PL:167:PHE:O | 1.96 | 0.65 |
| 41:QB:390:ARG:HG3 | 41:QB:391:ARG:HG2 | 1.78 | 0.65 |
| 41:QN:242:PHE:HB3 | 41:QN:356:ILE:HD13 | 1.79 | 0.65 |
| 40:SA:222:PRO:O | 41:SN:324:LYS:NZ | 2.30 | 0.65 |
| 40:TG:174:ALA:HB3 | 40:TG:178:SER:H | 1.61 | 0.65 |
| 41:UO:253:LEU:O | 41:UO:257:MET:HB2 | 1.97 | 0.65 |
| 41:VP:293:MET:HG2 | 41:VP:367:PHE:HB2 | 1.79 | 0.65 |
| 41:WB:347:ASN:ND2 | 40:WG:177:VAL:O | 2.30 | 0.65 |
| 7:1T:337:ASP:HA | 7:1T:592:ARG:HG3 | 1.79 | 0.64 |
| 8:1X:100:LEU:HD11 | 11:2I:251:TYR:H | 1.62 | 0.64 |
| 22:4I:626:GLN:HA | 22:4I:629:LYS:HD2 | 1.78 | 0.64 |
| 40:BG:109:THR:HG23 | 40:BG:110:ILE:HG12 | 1.79 | 0.64 |
| 40:CI:75:ILE:HG23 | 40:CI:92:LEU:HD12 | 1.79 | 0.64 |
| 40:DI:175:PRO:HG2 | 40:DI:176:GLN:HE21 | 1.61 | 0.64 |
| 40:EF:274:PRO:HD2 | 40:EF:291:ILE:HG13 | 1.80 | 0.64 |
| 40:FA:219:ILE:HB | 40:FA:222:PRO:CD | 2.27 | 0.64 |
| 40:GA:141:PHE:HB2 | 40:GA:173:PRO:HD3 | 1.79 | 0.64 |
| 41:GO:248:ALA:HA | 41:GO:252:LYS:HG2 | 1.78 | 0.64 |
| 40:HE:273:ALA:HB2 | 40:HE:374:VAL:HG12 | 1.77 | 0.64 |
| 40:HH:188:ILE:HD12 | 40:HH:424:MET:HG3 | 1.77 | 0.64 |
| 41:JB:406:MET:HG2 | 41:NB:306:ARG:HB3 | 1.79 | 0.64 |
| 40:MF:228:ASN:HB3 | 42:MM:501:GTP:N2 | 2.12 | 0.64 |
| 41:MN:386:THR:O | 41:MN:390:ARG:HB2 | 1.97 | 0.64 |
| 40:NA:93:ILE:HD13 | 40:NA:118:VAL:HG12 | 1.78 | 0.64 |
| 40:OF:177:VAL:HG11 | 41:OM:327:ASP:HB3 | 1.77 | 0.64 |
| 40:OH:129:CYS:SG | 40:OH:132:LEU:HB3 | 2.37 | 0.64 |
| 41:OP:253:LEU:O | 41:OP:257:MET:HB3 | 1.96 | 0.64 |
| 41:PB:42:LEU:HD11 | 41:PB:243:PRO:HG2 | 1.78 | 0.64 |
| 40:PE:55:GLU:O | 40:QE:285:GLN:NE2 | 2.29 | 0.64 |
| 41:QM:139:LEU:HD12 | 41:QM:170:VAL:HG12 | 1.79 | 0.64 |
| 40:RE:236:SER:O | 40:RE:240:ALA:HB2 | 1.97 | 0.64 |
| 41:UP:69:GLU:HB2 | 41:UP:96:GLY:HA2 | 1.77 | 0.64 |
| 12:2M:145:VAL:HG12 | 12:2M:149:LEU:HD23 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2X:74:PRO:HD2 | 13:2X:169:ASP:HA | 1.78 | 0.64 |
| 21:4E:212:TYR:O | 21:4E:216:ARG:HB2 | 1.97 | 0.64 |
| 22:4H:295:PRO:HB2 | 41:CL:215:LEU:HD21 | 1.79 | 0.64 |
| 23:4M:98:VAL:HG11 | 23:4M:113:TRP:HD1 | 1.63 | 0.64 |
| 41:BB:322:SER:HA | 40:BG:223:THR:HG22 | 1.79 | 0.64 |
| 41:CN:330:MET:HG3 | 41:CN:351:THR:HG21 | 1.79 | 0.64 |
| 41:DP:226:ASN:ND2 | 43:DP:501:GDP:N1 | 2.45 | 0.64 |
| 41:FO:341:PHE:HB3 | 41:FO:348:ASN:HD21 | 1.61 | 0.64 |
| 40:HA:254:GLU:OE1 | 41:HB:99:ASN:ND2 | 2.31 | 0.64 |
| 40:HA:328:VAL:HG11 | 40:HA:353:VAL:HG21 | 1.79 | 0.64 |
| 41:JO:52:ASN:ND2 | 41:JO:123:GLU:OE2 | 2.30 | 0.64 |
| 41:KL:417:ASP:O | 41:KL:420:ASN:N | 2.27 | 0.64 |
| 40:NA:204:VAL:HG11 | 40:NA:231:ILE:HD11 | 1.79 | 0.64 |
| 40:ND:88:HIS:HB2 | 40:OD:283:HIS:HB3 | 1.80 | 0.64 |
| 40:OH:88:HIS:HB3 | 40:OH:91:GLN:CB | 2.24 | 0.64 |
| 40:PG:27:GLU:OE2 | 40:PG:243:ARG:NH1 | 2.31 | 0.64 |
| 40:RI:120:ASP:O | 40:RI:123:ARG:NH2 | 2.30 | 0.64 |
| 40:TE:49:PHE:HB2 | 40:TE:53:PHE:HB2 | 1.79 | 0.64 |
| 40:TI:371:GLN:HG2 | 40:TI:372:ARG:HD2 | 1.79 | 0.64 |
| 41:TN:179:VAL:HG23 | 41:TN:180:VAL:HG13 | 1.80 | 0.64 |
| 41:UO:384:GLN:O | 41:UO:388:MET:CB | 2.45 | 0.64 |
| 12:2O:67:THR:HG22 | 12:2O:159:LEU:HD11 | 1.79 | 0.64 |
| 14:3C:14:PHE:HD1 | 41:MO:174:LYS:HG3 | 1.62 | 0.64 |
| 23:4M:251:PRO:HD2 | 23:4M:268:ALA:HB1 | 1.80 | 0.64 |
| 31:5J:782:ARG:NH1 | 41:HM:74:ASP:OD2 | 2.27 | 0.64 |
| 36:5X:21:ARG:NH1 | 40:ND:37:PRO:HB3 | 2.12 | 0.64 |
| 41:AM:248:ALA:HA | 41:AM:252:LYS:HD3 | 1.79 | 0.64 |
| 41:AP:100:ASN:HB3 | 41:AP:103:LYS:HB2 | 1.79 | 0.64 |
| 40:BE:177:VAL:HG13 | 40:BE:178:SER:H | 1.62 | 0.64 |
| 40:BE:326:LYS:NZ | 41:BM:208:TYR:HB2 | 2.12 | 0.64 |
| 40:BF:188:ILE:HD12 | 40:BF:424:MET:HG3 | 1.78 | 0.64 |
| 41:BM:98:GLY:O | 41:BM:99:ASN:C | 2.36 | 0.64 |
| 40:DI:14:VAL:HG11 | 40:DI:75:ILE:HG12 | 1.79 | 0.64 |
| 41:GN:113:VAL:HG11 | 41:GN:150:LEU:HD13 | 1.79 | 0.64 |
| 41:HM:287:PRO:HG3 | 41:HM:329:GLN:HE22 | 1.62 | 0.64 |
| 40:LA:318:LEU:O | 40:LA:374:VAL:HA | 1.97 | 0.64 |
| 40:MF:139:HIS:H | 40:MF:139:HIS:CD2 | 2.14 | 0.64 |
| 41:MO:248:ALA:HA | 41:MO:252:LYS:HE3 | 1.79 | 0.64 |
| 40:NH:204:VAL:HG11 | 40:NH:231:ILE:HD11 | 1.79 | 0.64 |
| 41:NP:134:GLN:HA | 41:NP:165:ASN:O | 1.96 | 0.64 |
| 41:RB:8:GLN:HE21 | 41:RB:65:LEU:HG | 1.61 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SP:272:PRO:HG3 | 41:SP:364:SER:HA | 1.78 | 0.64 |
| 40:UE:98:ASP:O | 40:UE:105:ARG:NH1 | 2.30 | 0.64 |
| 41:UP:6:HIS:HD1 | 41:UP:21:TRP:HE1 | 1.45 | 0.64 |
| 12:2N:47:MET:HG3 | 41:AN:336:LYS:HG3 | 1.80 | 0.64 |
| 17:3O:267:ILE:HG23 | 17:3P:402:GLU:HG3 | 1.78 | 0.64 |
| 22:4J:637:ARG:HH21 | 22:4J:638:LEU:HA | 1.62 | 0.64 |
| 40:AF:298:PRO:HB3 | 40:AF:307:PRO:HD2 | 1.80 | 0.64 |
| 41:AO:170:VAL:HG11 | 41:AO:377:LEU:HD21 | 1.78 | 0.64 |
| 40:BH:56:THR:OG1 | 40:BH:57:GLY:N | 2.31 | 0.64 |
| 40:BH:329:ASN:OD1 | 41:BP:174:LYS:HE2 | 1.97 | 0.64 |
| 40:CG:51:THR:HG21 | 40:CG:243:ARG:HA | 1.78 | 0.64 |
| 40:DI:31:GLN:HG3 | 40:DI:37:PRO:HD3 | 1.77 | 0.64 |
| 41:EM:12:CYS:HB2 | 43:EM:501:GDP:C8 | 2.32 | 0.64 |
| 41:EO:253:LEU:HA | 41:EO:350:LYS:HZ1 | 1.62 | 0.64 |
| 41:FO:204:ASN:ND2 | 43:FO:502:GDP:O2' | 2.29 | 0.64 |
| 41:FP:16:ILE:HD13 | 41:FP:226:ASN:HD22 | 1.61 | 0.64 |
| 41:HB:165:ASN:HD21 | 41:HB:250:LEU:HD22 | 1.61 | 0.64 |
| 40:HH:212:ILE:HD11 | 40:HH:300:ASN:HA | 1.80 | 0.64 |
| 40:JA:65:ALA:O | 40:JA:91:GLN:NE2 | 2.30 | 0.64 |
| 40:LH:178:SER:OG | 41:LO:347:ASN:ND2 | 2.30 | 0.64 |
| 41:LM:248:ALA:HA | 41:LM:252:LYS:HD3 | 1.77 | 0.64 |
| 40:MH:256:GLN:HB3 | 41:MP:397:TRP:HH2 | 1.61 | 0.64 |
| 41:ML:313:VAL:O | 41:ML:349:VAL:HA | 1.97 | 0.64 |
| 41:NP:282:ARG:HG2 | 41:NP:283:ALA:H | 1.62 | 0.64 |
| 41:OL:8:GLN:HE21 | 41:OL:65:LEU:HD22 | 1.63 | 0.64 |
| 41:PB:309:ARG:H | 41:PB:372:THR:HB | 1.62 | 0.64 |
| 41:PP:232:THR:HG22 | 41:PP:270:PHE:HB2 | 1.77 | 0.64 |
| 41:QO:49:VAL:O | 41:QO:62:ARG:NH2 | 2.31 | 0.64 |
| 41:QP:66:VAL:CG1 | 41:QP:91:VAL:HG21 | 2.25 | 0.64 |
| 41:RB:178:THR:HG22 | 41:RB:180:VAL:H | 1.60 | 0.64 |
| 41:RL:232:THR:HG23 | 41:RL:270:PHE:HB2 | 1.80 | 0.64 |
| 40:SG:326:LYS:HZ3 | 41:SO:208:TYR:HB2 | 1.62 | 0.64 |
| 40:SI:88:HIS:HE1 | 40:TI:280:LYS:HG3 | 1.62 | 0.64 |
| 40:SI:273:ALA:HB3 | 40:SI:374:VAL:H | 1.62 | 0.64 |
| 40:WG:7:VAL:HB | 40:WG:137:ILE:HG22 | 1.79 | 0.64 |
| 12:2M:254:CYS:SG | 12:2M:255:LEU:N | 2.70 | 0.64 |
| 23:4N:185:SER:HA | 23:4N:202:PHE:HD2 | 1.62 | 0.64 |
| 30:5G:86:VAL:O | 30:5G:90:HIS:ND1 | 2.31 | 0.64 |
| 36:5X:130:LEU:HD23 | 36:5X:136:ASN:HA | 1.79 | 0.64 |
| 41:BL:6:HIS:O | 41:BL:63:ALA:HA | 1.97 | 0.64 |
| 40:CE:319:TYR:HB3 | 40:CE:323:VAL:HG21 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DA:180:ALA:HB3 | 40:DA:183:GLU:HB2 | 1.79 | 0.64 |
| 40:DI:3:GLU:HG3 | 40:DI:129:CYS:HB3 | 1.78 | 0.64 |
| 41:DL:132:GLY:HA3 | 41:DL:163:ILE:HB | 1.80 | 0.64 |
| 41:EP:98:GLY:O | 41:EP:99:ASN:C | 2.36 | 0.64 |
| 40:JE:133:GLN:NE2 | 40:JE:251:ASP:OD2 | 2.31 | 0.64 |
| 40:KA:254:GLU:HG2 | 41:KB:98:GLY:HA2 | 1.78 | 0.64 |
| 41:KN:100:ASN:HB3 | 41:KN:103:LYS:HB2 | 1.79 | 0.64 |
| 41:LB:318:ARG:HD3 | 41:LB:358:PRO:HD3 | 1.77 | 0.64 |
| 40:LG:332:ILE:HG23 | 40:LG:351:PHE:HD2 | 1.61 | 0.64 |
| 41:LO:318:ARG:HB3 | 41:LO:364:SER:HB2 | 1.80 | 0.64 |
| 41:LP:30:ILE:HD11 | 41:LP:47:ILE:HD11 | 1.79 | 0.64 |
| 41:QB:312:THR:HG23 | 41:QB:370:ASN:HB3 | 1.79 | 0.64 |
| 41:QO:269:GLY:HA3 | 41:QO:367:PHE:HB3 | 1.79 | 0.64 |
| 41:QP:427:ALA:O | 41:QP:428:CYS:C | 2.34 | 0.64 |
| 40:SA:231:ILE:HA | 40:SA:234:ILE:HD12 | 1.80 | 0.64 |
| 41:UM:100:ASN:HB3 | 41:UM:103:LYS:HB2 | 1.80 | 0.64 |
| 41:WP:293:MET:HG2 | 41:WP:367:PHE:HB2 | 1.80 | 0.64 |
| 41:WQ:136:THR:HG22 | 41:WQ:167:PHE:HB2 | 1.79 | 0.64 |
| 16:3L:8:PRO:HD3 | 18:3T:326:LEU:HB3 | 1.78 | 0.64 |
| 23:4M:98:VAL:HG11 | 23:4M:113:TRP:CD1 | 2.33 | 0.64 |
| 23:4N:18:TYR:CZ | 23:4N:22:TYR:CE2 | 2.86 | 0.64 |
| 40:AF:76:ASP:HA | 40:AF:79:ARG:HG2 | 1.80 | 0.64 |
| 41:AM:178:THR:HB | 41:AM:181:GLU:HG3 | 1.80 | 0.64 |
| 40:BG:119:LEU:HD21 | 40:BG:156:ARG:HB3 | 1.80 | 0.64 |
| 40:CE:356:ASN:OD1 | 40:CE:358:GLN:NE2 | 2.30 | 0.64 |
| 41:DL:8:GLN:HB2 | 41:DL:65:LEU:HA | 1.78 | 0.64 |
| 40:EE:229:ARG:HH22 | 40:EE:365:GLY:HA3 | 1.62 | 0.64 |
| 41:EP:108:GLU:O | 41:EP:111:GLU:HG2 | 1.98 | 0.64 |
| 40:FA:400:LYS:O | 40:FA:401:ARG:C | 2.36 | 0.64 |
| 40:GF:222:PRO:HD2 | 41:GM:324:LYS:HE3 | 1.80 | 0.64 |
| 40:GH:102:ASN:HB3 | 40:GH:105:ARG:HB2 | 1.79 | 0.64 |
| 40:GH:311:LYS:H | 40:GH:381:THR:HG22 | 1.62 | 0.64 |
| 40:HF:326:LYS:HZ1 | 41:HN:208:TYR:HB2 | 1.62 | 0.64 |
| 40:MH:210:TYR:CD1 | 41:MO:324:LYS:HG2 | 2.32 | 0.64 |
| 41:NB:178:THR:HB | 41:NB:181:GLU:HG3 | 1.79 | 0.64 |
| 41:PB:341:PHE:HB3 | 41:PB:348:ASN:HD21 | 1.60 | 0.64 |
| 41:PO:27:GLU:OE2 | 41:PO:318:ARG:NH2 | 2.31 | 0.64 |
| 41:QB:186:THR:HG21 | 41:QB:385:PHE:HB2 | 1.79 | 0.64 |
| 41:QL:163:ILE:HG21 | 41:QL:250:LEU:HB3 | 1.79 | 0.64 |
| 41:QL:178:THR:HG22 | 41:QL:180:VAL:H | 1.61 | 0.64 |
| 41:QM:178:THR:HB | 41:QM:181:GLU:HG3 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SI:70:LEU:HD12 | 40:SI:99:ALA:HB2 | 1.80 | 0.64 |
| 41:SP:271:ALA:HB1 | 41:SP:292:GLN:HG3 | 1.79 | 0.64 |
| 40:TF:11:GLN:HG3 | 40:TF:74:VAL:HG21 | 1.80 | 0.64 |
| 40:TF:168:GLU:HB2 | 40:TF:201:ALA:HA | 1.80 | 0.64 |
| 40:TH:205:ASP:HB3 | 40:TH:303:VAL:HA | 1.78 | 0.64 |
| 41:TN:105:HIS:HD2 | 41:TN:150:LEU:HD12 | 1.62 | 0.64 |
| 41:UB:131:GLN:HE22 | 41:UB:249:ASP:HB2 | 1.63 | 0.64 |
| 40:UI:188:ILE:HG13 | 40:UI:424:MET:HG3 | 1.80 | 0.64 |
| 40:VA:326:LYS:NZ | 41:VB:220:PRO:O | 2.30 | 0.64 |
| 40:WF:326:LYS:NZ | 41:WN:208:TYR:HB2 | 2.12 | 0.64 |
| 7:1S:459:GLU:HG3 | 7:1S:495:ARG:HD3 | 1.79 | 0.64 |
| 23:4R:94:TYR:CZ | 23:4R:96:GLY:HA3 | 2.33 | 0.64 |
| 35:5T:162:MET:SD | 41:KL:245:GLN:NE2 | 2.71 | 0.64 |
| 41:AP:7:LEU:HD12 | 41:AP:151:LEU:HD21 | 1.79 | 0.64 |
| 40:BA:73:THR:HA | 40:BA:76:ASP:HB2 | 1.80 | 0.64 |
| 40:CE:259:LEU:HD11 | 40:CE:316:CYS:HB2 | 1.79 | 0.64 |
| 40:CF:51:THR:HG21 | 40:CF:243:ARG:HG2 | 1.79 | 0.64 |
| 41:CN:170:VAL:HG21 | 41:CN:377:LEU:HG | 1.79 | 0.64 |
| 40:DI:72:PRO:HD2 | 41:DP:2:ARG:HH22 | 1.62 | 0.64 |
| 41:DP:16:ILE:HG13 | 41:DP:226:ASN:ND2 | 2.12 | 0.64 |
| 40:EA:98:ASP:O | 40:EA:105:ARG:NH2 | 2.29 | 0.64 |
| 40:EI:295:CYS:HB3 | 40:EI:376:MET:HE2 | 1.78 | 0.64 |
| 41:FM:317:PHE:HB2 | 41:FM:353:VAL:HG12 | 1.80 | 0.64 |
| 40:GA:219:ILE:HG23 | 40:GA:222:PRO:HG3 | 1.80 | 0.64 |
| 41:GB:3:GLU:HB3 | 41:GB:130:LEU:HA | 1.79 | 0.64 |
| 41:IM:22:GLU:HG3 | 41:IM:81:PHE:HD2 | 1.63 | 0.64 |
| 41:JM:86:ARG:HG3 | 41:JM:88:ASP:H | 1.61 | 0.64 |
| 40:KA:51:THR:HG21 | 40:KA:243:ARG:HG2 | 1.79 | 0.64 |
| 40:KF:2:ARG:HH22 | 41:KN:69:GLU:HB3 | 1.62 | 0.64 |
| 40:LG:273:ALA:HB3 | 40:LG:374:VAL:H | 1.63 | 0.64 |
| 40:NG:199:ASP:OD1 | 40:NG:256:GLN:NE2 | 2.31 | 0.64 |
| 41:NM:341:PHE:HB3 | 41:NM:348:ASN:HD21 | 1.62 | 0.64 |
| 41:NO:248:ALA:HA | 41:NO:252:LYS:HD3 | 1.79 | 0.64 |
| 41:PB:19:LYS:HZ1 | 41:PB:227:HIS:HA | 1.61 | 0.64 |
| 40:PG:271:THR:HG22 | 40:PG:301:GLN:HA | 1.78 | 0.64 |
| 41:QB:350:LYS:HE2 | 40:QG:180:ALA:HA | 1.80 | 0.64 |
| 40:QH:320:ARG:HG2 | 40:QH:356:ASN:HB3 | 1.80 | 0.64 |
| 40:RE:298:PRO:HA | 40:RE:301:GLN:HE22 | 1.62 | 0.64 |
| 40:RG:236:SER:O | 40:RG:240:ALA:HB2 | 1.97 | 0.64 |
| 41:RN:62:ARG:NH2 | 41:RN:127:CYS:SG | 2.69 | 0.64 |
| 41:TP:49:VAL:HG21 | 41:TP:241:ARG:HG2 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VN:156:ARG:NH1 | 41:VN:195:ASN:O | 2.30 | 0.64 |
| 41:VQ:62:ARG:NH1 | 41:VQ:127:CYS:SG | 2.71 | 0.64 |
| 11:2I:161:ARG:HH22 | 40:MG:399:ALA:HA | 1.62 | 0.64 |
| 17:3P:287:VAL:HG21 | 17:3Q:397:GLN:HA | 1.79 | 0.64 |
| 19:3Y:130:ARG:HB3 | 41:LB:279:GLN:HG2 | 1.78 | 0.64 |
| 34:5R:410:LYS:NZ | 34:5R:414:GLU:HB2 | 2.12 | 0.64 |
| 41:AB:347:ASN:ND2 | 40:AG:177:VAL:O | 2.31 | 0.64 |
| 40:AF:332:ILE:HG23 | 40:AF:351:PHE:HD2 | 1.62 | 0.64 |
| 40:CF:64:ARG:NH1 | 40:CF:128:GLN:O | 2.30 | 0.64 |
| 41:DB:91:VAL:HG21 | 41:DB:116:VAL:HG22 | 1.79 | 0.64 |
| 40:DF:288:VAL:HA | 40:DF:291:ILE:HD13 | 1.80 | 0.64 |
| 40:DG:70:LEU:HD23 | 40:DG:114:LEU:HD12 | 1.80 | 0.64 |
| 41:DL:212:PHE:HE2 | 41:DL:220:PRO:HD2 | 1.63 | 0.64 |
| 41:DN:193:VAL:HG13 | 41:DN:264:HIS:HE1 | 1.62 | 0.64 |
| 41:EP:163:ILE:HD13 | 41:EP:250:LEU:HB2 | 1.80 | 0.64 |
| 41:GB:100:ASN:HB3 | 41:GB:103:LYS:HB2 | 1.80 | 0.64 |
| 41:GN:70:PRO:HG2 | 41:GN:94:GLN:HG3 | 1.79 | 0.64 |
| 41:HM:7:LEU:HD22 | 41:HM:151:LEU:HD21 | 1.80 | 0.64 |
| 40:IA:76:ASP:OD2 | 41:IN:46:ARG:NH2 | 2.31 | 0.64 |
| 40:OD:228:ASN:HD21 | 42:OD:501:GTP:HN1 | 1.45 | 0.64 |
| 40:OG:271:THR:O | 40:OG:375:CYS:HA | 1.98 | 0.64 |
| 41:PP:330:MET:HA | 41:PP:333:VAL:HG12 | 1.80 | 0.64 |
| 40:QE:278:ALA:H | 40:QE:368:ALA:HB2 | 1.63 | 0.64 |
| 40:SA:76:ASP:HA | 40:SA:79:ARG:HG2 | 1.80 | 0.64 |
| 41:SB:291:GLN:O | 41:SB:295:ASP:HB2 | 1.98 | 0.64 |
| 40:TE:107:HIS:HA | 40:TE:152:LEU:HD23 | 1.80 | 0.64 |
| 41:TM:10:GLY:O | 41:TM:14:ASN:HB2 | 1.98 | 0.64 |
| 40:UA:257:THR:HA | 41:UB:397:TRP:HZ3 | 1.61 | 0.64 |
| 41:UB:260:PHE:HB2 | 41:UB:263:LEU:HD23 | 1.80 | 0.64 |
| 40:WI:319:TYR:HB2 | 40:WI:355:ILE:HG22 | 1.79 | 0.64 |
| 33:5N:319:VAL:HG23 | 34:5Q:131:LYS:HE2 | 1.80 | 0.64 |
| 35:5T:123:LEU:HD13 | 35:5T:128:LYS:HD2 | 1.80 | 0.64 |
| 36:5X:216:GLU:HB3 | 36:5X:221:GLN:HE22 | 1.63 | 0.64 |
| 40:AG:133:GLN:NE2 | 40:AG:251:ASP:OD1 | 2.30 | 0.64 |
| 41:BM:207:LEU:HB3 | 41:BM:225:LEU:HG | 1.79 | 0.64 |
| 40:CA:402:ALA:O | 40:CA:404:VAL:N | 2.31 | 0.64 |
| 40:CG:105:ARG:HG2 | 40:CG:410:GLU:HG2 | 1.79 | 0.64 |
| 40:DE:210:TYR:HB2 | 41:DL:324:LYS:HD3 | 1.79 | 0.64 |
| 40:EA:6:SER:O | 40:EA:65:ALA:HA | 1.98 | 0.64 |
| 41:EM:3:GLU:HG2 | 41:EM:62:ARG:HH22 | 1.63 | 0.64 |
| 40:FE:191:THR:O | 40:FE:195:LEU:HB2 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FH:76:ASP:OD2 | 41:FO:46:ARG:NH2 | 2.29 | 0.64 |
| 41:FM:222:TYR:O | 41:FM:226:ASN:ND2 | 2.30 | 0.64 |
| 40:HH:9:VAL:HG22 | 40:HH:68:VAL:HB | 1.80 | 0.64 |
| 40:JA:76:ASP:HA | 40:JA:79:ARG:HG2 | 1.80 | 0.64 |
| 40:JE:352:LYS:HZ3 | 41:JM:178:THR:C | 2.01 | 0.64 |
| 41:KL:42:LEU:HD22 | 41:KL:356:ILE:HG13 | 1.80 | 0.64 |
| 41:KN:274:THR:OG1 | 41:KN:282:ARG:NH1 | 2.31 | 0.64 |
| 41:KP:420:ASN:HA | 41:KP:423:VAL:HG12 | 1.78 | 0.64 |
| 40:LA:326:LYS:HD2 | 41:LB:220:PRO:HD2 | 1.79 | 0.64 |
| 40:LD:6:SER:O | 40:LD:65:ALA:HA | 1.98 | 0.64 |
| 40:ME:76:ASP:HA | 40:ME:79:ARG:HG2 | 1.79 | 0.64 |
| 41:NM:337:ASN:HB3 | 41:NM:340:TYR:HB2 | 1.80 | 0.64 |
| 41:NN:62:ARG:NH1 | 41:NN:127:CYS:SG | 2.71 | 0.64 |
| 40:OF:264:ARG:NH1 | 40:OF:430:ASP:OD2 | 2.30 | 0.64 |
| 41:QB:308:GLY:HA3 | 41:QB:373:ALA:HB2 | 1.78 | 0.64 |
| 40:RE:134:GLY:HA3 | 40:RE:252:LEU:HD11 | 1.78 | 0.64 |
| 40:SE:276:ILE:HD13 | 40:SE:286:LEU:HD11 | 1.80 | 0.64 |
| 41:SM:407:GLU:HA | 41:SM:410:GLU:HG3 | 1.77 | 0.64 |
| 41:UP:55:THR:H | 41:VQ:283:ALA:HA | 1.63 | 0.64 |
| 8:1Z:400:TRP:HH2 | 41:UP:276:ARG:HB3 | 1.63 | 0.64 |
| 11:2J:210:GLU:HG3 | 11:2J:230:LEU:HD11 | 1.80 | 0.64 |
| 17:3R:232:ARG:NH2 | 17:3R:328:LEU:HA | 2.07 | 0.64 |
| 21:4D:242:VAL:HG12 | 21:4D:267:TYR:HA | 1.79 | 0.64 |
| 23:4P:187:PHE:HA | 40:CA:79:ARG:HD3 | 1.80 | 0.64 |
| 40:BF:194:THR:O | 40:BF:198:SER:CB | 2.45 | 0.64 |
| 41:BP:44:LEU:HA | 41:BP:47:ILE:HG13 | 1.79 | 0.64 |
| 40:EA:203:MET:HG2 | 40:EA:303:VAL:HG21 | 1.80 | 0.64 |
| 41:EP:103:LYS:HG3 | 41:EP:401:GLU:HG3 | 1.80 | 0.64 |
| 40:FF:50:ASN:O | 40:FF:64:ARG:NH1 | 2.30 | 0.64 |
| 40:FF:228:ASN:HD21 | 42:FM:501:GTP:HN1 | 1.45 | 0.64 |
| 40:GE:285:GLN:O | 40:GE:286:LEU:C | 2.37 | 0.64 |
| 40:GF:352:LYS:HD2 | 41:GN:179:VAL:HG13 | 1.79 | 0.64 |
| 40:HE:54:SER:HB3 | 40:HE:64:ARG:HE | 1.62 | 0.64 |
| 40:HE:333:ALA:HA | 40:HE:336:LYS:HD2 | 1.80 | 0.64 |
| 41:HQ:317:PHE:HB2 | 41:HQ:353:VAL:HG12 | 1.79 | 0.64 |
| 41:KL:398:TYR:HB3 | 41:KL:408:PHE:HZ | 1.61 | 0.64 |
| 41:MB:8:GLN:HE21 | 41:MB:65:LEU:HG | 1.63 | 0.64 |
| 41:OB:322:SER:HB2 | 40:OG:221:ARG:HB2 | 1.79 | 0.64 |
| 41:PL:100:ASN:HB3 | 41:PL:103:LYS:HG2 | 1.80 | 0.64 |
| 41:QM:375:GLN:HE21 | 41:QM:379:LYS:HG3 | 1.62 | 0.64 |
| 41:QP:322:SER:O | 41:QP:323:MET:HB3 | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SN:313:VAL:HB | 41:SN:349:VAL:HG22 | 1.80 | 0.64 |
| 41:TL:318:ARG:HB3 | 41:TL:364:SER:HB3 | 1.78 | 0.64 |
| 7:1U:353:LYS:HA | 7:1U:376:THR:HG23 | 1.80 | 0.63 |
| 7:1U:530:GLU:HG3 | 7:1U:532:PHE:H | 1.62 | 0.63 |
| 9:2B:394:ARG:NH1 | 9:2B:394:ARG:O | 2.30 | 0.63 |
| 15:3E:269:LYS:HD3 | 16:3J:73:ARG:HH12 | 1.63 | 0.63 |
| 20:4A:34:ARG:HG2 | 25:4T:439:LEU:HD23 | 1.80 | 0.63 |
| 39:6K:59:CYS:HB3 | 39:6K:64:ASP:HB3 | 1.79 | 0.63 |
| 41:BO:61:PRO:HD2 | 41:BO:84:ILE:O | 1.98 | 0.63 |
| 41:BO:135:LEU:HB3 | 41:BO:166:THR:HG22 | 1.79 | 0.63 |
| 41:DP:2:ARG:HB3 | 41:DP:131:GLN:HE21 | 1.63 | 0.63 |
| 40:EE:260:VAL:HB | 41:EM:397:TRP:CH2 | 2.33 | 0.63 |
| 40:EH:99:ALA:HA | 40:EH:110:ILE:HD11 | 1.79 | 0.63 |
| 40:GA:396:LEU:HD23 | 41:GN:346:PRO:HG3 | 1.79 | 0.63 |
| 40:GF:214:ARG:HD3 | 41:GM:324:LYS:HE2 | 1.79 | 0.63 |
| 40:HE:106:GLY:CA | 40:HE:148:GLY:HA3 | 2.18 | 0.63 |
| 41:IQ:19:LYS:HD2 | 41:IQ:226:ASN:HB2 | 1.80 | 0.63 |
| 40:JA:359:PRO:HB3 | 40:JA:371:GLN:HA | 1.79 | 0.63 |
| 41:JO:86:ARG:HG3 | 41:JO:88:ASP:H | 1.62 | 0.63 |
| 40:KD:3:GLU:HA | 40:KD:51:THR:HA | 1.80 | 0.63 |
| 40:LF:142:GLY:O | 42:LM:501:GTP:H5' | 1.98 | 0.63 |
| 42:MB:502:GTP:HN21 | 40:MG:228:ASN:HD22 | 1.46 | 0.63 |
| 41:QB:202:ILE:HG23 | 41:QB:229:VAL:HG11 | 1.79 | 0.63 |
| 40:QF:70:LEU:HD23 | 40:QF:114:LEU:HD12 | 1.80 | 0.63 |
| 40:SA:55:GLU:O | 40:TA:285:GLN:NE2 | 2.31 | 0.63 |
| 40:VI:73:THR:HA | 40:VI:76:ASP:HB2 | 1.79 | 0.63 |
| 40:WI:3:GLU:HG3 | 40:WI:51:THR:HA | 1.80 | 0.63 |
| 14:3A:110:ARG:HH22 | 40:MF:339:ARG:CZ | 2.11 | 0.63 |
| 18:3U:163:GLN:HB2 | 18:3U:418:VAL:HG13 | 1.80 | 0.63 |
| 20:4A:70:GLN:HE22 | 41:MN:361:LEU:HA | 1.63 | 0.63 |
| 36:5Y:76:LEU:HB3 | 40:OG:282:TYR:HE2 | 1.63 | 0.63 |
| 39:6I:138:GLY:HA2 | 39:6I:141:SER:HB2 | 1.80 | 0.63 |
| 41:AL:202:ILE:HG23 | 41:AL:300:MET:HB3 | 1.81 | 0.63 |
| 40:BA:43:GLY:HA3 | 40:BA:358:GLN:HE22 | 1.62 | 0.63 |
| 40:DE:102:ASN:HB3 | 40:DE:105:ARG:HB2 | 1.79 | 0.63 |
| 40:DE:143:GLY:HA3 | 42:DE:501:GTP:O2A | 1.98 | 0.63 |
| 41:DM:372:THR:HA | 41:DM:422:VAL:HG22 | 1.78 | 0.63 |
| 41:DP:137:HIS:CE1 | 41:DP:168:SER:HB3 | 2.33 | 0.63 |
| 40:EH:273:ALA:O | 40:EH:274:PRO:C | 2.37 | 0.63 |
| 41:FB:2:ARG:HH21 | 41:FB:240:LEU:HA | 1.63 | 0.63 |
| 40:FI:305:CYS:HB3 | 40:FI:386:ALA:HB2 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GE:407:TYR:HB3 | 40:GE:412:MET:HG2 | 1.79 | 0.63 |
| 40:HH:70:LEU:HD23 | 40:HH:145:THR:HG23 | 1.80 | 0.63 |
| 40:HI:102:ASN:HB3 | 40:HI:105:ARG:HB3 | 1.80 | 0.63 |
| 40:IA:408:VAL:HA | 40:IA:412:MET:HB3 | 1.78 | 0.63 |
| 42:JB:502:GTP:O2' | 40:JG:206:ASN:OD1 | 2.15 | 0.63 |
| 40:JG:188:ILE:HD12 | 40:JG:424:MET:HG3 | 1.79 | 0.63 |
| 41:JM:293:MET:HG2 | 41:JM:367:PHE:HB2 | 1.80 | 0.63 |
| 41:KB:375:GLN:HE21 | 41:KB:379:LYS:HG3 | 1.61 | 0.63 |
| 40:KG:51:THR:HG21 | 40:KG:243:ARG:HG2 | 1.81 | 0.63 |
| 41:LL:334:GLN:NE2 | 41:LL:347:ASN:OD1 | 2.32 | 0.63 |
| 40:OE:226:ASN:ND2 | 40:OE:366:ASP:OD2 | 2.32 | 0.63 |
| 41:PB:325:GLU:HA | 41:PB:328:GLU:HB3 | 1.80 | 0.63 |
| 40:PF:271:THR:O | 40:PF:375:CYS:HA | 1.98 | 0.63 |
| 41:QP:192:LEU:HB2 | 41:QP:196:THR:HB | 1.80 | 0.63 |
| 40:RI:228:ASN:HD21 | 42:RP:501:GTP:HN1 | 1.44 | 0.63 |
| 40:SE:115:ILE:HG21 | 40:SE:152:LEU:HD22 | 1.79 | 0.63 |
| 40:TF:76:ASP:OD1 | 41:TM:46:ARG:NH2 | 2.32 | 0.63 |
| 41:TL:210:ILE:O | 41:TL:214:THR:HB | 1.98 | 0.63 |
| 41:TP:137:HIS:O | 41:TP:168:SER:HA | 1.98 | 0.63 |
| 40:UI:143:GLY:N | 42:UI:501:GTP:O2A | 2.28 | 0.63 |
| 41:UO:178:THR:HB | 41:UO:181:GLU:HB2 | 1.80 | 0.63 |
| 40:WG:27:GLU:OE1 | 40:WG:243:ARG:NH2 | 2.31 | 0.63 |
| 40:WG:137:ILE:HD11 | 40:WG:168:GLU:HG2 | 1.80 | 0.63 |
| 41:WQ:178:THR:HB | 41:WQ:181:GLU:HG3 | 1.80 | 0.63 |
| 7:1U:116:ALA:HB3 | 7:1U:129:LEU:HB3 | 1.81 | 0.63 |
| 17:3R:181:LEU:HD13 | 17:3R:328:LEU:HD21 | 1.80 | 0.63 |
| 18:3W:131:LEU:HB3 | 18:3W:201:ILE:HD11 | 1.80 | 0.63 |
| 23:4N:198:PHE:HB2 | 40:DF:221:ARG:HB2 | 1.79 | 0.63 |
| 23:4P:240:LEU:HD22 | 23:4P:266:HIS:CB | 2.28 | 0.63 |
| 40:AE:76:ASP:OD2 | 41:AL:46:ARG:NH2 | 2.31 | 0.63 |
| 41:AO:173:PRO:HA | 41:AO:380:ARG:HD3 | 1.80 | 0.63 |
| 41:AO:293:MET:HG2 | 41:AO:367:PHE:HB2 | 1.81 | 0.63 |
| 40:DI:70:LEU:HB2 | 40:DI:145:THR:HG23 | 1.80 | 0.63 |
| 40:EG:21:TRP:HH2 | 40:EG:52:PHE:HB3 | 1.63 | 0.63 |
| 40:FA:394:PHE:HZ | 40:FA:417:PHE:HB3 | 1.62 | 0.63 |
| 41:GB:253:LEU:O | 41:GB:257:MET:HB3 | 1.97 | 0.63 |
| 40:GI:104:ALA:HA | 40:GI:108:TYR:HD2 | 1.62 | 0.63 |
| 41:HO:317:PHE:HB2 | 41:HO:353:VAL:HG12 | 1.80 | 0.63 |
| 40:JF:259:LEU:HD21 | 40:JF:316:CYS:HB2 | 1.81 | 0.63 |
| 41:KN:289:LEU:HD11 | 41:KN:363:MET:HB3 | 1.79 | 0.63 |
| 41:LN:239:CYS:HB3 | 41:LN:247:ASN:HB2 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MG:204:VAL:HG22 | 40:MG:209:ILE:HD11 | 1.80 | 0.63 |
| 40:NE:79:ARG:HG2 | 40:NE:92:LEU:HD13 | 1.80 | 0.63 |
| 41:OB:350:LYS:HZ3 | 40:OG:181:VAL:H | 1.46 | 0.63 |
| 40:OG:254:GLU:OE1 | 40:OG:258:ASN:ND2 | 2.31 | 0.63 |
| 41:ON:165:ASN:HA | 41:ON:198:GLU:O | 1.98 | 0.63 |
| 40:PA:252:LEU:O | 40:PA:256:GLN:NE2 | 2.31 | 0.63 |
| 41:RB:30:ILE:HD11 | 41:RB:47:ILE:HD11 | 1.79 | 0.63 |
| 40:SF:16:ILE:HA | 40:SF:228:ASN:HB3 | 1.80 | 0.63 |
| 40:SH:406:TRP:HH2 | 41:SO:258:VAL:HG13 | 1.63 | 0.63 |
| 40:SI:151:SER:HG | 40:SI:190:THR:HG1 | 1.46 | 0.63 |
| 41:SL:66:VAL:HG12 | 41:SL:91:VAL:HB | 1.80 | 0.63 |
| 40:TA:278:ALA:H | 40:TA:368:ALA:HB2 | 1.63 | 0.63 |
| 40:VF:301:GLN:NE2 | 40:VF:303:VAL:O | 2.29 | 0.63 |
| 41:VQ:238:THR:OG1 | 41:VQ:318:ARG:NH1 | 2.32 | 0.63 |
| 41:WP:330:MET:HE2 | 41:WP:349:VAL:HG11 | 1.79 | 0.63 |
| 8:1X:123:GLU:HA | 8:1X:126:GLU:HB3 | 1.81 | 0.63 |
| 11:2I:218:ILE:HA | 11:2I:223:LYS:HE2 | 1.78 | 0.63 |
| 17:3R:156:TRP:HA | 17:3R:156:TRP:CE3 | 2.32 | 0.63 |
| 20:4A:149:ARG:HH22 | 20:4A:150:SER:HA | 1.63 | 0.63 |
| 23:4N:240:LEU:HD22 | 23:4N:266:HIS:CB | 2.28 | 0.63 |
| 23:4R:250:VAL:HG13 | 23:4R:253:TYR:HB2 | 1.79 | 0.63 |
| 36:5W:100:HIS:O | 41:ON:279:GLN:NE2 | 2.32 | 0.63 |
| 40:CE:75:ILE:HG23 | 40:CE:92:LEU:HD12 | 1.81 | 0.63 |
| 40:CE:318:LEU:O | 40:CE:374:VAL:HA | 1.97 | 0.63 |
| 40:DH:214:ARG:HA | 40:DH:219:ILE:O | 1.99 | 0.63 |
| 40:EG:88:HIS:HB3 | 40:EG:91:GLN:HG2 | 1.78 | 0.63 |
| 40:FG:6:SER:O | 40:FG:65:ALA:HA | 1.99 | 0.63 |
| 40:FI:70:LEU:HD23 | 40:FI:114:LEU:HD12 | 1.81 | 0.63 |
| 41:FP:292:GLN:O | 41:FP:298:ASN:ND2 | 2.30 | 0.63 |
| 40:GA:28:HIS:CE1 | 40:GA:243:ARG:HD3 | 2.33 | 0.63 |
| 40:GE:325:PRO:HB3 | 41:GM:222:TYR:HE1 | 1.64 | 0.63 |
| 40:HI:273:ALA:HB3 | 40:HI:374:VAL:H | 1.63 | 0.63 |
| 40:JH:51:THR:HG21 | 40:JH:243:ARG:HG2 | 1.80 | 0.63 |
| 40:KH:3:GLU:HA | 40:KH:51:THR:HA | 1.79 | 0.63 |
| 40:LD:239:THR:O | 40:LD:243:ARG:NH1 | 2.31 | 0.63 |
| 40:ND:435:GLY:O | 40:ND:436:MET:C | 2.36 | 0.63 |
| 41:OO:354:CYS:SG | 41:OO:355:ASP:N | 2.71 | 0.63 |
| 41:QB:395:LEU:O | 41:QB:396:HIS:C | 2.36 | 0.63 |
| 41:RL:100:ASN:HB3 | 41:RL:103:LYS:HB2 | 1.80 | 0.63 |
| 41:SO:242:PHE:HB3 | 41:SO:356:ILE:CG1 | 2.28 | 0.63 |
| 40:TE:285:GLN:O | 40:TE:372:ARG:NH2 | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TO:139:LEU:HB2 | 41:TO:168:SER:HB3 | 1.80 | 0.63 |
| 40:VF:319:TYR:HB3 | 40:VF:323:VAL:HG11 | 1.80 | 0.63 |
| 40:VI:326:LYS:NZ | 41:VQ:204:ASN:O | 2.31 | 0.63 |
| 40:WF:352:LYS:HE3 | 41:WN:179:VAL:HG23 | 1.80 | 0.63 |
| 7:1S:466:CYS:SG | 7:1S:468:ARG:NH1 | 2.72 | 0.63 |
| 7:1T:524:ARG:HH22 | 7:1T:546:GLY:H | 1.47 | 0.63 |
| 8:1X:160:LEU:HG | 8:1X:164:GLU:HB3 | 1.80 | 0.63 |
| 13:2X:87:PHE:HE2 | 13:2X:156:ILE:HG23 | 1.60 | 0.63 |
| 14:3B:8:ASN:HB3 | 41:ML:304:ASP:HB2 | 1.79 | 0.63 |
| 17:3R:231:GLU:HA | 17:3R:234:LYS:HD2 | 1.80 | 0.63 |
| 19:3Y:167:TRP:CZ2 | 25:4T:399:GLU:HB3 | 2.33 | 0.63 |
| 22:4J:87:ASP:OD1 | 22:4J:98:ARG:NH2 | 2.32 | 0.63 |
| 36:5X:247:LEU:HD13 | 40:LF:262:TYR:HB3 | 1.80 | 0.63 |
| 40:CI:31:GLN:HG3 | 40:CI:37:PRO:HD3 | 1.81 | 0.63 |
| 41:CP:60:VAL:HG11 | 41:DP:281:TYR:CA | 2.28 | 0.63 |
| 41:DB:132:GLY:HA2 | 41:DB:162:ARG:HG2 | 1.80 | 0.63 |
| 40:DE:188:ILE:HD13 | 40:DE:394:PHE:HB2 | 1.78 | 0.63 |
| 40:DI:76:ASP:HA | 40:DI:79:ARG:HE | 1.63 | 0.63 |
| 41:DN:308:GLY:HA3 | 41:DN:373:ALA:HB2 | 1.80 | 0.63 |
| 40:EI:103:TYR:HD2 | 40:EI:147:SER:HB2 | 1.64 | 0.63 |
| 41:FN:131:GLN:HA | 41:FN:162:ARG:HH21 | 1.64 | 0.63 |
| 41:GN:237:THR:HB | 41:GN:240:LEU:HD11 | 1.80 | 0.63 |
| 41:JB:62:ARG:NH2 | 41:JB:127:CYS:SG | 2.71 | 0.63 |
| 40:JH:73:THR:HA | 40:JH:76:ASP:HB2 | 1.80 | 0.63 |
| 41:JL:139:LEU:HG | 41:JL:168:SER:HB3 | 1.80 | 0.63 |
| 40:LA:276:ILE:HG23 | 40:LA:280:LYS:HB2 | 1.81 | 0.63 |
| 41:LL:256:ASN:HD22 | 41:LL:350:LYS:HD2 | 1.63 | 0.63 |
| 41:MP:273:LEU:O | 41:MP:292:GLN:NE2 | 2.31 | 0.63 |
| 40:NH:238:ILE:HG23 | 40:NH:239:THR:HG23 | 1.79 | 0.63 |
| 41:OM:137:HIS:O | 41:OM:168:SER:HA | 1.98 | 0.63 |
| 40:PH:97:GLU:OE1 | 40:PH:105:ARG:NH1 | 2.31 | 0.63 |
| 41:QO:63:ALA:O | 41:QO:89:ASN:ND2 | 2.32 | 0.63 |
| 40:UI:83:TYR:HD2 | 40:UI:86:LEU:HD22 | 1.64 | 0.63 |
| 40:UI:238:ILE:HG22 | 40:UI:239:THR:HG23 | 1.81 | 0.63 |
| 40:WF:323:VAL:HG22 | 40:WF:372:ARG:HG3 | 1.80 | 0.63 |
| 13:2V:48:GLU:HG2 | 13:2V:161:ARG:HG2 | 1.80 | 0.63 |
| 18:3T:247:PHE:O | 18:3W:374:GLN:NE2 | 2.32 | 0.63 |
| 20:4B:279:PRO:HA | 20:4B:282:ARG:HD2 | 1.79 | 0.63 |
| 21:4E:424:ALA:HB2 | 21:4E:505:ILE:HD13 | 1.79 | 0.63 |
| 21:4E:480:GLU:O | 21:4E:481:ASN:C | 2.37 | 0.63 |
| 22:4K:560:ARG:HA | 22:4K:563:LYS:HE2 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4Q:173:SER:HB2 | 23:4Q:181:LYS:CA | 2.29 | 0.63 |
| 27:4Z:4:ASN:O | 40:JG:285:GLN:NE2 | 2.32 | 0.63 |
| 36:5Y:131:VAL:HG23 | 36:5Y:132:THR:HG23 | 1.80 | 0.63 |
| 39:6K:138:GLY:HA2 | 39:6K:141:SER:HB2 | 1.80 | 0.63 |
| 40:BA:16:ILE:HD11 | 40:BA:171:ILE:HD11 | 1.80 | 0.63 |
| 40:DF:319:TYR:HB3 | 40:DF:323:VAL:HG11 | 1.80 | 0.63 |
| 40:EI:139:HIS:CE1 | 40:EI:170:SER:HB3 | 2.33 | 0.63 |
| 41:FM:235:GLY:HA3 | 41:FM:366:THR:HG21 | 1.80 | 0.63 |
| 41:FN:170:VAL:HG11 | 41:FN:377:LEU:HD21 | 1.81 | 0.63 |
| 40:GF:70:LEU:HD23 | 40:GF:145:THR:HG23 | 1.81 | 0.63 |
| 40:GI:278:ALA:O | 40:GI:280:LYS:N | 2.32 | 0.63 |
| 40:HA:225:THR:HG22 | 40:HA:229:ARG:HH21 | 1.64 | 0.63 |
| 40:HE:106:GLY:HA3 | 40:HE:148:GLY:CA | 2.17 | 0.63 |
| 41:HM:316:VAL:HG12 | 41:HM:352:ALA:HB3 | 1.81 | 0.63 |
| 41:HO:103:LYS:HA | 41:HO:107:THR:HB | 1.79 | 0.63 |
| 40:JG:91:GLN:HE22 | 40:JG:125:LEU:HD21 | 1.64 | 0.63 |
| 40:LD:260:VAL:HG13 | 41:LL:397:TRP:HH2 | 1.63 | 0.63 |
| 41:ML:317:PHE:HB2 | 41:ML:353:VAL:HG12 | 1.81 | 0.63 |
| 41:MM:236:VAL:HG22 | 41:MM:368:ILE:HD11 | 1.79 | 0.63 |
| 41:MM:248:ALA:HA | 41:MM:252:LYS:HD3 | 1.80 | 0.63 |
| 40:ND:109:THR:O | 40:ND:110:ILE:C | 2.36 | 0.63 |
| 40:PH:73:THR:OG1 | 41:PO:46:ARG:NH1 | 2.32 | 0.63 |
| 41:PO:421:PRO:HA | 41:PO:424:THR:HG22 | 1.80 | 0.63 |
| 41:QB:69:GLU:HB2 | 41:QB:96:GLY:HA2 | 1.79 | 0.63 |
| 41:QB:182:PRO:HB3 | 41:QB:384:GLN:HB3 | 1.81 | 0.63 |
| 41:QL:306:ARG:HA | 41:QL:340:TYR:HE1 | 1.63 | 0.63 |
| 41:QP:87:PRO:HA | 41:QP:90:PHE:HD1 | 1.63 | 0.63 |
| 41:SM:139:LEU:HD12 | 41:SM:170:VAL:HG12 | 1.79 | 0.63 |
| 41:UP:58:LYS:O | 41:UP:59:TYR:C | 2.35 | 0.63 |
| 40:VG:56:THR:HG22 | 40:WF:285:GLN:HG2 | 1.80 | 0.63 |
| 41:WN:245:GLN:O | 41:WN:246:LEU:C | 2.36 | 0.63 |
| 41:WO:268:PRO:HG2 | 41:WO:300:MET:HB2 | 1.79 | 0.63 |
| 9:2B:45:GLN:HB3 | 11:2K:247:HIS:CE1 | 2.34 | 0.63 |
| 11:2K:187:ARG:HE | 11:2K:251:TYR:HE1 | 1.47 | 0.63 |
| 23:4N:189:GLY:HA2 | 41:CM:46:ARG:NH1 | 2.14 | 0.63 |
| 38:6D:243:LYS:HG2 | 40:VF:215:ARG:HG3 | 1.80 | 0.63 |
| 40:AG:73:THR:HA | 40:AG:76:ASP:HB2 | 1.81 | 0.63 |
| 40:BI:222:PRO:HG2 | 41:BP:324:LYS:HE3 | 1.81 | 0.63 |
| 41:BP:319:GLY:HA2 | 41:BP:357:PRO:HB3 | 1.79 | 0.63 |
| 40:CI:120:ASP:OD2 | 40:CI:124:LYS:NZ | 2.32 | 0.63 |
| 41:CM:86:ARG:NH1 | 41:DM:281:TYR:O | 2.32 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CN:60:VAL:HG11 | 41:DN:281:TYR:HB3 | 1.80 | 0.63 |
| 40:DA:9:VAL:HG13 | 40:DA:68:VAL:HG13 | 1.81 | 0.63 |
| 40:DE:139:HIS:HB3 | 40:DE:150:THR:HG21 | 1.81 | 0.63 |
| 40:DH:71:GLU:HB3 | 40:DH:98:ASP:HB2 | 1.80 | 0.63 |
| 41:DL:19:LYS:HA | 41:DL:22:GLU:HB3 | 1.81 | 0.63 |
| 41:DN:237:THR:HA | 41:DN:240:LEU:HD21 | 1.81 | 0.63 |
| 40:FA:188:ILE:HG23 | 40:FA:424:MET:HG3 | 1.80 | 0.63 |
| 40:GE:175:PRO:HG3 | 40:GE:304:LYS:HB2 | 1.80 | 0.63 |
| 40:JG:2:ARG:HH22 | 40:JG:47:ASP:HB2 | 1.64 | 0.63 |
| 41:JL:2:ARG:HD2 | 41:JL:240:LEU:HD22 | 1.81 | 0.63 |
| 41:JO:207:LEU:HB3 | 41:JO:225:LEU:HD22 | 1.80 | 0.63 |
| 40:LG:352:LYS:HD2 | 41:LO:178:THR:CA | 2.28 | 0.63 |
| 41:NB:341:PHE:HB3 | 41:NB:348:ASN:HD21 | 1.64 | 0.63 |
| 40:NE:269:LEU:O | 40:NE:377:LEU:HA | 1.99 | 0.63 |
| 40:NG:119:LEU:HD11 | 40:NG:156:ARG:HG2 | 1.81 | 0.63 |
| 41:OB:317:PHE:HB2 | 41:OB:353:VAL:HG12 | 1.80 | 0.63 |
| 41:OO:236:VAL:HG23 | 41:OO:237:THR:HG23 | 1.81 | 0.63 |
| 41:PB:101:TRP:CZ3 | 41:PB:187:LEU:HB3 | 2.34 | 0.63 |
| 41:QM:49:VAL:O | 41:QM:62:ARG:NH2 | 2.31 | 0.63 |
| 41:QN:316:VAL:HA | 41:QN:352:ALA:HB3 | 1.80 | 0.63 |
| 40:RF:229:ARG:HH12 | 40:RF:365:GLY:HA3 | 1.63 | 0.63 |
| 41:RO:156:ARG:NH1 | 41:RO:195:ASN:O | 2.32 | 0.63 |
| 41:TB:31:ASP:OD2 | 41:TB:37:HIS:ND1 | 2.31 | 0.63 |
| 41:TL:3:GLU:OE1 | 41:TL:62:ARG:NH1 | 2.32 | 0.63 |
| 40:UF:100:ALA:CA | 41:UM:252:LYS:HB3 | 2.27 | 0.63 |
| 40:UG:273:ALA:HB2 | 40:UG:295:CYS:HB2 | 1.80 | 0.63 |
| 40:VI:90:GLU:O | 40:VI:121:ARG:NH1 | 2.32 | 0.63 |
| 40:VJ:72:PRO:HD2 | 41:VQ:2:ARG:HH12 | 1.64 | 0.63 |
| 40:WA:219:ILE:HG13 | 40:WA:222:PRO:HD3 | 1.80 | 0.63 |
| 7:1S:568:LEU:HD23 | 7:1S:570:LYS:HG2 | 1.79 | 0.63 |
| 8:1W:367:ILE:O | 40:VH:369:LYS:NZ | 2.31 | 0.63 |
| 13:2W:34:ILE:HA | 13:2W:48:GLU:O | 1.99 | 0.63 |
| 16:3L:100:GLU:OE2 | 18:3U:157:GLN:NE2 | 2.27 | 0.63 |
| 22:4J:92:LYS:N | 41:BN:280:GLN:H | 1.96 | 0.63 |
| 23:4N:246:TYR:HA | 40:DF:79:ARG:HE | 1.63 | 0.63 |
| 27:4Z:43:ASN:O | 27:4Z:45:ARG:N | 2.31 | 0.63 |
| 30:5G:33:ASN:HD21 | 30:5G:37:SER:HB3 | 1.62 | 0.63 |
| 36:5W:245:PRO:HA | 40:LG:429:LYS:HD2 | 1.81 | 0.63 |
| 36:5W:253:GLU:OE1 | 36:5W:257:GLN:NE2 | 2.32 | 0.63 |
| 40:AE:102:ASN:HB3 | 40:AE:105:ARG:HB2 | 1.81 | 0.63 |
| 40:BG:188:ILE:HD12 | 40:BG:424:MET:HG3 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BP:236:VAL:HG23 | 41:BP:237:THR:HG23 | 1.81 | 0.63 |
| 41:CB:65:LEU:HD22 | 41:CB:90:PHE:HE2 | 1.63 | 0.63 |
| 40:CH:68:VAL:HA | 40:CH:93:ILE:O | 1.98 | 0.63 |
| 40:CH:105:ARG:HA | 40:CH:109:THR:HG23 | 1.81 | 0.63 |
| 41:DN:123:GLU:O | 41:DN:124:ALA:C | 2.37 | 0.63 |
| 41:DO:30:ILE:HD11 | 41:DO:47:ILE:HD11 | 1.80 | 0.63 |
| 41:DO:163:ILE:HD11 | 41:DO:251:ARG:HD3 | 1.80 | 0.63 |
| 40:EG:239:THR:O | 40:EG:243:ARG:NH1 | 2.31 | 0.63 |
| 40:FE:273:ALA:HB2 | 40:FE:374:VAL:H | 1.62 | 0.63 |
| 41:IB:252:LYS:NZ | 42:IG:501:GTP:O1G | 2.32 | 0.63 |
| 40:KG:438:SER:HB2 | 41:KO:391:ARG:HD3 | 1.81 | 0.63 |
| 40:OH:222:PRO:HD2 | 41:OO:324:LYS:HZ2 | 1.64 | 0.63 |
| 40:QF:323:VAL:HA | 40:QF:372:ARG:HH21 | 1.63 | 0.63 |
| 41:RP:178:THR:HG22 | 41:RP:180:VAL:H | 1.63 | 0.63 |
| 40:SA:115:ILE:HG21 | 40:SA:152:LEU:HD22 | 1.80 | 0.63 |
| 41:TO:239:CYS:HB3 | 41:TO:247:ASN:HB2 | 1.80 | 0.63 |
| 40:UI:264:ARG:O | 40:UI:266:HIS:N | 2.32 | 0.63 |
| 40:WH:76:ASP:OD1 | 41:WO:46:ARG:NH2 | 2.26 | 0.63 |
| 41:WM:64:VAL:HG21 | 41:WM:120:VAL:HG22 | 1.81 | 0.63 |
| 41:WM:67:ASP:HA | 41:WM:143:THR:HG21 | 1.80 | 0.63 |
| 41:WP:309:ARG:NH1 | 41:WP:339:SER:O | 2.31 | 0.63 |
| 7:1T:116:ALA:HB3 | 7:1T:129:LEU:HB3 | 1.81 | 0.63 |
| 7:1T:498:MET:SD | 40:VG:84:ARG:NH2 | 2.71 | 0.63 |
| 9:2B:397:GLU:O | 9:2B:401:GLN:HB2 | 1.99 | 0.63 |
| 17:3R:183:ARG:HH22 | 17:3R:187:GLU:HB3 | 1.64 | 0.63 |
| 20:4A:149:ARG:NH1 | 20:4A:150:SER:CB | 2.61 | 0.63 |
| 40:CA:384:ALA:HA | 40:CA:387:TRP:CD1 | 2.34 | 0.63 |
| 40:CG:265:ILE:HD13 | 40:CG:434:VAL:HG21 | 1.81 | 0.63 |
| 40:CH:190:THR:HA | 40:CH:193:THR:HG22 | 1.81 | 0.63 |
| 40:DA:224:TYR:HB3 | 42:DA:501:GTP:N1 | 2.14 | 0.63 |
| 41:DN:68:LEU:HB2 | 41:DN:143:THR:OG1 | 1.99 | 0.63 |
| 40:GE:7:VAL:HG13 | 40:GE:66:VAL:HG13 | 1.80 | 0.63 |
| 41:HN:267:MET:HB3 | 41:HN:301:ALA:HB3 | 1.80 | 0.63 |
| 40:IH:178:SER:OG | 41:IO:347:ASN:ND2 | 2.30 | 0.63 |
| 40:II:259:LEU:O | 40:II:379:ASN:ND2 | 2.32 | 0.63 |
| 41:JB:204:ASN:ND2 | 43:JB:501:GDP:O2' | 2.32 | 0.63 |
| 41:KL:42:LEU:HD21 | 41:KL:243:PRO:HD2 | 1.81 | 0.63 |
| 41:KP:11:GLN:HA | 41:KP:72:THR:HG21 | 1.81 | 0.63 |
| 40:LA:16:ILE:HA | 40:LA:228:ASN:HB3 | 1.80 | 0.63 |
| 40:NG:142:GLY:O | 40:NG:186:ASN:ND2 | 2.32 | 0.63 |
| 41:ON:330:MET:O | 41:ON:334:GLN:NE2 | 2.32 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OO:187:LEU:O | 41:OO:191:GLN:NE2 | 2.30 | 0.63 |
| 41:PL:73:MET:HA | 41:PL:76:VAL:HG12 | 1.79 | 0.63 |
| 40:QG:76:ASP:HA | 40:QG:79:ARG:HE | 1.63 | 0.63 |
| 40:SH:76:ASP:OD1 | 40:SH:79:ARG:NH1 | 2.32 | 0.63 |
| 41:SL:282:ARG:HH12 | 41:SL:288:GLU:HG3 | 1.64 | 0.63 |
| 40:TG:298:PRO:HB3 | 40:TG:307:PRO:HD2 | 1.81 | 0.63 |
| 40:UG:332:ILE:HG23 | 40:UG:351:PHE:HD2 | 1.63 | 0.63 |
| 40:VA:73:THR:OG1 | 41:VO:46:ARG:NH1 | 2.28 | 0.63 |
| 41:WO:170:VAL:HG21 | 41:WO:377:LEU:HD11 | 1.80 | 0.63 |
| 4:1J:160:ASP:OD2 | 41:HM:306:ARG:NH1 | 2.31 | 0.62 |
| 16:3J:366:LEU:HD22 | 16:3L:31:GLN:HG3 | 1.80 | 0.62 |
| 17:3P:94:TYR:HB3 | 17:3P:98:ASP:HB2 | 1.80 | 0.62 |
| 21:4F:472:VAL:HG21 | 21:4F:498:VAL:HA | 1.80 | 0.62 |
| 22:4J:660:ARG:HH12 | 41:EM:38:GLY:H | 1.45 | 0.62 |
| 23:4M:90:MET:HB2 | 23:4M:113:TRP:CZ3 | 2.34 | 0.62 |
| 23:4Q:201:SER:HA | 40:DH:219:ILE:HA | 1.81 | 0.62 |
| 35:5T:183:PRO:HB2 | 35:5T:186:PRO:HD2 | 1.80 | 0.62 |
| 40:BH:252:LEU:HA | 40:BH:255:PHE:HD2 | 1.63 | 0.62 |
| 41:CB:316:VAL:HA | 41:CB:352:ALA:HB3 | 1.80 | 0.62 |
| 40:CH:276:ILE:HD11 | 40:CH:286:LEU:HD21 | 1.80 | 0.62 |
| 41:CL:354:CYS:SG | 41:CL:355:ASP:N | 2.72 | 0.62 |
| 40:DF:181:VAL:H | 41:DM:256:ASN:HD21 | 1.45 | 0.62 |
| 41:DP:242:PHE:HB3 | 41:DP:356:ILE:HB | 1.81 | 0.62 |
| 40:EI:90:GLU:O | 40:EI:91:GLN:C | 2.37 | 0.62 |
| 40:GE:167:LEU:HD22 | 40:GE:200:CYS:HB2 | 1.81 | 0.62 |
| 40:KD:258:ASN:HD21 | 41:KL:180:VAL:HG22 | 1.63 | 0.62 |
| 40:KH:221:ARG:NH1 | 41:KO:325:GLU:OE1 | 2.32 | 0.62 |
| 40:KH:285:GLN:HE22 | 40:KH:287:SER:HB3 | 1.62 | 0.62 |
| 42:MB:502:GTP:N1 | 40:MG:224:TYR:HB3 | 2.14 | 0.62 |
| 40:OH:88:HIS:CB | 40:OH:91:GLN:HB3 | 2.25 | 0.62 |
| 40:OH:213:CYS:HB3 | 40:OH:219:ILE:HG23 | 1.81 | 0.62 |
| 41:PB:324:LYS:HZ3 | 40:PG:222:PRO:HD2 | 1.64 | 0.62 |
| 40:PG:213:CYS:HA | 40:PG:217:LEU:HD23 | 1.81 | 0.62 |
| 40:QE:345:ASP:OD1 | 41:QM:390:ARG:NH2 | 2.32 | 0.62 |
| 40:QF:73:THR:OG1 | 41:QM:46:ARG:NH1 | 2.30 | 0.62 |
| 40:RA:98:ASP:O | 40:RA:105:ARG:NH2 | 2.32 | 0.62 |
| 40:RG:75:ILE:HD13 | 40:RG:94:THR:HB | 1.81 | 0.62 |
| 40:SG:271:THR:HG22 | 40:SG:301:GLN:HA | 1.81 | 0.62 |
| 40:SH:27:GLU:HA | 40:SH:361:THR:HG21 | 1.81 | 0.62 |
| 41:SL:253:LEU:O | 41:SL:257:MET:CB | 2.47 | 0.62 |
| 41:TL:134:GLN:HG2 | 41:TL:165:ASN:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UA:352:LYS:HD2 | 41:UB:179:VAL:HG23 | 1.81 | 0.62 |
| 8:1W:516:LYS:NZ | 8:1Y:188:GLU:OE2 | 2.32 | 0.62 |
| 8:1X:76:THR:HB | 8:1X:87:GLU:HG3 | 1.80 | 0.62 |
| 13:2X:30:ARG:HB3 | 13:2X:56:THR:HB | 1.81 | 0.62 |
| 16:3J:332:ASP:HA | 16:3L:215:LEU:HD21 | 1.82 | 0.62 |
| 16:3L:355:LYS:NZ | 16:3M:41:GLU:OE2 | 2.32 | 0.62 |
| 17:3O:395:VAL:HG22 | 17:3R:281:ILE:HD12 | 1.81 | 0.62 |
| 22:4H:33:ARG:NH2 | 41:ML:115:SER:OG | 2.32 | 0.62 |
| 23:4M:92:PRO:CB | 40:AG:89:PRO:CB | 2.78 | 0.62 |
| 31:5I:503:ASP:OD2 | 31:5I:505:ARG:NH1 | 2.33 | 0.62 |
| 36:5Y:123:ARG:NH1 | 40:KH:399:ALA:O | 2.32 | 0.62 |
| 40:BA:26:LEU:HD21 | 40:BA:363:VAL:HG12 | 1.81 | 0.62 |
| 41:BL:131:GLN:HE22 | 41:BL:240:LEU:HD22 | 1.64 | 0.62 |
| 40:CE:326:LYS:HZ2 | 41:CM:208:TYR:HB2 | 1.63 | 0.62 |
| 40:GH:195:LEU:HD11 | 40:GH:264:ARG:HG2 | 1.80 | 0.62 |
| 41:GN:323:MET:HE1 | 41:GN:353:VAL:HG21 | 1.80 | 0.62 |
| 40:HG:3:GLU:HA | 40:HG:51:THR:HA | 1.81 | 0.62 |
| 41:HP:178:THR:HB | 41:HP:181:GLU:HB2 | 1.78 | 0.62 |
| 40:IG:141:PHE:HB2 | 40:IG:173:PRO:HD3 | 1.81 | 0.62 |
| 40:JA:108:TYR:O | 40:JA:112:LYS:NZ | 2.31 | 0.62 |
| 41:JM:284:LEU:HG | 41:JM:363:MET:HG3 | 1.80 | 0.62 |
| 41:LL:6:HIS:O | 41:LL:63:ALA:HA | 1.99 | 0.62 |
| 41:MB:252:LYS:HA | 41:MB:255:VAL:HG12 | 1.81 | 0.62 |
| 40:MF:275:VAL:HA | 40:MF:367:LEU:HD21 | 1.80 | 0.62 |
| 40:OH:236:SER:HA | 40:OH:243:ARG:HH12 | 1.64 | 0.62 |
| 40:PF:213:CYS:HA | 40:PF:217:LEU:HD13 | 1.79 | 0.62 |
| 41:QP:124:ALA:O | 41:QP:125:GLU:C | 2.37 | 0.62 |
| 40:RG:75:ILE:HD11 | 40:RG:92:LEU:HB3 | 1.81 | 0.62 |
| 40:RH:260:VAL:HB | 41:RP:397:TRP:HZ2 | 1.64 | 0.62 |
| 41:SO:289:LEU:HD11 | 41:SO:363:MET:HB3 | 1.81 | 0.62 |
| 41:TN:174:LYS:HD2 | 41:TN:175:VAL:HG12 | 1.80 | 0.62 |
| 40:UG:205:ASP:OD1 | 40:UG:206:ASN:N | 2.32 | 0.62 |
| 40:UI:183:GLU:HB3 | 40:UI:184:PRO:HD3 | 1.80 | 0.62 |
| 12:2Q:161:ASN:HB3 | 12:2Q:164:VAL:HG12 | 1.81 | 0.62 |
| 13:2V:115:LYS:HD2 | 40:AH:264:ARG:NE | 2.08 | 0.62 |
| 13:2V:115:LYS:HB2 | 13:2V:116:PRO:HD2 | 1.81 | 0.62 |
| 18:3U:363:ARG:HD2 | 18:3U:367:GLU:HB3 | 1.79 | 0.62 |
| 19:3Y:179:ARG:HB3 | 19:3Y:183:LYS:NZ | 2.15 | 0.62 |
| 40:BF:88:HIS:HE1 | 40:CF:280:LYS:HB3 | 1.64 | 0.62 |
| 40:BH:63:PRO:HD3 | 40:BH:86:LEU:HG | 1.80 | 0.62 |
| 40:BI:20:CYS:HA | 40:BI:232:SER:HB2 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BO:12:CYS:HB3 | 41:BO:138:SER:HB3 | 1.82 | 0.62 |
| 41:BO:100:ASN:HB3 | 41:BO:103:LYS:HB2 | 1.82 | 0.62 |
| 41:DM:34:GLY:HA3 | 41:DM:58:LYS:HE3 | 1.82 | 0.62 |
| 40:EA:274:PRO:HA | 40:EA:276:ILE:HD12 | 1.80 | 0.62 |
| 40:EI:7:VAL:HG13 | 40:EI:122:ILE:HD11 | 1.81 | 0.62 |
| 41:FN:62:ARG:NH2 | 41:FN:127:CYS:SG | 2.72 | 0.62 |
| 40:HE:195:LEU:HD11 | 40:HE:264:ARG:HG3 | 1.81 | 0.62 |
| 40:HF:27:GLU:OE1 | 40:HF:243:ARG:NH2 | 2.32 | 0.62 |
| 41:KL:375:GLN:HG2 | 41:KL:422:VAL:HG23 | 1.81 | 0.62 |
| 41:KO:51:TYR:HB3 | 41:KO:59:TYR:HB3 | 1.81 | 0.62 |
| 41:LM:30:ILE:HD11 | 41:LM:47:ILE:HD11 | 1.80 | 0.62 |
| 40:MA:20:CYS:HA | 40:MA:232:SER:HB2 | 1.81 | 0.62 |
| 40:MF:317:LEU:HG | 40:MF:376:MET:HG3 | 1.81 | 0.62 |
| 41:ON:178:THR:HG22 | 41:ON:180:VAL:H | 1.64 | 0.62 |
| 40:QE:225:THR:HG22 | 40:QE:229:ARG:HD2 | 1.79 | 0.62 |
| 40:SG:76:ASP:HA | 40:SG:79:ARG:HG2 | 1.81 | 0.62 |
| 41:TM:252:LYS:HA | 41:TM:255:VAL:HG12 | 1.81 | 0.62 |
| 41:TO:7:LEU:HD12 | 41:TO:151:LEU:HD21 | 1.81 | 0.62 |
| 40:UF:238:ILE:HG23 | 40:UF:239:THR:HG23 | 1.80 | 0.62 |
| 40:VA:329:ASN:HB2 | 41:VB:175:VAL:HG11 | 1.80 | 0.62 |
| 41:WB:4:ILE:HB | 41:WB:50:TYR:HE1 | 1.65 | 0.62 |
| 41:WN:295:ASP:HB2 | 41:WN:297:LYS:HE2 | 1.80 | 0.62 |
| 7:1T:373:PRO:HB3 | 10:2E:137:LYS:HG3 | 1.80 | 0.62 |
| 7:1U:243:GLY:HA2 | 7:1U:281:TYR:CD1 | 2.34 | 0.62 |
| 8:1W:277:ARG:HH22 | 41:UP:57:GLY:HA3 | 1.63 | 0.62 |
| 16:3L:8:PRO:HG2 | 18:3T:327:ARG:HD2 | 1.81 | 0.62 |
| 22:4J:642:CYS:HB3 | 22:4J:690:TYR:HB3 | 1.81 | 0.62 |
| 39:6L:131:GLU:HB3 | 39:6L:136:TYR:HB2 | 1.82 | 0.62 |
| 41:AN:49:VAL:HG11 | 41:AN:241:ARG:HG2 | 1.81 | 0.62 |
| 40:DA:333:ALA:HB2 | 41:DB:175:VAL:HG11 | 1.81 | 0.62 |
| 40:DH:346:TRP:HZ2 | 40:DH:434:VAL:HG13 | 1.65 | 0.62 |
| 41:DP:240:LEU:HD22 | 41:DP:249:ASP:HB2 | 1.82 | 0.62 |
| 41:GB:6:HIS:O | 41:GB:63:ALA:HA | 2.00 | 0.62 |
| 40:GE:325:PRO:HB3 | 41:GM:222:TYR:CE1 | 2.34 | 0.62 |
| 40:GG:273:ALA:HB1 | 40:GG:274:PRO:HD2 | 1.82 | 0.62 |
| 41:HM:237:THR:HG22 | 41:HM:250:LEU:HD21 | 1.80 | 0.62 |
| 41:HN:271:ALA:HB1 | 41:HN:289:LEU:HG | 1.79 | 0.62 |
| 41:IP:2:ARG:HD2 | 41:IP:240:LEU:HB2 | 1.81 | 0.62 |
| 41:JL:105:HIS:HA | 41:JL:150:LEU:HD21 | 1.81 | 0.62 |
| 41:JL:292:GLN:O | 41:JL:298:ASN:ND2 | 2.32 | 0.62 |
| 41:JO:131:GLN:HE22 | 41:JO:249:ASP:HB3 | 1.63 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KN:207:LEU:HB3 | 41:KN:225:LEU:HD22 | 1.81 | 0.62 |
| 41:KP:165:ASN:ND2 | 41:KP:198:GLU:OE2 | 2.31 | 0.62 |
| 40:MG:352:LYS:HZ2 | 41:MO:179:VAL:HG23 | 1.62 | 0.62 |
| 41:NB:314:ALA:HB3 | 41:NB:368:ILE:HB | 1.81 | 0.62 |
| 40:NE:228:ASN:HD21 | 42:NE:501:GTP:HN1 | 1.47 | 0.62 |
| 40:NF:356:ASN:OD1 | 40:NF:358:GLN:NE2 | 2.32 | 0.62 |
| 41:OB:222:TYR:O | 41:OB:226:ASN:ND2 | 2.33 | 0.62 |
| 41:QB:261:PRO:HD3 | 40:QG:405:HIS:CD2 | 2.34 | 0.62 |
| 41:RL:2:ARG:HH12 | 41:RL:240:LEU:HB2 | 1.65 | 0.62 |
| 41:RM:43:GLN:O | 41:RM:47:ILE:HB | 2.00 | 0.62 |
| 41:SB:395:LEU:O | 41:SB:397:TRP:N | 2.32 | 0.62 |
| 40:SE:210:TYR:HE2 | 41:SL:324:LYS:HA | 1.64 | 0.62 |
| 41:TL:244:GLY:HA3 | 41:TL:354:CYS:HA | 1.81 | 0.62 |
| 40:WI:194:THR:HG22 | 40:WI:198:SER:HB2 | 1.81 | 0.62 |
| 4:1H:76:ILE:O | 40:HA:342:GLN:NE2 | 2.33 | 0.62 |
| 7:1T:276:CYS:HB2 | 7:1T:281:TYR:HA | 1.82 | 0.62 |
| 8:1X:100:LEU:HD13 | 11:2I:250:ILE:HA | 1.82 | 0.62 |
| 13:2T:2:PHE:O | 13:2T:7:GLN:NE2 | 2.32 | 0.62 |
| 13:2X:45:LEU:HD12 | 41:WM:125:GLU:HB2 | 1.81 | 0.62 |
| 15:3F:320:ARG:NH2 | 15:3F:331:ASP:OD2 | 2.33 | 0.62 |
| 18:3U:94:ARG:NH1 | 18:3U:98:ASP:OD1 | 2.32 | 0.62 |
| 40:BG:258:ASN:HD22 | 41:BO:179:VAL:HB | 1.64 | 0.62 |
| 40:CA:209:ILE:HB | 40:CA:227:LEU:HD13 | 1.81 | 0.62 |
| 40:CF:294:ALA:O | 40:CF:300:ASN:ND2 | 2.32 | 0.62 |
| 41:CN:86:ARG:HH22 | 41:DN:282:ARG:HB2 | 1.65 | 0.62 |
| 40:DA:154:MET:HB3 | 40:DA:197:HIS:HB3 | 1.81 | 0.62 |
| 41:DB:391:ARG:O | 41:DB:392:LYS:C | 2.37 | 0.62 |
| 40:DH:102:ASN:O | 40:DH:103:TYR:C | 2.38 | 0.62 |
| 41:DM:259:PRO:HG3 | 41:DM:311:LEU:HD21 | 1.82 | 0.62 |
| 41:EB:28:HIS:O | 41:EB:43:GLN:NE2 | 2.33 | 0.62 |
| 41:EB:156:ARG:NH1 | 41:EB:195:ASN:O | 2.32 | 0.62 |
| 40:FI:171:ILE:HD12 | 40:FI:206:ASN:HD21 | 1.63 | 0.62 |
| 40:HA:204:VAL:HG23 | 40:HA:302:MET:HB3 | 1.82 | 0.62 |
| 40:IA:254:GLU:OE2 | 41:IB:99:ASN:ND2 | 2.32 | 0.62 |
| 41:IQ:47:ILE:HG12 | 41:IQ:51:TYR:HB2 | 1.81 | 0.62 |
| 41:JM:7:LEU:HD12 | 41:JM:135:LEU:HB2 | 1.82 | 0.62 |
| 40:LA:73:THR:HA | 40:LA:76:ASP:HB2 | 1.80 | 0.62 |
| 41:MM:178:THR:HB | 41:MM:181:GLU:HG3 | 1.80 | 0.62 |
| 40:NG:90:GLU:HB3 | 40:NG:121:ARG:HH12 | 1.64 | 0.62 |
| 40:NH:73:THR:HA | 40:NH:76:ASP:HB2 | 1.81 | 0.62 |
| 41:NL:272:PRO:HG3 | 41:NL:364:SER:HA | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:NM:27:GLU:OE2 | 41:NM:318:ARG:NH2 | 2.33 | 0.62 |
| 41:OP:133:PHE:HB2 | 41:OP:164:MET:HB2 | 1.81 | 0.62 |
| 40:RH:11:GLN:O | 40:RH:15:GLN:NE2 | 2.33 | 0.62 |
| 40:RI:91:GLN:OE1 | 40:RI:121:ARG:NH2 | 2.33 | 0.62 |
| 40:SF:238:ILE:HD13 | 40:SF:377:LEU:HD11 | 1.81 | 0.62 |
| 40:SG:285:GLN:O | 40:SG:372:ARG:NH2 | 2.31 | 0.62 |
| 40:TH:276:ILE:HD11 | 40:TH:280:LYS:HG3 | 1.81 | 0.62 |
| 40:UI:174:ALA:HB1 | 40:UI:207:GLU:HG3 | 1.80 | 0.62 |
| 41:UO:232:THR:HG22 | 41:UO:270:PHE:HB2 | 1.81 | 0.62 |
| 41:UO:248:ALA:HA | 41:UO:252:LYS:HD2 | 1.81 | 0.62 |
| 41:WB:60:VAL:HG11 | 41:WB:86:ARG:HG3 | 1.81 | 0.62 |
| 40:WH:326:LYS:HE2 | 41:WP:220:PRO:HD2 | 1.82 | 0.62 |
| 5:1M:241:LEU:HB3 | 40:GH:159:VAL:HG21 | 1.81 | 0.62 |
| 13:2V:77:VAL:HG22 | 13:2V:133:GLN:HG3 | 1.81 | 0.62 |
| 21:4D:534:HIS:O | 21:4D:535:ILE:C | 2.37 | 0.62 |
| 40:AF:352:LYS:HD2 | 41:AN:179:VAL:HG23 | 1.81 | 0.62 |
| 41:CB:77:ARG:NH1 | 41:CB:82:GLY:O | 2.32 | 0.62 |
| 41:CP:310:TYR:CD1 | 41:CP:371:SER:HB2 | 2.34 | 0.62 |
| 40:DA:88:HIS:HD2 | 40:EA:283:HIS:HB2 | 1.64 | 0.62 |
| 41:DM:68:LEU:HB2 | 41:DM:143:THR:HG23 | 1.82 | 0.62 |
| 41:EN:313:VAL:HB | 41:EN:349:VAL:HG22 | 1.80 | 0.62 |
| 40:FF:88:HIS:HB3 | 40:FF:91:GLN:HB2 | 1.80 | 0.62 |
| 41:FO:248:ALA:HA | 41:FO:252:LYS:HD3 | 1.80 | 0.62 |
| 41:GN:202:ILE:HG23 | 41:GN:268:PRO:HG3 | 1.81 | 0.62 |
| 40:HF:98:ASP:O | 40:HF:105:ARG:NH1 | 2.33 | 0.62 |
| 40:HH:6:SER:O | 40:HH:65:ALA:HA | 1.99 | 0.62 |
| 40:IF:64:ARG:NH1 | 40:IF:129:CYS:SG | 2.72 | 0.62 |
| 40:II:142:GLY:HA2 | 40:II:183:GLU:HG3 | 1.81 | 0.62 |
| 41:IM:392:LYS:HD3 | 41:IM:395:LEU:HD23 | 1.82 | 0.62 |
| 40:JE:88:HIS:HB3 | 40:JE:91:GLN:HB2 | 1.80 | 0.62 |
| 40:LH:3:GLU:HA | 40:LH:51:THR:HA | 1.82 | 0.62 |
| 41:LL:68:LEU:HD12 | 41:LL:97:ALA:HB2 | 1.82 | 0.62 |
| 41:LO:334:GLN:NE2 | 41:LO:348:ASN:OD1 | 2.32 | 0.62 |
| 40:MH:177:VAL:CG2 | 41:MO:327:ASP:HB3 | 2.30 | 0.62 |
| 41:MN:237:THR:HG22 | 41:MN:250:LEU:HD21 | 1.82 | 0.62 |
| 41:MO:5:VAL:HG23 | 41:MO:130:LEU:HD11 | 1.80 | 0.62 |
| 40:OE:376:MET:SD | 40:OE:378:SER:OG | 2.52 | 0.62 |
| 40:OF:133:GLN:NE2 | 40:OF:251:ASP:OD2 | 2.32 | 0.62 |
| 40:QE:140:SER:HA | 40:QE:171:ILE:HB | 1.80 | 0.62 |
| 40:RI:73:THR:HG22 | 41:RP:46:ARG:HE | 1.63 | 0.62 |
| 41:RO:8:GLN:NE2 | 41:RO:14:ASN:OD1 | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SF:177:VAL:HG21 | 41:SM:327:ASP:HB2 | 1.81 | 0.62 |
| 41:SP:248:ALA:HA | 41:SP:252:LYS:HD3 | 1.81 | 0.62 |
| 41:TB:16:ILE:HD13 | 41:TB:226:ASN:HD21 | 1.64 | 0.62 |
| 40:UF:21:TRP:HA | 40:UF:24:TYR:HB2 | 1.82 | 0.62 |
| 40:VF:120:ASP:OD1 | 40:VF:124:LYS:NZ | 2.31 | 0.62 |
| 41:VN:289:LEU:HD11 | 41:VN:363:MET:HB3 | 1.81 | 0.62 |
| 41:VO:55:THR:HG23 | 41:WN:283:ALA:HA | 1.81 | 0.62 |
| 22:4I:456:TYR:HD1 | 22:4I:458:LEU:H | 1.47 | 0.62 |
| 23:4N:250:VAL:HG13 | 23:4N:253:TYR:CB | 2.29 | 0.62 |
| 24:4O:257:PHE:HD1 | 40:EE:221:ARG:HG2 | 1.64 | 0.62 |
| 23:4P:250:VAL:HG13 | 23:4P:253:TYR:CB | 2.29 | 0.62 |
| 31:5I:721:LYS:HB2 | 31:5I:728:LYS:HB3 | 1.79 | 0.62 |
| 40:BA:188:ILE:HD12 | 40:BA:424:MET:HG3 | 1.81 | 0.62 |
| 40:BG:224:TYR:O | 40:BG:228:ASN:ND2 | 2.25 | 0.62 |
| 40:BI:274:PRO:HD2 | 40:BI:291:ILE:HB | 1.80 | 0.62 |
| 41:BN:398:TYR:HB3 | 41:BN:403:MET:HG3 | 1.80 | 0.62 |
| 41:BO:268:PRO:HG2 | 41:BO:300:MET:HB2 | 1.82 | 0.62 |
| 41:DB:245:GLN:O | 41:DB:246:LEU:C | 2.38 | 0.62 |
| 41:DB:337:ASN:O | 41:DB:338:SER:C | 2.38 | 0.62 |
| 41:DM:42:LEU:HD22 | 41:DM:356:ILE:HD11 | 1.80 | 0.62 |
| 41:DO:317:PHE:HB2 | 41:DO:353:VAL:HG12 | 1.81 | 0.62 |
| 41:EN:222:TYR:O | 41:EN:226:ASN:HB2 | 2.00 | 0.62 |
| 41:EP:420:ASN:O | 41:EP:423:VAL:N | 2.32 | 0.62 |
| 40:FA:182:VAL:HG22 | 41:FN:256:ASN:HD21 | 1.64 | 0.62 |
| 41:FP:209:ASP:OD1 | 41:FP:213:ARG:NH1 | 2.33 | 0.62 |
| 40:GA:104:ALA:O | 40:GA:108:TYR:HB2 | 2.00 | 0.62 |
| 40:GE:23:LEU:HD21 | 40:GE:236:SER:HB2 | 1.80 | 0.62 |
| 40:GE:393:LYS:HA | 40:GE:396:LEU:HD12 | 1.81 | 0.62 |
| 40:IA:97:GLU:OE1 | 40:IA:105:ARG:NH2 | 2.33 | 0.62 |
| 40:IF:195:LEU:HD12 | 40:IF:266:HIS:HE1 | 1.65 | 0.62 |
| 41:IQ:132:GLY:HA2 | 41:IQ:163:ILE:O | 2.00 | 0.62 |
| 40:ME:174:ALA:HB3 | 40:ME:178:SER:H | 1.65 | 0.62 |
| 41:OL:16:ILE:HA | 41:OL:226:ASN:HB3 | 1.81 | 0.62 |
| 41:QB:121:ARG:O | 41:QB:122:LYS:C | 2.38 | 0.62 |
| 41:QB:417:ASP:O | 41:QB:421:PRO:HD2 | 1.98 | 0.62 |
| 41:RO:257:MET:O | 41:RO:370:ASN:ND2 | 2.32 | 0.62 |
| 40:TG:219:ILE:HD12 | 40:TG:222:PRO:HB3 | 1.82 | 0.62 |
| 41:UP:258:VAL:HG22 | 41:UP:266:PHE:CZ | 2.33 | 0.62 |
| 40:VF:79:ARG:HH21 | 40:VF:92:LEU:HB3 | 1.65 | 0.62 |
| 41:WP:204:ASN:ND2 | 43:WP:501:GDP:O2' | 2.33 | 0.62 |
| 16:3J:317:ARG:NH1 | 16:3L:57:GLU:OE1 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4E:260:ARG:HD2 | 21:4E:285:ARG:HH12 | 1.65 | 0.62 |
| 23:4M:171:PRO:HD3 | 41:CB:44:LEU:HD23 | 1.82 | 0.62 |
| 36:5Z:216:GLU:OE1 | 36:5Z:221:GLN:NE2 | 2.32 | 0.62 |
| 41:AB:316:VAL:HG12 | 41:AB:352:ALA:HB3 | 1.82 | 0.62 |
| 41:AP:421:PRO:HA | 41:AP:424:THR:HG22 | 1.80 | 0.62 |
| 41:BM:358:PRO:HG3 | 41:BM:364:SER:HB3 | 1.82 | 0.62 |
| 41:BP:243:PRO:HD2 | 41:BP:356:ILE:HG13 | 1.80 | 0.62 |
| 40:CA:174:ALA:HB1 | 40:CA:175:PRO:HD2 | 1.81 | 0.62 |
| 41:CM:310:TYR:HA | 41:CM:371:SER:HA | 1.80 | 0.62 |
| 41:CP:357:PRO:HB2 | 41:CP:358:PRO:HD2 | 1.80 | 0.62 |
| 40:DA:37:PRO:O | 40:DA:38:SER:C | 2.38 | 0.62 |
| 40:GE:238:ILE:HG13 | 40:GE:239:THR:HG23 | 1.81 | 0.62 |
| 41:GN:198:GLU:HG2 | 41:GN:266:PHE:HE2 | 1.64 | 0.62 |
| 40:JA:11:GLN:NE2 | 40:JA:71:GLU:OE2 | 2.33 | 0.62 |
| 40:JA:76:ASP:OD1 | 41:JN:46:ARG:NH2 | 2.32 | 0.62 |
| 41:JN:193:VAL:HG11 | 41:JN:262:ARG:HH21 | 1.64 | 0.62 |
| 40:KF:264:ARG:NH2 | 40:KF:423:ASP:OD1 | 2.33 | 0.62 |
| 40:LF:37:PRO:O | 40:LF:38:SER:C | 2.38 | 0.62 |
| 41:LM:33:THR:O | 41:LM:58:LYS:NZ | 2.32 | 0.62 |
| 41:MB:101:TRP:HB2 | 41:MB:184:ASN:HD22 | 1.65 | 0.62 |
| 40:ND:273:ALA:O | 40:ND:274:PRO:C | 2.38 | 0.62 |
| 41:OL:149:THR:HA | 41:OL:152:ILE:HG22 | 1.81 | 0.62 |
| 40:PA:240:ALA:O | 40:PA:356:ASN:ND2 | 2.32 | 0.62 |
| 40:RI:70:LEU:HD12 | 40:RI:145:THR:HG22 | 1.81 | 0.62 |
| 41:RP:191:GLN:O | 41:RP:195:ASN:ND2 | 2.33 | 0.62 |
| 40:SF:11:GLN:NE2 | 41:SM:247:ASN:OD1 | 2.32 | 0.62 |
| 41:SO:102:ALA:HB1 | 41:SO:401:GLU:HG2 | 1.81 | 0.62 |
| 41:SO:211:CYS:HA | 41:SO:215:LEU:HB2 | 1.81 | 0.62 |
| 40:TH:175:PRO:O | 40:TH:389:ARG:NH2 | 2.31 | 0.62 |
| 40:UE:318:LEU:HB2 | 40:UE:375:CYS:HB3 | 1.80 | 0.62 |
| 40:UI:28:HIS:O | 40:UI:30:ILE:N | 2.32 | 0.62 |
| 41:UM:424:THR:OG1 | 41:UM:425:ARG:NH1 | 2.33 | 0.62 |
| 40:VJ:20:CYS:HA | 40:VJ:232:SER:HB2 | 1.82 | 0.62 |
| 7:1S:602:ILE:HG23 | 7:1S:614:TRP:HB2 | 1.81 | 0.62 |
| 8:1X:100:LEU:CD1 | 11:2I:251:TYR:H | 2.13 | 0.62 |
| 10:2E:97:GLN:O | 10:2E:101:GLN:HB2 | 1.99 | 0.62 |
| 12:2O:254:CYS:SG | 12:2O:255:LEU:N | 2.71 | 0.62 |
| 21:4D:473:VAL:HA | 21:4D:483:ILE:O | 2.00 | 0.62 |
| 24:4O:235:THR:HG22 | 24:4O:268:ALA:HB2 | 1.81 | 0.62 |
| 23:4P:257:PHE:HB3 | 41:EN:322:SER:HB3 | 1.82 | 0.62 |
| 35:5T:162:MET:HE3 | 41:KL:320:ARG:HA | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AP:374:ILE:HG22 | 41:AP:422:VAL:HG21 | 1.82 | 0.62 |
| 40:CH:317:LEU:HD23 | 40:CH:376:MET:HE3 | 1.82 | 0.62 |
| 40:CH:405:HIS:O | 40:CH:407:TYR:N | 2.33 | 0.62 |
| 41:CM:303:CYS:O | 41:CM:304:ASP:C | 2.37 | 0.62 |
| 40:DA:295:CYS:HB3 | 40:DA:376:MET:HG2 | 1.81 | 0.62 |
| 40:DE:380:THR:HG23 | 40:DE:383:ILE:HB | 1.81 | 0.62 |
| 41:DP:245:GLN:O | 41:DP:246:LEU:C | 2.38 | 0.62 |
| 40:FH:324:VAL:HG12 | 40:FH:326:LYS:H | 1.64 | 0.62 |
| 41:GN:1:MET:HG2 | 41:GN:48:ASN:HB2 | 1.82 | 0.62 |
| 41:GN:58:LYS:O | 41:GN:59:TYR:C | 2.38 | 0.62 |
| 41:GN:298:ASN:O | 41:GN:299:MET:C | 2.38 | 0.62 |
| 41:GN:304:ASP:HB3 | 41:GN:307:HIS:CE1 | 2.34 | 0.62 |
| 41:GP:73:MET:HG3 | 41:GP:92:PHE:HB3 | 1.82 | 0.62 |
| 41:KL:417:ASP:O | 41:KL:421:PRO:HD2 | 2.00 | 0.62 |
| 41:KP:156:ARG:HH21 | 41:KP:164:MET:HG2 | 1.65 | 0.62 |
| 41:MB:247:ASN:O | 41:MB:252:LYS:NZ | 2.32 | 0.62 |
| 40:NH:205:ASP:HB3 | 40:NH:303:VAL:HA | 1.82 | 0.62 |
| 40:PF:271:THR:HB | 40:PF:376:MET:HB2 | 1.82 | 0.62 |
| 41:QB:192:LEU:HD22 | 41:QB:196:THR:HB | 1.80 | 0.62 |
| 41:QO:404:ASP:HB3 | 41:QO:407:GLU:HG3 | 1.82 | 0.62 |
| 41:RL:267:MET:HG3 | 41:RL:367:PHE:HE1 | 1.64 | 0.62 |
| 40:SE:76:ASP:HA | 40:SE:79:ARG:HG2 | 1.81 | 0.62 |
| 41:SL:165:ASN:ND2 | 41:SL:198:GLU:OE1 | 2.33 | 0.62 |
| 41:SL:282:ARG:HD2 | 41:SL:283:ALA:H | 1.65 | 0.62 |
| 41:TB:131:GLN:HE22 | 41:TB:240:LEU:HD22 | 1.64 | 0.62 |
| 41:UN:3:GLU:OE2 | 41:UN:62:ARG:NH2 | 2.31 | 0.62 |
| 41:UO:252:LYS:O | 41:UO:256:ASN:ND2 | 2.33 | 0.62 |
| 41:VN:20:PHE:HA | 41:VN:230:SER:HB2 | 1.81 | 0.62 |
| 41:VO:341:PHE:HB3 | 41:VO:348:ASN:HD21 | 1.65 | 0.62 |
| 41:VP:248:ALA:HA | 41:VP:252:LYS:HD2 | 1.81 | 0.62 |
| 10:2G:101:GLN:NE2 | 10:2G:102:ASP:OD1 | 2.32 | 0.62 |
| 22:4I:434:LEU:O | 22:4I:455:SER:HA | 2.00 | 0.62 |
| 23:4M:89:SER:O | 40:AG:84:ARG:HD2 | 1.99 | 0.62 |
| 41:AN:52:ASN:OD1 | 41:AN:62:ARG:NH1 | 2.31 | 0.62 |
| 40:BF:14:VAL:O | 40:BF:18:ASN:ND2 | 2.32 | 0.62 |
| 40:CH:317:LEU:HB2 | 40:CH:319:TYR:CE2 | 2.35 | 0.62 |
| 41:CP:135:LEU:HD23 | 41:CP:166:THR:HG22 | 1.82 | 0.62 |
| 41:DB:262:ARG:HE | 41:DB:418:LEU:HD13 | 1.63 | 0.62 |
| 40:EA:380:THR:HG22 | 40:EA:382:ALA:H | 1.65 | 0.62 |
| 41:EB:11:GLN:HA | 41:EB:72:THR:HG21 | 1.82 | 0.62 |
| 41:EL:132:GLY:HA3 | 41:EL:163:ILE:O | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FB:137:HIS:O | 41:FB:168:SER:HA | 2.00 | 0.62 |
| 40:FE:73:THR:HA | 40:FE:76:ASP:HB2 | 1.81 | 0.62 |
| 41:IO:341:PHE:HB3 | 41:IO:348:ASN:HD21 | 1.63 | 0.62 |
| 40:KF:168:GLU:HB3 | 40:KF:201:ALA:HA | 1.82 | 0.62 |
| 40:OD:121:ARG:HD2 | 40:OD:124:LYS:HZ3 | 1.65 | 0.62 |
| 40:OH:101:ASN:HA | 40:OH:144:GLY:H | 1.64 | 0.62 |
| 41:PO:156:ARG:NH1 | 41:PO:195:ASN:O | 2.33 | 0.62 |
| 40:QF:320:ARG:HG2 | 40:QF:356:ASN:HD21 | 1.65 | 0.62 |
| 41:WO:42:LEU:HD12 | 41:WO:45:GLU:HG3 | 1.82 | 0.62 |
| 11:2K:231:GLU:HA | 11:2K:234:MET:HE2 | 1.81 | 0.61 |
| 12:2M:157:LEU:HD23 | 12:2M:196:ILE:HB | 1.81 | 0.61 |
| 12:2N:254:CYS:SG | 12:2N:255:LEU:N | 2.73 | 0.61 |
| 13:2U:156:ILE:HD11 | 13:2U:165:VAL:HG21 | 1.82 | 0.61 |
| 23:4M:108:ASN:ND2 | 23:4M:111:GLN:HB2 | 2.15 | 0.61 |
| 23:4M:249:TYR:CZ | 23:4M:251:PRO:HA | 2.35 | 0.61 |
| 23:4R:218:SER:O | 23:4R:219:GLN:C | 2.38 | 0.61 |
| 36:5X:118:TYR:CE2 | 41:KL:421:PRO:HD3 | 2.34 | 0.61 |
| 40:BA:222:PRO:O | 41:BN:324:LYS:NZ | 2.33 | 0.61 |
| 40:BG:215:ARG:NH2 | 40:BG:299:ALA:O | 2.33 | 0.61 |
| 41:CO:245:GLN:O | 41:CO:246:LEU:C | 2.39 | 0.61 |
| 41:CO:354:CYS:SG | 41:CO:355:ASP:N | 2.73 | 0.61 |
| 40:DE:261:PRO:HB3 | 40:DE:346:TRP:HH2 | 1.65 | 0.61 |
| 40:DH:69:ASP:HB3 | 40:DH:75:ILE:HG13 | 1.82 | 0.61 |
| 41:DN:266:PHE:HB3 | 41:DN:369:GLY:C | 2.20 | 0.61 |
| 41:DO:190:HIS:HD2 | 41:DO:411:ALA:HA | 1.65 | 0.61 |
| 41:EL:320:ARG:NH2 | 41:EL:355:ASP:OD1 | 2.33 | 0.61 |
| 40:FA:394:PHE:CZ | 40:FA:417:PHE:HB3 | 2.35 | 0.61 |
| 40:GI:188:ILE:HG13 | 40:GI:394:PHE:HB2 | 1.82 | 0.61 |
| 40:IA:71:GLU:HB3 | 40:IA:98:ASP:HA | 1.82 | 0.61 |
| 41:JL:67:ASP:OD1 | 41:JL:69:GLU:N | 2.30 | 0.61 |
| 40:LG:273:ALA:CB | 40:LG:274:PRO:HD2 | 2.27 | 0.61 |
| 40:LG:352:LYS:HE3 | 41:LO:179:VAL:HA | 1.81 | 0.61 |
| 40:MH:273:ALA:CB | 40:MH:374:VAL:HG12 | 2.22 | 0.61 |
| 41:MO:107:THR:OG1 | 41:MO:108:GLU:N | 2.33 | 0.61 |
| 41:MP:398:TYR:HB3 | 41:MP:403:MET:HG3 | 1.82 | 0.61 |
| 40:OA:166:LYS:HD2 | 40:OA:198:SER:HA | 1.82 | 0.61 |
| 40:OF:318:LEU:O | 40:OF:374:VAL:HA | 2.00 | 0.61 |
| 41:OP:103:LYS:HA | 41:OP:107:THR:HB | 1.82 | 0.61 |
| 41:PB:238:THR:HG21 | 41:PB:318:ARG:HD2 | 1.82 | 0.61 |
| 41:PL:178:THR:HG22 | 41:PL:180:VAL:H | 1.64 | 0.61 |
| 40:QA:273:ALA:HB1 | 40:QA:291:ILE:HB | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RH:288:VAL:HA | 40:RH:291:ILE:HG12 | 1.82 | 0.61 |
| 41:RP:7:LEU:O | 41:RP:135:LEU:HA | 2.00 | 0.61 |
| 40:SA:206:ASN:OD1 | 42:SN:501:GTP:O2' | 2.17 | 0.61 |
| 41:SB:191:GLN:NE2 | 41:SB:195:ASN:OD1 | 2.32 | 0.61 |
| 40:SF:298:PRO:HA | 40:SF:301:GLN:HE22 | 1.65 | 0.61 |
| 40:SF:406:TRP:CZ3 | 41:SM:255:VAL:HA | 2.35 | 0.61 |
| 41:SL:170:VAL:HG11 | 41:SL:377:LEU:HD21 | 1.80 | 0.61 |
| 41:SN:137:HIS:O | 41:SN:168:SER:HA | 1.99 | 0.61 |
| 41:SP:2:ARG:HB3 | 41:SP:131:GLN:HB2 | 1.82 | 0.61 |
| 41:TB:292:GLN:O | 41:TB:298:ASN:ND2 | 2.33 | 0.61 |
| 41:UP:290:THR:HG21 | 41:UP:329:GLN:HB3 | 1.82 | 0.61 |
| 41:VN:11:GLN:NE2 | 41:VN:15:GLN:OE1 | 2.33 | 0.61 |
| 41:WM:8:GLN:HG3 | 41:WM:65:LEU:HA | 1.82 | 0.61 |
| 41:WQ:222:TYR:O | 41:WQ:226:ASN:ND2 | 2.33 | 0.61 |
| 7:1T:602:ILE:HG23 | 7:1T:614:TRP:HB2 | 1.83 | 0.61 |
| 8:1X:320:ASN:OD1 | 8:1X:323:GLN:NE2 | 2.33 | 0.61 |
| 12:2N:116:LEU:HD13 | 12:2N:168:THR:HG22 | 1.81 | 0.61 |
| 19:3Y:216:ALA:HB2 | 40:KF:58:ALA:HB2 | 1.81 | 0.61 |
| 21:4F:27:ARG:HH21 | 40:LD:245:ASP:HA | 1.65 | 0.61 |
| 36:5X:53:ASP:O | 36:5X:57:GLN:NE2 | 2.31 | 0.61 |
| 38:6C:140:ASN:OD1 | 41:VP:306:ARG:NH2 | 2.33 | 0.61 |
| 40:BI:262:TYR:HB2 | 40:BI:265:ILE:HG13 | 1.82 | 0.61 |
| 41:CN:87:PRO:HD3 | 41:DN:281:TYR:HD2 | 1.64 | 0.61 |
| 41:CP:313:VAL:HB | 41:CP:367:PHE:HE1 | 1.65 | 0.61 |
| 41:DB:135:LEU:HD13 | 41:DB:152:ILE:HG12 | 1.82 | 0.61 |
| 41:DN:202:ILE:HG21 | 41:DN:229:VAL:HB | 1.81 | 0.61 |
| 40:EE:346:TRP:CH2 | 41:EM:393:ALA:HB3 | 2.35 | 0.61 |
| 41:EM:107:THR:OG1 | 41:EM:108:GLU:N | 2.33 | 0.61 |
| 40:FA:273:ALA:CB | 40:FA:274:PRO:HD2 | 2.24 | 0.61 |
| 41:FB:52:ASN:OD1 | 41:FB:62:ARG:NH2 | 2.34 | 0.61 |
| 40:GH:402:ALA:O | 40:GH:403:PHE:C | 2.38 | 0.61 |
| 41:HQ:222:TYR:O | 41:HQ:226:ASN:ND2 | 2.32 | 0.61 |
| 41:IO:163:ILE:HD11 | 41:IO:251:ARG:HD3 | 1.83 | 0.61 |
| 40:JE:228:ASN:HD21 | 42:JE:501:GTP:HN1 | 1.48 | 0.61 |
| 41:KL:258:VAL:HG22 | 41:KL:266:PHE:CZ | 2.34 | 0.61 |
| 40:MF:271:THR:HA | 40:MF:302:MET:HG3 | 1.82 | 0.61 |
| 40:ND:59:GLY:HA2 | 40:ND:61:HIS:CE1 | 2.34 | 0.61 |
| 40:NH:123:ARG:HH22 | 40:OH:338:LYS:NZ | 1.98 | 0.61 |
| 40:OG:240:ALA:HB1 | 40:OG:356:ASN:HD22 | 1.65 | 0.61 |
| 40:OH:259:LEU:HD21 | 40:OH:316:CYS:HB2 | 1.81 | 0.61 |
| 41:ON:5:VAL:HG12 | 41:ON:62:ARG:HD2 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:PG:69:ASP:HA | 40:PG:145:THR:HG21 | 1.83 | 0.61 |
| 40:PH:64:ARG:NH2 | 40:PH:129:CYS:SG | 2.73 | 0.61 |
| 40:QH:362:VAL:HG21 | 40:QH:369:LYS:HA | 1.81 | 0.61 |
| 41:QM:7:LEU:HD13 | 41:QM:64:VAL:HB | 1.82 | 0.61 |
| 40:RG:15:GLN:O | 40:RG:228:ASN:ND2 | 2.33 | 0.61 |
| 40:RI:88:HIS:HB3 | 40:RI:91:GLN:HG2 | 1.80 | 0.61 |
| 40:SF:98:ASP:O | 40:SF:105:ARG:NH1 | 2.33 | 0.61 |
| 41:SP:134:GLN:HA | 41:SP:165:ASN:O | 2.00 | 0.61 |
| 40:TG:205:ASP:HB3 | 40:TG:303:VAL:HA | 1.82 | 0.61 |
| 40:TH:177:VAL:HG21 | 41:TO:327:ASP:HB2 | 1.81 | 0.61 |
| 41:UP:98:GLY:O | 41:UP:99:ASN:C | 2.38 | 0.61 |
| 40:VI:205:ASP:HB2 | 40:VI:303:VAL:HG12 | 1.81 | 0.61 |
| 41:VP:236:VAL:HG22 | 41:VP:368:ILE:HD11 | 1.82 | 0.61 |
| 41:VQ:318:ARG:HE | 41:VQ:358:PRO:HD3 | 1.62 | 0.61 |
| 40:WA:96:LYS:NZ | 41:WN:1:MET:HG2 | 2.09 | 0.61 |
| 21:4D:427:GLU:HB2 | 21:4D:502:ARG:HD2 | 1.82 | 0.61 |
| 22:4I:232:PHE:HB2 | 22:4I:251:LEU:HB3 | 1.80 | 0.61 |
| 22:4J:90:PRO:HG2 | 41:BN:284:LEU:H | 1.65 | 0.61 |
| 26:4W:353:ASN:ND2 | 26:4W:355:VAL:O | 2.34 | 0.61 |
| 38:6C:45:GLN:NE2 | 41:VO:295:ASP:OD2 | 2.33 | 0.61 |
| 39:6F:129:CYS:SG | 39:6F:133:ARG:NH2 | 2.73 | 0.61 |
| 41:AM:198:GLU:HG2 | 41:AM:266:PHE:HE2 | 1.65 | 0.61 |
| 40:BA:257:THR:HA | 41:BB:397:TRP:CE2 | 2.35 | 0.61 |
| 40:BG:7:VAL:O | 40:BG:137:ILE:HA | 2.01 | 0.61 |
| 40:BH:177:VAL:HG21 | 41:BO:327:ASP:HB3 | 1.82 | 0.61 |
| 40:CI:26:LEU:HD21 | 40:CI:363:VAL:HG12 | 1.83 | 0.61 |
| 41:CL:173:PRO:O | 41:CL:174:LYS:C | 2.38 | 0.61 |
| 41:CO:178:THR:HG22 | 41:CO:181:GLU:H | 1.64 | 0.61 |
| 40:GA:17:GLY:HA2 | 40:GA:20:CYS:HB2 | 1.81 | 0.61 |
| 40:GE:263:PRO:HB3 | 41:GM:396:HIS:CD2 | 2.36 | 0.61 |
| 40:IH:228:ASN:HD21 | 42:IH:501:GTP:HN1 | 1.47 | 0.61 |
| 40:II:221:ARG:NE | 41:IP:325:GLU:OE2 | 2.33 | 0.61 |
| 41:IP:253:LEU:O | 41:IP:257:MET:CB | 2.49 | 0.61 |
| 41:JN:51:TYR:HB3 | 41:JN:59:TYR:HB3 | 1.82 | 0.61 |
| 40:LD:188:ILE:HD12 | 40:LD:424:MET:HG3 | 1.82 | 0.61 |
| 40:MA:101:ASN:HD22 | 41:MN:256:ASN:HD21 | 1.46 | 0.61 |
| 41:MB:33:THR:O | 41:MB:58:LYS:NZ | 2.32 | 0.61 |
| 40:MD:50:ASN:O | 40:MD:64:ARG:NH1 | 2.33 | 0.61 |
| 40:MD:123:ARG:NH2 | 40:MD:160:ASP:OD2 | 2.33 | 0.61 |
| 41:OO:421:PRO:HA | 41:OO:424:THR:HG22 | 1.83 | 0.61 |
| 40:QG:246:GLY:HA3 | 40:QG:356:ASN:HA | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RH:174:ALA:HB3 | 40:RH:178:SER:H | 1.65 | 0.61 |
| 41:RO:7:LEU:O | 41:RO:135:LEU:HA | 2.01 | 0.61 |
| 40:SG:269:LEU:HD21 | 40:SG:301:GLN:HB3 | 1.82 | 0.61 |
| 41:SL:257:MET:HG3 | 41:SL:266:PHE:HE2 | 1.65 | 0.61 |
| 41:SM:272:PRO:HG3 | 41:SM:364:SER:HA | 1.82 | 0.61 |
| 40:TI:406:TRP:HE1 | 41:TP:258:VAL:HB | 1.65 | 0.61 |
| 41:TL:278:SER:O | 41:TL:282:ARG:NH1 | 2.33 | 0.61 |
| 41:TM:286:VAL:HG11 | 41:TM:326:VAL:HG22 | 1.81 | 0.61 |
| 41:VP:27:GLU:OE2 | 41:VP:318:ARG:NH2 | 2.32 | 0.61 |
| 41:WN:193:VAL:HG23 | 41:WN:265:PHE:HE1 | 1.64 | 0.61 |
| 12:2P:197:LEU:HD13 | 12:2P:225:ILE:HG12 | 1.82 | 0.61 |
| 13:2W:42:ILE:HD13 | 13:2W:183:LEU:HD11 | 1.82 | 0.61 |
| 13:2X:62:PRO:HG3 | 13:2X:69:LEU:HD23 | 1.82 | 0.61 |
| 15:3E:162:ARG:NH1 | 21:4D:197:GLN:O | 2.34 | 0.61 |
| 17:3O:93:ARG:HB2 | 17:3P:212:HIS:HB2 | 1.81 | 0.61 |
| 21:4F:407:LYS:NZ | 21:4F:410:ILE:HD12 | 2.16 | 0.61 |
| 27:4Y:11:ARG:NH1 | 41:IM:45:GLU:OE1 | 2.34 | 0.61 |
| 41:AB:11:GLN:HA | 41:AB:72:THR:HG21 | 1.81 | 0.61 |
| 41:CN:244:GLY:HA3 | 41:CN:354:CYS:HA | 1.80 | 0.61 |
| 40:DA:90:GLU:O | 40:DA:92:LEU:N | 2.33 | 0.61 |
| 40:DH:217:LEU:HB2 | 40:DH:219:ILE:HG12 | 1.83 | 0.61 |
| 41:EP:49:VAL:HG11 | 41:EP:241:ARG:HG2 | 1.82 | 0.61 |
| 40:FH:88:HIS:HB3 | 40:FH:91:GLN:HG2 | 1.80 | 0.61 |
| 41:FP:248:ALA:HA | 41:FP:252:LYS:HD3 | 1.82 | 0.61 |
| 40:GE:237:SER:HA | 40:GE:320:ARG:HD3 | 1.83 | 0.61 |
| 40:HH:139:HIS:NE2 | 40:HH:168:GLU:OE2 | 2.32 | 0.61 |
| 40:IA:239:THR:O | 40:IA:243:ARG:NH1 | 2.33 | 0.61 |
| 40:IF:254:GLU:HG3 | 41:IN:98:GLY:HA2 | 1.81 | 0.61 |
| 41:KB:262:ARG:HD2 | 41:KB:421:PRO:HG2 | 1.83 | 0.61 |
| 41:KP:60:VAL:HG21 | 41:KP:86:ARG:HG2 | 1.82 | 0.61 |
| 40:LE:178:SER:HB3 | 41:LL:347:ASN:HD22 | 1.66 | 0.61 |
| 41:LN:207:LEU:HB3 | 41:LN:225:LEU:HD22 | 1.82 | 0.61 |
| 41:LP:8:GLN:OE1 | 41:LP:17:GLY:HA3 | 2.00 | 0.61 |
| 40:NA:98:ASP:O | 40:NA:105:ARG:NH2 | 2.33 | 0.61 |
| 41:NL:387:ALA:HA | 41:NL:390:ARG:HH21 | 1.64 | 0.61 |
| 41:NM:248:ALA:HA | 41:NM:252:LYS:HG3 | 1.81 | 0.61 |
| 41:NM:421:PRO:HA | 41:NM:424:THR:HG22 | 1.83 | 0.61 |
| 41:OL:44:LEU:HA | 41:OL:47:ILE:HG23 | 1.82 | 0.61 |
| 41:PN:263:LEU:HD21 | 41:PN:422:VAL:HG22 | 1.83 | 0.61 |
| 40:QE:60:LYS:NZ | 40:RE:283:HIS:HA | 2.16 | 0.61 |
| 40:RG:26:LEU:HD21 | 40:RG:363:VAL:HG13 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SA:73:THR:HA | 40:SA:76:ASP:HB2 | 1.83 | 0.61 |
| 40:SH:276:ILE:HG23 | 40:SH:280:LYS:HG3 | 1.82 | 0.61 |
| 40:SH:317:LEU:HD22 | 40:SH:319:TYR:HE1 | 1.64 | 0.61 |
| 41:SP:86:ARG:HG3 | 41:SP:89:ASN:H | 1.66 | 0.61 |
| 40:UF:293:ASN:HA | 40:UF:335:ILE:HD11 | 1.82 | 0.61 |
| 40:WA:258:ASN:HD22 | 41:WB:179:VAL:HG22 | 1.66 | 0.61 |
| 40:WI:15:GLN:NE2 | 42:WI:501:GTP:O6 | 2.32 | 0.61 |
| 8:1X:254:ARG:HD2 | 8:1X:258:HIS:HE1 | 1.65 | 0.61 |
| 10:2G:58:ARG:HH21 | 41:MP:397:TRP:HE1 | 1.48 | 0.61 |
| 12:2Q:41:GLY:HA3 | 41:AO:306:ARG:HD2 | 1.81 | 0.61 |
| 23:4Q:237:PRO:O | 23:4Q:238:HIS:C | 2.38 | 0.61 |
| 36:5X:69:PRO:HA | 40:OD:219:ILE:HD13 | 1.82 | 0.61 |
| 40:BE:177:VAL:HG23 | 41:BL:327:ASP:HB3 | 1.80 | 0.61 |
| 40:BH:11:GLN:HA | 40:BH:74:VAL:HG11 | 1.81 | 0.61 |
| 40:CG:258:ASN:HD21 | 41:CO:179:VAL:H | 1.49 | 0.61 |
| 40:DA:214:ARG:HD3 | 41:DN:324:LYS:HE2 | 1.83 | 0.61 |
| 40:DA:279:GLU:O | 40:DA:280:LYS:C | 2.38 | 0.61 |
| 41:EB:6:HIS:O | 41:EB:63:ALA:HA | 2.00 | 0.61 |
| 41:EM:169:VAL:HG22 | 41:EM:202:ILE:HD11 | 1.82 | 0.61 |
| 41:GO:10:GLY:O | 41:GO:14:ASN:HB2 | 2.00 | 0.61 |
| 41:IM:257:MET:O | 41:IM:370:ASN:ND2 | 2.33 | 0.61 |
| 41:IN:207:LEU:HG | 41:IN:225:LEU:HG | 1.82 | 0.61 |
| 40:KH:255:PHE:O | 40:KH:259:LEU:HB2 | 2.01 | 0.61 |
| 41:KO:262:ARG:NH1 | 41:KO:417:ASP:OD2 | 2.32 | 0.61 |
| 41:LL:421:PRO:HA | 41:LL:424:THR:HG22 | 1.81 | 0.61 |
| 41:MN:248:ALA:HA | 41:MN:252:LYS:HD3 | 1.82 | 0.61 |
| 41:NB:324:LYS:HE3 | 40:NG:210:TYR:HA | 1.83 | 0.61 |
| 40:NF:224:TYR:HA | 40:NF:227:LEU:HB2 | 1.82 | 0.61 |
| 41:NN:421:PRO:HA | 41:NN:424:THR:HG22 | 1.83 | 0.61 |
| 41:OB:354:CYS:SG | 41:OB:355:ASP:N | 2.73 | 0.61 |
| 40:OH:220:GLU:C | 41:OO:324:LYS:NZ | 2.53 | 0.61 |
| 40:PA:259:LEU:O | 40:PA:379:ASN:ND2 | 2.33 | 0.61 |
| 41:PB:62:ARG:NH1 | 41:PB:127:CYS:SG | 2.74 | 0.61 |
| 40:PD:50:ASN:O | 40:PD:64:ARG:NH1 | 2.32 | 0.61 |
| 40:PH:332:ILE:HG23 | 40:PH:351:PHE:HD2 | 1.65 | 0.61 |
| 41:PO:178:THR:HB | 41:PO:181:GLU:HB2 | 1.81 | 0.61 |
| 41:QM:209:ASP:OD1 | 41:QM:213:ARG:NH2 | 2.34 | 0.61 |
| 41:QO:209:ASP:OD1 | 41:QO:213:ARG:NH2 | 2.33 | 0.61 |
| 40:SF:50:ASN:O | 40:SF:64:ARG:NH1 | 2.34 | 0.61 |
| 40:SH:97:GLU:OE2 | 40:SH:105:ARG:NH2 | 2.34 | 0.61 |
| 40:SH:228:ASN:HD21 | 42:SH:501:GTP:HN1 | 1.47 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TB:245:GLN:HG2 | 42:TG:501:GTP:N7 | 2.15 | 0.61 |
| 40:VI:76:ASP:HA | 40:VI:79:ARG:HG2 | 1.81 | 0.61 |
| 41:VN:252:LYS:HA | 41:VN:255:VAL:HG12 | 1.82 | 0.61 |
| 40:WI:273:ALA:HB3 | 40:WI:374:VAL:H | 1.65 | 0.61 |
| 41:WP:341:PHE:HB3 | 41:WP:348:ASN:HD21 | 1.66 | 0.61 |
| 8:1X:260:VAL:HA | 40:UF:282:TYR:OH | 2.00 | 0.61 |
| 15:3E:254:GLN:HB2 | 15:3E:400:ARG:HH12 | 1.65 | 0.61 |
| 18:3T:81:SER:OG | 18:3W:335:ASN:ND2 | 2.30 | 0.61 |
| 34:5Q:269:GLU:OE2 | 41:GM:276:ARG:NH1 | 2.33 | 0.61 |
| 40:AH:397:MET:HG3 | 41:AO:346:PRO:HD2 | 1.82 | 0.61 |
| 41:BL:163:ILE:HG21 | 41:BL:250:LEU:HB3 | 1.82 | 0.61 |
| 41:BP:16:ILE:HD13 | 41:BP:229:VAL:HG11 | 1.82 | 0.61 |
| 41:BP:285:THR:H | 41:BP:288:GLU:HG2 | 1.64 | 0.61 |
| 40:CA:222:PRO:HD2 | 41:CN:324:LYS:HG3 | 1.81 | 0.61 |
| 40:CH:181:VAL:HG13 | 41:CO:256:ASN:OD1 | 2.00 | 0.61 |
| 40:FE:188:ILE:HD12 | 40:FE:424:MET:HG3 | 1.81 | 0.61 |
| 41:GM:131:GLN:HE22 | 41:GM:249:ASP:HB3 | 1.66 | 0.61 |
| 40:HH:51:THR:HG21 | 40:HH:243:ARG:HG2 | 1.82 | 0.61 |
| 40:IH:88:HIS:HB3 | 40:IH:91:GLN:HB2 | 1.82 | 0.61 |
| 41:IO:193:VAL:HG11 | 41:IO:418:LEU:HD11 | 1.83 | 0.61 |
| 40:JD:16:ILE:HD13 | 40:JD:228:ASN:HB3 | 1.83 | 0.61 |
| 41:JO:2:ARG:HH21 | 41:JO:240:LEU:HA | 1.65 | 0.61 |
| 41:KM:101:TRP:NE1 | 41:KM:188:SER:OG | 2.33 | 0.61 |
| 41:NP:186:THR:HG23 | 41:NP:415:MET:HG3 | 1.83 | 0.61 |
| 40:OE:2:ARG:CB | 40:OE:133:GLN:HE22 | 2.12 | 0.61 |
| 41:OM:44:LEU:HA | 41:OM:47:ILE:HG23 | 1.81 | 0.61 |
| 41:ON:2:ARG:HH21 | 41:ON:240:LEU:HA | 1.66 | 0.61 |
| 40:PD:112:LYS:HA | 40:PD:115:ILE:HB | 1.81 | 0.61 |
| 41:PP:325:GLU:HA | 41:PP:328:GLU:HG3 | 1.82 | 0.61 |
| 40:RG:2:ARG:NH1 | 40:RG:242:LEU:O | 2.33 | 0.61 |
| 41:RO:66:VAL:HG12 | 41:RO:91:VAL:HB | 1.81 | 0.61 |
| 41:SO:55:THR:N | 41:TO:283:ALA:HA | 2.08 | 0.61 |
| 40:UA:319:TYR:HB3 | 40:UA:323:VAL:HG21 | 1.81 | 0.61 |
| 40:VA:35:GLN:HG2 | 40:VA:60:LYS:H | 1.65 | 0.61 |
| 10:2F:97:GLN:O | 10:2F:101:GLN:HB2 | 2.01 | 0.61 |
| 23:4N:37:TYR:CE2 | 23:4N:41:THR:CG2 | 2.81 | 0.61 |
| 23:4Q:240:LEU:HA | 23:4Q:266:HIS:HA | 1.81 | 0.61 |
| 28:5B:186:ARG:HD2 | 28:5B:196:LYS:HB3 | 1.81 | 0.61 |
| 38:6C:140:ASN:ND2 | 41:UO:118:ASP:OD1 | 2.34 | 0.61 |
| 41:AB:178:THR:HB | 41:AB:181:GLU:HG3 | 1.83 | 0.61 |
| 40:BE:181:VAL:HG13 | 41:BL:348:ASN:HA | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CP:21:TRP:CE3 | 41:CP:24:ILE:HD11 | 2.36 | 0.61 |
| 40:DH:219:ILE:C | 40:DH:221:ARG:N | 2.49 | 0.61 |
| 41:DO:271:ALA:O | 41:DO:292:GLN:NE2 | 2.33 | 0.61 |
| 40:EE:222:PRO:HD2 | 41:EL:324:LYS:HG3 | 1.82 | 0.61 |
| 40:EI:81:GLY:H | 40:EI:84:ARG:HB3 | 1.66 | 0.61 |
| 41:EM:258:VAL:HG22 | 41:EM:266:PHE:HZ | 1.65 | 0.61 |
| 40:FH:6:SER:O | 40:FH:65:ALA:HA | 2.01 | 0.61 |
| 41:FM:51:TYR:HA | 41:FM:60:VAL:O | 2.01 | 0.61 |
| 40:HG:173:PRO:HG2 | 40:HG:390:LEU:HD21 | 1.83 | 0.61 |
| 40:IA:223:THR:HG22 | 41:IN:322:SER:HA | 1.82 | 0.61 |
| 40:JF:181:VAL:HG23 | 41:JM:346:PRO:O | 2.01 | 0.61 |
| 41:KN:311:LEU:HD21 | 41:KN:425:ARG:HB3 | 1.82 | 0.61 |
| 40:LF:353:VAL:HG23 | 41:LN:177:ASP:HA | 1.83 | 0.61 |
| 41:LM:289:LEU:HD11 | 41:LM:363:MET:HG2 | 1.83 | 0.61 |
| 41:LO:284:LEU:HD22 | 41:LO:362:LYS:HE3 | 1.82 | 0.61 |
| 41:NP:222:TYR:O | 41:NP:226:ASN:ND2 | 2.33 | 0.61 |
| 40:OH:352:LYS:HD2 | 41:OP:178:THR:HA | 1.83 | 0.61 |
| 40:OH:363:VAL:HG12 | 40:OH:364:PRO:HD2 | 1.83 | 0.61 |
| 41:PP:14:ASN:HB2 | 41:PP:65:LEU:HD23 | 1.81 | 0.61 |
| 41:QB:331:LEU:HB3 | 40:QG:177:VAL:HG23 | 1.82 | 0.61 |
| 40:RI:141:PHE:HB2 | 40:RI:173:PRO:HD3 | 1.82 | 0.61 |
| 41:RM:139:LEU:HG | 41:RM:168:SER:HB2 | 1.83 | 0.61 |
| 40:UF:257:THR:HB | 41:UN:397:TRP:CD1 | 2.35 | 0.61 |
| 41:UN:275:SER:HB2 | 41:UN:278:SER:HB3 | 1.83 | 0.61 |
| 40:VG:236:SER:OG | 40:VG:243:ARG:NH2 | 2.34 | 0.61 |
| 40:VI:68:VAL:HG22 | 40:VI:93:ILE:HB | 1.81 | 0.61 |
| 40:WA:8:HIS:HE1 | 40:WA:21:TRP:HE1 | 1.48 | 0.61 |
| 40:WH:319:TYR:HE2 | 40:WH:328:VAL:HG13 | 1.65 | 0.61 |
| 41:WQ:392:LYS:NZ | 41:WQ:405:GLU:OE1 | 2.33 | 0.61 |
| 21:4E:429:PRO:HD2 | 21:4E:430:ILE:HD13 | 1.83 | 0.61 |
| 22:4J:537:SER:HA | 22:4J:540:PHE:HB2 | 1.83 | 0.61 |
| 36:5X:118:TYR:HA | 36:5X:121:MET:HB2 | 1.83 | 0.61 |
| 41:AO:358:PRO:HG3 | 41:AO:364:SER:CB | 2.31 | 0.61 |
| 40:BA:318:LEU:O | 40:BA:374:VAL:HA | 2.01 | 0.61 |
| 40:DH:90:GLU:O | 40:DH:92:LEU:N | 2.33 | 0.61 |
| 40:DI:238:ILE:HG22 | 40:DI:239:THR:HG23 | 1.82 | 0.61 |
| 41:DP:104:GLY:O | 41:DP:109:GLY:HA3 | 2.01 | 0.61 |
| 41:EM:112:LEU:O | 41:EM:113:VAL:C | 2.39 | 0.61 |
| 41:EM:173:PRO:O | 41:EM:174:LYS:C | 2.38 | 0.61 |
| 40:FA:109:THR:O | 40:FA:110:ILE:C | 2.39 | 0.61 |
| 41:FO:337:ASN:HB3 | 41:FO:340:TYR:HB2 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IG:188:ILE:HD11 | 40:IG:424:MET:HG3 | 1.82 | 0.61 |
| 40:KE:100:ALA:O | 41:KL:255:VAL:HG11 | 2.01 | 0.61 |
| 40:KG:90:GLU:HG3 | 40:KG:121:ARG:HH12 | 1.66 | 0.61 |
| 41:NN:30:ILE:HG13 | 41:NN:51:TYR:HE2 | 1.65 | 0.61 |
| 41:OB:253:LEU:O | 41:OB:257:MET:HB3 | 2.01 | 0.61 |
| 40:OE:174:ALA:HB3 | 40:OE:178:SER:H | 1.66 | 0.61 |
| 41:QN:49:VAL:O | 41:QN:62:ARG:NH2 | 2.34 | 0.61 |
| 41:QP:5:VAL:HG13 | 41:QP:62:ARG:HD3 | 1.81 | 0.61 |
| 41:RB:21:TRP:HA | 41:RB:24:ILE:HG22 | 1.82 | 0.61 |
| 41:SB:415:MET:O | 41:SB:418:LEU:HB2 | 2.01 | 0.61 |
| 40:SE:278:ALA:H | 40:SE:368:ALA:HB2 | 1.66 | 0.61 |
| 41:SL:248:ALA:HA | 41:SL:252:LYS:HD3 | 1.82 | 0.61 |
| 40:UF:269:LEU:HD22 | 40:UF:303:VAL:HG21 | 1.82 | 0.61 |
| 40:WF:121:ARG:HH12 | 40:WF:124:LYS:HD2 | 1.65 | 0.61 |
| 7:1S:502:ASN:HD21 | 41:VB:40:SER:HA | 1.66 | 0.61 |
| 20:4A:81:GLU:HA | 20:4A:84:GLN:HG3 | 1.81 | 0.61 |
| 22:4J:551:LYS:HZ3 | 22:4J:594:LEU:HB3 | 1.66 | 0.61 |
| 40:AH:101:ASN:ND2 | 41:AO:252:LYS:HD2 | 2.16 | 0.61 |
| 41:BN:248:ALA:HA | 41:BN:252:LYS:HD2 | 1.82 | 0.61 |
| 40:CE:10:GLY:HA2 | 40:CE:145:THR:HG23 | 1.82 | 0.61 |
| 41:CL:58:LYS:O | 41:CL:59:TYR:C | 2.38 | 0.61 |
| 41:CP:171:PRO:HG3 | 41:CP:185:ALA:HB2 | 1.81 | 0.61 |
| 40:DA:62:VAL:HG11 | 40:EA:283:HIS:HB3 | 1.83 | 0.61 |
| 40:DG:274:PRO:HG3 | 40:DG:286:LEU:HD22 | 1.83 | 0.61 |
| 40:DG:314:ALA:HB3 | 40:DG:379:ASN:HB3 | 1.83 | 0.61 |
| 40:DI:212:ILE:HG23 | 40:DI:216:ASN:HD21 | 1.64 | 0.61 |
| 41:EM:72:THR:O | 41:EM:76:VAL:HG23 | 2.00 | 0.61 |
| 40:FA:275:VAL:HA | 40:FA:367:LEU:HD21 | 1.81 | 0.61 |
| 40:FH:195:LEU:HD21 | 40:FH:264:ARG:HH11 | 1.65 | 0.61 |
| 41:FN:316:VAL:HG12 | 41:FN:352:ALA:HB3 | 1.81 | 0.61 |
| 40:GG:73:THR:HA | 40:GG:76:ASP:HB2 | 1.83 | 0.61 |
| 41:GM:275:SER:HG | 41:GM:278:SER:HG | 1.49 | 0.61 |
| 41:GN:303:CYS:O | 41:GN:304:ASP:C | 2.39 | 0.61 |
| 40:HI:72:PRO:HB2 | 41:HP:46:ARG:HH12 | 1.66 | 0.61 |
| 40:IH:395:ASP:OD1 | 40:IH:421:ARG:NH1 | 2.33 | 0.61 |
| 41:IM:341:PHE:HB3 | 41:IM:348:ASN:HD21 | 1.66 | 0.61 |
| 41:IP:107:THR:O | 41:IP:110:ALA:N | 2.34 | 0.61 |
| 40:JA:91:GLN:HE22 | 40:JA:125:LEU:HD11 | 1.66 | 0.61 |
| 40:JE:137:ILE:HD11 | 40:JE:168:GLU:HG2 | 1.81 | 0.61 |
| 40:KA:139:HIS:NE2 | 40:KA:168:GLU:OE2 | 2.32 | 0.61 |
| 40:KE:217:LEU:HD21 | 40:KE:367:LEU:HD23 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LE:98:ASP:O | 40:LE:105:ARG:NH2 | 2.34 | 0.61 |
| 40:MF:172:TYR:HE2 | 40:MF:386:ALA:HB1 | 1.65 | 0.61 |
| 40:NA:30:ILE:HG22 | 40:NA:36:MET:HB2 | 1.83 | 0.61 |
| 41:NP:101:TRP:CZ3 | 41:NP:187:LEU:HB3 | 2.36 | 0.61 |
| 41:OL:139:LEU:HD12 | 41:OL:170:VAL:HG23 | 1.83 | 0.61 |
| 41:OM:164:MET:SD | 41:OM:196:THR:OG1 | 2.53 | 0.61 |
| 41:RL:10:GLY:O | 41:RL:14:ASN:HB2 | 2.01 | 0.61 |
| 40:SE:2:ARG:NH2 | 41:SM:69:GLU:OE1 | 2.34 | 0.61 |
| 41:SO:318:ARG:HA | 41:SO:354:CYS:HB3 | 1.83 | 0.61 |
| 40:TH:174:ALA:HB3 | 40:TH:178:SER:H | 1.66 | 0.61 |
| 41:TM:292:GLN:O | 41:TM:298:ASN:ND2 | 2.33 | 0.61 |
| 40:UH:319:TYR:HB3 | 40:UH:323:VAL:HG21 | 1.83 | 0.61 |
| 41:VN:271:ALA:HB1 | 41:VN:292:GLN:HB3 | 1.83 | 0.61 |
| 41:WO:26:ASP:O | 41:WO:359:ARG:NH1 | 2.33 | 0.61 |
| 7:1U:554:THR:HG23 | 7:1U:557:GLY:H | 1.66 | 0.61 |
| 8:1Z:407:ASN:OD1 | 8:1Z:410:LYS:NZ | 2.31 | 0.61 |
| 9:2B:174:GLN:NE2 | 40:TH:365:GLY:O | 2.34 | 0.61 |
| 18:3U:321:HIS:O | 18:3V:71:ARG:NH2 | 2.34 | 0.61 |
| 19:3Y:190:LEU:HD22 | 41:KN:56:GLY:HA3 | 1.82 | 0.61 |
| 23:4M:19:ILE:CD1 | 40:BG:79:ARG:HB3 | 2.30 | 0.61 |
| 41:DL:86:ARG:HG2 | 41:DL:88:ASP:H | 1.66 | 0.61 |
| 41:DP:420:ASN:HB2 | 41:DP:421:PRO:HD3 | 1.83 | 0.61 |
| 40:HA:235:VAL:HA | 40:HA:238:ILE:HG22 | 1.83 | 0.61 |
| 40:HE:184:PRO:HB2 | 40:HE:397:MET:HE1 | 1.83 | 0.61 |
| 40:HI:100:ALA:HA | 41:HP:252:LYS:HE2 | 1.83 | 0.61 |
| 41:IB:61:PRO:HD3 | 41:IB:84:ILE:HG13 | 1.82 | 0.61 |
| 40:IG:213:CYS:HA | 40:IG:217:LEU:HB2 | 1.83 | 0.61 |
| 40:JA:438:SER:HB3 | 41:JB:391:ARG:HD2 | 1.83 | 0.61 |
| 41:JM:178:THR:HB | 41:JM:181:GLU:HG3 | 1.81 | 0.61 |
| 41:KB:213:ARG:HH12 | 41:KB:297:LYS:HE3 | 1.66 | 0.61 |
| 41:LN:292:GLN:O | 41:LN:298:ASN:ND2 | 2.33 | 0.61 |
| 41:LO:1:MET:SD | 41:LO:48:ASN:ND2 | 2.74 | 0.61 |
| 40:MG:273:ALA:HB1 | 40:MG:274:PRO:CD | 2.28 | 0.61 |
| 41:MO:70:PRO:HD3 | 41:MO:92:PHE:HB2 | 1.81 | 0.61 |
| 40:NE:7:VAL:HB | 40:NE:137:ILE:HG22 | 1.83 | 0.61 |
| 41:NL:320:ARG:NH2 | 41:NL:355:ASP:OD1 | 2.34 | 0.61 |
| 41:PL:274:THR:OG1 | 41:PL:282:ARG:NH1 | 2.34 | 0.61 |
| 41:PO:341:PHE:HB3 | 41:PO:348:ASN:HD21 | 1.65 | 0.61 |
| 41:QB:102:ALA:HB3 | 41:QB:103:LYS:HE3 | 1.83 | 0.61 |
| 40:QG:20:CYS:HA | 40:QG:232:SER:HB2 | 1.83 | 0.61 |
| 41:QP:405:GLU:HA | 41:QP:408:PHE:CD2 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SN:159:TYR:HB3 | 41:SN:162:ARG:HD3 | 1.83 | 0.61 |
| 41:SO:139:LEU:HB3 | 41:SO:171:PRO:HD3 | 1.83 | 0.61 |
| 41:TB:46:ARG:NH2 | 40:TG:76:ASP:OD2 | 2.34 | 0.61 |
| 40:TF:278:ALA:H | 40:TF:368:ALA:HB2 | 1.65 | 0.61 |
| 41:TM:113:VAL:HG11 | 41:TM:150:LEU:HD11 | 1.82 | 0.61 |
| 41:TO:27:GLU:OE1 | 41:TO:318:ARG:NH2 | 2.34 | 0.61 |
| 40:VF:71:GLU:HB3 | 40:VF:98:ASP:HA | 1.81 | 0.61 |
| 40:VH:139:HIS:NE2 | 40:VH:168:GLU:OE2 | 2.31 | 0.61 |
| 40:WI:73:THR:HA | 40:WI:76:ASP:HB2 | 1.83 | 0.61 |
| 41:WM:137:HIS:CE1 | 41:WM:192:LEU:HD11 | 2.36 | 0.61 |
| 13:2T:88:THR:HG23 | 13:2T:157:HIS:HB2 | 1.83 | 0.60 |
| 16:3J:110:LEU:HB2 | 16:3J:144:ILE:HG21 | 1.83 | 0.60 |
| 16:3K:216:GLN:NE2 | 16:3K:220:ASP:OD2 | 2.33 | 0.60 |
| 22:4J:231:ARG:HA | 22:4J:251:LEU:O | 2.01 | 0.60 |
| 34:5Q:265:GLN:OE1 | 41:GM:276:ARG:NH2 | 2.34 | 0.60 |
| 41:BB:252:LYS:HG3 | 40:BG:100:ALA:HA | 1.83 | 0.60 |
| 40:BH:181:VAL:HG13 | 41:BO:256:ASN:HB2 | 1.82 | 0.60 |
| 41:BN:178:THR:HB | 41:BN:181:GLU:HG3 | 1.83 | 0.60 |
| 41:CB:292:GLN:O | 41:CB:298:ASN:ND2 | 2.34 | 0.60 |
| 40:CF:250:VAL:HG23 | 40:CF:254:GLU:HG2 | 1.83 | 0.60 |
| 40:CF:385:GLU:OE1 | 40:CF:389:ARG:NH1 | 2.34 | 0.60 |
| 40:CI:96:LYS:HZ3 | 41:CP:1:MET:HB2 | 1.66 | 0.60 |
| 41:CM:271:ALA:HB3 | 41:CM:272:PRO:HD3 | 1.81 | 0.60 |
| 40:DA:65:ALA:H | 40:DA:91:GLN:HE21 | 1.49 | 0.60 |
| 40:DH:89:PRO:HG2 | 40:EH:280:LYS:HB3 | 1.82 | 0.60 |
| 41:DN:245:GLN:O | 41:DN:247:ASN:N | 2.34 | 0.60 |
| 41:EO:91:VAL:HG11 | 41:EO:116:VAL:HG22 | 1.83 | 0.60 |
| 40:FA:205:ASP:HB2 | 40:FA:303:VAL:HG13 | 1.81 | 0.60 |
| 40:GH:31:GLN:O | 40:GH:33:ASP:N | 2.34 | 0.60 |
| 40:GI:265:ILE:HG23 | 40:GI:431:TYR:CE2 | 2.36 | 0.60 |
| 41:HB:134:GLN:HA | 41:HB:165:ASN:O | 2.01 | 0.60 |
| 40:KF:50:ASN:O | 40:KF:64:ARG:NH1 | 2.34 | 0.60 |
| 40:KH:42:ILE:HG12 | 40:KH:46:ASP:HB3 | 1.82 | 0.60 |
| 41:LB:27:GLU:OE1 | 41:LB:241:ARG:NH2 | 2.34 | 0.60 |
| 40:LG:285:GLN:O | 40:LG:286:LEU:C | 2.39 | 0.60 |
| 41:LP:134:GLN:NE2 | 41:LP:233:MET:SD | 2.74 | 0.60 |
| 40:MH:11:GLN:HA | 40:MH:74:VAL:HG11 | 1.82 | 0.60 |
| 40:ND:101:ASN:HA | 40:ND:144:GLY:N | 2.15 | 0.60 |
| 40:NH:191:THR:O | 40:NH:195:LEU:HB2 | 2.00 | 0.60 |
| 41:NM:139:LEU:HD12 | 41:NM:170:VAL:HG12 | 1.83 | 0.60 |
| 40:OE:16:ILE:HA | 40:OE:228:ASN:HB3 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OE:73:THR:HA | 40:OE:76:ASP:HB2 | 1.83 | 0.60 |
| 40:OH:15:GLN:HE21 | 41:OO:245:GLN:HG3 | 1.65 | 0.60 |
| 40:OH:107:HIS:HA | 40:OH:152:LEU:HD22 | 1.81 | 0.60 |
| 41:OL:275:SER:O | 41:OL:279:GLN:HB2 | 2.01 | 0.60 |
| 40:PD:294:ALA:O | 40:PD:300:ASN:ND2 | 2.34 | 0.60 |
| 41:QP:173:PRO:O | 41:QP:174:LYS:C | 2.39 | 0.60 |
| 40:SH:213:CYS:HB3 | 40:SH:222:PRO:HG2 | 1.82 | 0.60 |
| 40:TE:339:ARG:O | 40:TE:342:GLN:NE2 | 2.32 | 0.60 |
| 40:VA:76:ASP:HA | 40:VA:79:ARG:HG2 | 1.82 | 0.60 |
| 40:WF:76:ASP:HA | 40:WF:79:ARG:HG2 | 1.83 | 0.60 |
| 41:WN:268:PRO:HG2 | 41:WN:300:MET:HB2 | 1.83 | 0.60 |
| 8:1X:263:MET:HG3 | 40:UF:282:TYR:CE2 | 2.36 | 0.60 |
| 11:2K:244:LEU:HD13 | 11:2K:250:ILE:HD12 | 1.83 | 0.60 |
| 23:4N:254:LYS:CD | 41:DM:53:GLU:HB2 | 2.31 | 0.60 |
| 23:4R:58:ARG:CZ | 41:BP:42:LEU:HD23 | 2.31 | 0.60 |
| 23:4R:187:PHE:HB3 | 23:4R:202:PHE:HZ | 1.66 | 0.60 |
| 39:6K:25:PHE:N | 41:OL:41:ASP:OD2 | 2.34 | 0.60 |
| 41:AO:372:THR:HA | 41:AO:422:VAL:HG22 | 1.83 | 0.60 |
| 41:BB:98:GLY:O | 41:BB:99:ASN:C | 2.40 | 0.60 |
| 40:BH:138:PHE:HE2 | 40:BH:235:VAL:HG21 | 1.66 | 0.60 |
| 40:CA:104:ALA:HB1 | 40:CA:410:GLU:HB3 | 1.83 | 0.60 |
| 41:DB:36:TYR:CZ | 41:DB:38:GLY:HA3 | 2.36 | 0.60 |
| 40:DH:28:HIS:CE1 | 40:DH:243:ARG:HD2 | 2.37 | 0.60 |
| 42:DI:501:GTP:H5" | 41:DP:246:LEU:HD21 | 1.84 | 0.60 |
| 41:DL:81:PHE:HB3 | 41:DL:84:ILE:HD12 | 1.83 | 0.60 |
| 40:EA:318:LEU:O | 40:EA:374:VAL:HA | 2.01 | 0.60 |
| 40:EF:75:ILE:HD11 | 40:EF:92:LEU:HD22 | 1.81 | 0.60 |
| 40:EH:271:THR:HA | 40:EH:302:MET:HG3 | 1.81 | 0.60 |
| 40:GE:104:ALA:HA | 40:GE:108:TYR:CD2 | 2.37 | 0.60 |
| 40:GE:440:GLU:HB2 | 41:GM:390:ARG:HH12 | 1.67 | 0.60 |
| 40:GI:174:ALA:HB1 | 40:GI:177:VAL:HG23 | 1.83 | 0.60 |
| 41:GP:257:MET:HA | 41:GP:312:THR:HG21 | 1.82 | 0.60 |
| 40:HE:261:PRO:HA | 41:HM:394:PHE:CE2 | 2.36 | 0.60 |
| 40:II:180:ALA:HB3 | 40:II:183:GLU:HB2 | 1.83 | 0.60 |
| 40:KH:235:VAL:HA | 40:KH:238:ILE:HG22 | 1.83 | 0.60 |
| 40:MH:210:TYR:CD1 | 40:MH:222:PRO:HB2 | 2.37 | 0.60 |
| 41:MM:341:PHE:HB3 | 41:MM:348:ASN:HD21 | 1.65 | 0.60 |
| 41:NM:30:ILE:HD11 | 41:NM:47:ILE:HD11 | 1.81 | 0.60 |
| 41:NO:163:ILE:HG21 | 41:NO:250:LEU:HB3 | 1.81 | 0.60 |
| 40:OD:329:ASN:OD1 | 41:OL:174:LYS:NZ | 2.32 | 0.60 |
| 41:PB:292:GLN:O | 41:PB:298:ASN:ND2 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PN:341:PHE:HB3 | 41:PN:348:ASN:HD21 | 1.65 | 0.60 |
| 41:QB:293:MET:HG2 | 41:QB:367:PHE:HB2 | 1.83 | 0.60 |
| 40:QH:207:GLU:OE1 | 40:QH:304:LYS:NZ | 2.25 | 0.60 |
| 41:QP:192:LEU:O | 41:QP:193:VAL:C | 2.38 | 0.60 |
| 40:RF:254:GLU:HG2 | 41:RN:98:GLY:HA2 | 1.82 | 0.60 |
| 40:SH:90:GLU:O | 40:SH:121:ARG:NH1 | 2.32 | 0.60 |
| 40:SH:141:PHE:HB2 | 40:SH:173:PRO:HD3 | 1.83 | 0.60 |
| 41:SM:202:ILE:HG23 | 41:SM:300:MET:HB3 | 1.83 | 0.60 |
| 40:TE:248:LEU:HB2 | 40:TE:355:ILE:H | 1.66 | 0.60 |
| 40:TF:427:LEU:O | 40:TF:431:TYR:HB2 | 2.01 | 0.60 |
| 40:TI:226:ASN:ND2 | 40:TI:366:ASP:OD2 | 2.34 | 0.60 |
| 41:UM:252:LYS:HA | 41:UM:255:VAL:HG12 | 1.83 | 0.60 |
| 41:WO:51:TYR:HB3 | 41:WO:59:TYR:HB3 | 1.82 | 0.60 |
| 9:2B:47:THR:HG23 | 11:2K:247:HIS:HB3 | 1.83 | 0.60 |
| 13:2U:74:PRO:HD2 | 13:2U:169:ASP:HA | 1.83 | 0.60 |
| 15:3H:173:LYS:HD2 | 15:3H:176:ARG:HH12 | 1.66 | 0.60 |
| 34:5R:373:ALA:HA | 34:5R:376:ASP:HB3 | 1.83 | 0.60 |
| 41:BO:86:ARG:HB3 | 41:BO:89:ASN:HB2 | 1.83 | 0.60 |
| 41:CL:56:GLY:O | 41:CL:57:GLY:C | 2.39 | 0.60 |
| 41:CO:215:LEU:HD21 | 41:CO:273:LEU:HD22 | 1.82 | 0.60 |
| 40:GH:276:ILE:HD11 | 40:GH:280:LYS:HB3 | 1.83 | 0.60 |
| 41:GM:191:GLN:OE1 | 41:GM:195:ASN:ND2 | 2.34 | 0.60 |
| 40:HF:228:ASN:HD21 | 42:HM:501:GTP:HN1 | 1.49 | 0.60 |
| 40:HH:11:GLN:HE22 | 41:HO:247:ASN:H | 1.47 | 0.60 |
| 40:IA:64:ARG:NH1 | 40:IA:129:CYS:SG | 2.74 | 0.60 |
| 40:IE:322:ASP:O | 40:IE:372:ARG:NH1 | 2.34 | 0.60 |
| 41:JM:389:PHE:CZ | 41:JM:405:GLU:HG2 | 2.37 | 0.60 |
| 40:KD:70:LEU:HD12 | 40:KD:99:ALA:HB2 | 1.82 | 0.60 |
| 40:KH:76:ASP:OD2 | 41:KO:46:ARG:NH2 | 2.34 | 0.60 |
| 40:MF:177:VAL:HG12 | 41:MM:327:ASP:HB3 | 1.81 | 0.60 |
| 40:MF:224:TYR:HB3 | 42:MM:501:GTP:N1 | 2.16 | 0.60 |
| 40:MH:177:VAL:HG13 | 40:MH:178:SER:H | 1.65 | 0.60 |
| 40:NA:65:ALA:O | 40:NA:91:GLN:NE2 | 2.33 | 0.60 |
| 40:NF:298:PRO:HB3 | 40:NF:307:PRO:HD2 | 1.84 | 0.60 |
| 41:NL:147:MET:O | 41:NL:151:LEU:HB2 | 2.00 | 0.60 |
| 41:ON:122:LYS:NZ | 41:PN:291:GLN:O | 2.33 | 0.60 |
| 40:PA:8:HIS:HB3 | 40:PA:138:PHE:HD1 | 1.65 | 0.60 |
| 40:RA:20:CYS:HA | 40:RA:232:SER:HB2 | 1.83 | 0.60 |
| 40:RH:138:PHE:HZ | 40:RH:235:VAL:HG21 | 1.65 | 0.60 |
| 41:RN:193:VAL:HG11 | 41:RN:418:LEU:HD21 | 1.82 | 0.60 |
| 40:SI:226:ASN:ND2 | 40:SI:366:ASP:OD2 | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UB:354:CYS:SG | 41:UB:355:ASP:N | 2.75 | 0.60 |
| 40:UF:163:LYS:O | 40:UF:164:LYS:C | 2.39 | 0.60 |
| 40:UI:49:PHE:O | 40:UI:50:ASN:C | 2.39 | 0.60 |
| 40:VJ:185:TYR:HE2 | 40:VJ:403:PHE:HB2 | 1.66 | 0.60 |
| 41:VN:237:THR:O | 41:VN:241:ARG:NH1 | 2.34 | 0.60 |
| 41:VO:133:PHE:HB2 | 41:VO:164:MET:HG2 | 1.83 | 0.60 |
| 41:WN:154:LYS:O | 41:WN:157:GLU:HG3 | 2.01 | 0.60 |
| 7:1T:84:VAL:HG12 | 7:1T:113:LYS:HB2 | 1.83 | 0.60 |
| 21:4F:447:ASP:HB3 | 21:4F:471:LYS:HE3 | 1.83 | 0.60 |
| 26:4W:370:TYR:HA | 26:4W:374:ILE:CG1 | 2.32 | 0.60 |
| 29:5E:106:SER:OG | 29:5E:107:ILE:N | 2.34 | 0.60 |
| 40:AF:260:VAL:HB | 41:AN:397:TRP:HH2 | 1.66 | 0.60 |
| 40:BF:319:TYR:HB3 | 40:BF:323:VAL:HG21 | 1.83 | 0.60 |
| 41:BP:12:CYS:HB3 | 41:BP:138:SER:HB2 | 1.83 | 0.60 |
| 40:CG:98:ASP:O | 40:CG:105:ARG:NH1 | 2.34 | 0.60 |
| 41:CL:311:LEU:HD23 | 41:CL:344:TRP:HZ2 | 1.65 | 0.60 |
| 40:DG:68:VAL:HA | 40:DG:93:ILE:HB | 1.83 | 0.60 |
| 40:EI:99:ALA:HB2 | 40:EI:110:ILE:HD11 | 1.83 | 0.60 |
| 41:EM:137:HIS:CE1 | 41:EM:168:SER:HB2 | 2.36 | 0.60 |
| 41:EP:152:ILE:O | 41:EP:155:ILE:HG12 | 2.02 | 0.60 |
| 40:FE:209:ILE:HG22 | 40:FE:227:LEU:HD22 | 1.83 | 0.60 |
| 41:GN:215:LEU:HD21 | 41:GN:273:LEU:HD22 | 1.83 | 0.60 |
| 40:HA:229:ARG:HD2 | 40:HA:363:VAL:HG21 | 1.83 | 0.60 |
| 40:KD:55:GLU:O | 40:LD:285:GLN:NE2 | 2.34 | 0.60 |
| 40:LE:211:ASP:OD1 | 40:LE:214:ARG:NH1 | 2.34 | 0.60 |
| 40:LH:181:VAL:HG23 | 40:LH:182:VAL:HG23 | 1.83 | 0.60 |
| 41:MB:87:PRO:HA | 41:MB:90:PHE:HD2 | 1.66 | 0.60 |
| 40:NA:213:CYS:HA | 40:NA:217:LEU:HB2 | 1.83 | 0.60 |
| 40:NF:181:VAL:HG23 | 40:NF:182:VAL:HG13 | 1.84 | 0.60 |
| 41:NL:166:THR:HG23 | 41:NL:199:THR:HG23 | 1.82 | 0.60 |
| 41:NN:222:TYR:HB3 | 43:NN:502:GDP:C6 | 2.36 | 0.60 |
| 41:NN:334:GLN:HE21 | 41:NN:349:VAL:HG13 | 1.65 | 0.60 |
| 40:PH:88:HIS:HB3 | 40:PH:91:GLN:HG2 | 1.82 | 0.60 |
| 41:QB:265:PHE:HB3 | 41:QB:374:ILE:HG12 | 1.82 | 0.60 |
| 40:RH:90:GLU:HB2 | 40:SH:280:LYS:HZ1 | 1.66 | 0.60 |
| 40:SA:265:ILE:HB | 40:SA:431:TYR:HE1 | 1.66 | 0.60 |
| 41:SN:293:MET:HE3 | 41:SN:367:PHE:HD1 | 1.66 | 0.60 |
| 41:TM:86:ARG:NH1 | 41:UM:281:TYR:O | 2.35 | 0.60 |
| 40:UE:352:LYS:NZ | 41:UM:176:SER:OG | 2.34 | 0.60 |
| 40:UG:270:ALA:HA | 40:UG:377:LEU:HD23 | 1.83 | 0.60 |
| 40:UI:144:GLY:N | 42:UI:501:GTP:O2G | 2.35 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UI:219:ILE:HB | 40:UI:222:PRO:HG3 | 1.82 | 0.60 |
| 41:WM:21:TRP:O | 41:WM:25:SER:HB2 | 2.01 | 0.60 |
| 7:1T:113:LYS:HG2 | 7:1T:131:GLY:HA3 | 1.82 | 0.60 |
| 7:1T:116:ALA:HB1 | 7:1T:164:VAL:HG22 | 1.83 | 0.60 |
| 11:2I:197:LEU:HD21 | 11:2I:244:LEU:HB3 | 1.83 | 0.60 |
| 12:2M:146:ILE:HD13 | 12:2M:149:LEU:HD21 | 1.83 | 0.60 |
| 12:2P:120:THR:HG22 | 12:2P:122:PRO:HD2 | 1.84 | 0.60 |
| 14:3C:14:PHE:CD1 | 41:MO:174:LYS:HG3 | 2.36 | 0.60 |
| 17:3P:364:HIS:HA | 17:3P:367:LYS:HD2 | 1.81 | 0.60 |
| 22:4H:304:LEU:HG | 22:4H:321:ASP:HB2 | 1.82 | 0.60 |
| 22:4I:659:LYS:HB2 | 22:4I:678:LEU:HD11 | 1.82 | 0.60 |
| 23:4Q:240:LEU:HB3 | 23:4Q:266:HIS:HA | 1.83 | 0.60 |
| 31:5I:507:MET:HA | 31:5I:510:THR:HG22 | 1.82 | 0.60 |
| 34:5Q:215:ARG:HH22 | 41:GN:217:LEU:HD11 | 1.66 | 0.60 |
| 36:5W:218:ARG:NH2 | 41:KB:157:GLU:OE2 | 2.33 | 0.60 |
| 41:BB:58:LYS:O | 41:BB:59:TYR:C | 2.39 | 0.60 |
| 40:BI:171:ILE:HG21 | 42:BI:501:GTP:H1' | 1.84 | 0.60 |
| 41:CB:113:VAL:HA | 41:CB:116:VAL:HG12 | 1.82 | 0.60 |
| 41:CM:268:PRO:HA | 41:CM:368:ILE:HD13 | 1.82 | 0.60 |
| 41:EB:169:VAL:HG22 | 41:EB:202:ILE:HD11 | 1.82 | 0.60 |
| 40:EF:326:LYS:HE3 | 41:EN:208:TYR:HB2 | 1.83 | 0.60 |
| 41:EM:87:PRO:HD3 | 41:FM:281:TYR:HD2 | 1.67 | 0.60 |
| 40:FA:271:THR:HG23 | 40:FA:376:MET:HB3 | 1.83 | 0.60 |
| 41:FM:163:ILE:HD11 | 41:FM:251:ARG:HG3 | 1.83 | 0.60 |
| 40:GE:71:GLU:HB3 | 40:GE:98:ASP:HB2 | 1.82 | 0.60 |
| 40:GF:101:ASN:HA | 40:GF:144:GLY:H | 1.65 | 0.60 |
| 40:GF:138:PHE:HZ | 40:GF:235:VAL:HG21 | 1.66 | 0.60 |
| 41:GM:139:LEU:HB2 | 41:GM:168:SER:HB3 | 1.82 | 0.60 |
| 40:II:16:ILE:HA | 40:II:228:ASN:HB3 | 1.83 | 0.60 |
| 41:IQ:341:PHE:HB3 | 41:IQ:348:ASN:HD21 | 1.67 | 0.60 |
| 41:JN:252:LYS:O | 41:JN:256:ASN:ND2 | 2.34 | 0.60 |
| 40:KE:215:ARG:HH12 | 40:KE:299:ALA:HB1 | 1.66 | 0.60 |
| 40:KF:212:ILE:HD11 | 40:KF:300:ASN:HA | 1.83 | 0.60 |
| 41:KO:213:ARG:HD2 | 41:KO:297:LYS:HD2 | 1.84 | 0.60 |
| 40:LD:421:ARG:HH12 | 40:LD:425:ALA:HB2 | 1.66 | 0.60 |
| 41:LL:237:THR:HG22 | 41:LL:250:LEU:HD21 | 1.83 | 0.60 |
| 40:MF:273:ALA:CB | 40:MF:374:VAL:HG13 | 2.32 | 0.60 |
| 41:MN:313:VAL:HB | 41:MN:349:VAL:HG22 | 1.82 | 0.60 |
| 40:NH:167:LEU:HD11 | 40:NH:252:LEU:HD11 | 1.83 | 0.60 |
| 40:OE:318:LEU:O | 40:OE:374:VAL:HA | 2.01 | 0.60 |
| 41:OM:27:GLU:OE2 | 41:OM:318:ARG:NH1 | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OM:237:THR:HG23 | 41:OM:241:ARG:HH12 | 1.66 | 0.60 |
| 41:QB:173:PRO:O | 41:QB:174:LYS:C | 2.39 | 0.60 |
| 41:QM:133:PHE:O | 41:QM:164:MET:HA | 2.02 | 0.60 |
| 40:SE:326:LYS:NZ | 41:SM:204:ASN:O | 2.34 | 0.60 |
| 40:SH:318:LEU:O | 40:SH:374:VAL:HA | 2.00 | 0.60 |
| 41:SP:285:THR:HG22 | 41:SP:287:PRO:HD2 | 1.83 | 0.60 |
| 40:WH:247:ALA:O | 41:WP:11:GLN:NE2 | 2.34 | 0.60 |
| 4:1I:80:GLN:NE2 | 40:HI:341:ILE:O | 2.34 | 0.60 |
| 7:1S:487:ILE:HB | 7:1S:497:GLN:HB2 | 1.84 | 0.60 |
| 17:3O:397:GLN:HA | 17:3R:287:VAL:HG21 | 1.83 | 0.60 |
| 23:4Q:194:ALA:HB2 | 23:4Q:209:ALA:CB | 2.32 | 0.60 |
| 34:5R:314:THR:O | 34:5R:318:LEU:HG | 2.01 | 0.60 |
| 35:5U:26:ARG:NH1 | 41:IQ:44:LEU:HB3 | 2.16 | 0.60 |
| 40:BA:326:LYS:HA | 40:BA:329:ASN:HB2 | 1.83 | 0.60 |
| 40:BF:173:PRO:HG2 | 40:BF:390:LEU:HD21 | 1.82 | 0.60 |
| 41:BP:173:PRO:O | 41:BP:174:LYS:C | 2.40 | 0.60 |
| 41:CB:4:ILE:HB | 41:CB:50:TYR:HE1 | 1.67 | 0.60 |
| 41:DM:7:LEU:HD11 | 41:DM:133:PHE:HB3 | 1.83 | 0.60 |
| 41:DP:270:PHE:H | 41:DP:298:ASN:HD21 | 1.49 | 0.60 |
| 40:EH:400:LYS:O | 40:EH:401:ARG:C | 2.40 | 0.60 |
| 40:EI:88:HIS:CE1 | 40:EI:90:GLU:HB2 | 2.36 | 0.60 |
| 41:EM:316:VAL:HA | 41:EM:352:ALA:HB3 | 1.82 | 0.60 |
| 41:EP:319:GLY:O | 41:EP:320:ARG:C | 2.39 | 0.60 |
| 40:FE:56:THR:HA | 40:GE:285:GLN:HG2 | 1.84 | 0.60 |
| 40:GI:191:THR:HG21 | 40:GI:424:MET:HG3 | 1.84 | 0.60 |
| 41:HM:10:GLY:O | 41:HM:14:ASN:HB2 | 2.00 | 0.60 |
| 41:HO:100:ASN:HB3 | 41:HO:103:LYS:HB2 | 1.83 | 0.60 |
| 40:IA:262:TYR:HB2 | 40:IA:265:ILE:HG12 | 1.82 | 0.60 |
| 40:JE:401:ARG:NH2 | 40:JE:414:GLU:OE2 | 2.33 | 0.60 |
| 41:LB:15:GLN:NE2 | 43:LB:501:GDP:O6 | 2.35 | 0.60 |
| 40:LH:98:ASP:O | 40:LH:105:ARG:NH1 | 2.35 | 0.60 |
| 40:MA:303:VAL:O | 40:MA:305:CYS:N | 2.34 | 0.60 |
| 40:MH:353:VAL:HG13 | 41:MP:177:ASP:HA | 1.84 | 0.60 |
| 40:NF:255:PHE:HE1 | 40:NF:318:LEU:HD11 | 1.67 | 0.60 |
| 40:NH:141:PHE:HB2 | 40:NH:173:PRO:HD3 | 1.82 | 0.60 |
| 40:NH:177:VAL:O | 41:NO:347:ASN:ND2 | 2.35 | 0.60 |
| 40:OH:370:VAL:HG23 | 40:OH:372:ARG:H | 1.66 | 0.60 |
| 41:ON:314:ALA:HB3 | 41:ON:368:ILE:HB | 1.83 | 0.60 |
| 41:PL:46:ARG:HH21 | 41:PL:48:ASN:HD21 | 1.47 | 0.60 |
| 41:QP:45:GLU:HG2 | 41:QP:46:ARG:H | 1.67 | 0.60 |
| 40:RA:76:ASP:OD2 | 41:RN:46:ARG:NH2 | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RB:186:THR:HG21 | 41:RB:385:PHE:HB2 | 1.84 | 0.60 |
| 40:RF:98:ASP:O | 40:RF:105:ARG:NH2 | 2.34 | 0.60 |
| 41:RO:222:TYR:O | 41:RO:226:ASN:ND2 | 2.33 | 0.60 |
| 41:TB:113:VAL:HA | 41:TB:116:VAL:HG12 | 1.82 | 0.60 |
| 40:VG:180:ALA:HB3 | 40:VG:183:GLU:HG3 | 1.84 | 0.60 |
| 41:VO:142:GLY:O | 41:VO:144:GLY:N | 2.34 | 0.60 |
| 41:VQ:273:LEU:O | 41:VQ:292:GLN:NE2 | 2.24 | 0.60 |
| 41:WP:238:THR:OG1 | 41:WP:318:ARG:NH1 | 2.30 | 0.60 |
| 7:1S:506:GLN:NE2 | 7:1S:549:ASN:OD1 | 2.34 | 0.60 |
| 7:1U:467:ILE:HG12 | 7:1U:478:THR:HG22 | 1.84 | 0.60 |
| 9:2B:231:ARG:HE | 9:2B:232:ARG:HH22 | 1.48 | 0.60 |
| 12:2N:209:ASP:OD1 | 13:2T:22:LEU:N | 2.34 | 0.60 |
| 18:3U:352:VAL:HG12 | 18:3V:238:VAL:HG11 | 1.84 | 0.60 |
| 20:4B:339:LEU:HD13 | 40:MG:371:GLN:HG2 | 1.82 | 0.60 |
| 20:4B:358:ASN:O | 20:4B:359:SER:C | 2.39 | 0.60 |
| 22:4J:583:ARG:NH1 | 22:4J:596:ASP:OD1 | 2.35 | 0.60 |
| 24:4O:250:VAL:HG13 | 24:4O:253:TYR:HB2 | 1.82 | 0.60 |
| 23:4P:244:PRO:O | 23:4P:245:LYS:C | 2.39 | 0.60 |
| 23:4R:48:SER:HG | 23:4R:53:TRP:N | 1.98 | 0.60 |
| 31:5I:687:ILE:HG22 | 31:5I:688:ILE:HG22 | 1.82 | 0.60 |
| 36:5W:104:PHE:HB2 | 41:NN:56:GLY:HA3 | 1.83 | 0.60 |
| 36:5W:218:ARG:HH21 | 36:5W:222:LEU:HD11 | 1.67 | 0.60 |
| 40:BF:438:SER:OG | 41:BN:390:ARG:NH1 | 2.34 | 0.60 |
| 40:BH:335:ILE:HG23 | 40:BH:341:ILE:HD13 | 1.83 | 0.60 |
| 41:BP:142:GLY:O | 41:BP:143:THR:C | 2.40 | 0.60 |
| 41:CB:191:GLN:O | 41:CB:195:ASN:ND2 | 2.34 | 0.60 |
| 40:CF:326:LYS:HD2 | 41:CN:208:TYR:CD1 | 2.36 | 0.60 |
| 40:DA:96:LYS:HE3 | 41:DN:128:ASP:HB3 | 1.83 | 0.60 |
| 40:DA:224:TYR:HB3 | 42:DA:501:GTP:C2 | 2.36 | 0.60 |
| 40:DF:31:GLN:C | 40:DF:33:ASP:H | 2.05 | 0.60 |
| 40:DI:9:VAL:HG13 | 40:DI:68:VAL:HG23 | 1.82 | 0.60 |
| 40:EE:57:GLY:O | 40:EE:60:LYS:NZ | 2.30 | 0.60 |
| 41:EO:156:ARG:NH1 | 41:EO:195:ASN:O | 2.35 | 0.60 |
| 40:GI:273:ALA:CB | 40:GI:274:PRO:HD2 | 2.25 | 0.60 |
| 40:HA:278:ALA:H | 40:HA:368:ALA:HB2 | 1.67 | 0.60 |
| 40:HE:319:TYR:HB3 | 40:HE:323:VAL:HG21 | 1.84 | 0.60 |
| 41:HO:170:VAL:HG11 | 41:HO:377:LEU:HD21 | 1.83 | 0.60 |
| 41:HO:238:THR:HG1 | 41:HO:354:CYS:HG | 1.45 | 0.60 |
| 41:HO:292:GLN:O | 41:HO:298:ASN:ND2 | 2.34 | 0.60 |
| 41:KP:7:LEU:O | 41:KP:135:LEU:HA | 2.01 | 0.60 |
| 40:ND:11:GLN:HA | 40:ND:74:VAL:HG11 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NF:236:SER:O | 40:NF:243:ARG:NH2 | 2.34 | 0.60 |
| 41:NP:213:ARG:O | 41:NP:216:LYS:NZ | 2.35 | 0.60 |
| 40:OD:89:PRO:HG2 | 40:PD:283:HIS:HD1 | 1.67 | 0.60 |
| 40:OF:320:ARG:HG3 | 40:OF:356:ASN:HB3 | 1.84 | 0.60 |
| 41:OL:170:VAL:HG21 | 41:OL:377:LEU:HD21 | 1.84 | 0.60 |
| 40:PF:151:SER:HA | 40:PF:154:MET:HG2 | 1.82 | 0.60 |
| 41:QB:184:ASN:HA | 41:QB:187:LEU:HD12 | 1.83 | 0.60 |
| 41:QB:322:SER:O | 41:QB:325:GLU:HG3 | 2.02 | 0.60 |
| 40:QE:16:ILE:HG13 | 40:QE:228:ASN:HD22 | 1.67 | 0.60 |
| 40:QE:97:GLU:OE2 | 40:QE:105:ARG:NH2 | 2.34 | 0.60 |
| 40:SA:6:SER:OG | 40:SA:8:HIS:NE2 | 2.34 | 0.60 |
| 40:SI:270:ALA:HA | 40:SI:376:MET:O | 2.02 | 0.60 |
| 41:SM:167:PHE:HE2 | 41:SM:233:MET:HG3 | 1.67 | 0.60 |
| 41:SO:405:GLU:HA | 41:SO:408:PHE:HD1 | 1.67 | 0.60 |
| 40:TA:319:TYR:HB3 | 40:TA:323:VAL:HG21 | 1.84 | 0.60 |
| 41:TM:237:THR:HG22 | 41:TM:250:LEU:HD21 | 1.84 | 0.60 |
| 40:VH:254:GLU:OE1 | 41:VP:99:ASN:ND2 | 2.34 | 0.60 |
| 41:VO:282:ARG:NH2 | 41:VO:292:GLN:OE1 | 2.35 | 0.60 |
| 40:WF:73:THR:HA | 40:WF:76:ASP:HB2 | 1.84 | 0.60 |
| 8:1Y:101:ILE:HD11 | 11:2J:251:TYR:CE2 | 2.37 | 0.60 |
| 22:4I:486:VAL:HG11 | 22:4I:515:VAL:HG12 | 1.84 | 0.60 |
| 23:4P:243:LEU:HD13 | 40:DA:79:ARG:O | 2.02 | 0.60 |
| 26:4W:301:THR:O | 26:4W:305:SER:HB2 | 2.01 | 0.60 |
| 28:5B:206:GLU:O | 41:KP:77:ARG:NH2 | 2.34 | 0.60 |
| 32:5L:43:ARG:HE | 41:JO:78:SER:HB2 | 1.66 | 0.60 |
| 41:AN:156:ARG:NH1 | 41:AN:195:ASN:O | 2.35 | 0.60 |
| 41:AO:358:PRO:O | 41:AO:359:ARG:C | 2.39 | 0.60 |
| 40:BI:63:PRO:HG3 | 40:BI:86:LEU:HG | 1.82 | 0.60 |
| 41:CN:138:SER:HA | 41:CN:169:VAL:HG22 | 1.83 | 0.60 |
| 40:DA:73:THR:O | 40:DA:76:ASP:N | 2.31 | 0.60 |
| 40:DA:296:PHE:HB3 | 40:DA:341:ILE:HD13 | 1.84 | 0.60 |
| 40:DE:291:ILE:HG12 | 40:DE:292:THR:N | 2.14 | 0.60 |
| 40:DG:228:ASN:HD21 | 42:DG:501:GTP:HN1 | 1.48 | 0.60 |
| 41:DL:314:ALA:HB1 | 41:DL:350:LYS:HB3 | 1.84 | 0.60 |
| 41:DN:5:VAL:HG23 | 41:DN:130:LEU:HD11 | 1.83 | 0.60 |
| 41:DN:193:VAL:O | 41:DN:195:ASN:N | 2.35 | 0.60 |
| 41:DP:19:LYS:HA | 41:DP:22:GLU:HB2 | 1.82 | 0.60 |
| 41:EO:7:LEU:O | 41:EO:135:LEU:HA | 2.01 | 0.60 |
| 40:FF:221:ARG:NH1 | 41:FM:325:GLU:OE2 | 2.35 | 0.60 |
| 40:FH:278:ALA:H | 40:FH:368:ALA:HB2 | 1.67 | 0.60 |
| 41:GP:139:LEU:HD12 | 41:GP:170:VAL:HG12 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HO:107:THR:HG22 | 41:HO:108:GLU:H | 1.66 | 0.60 |
| 40:JA:240:ALA:HA | 40:JA:243:ARG:HE | 1.67 | 0.60 |
| 41:JM:256:ASN:HB3 | 41:JM:350:LYS:HG2 | 1.83 | 0.60 |
| 41:ML:42:LEU:HD13 | 41:ML:356:ILE:HD11 | 1.84 | 0.60 |
| 40:ND:264:ARG:O | 40:ND:265:ILE:C | 2.40 | 0.60 |
| 40:NF:259:LEU:O | 40:NF:379:ASN:ND2 | 2.34 | 0.60 |
| 40:OE:319:TYR:HB3 | 40:OE:323:VAL:HG21 | 1.84 | 0.60 |
| 40:OF:228:ASN:HD21 | 42:OM:501:GTP:HN1 | 1.48 | 0.60 |
| 41:OP:132:GLY:HA2 | 41:OP:163:ILE:O | 2.01 | 0.60 |
| 41:PM:121:ARG:NH1 | 41:PM:159:TYR:OH | 2.35 | 0.60 |
| 41:QM:271:ALA:HB1 | 41:QM:292:GLN:HB3 | 1.83 | 0.60 |
| 40:RF:246:GLY:HA3 | 40:RF:356:ASN:HA | 1.83 | 0.60 |
| 41:RM:289:LEU:HD23 | 41:RM:292:GLN:HE21 | 1.66 | 0.60 |
| 41:SB:273:LEU:O | 41:SB:292:GLN:NE2 | 2.31 | 0.60 |
| 40:TA:213:CYS:HA | 40:TA:217:LEU:HD13 | 1.82 | 0.60 |
| 40:UA:239:THR:O | 40:UA:243:ARG:NH1 | 2.35 | 0.60 |
| 40:UI:126:ALA:HA | 40:UI:129:CYS:HB2 | 1.84 | 0.60 |
| 40:VG:133:GLN:NE2 | 40:VG:251:ASP:OD1 | 2.35 | 0.60 |
| 40:VH:51:THR:HG21 | 40:VH:243:ARG:HA | 1.84 | 0.60 |
| 41:WM:100:ASN:O | 41:WM:101:TRP:C | 2.40 | 0.60 |
| 41:WQ:27:GLU:O | 41:WQ:43:GLN:NE2 | 2.34 | 0.60 |
| 7:1T:278:SER:O | 7:1T:279:PRO:C | 2.40 | 0.60 |
| 14:3C:81:LEU:HD23 | 14:3C:89:ALA:HB1 | 1.84 | 0.60 |
| 17:3O:413:ARG:HH12 | 17:3R:294:VAL:H | 1.49 | 0.60 |
| 22:4J:113:ILE:HD11 | 22:4J:136:ILE:HD12 | 1.83 | 0.60 |
| 27:4Y:148:ARG:NH1 | 27:4Y:187:ASP:OD1 | 2.34 | 0.60 |
| 40:BE:102:ASN:HB3 | 40:BE:105:ARG:HG3 | 1.83 | 0.60 |
| 41:CM:70:PRO:HD3 | 41:CM:94:GLN:HA | 1.84 | 0.60 |
| 41:CM:309:ARG:H | 41:CM:372:THR:HG22 | 1.67 | 0.60 |
| 41:CP:248:ALA:HA | 41:CP:252:LYS:HE3 | 1.83 | 0.60 |
| 41:DB:87:PRO:O | 41:DB:88:ASP:C | 2.40 | 0.60 |
| 40:DE:124:LYS:O | 40:DE:127:ASP:HB2 | 2.01 | 0.60 |
| 40:DE:180:ALA:HB3 | 40:DE:183:GLU:HG3 | 1.83 | 0.60 |
| 40:DF:13:GLY:HA2 | 40:DF:16:ILE:HD13 | 1.83 | 0.60 |
| 40:DF:239:THR:HG23 | 40:DF:243:ARG:HH21 | 1.64 | 0.60 |
| 40:DH:402:ALA:HA | 41:DO:260:PHE:HE1 | 1.66 | 0.60 |
| 40:EG:260:VAL:HB | 41:EO:397:TRP:HH2 | 1.67 | 0.60 |
| 41:EM:267:MET:HE3 | 41:EM:301:ALA:HB3 | 1.84 | 0.60 |
| 40:FA:5:ILE:HG13 | 40:FA:132:LEU:HD11 | 1.83 | 0.60 |
| 40:GH:257:THR:HG21 | 41:GP:98:GLY:O | 2.02 | 0.60 |
| 41:IN:421:PRO:HA | 41:IN:424:THR:HG22 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JB:237:THR:HG22 | 41:JB:250:LEU:HD21 | 1.83 | 0.60 |
| 41:JB:256:ASN:HD22 | 41:JB:350:LYS:HD3 | 1.67 | 0.60 |
| 41:KO:296:ALA:HB3 | 41:KO:306:ARG:HH12 | 1.65 | 0.60 |
| 41:LB:204:ASN:ND2 | 43:LB:501:GDP:O2' | 2.34 | 0.60 |
| 40:ME:236:SER:O | 40:ME:240:ALA:HB2 | 2.02 | 0.60 |
| 41:MN:51:TYR:HB3 | 41:MN:59:TYR:HB3 | 1.83 | 0.60 |
| 41:NL:165:ASN:HD21 | 41:NL:250:LEU:HD13 | 1.65 | 0.60 |
| 41:NM:334:GLN:HE21 | 41:NM:349:VAL:HG13 | 1.66 | 0.60 |
| 41:OL:317:PHE:HB2 | 41:OL:353:VAL:HG12 | 1.84 | 0.60 |
| 41:PL:49:VAL:O | 41:PL:62:ARG:NH2 | 2.34 | 0.60 |
| 41:QB:61:PRO:HG2 | 41:QB:84:ILE:HD12 | 1.83 | 0.60 |
| 40:QE:254:GLU:OE2 | 41:QM:99:ASN:ND2 | 2.35 | 0.60 |
| 40:RI:31:GLN:HE22 | 40:RI:35:GLN:HB3 | 1.67 | 0.60 |
| 41:SB:247:ASN:OD1 | 40:SG:11:GLN:NE2 | 2.35 | 0.60 |
| 40:SH:406:TRP:CH2 | 41:SO:255:VAL:HA | 2.37 | 0.60 |
| 41:SP:178:THR:HB | 41:SP:181:GLU:HB2 | 1.82 | 0.60 |
| 41:TB:282:ARG:NH2 | 41:TB:288:GLU:OE2 | 2.32 | 0.60 |
| 41:VO:252:LYS:HA | 41:VO:255:VAL:HG12 | 1.83 | 0.60 |
| 41:VP:26:ASP:HB3 | 41:VP:359:ARG:HH21 | 1.67 | 0.60 |
| 41:VP:375:GLN:HE21 | 41:VP:423:VAL:HG22 | 1.67 | 0.60 |
| 40:WG:97:GLU:HG2 | 40:WG:105:ARG:HH21 | 1.67 | 0.60 |
| 7:1U:570:LYS:HG2 | 7:1U:582:VAL:HG22 | 1.84 | 0.60 |
| 18:3T:136:GLN:HG3 | 18:3T:140:ARG:NH1 | 2.17 | 0.60 |
| 21:4F:310:GLN:HB2 | 41:CM:359:ARG:CZ | 2.32 | 0.60 |
| 23:4N:244:PRO:O | 23:4N:245:LYS:C | 2.39 | 0.60 |
| 36:5X:176:THR:OG1 | 41:OM:276:ARG:NH2 | 2.32 | 0.60 |
| 41:AO:103:LYS:HG2 | 41:AO:108:GLU:HG2 | 1.83 | 0.60 |
| 41:BB:324:LYS:HD2 | 40:BG:222:PRO:HD2 | 1.83 | 0.60 |
| 40:BF:142:GLY:HA2 | 40:BF:183:GLU:HG2 | 1.84 | 0.60 |
| 40:BI:100:ALA:O | 40:BI:101:ASN:C | 2.40 | 0.60 |
| 40:DE:281:ALA:O | 40:DE:282:TYR:C | 2.40 | 0.60 |
| 41:DM:12:CYS:HB3 | 41:DM:138:SER:HB2 | 1.84 | 0.60 |
| 41:DP:259:PRO:HG2 | 41:DP:311:LEU:HD23 | 1.82 | 0.60 |
| 40:EH:274:PRO:HB3 | 40:EH:370:VAL:HG21 | 1.84 | 0.60 |
| 40:FE:88:HIS:HB3 | 40:FE:91:GLN:HB2 | 1.82 | 0.60 |
| 40:GE:259:LEU:O | 40:GE:260:VAL:C | 2.40 | 0.60 |
| 40:GI:285:GLN:O | 40:GI:286:LEU:C | 2.40 | 0.60 |
| 41:HN:271:ALA:HB3 | 41:HN:272:PRO:HD3 | 1.83 | 0.60 |
| 41:IB:46:ARG:NH2 | 40:IG:76:ASP:OD2 | 2.34 | 0.60 |
| 41:IQ:189:VAL:HA | 41:IQ:192:LEU:HB2 | 1.82 | 0.60 |
| 40:JH:212:ILE:HD11 | 40:JH:300:ASN:HA | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JN:292:GLN:OE1 | 41:JN:298:ASN:ND2 | 2.34 | 0.60 |
| 40:LF:269:LEU:HD12 | 40:LF:303:VAL:HG21 | 1.83 | 0.60 |
| 40:NH:223:THR:HG22 | 40:NH:225:THR:H | 1.66 | 0.60 |
| 41:OB:275:SER:O | 41:OB:279:GLN:HB2 | 2.01 | 0.60 |
| 41:OB:292:GLN:O | 41:OB:298:ASN:ND2 | 2.33 | 0.60 |
| 40:OD:206:ASN:OD1 | 42:OD:501:GTP:O2' | 2.17 | 0.60 |
| 40:OG:297:GLU:O | 40:OG:301:GLN:NE2 | 2.35 | 0.60 |
| 41:PB:317:PHE:HB2 | 41:PB:353:VAL:HG12 | 1.84 | 0.60 |
| 40:PH:317:LEU:HD23 | 40:PH:376:MET:HG2 | 1.84 | 0.60 |
| 41:PL:179:VAL:HG23 | 41:PL:180:VAL:HG13 | 1.84 | 0.60 |
| 40:QF:247:ALA:O | 41:QN:11:GLN:NE2 | 2.34 | 0.60 |
| 41:QP:25:SER:O | 41:QP:29:GLY:N | 2.34 | 0.60 |
| 40:RI:145:THR:OG1 | 42:RP:501:GTP:O2B | 2.19 | 0.60 |
| 41:SM:4:ILE:HB | 41:SM:50:TYR:HE2 | 1.66 | 0.60 |
| 41:SM:51:TYR:HB3 | 41:SM:59:TYR:HB3 | 1.84 | 0.60 |
| 40:TA:76:ASP:OD2 | 41:TN:46:ARG:NH2 | 2.35 | 0.60 |
| 41:TO:3:GLU:HA | 41:TO:49:VAL:HG23 | 1.84 | 0.60 |
| 40:VA:304:LYS:O | 40:VA:389:ARG:NH2 | 2.35 | 0.60 |
| 4:1H:80:GLN:HG2 | 40:HA:339:ARG:HA | 1.83 | 0.59 |
| 7:1T:94:ILE:HD13 | 7:1T:106:ARG:HH21 | 1.67 | 0.59 |
| 15:3F:205:VAL:HG13 | 15:3G:338:ILE:HD12 | 1.82 | 0.59 |
| 15:3F:310:ALA:HB2 | 15:3F:344:ILE:HG21 | 1.83 | 0.59 |
| 18:3W:312:GLU:OE1 | 18:3W:315:ARG:NH1 | 2.35 | 0.59 |
| 21:4F:511:TYR:N | 40:EE:39:ASP:OD1 | 2.35 | 0.59 |
| 23:4Q:259:ARG:NH1 | 40:EH:365:GLY:HA3 | 2.17 | 0.59 |
| 41:BB:189:VAL:O | 41:BB:193:VAL:HG23 | 2.02 | 0.59 |
| 40:CA:89:PRO:HG2 | 40:DA:280:LYS:HA | 1.82 | 0.59 |
| 40:CH:195:LEU:HD21 | 40:CH:427:LEU:HD13 | 1.84 | 0.59 |
| 41:CL:215:LEU:HD11 | 41:CL:273:LEU:HD22 | 1.84 | 0.59 |
| 41:CN:2:ARG:HA | 41:CN:131:GLN:HB3 | 1.84 | 0.59 |
| 41:CP:354:CYS:SG | 41:CP:355:ASP:N | 2.75 | 0.59 |
| 40:DA:12:ALA:HA | 40:DA:15:GLN:HG3 | 1.83 | 0.59 |
| 40:DF:405:HIS:HE1 | 41:DM:258:VAL:HG12 | 1.66 | 0.59 |
| 40:DG:272:TYR:HD2 | 40:DG:275:VAL:HG22 | 1.66 | 0.59 |
| 40:DH:278:ALA:HA | 40:DH:368:ALA:HB2 | 1.82 | 0.59 |
| 41:DL:311:LEU:HB2 | 41:DL:370:ASN:HB3 | 1.84 | 0.59 |
| 41:DN:262:ARG:O | 41:DN:263:LEU:C | 2.40 | 0.59 |
| 40:FA:101:ASN:OD1 | 40:FA:143:GLY:HA2 | 2.01 | 0.59 |
| 40:FA:222:PRO:N | 41:FN:324:LYS:HZ1 | 2.00 | 0.59 |
| 40:FI:71:GLU:OE2 | 41:FP:2:ARG:NH1 | 2.35 | 0.59 |
| 40:GE:201:ALA:O | 40:GE:203:MET:N | 2.34 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GN:420:ASN:HB2 | 41:GN:421:PRO:HD3 | 1.82 | 0.59 |
| 41:HO:26:ASP:O | 41:HO:359:ARG:NH2 | 2.35 | 0.59 |
| 41:IB:272:PRO:HG3 | 41:IB:364:SER:HA | 1.83 | 0.59 |
| 40:IF:352:LYS:NZ | 41:IN:177:ASP:O | 2.25 | 0.59 |
| 41:IN:390:ARG:HG3 | 41:IN:391:ARG:HG2 | 1.83 | 0.59 |
| 41:IP:317:PHE:HB2 | 41:IP:353:VAL:HG12 | 1.84 | 0.59 |
| 40:JE:55:GLU:O | 40:KE:285:GLN:NE2 | 2.34 | 0.59 |
| 40:JF:320:ARG:HG2 | 40:JF:356:ASN:HB2 | 1.84 | 0.59 |
| 40:LF:104:ALA:HB1 | 40:LF:410:GLU:HG2 | 1.84 | 0.59 |
| 40:LH:258:ASN:OD1 | 40:LH:352:LYS:NZ | 2.35 | 0.59 |
| 41:LM:237:THR:O | 41:LM:241:ARG:NH1 | 2.35 | 0.59 |
| 41:LO:86:ARG:HD2 | 41:MO:281:TYR:HB3 | 1.84 | 0.59 |
| 40:MF:122:ILE:HG21 | 40:MF:157:LEU:HD21 | 1.84 | 0.59 |
| 40:QE:424:MET:HA | 40:QE:427:LEU:HD23 | 1.83 | 0.59 |
| 41:QP:138:SER:HA | 41:QP:169:VAL:HB | 1.83 | 0.59 |
| 41:SB:417:ASP:O | 41:SB:421:PRO:HD3 | 2.02 | 0.59 |
| 40:SF:185:TYR:HE2 | 40:SF:403:PHE:HB2 | 1.67 | 0.59 |
| 40:SG:102:ASN:HB3 | 40:SG:105:ARG:HB2 | 1.84 | 0.59 |
| 41:SL:130:LEU:HB3 | 41:SL:162:ARG:HH21 | 1.67 | 0.59 |
| 41:SO:309:ARG:HG3 | 41:SO:372:THR:HG21 | 1.84 | 0.59 |
| 40:TE:98:ASP:O | 41:TL:251:ARG:NH2 | 2.34 | 0.59 |
| 40:TE:206:ASN:ND2 | 42:TL:501:GTP:O2' | 2.35 | 0.59 |
| 40:TI:211:ASP:OD2 | 40:TI:304:LYS:NZ | 2.35 | 0.59 |
| 41:UB:287:PRO:HA | 41:UB:329:GLN:HE22 | 1.65 | 0.59 |
| 40:UI:106:GLY:HA3 | 40:UI:148:GLY:HA3 | 1.83 | 0.59 |
| 41:UM:318:ARG:HB2 | 41:UM:364:SER:HB3 | 1.83 | 0.59 |
| 40:VG:142:GLY:HA2 | 40:VG:183:GLU:HG2 | 1.84 | 0.59 |
| 41:WB:282:ARG:NE | 41:WB:288:GLU:OE2 | 2.35 | 0.59 |
| 7:1T:228:ASP:HA | 7:1T:244:PRO:HD2 | 1.84 | 0.59 |
| 7:1T:392:ALA:HB2 | 7:1T:423:VAL:HG13 | 1.85 | 0.59 |
| 8:1Y:177:ARG:O | 8:1Y:181:LEU:HB2 | 2.03 | 0.59 |
| 12:2R:146:ILE:HD13 | 12:2R:149:LEU:HD21 | 1.84 | 0.59 |
| 16:3K:303:ASP:OD1 | 16:3K:306:ARG:NH2 | 2.34 | 0.59 |
| 20:4A:149:ARG:NH2 | 20:4A:150:SER:CA | 2.64 | 0.59 |
| 21:4D:429:PRO:HG3 | 22:4I:644:TYR:CG | 2.37 | 0.59 |
| 22:4K:545:ILE:HD11 | 22:4K:605:HIS:HB2 | 1.84 | 0.59 |
| 27:4Z:226:ARG:HE | 41:KO:80:PRO:HG2 | 1.66 | 0.59 |
| 33:5N:169:LEU:HD12 | 41:HQ:276:ARG:HG3 | 1.84 | 0.59 |
| 33:5N:279:GLN:NE2 | 33:5N:283:ASP:OD2 | 2.35 | 0.59 |
| 40:AA:318:LEU:O | 40:AA:374:VAL:HA | 2.03 | 0.59 |
| 41:AP:309:ARG:N | 41:AP:372:THR:OG1 | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BF:67:PHE:HB3 | 40:BF:75:ILE:HD12 | 1.84 | 0.59 |
| 40:BH:269:LEU:HD22 | 40:BH:303:VAL:HG21 | 1.84 | 0.59 |
| 40:CA:185:TYR:O | 40:CA:188:ILE:HG13 | 2.02 | 0.59 |
| 40:CF:254:GLU:HB3 | 41:CN:98:GLY:HA2 | 1.83 | 0.59 |
| 40:DA:177:VAL:HG13 | 40:DA:178:SER:H | 1.67 | 0.59 |
| 40:DE:83:TYR:O | 40:DE:84:ARG:C | 2.40 | 0.59 |
| 40:DH:139:HIS:HB2 | 40:DH:150:THR:HG21 | 1.84 | 0.59 |
| 40:EF:11:GLN:NE2 | 41:EM:245:GLN:O | 2.34 | 0.59 |
| 40:EF:229:ARG:HH22 | 40:EF:365:GLY:HA3 | 1.67 | 0.59 |
| 40:EI:63:PRO:HG3 | 40:EI:86:LEU:HG | 1.83 | 0.59 |
| 40:FA:30:ILE:HD12 | 40:FA:61:HIS:HB3 | 1.84 | 0.59 |
| 40:FE:260:VAL:HB | 41:FM:397:TRP:HH2 | 1.67 | 0.59 |
| 41:FP:172:SER:HB2 | 41:FP:205:GLU:HG3 | 1.85 | 0.59 |
| 40:HA:101:ASN:HB3 | 40:HA:182:VAL:HG21 | 1.83 | 0.59 |
| 40:JD:88:HIS:NE2 | 40:KD:284:GLU:OE1 | 2.30 | 0.59 |
| 41:JL:51:TYR:HB3 | 41:JL:59:TYR:HB3 | 1.82 | 0.59 |
| 40:KD:308:ARG:HB2 | 40:ND:282:TYR:OH | 2.02 | 0.59 |
| 41:KO:7:LEU:HD12 | 41:KO:135:LEU:HD13 | 1.83 | 0.59 |
| 40:MD:98:ASP:O | 40:MD:105:ARG:NH2 | 2.35 | 0.59 |
| 40:MH:393:LYS:HB3 | 41:MO:346:PRO:HG3 | 1.84 | 0.59 |
| 40:OA:16:ILE:HA | 40:OA:228:ASN:HB3 | 1.84 | 0.59 |
| 40:OH:70:LEU:HA | 40:OH:95:GLY:HA3 | 1.83 | 0.59 |
| 41:OO:268:PRO:HG2 | 41:OO:300:MET:HB2 | 1.83 | 0.59 |
| 41:PN:113:VAL:HG21 | 41:PN:150:LEU:HD22 | 1.83 | 0.59 |
| 41:PO:292:GLN:O | 41:PO:298:ASN:ND2 | 2.35 | 0.59 |
| 41:RN:73:MET:HG3 | 41:RN:77:ARG:HH21 | 1.65 | 0.59 |
| 41:RP:24:ILE:HA | 41:RP:27:GLU:HG3 | 1.83 | 0.59 |
| 40:SA:26:LEU:HD13 | 40:SA:363:VAL:HG12 | 1.84 | 0.59 |
| 40:SG:326:LYS:NZ | 41:SO:208:TYR:HB2 | 2.17 | 0.59 |
| 40:TI:221:ARG:NH1 | 41:TP:325:GLU:OE2 | 2.34 | 0.59 |
| 40:UE:105:ARG:HG2 | 40:UE:410:GLU:HG2 | 1.82 | 0.59 |
| 40:UG:213:CYS:HA | 40:UG:217:LEU:HB2 | 1.83 | 0.59 |
| 41:WN:178:THR:HG22 | 41:WN:180:VAL:H | 1.67 | 0.59 |
| 41:WP:252:LYS:HA | 41:WP:255:VAL:HG12 | 1.84 | 0.59 |
| 9:2B:242:ILE:HG13 | 9:2B:245:GLN:HE21 | 1.67 | 0.59 |
| 22:4I:260:ILE:HG13 | 22:4I:284:LEU:HB2 | 1.84 | 0.59 |
| 34:5R:397:ARG:HD2 | 40:GH:369:LYS:HD2 | 1.85 | 0.59 |
| 40:BH:3:GLU:HG2 | 40:BH:129:CYS:HB2 | 1.83 | 0.59 |
| 41:BM:260:PHE:HB3 | 41:BM:261:PRO:HD2 | 1.83 | 0.59 |
| 40:DI:73:THR:O | 40:DI:76:ASP:N | 2.29 | 0.59 |
| 40:EF:16:ILE:HD11 | 40:EF:138:PHE:HB3 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EO:284:LEU:HD21 | 41:EO:363:MET:HB2 | 1.84 | 0.59 |
| 40:GI:217:LEU:HA | 40:GI:277:SER:HB2 | 1.83 | 0.59 |
| 40:II:239:THR:O | 40:II:243:ARG:NH1 | 2.35 | 0.59 |
| 41:IO:178:THR:HB | 41:IO:181:GLU:HG3 | 1.84 | 0.59 |
| 40:JA:228:ASN:HD21 | 42:JA:501:GTP:HN1 | 1.50 | 0.59 |
| 41:JO:222:TYR:O | 41:JO:226:ASN:ND2 | 2.35 | 0.59 |
| 41:KB:27:GLU:OE2 | 41:KB:241:ARG:NH2 | 2.35 | 0.59 |
| 40:KD:405:HIS:HA | 40:KD:408:VAL:HG12 | 1.84 | 0.59 |
| 40:KE:228:ASN:HD21 | 42:KE:501:GTP:HN1 | 1.50 | 0.59 |
| 41:KO:7:LEU:O | 41:KO:135:LEU:HA | 2.02 | 0.59 |
| 41:KO:58:LYS:NZ | 41:LO:280:GLN:OE1 | 2.33 | 0.59 |
| 41:KP:89:ASN:ND2 | 41:KP:123:GLU:OE2 | 2.35 | 0.59 |
| 40:LA:30:ILE:HG13 | 40:LA:36:MET:HG3 | 1.85 | 0.59 |
| 41:LL:103:LYS:O | 41:LL:107:THR:OG1 | 2.20 | 0.59 |
| 40:MG:411:GLY:O | 40:MG:412:MET:C | 2.41 | 0.59 |
| 41:MN:309:ARG:NH2 | 41:MN:341:PHE:O | 2.35 | 0.59 |
| 40:OA:226:ASN:ND2 | 40:OA:366:ASP:OD2 | 2.35 | 0.59 |
| 41:ON:68:LEU:HD11 | 41:ON:109:GLY:HA2 | 1.83 | 0.59 |
| 41:ON:248:ALA:HA | 41:ON:252:LYS:HD3 | 1.85 | 0.59 |
| 40:QE:76:ASP:HA | 40:QE:79:ARG:HG2 | 1.84 | 0.59 |
| 40:QE:195:LEU:HD11 | 40:QE:427:LEU:HD21 | 1.84 | 0.59 |
| 40:QE:438:SER:OG | 41:QM:390:ARG:NH2 | 2.36 | 0.59 |
| 40:RF:265:ILE:HD13 | 40:RF:431:TYR:HE1 | 1.68 | 0.59 |
| 41:SM:295:ASP:OD1 | 41:SM:298:ASN:ND2 | 2.34 | 0.59 |
| 41:SO:313:VAL:HA | 41:SO:369:GLY:HA3 | 1.84 | 0.59 |
| 40:TG:195:LEU:HD21 | 40:TG:264:ARG:HE | 1.67 | 0.59 |
| 41:TL:179:VAL:HG23 | 41:TL:180:VAL:HG13 | 1.83 | 0.59 |
| 40:UF:55:GLU:HA | 40:UF:61:HIS:HA | 1.84 | 0.59 |
| 41:UM:354:CYS:SG | 41:UM:355:ASP:N | 2.74 | 0.59 |
| 41:UP:271:ALA:HB3 | 41:UP:272:PRO:HD3 | 1.84 | 0.59 |
| 40:VG:332:ILE:HG21 | 41:VO:175:VAL:HG23 | 1.85 | 0.59 |
| 40:VJ:397:MET:HG3 | 41:VQ:346:PRO:HD2 | 1.84 | 0.59 |
| 41:WM:310:TYR:O | 41:WM:311:LEU:C | 2.40 | 0.59 |
| 5:1N:164:ASN:ND2 | 41:HQ:339:SER:OG | 2.31 | 0.59 |
| 8:1X:175:LEU:HD11 | 41:UB:31:ASP:HB2 | 1.83 | 0.59 |
| 12:2M:45:LYS:HA | 12:2M:48:MET:HE3 | 1.84 | 0.59 |
| 12:2Q:78:ARG:HD2 | 13:2U:72:LYS:HD2 | 1.84 | 0.59 |
| 15:3F:363:LYS:HE3 | 22:4J:183:VAL:HG12 | 1.84 | 0.59 |
| 19:3Y:24:ARG:HH22 | 41:LP:80:PRO:HA | 1.68 | 0.59 |
| 22:4I:652:VAL:HB | 22:4I:687:GLN:HB3 | 1.83 | 0.59 |
| 23:4R:60:LEU:HB3 | 40:BI:84:ARG:CZ | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4R:236:TYR:HD1 | 23:4R:267:ASP:HB3 | 1.67 | 0.59 |
| 26:4V:113:ILE:HG23 | 26:4V:118:PHE:HD2 | 1.66 | 0.59 |
| 39:6H:24:GLN:NE2 | 39:6H:123:VAL:O | 2.36 | 0.59 |
| 40:AG:50:ASN:O | 40:AG:64:ARG:NH1 | 2.35 | 0.59 |
| 40:CE:11:GLN:HG3 | 40:CE:74:VAL:HG21 | 1.84 | 0.59 |
| 41:CO:268:PRO:HG2 | 41:CO:300:MET:HB2 | 1.84 | 0.59 |
| 40:DA:112:LYS:HE3 | 40:DA:152:LEU:HD22 | 1.84 | 0.59 |
| 40:DH:402:ALA:HA | 41:DO:260:PHE:CE1 | 2.37 | 0.59 |
| 41:DL:19:LYS:HB3 | 41:DL:226:ASN:ND2 | 2.17 | 0.59 |
| 41:DN:292:GLN:O | 41:DN:293:MET:C | 2.40 | 0.59 |
| 41:DO:421:PRO:HA | 41:DO:424:THR:HG22 | 1.85 | 0.59 |
| 40:EI:407:TYR:HB3 | 40:EI:417:PHE:HZ | 1.68 | 0.59 |
| 40:FA:30:ILE:HG23 | 40:FA:61:HIS:HB2 | 1.84 | 0.59 |
| 40:GF:205:ASP:HB3 | 40:GF:303:VAL:HA | 1.84 | 0.59 |
| 40:HE:3:GLU:HG3 | 40:HE:129:CYS:HB2 | 1.85 | 0.59 |
| 41:HN:288:GLU:HG3 | 41:HN:289:LEU:N | 2.17 | 0.59 |
| 41:HQ:385:PHE:O | 41:HQ:389:PHE:HB3 | 2.03 | 0.59 |
| 40:IG:185:TYR:HE2 | 40:IG:403:PHE:HB2 | 1.66 | 0.59 |
| 40:II:98:ASP:O | 40:II:105:ARG:NH2 | 2.32 | 0.59 |
| 41:IQ:316:VAL:HG12 | 41:IQ:352:ALA:HB3 | 1.85 | 0.59 |
| 41:JM:7:LEU:O | 41:JM:135:LEU:HA | 2.02 | 0.59 |
| 41:KL:391:ARG:O | 41:KL:392:LYS:C | 2.39 | 0.59 |
| 40:ME:142:GLY:HA2 | 40:ME:183:GLU:HG3 | 1.84 | 0.59 |
| 40:MF:9:VAL:HG12 | 40:MF:145:THR:HG22 | 1.83 | 0.59 |
| 40:NA:178:SER:OG | 41:NN:347:ASN:ND2 | 2.35 | 0.59 |
| 41:NB:324:LYS:HG3 | 40:NG:222:PRO:HD2 | 1.85 | 0.59 |
| 41:NL:178:THR:HB | 41:NL:181:GLU:HG3 | 1.84 | 0.59 |
| 41:OL:174:LYS:HD3 | 41:OL:175:VAL:HG13 | 1.82 | 0.59 |
| 41:PB:345:ILE:HG12 | 41:PB:425:ARG:HH22 | 1.66 | 0.59 |
| 41:PM:45:GLU:HG2 | 41:PM:46:ARG:HG2 | 1.84 | 0.59 |
| 40:QE:246:GLY:HA3 | 40:QE:356:ASN:HA | 1.82 | 0.59 |
| 40:RA:51:THR:HG21 | 40:RA:243:ARG:HG2 | 1.83 | 0.59 |
| 40:SA:11:GLN:HE22 | 41:SN:247:ASN:H | 1.50 | 0.59 |
| 40:SG:35:GLN:HG2 | 40:SG:60:LYS:HG3 | 1.84 | 0.59 |
| 40:UG:224:TYR:O | 40:UG:228:ASN:ND2 | 2.35 | 0.59 |
| 40:UI:224:TYR:HD2 | 41:UP:323:MET:HG3 | 1.67 | 0.59 |
| 40:UI:388:ALA:HA | 40:UI:391:ASP:HB2 | 1.84 | 0.59 |
| 40:VJ:298:PRO:HB3 | 40:VJ:307:PRO:HD2 | 1.83 | 0.59 |
| 41:VN:27:GLU:OE1 | 41:VN:241:ARG:NH2 | 2.35 | 0.59 |
| 41:VP:237:THR:HG22 | 41:VP:250:LEU:HD21 | 1.83 | 0.59 |
| 40:WI:235:VAL:HA | 40:WI:238:ILE:HG22 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1T:339:VAL:HG12 | 7:1T:380:ILE:HD12 | 1.85 | 0.59 |
| 8:1W:349:GLU:HA | 8:1W:352:PHE:HD2 | 1.66 | 0.59 |
| 8:1X:288:MET:SD | 41:UM:280:GLN:NE2 | 2.73 | 0.59 |
| 13:2W:173:SER:O | 13:2W:174:GLU:C | 2.41 | 0.59 |
| 16:3L:100:GLU:OE2 | 18:3U:161:ARG:NH2 | 2.35 | 0.59 |
| 17:3P:393:LEU:HB2 | 17:3P:427:VAL:HG11 | 1.85 | 0.59 |
| 21:4D:243:LEU:O | 21:4D:265:HIS:HA | 2.03 | 0.59 |
| 21:4D:484:TYR:O | 21:4D:485:TYR:C | 2.40 | 0.59 |
| 28:5B:124:ILE:O | 28:5B:127:ARG:NH1 | 2.36 | 0.59 |
| 40:BI:273:ALA:CB | 40:BI:274:PRO:HD2 | 2.31 | 0.59 |
| 41:CB:314:ALA:HB3 | 41:CB:368:ILE:HB | 1.84 | 0.59 |
| 40:CF:236:SER:O | 40:CF:243:ARG:NH2 | 2.35 | 0.59 |
| 41:CM:142:GLY:O | 41:CM:144:GLY:N | 2.35 | 0.59 |
| 41:CO:311:LEU:HA | 41:CO:342:VAL:HG22 | 1.85 | 0.59 |
| 40:DE:129:CYS:O | 40:DE:130:THR:C | 2.40 | 0.59 |
| 40:DH:225:THR:HA | 40:DH:228:ASN:ND2 | 2.17 | 0.59 |
| 41:DL:314:ALA:N | 41:DL:368:ILE:O | 2.36 | 0.59 |
| 41:DM:30:ILE:HD13 | 41:DM:59:TYR:HB2 | 1.85 | 0.59 |
| 41:DM:391:ARG:O | 41:DM:392:LYS:C | 2.40 | 0.59 |
| 41:DN:27:GLU:HA | 41:DN:359:ARG:HG2 | 1.85 | 0.59 |
| 41:DN:245:GLN:O | 41:DN:246:LEU:C | 2.40 | 0.59 |
| 40:EE:239:THR:HG23 | 40:EE:242:LEU:HD21 | 1.83 | 0.59 |
| 41:EM:170:VAL:HG11 | 41:EM:377:LEU:HD21 | 1.84 | 0.59 |
| 40:FA:228:ASN:OD1 | 42:FN:501:GTP:N2 | 2.34 | 0.59 |
| 40:FE:329:ASN:HB2 | 41:FM:175:VAL:HG11 | 1.85 | 0.59 |
| 40:FF:226:ASN:ND2 | 40:FF:366:ASP:OD2 | 2.31 | 0.59 |
| 40:FI:210:TYR:OH | 41:FP:323:MET:SD | 2.60 | 0.59 |
| 40:GG:138:PHE:HZ | 40:GG:235:VAL:HG21 | 1.68 | 0.59 |
| 41:GM:286:VAL:HG21 | 41:GM:326:VAL:HG22 | 1.84 | 0.59 |
| 40:IH:254:GLU:HA | 40:IH:257:THR:HG22 | 1.85 | 0.59 |
| 41:IP:282:ARG:NH1 | 41:IP:288:GLU:OE1 | 2.35 | 0.59 |
| 40:JE:406:TRP:HE1 | 41:JL:258:VAL:HG23 | 1.68 | 0.59 |
| 40:JH:319:TYR:HB3 | 40:JH:323:VAL:HG11 | 1.84 | 0.59 |
| 40:KE:133:GLN:NE2 | 40:KE:251:ASP:OD1 | 2.36 | 0.59 |
| 41:KL:61:PRO:HD2 | 41:KL:84:ILE:O | 2.03 | 0.59 |
| 41:LO:385:PHE:HZ | 41:LO:408:PHE:HB3 | 1.66 | 0.59 |
| 41:MO:314:ALA:HB3 | 41:MO:368:ILE:HB | 1.83 | 0.59 |
| 40:NE:107:HIS:HD2 | 40:NE:152:LEU:HB2 | 1.68 | 0.59 |
| 40:OH:63:PRO:HG3 | 40:OH:87:PHE:HD1 | 1.68 | 0.59 |
| 40:RI:11:GLN:OE1 | 42:RP:501:GTP:N7 | 2.35 | 0.59 |
| 41:RM:320:ARG:NH2 | 41:RM:355:ASP:OD1 | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SA:380:THR:HG22 | 40:SA:382:ALA:H | 1.67 | 0.59 |
| 41:SL:318:ARG:HG2 | 41:SL:354:CYS:HB3 | 1.83 | 0.59 |
| 40:TH:259:LEU:HD11 | 40:TH:377:LEU:HD23 | 1.85 | 0.59 |
| 40:UE:242:LEU:HD22 | 40:UE:252:LEU:HD23 | 1.85 | 0.59 |
| 41:UP:135:LEU:HD21 | 41:UP:137:HIS:HB3 | 1.85 | 0.59 |
| 41:WM:139:LEU:HD21 | 41:WM:189:VAL:HG22 | 1.83 | 0.59 |
| 41:WO:178:THR:HB | 41:WO:181:GLU:HG3 | 1.82 | 0.59 |
| 7:1S:573:ASP:HB3 | 7:1S:576:GLU:HB2 | 1.83 | 0.59 |
| 17:3Q:409:ILE:O | 17:3Q:410:GLU:C | 2.40 | 0.59 |
| 22:4I:642:CYS:HB3 | 22:4I:690:TYR:CE2 | 2.38 | 0.59 |
| 23:4M:18:TYR:HE1 | 40:BG:80:THR:HG22 | 1.67 | 0.59 |
| 26:4V:136:PHE:O | 26:4V:137:HIS:ND1 | 2.35 | 0.59 |
| 41:BM:355:ASP:O | 41:BM:356:ILE:C | 2.41 | 0.59 |
| 41:BN:274:THR:HA | 41:BN:278:SER:HB3 | 1.84 | 0.59 |
| 41:BO:58:LYS:O | 41:BO:59:TYR:C | 2.40 | 0.59 |
| 40:CA:136:LEU:HD22 | 40:CA:167:LEU:HB2 | 1.83 | 0.59 |
| 40:CA:402:ALA:O | 40:CA:403:PHE:C | 2.40 | 0.59 |
| 40:DG:60:LYS:NZ | 40:DG:85:GLN:O | 2.36 | 0.59 |
| 40:DH:217:LEU:O | 40:DH:219:ILE:N | 2.31 | 0.59 |
| 40:DH:250:VAL:HG12 | 40:DH:354:GLY:HA3 | 1.84 | 0.59 |
| 41:DL:42:LEU:HD12 | 41:DL:356:ILE:HD11 | 1.85 | 0.59 |
| 41:DM:21:TRP:CZ2 | 41:DM:63:ALA:HB2 | 2.38 | 0.59 |
| 40:EI:210:TYR:CD1 | 41:EP:324:LYS:HG2 | 2.38 | 0.59 |
| 40:EI:300:ASN:O | 40:EI:301:GLN:C | 2.40 | 0.59 |
| 40:EI:370:VAL:HG11 | 40:EI:373:ALA:HB2 | 1.83 | 0.59 |
| 41:EM:189:VAL:O | 41:EM:193:VAL:HG23 | 2.02 | 0.59 |
| 40:FA:297:GLU:HG3 | 40:FA:299:ALA:H | 1.68 | 0.59 |
| 40:FI:319:TYR:HD1 | 40:FI:323:VAL:HG11 | 1.67 | 0.59 |
| 41:GM:238:THR:HG21 | 41:GM:318:ARG:HD2 | 1.84 | 0.59 |
| 41:GO:100:ASN:HB2 | 41:GO:103:LYS:HB2 | 1.85 | 0.59 |
| 40:HA:403:PHE:CE2 | 41:HN:259:PRO:HA | 2.37 | 0.59 |
| 40:HE:10:GLY:HA2 | 40:HE:145:THR:HG23 | 1.83 | 0.59 |
| 40:II:259:LEU:HD11 | 40:II:377:LEU:HD23 | 1.83 | 0.59 |
| 40:JG:88:HIS:NE2 | 40:JG:90:GLU:OE1 | 2.35 | 0.59 |
| 41:JL:313:VAL:O | 41:JL:349:VAL:HA | 2.02 | 0.59 |
| 41:KB:159:TYR:HB3 | 41:KB:162:ARG:HD3 | 1.84 | 0.59 |
| 41:LB:42:LEU:HD23 | 41:LB:356:ILE:HD11 | 1.85 | 0.59 |
| 40:LD:210:TYR:HE1 | 40:LD:227:LEU:HD11 | 1.67 | 0.59 |
| 40:MG:20:CYS:HA | 40:MG:232:SER:HB2 | 1.83 | 0.59 |
| 41:MO:253:LEU:O | 41:MO:257:MET:HB2 | 2.03 | 0.59 |
| 41:NM:334:GLN:NE2 | 41:NM:348:ASN:OD1 | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OF:20:CYS:HA | 40:OF:232:SER:HB2 | 1.84 | 0.59 |
| 40:OH:222:PRO:HD2 | 41:OO:324:LYS:CE | 2.33 | 0.59 |
| 41:OO:238:THR:HG21 | 41:OO:318:ARG:HD2 | 1.85 | 0.59 |
| 40:PD:269:LEU:HD21 | 40:PD:301:GLN:HB2 | 1.83 | 0.59 |
| 40:PE:265:ILE:HG22 | 40:PE:379:ASN:HD21 | 1.68 | 0.59 |
| 41:RN:13:GLY:HA2 | 41:RN:16:ILE:HD12 | 1.83 | 0.59 |
| 41:RN:164:MET:O | 41:RN:198:GLU:HB3 | 2.02 | 0.59 |
| 40:SF:6:SER:OG | 40:SF:8:HIS:NE2 | 2.35 | 0.59 |
| 40:SH:177:VAL:HG11 | 41:SO:327:ASP:HB3 | 1.83 | 0.59 |
| 41:TM:314:ALA:HB3 | 41:TM:368:ILE:HB | 1.83 | 0.59 |
| 41:UN:325:GLU:O | 41:UN:329:GLN:HB2 | 2.02 | 0.59 |
| 40:VA:15:GLN:NE2 | 42:VA:501:GTP:O6 | 2.34 | 0.59 |
| 40:WE:254:GLU:HG2 | 41:WM:98:GLY:HA2 | 1.85 | 0.59 |
| 41:WP:222:TYR:O | 41:WP:226:ASN:ND2 | 2.36 | 0.59 |
| 7:1U:60:LEU:HG | 7:1U:96:TRP:CZ3 | 2.38 | 0.59 |
| 12:2M:250:THR:HG22 | 40:AG:401:ARG:HG2 | 1.84 | 0.59 |
| 22:4I:24:GLN:OE1 | 40:MG:1:GLN:N | 2.34 | 0.59 |
| 23:4P:243:LEU:HD11 | 40:DA:84:ARG:HG3 | 1.84 | 0.59 |
| 23:4Q:109:CYS:SG | 23:4Q:110:ASN:N | 2.76 | 0.59 |
| 27:4Z:74:ASN:ND2 | 27:4Z:263:HIS:O | 2.35 | 0.59 |
| 36:5Y:116:ARG:HA | 36:5Y:146:ARG:HA | 1.83 | 0.59 |
| 41:AN:30:ILE:HD11 | 41:AN:47:ILE:HD11 | 1.84 | 0.59 |
| 40:BH:177:VAL:HG13 | 40:BH:178:SER:H | 1.68 | 0.59 |
| 41:BM:87:PRO:HD3 | 41:CM:281:TYR:CD1 | 2.36 | 0.59 |
| 41:BO:21:TRP:CE3 | 41:BO:24:ILE:HD11 | 2.37 | 0.59 |
| 41:CL:165:ASN:HA | 41:CL:198:GLU:HB3 | 1.84 | 0.59 |
| 40:EA:238:ILE:HG23 | 40:EA:255:PHE:HE2 | 1.67 | 0.59 |
| 40:EA:259:LEU:HD12 | 40:EA:268:PRO:HB3 | 1.84 | 0.59 |
| 41:EN:138:SER:HA | 41:EN:169:VAL:HB | 1.85 | 0.59 |
| 40:FH:320:ARG:HB2 | 40:FH:373:ALA:HB3 | 1.85 | 0.59 |
| 41:FM:101:TRP:HB2 | 41:FM:184:ASN:HD22 | 1.68 | 0.59 |
| 41:FN:421:PRO:HA | 41:FN:424:THR:HG22 | 1.84 | 0.59 |
| 40:GI:60:LYS:O | 40:GI:61:HIS:C | 2.41 | 0.59 |
| 40:HE:435:GLY:O | 40:HE:436:MET:C | 2.41 | 0.59 |
| 41:HM:27:GLU:HA | 41:HM:359:ARG:HH12 | 1.68 | 0.59 |
| 41:JB:213:ARG:HH12 | 41:JB:297:LYS:HG3 | 1.66 | 0.59 |
| 41:JL:6:HIS:O | 41:JL:63:ALA:HA | 2.03 | 0.59 |
| 41:JM:391:ARG:O | 41:JM:392:LYS:C | 2.40 | 0.59 |
| 41:JO:172:SER:OG | 41:JO:175:VAL:O | 2.20 | 0.59 |
| 41:KB:46:ARG:NH2 | 40:KG:76:ASP:OD2 | 2.34 | 0.59 |
| 40:KG:255:PHE:O | 40:KG:259:LEU:HB2 | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:LP:390:ARG:NH1 | 41:LP:390:ARG:O | 2.34 | 0.59 |
| 40:NF:228:ASN:HD21 | 42:NM:501:GTP:HN1 | 1.49 | 0.59 |
| 41:NL:100:ASN:HB3 | 41:NL:103:LYS:HB2 | 1.84 | 0.59 |
| 41:NO:314:ALA:HB3 | 41:NO:368:ILE:HB | 1.83 | 0.59 |
| 40:OH:99:ALA:O | 40:OH:100:ALA:C | 2.40 | 0.59 |
| 41:OL:3:GLU:HB2 | 41:OL:130:LEU:HA | 1.83 | 0.59 |
| 41:PL:377:LEU:HD12 | 41:PL:380:ARG:HH12 | 1.67 | 0.59 |
| 40:QH:30:ILE:HA | 40:QH:36:MET:HG2 | 1.83 | 0.59 |
| 41:QO:237:THR:HG22 | 41:QO:250:LEU:HD21 | 1.84 | 0.59 |
| 41:RL:91:VAL:HG11 | 41:RL:116:VAL:HG22 | 1.84 | 0.59 |
| 40:SA:88:HIS:HE1 | 40:SA:90:GLU:HG3 | 1.67 | 0.59 |
| 40:SG:262:TYR:HB2 | 40:SG:265:ILE:HG22 | 1.84 | 0.59 |
| 41:SN:269:GLY:HA3 | 41:SN:367:PHE:HB3 | 1.83 | 0.59 |
| 40:UE:238:ILE:HG13 | 40:UE:239:THR:HG23 | 1.84 | 0.59 |
| 41:UO:134:GLN:HA | 41:UO:165:ASN:O | 2.02 | 0.59 |
| 41:VB:396:HIS:HA | 41:VB:399:THR:HG22 | 1.85 | 0.59 |
| 40:VH:98:ASP:O | 40:VH:105:ARG:NH1 | 2.36 | 0.59 |
| 40:VJ:73:THR:HA | 40:VJ:76:ASP:HB2 | 1.85 | 0.59 |
| 7:1T:373:PRO:HG2 | 10:2E:137:LYS:HA | 1.85 | 0.59 |
| 7:1U:416:HIS:HB2 | 7:1U:420:VAL:HG22 | 1.84 | 0.59 |
| 16:3J:100:GLU:HG3 | 18:3T:161:ARG:HH12 | 1.68 | 0.59 |
| 22:4J:155:ASN:HA | 22:4J:167:ILE:O | 2.02 | 0.59 |
| 22:4K:562:LEU:HD21 | 22:4K:589:LEU:HD11 | 1.83 | 0.59 |
| 23:4P:192:PRO:HG3 | 41:CN:44:LEU:HD21 | 1.83 | 0.59 |
| 40:AE:273:ALA:HB3 | 40:AE:374:VAL:H | 1.66 | 0.59 |
| 40:BA:261:PRO:HG3 | 41:BB:394:PHE:CZ | 2.38 | 0.59 |
| 40:BE:7:VAL:HG13 | 40:BE:66:VAL:HG13 | 1.85 | 0.59 |
| 40:BE:400:LYS:O | 40:BE:401:ARG:C | 2.40 | 0.59 |
| 40:CI:8:HIS:HD2 | 40:CI:138:PHE:HB2 | 1.68 | 0.59 |
| 41:CM:19:LYS:HA | 41:CM:22:GLU:HG3 | 1.85 | 0.59 |
| 40:DF:349:THR:HG21 | 41:DN:182:PRO:CD | 2.32 | 0.59 |
| 41:DL:62:ARG:HG2 | 41:DL:123:GLU:HG2 | 1.85 | 0.59 |
| 41:DM:174:LYS:CE | 41:DM:175:VAL:CG2 | 2.66 | 0.59 |
| 41:DO:252:LYS:HD2 | 41:DO:350:LYS:HE3 | 1.84 | 0.59 |
| 41:EN:316:VAL:HA | 41:EN:352:ALA:HB3 | 1.84 | 0.59 |
| 40:FE:90:GLU:OE1 | 40:FE:121:ARG:NH1 | 2.35 | 0.59 |
| 40:GH:16:ILE:HA | 40:GH:228:ASN:HB3 | 1.85 | 0.59 |
| 40:HA:108:TYR:O | 40:HA:112:LYS:NZ | 2.35 | 0.59 |
| 41:HN:86:ARG:HA | 41:IN:281:TYR:HD2 | 1.66 | 0.59 |
| 41:HO:16:ILE:HD11 | 41:HO:229:VAL:HG11 | 1.85 | 0.59 |
| 40:IF:35:GLN:NE2 | 40:IF:58:ALA:O | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IF:189:LEU:HD11 | 40:IF:417:PHE:HE1 | 1.68 | 0.59 |
| 40:II:70:LEU:HD23 | 40:II:145:THR:HG23 | 1.83 | 0.59 |
| 41:KB:282:ARG:HD3 | 41:KB:283:ALA:H | 1.68 | 0.59 |
| 40:LH:226:ASN:ND2 | 40:LH:366:ASP:OD2 | 2.36 | 0.59 |
| 41:LM:252:LYS:HG2 | 41:LM:350:LYS:HE2 | 1.84 | 0.59 |
| 40:ND:384:ALA:HA | 40:ND:387:TRP:HE3 | 1.68 | 0.59 |
| 41:NO:5:VAL:HG22 | 41:NO:62:ARG:HD3 | 1.83 | 0.59 |
| 40:OA:96:LYS:NZ | 41:ON:1:MET:SD | 2.75 | 0.59 |
| 41:OB:137:HIS:ND1 | 41:OB:144:GLY:O | 2.36 | 0.59 |
| 40:OH:288:VAL:HG11 | 40:OH:327:ASP:HB3 | 1.85 | 0.59 |
| 41:OM:248:ALA:HA | 41:OM:252:LYS:HD3 | 1.84 | 0.59 |
| 41:PO:253:LEU:O | 41:PO:257:MET:HB2 | 2.03 | 0.59 |
| 41:PP:132:GLY:HA3 | 41:PP:163:ILE:O | 2.02 | 0.59 |
| 41:QB:16:ILE:HG12 | 43:QB:501:GDP:C6 | 2.37 | 0.59 |
| 40:QF:15:GLN:OE1 | 40:QF:228:ASN:ND2 | 2.35 | 0.59 |
| 40:QG:68:VAL:HG12 | 40:QG:93:ILE:HB | 1.84 | 0.59 |
| 41:QP:1:MET:O | 41:QP:3:GLU:N | 2.36 | 0.59 |
| 41:QP:238:THR:HA | 41:QP:241:ARG:HB2 | 1.84 | 0.59 |
| 40:RA:102:ASN:HB3 | 40:RA:105:ARG:HB2 | 1.84 | 0.59 |
| 41:RM:30:ILE:HD11 | 41:RM:47:ILE:HD11 | 1.84 | 0.59 |
| 41:RO:242:PHE:HB3 | 41:RO:356:ILE:HD13 | 1.84 | 0.59 |
| 40:SH:221:ARG:HH22 | 41:SO:325:GLU:CB | 2.15 | 0.59 |
| 41:SO:142:GLY:O | 41:SO:143:THR:C | 2.41 | 0.59 |
| 40:UE:269:LEU:O | 40:UE:377:LEU:HA | 2.01 | 0.59 |
| 40:UI:50:ASN:O | 40:UI:52:PHE:N | 2.36 | 0.59 |
| 41:UP:211:CYS:SG | 41:UP:212:PHE:N | 2.76 | 0.59 |
| 40:VA:239:THR:O | 40:VA:243:ARG:NH1 | 2.35 | 0.59 |
| 40:VI:332:ILE:HG21 | 41:VQ:175:VAL:HG23 | 1.85 | 0.59 |
| 40:WF:217:LEU:HD11 | 40:WF:366:ASP:HB3 | 1.84 | 0.59 |
| 41:WN:249:ASP:H | 41:WN:252:LYS:HE3 | 1.67 | 0.59 |
| 8:1W:454:GLN:OE1 | 41:VO:276:ARG:NH2 | 2.35 | 0.59 |
| 16:3J:307:LYS:HD2 | 16:3J:348:THR:HG21 | 1.85 | 0.59 |
| 18:3W:188:GLU:HG3 | 18:3W:192:ARG:HH22 | 1.67 | 0.59 |
| 22:4J:10:SER:HB3 | 41:MN:215:LEU:HD13 | 1.84 | 0.59 |
| 23:4R:196:PHE:CE1 | 41:DP:283:ALA:HB1 | 2.38 | 0.59 |
| 29:5D:98:THR:HA | 41:HQ:295:ASP:HA | 1.85 | 0.59 |
| 35:5T:101:HIS:HB3 | 40:JE:225:THR:HG21 | 1.84 | 0.59 |
| 41:AB:237:THR:O | 41:AB:241:ARG:NH1 | 2.36 | 0.59 |
| 40:CE:400:LYS:HD2 | 41:CL:344:TRP:CB | 2.33 | 0.59 |
| 41:CL:86:ARG:HG3 | 41:DL:281:TYR:HB3 | 1.85 | 0.59 |
| 40:DF:271:THR:OG1 | 40:DF:301:GLN:HA | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DP:66:VAL:HG13 | 41:DP:91:VAL:HB | 1.84 | 0.59 |
| 40:EA:101:ASN:ND2 | 42:EA:501:GTP:O2G | 2.36 | 0.59 |
| 41:EB:66:VAL:HG12 | 41:EB:91:VAL:HB | 1.85 | 0.59 |
| 40:EH:131:GLY:O | 40:EH:132:LEU:C | 2.41 | 0.59 |
| 40:FA:70:LEU:HD12 | 40:FA:145:THR:HG22 | 1.83 | 0.59 |
| 40:FH:191:THR:HA | 40:FH:194:THR:HG22 | 1.84 | 0.59 |
| 40:GF:318:LEU:O | 40:GF:374:VAL:HA | 2.01 | 0.59 |
| 40:GH:85:GLN:O | 40:GH:86:LEU:C | 2.40 | 0.59 |
| 40:GI:160:ASP:O | 40:GI:162:GLY:N | 2.36 | 0.59 |
| 41:IM:207:LEU:HB3 | 41:IM:225:LEU:HD22 | 1.84 | 0.59 |
| 41:IP:237:THR:O | 41:IP:241:ARG:NE | 2.35 | 0.59 |
| 40:JG:251:ASP:HB3 | 40:JG:254:GLU:HG3 | 1.84 | 0.59 |
| 41:JO:178:THR:HB | 41:JO:181:GLU:HG3 | 1.85 | 0.59 |
| 41:KL:102:ALA:C | 41:KL:104:GLY:H | 2.06 | 0.59 |
| 40:LH:258:ASN:HD22 | 41:LP:179:VAL:HG22 | 1.67 | 0.59 |
| 40:MH:167:LEU:HD22 | 40:MH:200:CYS:HB2 | 1.84 | 0.59 |
| 40:ND:28:HIS:HD2 | 40:ND:49:PHE:HA | 1.66 | 0.59 |
| 40:OF:139:HIS:O | 40:OF:170:SER:HA | 2.02 | 0.59 |
| 40:OH:9:VAL:HG22 | 40:OH:68:VAL:HG13 | 1.85 | 0.59 |
| 41:OM:218:THR:HG23 | 41:OM:276:ARG:HH12 | 1.68 | 0.59 |
| 40:PA:26:LEU:HD21 | 40:PA:363:VAL:HG12 | 1.84 | 0.59 |
| 40:PE:97:GLU:OE1 | 40:PE:105:ARG:NH2 | 2.36 | 0.59 |
| 40:PE:276:ILE:HG23 | 40:PE:280:LYS:HG3 | 1.84 | 0.59 |
| 41:PO:107:THR:O | 41:PO:110:ALA:N | 2.36 | 0.59 |
| 41:QN:207:LEU:HB3 | 41:QN:225:LEU:HD22 | 1.84 | 0.59 |
| 41:QO:191:GLN:O | 41:QO:195:ASN:ND2 | 2.35 | 0.59 |
| 40:RG:248:LEU:HD23 | 40:RG:355:ILE:HD12 | 1.84 | 0.59 |
| 41:RP:233:MET:HA | 41:RP:236:VAL:HG22 | 1.83 | 0.59 |
| 40:SA:274:PRO:HG3 | 40:SA:286:LEU:HD12 | 1.83 | 0.59 |
| 40:SE:145:THR:OG1 | 42:SL:501:GTP:O2B | 2.20 | 0.59 |
| 40:SE:400:LYS:HG2 | 41:SL:425:ARG:HH22 | 1.67 | 0.59 |
| 40:UF:88:HIS:HB3 | 40:UF:91:GLN:HB3 | 1.85 | 0.59 |
| 41:UO:8:GLN:NE2 | 41:UO:64:VAL:O | 2.36 | 0.59 |
| 40:VF:55:GLU:OE2 | 40:VF:61:HIS:NE2 | 2.36 | 0.59 |
| 40:VG:16:ILE:HA | 40:VG:228:ASN:HB3 | 1.84 | 0.59 |
| 40:VG:177:VAL:HB | 41:VN:331:LEU:HD22 | 1.84 | 0.59 |
| 10:2F:69:LYS:HG3 | 10:2F:71:ASP:H | 1.68 | 0.59 |
| 10:2F:150:PRO:HD2 | 40:WG:221:ARG:HH12 | 1.67 | 0.59 |
| 13:2W:49:ILE:HD11 | 13:2W:162:ILE:HD11 | 1.83 | 0.59 |
| 15:3H:130:ASP:OD1 | 15:3H:131:GLU:N | 2.36 | 0.59 |
| 17:3R:215:VAL:O | 17:3R:216:GLU:C | 2.41 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4J:470:GLU:HG2 | 22:4J:471:ARG:H | 1.68 | 0.59 |
| 36:5W:248:ASP:OD1 | 36:5W:256:ARG:NH2 | 2.34 | 0.59 |
| 41:BB:226:ASN:ND2 | 43:BB:501:GDP:HN1 | 2.01 | 0.59 |
| 41:BM:135:LEU:HD22 | 41:BM:152:ILE:HD11 | 1.84 | 0.59 |
| 41:CL:8:GLN:HG2 | 41:CL:14:ASN:HA | 1.84 | 0.59 |
| 41:CM:273:LEU:HB2 | 41:CM:292:GLN:HE22 | 1.66 | 0.59 |
| 41:CN:138:SER:O | 41:CN:139:LEU:C | 2.41 | 0.59 |
| 41:DB:141:GLY:HA3 | 43:DB:501:GDP:O1A | 2.03 | 0.59 |
| 40:DH:168:GLU:HG3 | 40:DH:201:ALA:HA | 1.84 | 0.59 |
| 40:EH:407:TYR:HB3 | 40:EH:417:PHE:HZ | 1.68 | 0.59 |
| 40:FF:206:ASN:OD1 | 42:FM:501:GTP:O2' | 2.21 | 0.59 |
| 41:FO:62:ARG:NH2 | 41:FO:127:CYS:SG | 2.75 | 0.59 |
| 41:GB:107:THR:O | 41:GB:110:ALA:N | 2.36 | 0.59 |
| 40:GH:274:PRO:HB2 | 40:GH:370:VAL:HG11 | 1.85 | 0.59 |
| 40:GI:213:CYS:HB2 | 40:GI:222:PRO:HG3 | 1.85 | 0.59 |
| 41:GP:33:THR:O | 41:GP:58:LYS:NZ | 2.35 | 0.59 |
| 40:HI:228:ASN:HD21 | 42:HP:501:GTP:HN1 | 1.49 | 0.59 |
| 41:HM:273:LEU:O | 41:HM:292:GLN:NE2 | 2.33 | 0.59 |
| 41:HN:24:ILE:HA | 41:HN:27:GLU:HG2 | 1.85 | 0.59 |
| 40:IG:326:LYS:HD3 | 41:IO:208:TYR:HB2 | 1.84 | 0.59 |
| 41:IQ:172:SER:HB2 | 41:IQ:205:GLU:HG2 | 1.85 | 0.59 |
| 41:KL:178:THR:HB | 41:KL:181:GLU:HG2 | 1.85 | 0.59 |
| 40:NG:276:ILE:HG13 | 40:NG:368:ALA:HB3 | 1.85 | 0.59 |
| 40:OH:100:ALA:HA | 41:OO:252:LYS:HG2 | 1.83 | 0.59 |
| 40:PE:297:GLU:O | 40:PE:301:GLN:NE2 | 2.35 | 0.59 |
| 41:PM:101:TRP:HZ3 | 41:PM:187:LEU:HB3 | 1.67 | 0.59 |
| 41:QB:105:HIS:HB2 | 41:QB:146:GLY:HA2 | 1.85 | 0.59 |
| 40:QE:98:ASP:O | 40:QE:105:ARG:NH1 | 2.35 | 0.59 |
| 40:QG:138:PHE:HE1 | 40:QG:235:VAL:HG21 | 1.68 | 0.59 |
| 41:RB:159:TYR:HB3 | 41:RB:162:ARG:HD3 | 1.84 | 0.59 |
| 40:RH:288:VAL:HG11 | 40:RH:327:ASP:HB3 | 1.85 | 0.59 |
| 40:RI:224:TYR:CE1 | 41:RP:323:MET:HG3 | 2.38 | 0.59 |
| 41:SB:99:ASN:HB3 | 41:SB:178:THR:HG21 | 1.84 | 0.59 |
| 40:SG:51:THR:HG21 | 40:SG:243:ARG:HG2 | 1.85 | 0.59 |
| 41:SL:27:GLU:HA | 41:SL:359:ARG:HH12 | 1.66 | 0.59 |
| 41:SN:325:GLU:O | 41:SN:329:GLN:HB2 | 2.03 | 0.59 |
| 41:SP:314:ALA:HB3 | 41:SP:368:ILE:HB | 1.84 | 0.59 |
| 40:TH:223:THR:HG22 | 41:TO:322:SER:HA | 1.85 | 0.59 |
| 41:TO:314:ALA:HB3 | 41:TO:368:ILE:HB | 1.84 | 0.59 |
| 40:UE:240:ALA:HB1 | 40:UE:356:ASN:HD22 | 1.67 | 0.59 |
| 40:UI:180:ALA:HB3 | 40:UI:183:GLU:HB2 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UM:86:ARG:NH1 | 41:VN:281:TYR:O | 2.36 | 0.59 |
| 41:VB:62:ARG:NH1 | 41:VB:127:CYS:SG | 2.75 | 0.59 |
| 40:VH:239:THR:O | 40:VH:243:ARG:NH1 | 2.36 | 0.59 |
| 41:WN:97:ALA:HB1 | 41:WN:142:GLY:HA3 | 1.85 | 0.59 |
| 7:1T:591:THR:HG22 | 7:1T:592:ARG:HG2 | 1.83 | 0.58 |
| 11:2I:222:PRO:HA | 11:2I:225:MET:HE2 | 1.85 | 0.58 |
| 15:3F:114:LYS:HG3 | 15:3F:393:MET:HE1 | 1.84 | 0.58 |
| 21:4F:137:VAL:HG12 | 21:4F:145:GLN:HB3 | 1.85 | 0.58 |
| 31:5I:356:GLY:HA3 | 40:HA:80:THR:HG22 | 1.85 | 0.58 |
| 37:6A:113:ARG:O | 40:TH:46:ASP:N | 2.36 | 0.58 |
| 41:AO:2:ARG:HB3 | 41:AO:131:GLN:HB2 | 1.85 | 0.58 |
| 40:BF:194:THR:O | 40:BF:198:SER:HB3 | 2.03 | 0.58 |
| 40:BH:100:ALA:O | 40:BH:101:ASN:C | 2.41 | 0.58 |
| 41:BL:204:ASN:ND2 | 43:BL:502:GDP:O2' | 2.36 | 0.58 |
| 41:BP:98:GLY:O | 41:BP:99:ASN:C | 2.41 | 0.58 |
| 41:BP:360:GLY:O | 41:BP:361:LEU:C | 2.40 | 0.58 |
| 40:CA:191:THR:HB | 40:CA:424:MET:SD | 2.42 | 0.58 |
| 40:DI:111:GLY:O | 40:DI:113:GLU:N | 2.35 | 0.58 |
| 40:EF:229:ARG:HH21 | 40:EF:363:VAL:HG23 | 1.67 | 0.58 |
| 40:EI:231:ILE:HA | 40:EI:234:ILE:HD12 | 1.85 | 0.58 |
| 40:FE:102:ASN:HB3 | 40:FE:105:ARG:HB2 | 1.84 | 0.58 |
| 40:FG:3:GLU:HA | 40:FG:51:THR:HG23 | 1.85 | 0.58 |
| 40:GE:140:SER:HA | 40:GE:171:ILE:HG12 | 1.85 | 0.58 |
| 41:HM:156:ARG:NH1 | 41:HM:195:ASN:O | 2.35 | 0.58 |
| 40:II:101:ASN:ND2 | 41:IP:256:ASN:OD1 | 2.34 | 0.58 |
| 41:IM:77:ARG:O | 41:IM:83:GLN:NE2 | 2.35 | 0.58 |
| 41:IO:45:GLU:HG3 | 41:IO:46:ARG:HG2 | 1.84 | 0.58 |
| 41:JB:173:PRO:HB3 | 41:JB:380:ARG:HD3 | 1.83 | 0.58 |
| 41:JM:172:SER:HB2 | 41:JM:205:GLU:HB2 | 1.85 | 0.58 |
| 41:KP:54:ALA:HA | 41:LP:283:ALA:HB2 | 1.85 | 0.58 |
| 40:MG:360:PRO:HG2 | 40:MG:373:ALA:HB3 | 1.84 | 0.58 |
| 41:MO:1:MET:HB2 | 41:MO:128:ASP:HB2 | 1.85 | 0.58 |
| 40:ND:70:LEU:HA | 40:ND:95:GLY:HA3 | 1.85 | 0.58 |
| 41:OB:334:GLN:NE2 | 41:OB:348:ASN:OD1 | 2.35 | 0.58 |
| 41:OM:141:GLY:O | 41:OM:184:ASN:ND2 | 2.36 | 0.58 |
| 41:OO:130:LEU:HB2 | 41:OO:162:ARG:HH12 | 1.68 | 0.58 |
| 41:PP:8:GLN:HB2 | 41:PP:65:LEU:HA | 1.85 | 0.58 |
| 40:QE:200:CYS:HA | 40:QE:266:HIS:HB2 | 1.84 | 0.58 |
| 40:QG:188:ILE:HG22 | 40:QG:420:ALA:HB1 | 1.85 | 0.58 |
| 40:RE:180:ALA:HB3 | 40:RE:183:GLU:HG3 | 1.84 | 0.58 |
| 40:SA:261:PRO:HD2 | 40:SA:265:ILE:HG23 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SM:117:LEU:HA | 41:SM:120:VAL:HG12 | 1.85 | 0.58 |
| 41:TO:226:ASN:HA | 43:TO:501:GDP:HN21 | 1.68 | 0.58 |
| 40:UI:68:VAL:HG22 | 40:UI:93:ILE:HB | 1.84 | 0.58 |
| 41:UN:263:LEU:O | 41:UN:370:ASN:ND2 | 2.35 | 0.58 |
| 41:UP:107:THR:O | 41:UP:108:GLU:C | 2.41 | 0.58 |
| 40:WA:221:ARG:HH11 | 41:WN:322:SER:HB2 | 1.67 | 0.58 |
| 40:WE:27:GLU:OE1 | 40:WE:243:ARG:NH1 | 2.35 | 0.58 |
| 40:WF:256:GLN:HE21 | 41:WN:397:TRP:HZ2 | 1.51 | 0.58 |
| 41:WN:310:TYR:O | 41:WN:311:LEU:C | 2.40 | 0.58 |
| 7:1T:165:VAL:HG11 | 7:1T:211:ILE:HG13 | 1.84 | 0.58 |
| 8:1W:316:ILE:O | 8:1W:320:ASN:ND2 | 2.37 | 0.58 |
| 13:2X:7:GLN:HE21 | 13:2X:71:ILE:HD13 | 1.68 | 0.58 |
| 13:2X:87:PHE:CE2 | 13:2X:156:ILE:HG23 | 2.37 | 0.58 |
| 16:3J:214:THR:HG22 | 16:3J:217:GLN:HG3 | 1.85 | 0.58 |
| 31:5I:322:THR:HA | 31:5I:325:THR:HG22 | 1.85 | 0.58 |
| 36:5Y:131:VAL:HG12 | 40:KH:408:VAL:HG13 | 1.85 | 0.58 |
| 39:6K:50:GLN:NE2 | 39:6K:54:TYR:OH | 2.31 | 0.58 |
| 40:BF:6:SER:O | 40:BF:65:ALA:HA | 2.04 | 0.58 |
| 41:BM:44:LEU:O | 41:BM:45:GLU:C | 2.42 | 0.58 |
| 41:CL:258:VAL:HG22 | 41:CL:266:PHE:HZ | 1.68 | 0.58 |
| 40:DI:210:TYR:CD1 | 41:DP:324:LYS:HD3 | 2.38 | 0.58 |
| 40:DI:278:ALA:HA | 40:DI:368:ALA:HB2 | 1.85 | 0.58 |
| 41:DL:3:GLU:HB3 | 41:DL:130:LEU:HA | 1.84 | 0.58 |
| 41:DO:265:PHE:HB3 | 41:DO:374:ILE:HD13 | 1.85 | 0.58 |
| 41:DP:173:PRO:O | 41:DP:174:LYS:C | 2.42 | 0.58 |
| 40:EE:320:ARG:HE | 40:EE:360:PRO:HG3 | 1.68 | 0.58 |
| 40:FA:273:ALA:HB1 | 40:FA:274:PRO:CD | 2.26 | 0.58 |
| 40:FH:199:ASP:OD1 | 40:FH:256:GLN:NE2 | 2.30 | 0.58 |
| 41:FP:139:LEU:HD12 | 41:FP:170:VAL:HG12 | 1.83 | 0.58 |
| 40:GE:251:ASP:H | 40:GE:254:GLU:HG3 | 1.68 | 0.58 |
| 41:GP:100:ASN:HB3 | 41:GP:103:LYS:HB2 | 1.86 | 0.58 |
| 41:HB:211:CYS:HA | 41:HB:215:LEU:HB2 | 1.85 | 0.58 |
| 40:IA:316:CYS:HB3 | 40:IA:377:LEU:HB2 | 1.84 | 0.58 |
| 40:IA:405:HIS:HA | 40:IA:408:VAL:HG12 | 1.85 | 0.58 |
| 41:IN:8:GLN:NE2 | 41:IN:17:GLY:HA3 | 2.18 | 0.58 |
| 41:KL:107:THR:OG1 | 41:KL:108:GLU:N | 2.36 | 0.58 |
| 40:LF:3:GLU:HG3 | 40:LF:129:CYS:HB3 | 1.84 | 0.58 |
| 40:MF:224:TYR:HB3 | 42:MM:501:GTP:C6 | 2.38 | 0.58 |
| 40:ND:276:ILE:HG21 | 40:ND:281:ALA:HB2 | 1.84 | 0.58 |
| 40:NH:405:HIS:HA | 40:NH:408:VAL:HG12 | 1.84 | 0.58 |
| 41:NM:238:THR:OG1 | 41:NM:318:ARG:NH1 | 2.35 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:NO:86:ARG:NH1 | 41:OO:281:TYR:O | 2.36 | 0.58 |
| 40:OE:135:PHE:O | 40:OE:167:LEU:HB2 | 2.03 | 0.58 |
| 41:OM:176:SER:OG | 41:OM:178:THR:O | 2.21 | 0.58 |
| 41:PB:238:THR:HA | 41:PB:241:ARG:HH11 | 1.68 | 0.58 |
| 40:QG:36:MET:HG2 | 40:QG:61:HIS:CE1 | 2.38 | 0.58 |
| 40:QG:239:THR:O | 40:QG:243:ARG:NE | 2.32 | 0.58 |
| 41:QL:238:THR:HA | 41:QL:241:ARG:HE | 1.66 | 0.58 |
| 41:QN:136:THR:HG22 | 41:QN:167:PHE:HB2 | 1.84 | 0.58 |
| 40:RF:178:SER:OG | 40:RF:179:THR:N | 2.35 | 0.58 |
| 41:RL:122:LYS:NZ | 41:SL:295:ASP:OD2 | 2.35 | 0.58 |
| 40:SA:259:LEU:HD21 | 40:SA:377:LEU:HB2 | 1.85 | 0.58 |
| 41:SM:313:VAL:O | 41:SM:349:VAL:HA | 2.04 | 0.58 |
| 41:TB:229:VAL:HA | 41:TB:232:THR:HG22 | 1.84 | 0.58 |
| 40:UE:188:ILE:HD12 | 40:UE:424:MET:HG3 | 1.85 | 0.58 |
| 41:VO:229:VAL:HG12 | 41:VO:233:MET:HE2 | 1.84 | 0.58 |
| 41:VO:314:ALA:HA | 41:VO:350:LYS:HB3 | 1.85 | 0.58 |
| 40:WI:7:VAL:HB | 40:WI:137:ILE:HG12 | 1.85 | 0.58 |
| 40:WI:180:ALA:HB1 | 41:WP:256:ASN:HD21 | 1.67 | 0.58 |
| 41:WP:2:ARG:HB2 | 41:WP:240:LEU:HD11 | 1.84 | 0.58 |
| 41:WQ:309:ARG:H | 41:WQ:372:THR:HB | 1.68 | 0.58 |
| 7:1T:95:LEU:HD22 | 7:1T:107:LEU:HD11 | 1.86 | 0.58 |
| 9:2B:160:LEU:HA | 9:2B:163:VAL:HG12 | 1.85 | 0.58 |
| 12:2P:59:ALA:HB1 | 41:AL:423:VAL:HG13 | 1.86 | 0.58 |
| 15:3H:122:ARG:NH1 | 15:3H:126:ASP:O | 2.37 | 0.58 |
| 21:4E:164:HIS:HD2 | 21:4E:166:LYS:HG3 | 1.68 | 0.58 |
| 21:4E:352:ARG:HG3 | 21:4E:364:LEU:HD23 | 1.84 | 0.58 |
| 22:4I:276:SER:OG | 22:4I:277:LEU:N | 2.35 | 0.58 |
| 27:4Y:65:HIS:HA | 27:4Y:140:VAL:HA | 1.85 | 0.58 |
| 30:5G:115:PRO:O | 40:HG:215:ARG:NH1 | 2.35 | 0.58 |
| 40:AH:283:HIS:HD2 | 40:MH:62:VAL:HG23 | 1.68 | 0.58 |
| 40:BF:224:TYR:HA | 40:BF:227:LEU:HB2 | 1.83 | 0.58 |
| 41:CB:7:LEU:HD12 | 41:CB:151:LEU:HD21 | 1.85 | 0.58 |
| 41:CB:341:PHE:HB3 | 41:CB:348:ASN:HD21 | 1.68 | 0.58 |
| 40:CF:181:VAL:HG23 | 40:CF:182:VAL:HG13 | 1.84 | 0.58 |
| 40:CG:241:SER:OG | 40:CG:249:ASN:OD1 | 2.21 | 0.58 |
| 41:CN:5:VAL:HG23 | 41:CN:130:LEU:HD21 | 1.86 | 0.58 |
| 41:CP:391:ARG:O | 41:CP:392:LYS:C | 2.41 | 0.58 |
| 40:DE:141:PHE:O | 40:DE:143:GLY:N | 2.36 | 0.58 |
| 40:DI:1:GLN:HG2 | 40:DI:50:ASN:HB3 | 1.84 | 0.58 |
| 41:DN:263:LEU:HD11 | 41:DN:374:ILE:HG21 | 1.83 | 0.58 |
| 41:DN:395:LEU:O | 41:DN:396:HIS:C | 2.41 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DO:5:VAL:HG22 | 41:DO:62:ARG:HD2 | 1.85 | 0.58 |
| 40:EA:295:CYS:O | 40:EA:301:GLN:NE2 | 2.36 | 0.58 |
| 40:EF:239:THR:O | 40:EF:243:ARG:NH1 | 2.37 | 0.58 |
| 40:EG:15:GLN:NE2 | 42:EG:501:GTP:O6 | 2.37 | 0.58 |
| 40:EI:70:LEU:HD13 | 40:EI:110:ILE:HD12 | 1.85 | 0.58 |
| 41:EM:112:LEU:O | 41:EM:115:SER:N | 2.36 | 0.58 |
| 40:FA:81:GLY:O | 40:FA:82:THR:C | 2.41 | 0.58 |
| 41:FB:7:LEU:O | 41:FB:135:LEU:HA | 2.02 | 0.58 |
| 41:FO:186:THR:HG23 | 41:FO:415:MET:HG3 | 1.86 | 0.58 |
| 41:GB:317:PHE:HB2 | 41:GB:353:VAL:HG12 | 1.84 | 0.58 |
| 40:GI:247:ALA:O | 40:GI:248:LEU:C | 2.41 | 0.58 |
| 40:GI:284:GLU:HG2 | 40:GI:286:LEU:HD13 | 1.86 | 0.58 |
| 40:HF:320:ARG:HD3 | 40:HF:360:PRO:HG3 | 1.84 | 0.58 |
| 41:HN:279:GLN:HG2 | 41:HN:280:GLN:HG2 | 1.85 | 0.58 |
| 41:HQ:331:LEU:O | 41:HQ:335:ASN:ND2 | 2.36 | 0.58 |
| 40:IF:273:ALA:HB3 | 40:IF:374:VAL:H | 1.68 | 0.58 |
| 40:IG:234:ILE:HG13 | 40:IG:302:MET:HE1 | 1.85 | 0.58 |
| 40:JG:326:LYS:HE3 | 41:JO:208:TYR:HB2 | 1.85 | 0.58 |
| 41:JM:36:TYR:CZ | 41:JM:38:GLY:HA3 | 2.37 | 0.58 |
| 40:KA:239:THR:O | 40:KA:243:ARG:NE | 2.30 | 0.58 |
| 41:KP:1:MET:SD | 41:KP:48:ASN:ND2 | 2.77 | 0.58 |
| 40:LF:346:TRP:HB3 | 41:LN:391:ARG:HG3 | 1.85 | 0.58 |
| 40:MA:27:GLU:HA | 40:MA:361:THR:HG21 | 1.84 | 0.58 |
| 41:MB:7:LEU:O | 41:MB:135:LEU:HA | 2.03 | 0.58 |
| 40:ND:60:LYS:O | 40:ND:61:HIS:C | 2.40 | 0.58 |
| 40:NF:252:LEU:HA | 40:NF:255:PHE:HD2 | 1.69 | 0.58 |
| 40:OA:133:GLN:NE2 | 40:OA:251:ASP:OD2 | 2.36 | 0.58 |
| 40:OD:11:GLN:HG3 | 40:OD:74:VAL:HG11 | 1.85 | 0.58 |
| 41:OM:293:MET:HG3 | 41:OM:367:PHE:HB2 | 1.85 | 0.58 |
| 41:QO:311:LEU:HD23 | 41:QO:312:THR:HG23 | 1.85 | 0.58 |
| 40:RG:206:ASN:ND2 | 42:RG:501:GTP:O2' | 2.36 | 0.58 |
| 40:TG:291:ILE:HD13 | 40:TG:372:ARG:HB3 | 1.84 | 0.58 |
| 40:TH:255:PHE:HE1 | 40:TH:318:LEU:HD11 | 1.68 | 0.58 |
| 41:TL:180:VAL:HG23 | 41:TL:184:ASN:HD21 | 1.68 | 0.58 |
| 40:UI:317:LEU:HD11 | 40:UI:351:PHE:HD2 | 1.68 | 0.58 |
| 40:VF:102:ASN:ND2 | 40:VF:406:TRP:O | 2.36 | 0.58 |
| 40:WG:93:ILE:HD11 | 40:WG:121:ARG:HG3 | 1.84 | 0.58 |
| 40:WI:60:LYS:NZ | 40:WI:85:GLN:O | 2.33 | 0.58 |
| 41:WO:392:LYS:NZ | 41:WO:405:GLU:OE1 | 2.35 | 0.58 |
| 11:2I:104:ASN:ND2 | 11:2I:107:ASN:OD1 | 2.36 | 0.58 |
| 12:2Q:99:GLU:OE1 | 12:2Q:102:LYS:NZ | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2W:171:LEU:O | 13:2W:172:TYR:C | 2.42 | 0.58 |
| 13:2X:50:GLU:HG3 | 13:2X:159:ASN:HA | 1.84 | 0.58 |
| 16:3L:326:ASN:OD1 | 16:3L:327:VAL:N | 2.37 | 0.58 |
| 23:4M:95:THR:O | 41:AB:46:ARG:NH1 | 2.34 | 0.58 |
| 26:4W:370:TYR:O | 26:4W:375:LEU:HB2 | 2.04 | 0.58 |
| 36:5Y:132:THR:OG1 | 36:5Y:135:GLU:OE1 | 2.21 | 0.58 |
| 40:AA:76:ASP:OD2 | 41:AN:46:ARG:NH2 | 2.36 | 0.58 |
| 40:BA:98:ASP:O | 40:BA:105:ARG:NH1 | 2.36 | 0.58 |
| 41:BB:190:HIS:HD2 | 41:BB:411:ALA:HA | 1.67 | 0.58 |
| 41:BL:58:LYS:HG3 | 41:CL:280:GLN:HG3 | 1.86 | 0.58 |
| 40:CA:273:ALA:CB | 40:CA:374:VAL:HG13 | 2.33 | 0.58 |
| 40:CE:73:THR:HA | 40:CE:76:ASP:HB2 | 1.84 | 0.58 |
| 41:CP:104:GLY:HA2 | 41:CP:109:GLY:HA3 | 1.85 | 0.58 |
| 40:DA:256:GLN:HG3 | 41:DB:397:TRP:HZ2 | 1.69 | 0.58 |
| 40:DA:357:TYR:O | 40:DA:358:GLN:C | 2.41 | 0.58 |
| 40:DH:73:THR:O | 40:DH:74:VAL:C | 2.42 | 0.58 |
| 40:EH:90:GLU:O | 40:EH:91:GLN:C | 2.41 | 0.58 |
| 40:EI:397:MET:SD | 41:EP:346:PRO:HD2 | 2.44 | 0.58 |
| 41:EP:178:THR:HG22 | 41:EP:180:VAL:HG22 | 1.85 | 0.58 |
| 41:GM:121:ARG:NH1 | 41:GM:158:GLU:OE2 | 2.36 | 0.58 |
| 40:HE:85:GLN:O | 40:HE:86:LEU:C | 2.41 | 0.58 |
| 41:HO:66:VAL:HG12 | 41:HO:91:VAL:HB | 1.86 | 0.58 |
| 40:IA:207:GLU:HA | 40:IA:210:TYR:HD1 | 1.68 | 0.58 |
| 40:IE:326:LYS:HE2 | 41:IM:225:LEU:HD11 | 1.84 | 0.58 |
| 40:KF:228:ASN:HB3 | 40:KF:231:ILE:HD12 | 1.85 | 0.58 |
| 41:MP:341:PHE:HB3 | 41:MP:348:ASN:HD21 | 1.68 | 0.58 |
| 40:ND:269:LEU:HD21 | 40:ND:380:THR:HG22 | 1.85 | 0.58 |
| 41:OB:203:ASP:N | 41:OB:300:MET:O | 2.33 | 0.58 |
| 40:OD:77:GLU:HG3 | 40:OD:78:VAL:N | 2.18 | 0.58 |
| 41:ON:268:PRO:HG2 | 41:ON:300:MET:HB2 | 1.86 | 0.58 |
| 40:PG:264:ARG:NH1 | 40:PG:430:ASP:OD2 | 2.31 | 0.58 |
| 40:PH:265:ILE:HG13 | 40:PH:434:VAL:HG21 | 1.86 | 0.58 |
| 41:PL:8:GLN:HE22 | 41:PL:65:LEU:HG | 1.69 | 0.58 |
| 41:PM:248:ALA:HA | 41:PM:252:LYS:HD3 | 1.85 | 0.58 |
| 41:QB:318:ARG:HD3 | 41:QB:358:PRO:HD3 | 1.85 | 0.58 |
| 41:QB:427:ALA:O | 41:QB:428:CYS:C | 2.42 | 0.58 |
| 41:QN:248:ALA:HA | 41:QN:252:LYS:HG2 | 1.85 | 0.58 |
| 41:QP:226:ASN:HB2 | 43:QP:501:GDP:HN1 | 1.68 | 0.58 |
| 41:RO:100:ASN:HB3 | 41:RO:103:LYS:HB2 | 1.85 | 0.58 |
| 40:SI:370:VAL:HG22 | 40:SI:372:ARG:H | 1.69 | 0.58 |
| 40:UI:223:THR:HG22 | 41:UP:322:SER:HA | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UN:2:ARG:HE | 41:UN:240:LEU:HD22 | 1.68 | 0.58 |
| 40:VF:274:PRO:HG3 | 40:VF:286:LEU:HD12 | 1.84 | 0.58 |
| 41:WB:193:VAL:HG11 | 41:WB:262:ARG:HH21 | 1.67 | 0.58 |
| 41:WP:248:ALA:HA | 41:WP:252:LYS:HE3 | 1.86 | 0.58 |
| 7:1U:470:LYS:HG3 | 7:1U:514:GLU:HG2 | 1.86 | 0.58 |
| 7:1U:569:VAL:HG23 | 7:1U:586:HIS:HE1 | 1.69 | 0.58 |
| 8:1X:119:ARG:HA | 8:1X:122:LEU:HD12 | 1.84 | 0.58 |
| 10:2G:83:HIS:HB2 | 40:AH:305:CYS:HA | 1.84 | 0.58 |
| 12:2P:68:LYS:HD2 | 12:2P:69:PRO:HD2 | 1.84 | 0.58 |
| 13:2V:61:CYS:HB2 | 13:2V:154:VAL:HG13 | 1.85 | 0.58 |
| 14:3B:46:ARG:HH22 | 40:MD:264:ARG:HE | 1.50 | 0.58 |
| 21:4F:281:ARG:HB2 | 41:DM:219:THR:HG21 | 1.85 | 0.58 |
| 27:4Z:136:VAL:HG23 | 27:4Z:138:GLY:H | 1.68 | 0.58 |
| 38:6C:113:TYR:HE1 | 40:VH:215:ARG:HH21 | 1.50 | 0.58 |
| 41:AB:396:HIS:HA | 41:AB:399:THR:HG22 | 1.86 | 0.58 |
| 40:AH:143:GLY:H | 42:AH:501:GTP:H5' | 1.68 | 0.58 |
| 41:AL:11:GLN:HA | 41:AL:72:THR:HG21 | 1.86 | 0.58 |
| 41:AO:420:ASN:HB2 | 41:AO:421:PRO:HD3 | 1.85 | 0.58 |
| 41:CM:218:THR:O | 41:CM:220:PRO:HD3 | 2.03 | 0.58 |
| 40:DE:163:LYS:O | 40:DE:164:LYS:C | 2.42 | 0.58 |
| 40:DF:67:PHE:HB2 | 40:DF:92:LEU:HD12 | 1.85 | 0.58 |
| 40:FA:100:ALA:HA | 41:FN:252:LYS:HE2 | 1.85 | 0.58 |
| 40:FE:319:TYR:HB3 | 40:FE:323:VAL:HG21 | 1.85 | 0.58 |
| 40:FH:326:LYS:HD2 | 41:FP:208:TYR:HD1 | 1.67 | 0.58 |
| 40:FI:76:ASP:HA | 40:FI:79:ARG:HG2 | 1.84 | 0.58 |
| 41:HO:143:THR:OG1 | 43:HO:501:GDP:O1B | 2.21 | 0.58 |
| 40:IH:255:PHE:HE1 | 40:IH:318:LEU:HD21 | 1.68 | 0.58 |
| 41:IM:172:SER:HB2 | 41:IM:205:GLU:HG2 | 1.85 | 0.58 |
| 40:JA:26:LEU:HD21 | 40:JA:363:VAL:HG22 | 1.84 | 0.58 |
| 41:JB:207:LEU:HB3 | 41:JB:225:LEU:HD22 | 1.85 | 0.58 |
| 40:KA:50:ASN:O | 40:KA:64:ARG:NH1 | 2.36 | 0.58 |
| 40:LA:228:ASN:HD21 | 42:LA:501:GTP:HN1 | 1.51 | 0.58 |
| 40:LH:319:TYR:HB3 | 40:LH:323:VAL:HG11 | 1.84 | 0.58 |
| 41:MB:347:ASN:ND2 | 40:MG:178:SER:HB3 | 2.19 | 0.58 |
| 40:MF:224:TYR:O | 42:MM:501:GTP:N2 | 2.36 | 0.58 |
| 40:OG:165:SER:OG | 40:OG:256:GLN:NE2 | 2.37 | 0.58 |
| 41:OL:87:PRO:HD3 | 41:PL:281:TYR:HD2 | 1.68 | 0.58 |
| 41:OM:354:CYS:SG | 41:OM:355:ASP:N | 2.76 | 0.58 |
| 41:OO:222:TYR:O | 41:OO:226:ASN:ND2 | 2.37 | 0.58 |
| 40:PA:292:THR:HG1 | 40:PA:319:TYR:HH | 1.50 | 0.58 |
| 41:PB:258:VAL:HB | 40:PG:406:TRP:HE1 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:PH:316:CYS:HA | 40:PH:352:LYS:HB2 | 1.85 | 0.58 |
| 41:PP:276:ARG:NH1 | 41:PP:279:GLN:OE1 | 2.32 | 0.58 |
| 40:QG:212:ILE:HG23 | 40:QG:216:ASN:HD21 | 1.69 | 0.58 |
| 40:QH:269:LEU:HD21 | 40:QH:383:ILE:HD12 | 1.85 | 0.58 |
| 41:QP:101:TRP:N | 41:QP:184:ASN:HB3 | 2.11 | 0.58 |
| 41:QP:267:MET:HE1 | 41:QP:367:PHE:HE2 | 1.68 | 0.58 |
| 41:RP:165:ASN:ND2 | 41:RP:198:GLU:OE1 | 2.37 | 0.58 |
| 40:SE:185:TYR:HE2 | 40:SE:403:PHE:HB2 | 1.69 | 0.58 |
| 40:SH:16:ILE:HA | 40:SH:228:ASN:HB3 | 1.85 | 0.58 |
| 40:SH:277:SER:H | 40:SH:280:LYS:HB3 | 1.67 | 0.58 |
| 41:SO:242:PHE:HB3 | 41:SO:356:ILE:CB | 2.34 | 0.58 |
| 41:SP:174:LYS:HG3 | 41:SP:175:VAL:HG13 | 1.86 | 0.58 |
| 40:UG:205:ASP:HB2 | 40:UG:303:VAL:HG23 | 1.84 | 0.58 |
| 41:UP:318:ARG:HE | 41:UP:358:PRO:HG3 | 1.68 | 0.58 |
| 41:VB:7:LEU:HD13 | 41:VB:64:VAL:HB | 1.85 | 0.58 |
| 7:1T:467:ILE:HG12 | 7:1T:478:THR:HG22 | 1.84 | 0.58 |
| 12:2O:82:PRO:HA | 12:2O:97:LYS:HE2 | 1.86 | 0.58 |
| 13:2V:14:LEU:O | 13:2V:164:ARG:HA | 2.03 | 0.58 |
| 15:3E:310:ALA:HB2 | 15:3E:344:ILE:HG21 | 1.84 | 0.58 |
| 21:4E:525:PRO:HA | 21:4E:528:LEU:HB2 | 1.84 | 0.58 |
| 22:4J:272:ARG:CZ | 41:DN:277:GLY:HA2 | 2.33 | 0.58 |
| 38:6D:244:ALA:O | 40:VF:214:ARG:NH2 | 2.36 | 0.58 |
| 38:6D:285:ILE:HD12 | 40:UF:90:GLU:HG3 | 1.86 | 0.58 |
| 40:AE:380:THR:HG22 | 40:AE:382:ALA:H | 1.67 | 0.58 |
| 40:AG:188:ILE:HD12 | 40:AG:424:MET:HG3 | 1.86 | 0.58 |
| 40:BH:96:LYS:HD2 | 41:BO:129:CYS:HB2 | 1.85 | 0.58 |
| 41:BM:290:THR:HG21 | 41:BM:329:GLN:HE21 | 1.68 | 0.58 |
| 41:BN:252:LYS:HG2 | 41:BN:350:LYS:HZ1 | 1.69 | 0.58 |
| 41:CB:52:ASN:OD1 | 41:CB:62:ARG:NH2 | 2.36 | 0.58 |
| 40:DA:320:ARG:HB3 | 40:DA:356:ASN:HD22 | 1.68 | 0.58 |
| 41:DB:68:LEU:HB2 | 41:DB:143:THR:OG1 | 2.03 | 0.58 |
| 40:DH:310:GLY:HA3 | 40:DH:382:ALA:HB2 | 1.85 | 0.58 |
| 40:DI:110:ILE:HD12 | 40:DI:110:ILE:H | 1.69 | 0.58 |
| 40:DI:210:TYR:HB2 | 41:DP:324:LYS:HZ3 | 1.67 | 0.58 |
| 41:DL:25:SER:HA | 41:DL:30:ILE:HG23 | 1.86 | 0.58 |
| 41:EB:317:PHE:HB2 | 41:EB:353:VAL:HG12 | 1.85 | 0.58 |
| 40:EE:100:ALA:HA | 41:EL:252:LYS:HG3 | 1.84 | 0.58 |
| 40:FG:224:TYR:O | 40:FG:228:ASN:ND2 | 2.37 | 0.58 |
| 41:FO:3:GLU:OE1 | 41:FO:62:ARG:NH1 | 2.37 | 0.58 |
| 41:GB:2:ARG:HG2 | 41:GB:131:GLN:HE21 | 1.68 | 0.58 |
| 40:GE:72:PRO:O | 40:GE:73:THR:C | 2.42 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GI:316:CYS:HA | 40:GI:352:LYS:HB3 | 1.84 | 0.58 |
| 41:GM:134:GLN:HA | 41:GM:165:ASN:O | 2.04 | 0.58 |
| 40:HE:63:PRO:HD3 | 40:HE:86:LEU:HG | 1.84 | 0.58 |
| 40:HE:326:LYS:O | 40:HE:329:ASN:N | 2.36 | 0.58 |
| 40:HI:2:ARG:NH2 | 41:HQ:69:GLU:OE2 | 2.37 | 0.58 |
| 41:HM:26:ASP:O | 41:HM:359:ARG:NH2 | 2.36 | 0.58 |
| 41:HN:16:ILE:HG21 | 41:HN:136:THR:HB | 1.86 | 0.58 |
| 41:JM:248:ALA:HB2 | 41:JM:352:ALA:HB1 | 1.86 | 0.58 |
| 41:JO:253:LEU:O | 41:JO:257:MET:HB2 | 2.03 | 0.58 |
| 40:KE:102:ASN:HD22 | 40:KE:105:ARG:HD3 | 1.69 | 0.58 |
| 40:KF:326:LYS:HD2 | 41:KN:208:TYR:HB2 | 1.84 | 0.58 |
| 40:MF:93:ILE:HD13 | 40:MF:118:VAL:HA | 1.86 | 0.58 |
| 40:ND:180:ALA:HB3 | 40:ND:183:GLU:HB2 | 1.84 | 0.58 |
| 40:NE:180:ALA:HB3 | 40:NE:183:GLU:HG3 | 1.84 | 0.58 |
| 41:NL:407:GLU:HA | 41:NL:410:GLU:HG2 | 1.86 | 0.58 |
| 40:OA:311:LYS:NZ | 40:OA:437:ASP:OD1 | 2.36 | 0.58 |
| 40:OD:132:LEU:HB3 | 40:OD:164:LYS:HE3 | 1.86 | 0.58 |
| 41:OO:153:SER:HA | 41:OO:195:ASN:HD21 | 1.67 | 0.58 |
| 41:PB:237:THR:HG22 | 41:PB:250:LEU:HD21 | 1.84 | 0.58 |
| 40:PH:329:ASN:HD22 | 41:PP:175:VAL:HG21 | 1.69 | 0.58 |
| 41:PL:191:GLN:O | 41:PL:195:ASN:ND2 | 2.36 | 0.58 |
| 41:PO:319:GLY:HA2 | 41:PO:357:PRO:HG3 | 1.85 | 0.58 |
| 41:QB:358:PRO:HG2 | 41:QB:361:LEU:HD12 | 1.84 | 0.58 |
| 40:QF:259:LEU:O | 40:QF:379:ASN:ND2 | 2.36 | 0.58 |
| 41:QL:381:ILE:HA | 41:QL:384:GLN:HB2 | 1.85 | 0.58 |
| 40:RE:436:MET:O | 41:RM:391:ARG:NH2 | 2.36 | 0.58 |
| 41:RO:289:LEU:HD11 | 41:RO:363:MET:HG2 | 1.84 | 0.58 |
| 40:SA:210:TYR:HE1 | 41:SN:324:LYS:HA | 1.68 | 0.58 |
| 40:SA:262:TYR:O | 40:SA:264:ARG:N | 2.36 | 0.58 |
| 41:SN:207:LEU:HD13 | 41:SN:210:ILE:HD11 | 1.85 | 0.58 |
| 41:TB:137:HIS:O | 41:TB:168:SER:HA | 2.04 | 0.58 |
| 41:TM:252:LYS:O | 41:TM:256:ASN:ND2 | 2.34 | 0.58 |
| 40:UA:352:LYS:NZ | 41:UB:176:SER:OG | 2.37 | 0.58 |
| 41:UO:314:ALA:HB3 | 41:UO:368:ILE:HB | 1.85 | 0.58 |
| 41:UP:420:ASN:HB2 | 41:UP:421:PRO:HD3 | 1.85 | 0.58 |
| 40:VA:213:CYS:HA | 40:VA:217:LEU:HB2 | 1.85 | 0.58 |
| 40:VG:60:LYS:NZ | 40:VG:61:HIS:O | 2.35 | 0.58 |
| 8:1W:523:LEU:HD13 | 8:1Y:196:ILE:HG23 | 1.85 | 0.58 |
| 14:3B:65:MET:HE1 | 14:3B:102:LEU:HA | 1.84 | 0.58 |
| 23:4M:240:LEU:HD22 | 23:4M:266:HIS:HB3 | 1.85 | 0.58 |
| 23:4N:93:GLY:O | 23:4N:94:TYR:C | 2.41 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:4Y:38:LEU:HD12 | 27:4Y:41:GLN:H | 1.69 | 0.58 |
| 40:BH:328:VAL:HG11 | 40:BH:353:VAL:HG13 | 1.84 | 0.58 |
| 41:CN:354:CYS:SG | 41:CN:355:ASP:N | 2.76 | 0.58 |
| 41:CO:139:LEU:HD23 | 41:CO:168:SER:HB2 | 1.86 | 0.58 |
| 40:DF:36:MET:O | 40:DF:37:PRO:C | 2.42 | 0.58 |
| 40:FA:163:LYS:H | 40:FA:163:LYS:HE3 | 1.67 | 0.58 |
| 41:FB:191:GLN:O | 41:FB:195:ASN:ND2 | 2.36 | 0.58 |
| 41:FM:282:ARG:NH2 | 41:FM:292:GLN:OE1 | 2.36 | 0.58 |
| 41:FN:172:SER:HB2 | 41:FN:205:GLU:HG2 | 1.86 | 0.58 |
| 40:GE:172:TYR:N | 40:GE:204:VAL:O | 2.35 | 0.58 |
| 40:HE:105:ARG:HB3 | 40:HE:110:ILE:HG23 | 1.84 | 0.58 |
| 41:HO:117:LEU:HD21 | 41:HO:154:LYS:HB3 | 1.85 | 0.58 |
| 40:IH:174:ALA:HB3 | 40:IH:178:SER:H | 1.69 | 0.58 |
| 41:IM:100:ASN:HB3 | 41:IM:103:LYS:HG3 | 1.84 | 0.58 |
| 41:JM:216:LYS:HG3 | 41:JM:275:SER:HB2 | 1.85 | 0.58 |
| 41:KL:202:ILE:HG23 | 41:KL:300:MET:HB3 | 1.85 | 0.58 |
| 40:LD:244:PHE:HB2 | 40:LD:356:ASN:HD21 | 1.67 | 0.58 |
| 40:LH:329:ASN:HB3 | 41:LP:175:VAL:HG11 | 1.84 | 0.58 |
| 40:MA:380:THR:HG23 | 40:MA:382:ALA:H | 1.66 | 0.58 |
| 40:MG:116:ASP:OD1 | 40:MG:116:ASP:N | 2.37 | 0.58 |
| 40:ND:90:GLU:HB3 | 40:ND:121:ARG:HH22 | 1.68 | 0.58 |
| 40:ND:303:VAL:O | 40:ND:304:LYS:C | 2.42 | 0.58 |
| 41:OB:341:PHE:HB3 | 41:OB:348:ASN:HD21 | 1.67 | 0.58 |
| 41:OL:354:CYS:SG | 41:OL:355:ASP:N | 2.77 | 0.58 |
| 41:OO:87:PRO:HD3 | 41:PO:281:TYR:HD2 | 1.69 | 0.58 |
| 41:OO:292:GLN:O | 41:OO:298:ASN:ND2 | 2.35 | 0.58 |
| 40:QE:64:ARG:NH1 | 40:QE:129:CYS:SG | 2.77 | 0.58 |
| 41:QM:253:LEU:HD11 | 41:QM:368:ILE:HG13 | 1.84 | 0.58 |
| 40:RA:63:PRO:HG3 | 40:RA:87:PHE:HD1 | 1.69 | 0.58 |
| 40:RF:3:GLU:HA | 40:RF:51:THR:HA | 1.86 | 0.58 |
| 41:RL:253:LEU:O | 41:RL:257:MET:HB2 | 2.04 | 0.58 |
| 40:SH:55:GLU:OE2 | 40:SH:61:HIS:ND1 | 2.35 | 0.58 |
| 40:SH:221:ARG:CZ | 41:SO:322:SER:HB3 | 2.33 | 0.58 |
| 40:SH:262:TYR:HB2 | 40:SH:265:ILE:HG22 | 1.84 | 0.58 |
| 41:SL:325:GLU:HA | 41:SL:328:GLU:HG3 | 1.86 | 0.58 |
| 40:TE:264:ARG:NH1 | 40:TE:430:ASP:OD1 | 2.36 | 0.58 |
| 40:TH:166:LYS:HB2 | 40:TH:199:ASP:HB2 | 1.86 | 0.58 |
| 40:TI:7:VAL:HB | 40:TI:137:ILE:HG22 | 1.85 | 0.58 |
| 41:TM:165:ASN:HD21 | 41:TM:250:LEU:HD13 | 1.68 | 0.58 |
| 41:TN:159:TYR:HB3 | 41:TN:162:ARG:HD3 | 1.84 | 0.58 |
| 41:UP:100:ASN:HB3 | 41:UP:103:LYS:HG3 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VB:334:GLN:NE2 | 41:VB:348:ASN:OD1 | 2.36 | 0.58 |
| 40:VG:124:LYS:NZ | 40:WF:297:GLU:OE2 | 2.37 | 0.58 |
| 40:WG:50:ASN:O | 40:WG:64:ARG:NH1 | 2.36 | 0.58 |
| 40:WH:224:TYR:HA | 40:WH:227:LEU:HG | 1.86 | 0.58 |
| 7:1T:383:MET:O | 7:1T:384:ARG:C | 2.42 | 0.58 |
| 8:1W:425:GLN:NE2 | 40:VA:367:LEU:O | 2.36 | 0.58 |
| 10:2F:83:HIS:ND1 | 40:AA:385:GLU:OE1 | 2.37 | 0.58 |
| 12:2R:145:VAL:HG12 | 12:2R:149:LEU:HD23 | 1.85 | 0.58 |
| 17:3P:131:LYS:HG3 | 17:3Q:430:THR:HG23 | 1.86 | 0.58 |
| 21:4D:515:TYR:HA | 21:4D:518:SER:HB2 | 1.85 | 0.58 |
| 21:4F:456:VAL:HB | 21:4F:459:SER:HB3 | 1.85 | 0.58 |
| 22:4J:231:ARG:HH11 | 40:CF:41:THR:HB | 1.68 | 0.58 |
| 27:4Y:171:LYS:HA | 41:KL:276:ARG:HD3 | 1.86 | 0.58 |
| 36:5W:114:LEU:HB2 | 36:5W:146:ARG:HH21 | 1.69 | 0.58 |
| 36:5Y:82:ASN:OD1 | 40:OG:369:LYS:NZ | 2.36 | 0.58 |
| 40:AE:16:ILE:HD13 | 40:AE:228:ASN:HB2 | 1.85 | 0.58 |
| 41:BB:22:GLU:HG3 | 41:BB:81:PHE:HB2 | 1.86 | 0.58 |
| 40:BH:313:MET:HA | 40:BH:344:VAL:HG22 | 1.85 | 0.58 |
| 41:BM:391:ARG:O | 41:BM:392:LYS:C | 2.42 | 0.58 |
| 41:BP:58:LYS:O | 41:BP:59:TYR:C | 2.42 | 0.58 |
| 40:CA:228:ASN:OD1 | 42:CA:501:GTP:N2 | 2.33 | 0.58 |
| 41:CP:283:ALA:O | 41:CP:285:THR:N | 2.36 | 0.58 |
| 41:DB:198:GLU:HG2 | 41:DB:266:PHE:HZ | 1.67 | 0.58 |
| 40:DF:192:HIS:HE1 | 40:DF:419:GLU:HG3 | 1.68 | 0.58 |
| 41:DM:420:ASN:O | 41:DM:421:PRO:C | 2.42 | 0.58 |
| 40:EA:73:THR:HA | 40:EA:76:ASP:HB2 | 1.85 | 0.58 |
| 40:EF:324:VAL:HB | 40:EF:327:ASP:HB2 | 1.86 | 0.58 |
| 41:EM:16:ILE:HA | 41:EM:226:ASN:HD21 | 1.68 | 0.58 |
| 40:FA:99:ALA:O | 40:FA:100:ALA:C | 2.42 | 0.58 |
| 40:FF:322:ASP:O | 40:FF:372:ARG:NH1 | 2.37 | 0.58 |
| 40:GH:56:THR:O | 40:GH:58:ALA:N | 2.37 | 0.58 |
| 40:GH:66:VAL:O | 40:GH:67:PHE:C | 2.42 | 0.58 |
| 40:JD:274:PRO:HD2 | 40:JD:291:ILE:HG13 | 1.86 | 0.58 |
| 40:JE:332:ILE:HG21 | 41:JM:175:VAL:HG13 | 1.85 | 0.58 |
| 40:JG:88:HIS:HE1 | 40:KG:280:LYS:HG3 | 1.68 | 0.58 |
| 41:JM:243:PRO:HD2 | 41:JM:356:ILE:HD13 | 1.86 | 0.58 |
| 41:JN:274:THR:HG22 | 41:JN:282:ARG:HH11 | 1.68 | 0.58 |
| 40:KG:213:CYS:HA | 40:KG:217:LEU:HD12 | 1.84 | 0.58 |
| 41:KM:165:ASN:ND2 | 41:KM:198:GLU:OE1 | 2.37 | 0.58 |
| 40:LD:226:ASN:ND2 | 40:LD:366:ASP:OD2 | 2.36 | 0.58 |
| 41:NB:267:MET:HG2 | 41:NB:301:ALA:HB3 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:ND:72:PRO:O | 40:ND:74:VAL:N | 2.37 | 0.58 |
| 40:NE:90:GLU:HG3 | 40:NE:121:ARG:NH2 | 2.19 | 0.58 |
| 40:OH:101:ASN:HD22 | 41:OO:256:ASN:HD21 | 1.52 | 0.58 |
| 40:PF:329:ASN:HD22 | 41:PN:175:VAL:HG21 | 1.69 | 0.58 |
| 41:PL:107:THR:O | 41:PL:110:ALA:N | 2.37 | 0.58 |
| 40:RA:222:PRO:HD2 | 41:RN:324:LYS:HG2 | 1.85 | 0.58 |
| 40:RA:274:PRO:HG3 | 40:RA:286:LEU:HD12 | 1.86 | 0.58 |
| 40:TE:320:ARG:HH12 | 40:TE:360:PRO:HB3 | 1.69 | 0.58 |
| 40:UF:122:ILE:HG21 | 40:UF:157:LEU:HD21 | 1.85 | 0.58 |
| 40:UF:281:ALA:O | 40:UF:282:TYR:C | 2.42 | 0.58 |
| 40:VA:288:VAL:HA | 40:VA:291:ILE:HG12 | 1.84 | 0.58 |
| 40:WA:53:PHE:O | 40:WA:64:ARG:NH1 | 2.37 | 0.58 |
| 41:WB:327:ASP:HB3 | 40:WG:177:VAL:HG11 | 1.86 | 0.58 |
| 10:2E:150:PRO:HD2 | 40:WF:221:ARG:HH12 | 1.69 | 0.58 |
| 18:3U:347:GLU:OE1 | 18:3U:351:LYS:NZ | 2.37 | 0.58 |
| 23:4Q:194:ALA:HB2 | 23:4Q:209:ALA:HB2 | 1.84 | 0.58 |
| 36:5X:123:ARG:HD2 | 40:KE:400:LYS:HA | 1.86 | 0.58 |
| 39:6L:99:LEU:HB2 | 39:6L:153:TRP:HE1 | 1.69 | 0.58 |
| 41:CB:40:SER:HB2 | 41:CB:43:GLN:HG3 | 1.86 | 0.58 |
| 40:CE:252:LEU:HA | 40:CE:255:PHE:HD1 | 1.68 | 0.58 |
| 40:CG:73:THR:HA | 40:CG:76:ASP:HB2 | 1.84 | 0.58 |
| 40:CI:271:THR:HG22 | 40:CI:301:GLN:HA | 1.85 | 0.58 |
| 41:CO:142:GLY:O | 41:CO:144:GLY:N | 2.37 | 0.58 |
| 41:CP:358:PRO:HG3 | 41:CP:364:SER:HB2 | 1.86 | 0.58 |
| 40:DI:295:CYS:O | 40:DI:297:GLU:N | 2.36 | 0.58 |
| 40:EI:139:HIS:HE1 | 40:EI:168:GLU:HB3 | 1.68 | 0.58 |
| 41:EN:108:GLU:HA | 41:EN:111:GLU:HG2 | 1.85 | 0.58 |
| 40:FA:100:ALA:O | 40:FA:101:ASN:C | 2.41 | 0.58 |
| 40:FA:352:LYS:HE3 | 41:FB:179:VAL:HG22 | 1.84 | 0.58 |
| 41:FO:268:PRO:HD2 | 41:FO:300:MET:HB2 | 1.84 | 0.58 |
| 41:GM:207:LEU:HD22 | 41:GM:228:LEU:HD11 | 1.85 | 0.58 |
| 41:HB:42:LEU:HD23 | 41:HB:356:ILE:HD11 | 1.86 | 0.58 |
| 41:HM:100:ASN:HB3 | 41:HM:103:LYS:HB2 | 1.84 | 0.58 |
| 41:HO:262:ARG:NH2 | 41:HO:414:ASN:OD1 | 2.36 | 0.58 |
| 40:LA:320:ARG:NH1 | 40:LA:358:GLN:O | 2.37 | 0.58 |
| 40:LF:303:VAL:O | 40:LF:304:LYS:C | 2.42 | 0.58 |
| 40:LG:160:ASP:O | 40:LG:161:TYR:C | 2.41 | 0.58 |
| 41:LN:213:ARG:HH21 | 41:LN:297:LYS:HG2 | 1.68 | 0.58 |
| 41:LP:174:LYS:HG3 | 41:LP:175:VAL:HG13 | 1.86 | 0.58 |
| 40:MF:338:LYS:HB2 | 40:MF:341:ILE:HD12 | 1.86 | 0.58 |
| 40:NE:2:ARG:HH11 | 40:NE:242:LEU:HA | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OA:247:ALA:HB3 | 40:OA:355:ILE:HB | 1.86 | 0.58 |
| 40:OE:118:VAL:HG21 | 40:OE:149:PHE:HZ | 1.67 | 0.58 |
| 40:OF:133:GLN:HG2 | 40:OF:242:LEU:HD21 | 1.86 | 0.58 |
| 41:OP:107:THR:HG22 | 41:OP:108:GLU:H | 1.68 | 0.58 |
| 41:PO:163:ILE:HD13 | 41:PO:250:LEU:HB3 | 1.86 | 0.58 |
| 41:QB:322:SER:O | 41:QB:323:MET:C | 2.41 | 0.58 |
| 40:RF:70:LEU:HD23 | 40:RF:114:LEU:HD22 | 1.84 | 0.58 |
| 40:RH:90:GLU:OE1 | 40:RH:121:ARG:NH2 | 2.35 | 0.58 |
| 40:SE:16:ILE:HG13 | 40:SE:228:ASN:HD22 | 1.68 | 0.58 |
| 40:SF:226:ASN:ND2 | 40:SF:366:ASP:OD2 | 2.37 | 0.58 |
| 40:TA:222:PRO:HD2 | 41:TN:324:LYS:HG2 | 1.85 | 0.58 |
| 40:TH:221:ARG:NH1 | 41:TO:325:GLU:OE1 | 2.36 | 0.58 |
| 40:WA:436:MET:SD | 41:WB:391:ARG:NH1 | 2.77 | 0.58 |
| 41:WM:20:PHE:HA | 41:WM:230:SER:HB2 | 1.85 | 0.58 |
| 41:WN:30:ILE:HD11 | 41:WN:47:ILE:HD11 | 1.86 | 0.58 |
| 41:WQ:156:ARG:NH1 | 41:WQ:162:ARG:O | 2.37 | 0.58 |
| 2:1C:10:ARG:HB2 | 40:GF:401:ARG:HG3 | 1.84 | 0.58 |
| 2:1D:10:ARG:NH2 | 40:GH:398:TYR:HA | 2.19 | 0.58 |
| 7:1S:502:ASN:ND2 | 41:VB:39:ASP:O | 2.35 | 0.58 |
| 7:1T:14:LEU:O | 7:1T:15:GLU:HB2 | 2.03 | 0.58 |
| 7:1U:248:LYS:HB2 | 41:WP:33:THR:HG22 | 1.84 | 0.58 |
| 11:2I:113:VAL:HG21 | 40:LG:401:ARG:HB3 | 1.86 | 0.58 |
| 12:2M:213:TYR:HE2 | 41:WO:122:LYS:HB3 | 1.69 | 0.58 |
| 13:2X:32:GLY:HA3 | 13:2X:57:THR:HG21 | 1.83 | 0.58 |
| 20:4A:157:GLN:HG2 | 40:LE:58:ALA:N | 2.19 | 0.58 |
| 21:4F:255:MET:N | 21:4F:255:MET:SD | 2.70 | 0.58 |
| 21:4F:477:SER:HB2 | 21:4F:480:GLU:HB2 | 1.85 | 0.58 |
| 23:4Q:187:PHE:CZ | 23:4Q:189:GLY:HA3 | 2.39 | 0.58 |
| 23:4R:87:SER:HA | 23:4R:90:MET:HG3 | 1.86 | 0.58 |
| 34:5Q:60:ASP:HB3 | 41:KN:212:PHE:HE2 | 1.69 | 0.58 |
| 34:5R:367:GLU:HG2 | 41:GP:360:GLY:HA2 | 1.85 | 0.58 |
| 38:6C:48:PRO:HA | 41:VO:336:LYS:HZ1 | 1.68 | 0.58 |
| 39:6G:138:GLY:HA2 | 39:6G:141:SER:HB2 | 1.85 | 0.58 |
| 40:BI:222:PRO:HD2 | 41:BP:324:LYS:CE | 2.34 | 0.58 |
| 40:CA:350:GLY:HA2 | 41:CB:179:VAL:HG22 | 1.85 | 0.58 |
| 40:CF:235:VAL:HA | 40:CF:238:ILE:HG22 | 1.84 | 0.58 |
| 41:CL:271:ALA:O | 41:CL:273:LEU:N | 2.37 | 0.58 |
| 40:DF:132:LEU:O | 40:DF:133:GLN:C | 2.41 | 0.58 |
| 41:DM:49:VAL:HG11 | 41:DM:241:ARG:HG3 | 1.85 | 0.58 |
| 41:DN:135:LEU:HD23 | 41:DN:166:THR:HG22 | 1.86 | 0.58 |
| 40:EF:168:GLU:HB2 | 40:EF:201:ALA:HA | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EH:357:TYR:O | 40:EH:358:GLN:C | 2.42 | 0.58 |
| 40:EI:177:VAL:HA | 41:EP:331:LEU:HD22 | 1.85 | 0.58 |
| 40:FI:26:LEU:HD12 | 40:FI:363:VAL:HG12 | 1.86 | 0.58 |
| 40:GE:325:PRO:HG3 | 41:GM:222:TYR:CD1 | 2.38 | 0.58 |
| 41:GM:45:GLU:HG3 | 41:GM:46:ARG:HG3 | 1.85 | 0.58 |
| 40:HA:136:LEU:HD23 | 40:HA:167:LEU:HB2 | 1.86 | 0.58 |
| 40:HE:26:LEU:O | 40:HE:27:GLU:C | 2.42 | 0.58 |
| 41:HN:303:CYS:O | 41:HN:304:ASP:C | 2.43 | 0.58 |
| 41:IP:202:ILE:HG12 | 41:IP:268:PRO:HG3 | 1.85 | 0.58 |
| 40:JD:274:PRO:HG3 | 40:JD:286:LEU:HD12 | 1.86 | 0.58 |
| 40:KG:7:VAL:HG12 | 40:KG:66:VAL:HB | 1.85 | 0.58 |
| 41:KL:237:THR:HA | 41:KL:240:LEU:HD21 | 1.86 | 0.58 |
| 41:KL:393:ALA:O | 41:KL:394:PHE:C | 2.41 | 0.58 |
| 41:KN:323:MET:HA | 41:KN:326:VAL:HB | 1.86 | 0.58 |
| 40:LG:352:LYS:HD2 | 41:LO:178:THR:C | 2.25 | 0.58 |
| 41:LO:341:PHE:HB3 | 41:LO:348:ASN:HD21 | 1.67 | 0.58 |
| 40:MA:189:LEU:HD11 | 40:MA:417:PHE:HA | 1.86 | 0.58 |
| 40:MD:258:ASN:HD21 | 41:ML:178:THR:HG23 | 1.69 | 0.58 |
| 40:NA:259:LEU:O | 40:NA:379:ASN:ND2 | 2.34 | 0.58 |
| 41:NP:292:GLN:O | 41:NP:298:ASN:ND2 | 2.37 | 0.58 |
| 40:OA:105:ARG:HG2 | 40:OA:410:GLU:HG2 | 1.85 | 0.58 |
| 41:OM:107:THR:HG22 | 41:OM:108:GLU:H | 1.68 | 0.58 |
| 41:OO:305:PRO:HB3 | 41:OO:310:TYR:HE1 | 1.69 | 0.58 |
| 40:PA:258:ASN:HD22 | 41:PB:179:VAL:HG22 | 1.68 | 0.58 |
| 41:PP:414:ASN:HA | 41:PP:417:ASP:HB2 | 1.86 | 0.58 |
| 41:QB:290:THR:HG21 | 41:QB:329:GLN:HB3 | 1.85 | 0.58 |
| 41:QO:312:THR:OG1 | 41:QO:370:ASN:OD1 | 2.22 | 0.58 |
| 40:RA:142:GLY:HA2 | 40:RA:183:GLU:HG2 | 1.85 | 0.58 |
| 40:RG:6:SER:O | 40:RG:65:ALA:HA | 2.04 | 0.58 |
| 41:RM:236:VAL:HG13 | 41:RM:237:THR:HG23 | 1.86 | 0.58 |
| 41:RO:325:GLU:O | 41:RO:329:GLN:HB2 | 2.04 | 0.58 |
| 40:SE:50:ASN:OD1 | 40:SE:64:ARG:NH2 | 2.31 | 0.58 |
| 40:SE:226:ASN:ND2 | 40:SE:366:ASP:OD2 | 2.34 | 0.58 |
| 40:SF:141:PHE:HB2 | 40:SF:173:PRO:HD3 | 1.86 | 0.58 |
| 40:UE:315:CYS:O | 40:UE:351:PHE:HA | 2.04 | 0.58 |
| 40:VF:174:ALA:HB1 | 40:VF:207:GLU:HG2 | 1.86 | 0.58 |
| 40:VG:178:SER:OG | 40:VG:183:GLU:OE1 | 2.22 | 0.58 |
| 40:VJ:177:VAL:HB | 41:VQ:331:LEU:HD22 | 1.86 | 0.58 |
| 40:WA:206:ASN:OD1 | 42:WA:501:GTP:O2' | 2.22 | 0.58 |
| 40:WE:319:TYR:HB3 | 40:WE:323:VAL:HG11 | 1.86 | 0.58 |
| 41:WM:244:GLY:HA2 | 41:WM:355:ASP:HB2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:2G:88:LYS:HB3 | 10:2G:92:GLU:HB2 | 1.85 | 0.57 |
| 11:2J:113:VAL:HG11 | 40:LF:404:VAL:CG1 | 2.34 | 0.57 |
| 17:3R:93:ARG:O | 17:3R:94:TYR:C | 2.43 | 0.57 |
| 28:5B:212:ASN:HB2 | 28:5B:215:LEU:HD11 | 1.85 | 0.57 |
| 29:5E:116:THR:OG1 | 29:5E:118:TYR:O | 2.22 | 0.57 |
| 30:5G:76:PHE:HB2 | 34:5R:502:HIS:CE1 | 2.39 | 0.57 |
| 41:AL:421:PRO:HA | 41:AL:424:THR:HG22 | 1.85 | 0.57 |
| 41:AN:421:PRO:HA | 41:AN:424:THR:HG22 | 1.85 | 0.57 |
| 40:BF:207:GLU:HG2 | 40:BF:210:TYR:HD2 | 1.69 | 0.57 |
| 40:CA:195:LEU:HD21 | 40:CA:427:LEU:HD13 | 1.86 | 0.57 |
| 40:CF:326:LYS:HD2 | 41:CN:208:TYR:CG | 2.39 | 0.57 |
| 40:CH:434:VAL:HA | 41:CP:391:ARG:HH22 | 1.68 | 0.57 |
| 41:CN:1:MET:O | 41:CN:2:ARG:C | 2.43 | 0.57 |
| 40:DA:363:VAL:O | 40:DA:365:GLY:N | 2.37 | 0.57 |
| 40:DF:51:THR:HG21 | 40:DF:243:ARG:HG2 | 1.86 | 0.57 |
| 41:EL:314:ALA:HB3 | 41:EL:368:ILE:HB | 1.84 | 0.57 |
| 41:EM:226:ASN:CB | 43:EM:501:GDP:HN1 | 2.16 | 0.57 |
| 40:GE:88:HIS:C | 40:GE:90:GLU:H | 2.08 | 0.57 |
| 40:HH:298:PRO:HB3 | 40:HH:307:PRO:HD2 | 1.85 | 0.57 |
| 41:HN:309:ARG:H | 41:HN:372:THR:HG22 | 1.68 | 0.57 |
| 40:IE:195:LEU:HG | 40:IE:266:HIS:HE1 | 1.68 | 0.57 |
| 40:JD:262:TYR:HE1 | 41:JL:393:ALA:HA | 1.69 | 0.57 |
| 41:KM:7:LEU:HD23 | 41:KM:64:VAL:HB | 1.85 | 0.57 |
| 40:LF:323:VAL:HG13 | 40:LF:355:ILE:HG23 | 1.86 | 0.57 |
| 41:LL:47:ILE:HG12 | 41:LL:51:TYR:HB2 | 1.86 | 0.57 |
| 40:MF:188:ILE:HG23 | 40:MF:424:MET:HG3 | 1.84 | 0.57 |
| 40:MH:60:LYS:O | 40:MH:61:HIS:C | 2.41 | 0.57 |
| 41:MM:107:THR:O | 41:MM:110:ALA:N | 2.34 | 0.57 |
| 40:ND:326:LYS:HA | 41:NL:208:TYR:CE1 | 2.38 | 0.57 |
| 40:NH:104:ALA:HB2 | 40:NH:412:MET:HG2 | 1.86 | 0.57 |
| 41:NN:285:THR:OG1 | 41:NN:288:GLU:OE1 | 2.21 | 0.57 |
| 40:OD:20:CYS:HA | 40:OD:232:SER:HB2 | 1.86 | 0.57 |
| 41:OP:87:PRO:HD3 | 41:PP:281:TYR:HD2 | 1.69 | 0.57 |
| 41:OP:152:ILE:HA | 41:OP:155:ILE:HG22 | 1.86 | 0.57 |
| 40:QG:27:GLU:OE1 | 40:QG:243:ARG:NH1 | 2.37 | 0.57 |
| 41:QP:298:ASN:O | 41:QP:299:MET:C | 2.42 | 0.57 |
| 40:RE:385:GLU:OE1 | 40:RE:389:ARG:NH2 | 2.32 | 0.57 |
| 41:RO:313:VAL:HG23 | 41:RO:367:PHE:HE2 | 1.68 | 0.57 |
| 41:SB:341:PHE:HB3 | 41:SB:348:ASN:HD21 | 1.68 | 0.57 |
| 41:TL:191:GLN:O | 41:TL:195:ASN:ND2 | 2.37 | 0.57 |
| 40:UG:98:ASP:O | 40:UG:105:ARG:NH2 | 2.31 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UN:113:VAL:HG21 | 41:UN:150:LEU:HG | 1.86 | 0.57 |
| 41:UP:264:HIS:O | 41:UP:265:PHE:C | 2.42 | 0.57 |
| 41:VP:172:SER:OG | 41:VP:175:VAL:O | 2.21 | 0.57 |
| 41:VP:193:VAL:HG13 | 41:VP:194:GLU:HG3 | 1.86 | 0.57 |
| 40:WF:186:ASN:OD1 | 40:WF:407:TYR:OH | 2.21 | 0.57 |
| 41:WO:4:ILE:HB | 41:WO:50:TYR:HE1 | 1.69 | 0.57 |
| 14:3C:10:TYR:CE1 | 41:MO:297:LYS:HA | 2.35 | 0.57 |
| 17:3R:174:LEU:HD23 | 17:3R:244:LEU:HG | 1.86 | 0.57 |
| 21:4D:420:LEU:HG | 21:4D:444:LEU:HD11 | 1.85 | 0.57 |
| 21:4F:435:GLY:O | 21:4F:436:ARG:C | 2.41 | 0.57 |
| 22:4I:98:ARG:NH2 | 41:BO:276:ARG:O | 2.37 | 0.57 |
| 25:4T:341:ARG:HD3 | 26:4W:374:ILE:HD12 | 1.86 | 0.57 |
| 35:5T:100:ASP:OD2 | 41:JL:320:ARG:NH2 | 2.38 | 0.57 |
| 36:5X:82:ASN:OD1 | 40:OD:371:GLN:NE2 | 2.37 | 0.57 |
| 36:5Y:66:LEU:HB3 | 40:OG:221:ARG:HH11 | 1.69 | 0.57 |
| 40:BI:142:GLY:O | 40:BI:186:ASN:HB3 | 2.05 | 0.57 |
| 40:CI:226:ASN:ND2 | 40:CI:366:ASP:OD2 | 2.37 | 0.57 |
| 41:CL:342:VAL:HB | 41:CL:344:TRP:CD1 | 2.39 | 0.57 |
| 41:CN:375:GLN:HB3 | 41:CN:422:VAL:HG21 | 1.86 | 0.57 |
| 41:CP:226:ASN:ND2 | 43:CP:501:GDP:HN1 | 2.02 | 0.57 |
| 40:DE:167:LEU:HB3 | 40:DE:202:PHE:HE2 | 1.69 | 0.57 |
| 40:DF:88:HIS:HD2 | 40:EF:283:HIS:HB2 | 1.69 | 0.57 |
| 40:DF:159:VAL:O | 40:DF:160:ASP:C | 2.41 | 0.57 |
| 41:DM:245:GLN:O | 41:DM:247:ASN:N | 2.37 | 0.57 |
| 41:DO:182:PRO:HA | 41:DO:381:ILE:HD11 | 1.85 | 0.57 |
| 41:DP:193:VAL:HA | 41:DP:264:HIS:CE1 | 2.39 | 0.57 |
| 40:EE:101:ASN:HD22 | 40:EE:143:GLY:HA2 | 1.69 | 0.57 |
| 40:EH:409:GLY:O | 40:EH:410:GLU:C | 2.41 | 0.57 |
| 40:GA:217:LEU:HB3 | 40:GA:219:ILE:HG22 | 1.87 | 0.57 |
| 40:GI:33:ASP:HA | 40:GI:85:GLN:HG3 | 1.86 | 0.57 |
| 40:GI:135:PHE:HB2 | 40:GI:166:LYS:HG3 | 1.84 | 0.57 |
| 40:GI:213:CYS:CB | 40:GI:222:PRO:HG3 | 2.33 | 0.57 |
| 41:HB:248:ALA:HA | 41:HB:252:LYS:HG3 | 1.86 | 0.57 |
| 40:IA:278:ALA:H | 40:IA:368:ALA:HB2 | 1.69 | 0.57 |
| 40:IE:27:GLU:OE1 | 40:IE:243:ARG:NH1 | 2.31 | 0.57 |
| 41:IM:113:VAL:HA | 41:IM:116:VAL:HG12 | 1.87 | 0.57 |
| 40:JA:112:LYS:HA | 40:JA:115:ILE:HG22 | 1.87 | 0.57 |
| 40:JE:332:ILE:HG23 | 40:JE:351:PHE:HD2 | 1.69 | 0.57 |
| 40:KF:98:ASP:O | 40:KF:105:ARG:NH1 | 2.37 | 0.57 |
| 40:LH:180:ALA:HB3 | 40:LH:183:GLU:HG3 | 1.84 | 0.57 |
| 41:LP:170:VAL:HG21 | 41:LP:377:LEU:HD11 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:MB:103:LYS:O | 41:MB:107:THR:OG1 | 2.22 | 0.57 |
| 41:MP:107:THR:O | 41:MP:110:ALA:N | 2.36 | 0.57 |
| 40:NE:319:TYR:HB3 | 40:NE:323:VAL:HG21 | 1.86 | 0.57 |
| 41:NN:262:ARG:HH22 | 41:NN:421:PRO:HG3 | 1.68 | 0.57 |
| 41:OB:163:ILE:HD13 | 41:OB:251:ARG:HG3 | 1.84 | 0.57 |
| 41:OP:292:GLN:O | 41:OP:298:ASN:ND2 | 2.35 | 0.57 |
| 40:PF:96:LYS:NZ | 41:PM:1:MET:SD | 2.77 | 0.57 |
| 40:PH:176:GLN:HG3 | 41:PO:331:LEU:HD11 | 1.85 | 0.57 |
| 41:PM:209:ASP:HA | 41:PM:213:ARG:HH21 | 1.69 | 0.57 |
| 41:PP:139:LEU:HG | 41:PP:168:SER:HB3 | 1.85 | 0.57 |
| 40:QG:174:ALA:HB3 | 40:QG:178:SER:H | 1.69 | 0.57 |
| 40:QG:254:GLU:OE1 | 41:QO:99:ASN:ND2 | 2.37 | 0.57 |
| 40:RF:93:ILE:HD11 | 40:RF:121:ARG:HD2 | 1.86 | 0.57 |
| 40:RH:76:ASP:OD2 | 41:RO:46:ARG:NH2 | 2.37 | 0.57 |
| 41:RN:271:ALA:HB1 | 41:RN:292:GLN:HB3 | 1.85 | 0.57 |
| 41:RO:198:GLU:HG2 | 41:RO:266:PHE:HE2 | 1.69 | 0.57 |
| 40:TG:11:GLN:HG3 | 40:TG:74:VAL:HG21 | 1.85 | 0.57 |
| 40:UA:88:HIS:HD2 | 40:UA:89:PRO:HD2 | 1.70 | 0.57 |
| 40:UF:277:SER:HB2 | 40:UF:279:GLU:HG2 | 1.85 | 0.57 |
| 40:UI:384:ALA:HA | 40:UI:387:TRP:HD1 | 1.68 | 0.57 |
| 40:WI:16:ILE:HA | 40:WI:228:ASN:HB3 | 1.85 | 0.57 |
| 41:WO:228:LEU:HD11 | 41:WO:273:LEU:HD21 | 1.85 | 0.57 |
| 41:WQ:99:ASN:HD21 | 41:WQ:178:THR:HG23 | 1.69 | 0.57 |
| 41:WQ:313:VAL:HG13 | 41:WQ:367:PHE:HE1 | 1.69 | 0.57 |
| 7:1S:441:VAL:HG11 | 7:1S:478:THR:HG21 | 1.86 | 0.57 |
| 10:2G:157:ARG:HH21 | 41:VQ:59:TYR:HB3 | 1.70 | 0.57 |
| 13:2W:88:THR:O | 13:2W:157:HIS:HB2 | 2.04 | 0.57 |
| 17:3Q:358:LYS:HD3 | 17:3Q:466:LEU:HD23 | 1.84 | 0.57 |
| 20:4B:321:ALA:HA | 20:4B:324:LEU:HD23 | 1.86 | 0.57 |
| 21:4E:243:LEU:HD22 | 21:4E:351:THR:HG23 | 1.87 | 0.57 |
| 22:4J:236:TRP:HB2 | 22:4J:351:VAL:HG12 | 1.87 | 0.57 |
| 22:4J:650:LYS:O | 22:4J:652:VAL:N | 2.37 | 0.57 |
| 36:5Y:130:LEU:HD23 | 36:5Y:136:ASN:HA | 1.85 | 0.57 |
| 40:AH:326:LYS:HD3 | 41:AP:220:PRO:HD2 | 1.86 | 0.57 |
| 40:BH:109:THR:O | 40:BH:110:ILE:C | 2.43 | 0.57 |
| 40:CF:403:PHE:HZ | 41:CM:312:THR:HG21 | 1.69 | 0.57 |
| 41:CO:2:ARG:HB2 | 41:CO:131:GLN:HB2 | 1.85 | 0.57 |
| 41:CP:358:PRO:HD3 | 41:CP:364:SER:HB3 | 1.87 | 0.57 |
| 40:DA:138:PHE:HA | 40:DA:169:PHE:O | 2.05 | 0.57 |
| 40:DF:64:ARG:HH12 | 40:DF:129:CYS:HB2 | 1.69 | 0.57 |
| 41:DN:36:TYR:CZ | 41:DN:38:GLY:HA3 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DN:167:PHE:HZ | 41:DN:236:VAL:HG11 | 1.68 | 0.57 |
| 40:EH:109:THR:OG1 | 40:EH:110:ILE:N | 2.35 | 0.57 |
| 41:EO:169:VAL:HG22 | 41:EO:202:ILE:HD11 | 1.86 | 0.57 |
| 40:FA:348:PRO:HD2 | 41:FB:388:MET:HG3 | 1.86 | 0.57 |
| 40:FH:123:ARG:HH21 | 40:GH:338:LYS:HE3 | 1.69 | 0.57 |
| 40:FH:264:ARG:HH22 | 40:FH:427:LEU:HA | 1.68 | 0.57 |
| 41:FM:139:LEU:HD12 | 41:FM:170:VAL:HG12 | 1.86 | 0.57 |
| 41:FN:60:VAL:HG11 | 41:FN:86:ARG:HE | 1.70 | 0.57 |
| 40:GF:3:GLU:HG3 | 40:GF:51:THR:HA | 1.86 | 0.57 |
| 40:HE:438:SER:HB2 | 41:HM:391:ARG:HD2 | 1.85 | 0.57 |
| 40:HG:76:ASP:HA | 40:HG:79:ARG:HG2 | 1.86 | 0.57 |
| 40:HI:50:ASN:O | 40:HI:64:ARG:NH1 | 2.38 | 0.57 |
| 41:HQ:215:LEU:O | 41:HQ:275:SER:OG | 2.20 | 0.57 |
| 40:IH:102:ASN:HB3 | 40:IH:105:ARG:HB2 | 1.87 | 0.57 |
| 41:IN:341:PHE:HB3 | 41:IN:348:ASN:HD21 | 1.69 | 0.57 |
| 40:JH:7:VAL:HG12 | 40:JH:66:VAL:HB | 1.84 | 0.57 |
| 41:KN:156:ARG:NH1 | 41:KN:195:ASN:O | 2.37 | 0.57 |
| 41:KP:156:ARG:NH2 | 41:KP:162:ARG:O | 2.37 | 0.57 |
| 40:LG:9:VAL:HG23 | 40:LG:145:THR:HG22 | 1.86 | 0.57 |
| 41:LL:89:ASN:HA | 41:LL:119:VAL:HG21 | 1.85 | 0.57 |
| 40:MG:11:GLN:HA | 40:MG:74:VAL:HG11 | 1.85 | 0.57 |
| 40:NE:100:ALA:HA | 41:NL:252:LYS:HD3 | 1.85 | 0.57 |
| 41:NO:19:LYS:HE2 | 41:NO:223:GLY:HA2 | 1.86 | 0.57 |
| 40:OE:326:LYS:NZ | 41:OM:204:ASN:OD1 | 2.38 | 0.57 |
| 41:OP:238:THR:HG21 | 41:OP:318:ARG:HD3 | 1.85 | 0.57 |
| 40:PG:265:ILE:HG23 | 40:PG:431:TYR:HE1 | 1.69 | 0.57 |
| 41:PO:104:GLY:HA2 | 41:PO:109:GLY:HA3 | 1.86 | 0.57 |
| 41:QP:28:HIS:HA | 41:QP:47:ILE:HD13 | 1.86 | 0.57 |
| 40:RA:88:HIS:ND1 | 40:SA:284:GLU:OE2 | 2.37 | 0.57 |
| 40:SG:20:CYS:HA | 40:SG:232:SER:HB2 | 1.84 | 0.57 |
| 41:SM:8:GLN:HE21 | 41:SM:65:LEU:HG | 1.69 | 0.57 |
| 41:SM:61:PRO:HD3 | 41:SM:84:ILE:HG22 | 1.84 | 0.57 |
| 40:TA:239:THR:O | 40:TA:243:ARG:NH1 | 2.36 | 0.57 |
| 40:TE:332:ILE:HG12 | 40:TE:351:PHE:HD2 | 1.69 | 0.57 |
| 40:UF:201:ALA:O | 40:UF:202:PHE:C | 2.43 | 0.57 |
| 41:UO:107:THR:HG22 | 41:UO:108:GLU:H | 1.69 | 0.57 |
| 40:VG:147:SER:HB2 | 40:VG:190:THR:HB | 1.86 | 0.57 |
| 40:VJ:226:ASN:ND2 | 40:VJ:366:ASP:OD2 | 2.37 | 0.57 |
| 40:WG:186:ASN:OD1 | 40:WG:407:TYR:OH | 2.23 | 0.57 |
| 7:1U:573:ASP:HB3 | 7:1U:576:GLU:HB2 | 1.87 | 0.57 |
| 8:1W:277:ARG:HH12 | 41:UP:56:GLY:C | 2.07 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:2B:394:ARG:HH12 | 9:2B:398:ALA:HB2 | 1.69 | 0.57 |
| 13:2U:95:ASP:HB3 | 13:2U:146:THR:OG1 | 2.05 | 0.57 |
| 13:2V:83:LEU:HD11 | 13:2V:161:ARG:HG3 | 1.86 | 0.57 |
| 15:3H:82:GLU:HB2 | 17:3P:275:ARG:NH2 | 2.19 | 0.57 |
| 17:3O:393:LEU:HB3 | 17:3R:283:TYR:HE2 | 1.70 | 0.57 |
| 21:4F:248:ILE:HG22 | 21:4F:261:THR:HG22 | 1.87 | 0.57 |
| 23:4N:233:SER:N | 23:4N:246:TYR:HH | 2.01 | 0.57 |
| 23:4N:250:VAL:HG21 | 23:4N:265:THR:HG22 | 1.85 | 0.57 |
| 23:4P:233:SER:N | 23:4P:246:TYR:HH | 2.01 | 0.57 |
| 28:5B:163:PRO:HG2 | 40:JH:26:LEU:HD21 | 1.85 | 0.57 |
| 41:AB:170:VAL:HG21 | 41:AB:377:LEU:HD11 | 1.86 | 0.57 |
| 40:AH:326:LYS:NZ | 40:AH:327:ASP:OD1 | 2.37 | 0.57 |
| 41:AP:292:GLN:O | 41:AP:298:ASN:ND2 | 2.37 | 0.57 |
| 40:BE:260:VAL:HG13 | 40:BE:266:HIS:HB3 | 1.87 | 0.57 |
| 40:BF:213:CYS:HA | 40:BF:217:LEU:HB2 | 1.85 | 0.57 |
| 40:CH:180:ALA:HB3 | 40:CH:183:GLU:HG3 | 1.87 | 0.57 |
| 41:CO:4:ILE:HD13 | 41:CO:131:GLN:HB3 | 1.86 | 0.57 |
| 41:CO:268:PRO:HA | 41:CO:368:ILE:HD12 | 1.85 | 0.57 |
| 40:DA:181:VAL:HG22 | 41:DN:256:ASN:HB3 | 1.86 | 0.57 |
| 40:DA:350:GLY:CA | 41:DB:179:VAL:HG22 | 2.33 | 0.57 |
| 40:DI:246:GLY:HA2 | 40:DI:357:TYR:CD2 | 2.39 | 0.57 |
| 41:EP:129:CYS:O | 41:EP:130:LEU:C | 2.42 | 0.57 |
| 40:FG:209:ILE:HA | 40:FG:212:ILE:HG22 | 1.85 | 0.57 |
| 41:FO:424:THR:OG1 | 41:FO:425:ARG:NH1 | 2.37 | 0.57 |
| 40:GA:259:LEU:HD11 | 40:GA:316:CYS:HB2 | 1.87 | 0.57 |
| 40:GE:88:HIS:O | 40:GE:90:GLU:N | 2.37 | 0.57 |
| 40:HA:7:VAL:HB | 40:HA:137:ILE:HG22 | 1.86 | 0.57 |
| 40:IA:133:GLN:NE2 | 40:IA:251:ASP:OD2 | 2.35 | 0.57 |
| 41:IB:237:THR:O | 41:IB:241:ARG:NH1 | 2.34 | 0.57 |
| 40:IF:72:PRO:HB2 | 41:IM:46:ARG:HH12 | 1.70 | 0.57 |
| 40:IH:76:ASP:HA | 40:IH:79:ARG:HG2 | 1.85 | 0.57 |
| 40:II:90:GLU:HG3 | 40:II:121:ARG:HD3 | 1.86 | 0.57 |
| 40:JA:128:GLN:HE21 | 40:KA:290:GLU:HG3 | 1.69 | 0.57 |
| 41:JB:198:GLU:HG3 | 41:JB:266:PHE:CE2 | 2.39 | 0.57 |
| 40:KH:141:PHE:HB2 | 40:KH:173:PRO:HD3 | 1.86 | 0.57 |
| 40:MG:187:SER:HB2 | 40:MG:390:LEU:HD21 | 1.86 | 0.57 |
| 40:MG:273:ALA:CB | 40:MG:374:VAL:HG22 | 2.35 | 0.57 |
| 41:NB:134:GLN:HA | 41:NB:165:ASN:O | 2.03 | 0.57 |
| 41:NB:296:ALA:HB1 | 41:NB:305:PRO:HD2 | 1.86 | 0.57 |
| 40:NH:221:ARG:NH1 | 41:NO:325:GLU:OE2 | 2.36 | 0.57 |
| 41:NN:105:HIS:CD2 | 41:NN:150:LEU:HB2 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:PA:335:ILE:HD11 | 40:PA:341:ILE:HD13 | 1.86 | 0.57 |
| 40:PE:211:ASP:OD1 | 40:PE:214:ARG:NH1 | 2.37 | 0.57 |
| 41:PM:7:LEU:O | 41:PM:135:LEU:HA | 2.05 | 0.57 |
| 41:QB:249:ASP:H | 41:QB:252:LYS:HB3 | 1.69 | 0.57 |
| 41:QM:24:ILE:HG23 | 41:QM:241:ARG:HH22 | 1.70 | 0.57 |
| 41:RO:313:VAL:O | 41:RO:349:VAL:HA | 2.04 | 0.57 |
| 41:RO:372:THR:OG1 | 41:RO:422:VAL:O | 2.21 | 0.57 |
| 40:SG:88:HIS:HD2 | 40:TG:283:HIS:HB2 | 1.69 | 0.57 |
| 41:SO:70:PRO:HG3 | 41:SO:94:GLN:HG3 | 1.85 | 0.57 |
| 41:SO:417:ASP:O | 41:SO:420:ASN:N | 2.33 | 0.57 |
| 40:TE:16:ILE:HG13 | 40:TE:228:ASN:HD22 | 1.68 | 0.57 |
| 41:TP:73:MET:HA | 41:TP:76:VAL:HG12 | 1.87 | 0.57 |
| 41:UB:130:LEU:O | 41:UB:162:ARG:NH1 | 2.37 | 0.57 |
| 40:UE:174:ALA:HB3 | 40:UE:178:SER:H | 1.70 | 0.57 |
| 40:UH:226:ASN:ND2 | 40:UH:366:ASP:OD2 | 2.36 | 0.57 |
| 40:UH:306:ASP:OD2 | 40:UH:308:ARG:NH2 | 2.34 | 0.57 |
| 40:VJ:51:THR:HG21 | 40:VJ:243:ARG:HG2 | 1.85 | 0.57 |
| 40:WG:332:ILE:HG23 | 40:WG:351:PHE:HD2 | 1.69 | 0.57 |
| 40:WI:258:ASN:OD1 | 41:WQ:99:ASN:ND2 | 2.37 | 0.57 |
| 41:WM:12:CYS:SG | 41:WM:13:GLY:N | 2.77 | 0.57 |
| 41:WN:142:GLY:O | 41:WN:144:GLY:N | 2.37 | 0.57 |
| 8:1Z:356:GLN:OE1 | 8:1Z:360:ARG:NH1 | 2.38 | 0.57 |
| 13:2T:54:VAL:HG21 | 13:2T:86:TYR:HB2 | 1.85 | 0.57 |
| 19:3Z:364:ILE:HG21 | 41:LP:320:ARG:HH22 | 1.70 | 0.57 |
| 20:4A:87:ARG:HA | 20:4A:90:ARG:HE | 1.69 | 0.57 |
| 21:4D:301:LEU:HD11 | 21:4D:315:ILE:HD11 | 1.86 | 0.57 |
| 23:4R:20:PRO:HD2 | 40:BI:89:PRO:HB3 | 1.87 | 0.57 |
| 23:4R:109:CYS:HB2 | 23:4R:113:TRP:CZ2 | 2.40 | 0.57 |
| 26:4V:140:HIS:CE1 | 26:4V:143:ARG:HH21 | 2.22 | 0.57 |
| 31:5I:507:MET:HG2 | 41:IP:227:HIS:HB3 | 1.86 | 0.57 |
| 36:5X:258:ARG:HH12 | 40:LF:440:GLU:HA | 1.70 | 0.57 |
| 38:6C:48:PRO:HB3 | 41:VO:333:VAL:HG22 | 1.85 | 0.57 |
| 39:6J:66:ARG:NH2 | 41:OM:38:GLY:O | 2.37 | 0.57 |
| 41:AP:117:LEU:HA | 41:AP:120:VAL:HG12 | 1.85 | 0.57 |
| 41:BL:87:PRO:HD3 | 41:CL:281:TYR:HD2 | 1.70 | 0.57 |
| 40:DE:159:VAL:O | 40:DE:160:ASP:C | 2.42 | 0.57 |
| 40:DE:264:ARG:O | 40:DE:265:ILE:C | 2.43 | 0.57 |
| 40:DH:202:PHE:HE1 | 40:DH:377:LEU:HB3 | 1.69 | 0.57 |
| 41:DM:173:PRO:O | 41:DM:174:LYS:C | 2.43 | 0.57 |
| 41:DM:200:TYR:O | 41:DM:201:CYS:C | 2.43 | 0.57 |
| 41:DO:271:ALA:HB1 | 41:DO:292:GLN:HG3 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EI:415:GLY:O | 40:EI:416:GLU:C | 2.43 | 0.57 |
| 41:EM:167:PHE:CZ | 41:EM:236:VAL:HG11 | 2.38 | 0.57 |
| 41:EP:30:ILE:HG23 | 41:EP:34:GLY:HA2 | 1.86 | 0.57 |
| 40:FH:222:PRO:O | 41:FO:322:SER:OG | 2.23 | 0.57 |
| 41:FO:211:CYS:O | 41:FO:217:LEU:N | 2.35 | 0.57 |
| 41:FP:221:THR:HG23 | 41:FP:223:GLY:H | 1.69 | 0.57 |
| 40:GA:70:LEU:HD23 | 40:GA:114:LEU:HD12 | 1.87 | 0.57 |
| 41:HB:191:GLN:O | 41:HB:195:ASN:ND2 | 2.38 | 0.57 |
| 41:HB:237:THR:O | 41:HB:241:ARG:NH1 | 2.38 | 0.57 |
| 40:HF:73:THR:HA | 40:HF:76:ASP:HB2 | 1.84 | 0.57 |
| 41:IQ:399:THR:HA | 41:IQ:403:MET:HB2 | 1.85 | 0.57 |
| 41:KL:323:MET:SD | 41:KL:353:VAL:HG21 | 2.44 | 0.57 |
| 40:LA:180:ALA:HB3 | 40:LA:183:GLU:HG3 | 1.85 | 0.57 |
| 41:LB:232:THR:HG21 | 41:LB:268:PRO:HB2 | 1.85 | 0.57 |
| 40:LG:273:ALA:HB1 | 40:LG:274:PRO:CD | 2.31 | 0.57 |
| 41:LL:412:GLU:OE2 | 41:LL:416:ASN:ND2 | 2.37 | 0.57 |
| 40:MD:228:ASN:HA | 40:MD:231:ILE:HB | 1.87 | 0.57 |
| 41:MP:6:HIS:O | 41:MP:63:ALA:HA | 2.05 | 0.57 |
| 40:NE:238:ILE:HD12 | 40:NE:377:LEU:HD11 | 1.86 | 0.57 |
| 40:NF:15:GLN:NE2 | 42:NM:501:GTP:O6 | 2.36 | 0.57 |
| 40:NH:318:LEU:O | 40:NH:374:VAL:HA | 2.05 | 0.57 |
| 41:OB:24:ILE:HA | 41:OB:27:GLU:HB2 | 1.86 | 0.57 |
| 40:OF:65:ALA:O | 40:OF:91:GLN:NE2 | 2.37 | 0.57 |
| 40:OF:70:LEU:HD23 | 40:OF:145:THR:HG23 | 1.86 | 0.57 |
| 41:OL:350:LYS:HE3 | 41:OL:352:ALA:HB2 | 1.87 | 0.57 |
| 41:OM:187:LEU:O | 41:OM:191:GLN:NE2 | 2.33 | 0.57 |
| 40:PA:98:ASP:O | 40:PA:105:ARG:NH2 | 2.27 | 0.57 |
| 40:PE:217:LEU:HB3 | 40:PE:219:ILE:HD12 | 1.86 | 0.57 |
| 40:QF:53:PHE:HB3 | 40:QF:61:HIS:HB3 | 1.86 | 0.57 |
| 41:QL:164:MET:O | 41:QL:196:THR:OG1 | 2.21 | 0.57 |
| 41:QP:67:ASP:HA | 41:QP:143:THR:CG2 | 2.35 | 0.57 |
| 41:RM:7:LEU:HG | 41:RM:64:VAL:HB | 1.87 | 0.57 |
| 41:RN:362:LYS:HG3 | 41:RN:363:MET:HG2 | 1.85 | 0.57 |
| 40:SI:88:HIS:CE1 | 40:TI:280:LYS:HG3 | 2.39 | 0.57 |
| 41:SL:21:TRP:HA | 41:SL:24:ILE:HG12 | 1.86 | 0.57 |
| 41:SP:375:GLN:HE21 | 41:SP:379:LYS:HG3 | 1.69 | 0.57 |
| 41:TM:139:LEU:HG | 41:TM:168:SER:HB3 | 1.85 | 0.57 |
| 40:UF:221:ARG:HB2 | 41:UM:322:SER:CB | 2.34 | 0.57 |
| 40:VI:11:GLN:OE1 | 42:VP:501:GTP:N7 | 2.38 | 0.57 |
| 40:VJ:55:GLU:O | 40:WI:285:GLN:NE2 | 2.37 | 0.57 |
| 41:WB:238:THR:HG21 | 41:WB:318:ARG:HG2 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:WF:70:LEU:HD23 | 40:WF:114:LEU:HD22 | 1.87 | 0.57 |
| 41:WM:137:HIS:HE1 | 41:WM:192:LEU:HD11 | 1.68 | 0.57 |
| 8:1Y:104:PRO:CG | 11:2J:253:ALA:HB3 | 2.34 | 0.57 |
| 12:2O:78:ARG:NH2 | 13:2X:149:ILE:O | 2.37 | 0.57 |
| 18:3U:162:ARG:HH11 | 18:3U:307:ARG:HH21 | 1.52 | 0.57 |
| 18:3V:116:GLU:OE1 | 18:3V:119:ARG:NH2 | 2.36 | 0.57 |
| 23:4M:91:ILE:CD1 | 40:AG:79:ARG:HB2 | 2.34 | 0.57 |
| 23:4R:188:THR:HG23 | 40:CI:79:ARG:HH12 | 1.70 | 0.57 |
| 28:5B:33:LEU:HA | 41:IO:122:LYS:HZ2 | 1.70 | 0.57 |
| 36:5Y:96:GLU:O | 41:OO:276:ARG:NH1 | 2.37 | 0.57 |
| 40:BA:241:SER:OG | 40:BA:250:VAL:O | 2.20 | 0.57 |
| 41:BB:99:ASN:HA | 41:BB:142:GLY:HA3 | 1.85 | 0.57 |
| 41:BB:273:LEU:HB2 | 41:BB:292:GLN:HE22 | 1.69 | 0.57 |
| 40:BE:100:ALA:O | 40:BE:101:ASN:C | 2.43 | 0.57 |
| 40:BG:319:TYR:HB3 | 40:BG:323:VAL:HG21 | 1.85 | 0.57 |
| 40:BH:258:ASN:O | 41:BP:179:VAL:HG21 | 2.04 | 0.57 |
| 41:BL:121:ARG:NH1 | 41:BL:158:GLU:OE1 | 2.38 | 0.57 |
| 41:BL:421:PRO:HA | 41:BL:424:THR:HG22 | 1.86 | 0.57 |
| 41:CB:46:ARG:NH2 | 40:CG:76:ASP:OD2 | 2.36 | 0.57 |
| 40:CI:101:ASN:OD1 | 40:CI:186:ASN:ND2 | 2.38 | 0.57 |
| 41:CP:309:ARG:O | 41:CP:310:TYR:C | 2.43 | 0.57 |
| 40:DE:146:GLY:O | 40:DE:147:SER:C | 2.42 | 0.57 |
| 40:DF:252:LEU:HD23 | 40:DF:255:PHE:HE2 | 1.69 | 0.57 |
| 40:DH:231:ILE:HA | 40:DH:234:ILE:HD12 | 1.85 | 0.57 |
| 40:EF:76:ASP:OD1 | 40:EF:79:ARG:NH1 | 2.37 | 0.57 |
| 40:EI:258:ASN:HB3 | 40:EI:352:LYS:HD2 | 1.87 | 0.57 |
| 40:FF:141:PHE:HB2 | 40:FF:173:PRO:HD3 | 1.86 | 0.57 |
| 40:FF:225:THR:O | 40:FF:229:ARG:HB2 | 2.04 | 0.57 |
| 41:FN:8:GLN:HE21 | 41:FN:14:ASN:HA | 1.68 | 0.57 |
| 40:GE:104:ALA:HA | 40:GE:108:TYR:HD2 | 1.70 | 0.57 |
| 40:GF:316:CYS:HA | 40:GF:352:LYS:HB2 | 1.86 | 0.57 |
| 41:GM:193:VAL:HG21 | 41:GM:418:LEU:HD21 | 1.86 | 0.57 |
| 41:GM:341:PHE:HB3 | 41:GM:348:ASN:HD21 | 1.70 | 0.57 |
| 41:GO:45:GLU:OE2 | 41:GO:46:ARG:NH1 | 2.36 | 0.57 |
| 40:HI:141:PHE:HB2 | 40:HI:173:PRO:HD3 | 1.86 | 0.57 |
| 41:HN:158:GLU:O | 41:HN:159:TYR:C | 2.42 | 0.57 |
| 41:IB:325:GLU:O | 41:IB:329:GLN:HB2 | 2.04 | 0.57 |
| 40:JA:319:TYR:HB2 | 40:JA:355:ILE:HG22 | 1.86 | 0.57 |
| 40:JH:246:GLY:HA3 | 40:JH:356:ASN:HA | 1.86 | 0.57 |
| 41:JN:313:VAL:HG13 | 41:JN:367:PHE:HE1 | 1.68 | 0.57 |
| 40:KG:236:SER:O | 40:KG:240:ALA:HB2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KN:95:SER:OG | 41:KN:96:GLY:N | 2.38 | 0.57 |
| 40:LA:139:HIS:O | 40:LA:170:SER:HA | 2.05 | 0.57 |
| 40:MF:326:LYS:O | 40:MF:327:ASP:C | 2.42 | 0.57 |
| 40:MF:400:LYS:O | 40:MF:401:ARG:C | 2.43 | 0.57 |
| 40:MG:11:GLN:HB2 | 40:MG:74:VAL:HG21 | 1.85 | 0.57 |
| 41:MP:7:LEU:HB2 | 41:MP:135:LEU:HD12 | 1.87 | 0.57 |
| 40:ND:273:ALA:HB1 | 40:ND:274:PRO:CD | 2.30 | 0.57 |
| 41:NP:118:ASP:OD1 | 41:NP:121:ARG:NH1 | 2.37 | 0.57 |
| 40:OD:99:ALA:HA | 40:OD:105:ARG:HG2 | 1.87 | 0.57 |
| 40:OG:139:HIS:ND1 | 40:OG:140:SER:O | 2.37 | 0.57 |
| 41:OP:232:THR:HG21 | 41:OP:268:PRO:HB2 | 1.86 | 0.57 |
| 40:PA:236:SER:O | 40:PA:240:ALA:HB2 | 2.05 | 0.57 |
| 40:PD:140:SER:HA | 40:PD:171:ILE:H | 1.70 | 0.57 |
| 40:PE:68:VAL:HG11 | 40:PE:118:VAL:HG22 | 1.87 | 0.57 |
| 40:QG:319:TYR:HB3 | 40:QG:323:VAL:HG11 | 1.87 | 0.57 |
| 40:QG:394:PHE:HD2 | 40:QG:421:ARG:HD3 | 1.69 | 0.57 |
| 40:RF:15:GLN:OE1 | 40:RF:228:ASN:ND2 | 2.38 | 0.57 |
| 40:RH:191:THR:O | 40:RH:195:LEU:HB2 | 2.05 | 0.57 |
| 41:RN:7:LEU:O | 41:RN:135:LEU:HA | 2.05 | 0.57 |
| 41:RO:48:ASN:OD1 | 41:RO:62:ARG:NH2 | 2.38 | 0.57 |
| 40:UE:2:ARG:HA | 40:UE:133:GLN:HE22 | 1.69 | 0.57 |
| 41:UM:375:GLN:HE21 | 41:UM:423:VAL:HG23 | 1.70 | 0.57 |
| 40:WA:393:LYS:HE3 | 41:WN:346:PRO:HB2 | 1.86 | 0.57 |
| 40:WF:16:ILE:HA | 40:WF:228:ASN:HB3 | 1.86 | 0.57 |
| 40:WF:349:THR:HG21 | 41:WN:182:PRO:HD3 | 1.87 | 0.57 |
| 41:WN:7:LEU:HB2 | 41:WN:135:LEU:HD13 | 1.86 | 0.57 |
| 13:2T:115:LYS:HB3 | 13:2T:116:PRO:HD2 | 1.86 | 0.57 |
| 13:2U:2:PHE:HZ | 13:2U:11:LEU:HD11 | 1.68 | 0.57 |
| 14:3B:46:ARG:HH22 | 40:MD:264:ARG:NE | 2.03 | 0.57 |
| 16:3M:203:ILE:HG13 | 18:3V:121:VAL:HG11 | 1.86 | 0.57 |
| 17:3R:183:ARG:NH2 | 17:3R:187:GLU:HB3 | 2.20 | 0.57 |
| 21:4D:475:PRO:HD2 | 21:4D:483:ILE:CG2 | 2.33 | 0.57 |
| 21:4F:444:LEU:HD21 | 21:4F:515:TYR:CZ | 2.40 | 0.57 |
| 21:4F:484:TYR:O | 21:4F:486:GLY:N | 2.37 | 0.57 |
| 21:4F:491:PHE:HD2 | 21:4F:494:ALA:HB2 | 1.68 | 0.57 |
| 26:4W:193:ARG:NH2 | 26:4W:205:ALA:O | 2.36 | 0.57 |
| 39:6J:61:ASN:HA | 41:OM:56:GLY:HA2 | 1.86 | 0.57 |
| 40:BG:248:LEU:HD13 | 40:BG:355:ILE:HD12 | 1.85 | 0.57 |
| 41:BM:211:CYS:HA | 41:BM:215:LEU:HB2 | 1.87 | 0.57 |
| 41:CB:113:VAL:HG21 | 41:CB:150:LEU:HD23 | 1.86 | 0.57 |
| 40:CF:292:THR:HG22 | 40:CF:335:ILE:HD11 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CI:20:CYS:HA | 40:CI:232:SER:HB2 | 1.87 | 0.57 |
| 41:CL:245:GLN:O | 41:CL:246:LEU:C | 2.42 | 0.57 |
| 41:CN:129:CYS:O | 41:CN:130:LEU:C | 2.43 | 0.57 |
| 40:EF:208:ALA:HB2 | 40:EF:304:LYS:HG2 | 1.85 | 0.57 |
| 40:EH:100:ALA:O | 41:EO:255:VAL:HG11 | 2.03 | 0.57 |
| 40:FF:318:LEU:HB2 | 40:FF:375:CYS:HB3 | 1.85 | 0.57 |
| 41:FP:178:THR:HG22 | 41:FP:180:VAL:H | 1.69 | 0.57 |
| 40:GA:16:ILE:HA | 40:GA:228:ASN:ND2 | 2.20 | 0.57 |
| 40:GI:288:VAL:O | 40:GI:291:ILE:HG12 | 2.05 | 0.57 |
| 40:HE:258:ASN:HD21 | 41:HM:99:ASN:HD21 | 1.52 | 0.57 |
| 40:IF:276:ILE:HD12 | 40:IF:281:ALA:HA | 1.86 | 0.57 |
| 41:IM:139:LEU:HD12 | 41:IM:170:VAL:HG12 | 1.86 | 0.57 |
| 41:IM:248:ALA:HA | 41:IM:252:LYS:HD2 | 1.86 | 0.57 |
| 40:KH:219:ILE:HG13 | 40:KH:222:PRO:HG3 | 1.87 | 0.57 |
| 41:KL:305:PRO:O | 41:KL:308:GLY:N | 2.37 | 0.57 |
| 40:LD:154:MET:HE3 | 40:LD:166:LYS:HD2 | 1.86 | 0.57 |
| 40:LF:100:ALA:O | 40:LF:101:ASN:C | 2.42 | 0.57 |
| 41:LP:314:ALA:HB3 | 41:LP:368:ILE:HB | 1.86 | 0.57 |
| 40:MD:224:TYR:HE2 | 42:MD:501:GTP:H2' | 1.70 | 0.57 |
| 40:NG:205:ASP:HB2 | 40:NG:303:VAL:HG22 | 1.84 | 0.57 |
| 40:NH:332:ILE:HG23 | 40:NH:351:PHE:HD2 | 1.68 | 0.57 |
| 41:OB:19:LYS:HE2 | 41:OB:223:GLY:HA2 | 1.87 | 0.57 |
| 40:OE:391:ASP:HB3 | 40:OE:421:ARG:HH12 | 1.69 | 0.57 |
| 40:OH:100:ALA:O | 40:OH:101:ASN:C | 2.42 | 0.57 |
| 40:OH:213:CYS:HA | 40:OH:217:LEU:HG | 1.87 | 0.57 |
| 41:OM:107:THR:O | 41:OM:110:ALA:N | 2.37 | 0.57 |
| 40:PA:286:LEU:O | 40:PA:372:ARG:NH1 | 2.37 | 0.57 |
| 40:PH:260:VAL:HG13 | 41:PP:397:TRP:HE1 | 1.70 | 0.57 |
| 41:PN:8:GLN:HE21 | 41:PN:65:LEU:HG | 1.68 | 0.57 |
| 41:PO:2:ARG:HD2 | 41:PO:240:LEU:HB2 | 1.86 | 0.57 |
| 40:QA:60:LYS:HD2 | 40:RA:283:HIS:HA | 1.86 | 0.57 |
| 40:QH:228:ASN:HD21 | 42:QO:501:GTP:HN1 | 1.51 | 0.57 |
| 41:QP:246:LEU:O | 41:QP:352:ALA:HA | 2.05 | 0.57 |
| 40:RF:358:GLN:NE2 | 40:RF:359:PRO:O | 2.33 | 0.57 |
| 40:RI:90:GLU:OE1 | 40:SI:280:LYS:NZ | 2.36 | 0.57 |
| 40:SA:11:GLN:O | 40:SA:15:GLN:NE2 | 2.38 | 0.57 |
| 40:SE:20:CYS:HG | 40:SE:24:TYR:HE2 | 1.53 | 0.57 |
| 40:SE:91:GLN:HE22 | 40:SE:125:LEU:HD21 | 1.69 | 0.57 |
| 40:SE:202:PHE:HE2 | 40:SE:238:ILE:HG12 | 1.70 | 0.57 |
| 40:SF:238:ILE:HG23 | 40:SF:239:THR:HG23 | 1.86 | 0.57 |
| 41:TB:73:MET:HA | 41:TB:76:VAL:HG12 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UF:100:ALA:O | 40:UF:101:ASN:C | 2.43 | 0.57 |
| 40:UF:204:VAL:HG22 | 40:UF:209:ILE:HD11 | 1.87 | 0.57 |
| 40:UF:274:PRO:O | 40:UF:276:ILE:N | 2.37 | 0.57 |
| 40:UH:136:LEU:HD11 | 40:UH:239:THR:HG21 | 1.87 | 0.57 |
| 41:UP:165:ASN:HB3 | 41:UP:200:TYR:HE2 | 1.68 | 0.57 |
| 40:VI:318:LEU:O | 40:VI:374:VAL:HA | 2.05 | 0.57 |
| 40:WG:407:TYR:HB3 | 40:WG:412:MET:HG3 | 1.87 | 0.57 |
| 40:WI:154:MET:HG3 | 40:WI:194:THR:HG23 | 1.86 | 0.57 |
| 8:1X:104:PRO:HA | 11:2I:253:ALA:HB3 | 1.86 | 0.57 |
| 11:2J:88:VAL:HB | 11:2J:92:THR:HG21 | 1.87 | 0.57 |
| 21:4E:440:LEU:HD11 | 21:4E:449:ILE:HG12 | 1.86 | 0.57 |
| 23:4P:250:VAL:HG21 | 23:4P:265:THR:HG22 | 1.85 | 0.57 |
| 29:5D:97:ASN:HD21 | 41:HQ:297:LYS:HG2 | 1.69 | 0.57 |
| 41:BB:44:LEU:O | 41:BB:45:GLU:C | 2.43 | 0.57 |
| 40:CH:102:ASN:HB3 | 40:CH:105:ARG:HG3 | 1.87 | 0.57 |
| 40:CH:328:VAL:HG11 | 40:CH:353:VAL:CG1 | 2.34 | 0.57 |
| 41:CL:141:GLY:HA3 | 43:CL:501:GDP:O1A | 2.05 | 0.57 |
| 41:CO:11:GLN:N | 43:CO:501:GDP:O2B | 2.38 | 0.57 |
| 41:DB:113:VAL:HG12 | 41:DB:147:MET:HG3 | 1.85 | 0.57 |
| 41:DB:218:THR:O | 41:DB:220:PRO:HD3 | 2.04 | 0.57 |
| 40:DF:261:PRO:HG3 | 40:DF:313:MET:SD | 2.45 | 0.57 |
| 41:DL:245:GLN:O | 41:DL:246:LEU:C | 2.42 | 0.57 |
| 41:DM:109:GLY:HA2 | 41:DM:147:MET:HE2 | 1.86 | 0.57 |
| 41:DP:419:GLY:O | 41:DP:423:VAL:HG13 | 2.04 | 0.57 |
| 40:EA:70:LEU:HB2 | 40:EA:145:THR:HG22 | 1.87 | 0.57 |
| 40:EH:177:VAL:HG12 | 41:EO:327:ASP:HB3 | 1.86 | 0.57 |
| 40:FA:109:THR:O | 40:FA:111:GLY:N | 2.38 | 0.57 |
| 41:FN:100:ASN:HB2 | 41:FN:103:LYS:HB2 | 1.87 | 0.57 |
| 41:GO:2:ARG:NH1 | 41:GO:249:ASP:OD2 | 2.34 | 0.57 |
| 41:HN:108:GLU:HG3 | 41:HN:109:GLY:N | 2.20 | 0.57 |
| 40:II:262:TYR:OH | 41:IQ:391:ARG:NH1 | 2.38 | 0.57 |
| 40:JH:90:GLU:O | 40:JH:121:ARG:NH1 | 2.38 | 0.57 |
| 40:JH:128:GLN:NE2 | 40:KH:290:GLU:OE2 | 2.38 | 0.57 |
| 40:JH:278:ALA:H | 40:JH:368:ALA:HB2 | 1.70 | 0.57 |
| 41:JM:69:GLU:O | 41:JM:71:GLY:N | 2.38 | 0.57 |
| 41:KB:237:THR:O | 41:KB:241:ARG:NH1 | 2.38 | 0.57 |
| 41:KM:318:ARG:HD3 | 41:KM:358:PRO:HD3 | 1.85 | 0.57 |
| 41:MO:116:VAL:HG11 | 41:MO:151:LEU:HD11 | 1.85 | 0.57 |
| 40:NF:401:ARG:NH1 | 40:NF:414:GLU:OE2 | 2.36 | 0.57 |
| 40:OH:109:THR:OG1 | 40:OH:410:GLU:HB3 | 2.05 | 0.57 |
| 40:OH:222:PRO:HB2 | 41:OO:324:LYS:HD3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QB:259:PRO:O | 40:QG:405:HIS:NE2 | 2.38 | 0.57 |
| 41:QP:144:GLY:O | 41:QP:145:SER:C | 2.43 | 0.57 |
| 40:SG:73:THR:HA | 40:SG:76:ASP:HB3 | 1.87 | 0.57 |
| 40:TA:229:ARG:HD3 | 40:TA:363:VAL:HG11 | 1.86 | 0.57 |
| 41:TP:317:PHE:HB2 | 41:TP:353:VAL:HG12 | 1.86 | 0.57 |
| 40:UE:298:PRO:HB3 | 40:UE:307:PRO:HD2 | 1.85 | 0.57 |
| 40:UE:326:LYS:HG2 | 41:UM:220:PRO:HD2 | 1.87 | 0.57 |
| 40:VA:267:PHE:HE2 | 40:VA:427:LEU:HD21 | 1.70 | 0.57 |
| 41:VB:348:ASN:HA | 40:VH:181:VAL:HG12 | 1.87 | 0.57 |
| 41:WB:377:LEU:HD23 | 41:WB:380:ARG:HH12 | 1.68 | 0.57 |
| 8:1Y:208:GLN:NE2 | 40:VF:367:LEU:O | 2.38 | 0.57 |
| 8:1Z:367:ILE:HG22 | 8:1Z:371:ARG:HH21 | 1.70 | 0.57 |
| 12:2P:204:ASN:HA | 12:2P:220:ASN:HD21 | 1.70 | 0.57 |
| 12:2R:70:THR:OG1 | 12:2R:118:GLU:OE2 | 2.21 | 0.57 |
| 13:2X:13:ILE:HG13 | 13:2X:25:TRP:CZ2 | 2.39 | 0.57 |
| 17:3P:157:LYS:HG3 | 17:3P:258:LEU:HD21 | 1.87 | 0.57 |
| 22:4J:676:ALA:O | 22:4J:677:LEU:C | 2.42 | 0.57 |
| 26:4W:178:PRO:O | 26:4W:193:ARG:NH1 | 2.37 | 0.57 |
| 38:6D:295:ARG:NH2 | 41:UM:41:ASP:OD2 | 2.37 | 0.57 |
| 40:BE:174:ALA:HB1 | 40:BE:175:PRO:HD2 | 1.85 | 0.57 |
| 41:BO:288:GLU:HG3 | 41:BO:289:LEU:N | 2.20 | 0.57 |
| 40:CG:248:LEU:HB2 | 40:CG:355:ILE:H | 1.69 | 0.57 |
| 40:CI:121:ARG:HE | 40:CI:124:LYS:HD2 | 1.69 | 0.57 |
| 41:CM:213:ARG:O | 41:CM:214:THR:C | 2.44 | 0.57 |
| 41:CN:100:ASN:O | 41:CN:101:TRP:C | 2.43 | 0.57 |
| 41:CP:139:LEU:HD23 | 41:CP:185:ALA:HA | 1.87 | 0.57 |
| 40:DH:101:ASN:HB3 | 40:DH:182:VAL:HG21 | 1.87 | 0.57 |
| 41:DN:136:THR:HA | 41:DN:167:PHE:O | 2.04 | 0.57 |
| 41:DP:7:LEU:HB3 | 41:DP:135:LEU:HD12 | 1.86 | 0.57 |
| 40:EH:234:ILE:HD11 | 40:EH:272:TYR:HB2 | 1.87 | 0.57 |
| 40:EH:258:ASN:ND2 | 40:EH:352:LYS:HB2 | 2.20 | 0.57 |
| 41:EP:200:TYR:CE1 | 41:EP:236:VAL:HG21 | 2.39 | 0.57 |
| 40:FH:102:ASN:HB2 | 40:FH:105:ARG:HB2 | 1.86 | 0.57 |
| 40:FH:352:LYS:HD2 | 41:FP:179:VAL:HG13 | 1.87 | 0.57 |
| 41:FM:19:LYS:HG3 | 41:FM:226:ASN:HB2 | 1.87 | 0.57 |
| 41:FN:14:ASN:ND2 | 41:FN:67:ASP:OD2 | 2.37 | 0.57 |
| 40:GI:109:THR:O | 40:GI:111:GLY:N | 2.37 | 0.57 |
| 40:GI:394:PHE:HD2 | 40:GI:421:ARG:HD3 | 1.70 | 0.57 |
| 40:HE:122:ILE:HG12 | 40:HE:123:ARG:N | 2.20 | 0.57 |
| 41:HO:237:THR:HG22 | 41:HO:250:LEU:HD21 | 1.87 | 0.57 |
| 40:IE:324:VAL:HB | 40:IE:327:ASP:HB2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IF:212:ILE:HD11 | 40:IF:300:ASN:HA | 1.86 | 0.57 |
| 40:II:140:SER:OG | 42:II:501:GTP:O2A | 2.20 | 0.57 |
| 40:JD:235:VAL:HA | 40:JD:238:ILE:HG12 | 1.86 | 0.57 |
| 40:JH:64:ARG:NH1 | 40:JH:128:GLN:O | 2.37 | 0.57 |
| 41:JM:270:PHE:HB3 | 41:JM:273:LEU:HD11 | 1.87 | 0.57 |
| 41:KM:35:THR:HG23 | 41:KM:37:HIS:CE1 | 2.40 | 0.57 |
| 41:LN:421:PRO:HA | 41:LN:424:THR:HG22 | 1.87 | 0.57 |
| 40:ME:90:GLU:OE1 | 40:ME:121:ARG:NH2 | 2.37 | 0.57 |
| 40:MH:348:PRO:HD2 | 41:MP:388:MET:HG2 | 1.87 | 0.57 |
| 40:NF:217:LEU:HD12 | 40:NF:277:SER:HB3 | 1.87 | 0.57 |
| 40:NG:259:LEU:O | 40:NG:379:ASN:ND2 | 2.38 | 0.57 |
| 41:NM:63:ALA:O | 41:NM:89:ASN:ND2 | 2.37 | 0.57 |
| 40:OE:79:ARG:NH2 | 40:OE:92:LEU:O | 2.38 | 0.57 |
| 40:PE:319:TYR:HB3 | 40:PE:323:VAL:HG21 | 1.85 | 0.57 |
| 40:RE:101:ASN:O | 40:RE:186:ASN:ND2 | 2.38 | 0.57 |
| 40:TA:251:ASP:OD1 | 40:TA:252:LEU:N | 2.38 | 0.57 |
| 40:TE:398:TYR:O | 40:TE:401:ARG:NH1 | 2.38 | 0.57 |
| 40:TF:352:LYS:HD2 | 41:TN:179:VAL:HG13 | 1.86 | 0.57 |
| 40:TH:395:ASP:OD1 | 40:TH:421:ARG:NE | 2.31 | 0.57 |
| 40:UE:88:HIS:HD2 | 40:VF:283:HIS:HB2 | 1.69 | 0.57 |
| 40:UH:254:GLU:HG2 | 40:UH:352:LYS:HE3 | 1.86 | 0.57 |
| 40:UI:71:GLU:HB2 | 40:UI:98:ASP:HA | 1.86 | 0.57 |
| 40:VF:220:GLU:HG2 | 40:VF:221:ARG:HG2 | 1.86 | 0.57 |
| 40:VG:98:ASP:O | 40:VG:105:ARG:NH1 | 2.37 | 0.57 |
| 40:VJ:101:ASN:HD22 | 41:VQ:256:ASN:HD21 | 1.51 | 0.57 |
| 41:VP:273:LEU:O | 41:VP:292:GLN:NE2 | 2.38 | 0.57 |
| 41:WB:107:THR:O | 41:WB:110:ALA:N | 2.38 | 0.57 |
| 40:WE:319:TYR:HE2 | 40:WE:328:VAL:HG13 | 1.70 | 0.57 |
| 40:WF:238:ILE:HA | 40:WF:318:LEU:HD22 | 1.85 | 0.57 |
| 9:2B:245:GLN:NE2 | 9:2B:246:ASN:OD1 | 2.38 | 0.57 |
| 15:3F:198:ILE:HG12 | 15:3G:311:LYS:HB3 | 1.86 | 0.57 |
| 17:3R:163:GLU:HB3 | 17:3R:254:LEU:HD11 | 1.86 | 0.57 |
| 20:4A:93:LYS:HZ2 | 40:LF:58:ALA:HA | 1.70 | 0.57 |
| 21:4D:170:ARG:HE | 21:4D:201:LEU:HB3 | 1.68 | 0.57 |
| 21:4E:11:PHE:O | 41:LO:227:HIS:NE2 | 2.38 | 0.57 |
| 23:4P:234:ARG:O | 23:4P:235:THR:HB | 2.05 | 0.57 |
| 32:5L:98:VAL:H | 32:5L:101:LEU:HD13 | 1.70 | 0.57 |
| 41:AL:318:ARG:HD3 | 41:AL:358:PRO:HD3 | 1.87 | 0.57 |
| 41:AO:215:LEU:O | 41:AO:216:LYS:C | 2.42 | 0.57 |
| 41:BB:61:PRO:HG2 | 41:BB:84:ILE:HG23 | 1.85 | 0.57 |
| 41:BO:135:LEU:HD22 | 41:BO:152:ILE:HD11 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CA:45:GLY:O | 40:CA:47:ASP:N | 2.38 | 0.57 |
| 40:CE:335:ILE:HD13 | 40:CE:338:LYS:HZ1 | 1.67 | 0.57 |
| 41:CO:357:PRO:HG3 | 41:CO:362:LYS:HD2 | 1.85 | 0.57 |
| 40:DA:327:ASP:O | 40:DA:328:VAL:C | 2.43 | 0.57 |
| 40:DE:5:ILE:HD13 | 40:DE:64:ARG:HB3 | 1.86 | 0.57 |
| 40:DE:104:ALA:C | 40:DE:106:GLY:H | 2.07 | 0.57 |
| 40:DE:400:LYS:O | 40:DE:401:ARG:C | 2.43 | 0.57 |
| 40:DH:21:TRP:CZ3 | 40:DH:63:PRO:HB3 | 2.40 | 0.57 |
| 40:EG:55:GLU:OE2 | 40:EG:61:HIS:NE2 | 2.37 | 0.57 |
| 40:EG:238:ILE:HA | 40:EG:318:LEU:HD22 | 1.85 | 0.57 |
| 41:EL:292:GLN:O | 41:EL:298:ASN:ND2 | 2.36 | 0.57 |
| 41:EM:87:PRO:O | 41:EM:88:ASP:C | 2.42 | 0.57 |
| 40:FA:285:GLN:O | 40:FA:286:LEU:C | 2.43 | 0.57 |
| 40:FF:257:THR:HA | 41:FN:397:TRP:HZ3 | 1.69 | 0.57 |
| 40:FG:401:ARG:HG3 | 40:FG:404:VAL:HG11 | 1.86 | 0.57 |
| 40:FI:72:PRO:HB2 | 41:FP:46:ARG:HH12 | 1.69 | 0.57 |
| 40:FI:222:PRO:HD2 | 41:FP:324:LYS:HB2 | 1.85 | 0.57 |
| 41:FO:178:THR:HB | 41:FO:181:GLU:HB3 | 1.85 | 0.57 |
| 40:GE:50:ASN:O | 40:GE:51:THR:C | 2.43 | 0.57 |
| 40:GF:238:ILE:HA | 40:GF:318:LEU:HD22 | 1.87 | 0.57 |
| 40:GI:400:LYS:O | 40:GI:401:ARG:C | 2.42 | 0.57 |
| 40:IH:124:LYS:HE3 | 41:JB:282:ARG:HH12 | 1.69 | 0.57 |
| 41:IM:319:GLY:HA2 | 41:IM:357:PRO:HG3 | 1.86 | 0.57 |
| 41:JB:27:GLU:OE1 | 41:JB:318:ARG:NH2 | 2.29 | 0.57 |
| 41:JB:194:GLU:OE2 | 41:JB:262:ARG:NH1 | 2.37 | 0.57 |
| 40:JH:51:THR:HG23 | 40:JH:52:PHE:HD2 | 1.69 | 0.57 |
| 40:LE:206:ASN:OD1 | 42:LL:501:GTP:O2' | 2.22 | 0.57 |
| 40:LF:276:ILE:HG13 | 40:LF:286:LEU:HD21 | 1.87 | 0.57 |
| 40:LG:305:CYS:O | 40:LG:306:ASP:C | 2.43 | 0.57 |
| 41:LN:107:THR:O | 41:LN:110:ALA:N | 2.37 | 0.57 |
| 40:ME:206:ASN:OD1 | 42:ML:501:GTP:O2' | 2.23 | 0.57 |
| 41:MO:6:HIS:HD1 | 41:MO:21:TRP:HE1 | 1.53 | 0.57 |
| 41:NB:156:ARG:NH1 | 41:NB:195:ASN:O | 2.38 | 0.57 |
| 40:NF:306:ASP:OD2 | 40:NF:309:HIS:ND1 | 2.38 | 0.57 |
| 41:NP:139:LEU:HD12 | 41:NP:170:VAL:HG12 | 1.87 | 0.57 |
| 41:OB:232:THR:HG21 | 41:OB:268:PRO:HB2 | 1.86 | 0.57 |
| 40:OF:127:ASP:OD1 | 40:PF:293:ASN:ND2 | 2.38 | 0.57 |
| 41:OP:237:THR:HG22 | 41:OP:250:LEU:HD21 | 1.87 | 0.57 |
| 41:PB:64:VAL:HA | 41:PB:89:ASN:HB3 | 1.85 | 0.57 |
| 41:PL:236:VAL:HG13 | 41:PL:237:THR:HG23 | 1.86 | 0.57 |
| 41:PN:183:TYR:OH | 41:PN:393:ALA:O | 2.20 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PP:392:LYS:HB3 | 41:PP:395:LEU:HD13 | 1.87 | 0.57 |
| 41:QP:354:CYS:SG | 41:QP:355:ASP:N | 2.78 | 0.57 |
| 40:RG:73:THR:HA | 40:RG:76:ASP:HB2 | 1.86 | 0.57 |
| 41:RM:27:GLU:HA | 41:RM:359:ARG:HH21 | 1.70 | 0.57 |
| 41:RM:74:ASP:OD1 | 41:RM:77:ARG:NH2 | 2.38 | 0.57 |
| 41:RP:51:TYR:HB3 | 41:RP:59:TYR:HB3 | 1.86 | 0.57 |
| 40:SE:11:GLN:HG3 | 40:SE:74:VAL:HG11 | 1.86 | 0.57 |
| 40:SH:255:PHE:HZ | 40:SH:318:LEU:HD21 | 1.70 | 0.57 |
| 41:TB:253:LEU:O | 41:TB:257:MET:HB2 | 2.05 | 0.57 |
| 40:UA:115:ILE:HA | 40:UA:118:VAL:HG22 | 1.85 | 0.57 |
| 41:UM:10:GLY:O | 41:UM:14:ASN:ND2 | 2.38 | 0.57 |
| 40:VF:329:ASN:HB3 | 41:VN:175:VAL:HG11 | 1.86 | 0.57 |
| 41:VP:292:GLN:O | 41:VP:298:ASN:ND2 | 2.37 | 0.57 |
| 7:1S:586:HIS:ND1 | 7:1S:606:SER:HB2 | 2.20 | 0.56 |
| 7:1U:395:ASP:HB3 | 7:1U:397:LYS:HG3 | 1.85 | 0.56 |
| 11:2J:185:MET:SD | 11:2J:187:ARG:NH2 | 2.78 | 0.56 |
| 12:2N:197:LEU:HD13 | 12:2N:225:ILE:HG12 | 1.86 | 0.56 |
| 13:2U:11:LEU:HD22 | 13:2U:71:ILE:HD11 | 1.86 | 0.56 |
| 13:2W:69:LEU:O | 13:2W:70:GLY:C | 2.43 | 0.56 |
| 16:3L:140:GLU:OE2 | 16:3L:394:ARG:NH2 | 2.38 | 0.56 |
| 22:4I:277:LEU:HD12 | 41:CO:78:SER:HB2 | 1.88 | 0.56 |
| 22:4K:555:GLU:HB2 | 22:4K:591:VAL:HG22 | 1.86 | 0.56 |
| 26:4V:250:ILE:HG22 | 26:4V:255:LEU:HB2 | 1.86 | 0.56 |
| 27:4Y:252:LEU:O | 27:4Y:259:LYS:NZ | 2.38 | 0.56 |
| 39:6J:24:GLN:N | 41:OM:41:ASP:OD2 | 2.38 | 0.56 |
| 40:AG:139:HIS:NE2 | 40:AG:168:GLU:OE1 | 2.38 | 0.56 |
| 41:AO:14:ASN:HB3 | 41:AO:76:VAL:HG21 | 1.87 | 0.56 |
| 40:BG:101:ASN:HA | 40:BG:144:GLY:H | 1.69 | 0.56 |
| 41:BM:189:VAL:O | 41:BM:193:VAL:HG23 | 2.05 | 0.56 |
| 40:CH:400:LYS:O | 40:CH:401:ARG:C | 2.43 | 0.56 |
| 41:CP:141:GLY:HA3 | 43:CP:501:GDP:O1A | 2.05 | 0.56 |
| 40:DA:190:THR:O | 40:DA:191:THR:C | 2.43 | 0.56 |
| 40:DE:240:ALA:O | 40:DE:241:SER:C | 2.41 | 0.56 |
| 41:DN:130:LEU:O | 41:DN:131:GLN:C | 2.41 | 0.56 |
| 41:DN:391:ARG:O | 41:DN:392:LYS:C | 2.43 | 0.56 |
| 40:EI:70:LEU:HB2 | 40:EI:145:THR:OG1 | 2.05 | 0.56 |
| 40:EI:99:ALA:HB3 | 40:EI:144:GLY:HA3 | 1.88 | 0.56 |
| 41:EM:30:ILE:HG13 | 41:EM:59:TYR:HB2 | 1.87 | 0.56 |
| 40:GE:274:PRO:HG2 | 40:GE:373:ALA:HA | 1.86 | 0.56 |
| 40:HF:126:ALA:HA | 40:HF:129:CYS:HB3 | 1.85 | 0.56 |
| 40:IA:255:PHE:O | 40:IA:259:LEU:HB2 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IH:258:ASN:HD21 | 41:IP:179:VAL:H | 1.52 | 0.56 |
| 41:JB:1:MET:SD | 41:JB:48:ASN:ND2 | 2.78 | 0.56 |
| 41:KB:309:ARG:H | 41:KB:372:THR:HB | 1.70 | 0.56 |
| 40:KD:205:ASP:HB2 | 40:KD:303:VAL:HG23 | 1.87 | 0.56 |
| 40:KF:206:ASN:OD1 | 42:KM:501:GTP:O2' | 2.17 | 0.56 |
| 41:KO:210:ILE:HG12 | 41:KO:298:ASN:HA | 1.87 | 0.56 |
| 40:LA:70:LEU:HD23 | 40:LA:114:LEU:HD12 | 1.87 | 0.56 |
| 40:LA:138:PHE:HZ | 40:LA:235:VAL:HG21 | 1.69 | 0.56 |
| 41:LB:172:SER:OG | 41:LB:175:VAL:O | 2.23 | 0.56 |
| 40:LE:311:LYS:NZ | 40:LE:437:ASP:OD1 | 2.38 | 0.56 |
| 40:LH:73:THR:HA | 40:LH:76:ASP:HB2 | 1.86 | 0.56 |
| 40:ME:259:LEU:O | 40:ME:379:ASN:ND2 | 2.35 | 0.56 |
| 40:MH:214:ARG:HH22 | 41:MO:324:LYS:CG | 2.13 | 0.56 |
| 40:NH:178:SER:HG | 41:NO:347:ASN:HD22 | 1.53 | 0.56 |
| 41:NM:314:ALA:HB3 | 41:NM:368:ILE:HB | 1.87 | 0.56 |
| 40:PG:24:TYR:HE1 | 40:PG:243:ARG:HH22 | 1.53 | 0.56 |
| 41:PP:237:THR:HG22 | 41:PP:250:LEU:HD21 | 1.87 | 0.56 |
| 41:QL:51:TYR:HB3 | 41:QL:59:TYR:HB3 | 1.87 | 0.56 |
| 41:QL:73:MET:HA | 41:QL:76:VAL:HG12 | 1.87 | 0.56 |
| 41:QM:135:LEU:HB3 | 41:QM:166:THR:HG22 | 1.87 | 0.56 |
| 41:SO:348:ASN:N | 41:SO:348:ASN:OD1 | 2.38 | 0.56 |
| 40:UA:228:ASN:HB3 | 40:UA:231:ILE:HD12 | 1.86 | 0.56 |
| 40:UI:17:GLY:HA2 | 40:UI:20:CYS:HB3 | 1.87 | 0.56 |
| 40:VG:30:ILE:HG12 | 40:VG:61:HIS:HD2 | 1.70 | 0.56 |
| 40:WF:269:LEU:HD11 | 40:WF:383:ILE:HD13 | 1.87 | 0.56 |
| 40:WH:7:VAL:HG12 | 40:WH:66:VAL:HB | 1.86 | 0.56 |
| 7:1T:40:ILE:HG12 | 7:1T:47:ILE:HG22 | 1.87 | 0.56 |
| 9:2B:327:ARG:O | 9:2B:329:ASN:N | 2.38 | 0.56 |
| 12:2O:59:ALA:HB1 | 41:AM:423:VAL:HG13 | 1.86 | 0.56 |
| 16:3J:100:GLU:HG3 | 18:3T:161:ARG:HH22 | 1.71 | 0.56 |
| 21:4F:412:MET:HA | 21:4F:415:ASN:HD21 | 1.70 | 0.56 |
| 23:4N:188:THR:HG21 | 40:CF:72:PRO:HB3 | 1.86 | 0.56 |
| 23:4N:234:ARG:O | 23:4N:235:THR:HB | 2.05 | 0.56 |
| 23:4N:253:TYR:CE2 | 40:EF:220:GLU:CD | 2.79 | 0.56 |
| 27:4Y:251:TYR:O | 27:4Y:262:ASN:ND2 | 2.38 | 0.56 |
| 31:5J:782:ARG:HB3 | 31:5J:785:ASP:HB2 | 1.88 | 0.56 |
| 34:5R:387:LYS:HD2 | 34:5R:391:ASN:HD21 | 1.70 | 0.56 |
| 38:6C:187:LEU:HB3 | 41:VQ:307:HIS:CD2 | 2.40 | 0.56 |
| 38:6C:204:ASP:HB2 | 38:6C:207:PRO:HG3 | 1.87 | 0.56 |
| 40:AA:178:SER:OG | 40:AA:179:THR:N | 2.38 | 0.56 |
| 40:BE:305:CYS:O | 40:BE:306:ASP:C | 2.42 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BM:303:CYS:O | 41:BM:304:ASP:C | 2.44 | 0.56 |
| 41:CL:399:THR:HA | 41:CL:403:MET:HB3 | 1.86 | 0.56 |
| 40:DE:335:ILE:HA | 40:DE:338:LYS:HD2 | 1.86 | 0.56 |
| 40:DF:195:LEU:HG | 40:DF:267:PHE:HZ | 1.70 | 0.56 |
| 40:DF:216:ASN:HB3 | 40:DF:275:VAL:O | 2.05 | 0.56 |
| 41:DN:311:LEU:HD21 | 41:DN:344:TRP:CZ2 | 2.40 | 0.56 |
| 40:EA:11:GLN:NE2 | 41:EN:247:ASN:OD1 | 2.38 | 0.56 |
| 40:EA:168:GLU:HB2 | 40:EA:201:ALA:HA | 1.87 | 0.56 |
| 40:EE:229:ARG:NH2 | 40:EE:366:ASP:OD1 | 2.38 | 0.56 |
| 40:EF:16:ILE:HA | 40:EF:228:ASN:HB3 | 1.87 | 0.56 |
| 40:EH:164:LYS:O | 40:EH:165:SER:C | 2.43 | 0.56 |
| 41:EM:318:ARG:HH21 | 41:EM:356:ILE:HG22 | 1.70 | 0.56 |
| 40:FA:88:HIS:O | 40:FA:89:PRO:C | 2.43 | 0.56 |
| 41:FO:334:GLN:HE22 | 41:FO:347:ASN:HA | 1.68 | 0.56 |
| 41:GM:260:PHE:HE2 | 41:GM:425:ARG:HE | 1.52 | 0.56 |
| 40:HI:342:GLN:NE2 | 40:HI:343:PHE:O | 2.38 | 0.56 |
| 40:IA:406:TRP:HE1 | 41:IN:258:VAL:HG13 | 1.70 | 0.56 |
| 41:IP:222:TYR:O | 41:IP:226:ASN:ND2 | 2.38 | 0.56 |
| 40:JA:88:HIS:NE2 | 40:JA:90:GLU:OE1 | 2.34 | 0.56 |
| 41:JM:3:GLU:HB2 | 41:JM:127:CYS:HB3 | 1.87 | 0.56 |
| 40:KD:51:THR:HG21 | 40:KD:243:ARG:HG2 | 1.86 | 0.56 |
| 40:KE:113:GLU:HG2 | 40:KE:114:LEU:HD12 | 1.87 | 0.56 |
| 40:KE:292:THR:HG21 | 40:KE:331:ALA:HB1 | 1.85 | 0.56 |
| 40:KH:88:HIS:HB3 | 40:KH:91:GLN:HG2 | 1.87 | 0.56 |
| 40:KH:157:LEU:O | 40:KH:161:TYR:HB2 | 2.05 | 0.56 |
| 40:KH:398:TYR:OH | 40:KH:414:GLU:OE2 | 2.23 | 0.56 |
| 41:KP:204:ASN:OD1 | 43:KP:501:GDP:O2' | 2.22 | 0.56 |
| 40:LF:296:PHE:HZ | 40:LF:351:PHE:HE2 | 1.51 | 0.56 |
| 40:LH:139:HIS:O | 40:LH:170:SER:HA | 2.05 | 0.56 |
| 40:MH:101:ASN:HD22 | 41:MO:256:ASN:ND2 | 1.92 | 0.56 |
| 40:NA:258:ASN:HD21 | 41:NB:178:THR:HG23 | 1.70 | 0.56 |
| 40:NE:6:SER:HA | 40:NE:136:LEU:O | 2.05 | 0.56 |
| 40:NE:224:TYR:HA | 40:NE:227:LEU:HB2 | 1.87 | 0.56 |
| 41:OL:165:ASN:HA | 41:OL:198:GLU:O | 2.05 | 0.56 |
| 41:PB:101:TRP:CD1 | 41:PB:105:HIS:HB2 | 2.40 | 0.56 |
| 40:PF:87:PHE:HB3 | 40:PF:92:LEU:HD21 | 1.86 | 0.56 |
| 41:QB:109:GLY:O | 41:QB:112:LEU:N | 2.32 | 0.56 |
| 41:QB:129:CYS:O | 41:QB:131:GLN:N | 2.38 | 0.56 |
| 41:QB:393:ALA:C | 41:QB:395:LEU:H | 2.08 | 0.56 |
| 40:QF:248:LEU:H | 40:QF:355:ILE:HB | 1.70 | 0.56 |
| 40:QG:155:GLU:OE2 | 40:QG:197:HIS:NE2 | 2.34 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QH:207:GLU:HA | 40:QH:210:TYR:HD2 | 1.69 | 0.56 |
| 41:QM:198:GLU:OE1 | 41:QM:200:TYR:OH | 2.21 | 0.56 |
| 41:QP:34:GLY:O | 41:QP:35:THR:C | 2.44 | 0.56 |
| 41:RB:421:PRO:HA | 41:RB:424:THR:HG22 | 1.86 | 0.56 |
| 40:RF:90:GLU:O | 40:RF:121:ARG:NH1 | 2.39 | 0.56 |
| 40:SG:141:PHE:HB2 | 40:SG:173:PRO:HD3 | 1.87 | 0.56 |
| 40:SG:267:PHE:HD2 | 40:SG:387:TRP:HH2 | 1.53 | 0.56 |
| 40:SH:50:ASN:O | 40:SH:64:ARG:NH1 | 2.37 | 0.56 |
| 41:SL:236:VAL:HG13 | 41:SL:237:THR:HG23 | 1.87 | 0.56 |
| 41:SP:131:GLN:HA | 41:SP:162:ARG:HH21 | 1.70 | 0.56 |
| 40:TE:288:VAL:HG21 | 40:TE:328:VAL:HG22 | 1.87 | 0.56 |
| 40:TI:93:ILE:HD13 | 40:TI:118:VAL:HG12 | 1.87 | 0.56 |
| 40:TI:182:VAL:O | 40:TI:186:ASN:ND2 | 2.38 | 0.56 |
| 40:UA:3:GLU:HA | 40:UA:51:THR:HA | 1.87 | 0.56 |
| 40:UF:137:ILE:HB | 40:UF:168:GLU:HG2 | 1.86 | 0.56 |
| 40:UI:406:TRP:CH2 | 41:UP:255:VAL:HA | 2.40 | 0.56 |
| 7:1T:574:TYR:O | 7:1T:575:ASN:C | 2.44 | 0.56 |
| 8:1Z:385:ASP:HA | 8:1Z:388:ARG:HG2 | 1.87 | 0.56 |
| 12:2N:230:GLU:OE2 | 12:2N:234:ARG:NH2 | 2.39 | 0.56 |
| 12:2O:98:VAL:HG21 | 12:2O:103:LEU:HD21 | 1.86 | 0.56 |
| 15:3E:316:ARG:NH2 | 15:3H:60:ASN:OD1 | 2.38 | 0.56 |
| 15:3H:195:SER:HB3 | 15:3H:198:ILE:HD11 | 1.87 | 0.56 |
| 17:3P:191:PRO:HB2 | 17:3P:226:ILE:HD12 | 1.87 | 0.56 |
| 17:3R:205:ARG:HB2 | 17:3R:210:LEU:HD13 | 1.88 | 0.56 |
| 17:3R:222:GLU:HG3 | 17:3R:339:GLN:HB3 | 1.88 | 0.56 |
| 18:3T:63:ARG:NH1 | 18:3W:415:ASP:OD2 | 2.38 | 0.56 |
| 20:4A:149:ARG:O | 20:4A:150:SER:C | 2.43 | 0.56 |
| 22:4I:361:LYS:HG2 | 22:4I:373:PHE:HD2 | 1.70 | 0.56 |
| 22:4J:89:VAL:N | 41:BN:280:GLN:HA | 2.20 | 0.56 |
| 23:4N:18:TYR:CE1 | 23:4N:22:TYR:CE2 | 2.92 | 0.56 |
| 23:4N:260:THR:HG23 | 23:4N:263:HIS:HE1 | 1.69 | 0.56 |
| 23:4P:243:LEU:HD22 | 40:DA:79:ARG:HG2 | 1.86 | 0.56 |
| 23:4P:254:LYS:HD3 | 41:DN:53:GLU:HB3 | 1.87 | 0.56 |
| 23:4P:260:THR:HG23 | 23:4P:263:HIS:HE1 | 1.69 | 0.56 |
| 23:4R:256:GLN:HB3 | 23:4R:264:LEU:HD13 | 1.87 | 0.56 |
| 25:4T:413:PRO:O | 41:LB:75:SER:OG | 2.24 | 0.56 |
| 27:4Y:234:LEU:HD11 | 27:4Y:245:GLU:HG2 | 1.87 | 0.56 |
| 36:5X:130:LEU:O | 36:5X:132:THR:N | 2.38 | 0.56 |
| 38:6C:116:THR:HG22 | 40:VH:214:ARG:HD3 | 1.88 | 0.56 |
| 38:6C:124:PHE:HB3 | 40:UG:123:ARG:HH22 | 1.70 | 0.56 |
| 40:AF:50:ASN:O | 40:AF:64:ARG:NH1 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AF:269:LEU:HD22 | 40:AF:303:VAL:HG11 | 1.87 | 0.56 |
| 41:AL:86:ARG:NH1 | 41:BL:281:TYR:O | 2.38 | 0.56 |
| 41:AL:170:VAL:HG11 | 41:AL:377:LEU:HD21 | 1.87 | 0.56 |
| 40:BE:103:TYR:HB3 | 40:BE:407:TYR:CE2 | 2.40 | 0.56 |
| 40:BG:139:HIS:ND1 | 40:BG:140:SER:O | 2.34 | 0.56 |
| 40:BI:200:CYS:HB3 | 40:BI:256:GLN:HE22 | 1.71 | 0.56 |
| 41:BL:174:LYS:HD2 | 41:BL:175:VAL:HG13 | 1.85 | 0.56 |
| 41:BP:103:LYS:HA | 41:BP:107:THR:CG2 | 2.36 | 0.56 |
| 40:CH:100:ALA:HB1 | 41:CO:252:LYS:HA | 1.87 | 0.56 |
| 41:CL:12:CYS:SG | 41:CL:169:VAL:HG21 | 2.45 | 0.56 |
| 41:CL:165:ASN:HB3 | 41:CL:198:GLU:HB3 | 1.87 | 0.56 |
| 41:CL:303:CYS:O | 41:CL:304:ASP:C | 2.42 | 0.56 |
| 41:CM:330:MET:HG2 | 41:CM:349:VAL:HG11 | 1.87 | 0.56 |
| 41:CN:309:ARG:HD3 | 41:CN:342:VAL:HA | 1.86 | 0.56 |
| 41:CO:215:LEU:HD11 | 41:CO:228:LEU:HD21 | 1.88 | 0.56 |
| 41:CP:237:THR:O | 41:CP:238:THR:C | 2.43 | 0.56 |
| 41:DB:392:LYS:HA | 41:DB:395:LEU:HD21 | 1.85 | 0.56 |
| 41:DB:398:TYR:HB3 | 41:DB:408:PHE:HZ | 1.70 | 0.56 |
| 40:DE:185:TYR:O | 40:DE:186:ASN:C | 2.44 | 0.56 |
| 40:DF:268:PRO:HA | 40:DF:379:ASN:HA | 1.86 | 0.56 |
| 40:DH:114:LEU:HB3 | 40:DH:149:PHE:CE1 | 2.41 | 0.56 |
| 40:DI:228:ASN:HB3 | 42:DI:501:GTP:N2 | 2.19 | 0.56 |
| 40:DI:357:TYR:O | 40:DI:358:GLN:C | 2.44 | 0.56 |
| 41:DM:68:LEU:HD12 | 41:DM:143:THR:HA | 1.87 | 0.56 |
| 41:DM:100:ASN:HB2 | 41:DM:103:LYS:HD3 | 1.86 | 0.56 |
| 41:DN:243:PRO:HD2 | 41:DN:356:ILE:HD13 | 1.88 | 0.56 |
| 40:EA:154:MET:HG3 | 40:EA:194:THR:HG22 | 1.86 | 0.56 |
| 40:EH:190:THR:O | 40:EH:191:THR:C | 2.44 | 0.56 |
| 40:EH:273:ALA:CB | 40:EH:274:PRO:HD2 | 2.31 | 0.56 |
| 41:EO:103:LYS:HG2 | 41:EO:107:THR:HG21 | 1.87 | 0.56 |
| 41:EP:162:ARG:O | 41:EP:163:ILE:C | 2.43 | 0.56 |
| 40:FF:2:ARG:NH1 | 40:FF:242:LEU:O | 2.38 | 0.56 |
| 40:FF:127:ASP:OD2 | 40:GF:293:ASN:ND2 | 2.37 | 0.56 |
| 41:FM:30:ILE:HD11 | 41:FM:47:ILE:HD11 | 1.87 | 0.56 |
| 40:GH:265:ILE:HG23 | 40:GH:431:TYR:CZ | 2.41 | 0.56 |
| 40:GH:339:ARG:O | 40:GH:340:SER:C | 2.43 | 0.56 |
| 41:GM:210:ILE:O | 41:GM:214:THR:OG1 | 2.24 | 0.56 |
| 40:HA:224:TYR:CZ | 41:HN:323:MET:HG2 | 2.40 | 0.56 |
| 40:HF:113:GLU:HG3 | 40:HF:114:LEU:HG | 1.87 | 0.56 |
| 40:HI:219:ILE:HG12 | 40:HI:222:PRO:HD3 | 1.86 | 0.56 |
| 41:HM:248:ALA:HA | 41:HM:252:LYS:HE3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HN:267:MET:HE1 | 41:HN:305:PRO:HG3 | 1.86 | 0.56 |
| 41:HP:354:CYS:SG | 41:HP:355:ASP:N | 2.77 | 0.56 |
| 40:IF:274:PRO:HG3 | 40:IF:286:LEU:HD22 | 1.87 | 0.56 |
| 40:IG:88:HIS:HB3 | 40:IG:91:GLN:HG2 | 1.85 | 0.56 |
| 40:IH:205:ASP:HB3 | 40:IH:303:VAL:HA | 1.87 | 0.56 |
| 40:II:172:TYR:OH | 40:II:386:ALA:O | 2.23 | 0.56 |
| 41:IN:273:LEU:O | 41:IN:292:GLN:NE2 | 2.39 | 0.56 |
| 41:IO:10:GLY:O | 41:IO:14:ASN:ND2 | 2.38 | 0.56 |
| 41:IO:86:ARG:HG2 | 41:IO:89:ASN:H | 1.70 | 0.56 |
| 41:IQ:100:ASN:HB3 | 41:IQ:103:LYS:HB2 | 1.87 | 0.56 |
| 41:JB:191:GLN:O | 41:JB:195:ASN:HB2 | 2.06 | 0.56 |
| 40:JE:75:ILE:HG22 | 40:JE:79:ARG:HH12 | 1.70 | 0.56 |
| 40:KG:120:ASP:OD1 | 40:KG:123:ARG:NH2 | 2.38 | 0.56 |
| 40:KH:206:ASN:ND2 | 42:KO:501:GTP:O2' | 2.35 | 0.56 |
| 40:KH:278:ALA:H | 40:KH:368:ALA:HB2 | 1.71 | 0.56 |
| 40:LE:215:ARG:NH2 | 40:LE:300:ASN:OD1 | 2.38 | 0.56 |
| 40:LF:188:ILE:HG23 | 40:LF:424:MET:HG3 | 1.85 | 0.56 |
| 40:LH:217:LEU:HA | 40:LH:277:SER:HB3 | 1.86 | 0.56 |
| 41:LN:130:LEU:O | 41:LN:162:ARG:NH1 | 2.39 | 0.56 |
| 40:MG:242:LEU:HD11 | 40:MG:252:LEU:HG | 1.87 | 0.56 |
| 41:MM:313:VAL:O | 41:MM:349:VAL:HA | 2.05 | 0.56 |
| 41:MO:391:ARG:O | 41:MO:392:LYS:C | 2.43 | 0.56 |
| 41:MP:237:THR:HG22 | 41:MP:250:LEU:HD21 | 1.87 | 0.56 |
| 40:NA:143:GLY:N | 42:NN:501:GTP:O2A | 2.35 | 0.56 |
| 41:NB:6:HIS:O | 41:NB:63:ALA:HA | 2.03 | 0.56 |
| 40:ND:8:HIS:CE1 | 40:ND:21:TRP:HE1 | 2.22 | 0.56 |
| 40:ND:413:GLU:O | 40:ND:414:GLU:C | 2.43 | 0.56 |
| 40:NF:204:VAL:HG13 | 40:NF:302:MET:HB3 | 1.86 | 0.56 |
| 40:NG:53:PHE:HB3 | 40:NG:61:HIS:HB3 | 1.86 | 0.56 |
| 40:NH:206:ASN:OD1 | 42:NO:501:GTP:O2' | 2.23 | 0.56 |
| 40:OD:438:SER:OG | 41:OL:391:ARG:NH1 | 2.35 | 0.56 |
| 40:OE:79:ARG:HH21 | 40:OE:92:LEU:HB3 | 1.70 | 0.56 |
| 40:OH:250:VAL:HG11 | 40:OH:318:LEU:HD21 | 1.87 | 0.56 |
| 40:PG:181:VAL:HG23 | 40:PG:182:VAL:HG13 | 1.86 | 0.56 |
| 41:PM:271:ALA:HB1 | 41:PM:292:GLN:HG3 | 1.87 | 0.56 |
| 41:PO:113:VAL:HA | 41:PO:116:VAL:HG12 | 1.86 | 0.56 |
| 40:QA:158:SER:OG | 40:QA:166:LYS:NZ | 2.39 | 0.56 |
| 40:QA:205:ASP:HB2 | 40:QA:303:VAL:HG22 | 1.88 | 0.56 |
| 41:QB:151:LEU:O | 41:QB:152:ILE:C | 2.43 | 0.56 |
| 41:QO:111:GLU:N | 41:QO:111:GLU:OE1 | 2.38 | 0.56 |
| 41:QP:393:ALA:C | 41:QP:395:LEU:H | 2.09 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RA:222:PRO:HG2 | 41:RN:324:LYS:HE3 | 1.87 | 0.56 |
| 40:RG:47:ASP:O | 40:RG:50:ASN:HB3 | 2.05 | 0.56 |
| 40:RH:254:GLU:O | 40:RH:258:ASN:ND2 | 2.38 | 0.56 |
| 41:RN:237:THR:HG22 | 41:RN:250:LEU:HD21 | 1.88 | 0.56 |
| 40:SF:405:HIS:CD2 | 41:SM:261:PRO:HG3 | 2.40 | 0.56 |
| 40:SH:226:ASN:ND2 | 40:SH:366:ASP:OD2 | 2.35 | 0.56 |
| 41:SM:21:TRP:HA | 41:SM:24:ILE:HG22 | 1.87 | 0.56 |
| 41:SM:209:ASP:OD1 | 41:SM:213:ARG:NH2 | 2.39 | 0.56 |
| 41:SP:27:GLU:OE1 | 41:SP:241:ARG:NH2 | 2.38 | 0.56 |
| 41:SP:193:VAL:HG12 | 41:SP:194:GLU:HG2 | 1.88 | 0.56 |
| 41:TB:193:VAL:HG21 | 41:TB:418:LEU:HD21 | 1.87 | 0.56 |
| 41:TM:271:ALA:HA | 41:TM:273:LEU:HD13 | 1.88 | 0.56 |
| 41:TP:293:MET:HG3 | 41:TP:367:PHE:HD2 | 1.70 | 0.56 |
| 41:UB:256:ASN:HD22 | 41:UB:350:LYS:HE2 | 1.70 | 0.56 |
| 40:UI:160:ASP:O | 40:UI:161:TYR:C | 2.43 | 0.56 |
| 41:UN:354:CYS:SG | 41:UN:355:ASP:N | 2.76 | 0.56 |
| 41:VB:107:THR:HG22 | 41:VB:108:GLU:H | 1.70 | 0.56 |
| 41:VB:237:THR:HB | 41:VB:240:LEU:HD11 | 1.88 | 0.56 |
| 40:VJ:6:SER:O | 40:VJ:65:ALA:HA | 2.04 | 0.56 |
| 41:VO:12:CYS:HB3 | 41:VO:138:SER:HB2 | 1.87 | 0.56 |
| 40:WE:217:LEU:HA | 40:WE:277:SER:HB3 | 1.87 | 0.56 |
| 7:1S:459:GLU:OE2 | 40:VH:85:GLN:NE2 | 2.39 | 0.56 |
| 9:2B:210:ARG:NH2 | 40:SG:56:THR:O | 2.37 | 0.56 |
| 9:2B:315:ALA:HA | 9:2B:318:HIS:CE1 | 2.39 | 0.56 |
| 17:3Q:406:ARG:HB3 | 17:3Q:410:GLU:HG3 | 1.86 | 0.56 |
| 17:3R:160:ILE:HG23 | 17:3R:254:LEU:HD22 | 1.87 | 0.56 |
| 23:4N:249:TYR:O | 23:4N:251:PRO:HD3 | 2.04 | 0.56 |
| 23:4P:249:TYR:O | 23:4P:251:PRO:HD3 | 2.04 | 0.56 |
| 27:4Z:14:ASN:ND2 | 27:4Z:17:GLU:OE1 | 2.38 | 0.56 |
| 33:5N:413:GLU:OE2 | 33:5N:417:ASN:ND2 | 2.39 | 0.56 |
| 34:5Q:164:LEU:HD23 | 34:5R:487:ILE:CD1 | 2.35 | 0.56 |
| 36:5Y:62:VAL:HG21 | 36:5Y:71:GLU:HB3 | 1.87 | 0.56 |
| 40:BI:160:ASP:O | 40:BI:162:GLY:N | 2.38 | 0.56 |
| 40:CA:114:LEU:HB3 | 40:CA:149:PHE:CZ | 2.41 | 0.56 |
| 41:CL:375:GLN:HB2 | 41:CL:422:VAL:HG11 | 1.87 | 0.56 |
| 41:CN:26:ASP:HB2 | 41:CN:359:ARG:CZ | 2.34 | 0.56 |
| 40:EE:177:VAL:HA | 41:EL:331:LEU:HD11 | 1.86 | 0.56 |
| 40:EI:243:ARG:O | 40:EI:244:PHE:C | 2.42 | 0.56 |
| 41:EL:24:ILE:HD12 | 41:EL:241:ARG:HH12 | 1.70 | 0.56 |
| 41:EP:116:VAL:O | 41:EP:120:VAL:HG13 | 2.06 | 0.56 |
| 41:FN:314:ALA:HB2 | 41:FN:350:LYS:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FP:31:ASP:OD2 | 41:FP:34:GLY:N | 2.37 | 0.56 |
| 41:FP:51:TYR:HB3 | 41:FP:59:TYR:HB3 | 1.87 | 0.56 |
| 40:GA:231:ILE:HA | 40:GA:234:ILE:HG22 | 1.87 | 0.56 |
| 40:GE:326:LYS:HE3 | 41:GM:225:LEU:HD11 | 1.87 | 0.56 |
| 40:GH:104:ALA:HB3 | 40:GH:410:GLU:HB3 | 1.88 | 0.56 |
| 40:HE:68:VAL:HG12 | 40:HE:93:ILE:HB | 1.86 | 0.56 |
| 40:HH:205:ASP:H | 40:HH:303:VAL:HG12 | 1.69 | 0.56 |
| 40:IA:402:ALA:HB2 | 41:IN:344:TRP:HZ3 | 1.71 | 0.56 |
| 40:II:408:VAL:HA | 40:II:412:MET:HB2 | 1.86 | 0.56 |
| 40:LA:235:VAL:HA | 40:LA:238:ILE:HG22 | 1.87 | 0.56 |
| 41:LL:170:VAL:HG11 | 41:LL:377:LEU:HD21 | 1.88 | 0.56 |
| 41:MB:134:GLN:NE2 | 41:MB:233:MET:SD | 2.78 | 0.56 |
| 40:NA:221:ARG:HH22 | 41:NN:325:GLU:H | 1.53 | 0.56 |
| 40:NH:8:HIS:HD2 | 40:NH:138:PHE:HB2 | 1.70 | 0.56 |
| 40:PD:270:ALA:HA | 40:PD:376:MET:O | 2.06 | 0.56 |
| 41:QB:108:GLU:O | 41:QB:111:GLU:N | 2.34 | 0.56 |
| 41:QB:271:ALA:HB2 | 41:QB:293:MET:HG3 | 1.87 | 0.56 |
| 40:QE:320:ARG:HB2 | 40:QE:373:ALA:HB3 | 1.86 | 0.56 |
| 40:QH:68:VAL:HG12 | 40:QH:93:ILE:HB | 1.87 | 0.56 |
| 41:RN:2:ARG:HB2 | 41:RN:131:GLN:HB2 | 1.87 | 0.56 |
| 41:SB:222:TYR:O | 41:SB:226:ASN:HB2 | 2.06 | 0.56 |
| 41:SL:139:LEU:HB2 | 41:SL:170:VAL:HA | 1.87 | 0.56 |
| 41:SL:169:VAL:HA | 41:SL:202:ILE:HB | 1.88 | 0.56 |
| 41:TB:46:ARG:NH1 | 40:TG:73:THR:OG1 | 2.38 | 0.56 |
| 40:TF:229:ARG:O | 40:TF:232:SER:OG | 2.24 | 0.56 |
| 40:TG:189:LEU:HD11 | 40:TG:417:PHE:HE1 | 1.71 | 0.56 |
| 40:TH:31:GLN:HG3 | 40:TH:37:PRO:HD3 | 1.87 | 0.56 |
| 40:TH:318:LEU:O | 40:TH:374:VAL:HA | 2.06 | 0.56 |
| 40:TI:71:GLU:OE2 | 41:TP:2:ARG:NH1 | 2.38 | 0.56 |
| 41:UB:8:GLN:HE22 | 41:UB:63:ALA:HB1 | 1.70 | 0.56 |
| 40:UI:21:TRP:CZ2 | 40:UI:65:ALA:HB2 | 2.40 | 0.56 |
| 40:UI:72:PRO:HD3 | 40:UI:96:LYS:HA | 1.88 | 0.56 |
| 40:VF:139:HIS:O | 40:VF:170:SER:HA | 2.05 | 0.56 |
| 40:WF:141:PHE:HB2 | 40:WF:173:PRO:HD3 | 1.87 | 0.56 |
| 40:WG:73:THR:HA | 40:WG:76:ASP:HB2 | 1.87 | 0.56 |
| 7:1S:59:PHE:HE1 | 7:1S:585:GLY:HA2 | 1.70 | 0.56 |
| 7:1T:330:CYS:SG | 7:1T:331:HIS:N | 2.79 | 0.56 |
| 10:2E:97:GLN:O | 10:2E:101:GLN:CB | 2.54 | 0.56 |
| 11:2I:88:VAL:HG21 | 41:LB:392:LYS:HB2 | 1.86 | 0.56 |
| 12:2N:250:THR:HA | 40:AA:401:ARG:HD2 | 1.87 | 0.56 |
| 15:3H:144:GLN:OE1 | 15:3H:147:ARG:NH1 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:3L:380:LYS:HE3 | 16:3M:17:TRP:HE1 | 1.70 | 0.56 |
| 18:3V:116:GLU:HB3 | 18:3V:265:LEU:HD21 | 1.87 | 0.56 |
| 19:3Y:323:ARG:HH22 | 27:4Y:204:LEU:HD11 | 1.70 | 0.56 |
| 21:4E:228:ASP:OD2 | 21:4E:233:LYS:NZ | 2.39 | 0.56 |
| 21:4E:473:VAL:HB | 21:4E:482:PRO:HG2 | 1.86 | 0.56 |
| 21:4F:264:ILE:HD13 | 21:4F:275:ILE:HG12 | 1.87 | 0.56 |
| 22:4I:635:PHE:HA | 22:4I:638:LEU:HD23 | 1.87 | 0.56 |
| 26:4V:59:ASP:O | 26:4V:64:ASN:ND2 | 2.38 | 0.56 |
| 26:4V:82:TYR:HB2 | 40:IH:39:ASP:HB3 | 1.88 | 0.56 |
| 40:AE:76:ASP:HA | 40:AE:79:ARG:HG2 | 1.87 | 0.56 |
| 40:AE:254:GLU:O | 40:AE:258:ASN:ND2 | 2.39 | 0.56 |
| 41:AO:67:ASP:HA | 41:AO:143:THR:HG21 | 1.87 | 0.56 |
| 41:AP:237:THR:HG22 | 41:AP:250:LEU:HD11 | 1.86 | 0.56 |
| 40:BA:122:ILE:HG21 | 40:BA:157:LEU:HD21 | 1.88 | 0.56 |
| 40:BF:73:THR:HA | 40:BF:76:ASP:HB2 | 1.86 | 0.56 |
| 41:CB:375:GLN:HE22 | 41:CB:423:VAL:HB | 1.68 | 0.56 |
| 41:CP:60:VAL:CG1 | 41:DP:281:TYR:HA | 2.33 | 0.56 |
| 40:DF:143:GLY:HA3 | 42:DF:501:GTP:O2A | 2.05 | 0.56 |
| 41:DL:5:VAL:HG23 | 41:DL:133:PHE:HB3 | 1.88 | 0.56 |
| 41:DL:156:ARG:HD3 | 41:DL:164:MET:HG2 | 1.87 | 0.56 |
| 41:DL:170:VAL:HB | 41:DL:171:PRO:HD2 | 1.87 | 0.56 |
| 41:DN:31:ASP:C | 41:DN:33:THR:H | 2.08 | 0.56 |
| 41:EB:2:ARG:HB3 | 41:EB:131:GLN:HG2 | 1.86 | 0.56 |
| 41:EB:114:ASP:HA | 41:EB:117:LEU:HD12 | 1.86 | 0.56 |
| 41:EB:327:ASP:HB3 | 40:EG:177:VAL:HG21 | 1.88 | 0.56 |
| 40:FF:108:TYR:O | 40:FF:112:LYS:NZ | 2.38 | 0.56 |
| 41:FN:54:ALA:HB3 | 41:FN:58:LYS:HB3 | 1.87 | 0.56 |
| 41:HB:10:GLY:O | 41:HB:14:ASN:CB | 2.53 | 0.56 |
| 41:HB:286:VAL:HG11 | 41:HB:326:VAL:HG22 | 1.87 | 0.56 |
| 40:HE:189:LEU:HD22 | 40:HE:416:GLU:HG3 | 1.88 | 0.56 |
| 40:IF:101:ASN:OD1 | 41:IM:256:ASN:ND2 | 2.39 | 0.56 |
| 40:II:270:ALA:HA | 40:II:376:MET:O | 2.06 | 0.56 |
| 41:KL:3:GLU:HA | 41:KL:49:VAL:HA | 1.86 | 0.56 |
| 41:KN:237:THR:HG23 | 41:KN:241:ARG:HH11 | 1.70 | 0.56 |
| 40:LA:264:ARG:NH1 | 40:LA:430:ASP:OD2 | 2.38 | 0.56 |
| 40:LD:51:THR:HG21 | 40:LD:243:ARG:HG2 | 1.87 | 0.56 |
| 41:LL:100:ASN:HB3 | 41:LL:103:LYS:HB3 | 1.87 | 0.56 |
| 40:MH:16:ILE:HG12 | 40:MH:228:ASN:HB3 | 1.86 | 0.56 |
| 40:MH:104:ALA:HA | 40:MH:108:TYR:HD1 | 1.69 | 0.56 |
| 41:ML:334:GLN:HE21 | 41:ML:349:VAL:HG23 | 1.70 | 0.56 |
| 41:MO:271:ALA:HB3 | 41:MO:272:PRO:HD3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NG:326:LYS:HG2 | 41:NO:220:PRO:HD2 | 1.87 | 0.56 |
| 41:NM:34:GLY:HA3 | 41:NM:58:LYS:HE3 | 1.86 | 0.56 |
| 41:NM:105:HIS:CE1 | 41:NM:150:LEU:HD13 | 2.40 | 0.56 |
| 41:NN:113:VAL:HA | 41:NN:116:VAL:HG12 | 1.87 | 0.56 |
| 40:PH:185:TYR:HE2 | 40:PH:403:PHE:HB2 | 1.69 | 0.56 |
| 41:PM:31:ASP:OD2 | 41:PM:35:THR:OG1 | 2.22 | 0.56 |
| 40:QE:89:PRO:HG2 | 40:RE:280:LYS:NZ | 2.20 | 0.56 |
| 40:QF:11:GLN:HG3 | 40:QF:74:VAL:HG11 | 1.86 | 0.56 |
| 40:RH:76:ASP:OD1 | 40:RH:79:ARG:NH1 | 2.38 | 0.56 |
| 41:RL:372:THR:OG1 | 41:RL:422:VAL:O | 2.24 | 0.56 |
| 41:RP:181:GLU:HA | 41:RP:184:ASN:HB2 | 1.87 | 0.56 |
| 40:SE:391:ASP:HA | 40:SE:421:ARG:HH12 | 1.71 | 0.56 |
| 40:SH:76:ASP:HA | 40:SH:79:ARG:HG2 | 1.87 | 0.56 |
| 40:SI:297:GLU:OE2 | 40:SI:300:ASN:ND2 | 2.38 | 0.56 |
| 41:SO:98:GLY:O | 41:SO:99:ASN:C | 2.43 | 0.56 |
| 40:TF:136:LEU:HD11 | 40:TF:239:THR:HG21 | 1.87 | 0.56 |
| 40:TI:207:GLU:HA | 40:TI:210:TYR:HB2 | 1.87 | 0.56 |
| 40:TI:217:LEU:HA | 40:TI:277:SER:HB3 | 1.87 | 0.56 |
| 41:TM:130:LEU:HG | 41:TM:162:ARG:HD2 | 1.87 | 0.56 |
| 41:TP:209:ASP:O | 41:TP:213:ARG:HB3 | 2.05 | 0.56 |
| 41:TP:374:ILE:HD11 | 41:TP:422:VAL:HG21 | 1.87 | 0.56 |
| 40:UA:255:PHE:HZ | 40:UA:318:LEU:HD21 | 1.71 | 0.56 |
| 41:UB:222:TYR:O | 41:UB:226:ASN:ND2 | 2.38 | 0.56 |
| 40:UG:320:ARG:HH21 | 40:UG:360:PRO:HA | 1.69 | 0.56 |
| 41:UP:40:SER:O | 41:UP:41:ASP:C | 2.43 | 0.56 |
| 40:VI:153:LEU:O | 40:VI:157:LEU:HB2 | 2.06 | 0.56 |
| 40:VJ:324:VAL:HG12 | 40:VJ:326:LYS:H | 1.71 | 0.56 |
| 41:VO:174:LYS:HG3 | 41:VO:175:VAL:HG12 | 1.87 | 0.56 |
| 41:WB:198:GLU:HG2 | 41:WB:266:PHE:HE2 | 1.70 | 0.56 |
| 40:WE:141:PHE:HB2 | 40:WE:173:PRO:HD3 | 1.86 | 0.56 |
| 7:1T:250:SER:HA | 41:WM:33:THR:HG21 | 1.86 | 0.56 |
| 17:3R:94:TYR:HB3 | 17:3R:98:ASP:HB2 | 1.88 | 0.56 |
| 31:5I:551:THR:OG1 | 40:HI:85:GLN:NE2 | 2.35 | 0.56 |
| 40:AA:98:ASP:O | 40:AA:105:ARG:NH1 | 2.39 | 0.56 |
| 40:BE:105:ARG:HA | 40:BE:109:THR:HG23 | 1.88 | 0.56 |
| 40:BI:218:ASP:O | 40:BI:219:ILE:C | 2.44 | 0.56 |
| 41:BN:392:LYS:HG2 | 41:BN:395:LEU:HD23 | 1.87 | 0.56 |
| 40:CH:276:ILE:HG22 | 40:CH:280:LYS:HE3 | 1.87 | 0.56 |
| 40:CI:179:THR:O | 41:CP:350:LYS:HA | 2.05 | 0.56 |
| 41:CO:103:LYS:HA | 41:CO:107:THR:HG23 | 1.88 | 0.56 |
| 41:CP:427:ALA:O | 41:CP:428:CYS:C | 2.44 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DA:59:GLY:O | 40:DA:60:LYS:C | 2.42 | 0.56 |
| 41:DB:413:SER:HA | 41:DB:416:ASN:HB3 | 1.86 | 0.56 |
| 40:DH:208:ALA:HB2 | 40:DH:304:LYS:H | 1.70 | 0.56 |
| 40:DH:276:ILE:HB | 40:DH:281:ALA:HB2 | 1.88 | 0.56 |
| 40:DI:73:THR:O | 40:DI:74:VAL:C | 2.42 | 0.56 |
| 41:DM:82:GLY:C | 41:DM:84:ILE:H | 2.09 | 0.56 |
| 41:DN:224:ASP:OD2 | 41:DN:224:ASP:N | 2.39 | 0.56 |
| 41:DO:172:SER:OG | 41:DO:175:VAL:O | 2.23 | 0.56 |
| 41:DP:100:ASN:HB3 | 41:DP:103:LYS:HG3 | 1.88 | 0.56 |
| 40:EA:16:ILE:HD11 | 40:EA:138:PHE:HB3 | 1.86 | 0.56 |
| 40:EA:142:GLY:HA3 | 42:EA:501:GTP:H5' | 1.87 | 0.56 |
| 41:EB:232:THR:HG22 | 41:EB:270:PHE:HB2 | 1.88 | 0.56 |
| 40:EH:135:PHE:O | 40:EH:136:LEU:C | 2.44 | 0.56 |
| 40:GE:288:VAL:HG21 | 40:GE:327:ASP:CG | 2.26 | 0.56 |
| 40:GH:285:GLN:O | 40:GH:286:LEU:C | 2.43 | 0.56 |
| 41:GP:262:ARG:NH2 | 41:GP:417:ASP:O | 2.38 | 0.56 |
| 40:HA:1:GLN:O | 41:HB:94:GLN:NE2 | 2.38 | 0.56 |
| 40:HA:182:VAL:HG22 | 41:HN:256:ASN:HD21 | 1.70 | 0.56 |
| 40:HI:60:LYS:HE2 | 40:II:283:HIS:CD2 | 2.41 | 0.56 |
| 41:HN:135:LEU:HD23 | 41:HN:166:THR:HG22 | 1.87 | 0.56 |
| 40:IF:319:TYR:HB3 | 40:IF:323:VAL:HG21 | 1.87 | 0.56 |
| 40:IH:288:VAL:HA | 40:IH:291:ILE:HG12 | 1.87 | 0.56 |
| 40:II:276:ILE:HG21 | 40:II:281:ALA:HB2 | 1.88 | 0.56 |
| 40:JH:185:TYR:HE2 | 40:JH:403:PHE:HB2 | 1.70 | 0.56 |
| 41:JL:27:GLU:OE1 | 41:JL:241:ARG:NH2 | 2.38 | 0.56 |
| 41:JM:157:GLU:O | 41:JM:158:GLU:C | 2.44 | 0.56 |
| 41:JO:237:THR:O | 41:JO:241:ARG:NH1 | 2.39 | 0.56 |
| 40:LE:30:ILE:HD13 | 40:LE:36:MET:HB2 | 1.88 | 0.56 |
| 40:LF:88:HIS:HB3 | 40:LF:91:GLN:HG3 | 1.88 | 0.56 |
| 40:LG:20:CYS:HA | 40:LG:232:SER:HB2 | 1.87 | 0.56 |
| 41:LO:271:ALA:HB1 | 41:LO:292:GLN:HG3 | 1.87 | 0.56 |
| 41:LP:178:THR:HB | 41:LP:181:GLU:HG3 | 1.85 | 0.56 |
| 40:MA:138:PHE:HZ | 40:MA:235:VAL:HG21 | 1.70 | 0.56 |
| 40:MF:167:LEU:HD22 | 40:MF:200:CYS:HB3 | 1.87 | 0.56 |
| 40:NE:178:SER:OG | 41:NL:347:ASN:ND2 | 2.39 | 0.56 |
| 40:NG:191:THR:O | 40:NG:195:LEU:HB2 | 2.05 | 0.56 |
| 41:OM:68:LEU:HD22 | 41:OM:108:GLU:HG3 | 1.88 | 0.56 |
| 41:PB:103:LYS:HA | 41:PB:107:THR:HB | 1.86 | 0.56 |
| 40:QA:64:ARG:NH1 | 40:QA:129:CYS:SG | 2.78 | 0.56 |
| 40:QA:319:TYR:HB3 | 40:QA:323:VAL:HG21 | 1.87 | 0.56 |
| 41:QB:215:LEU:O | 41:QB:216:LYS:C | 2.44 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RM:63:ALA:O | 41:RM:89:ASN:ND2 | 2.38 | 0.56 |
| 41:SB:324:LYS:NZ | 40:SG:210:TYR:O | 2.39 | 0.56 |
| 40:SE:221:ARG:NH2 | 41:SL:322:SER:O | 2.38 | 0.56 |
| 41:SM:27:GLU:HA | 41:SM:359:ARG:HH12 | 1.69 | 0.56 |
| 41:SO:178:THR:O | 41:SO:181:GLU:HB2 | 2.06 | 0.56 |
| 40:TA:440:GLU:HB2 | 41:TB:390:ARG:HH22 | 1.70 | 0.56 |
| 41:TB:137:HIS:ND1 | 41:TB:144:GLY:O | 2.39 | 0.56 |
| 41:TP:358:PRO:HD2 | 41:TP:361:LEU:HD11 | 1.87 | 0.56 |
| 40:VH:73:THR:HA | 40:VH:76:ASP:HB2 | 1.87 | 0.56 |
| 41:WM:135:LEU:HD22 | 41:WM:137:HIS:HB3 | 1.87 | 0.56 |
| 41:WP:178:THR:HB | 41:WP:181:GLU:HG3 | 1.87 | 0.56 |
| 7:1T:95:LEU:HD21 | 7:1T:142:ILE:HG22 | 1.88 | 0.56 |
| 8:1Z:371:ARG:HB3 | 40:UI:282:TYR:HE1 | 1.69 | 0.56 |
| 8:1Z:391:ARG:HD3 | 9:2B:118:ARG:HE | 1.70 | 0.56 |
| 11:2I:114:ILE:HD13 | 40:LG:414:GLU:HG2 | 1.88 | 0.56 |
| 12:2P:118:GLU:OE1 | 12:2P:120:THR:N | 2.37 | 0.56 |
| 12:2R:234:ARG:NH2 | 12:2R:254:CYS:SG | 2.79 | 0.56 |
| 21:4F:532:GLN:O | 21:4F:533:ASN:C | 2.43 | 0.56 |
| 22:4J:667:LEU:O | 22:4J:669:PHE:N | 2.38 | 0.56 |
| 24:4O:233:SER:HB3 | 24:4O:268:ALA:HB1 | 1.88 | 0.56 |
| 23:4Q:238:HIS:O | 23:4Q:239:ASN:C | 2.43 | 0.56 |
| 37:6A:66:ARG:O | 37:6A:70:LEU:HB2 | 2.06 | 0.56 |
| 40:AE:329:ASN:HB3 | 41:AM:175:VAL:HG11 | 1.87 | 0.56 |
| 40:AF:205:ASP:HB2 | 40:AF:303:VAL:HG23 | 1.86 | 0.56 |
| 41:AN:11:GLN:HA | 41:AN:72:THR:HG21 | 1.87 | 0.56 |
| 40:BE:104:ALA:HB1 | 40:BE:410:GLU:HB2 | 1.86 | 0.56 |
| 40:BI:231:ILE:HA | 40:BI:234:ILE:HD12 | 1.88 | 0.56 |
| 41:BM:226:ASN:ND2 | 43:BM:501:GDP:HN1 | 2.03 | 0.56 |
| 41:CB:178:THR:HB | 41:CB:181:GLU:HG2 | 1.87 | 0.56 |
| 40:CE:326:LYS:HZ3 | 41:CM:208:TYR:HB2 | 1.71 | 0.56 |
| 40:CG:139:HIS:ND1 | 40:CG:146:GLY:O | 2.37 | 0.56 |
| 40:CG:352:LYS:HA | 41:CO:177:ASP:O | 2.05 | 0.56 |
| 41:CP:99:ASN:HB2 | 41:CP:180:VAL:HG21 | 1.87 | 0.56 |
| 40:DA:164:LYS:O | 40:DA:165:SER:C | 2.44 | 0.56 |
| 40:DH:298:PRO:HB3 | 40:DH:307:PRO:HD2 | 1.88 | 0.56 |
| 41:DP:141:GLY:HA3 | 43:DP:501:GDP:O1A | 2.05 | 0.56 |
| 41:EB:139:LEU:HG | 41:EB:168:SER:HB3 | 1.88 | 0.56 |
| 40:EE:247:ALA:HB3 | 40:EE:355:ILE:HB | 1.88 | 0.56 |
| 40:EE:260:VAL:HB | 41:EM:397:TRP:CZ2 | 2.40 | 0.56 |
| 40:EF:180:ALA:HB3 | 40:EF:183:GLU:HG3 | 1.88 | 0.56 |
| 41:EP:267:MET:HE3 | 41:EP:301:ALA:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EP:311:LEU:HD12 | 41:EP:342:VAL:HG11 | 1.87 | 0.56 |
| 40:FA:297:GLU:HG2 | 40:FA:300:ASN:HB2 | 1.88 | 0.56 |
| 40:FF:251:ASP:HB2 | 40:FF:254:GLU:HG3 | 1.88 | 0.56 |
| 40:FG:98:ASP:O | 40:FG:105:ARG:NH1 | 2.39 | 0.56 |
| 40:GA:352:LYS:HD2 | 41:GB:178:THR:HA | 1.88 | 0.56 |
| 40:GH:238:ILE:HG13 | 40:GH:239:THR:HG23 | 1.87 | 0.56 |
| 40:GI:217:LEU:C | 40:GI:277:SER:HB2 | 2.26 | 0.56 |
| 40:GI:259:LEU:O | 40:GI:260:VAL:C | 2.44 | 0.56 |
| 41:GM:317:PHE:HB2 | 41:GM:353:VAL:HG12 | 1.88 | 0.56 |
| 41:GN:19:LYS:HG2 | 41:GN:226:ASN:HB3 | 1.87 | 0.56 |
| 41:GN:198:GLU:HG2 | 41:GN:266:PHE:CE2 | 2.40 | 0.56 |
| 41:GP:334:GLN:HE21 | 41:GP:349:VAL:HG23 | 1.71 | 0.56 |
| 41:HM:289:LEU:HD11 | 41:HM:363:MET:HB3 | 1.87 | 0.56 |
| 41:HP:256:ASN:OD1 | 41:HP:350:LYS:NZ | 2.33 | 0.56 |
| 40:IA:88:HIS:HB3 | 40:IA:91:GLN:HG3 | 1.87 | 0.56 |
| 40:IH:311:LYS:NZ | 40:IH:437:ASP:OD1 | 2.38 | 0.56 |
| 40:JE:318:LEU:O | 40:JE:374:VAL:HA | 2.06 | 0.56 |
| 40:JF:326:LYS:HG3 | 41:JN:220:PRO:HG2 | 1.86 | 0.56 |
| 40:KG:258:ASN:HD22 | 40:KG:352:LYS:HD2 | 1.70 | 0.56 |
| 40:LG:258:ASN:HB3 | 41:LO:179:VAL:HG23 | 1.87 | 0.56 |
| 40:ME:226:ASN:ND2 | 40:ME:366:ASP:OD2 | 2.33 | 0.56 |
| 41:MN:16:ILE:HA | 41:MN:226:ASN:HB3 | 1.87 | 0.56 |
| 40:NG:223:THR:HG23 | 40:NG:225:THR:H | 1.71 | 0.56 |
| 40:OA:24:TYR:HE1 | 40:OA:243:ARG:HH21 | 1.52 | 0.56 |
| 41:OB:191:GLN:O | 41:OB:195:ASN:ND2 | 2.33 | 0.56 |
| 41:OB:236:VAL:HG12 | 41:OB:368:ILE:HD11 | 1.87 | 0.56 |
| 40:PA:8:HIS:HB3 | 40:PA:138:PHE:HB2 | 1.88 | 0.56 |
| 40:PE:49:PHE:HE2 | 40:PE:55:GLU:HB3 | 1.71 | 0.56 |
| 41:QB:325:GLU:HG2 | 40:QG:221:ARG:HD3 | 1.88 | 0.56 |
| 41:QB:391:ARG:O | 41:QB:392:LYS:C | 2.44 | 0.56 |
| 41:RO:202:ILE:HG23 | 41:RO:300:MET:HB3 | 1.86 | 0.56 |
| 41:SB:255:VAL:HA | 40:SG:406:TRP:CZ3 | 2.41 | 0.56 |
| 40:SI:188:ILE:HD12 | 40:SI:424:MET:HG3 | 1.88 | 0.56 |
| 40:TE:265:ILE:HG22 | 40:TE:379:ASN:HD21 | 1.71 | 0.56 |
| 41:TM:236:VAL:HG23 | 41:TM:237:THR:HG23 | 1.87 | 0.56 |
| 41:UB:173:PRO:HB3 | 41:UB:380:ARG:HD3 | 1.87 | 0.56 |
| 40:UE:108:TYR:O | 40:UE:112:LYS:NZ | 2.39 | 0.56 |
| 40:UF:352:LYS:HE3 | 41:UN:179:VAL:HG22 | 1.87 | 0.56 |
| 40:UG:121:ARG:HH21 | 40:UG:124:LYS:HE2 | 1.71 | 0.56 |
| 40:UI:21:TRP:HA | 40:UI:24:TYR:HB2 | 1.86 | 0.56 |
| 41:UP:42:LEU:HA | 41:UP:45:GLU:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VI:20:CYS:HA | 40:VI:232:SER:HB2 | 1.87 | 0.56 |
| 40:VJ:317:LEU:HB2 | 40:VJ:353:VAL:HA | 1.88 | 0.56 |
| 41:VN:134:GLN:HG3 | 41:VN:167:PHE:HE1 | 1.69 | 0.56 |
| 40:WF:105:ARG:HG2 | 40:WF:410:GLU:HG2 | 1.86 | 0.56 |
| 40:WG:6:SER:O | 40:WG:65:ALA:HA | 2.05 | 0.56 |
| 41:WM:200:TYR:HE2 | 41:WM:368:ILE:HG12 | 1.71 | 0.56 |
| 7:1T:98:TYR:O | 7:1T:99:LYS:C | 2.44 | 0.56 |
| 11:2K:80:ARG:HG2 | 11:2K:81:HIS:H | 1.71 | 0.56 |
| 12:2O:94:ILE:HD11 | 12:2O:126:PHE:HA | 1.87 | 0.56 |
| 12:2P:168:THR:HA | 12:2P:171:VAL:HG12 | 1.88 | 0.56 |
| 12:2Q:172:LEU:HD23 | 12:2Q:232:PHE:HZ | 1.70 | 0.56 |
| 13:2X:173:SER:O | 13:2X:174:GLU:C | 2.43 | 0.56 |
| 18:3T:376:ARG:NH1 | 18:3T:379:SER:OG | 2.39 | 0.56 |
| 21:4E:299:LYS:HG2 | 21:4E:300:VAL:H | 1.71 | 0.56 |
| 22:4I:676:ALA:O | 22:4I:677:LEU:C | 2.44 | 0.56 |
| 22:4J:503:LYS:NZ | 22:4J:504:ALA:O | 2.39 | 0.56 |
| 23:4R:244:PRO:HD2 | 40:DI:89:PRO:HG2 | 1.86 | 0.56 |
| 31:5I:598:ARG:NH1 | 31:5I:671:PHE:O | 2.38 | 0.56 |
| 35:5T:155:GLU:HB3 | 35:5T:158:LEU:HB2 | 1.87 | 0.56 |
| 36:5W:38:ASP:O | 36:5W:40:ARG:NH1 | 2.30 | 0.56 |
| 41:AO:27:GLU:HA | 41:AO:359:ARG:HD3 | 1.88 | 0.56 |
| 40:BI:63:PRO:CG | 40:BI:86:LEU:HG | 2.35 | 0.56 |
| 40:CH:147:SER:HB2 | 40:CH:190:THR:HB | 1.87 | 0.56 |
| 40:CI:5:ILE:HD12 | 40:CI:125:LEU:HD23 | 1.88 | 0.56 |
| 40:DF:225:THR:HG22 | 40:DF:229:ARG:HE | 1.71 | 0.56 |
| 41:DL:239:CYS:HB3 | 41:DL:248:ALA:H | 1.71 | 0.56 |
| 41:DL:303:CYS:O | 41:DL:304:ASP:C | 2.43 | 0.56 |
| 41:DM:36:TYR:CZ | 41:DM:38:GLY:HA3 | 2.40 | 0.56 |
| 41:DM:420:ASN:O | 41:DM:423:VAL:N | 2.39 | 0.56 |
| 40:EF:26:LEU:HD22 | 40:EF:363:VAL:HG12 | 1.88 | 0.56 |
| 40:EG:395:ASP:OD1 | 40:EG:421:ARG:NH1 | 2.39 | 0.56 |
| 40:EI:157:LEU:HB3 | 40:EI:166:LYS:HE3 | 1.87 | 0.56 |
| 41:EM:200:TYR:CE2 | 41:EM:236:VAL:HG21 | 2.38 | 0.56 |
| 41:FB:54:ALA:HB3 | 41:FB:58:LYS:HB3 | 1.86 | 0.56 |
| 41:FM:318:ARG:HD3 | 41:FM:358:PRO:HD3 | 1.88 | 0.56 |
| 41:GB:134:GLN:HA | 41:GB:165:ASN:O | 2.06 | 0.56 |
| 40:HA:173:PRO:HB3 | 40:HA:183:GLU:HG2 | 1.86 | 0.56 |
| 40:HE:274:PRO:HB2 | 40:HE:370:VAL:HG21 | 1.88 | 0.56 |
| 40:HI:223:THR:HG23 | 40:HI:225:THR:H | 1.70 | 0.56 |
| 40:IF:188:ILE:HD12 | 40:IF:424:MET:HG3 | 1.88 | 0.56 |
| 40:JA:188:ILE:HD12 | 40:JA:424:MET:HG2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:LB:215:LEU:HD21 | 41:LB:273:LEU:HD22 | 1.88 | 0.56 |
| 40:LD:55:GLU:HG3 | 40:LD:57:GLY:H | 1.71 | 0.56 |
| 40:MG:273:ALA:O | 40:MG:274:PRO:C | 2.44 | 0.56 |
| 41:MM:273:LEU:O | 41:MM:292:GLN:NE2 | 2.38 | 0.56 |
| 40:ND:305:CYS:O | 40:ND:307:PRO:HD3 | 2.05 | 0.56 |
| 40:NH:60:LYS:NZ | 40:OH:282:TYR:HB2 | 2.21 | 0.56 |
| 41:NL:198:GLU:HA | 41:NL:264:HIS:HB2 | 1.86 | 0.56 |
| 41:NP:30:ILE:HD11 | 41:NP:47:ILE:HD11 | 1.87 | 0.56 |
| 41:QB:99:ASN:HD22 | 41:QB:178:THR:HG21 | 1.71 | 0.56 |
| 41:QL:101:TRP:HD1 | 41:QL:145:SER:HB2 | 1.71 | 0.56 |
| 41:QP:232:THR:HG21 | 41:QP:300:MET:HG3 | 1.88 | 0.56 |
| 41:RB:7:LEU:O | 41:RB:135:LEU:HA | 2.06 | 0.56 |
| 41:RO:73:MET:HG3 | 41:RO:92:PHE:HB3 | 1.87 | 0.56 |
| 40:SE:113:GLU:HG2 | 40:SE:114:LEU:HD12 | 1.87 | 0.56 |
| 41:TB:292:GLN:OE1 | 41:TB:298:ASN:ND2 | 2.36 | 0.56 |
| 40:TF:189:LEU:HD11 | 40:TF:417:PHE:HE1 | 1.70 | 0.56 |
| 40:TH:15:GLN:NE2 | 41:TO:245:GLN:OE1 | 2.39 | 0.56 |
| 40:TI:188:ILE:HG13 | 40:TI:424:MET:HG3 | 1.87 | 0.56 |
| 41:VP:107:THR:HG22 | 41:VP:108:GLU:H | 1.71 | 0.56 |
| 41:WQ:121:ARG:NH1 | 41:WQ:158:GLU:OE1 | 2.38 | 0.56 |
| 18:3T:166:ASP:OD2 | 18:3T:422:SER:OG | 2.21 | 0.56 |
| 21:4F:420:LEU:HD12 | 21:4F:512:VAL:HA | 1.88 | 0.56 |
| 22:4I:475:TYR:O | 41:FO:216:LYS:NZ | 2.35 | 0.56 |
| 23:4M:91:ILE:HD11 | 40:AG:79:ARG:HB2 | 1.87 | 0.56 |
| 23:4R:110:ASN:HA | 23:4R:113:TRP:CZ3 | 2.41 | 0.56 |
| 26:4V:271:ALA:O | 26:4V:311:MET:HA | 2.06 | 0.56 |
| 34:5R:497:LEU:HD12 | 34:5R:499:ARG:HB3 | 1.86 | 0.56 |
| 41:AN:130:LEU:O | 41:AN:162:ARG:NH1 | 2.39 | 0.56 |
| 40:BG:70:LEU:HD13 | 40:BG:145:THR:HG23 | 1.87 | 0.56 |
| 40:CE:136:LEU:HD13 | 40:CE:167:LEU:HB2 | 1.87 | 0.56 |
| 41:CL:313:VAL:HB | 41:CL:341:PHE:HZ | 1.71 | 0.56 |
| 41:CN:137:HIS:H | 41:CN:137:HIS:CD2 | 2.23 | 0.56 |
| 40:DE:70:LEU:H | 40:DE:145:THR:HG23 | 1.71 | 0.56 |
| 40:DI:114:LEU:HB3 | 40:DI:149:PHE:HE2 | 1.71 | 0.56 |
| 41:DM:103:LYS:HD2 | 41:DM:401:GLU:HG3 | 1.88 | 0.56 |
| 41:DN:112:LEU:HB3 | 41:DN:147:MET:SD | 2.46 | 0.56 |
| 41:DP:61:PRO:HD3 | 41:DP:84:ILE:HG12 | 1.87 | 0.56 |
| 40:EE:231:ILE:HA | 40:EE:234:ILE:HD12 | 1.88 | 0.56 |
| 41:EP:173:PRO:O | 41:EP:174:LYS:C | 2.44 | 0.56 |
| 41:FB:288:GLU:HA | 41:FB:291:GLN:HG3 | 1.87 | 0.56 |
| 40:FE:64:ARG:NH1 | 40:FE:129:CYS:SG | 2.79 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FM:142:GLY:O | 41:FM:144:GLY:N | 2.39 | 0.56 |
| 40:GE:11:GLN:HA | 40:GE:74:VAL:HG11 | 1.87 | 0.56 |
| 40:GE:188:ILE:HG13 | 40:GE:394:PHE:CD1 | 2.41 | 0.56 |
| 40:HA:75:ILE:HG23 | 40:HA:92:LEU:HD23 | 1.87 | 0.56 |
| 40:HE:326:LYS:O | 40:HE:327:ASP:C | 2.44 | 0.56 |
| 40:HI:174:ALA:HB3 | 40:HI:178:SER:H | 1.71 | 0.56 |
| 41:HM:4:ILE:HG21 | 41:HM:134:GLN:HG3 | 1.88 | 0.56 |
| 40:IF:164:LYS:O | 40:IF:166:LYS:NZ | 2.39 | 0.56 |
| 40:IG:319:TYR:HB3 | 40:IG:323:VAL:HG21 | 1.88 | 0.56 |
| 40:JD:89:PRO:HG2 | 40:KD:280:LYS:HG3 | 1.87 | 0.56 |
| 40:JD:266:HIS:CE1 | 40:JD:267:PHE:CE1 | 2.94 | 0.56 |
| 40:KA:319:TYR:HB3 | 40:KA:323:VAL:HG21 | 1.88 | 0.56 |
| 41:KO:237:THR:O | 41:KO:241:ARG:NH1 | 2.39 | 0.56 |
| 40:LF:363:VAL:O | 40:LF:365:GLY:N | 2.39 | 0.56 |
| 41:LL:379:LYS:NZ | 41:LL:383:GLU:OE2 | 2.37 | 0.56 |
| 41:MB:5:VAL:HG22 | 41:MB:62:ARG:HD3 | 1.88 | 0.56 |
| 40:ME:140:SER:OG | 42:ML:501:GTP:O2A | 2.22 | 0.56 |
| 40:MG:71:GLU:HG2 | 40:MG:98:ASP:HB2 | 1.88 | 0.56 |
| 40:MH:73:THR:O | 40:MH:76:ASP:N | 2.39 | 0.56 |
| 41:NN:103:LYS:NZ | 41:NN:108:GLU:OE2 | 2.36 | 0.56 |
| 40:OH:411:GLY:O | 40:OH:412:MET:C | 2.43 | 0.56 |
| 41:ON:7:LEU:O | 41:ON:135:LEU:HA | 2.06 | 0.56 |
| 41:OP:285:THR:HG23 | 41:OP:287:PRO:HD2 | 1.86 | 0.56 |
| 40:PA:238:ILE:HD11 | 40:PA:377:LEU:HD11 | 1.88 | 0.56 |
| 40:PE:251:ASP:N | 40:PE:254:GLU:OE1 | 2.39 | 0.56 |
| 40:PF:400:LYS:HD3 | 41:PM:425:ARG:HH22 | 1.71 | 0.56 |
| 41:QB:271:ALA:HA | 41:QB:298:ASN:HD21 | 1.70 | 0.56 |
| 41:QP:221:THR:O | 41:QP:222:TYR:C | 2.44 | 0.56 |
| 41:QP:269:GLY:HA3 | 41:QP:367:PHE:H | 1.70 | 0.56 |
| 41:QP:387:ALA:HA | 41:QP:390:ARG:HE | 1.70 | 0.56 |
| 40:RA:284:GLU:HG2 | 40:RA:286:LEU:HD22 | 1.87 | 0.56 |
| 41:RB:334:GLN:HA | 41:RB:341:PHE:HE2 | 1.71 | 0.56 |
| 40:SF:318:LEU:O | 40:SF:374:VAL:HA | 2.05 | 0.56 |
| 40:SI:185:TYR:HE2 | 40:SI:403:PHE:HB2 | 1.70 | 0.56 |
| 40:TE:76:ASP:OD2 | 41:TL:46:ARG:NH2 | 2.39 | 0.56 |
| 40:TF:182:VAL:O | 40:TF:186:ASN:ND2 | 2.38 | 0.56 |
| 41:TL:214:THR:OG1 | 41:TL:297:LYS:NZ | 2.35 | 0.56 |
| 41:TP:25:SER:OG | 41:TP:51:TYR:OH | 2.24 | 0.56 |
| 41:UB:375:GLN:HG3 | 41:UB:379:LYS:HE3 | 1.88 | 0.56 |
| 40:UF:329:ASN:HB3 | 41:UN:175:VAL:HG11 | 1.88 | 0.56 |
| 40:UI:187:SER:HB2 | 40:UI:390:LEU:HD21 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VA:11:GLN:HG3 | 40:VA:74:VAL:HG21 | 1.86 | 0.56 |
| 40:VG:142:GLY:O | 40:VG:186:ASN:ND2 | 2.38 | 0.56 |
| 40:WA:247:ALA:O | 41:WB:11:GLN:NE2 | 2.39 | 0.56 |
| 41:WM:141:GLY:HA3 | 43:WM:501:GDP:O1A | 2.06 | 0.56 |
| 7:1U:425:THR:HG22 | 7:1U:432:VAL:HG22 | 1.88 | 0.56 |
| 9:2B:193:GLU:HA | 9:2B:196:PHE:HD2 | 1.71 | 0.56 |
| 13:2U:62:PRO:HG3 | 13:2U:69:LEU:HD23 | 1.87 | 0.56 |
| 15:3F:383:ILE:O | 15:3F:387:GLU:HB3 | 2.06 | 0.56 |
| 17:3O:182:GLU:HA | 17:3O:185:LEU:HD23 | 1.87 | 0.56 |
| 22:4J:660:ARG:HH12 | 41:EM:38:GLY:N | 2.04 | 0.56 |
| 22:4K:511:ALA:O | 22:4K:521:LEU:HA | 2.05 | 0.56 |
| 29:5D:63:TYR:HE2 | 40:GI:19:ALA:HB2 | 1.70 | 0.56 |
| 31:5I:471:ASN:O | 40:IH:221:ARG:NH2 | 2.39 | 0.56 |
| 39:6L:4:ASN:OD1 | 39:6L:5:GLU:N | 2.38 | 0.56 |
| 40:AH:56:THR:HA | 40:BH:285:GLN:HG3 | 1.86 | 0.56 |
| 41:AM:164:MET:O | 41:AM:196:THR:OG1 | 2.23 | 0.56 |
| 41:AO:272:PRO:HB3 | 41:AO:284:LEU:HD11 | 1.88 | 0.56 |
| 40:BE:8:HIS:CE1 | 40:BE:17:GLY:HA3 | 2.40 | 0.56 |
| 40:BI:222:PRO:HD2 | 41:BP:324:LYS:NZ | 2.21 | 0.56 |
| 41:BO:372:THR:HA | 41:BO:422:VAL:HG22 | 1.88 | 0.56 |
| 41:BP:174:LYS:HG2 | 41:BP:205:GLU:HB2 | 1.87 | 0.56 |
| 40:CG:212:ILE:HD11 | 40:CG:300:ASN:HA | 1.88 | 0.56 |
| 41:CL:26:ASP:HB3 | 41:CL:359:ARG:HH22 | 1.71 | 0.56 |
| 41:CP:86:ARG:HB2 | 41:CP:89:ASN:HB2 | 1.87 | 0.56 |
| 41:DB:162:ARG:O | 41:DB:163:ILE:C | 2.45 | 0.56 |
| 40:DE:162:GLY:O | 40:DE:163:LYS:C | 2.44 | 0.56 |
| 40:DI:76:ASP:HA | 40:DI:79:ARG:NE | 2.21 | 0.56 |
| 41:EB:262:ARG:NH2 | 41:EB:414:ASN:OD1 | 2.39 | 0.56 |
| 40:EG:26:LEU:HD21 | 40:EG:363:VAL:HG23 | 1.88 | 0.56 |
| 40:EH:28:HIS:CE1 | 40:EH:243:ARG:HB2 | 2.41 | 0.56 |
| 40:EI:72:PRO:O | 40:EI:74:VAL:N | 2.39 | 0.56 |
| 40:FE:362:VAL:HG11 | 40:FE:369:LYS:HA | 1.88 | 0.56 |
| 40:FG:253:THR:HG22 | 41:FO:98:GLY:HA3 | 1.88 | 0.56 |
| 40:FI:332:ILE:HD11 | 40:FI:351:PHE:HB3 | 1.89 | 0.56 |
| 41:FO:282:ARG:HD3 | 41:FO:283:ALA:H | 1.70 | 0.56 |
| 41:GB:207:LEU:HB3 | 41:GB:225:LEU:HD22 | 1.86 | 0.56 |
| 40:GH:23:LEU:HD11 | 40:GH:233:GLN:HG2 | 1.88 | 0.56 |
| 40:GI:273:ALA:O | 40:GI:274:PRO:C | 2.44 | 0.56 |
| 41:HQ:50:TYR:HE1 | 41:HQ:241:ARG:HD2 | 1.70 | 0.56 |
| 40:IA:138:PHE:HZ | 40:IA:235:VAL:HG21 | 1.71 | 0.56 |
| 40:II:2:ARG:NH2 | 41:IQ:69:GLU:OE2 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IM:26:ASP:HB3 | 41:IM:359:ARG:HE | 1.71 | 0.56 |
| 41:IQ:213:ARG:HH22 | 41:IQ:297:LYS:HD2 | 1.71 | 0.56 |
| 41:JB:256:ASN:ND2 | 41:JB:350:LYS:HD3 | 2.21 | 0.56 |
| 41:JN:245:GLN:HG3 | 41:JN:353:VAL:HG23 | 1.88 | 0.56 |
| 41:LN:235:GLY:HA2 | 41:LN:318:ARG:HH21 | 1.70 | 0.56 |
| 41:LO:317:PHE:HB2 | 41:LO:353:VAL:HG12 | 1.88 | 0.56 |
| 41:MB:149:THR:HA | 41:MB:152:ILE:HD12 | 1.88 | 0.56 |
| 41:ML:215:LEU:HD21 | 41:ML:273:LEU:HD22 | 1.88 | 0.56 |
| 41:MO:292:GLN:HE21 | 41:MO:298:ASN:HD21 | 1.54 | 0.56 |
| 40:NG:264:ARG:NH2 | 40:NG:423:ASP:OD1 | 2.39 | 0.56 |
| 41:NN:211:CYS:HA | 41:NN:215:LEU:HB2 | 1.86 | 0.56 |
| 40:OH:106:GLY:HA3 | 40:OH:148:GLY:HA3 | 1.88 | 0.56 |
| 40:OH:295:CYS:SG | 40:OH:296:PHE:N | 2.79 | 0.56 |
| 41:ON:282:ARG:HD3 | 41:ON:283:ALA:H | 1.71 | 0.56 |
| 41:ON:377:LEU:HG | 41:ON:380:ARG:HH22 | 1.70 | 0.56 |
| 41:OP:91:VAL:HG21 | 41:OP:116:VAL:HG12 | 1.87 | 0.56 |
| 41:QP:52:ASN:O | 41:QP:60:VAL:N | 2.37 | 0.56 |
| 40:RG:205:ASP:OD2 | 40:RG:304:LYS:N | 2.38 | 0.56 |
| 41:RN:73:MET:SD | 41:RN:92:PHE:HB3 | 2.46 | 0.56 |
| 40:SH:352:LYS:HD2 | 41:SP:179:VAL:HG13 | 1.88 | 0.56 |
| 41:SL:216:LYS:O | 41:SL:276:ARG:NH1 | 2.34 | 0.56 |
| 41:SO:52:ASN:HD22 | 41:SO:86:ARG:HH22 | 1.53 | 0.56 |
| 40:TA:88:HIS:NE2 | 40:UA:284:GLU:OE2 | 2.32 | 0.56 |
| 40:TA:255:PHE:HZ | 40:TA:318:LEU:HD21 | 1.70 | 0.56 |
| 41:TB:100:ASN:HB2 | 41:TB:103:LYS:HB2 | 1.88 | 0.56 |
| 40:UE:28:HIS:CE1 | 40:UE:243:ARG:HD3 | 2.41 | 0.56 |
| 40:UG:306:ASP:OD2 | 40:UG:309:HIS:ND1 | 2.38 | 0.56 |
| 40:UH:254:GLU:HB2 | 41:UP:98:GLY:HA2 | 1.88 | 0.56 |
| 41:UM:313:VAL:HB | 41:UM:349:VAL:HG22 | 1.88 | 0.56 |
| 40:VG:20:CYS:HA | 40:VG:232:SER:HB2 | 1.88 | 0.56 |
| 40:VJ:271:THR:HA | 40:VJ:302:MET:HG2 | 1.87 | 0.56 |
| 41:WB:271:ALA:HB1 | 41:WB:292:GLN:HG2 | 1.88 | 0.56 |
| 40:WF:101:ASN:HD22 | 41:WM:256:ASN:HD21 | 1.53 | 0.56 |
| 40:WF:406:TRP:HE1 | 41:WM:258:VAL:HG23 | 1.71 | 0.56 |
| 40:WH:102:ASN:HB3 | 40:WH:105:ARG:HB3 | 1.88 | 0.56 |
| 7:1T:100:LYS:O | 7:1T:101:ARG:C | 2.44 | 0.55 |
| 7:1T:313:HIS:HE1 | 7:1T:357:ARG:HH12 | 1.52 | 0.55 |
| 9:2B:49:ILE:O | 11:2K:252:ILE:HD12 | 2.05 | 0.55 |
| 21:4D:214:GLU:OE2 | 21:4D:217:LYS:NZ | 2.35 | 0.55 |
| 23:4R:110:ASN:HD21 | 40:BI:279:GLU:CB | 2.17 | 0.55 |
| 28:5B:214:TYR:CE2 | 28:5B:215:LEU:HD23 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:5G:112:LEU:HD23 | 40:GG:113:GLU:HG2 | 1.87 | 0.55 |
| 34:5R:317:ALA:O | 34:5R:321:LEU:HG | 2.07 | 0.55 |
| 36:5X:100:HIS:O | 41:OL:279:GLN:NE2 | 2.40 | 0.55 |
| 36:5Y:181:LEU:HD22 | 41:OP:215:LEU:HD11 | 1.88 | 0.55 |
| 41:AN:27:GLU:OE2 | 41:AN:241:ARG:NH2 | 2.39 | 0.55 |
| 41:BB:210:ILE:HD11 | 41:BB:300:MET:HA | 1.87 | 0.55 |
| 40:BH:223:THR:OG1 | 40:BH:224:TYR:N | 2.39 | 0.55 |
| 41:BN:165:ASN:ND2 | 41:BN:198:GLU:OE2 | 2.39 | 0.55 |
| 40:CE:339:ARG:O | 40:CE:342:GLN:NE2 | 2.39 | 0.55 |
| 40:CG:180:ALA:HB3 | 40:CG:183:GLU:HG2 | 1.88 | 0.55 |
| 41:EL:248:ALA:HA | 41:EL:252:LYS:HD3 | 1.88 | 0.55 |
| 40:FI:274:PRO:HG3 | 40:FI:286:LEU:HD12 | 1.89 | 0.55 |
| 41:FO:274:THR:OG1 | 41:FO:282:ARG:NH1 | 2.40 | 0.55 |
| 40:HF:69:ASP:O | 40:HF:94:THR:HA | 2.06 | 0.55 |
| 41:HP:282:ARG:NH1 | 41:HP:288:GLU:OE2 | 2.39 | 0.55 |
| 40:IA:98:ASP:O | 40:IA:105:ARG:NH2 | 2.35 | 0.55 |
| 40:IF:7:VAL:HB | 40:IF:137:ILE:HG12 | 1.87 | 0.55 |
| 41:IP:253:LEU:O | 41:IP:257:MET:HB3 | 2.06 | 0.55 |
| 41:IP:307:HIS:ND1 | 41:IP:376:GLU:OE1 | 2.34 | 0.55 |
| 41:IQ:296:ALA:HB3 | 41:IQ:306:ARG:HH21 | 1.71 | 0.55 |
| 41:JB:179:VAL:HG23 | 41:JB:180:VAL:HG13 | 1.88 | 0.55 |
| 40:JE:270:ALA:HB3 | 40:JE:302:MET:HG2 | 1.88 | 0.55 |
| 41:JM:87:PRO:HD3 | 41:KM:281:TYR:CD2 | 2.40 | 0.55 |
| 41:KB:121:ARG:NH1 | 41:KB:158:GLU:OE2 | 2.39 | 0.55 |
| 40:KE:188:ILE:HD12 | 40:KE:424:MET:HG3 | 1.87 | 0.55 |
| 41:KL:87:PRO:HD3 | 41:LL:281:TYR:CD2 | 2.40 | 0.55 |
| 41:KM:313:VAL:O | 41:KM:349:VAL:HA | 2.06 | 0.55 |
| 41:KN:313:VAL:HB | 41:KN:349:VAL:HG22 | 1.87 | 0.55 |
| 41:KO:103:LYS:HA | 41:KO:107:THR:HB | 1.88 | 0.55 |
| 41:MB:23:VAL:HG23 | 41:MB:359:ARG:HH22 | 1.69 | 0.55 |
| 40:MF:326:LYS:HG2 | 41:MN:208:TYR:OH | 2.06 | 0.55 |
| 40:NF:207:GLU:HA | 40:NF:210:TYR:HB2 | 1.88 | 0.55 |
| 40:NG:401:ARG:NH2 | 40:NG:414:GLU:OE2 | 2.38 | 0.55 |
| 41:NM:252:LYS:O | 41:NM:256:ASN:ND2 | 2.39 | 0.55 |
| 41:NO:96:GLY:O | 41:NO:103:LYS:NZ | 2.39 | 0.55 |
| 41:NP:321:MET:N | 41:NP:321:MET:SD | 2.79 | 0.55 |
| 40:OD:429:LYS:HA | 40:OD:432:GLU:HG2 | 1.88 | 0.55 |
| 40:OH:115:ILE:HG13 | 40:OH:152:LEU:HG | 1.87 | 0.55 |
| 40:QA:108:TYR:O | 40:QA:112:LYS:NZ | 2.39 | 0.55 |
| 40:QF:155:GLU:OE2 | 40:QF:197:HIS:NE2 | 2.34 | 0.55 |
| 40:QH:141:PHE:HB2 | 40:QH:173:PRO:HD3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QO:232:THR:HG22 | 41:QO:270:PHE:HB2 | 1.87 | 0.55 |
| 40:RA:209:ILE:HA | 40:RA:212:ILE:HG12 | 1.87 | 0.55 |
| 40:RI:398:TYR:O | 40:RI:401:ARG:NH1 | 2.39 | 0.55 |
| 41:RM:222:TYR:O | 41:RM:226:ASN:HB2 | 2.05 | 0.55 |
| 41:RM:385:PHE:O | 41:RM:389:PHE:HB2 | 2.06 | 0.55 |
| 41:SL:209:ASP:OD1 | 41:SL:213:ARG:NH2 | 2.38 | 0.55 |
| 41:SN:132:GLY:HA2 | 41:SN:162:ARG:HB3 | 1.88 | 0.55 |
| 41:SO:155:ILE:HA | 41:SO:158:GLU:HG2 | 1.88 | 0.55 |
| 40:UA:100:ALA:HA | 41:UN:252:LYS:HB3 | 1.87 | 0.55 |
| 40:UH:88:HIS:CE1 | 40:UH:90:GLU:HG2 | 2.41 | 0.55 |
| 40:UI:4:CYS:HB2 | 40:UI:136:LEU:HD11 | 1.88 | 0.55 |
| 41:UN:139:LEU:HD12 | 41:UN:170:VAL:HG12 | 1.87 | 0.55 |
| 41:VO:62:ARG:NH1 | 41:VO:127:CYS:SG | 2.79 | 0.55 |
| 41:VO:215:LEU:HD21 | 41:VO:273:LEU:HD22 | 1.88 | 0.55 |
| 40:WH:397:MET:HG3 | 41:WO:346:PRO:HD2 | 1.89 | 0.55 |
| 40:WI:223:THR:HG23 | 40:WI:225:THR:H | 1.71 | 0.55 |
| 7:1S:511:HIS:CD2 | 7:1S:513:GLU:HG3 | 2.41 | 0.55 |
| 11:2I:119:LYS:NZ | 40:LG:408:VAL:O | 2.40 | 0.55 |
| 13:2T:42:ILE:HD13 | 13:2T:183:LEU:HD11 | 1.88 | 0.55 |
| 16:3M:200:SER:OG | 16:3M:202:LYS:NZ | 2.30 | 0.55 |
| 21:4F:414:MET:O | 21:4F:415:ASN:C | 2.45 | 0.55 |
| 26:4W:349:THR:HG22 | 26:4W:350:LYS:H | 1.71 | 0.55 |
| 31:5I:432:PHE:O | 40:IG:371:GLN:NE2 | 2.38 | 0.55 |
| 40:AF:27:GLU:OE1 | 40:AF:243:ARG:NH1 | 2.40 | 0.55 |
| 41:AO:358:PRO:HG2 | 41:AO:361:LEU:HB2 | 1.88 | 0.55 |
| 41:BP:54:ALA:O | 41:BP:55:THR:C | 2.44 | 0.55 |
| 40:CH:51:THR:HG21 | 40:CH:243:ARG:HB3 | 1.89 | 0.55 |
| 41:CM:164:MET:HB3 | 41:CM:196:THR:HA | 1.88 | 0.55 |
| 40:DA:176:GLN:O | 40:DA:177:VAL:C | 2.44 | 0.55 |
| 40:DF:6:SER:HB3 | 40:DF:138:PHE:HE1 | 1.70 | 0.55 |
| 40:DG:297:GLU:O | 40:DG:301:GLN:NE2 | 2.39 | 0.55 |
| 40:DI:163:LYS:O | 40:DI:164:LYS:C | 2.44 | 0.55 |
| 41:DL:130:LEU:O | 41:DL:132:GLY:N | 2.36 | 0.55 |
| 40:EG:185:TYR:HE2 | 40:EG:403:PHE:HB2 | 1.70 | 0.55 |
| 41:EL:192:LEU:O | 41:EL:264:HIS:NE2 | 2.40 | 0.55 |
| 41:EP:102:ALA:O | 41:EP:104:GLY:N | 2.40 | 0.55 |
| 40:FA:143:GLY:O | 40:FA:144:GLY:C | 2.44 | 0.55 |
| 40:FH:318:LEU:O | 40:FH:374:VAL:HA | 2.07 | 0.55 |
| 41:GN:200:TYR:O | 41:GN:201:CYS:C | 2.45 | 0.55 |
| 40:HE:16:ILE:HD11 | 40:HE:171:ILE:HD11 | 1.88 | 0.55 |
| 40:HE:47:ASP:O | 40:HE:48:SER:C | 2.44 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HE:102:ASN:HB3 | 40:HE:105:ARG:HG3 | 1.88 | 0.55 |
| 40:IA:262:TYR:OH | 41:IB:391:ARG:O | 2.21 | 0.55 |
| 40:IH:16:ILE:HA | 40:IH:228:ASN:HB3 | 1.88 | 0.55 |
| 41:IP:8:GLN:HE21 | 41:IP:65:LEU:HG | 1.71 | 0.55 |
| 41:IQ:134:GLN:HG2 | 41:IQ:165:ASN:HB2 | 1.88 | 0.55 |
| 40:JA:137:ILE:HG21 | 40:JA:154:MET:HE2 | 1.87 | 0.55 |
| 41:JB:103:LYS:O | 41:JB:107:THR:OG1 | 2.24 | 0.55 |
| 40:JE:322:ASP:O | 40:JE:372:ARG:NH1 | 2.40 | 0.55 |
| 40:JH:181:VAL:HG12 | 41:JO:348:ASN:HA | 1.86 | 0.55 |
| 41:JO:358:PRO:HG2 | 41:JO:361:LEU:HB2 | 1.89 | 0.55 |
| 41:KO:211:CYS:HA | 41:KO:215:LEU:HD12 | 1.88 | 0.55 |
| 40:LD:88:HIS:HD2 | 40:LD:90:GLU:H | 1.54 | 0.55 |
| 40:LE:183:GLU:HG3 | 40:LE:184:PRO:HD3 | 1.87 | 0.55 |
| 40:LG:273:ALA:CB | 40:LG:374:VAL:HG12 | 2.36 | 0.55 |
| 40:LG:352:LYS:HE3 | 41:LO:179:VAL:HG22 | 1.88 | 0.55 |
| 40:OD:84:ARG:O | 40:OD:86:LEU:N | 2.39 | 0.55 |
| 40:OH:100:ALA:HA | 41:OO:252:LYS:CG | 2.37 | 0.55 |
| 41:ON:289:LEU:O | 41:ON:293:MET:HB2 | 2.06 | 0.55 |
| 41:QB:212:PHE:HB3 | 41:QB:213:ARG:HH11 | 1.69 | 0.55 |
| 40:QG:269:LEU:HD13 | 40:QG:303:VAL:HG22 | 1.89 | 0.55 |
| 41:QM:207:LEU:HB3 | 41:QM:225:LEU:HD22 | 1.88 | 0.55 |
| 40:RE:326:LYS:O | 41:RM:208:TYR:OH | 2.22 | 0.55 |
| 41:RL:282:ARG:HE | 41:RL:283:ALA:H | 1.51 | 0.55 |
| 41:RP:199:THR:HB | 41:RP:265:PHE:HA | 1.88 | 0.55 |
| 40:TE:271:THR:HB | 40:TE:376:MET:HB3 | 1.87 | 0.55 |
| 40:TG:167:LEU:HD22 | 40:TG:200:CYS:HB3 | 1.88 | 0.55 |
| 41:TP:51:TYR:HB3 | 41:TP:59:TYR:HB3 | 1.88 | 0.55 |
| 41:TP:245:GLN:HE22 | 41:TP:246:LEU:HD23 | 1.71 | 0.55 |
| 40:UG:167:LEU:HD22 | 40:UG:202:PHE:HE1 | 1.71 | 0.55 |
| 41:UN:87:PRO:HA | 41:UN:90:PHE:HD2 | 1.72 | 0.55 |
| 41:UN:215:LEU:HD13 | 41:UN:273:LEU:HD23 | 1.89 | 0.55 |
| 40:VI:298:PRO:HB3 | 40:VI:307:PRO:HD2 | 1.87 | 0.55 |
| 40:VJ:401:ARG:NH1 | 40:VJ:414:GLU:OE2 | 2.39 | 0.55 |
| 41:WB:64:VAL:HG21 | 41:WB:120:VAL:HG22 | 1.87 | 0.55 |
| 41:WM:202:ILE:HG22 | 41:WM:207:LEU:HD21 | 1.88 | 0.55 |
| 41:WN:354:CYS:SG | 41:WN:355:ASP:N | 2.79 | 0.55 |
| 41:WO:282:ARG:HD3 | 41:WO:283:ALA:H | 1.71 | 0.55 |
| 7:1T:122:ASN:O | 7:1T:123:ASP:C | 2.44 | 0.55 |
| 7:1U:78:TYR:HD2 | 7:1U:95:LEU:HD11 | 1.71 | 0.55 |
| 9:2C:431:GLN:HE22 | 40:TI:370:VAL:HA | 1.71 | 0.55 |
| 10:2F:35:THR:O | 10:2F:39:GLN:HB2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:3O:191:PRO:HA | 17:3O:194:VAL:HG12 | 1.88 | 0.55 |
| 18:3W:340:LYS:HD3 | 18:3W:395:LEU:HD11 | 1.88 | 0.55 |
| 23:4Q:233:SER:N | 23:4Q:246:TYR:HH | 2.04 | 0.55 |
| 25:4T:379:ARG:HA | 40:KA:82:THR:HG21 | 1.87 | 0.55 |
| 27:4Z:237:SER:HB3 | 27:4Z:242:LYS:HG3 | 1.89 | 0.55 |
| 34:5R:365:GLU:HG3 | 34:5R:366:LYS:N | 2.21 | 0.55 |
| 38:6C:142:TYR:OH | 41:UO:118:ASP:OD1 | 2.25 | 0.55 |
| 40:AA:397:MET:HG3 | 41:AN:346:PRO:HD2 | 1.87 | 0.55 |
| 41:AB:172:SER:OG | 41:AB:175:VAL:O | 2.24 | 0.55 |
| 40:AE:26:LEU:HD21 | 40:AE:363:VAL:HG12 | 1.88 | 0.55 |
| 40:AF:81:GLY:O | 40:AF:84:ARG:NH1 | 2.40 | 0.55 |
| 40:BA:221:ARG:HG2 | 41:BN:322:SER:HB2 | 1.87 | 0.55 |
| 40:BA:239:THR:O | 40:BA:243:ARG:NH1 | 2.40 | 0.55 |
| 40:BH:435:GLY:O | 40:BH:436:MET:C | 2.45 | 0.55 |
| 40:BI:36:MET:O | 40:BI:37:PRO:C | 2.43 | 0.55 |
| 41:BL:132:GLY:HA3 | 41:BL:163:ILE:O | 2.07 | 0.55 |
| 41:BO:358:PRO:HG2 | 41:BO:361:LEU:HB2 | 1.88 | 0.55 |
| 41:BP:284:LEU:HA | 41:BP:288:GLU:HG2 | 1.89 | 0.55 |
| 41:CB:208:TYR:HE1 | 41:CB:225:LEU:HD21 | 1.70 | 0.55 |
| 41:CL:308:GLY:HA3 | 41:CL:372:THR:HG22 | 1.89 | 0.55 |
| 41:CM:391:ARG:O | 41:CM:392:LYS:C | 2.44 | 0.55 |
| 41:CN:391:ARG:O | 41:CN:392:LYS:C | 2.45 | 0.55 |
| 40:DA:129:CYS:O | 40:DA:130:THR:C | 2.44 | 0.55 |
| 40:DE:255:PHE:HE1 | 40:DE:318:LEU:HD21 | 1.72 | 0.55 |
| 40:DF:176:GLN:O | 40:DF:177:VAL:C | 2.45 | 0.55 |
| 40:DF:310:GLY:HA3 | 40:DF:382:ALA:HB2 | 1.87 | 0.55 |
| 41:DL:22:GLU:HG3 | 41:DL:23:VAL:N | 2.22 | 0.55 |
| 41:DP:48:ASN:O | 41:DP:49:VAL:C | 2.45 | 0.55 |
| 41:DP:271:ALA:HB2 | 41:DP:293:MET:HE3 | 1.88 | 0.55 |
| 42:EH:501:GTP:O1G | 41:EO:252:LYS:NZ | 2.39 | 0.55 |
| 41:EL:211:CYS:HA | 41:EL:215:LEU:HD12 | 1.87 | 0.55 |
| 41:FB:4:ILE:HA | 41:FB:132:GLY:O | 2.07 | 0.55 |
| 40:FE:68:VAL:HG22 | 40:FE:93:ILE:HB | 1.88 | 0.55 |
| 40:FF:70:LEU:HD13 | 40:FF:114:LEU:HD12 | 1.88 | 0.55 |
| 40:FI:390:LEU:HD23 | 40:FI:393:LYS:HD2 | 1.88 | 0.55 |
| 41:FN:114:ASP:OD2 | 41:FN:115:SER:N | 2.38 | 0.55 |
| 41:GP:287:PRO:HA | 41:GP:329:GLN:HE22 | 1.71 | 0.55 |
| 41:GP:328:GLU:OE1 | 41:GP:332:ASN:ND2 | 2.38 | 0.55 |
| 41:HN:158:GLU:O | 41:HN:160:PRO:N | 2.39 | 0.55 |
| 40:IG:234:ILE:HD11 | 40:IG:272:TYR:HB2 | 1.88 | 0.55 |
| 42:KB:502:GTP:O2' | 40:KG:206:ASN:OD1 | 2.23 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KF:297:GLU:C | 40:KF:298:PRO:HG2 | 2.26 | 0.55 |
| 41:KL:218:THR:C | 41:KL:220:PRO:HD3 | 2.26 | 0.55 |
| 40:LG:352:LYS:HG2 | 41:LO:179:VAL:HG23 | 1.87 | 0.55 |
| 41:LN:139:LEU:HD12 | 41:LN:170:VAL:HG12 | 1.88 | 0.55 |
| 40:MD:180:ALA:HB3 | 40:MD:183:GLU:HG3 | 1.89 | 0.55 |
| 40:NA:135:PHE:HD2 | 40:NA:166:LYS:HG2 | 1.70 | 0.55 |
| 40:NH:195:LEU:HD21 | 40:NH:264:ARG:NE | 2.22 | 0.55 |
| 41:NN:178:THR:HB | 41:NN:181:GLU:HG3 | 1.88 | 0.55 |
| 41:OP:273:LEU:O | 41:OP:292:GLN:NE2 | 2.36 | 0.55 |
| 40:PF:252:LEU:HA | 40:PF:255:PHE:HD2 | 1.70 | 0.55 |
| 41:QM:132:GLY:HA2 | 41:QM:162:ARG:HB3 | 1.88 | 0.55 |
| 41:QP:335:ASN:O | 41:QP:336:LYS:C | 2.44 | 0.55 |
| 41:QP:384:GLN:O | 41:QP:385:PHE:C | 2.43 | 0.55 |
| 41:RB:135:LEU:O | 41:RB:166:THR:HA | 2.07 | 0.55 |
| 41:RB:203:ASP:N | 41:RB:300:MET:O | 2.38 | 0.55 |
| 40:SF:222:PRO:O | 41:SM:322:SER:OG | 2.21 | 0.55 |
| 41:SP:267:MET:HE1 | 41:SP:299:MET:HB3 | 1.87 | 0.55 |
| 40:TF:98:ASP:O | 40:TF:105:ARG:NH1 | 2.37 | 0.55 |
| 40:TG:217:LEU:HA | 40:TG:277:SER:HB3 | 1.88 | 0.55 |
| 41:TP:248:ALA:HA | 41:TP:252:LYS:HD3 | 1.88 | 0.55 |
| 40:UF:102:ASN:HB3 | 40:UF:105:ARG:HG3 | 1.88 | 0.55 |
| 40:UF:214:ARG:HA | 40:UF:219:ILE:H | 1.71 | 0.55 |
| 40:VG:102:ASN:HB3 | 40:VG:105:ARG:HG3 | 1.88 | 0.55 |
| 40:VG:180:ALA:O | 41:VN:347:ASN:ND2 | 2.39 | 0.55 |
| 41:VP:6:HIS:O | 41:VP:63:ALA:HA | 2.06 | 0.55 |
| 41:VQ:156:ARG:NH1 | 41:VQ:162:ARG:O | 2.39 | 0.55 |
| 40:WA:73:THR:HA | 40:WA:76:ASP:HB2 | 1.88 | 0.55 |
| 40:WI:20:CYS:HA | 40:WI:232:SER:HB2 | 1.89 | 0.55 |
| 7:1U:222:LEU:HD12 | 7:1U:230:LEU:HD11 | 1.88 | 0.55 |
| 8:1W:515:ILE:HG13 | 8:1W:518:LYS:HD3 | 1.88 | 0.55 |
| 9:2B:143:TYR:HB3 | 41:TP:80:PRO:HG3 | 1.88 | 0.55 |
| 15:3H:135:GLU:HB3 | 15:3H:260:VAL:HG22 | 1.88 | 0.55 |
| 17:3O:240:ALA:HA | 17:3O:321:LEU:HD21 | 1.88 | 0.55 |
| 20:4A:149:ARG:NH1 | 20:4A:150:SER:CA | 2.69 | 0.55 |
| 21:4F:510:ASP:O | 21:4F:513:LEU:HG | 2.06 | 0.55 |
| 26:4V:329:ALA:O | 26:4V:353:ASN:ND2 | 2.39 | 0.55 |
| 26:4W:118:PHE:HB3 | 26:4W:163:ILE:HG23 | 1.88 | 0.55 |
| 34:5Q:164:LEU:CD2 | 34:5R:487:ILE:CD1 | 2.85 | 0.55 |
| 39:6L:24:GLN:HG2 | 39:6L:126:HIS:NE2 | 2.22 | 0.55 |
| 40:BE:223:THR:OG1 | 40:BE:224:TYR:N | 2.40 | 0.55 |
| 40:BE:326:LYS:HZ3 | 41:BM:208:TYR:HB2 | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BP:317:PHE:HB3 | 41:BP:321:MET:SD | 2.46 | 0.55 |
| 41:BP:371:SER:C | 41:BP:373:ALA:H | 2.08 | 0.55 |
| 41:CO:391:ARG:O | 41:CO:392:LYS:C | 2.43 | 0.55 |
| 41:CP:54:ALA:O | 41:CP:56:GLY:N | 2.40 | 0.55 |
| 40:DF:2:ARG:HB3 | 40:DF:133:GLN:HE21 | 1.72 | 0.55 |
| 41:DN:115:SER:HA | 41:DN:118:ASP:HB3 | 1.86 | 0.55 |
| 40:EE:6:SER:O | 40:EE:65:ALA:HA | 2.05 | 0.55 |
| 40:GF:73:THR:HA | 40:GF:76:ASP:HB2 | 1.88 | 0.55 |
| 40:GH:20:CYS:HA | 40:GH:232:SER:HB2 | 1.89 | 0.55 |
| 40:HG:319:TYR:HB2 | 40:HG:355:ILE:HG22 | 1.87 | 0.55 |
| 41:HN:3:GLU:HG2 | 41:HN:130:LEU:HA | 1.88 | 0.55 |
| 41:HN:391:ARG:O | 41:HN:392:LYS:C | 2.44 | 0.55 |
| 41:IP:180:VAL:HG23 | 41:IP:184:ASN:HD21 | 1.71 | 0.55 |
| 40:JA:318:LEU:O | 40:JA:374:VAL:HA | 2.07 | 0.55 |
| 40:KA:109:THR:OG1 | 40:KA:410:GLU:O | 2.24 | 0.55 |
| 40:KG:139:HIS:NE2 | 40:KG:168:GLU:OE2 | 2.39 | 0.55 |
| 40:LA:329:ASN:HB2 | 41:LB:175:VAL:HG11 | 1.88 | 0.55 |
| 40:LD:180:ALA:HB3 | 40:LD:183:GLU:HG3 | 1.87 | 0.55 |
| 40:LE:226:ASN:ND2 | 40:LE:366:ASP:OD2 | 2.39 | 0.55 |
| 41:LM:252:LYS:O | 41:LM:256:ASN:ND2 | 2.40 | 0.55 |
| 40:MF:363:VAL:O | 40:MF:365:GLY:N | 2.40 | 0.55 |
| 40:MH:139:HIS:CD2 | 40:MH:170:SER:HB2 | 2.42 | 0.55 |
| 41:MN:272:PRO:HG2 | 41:MN:364:SER:HB2 | 1.87 | 0.55 |
| 40:NA:298:PRO:HB3 | 40:NA:307:PRO:HD2 | 1.88 | 0.55 |
| 40:ND:352:LYS:HZ3 | 41:NL:99:ASN:ND2 | 2.04 | 0.55 |
| 40:NF:318:LEU:O | 40:NF:374:VAL:HA | 2.05 | 0.55 |
| 40:OF:217:LEU:HA | 40:OF:277:SER:HB3 | 1.88 | 0.55 |
| 40:OG:247:ALA:HB3 | 40:OG:355:ILE:HB | 1.88 | 0.55 |
| 40:OH:415:GLY:O | 40:OH:416:GLU:C | 2.45 | 0.55 |
| 41:OM:95:SER:OG | 41:OM:96:GLY:N | 2.39 | 0.55 |
| 40:PF:79:ARG:NH2 | 40:PF:92:LEU:O | 2.39 | 0.55 |
| 41:PP:103:LYS:HA | 41:PP:107:THR:HB | 1.88 | 0.55 |
| 40:QF:185:TYR:HE2 | 40:QF:403:PHE:HB2 | 1.72 | 0.55 |
| 40:QF:332:ILE:HA | 40:QF:335:ILE:HG22 | 1.88 | 0.55 |
| 41:QL:309:ARG:NH1 | 41:QL:339:SER:O | 2.39 | 0.55 |
| 40:RH:206:ASN:O | 41:RO:324:LYS:NZ | 2.35 | 0.55 |
| 40:RI:154:MET:HG3 | 40:RI:194:THR:HG22 | 1.88 | 0.55 |
| 41:RM:274:THR:HG21 | 41:RM:282:ARG:HG2 | 1.89 | 0.55 |
| 40:SG:258:ASN:HA | 41:SO:179:VAL:CG2 | 2.36 | 0.55 |
| 41:SO:313:VAL:HA | 41:SO:369:GLY:CA | 2.37 | 0.55 |
| 40:TF:287:SER:N | 40:TF:290:GLU:OE1 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:TG:141:PHE:HB2 | 40:TG:173:PRO:HD3 | 1.88 | 0.55 |
| 41:TN:173:PRO:HB3 | 41:TN:380:ARG:HD3 | 1.86 | 0.55 |
| 41:TP:242:PHE:HB3 | 41:TP:356:ILE:HD12 | 1.88 | 0.55 |
| 41:UB:314:ALA:HB3 | 41:UB:368:ILE:HB | 1.89 | 0.55 |
| 40:UE:431:TYR:HA | 40:UE:434:VAL:HG12 | 1.88 | 0.55 |
| 40:UF:123:ARG:HA | 40:UF:161:TYR:OH | 2.06 | 0.55 |
| 40:UI:175:PRO:HB3 | 40:UI:389:ARG:HD2 | 1.88 | 0.55 |
| 41:UN:139:LEU:HG | 41:UN:168:SER:HB3 | 1.89 | 0.55 |
| 41:UN:285:THR:HG23 | 41:UN:287:PRO:HD2 | 1.87 | 0.55 |
| 41:WB:189:VAL:HA | 41:WB:192:LEU:HB2 | 1.89 | 0.55 |
| 40:WE:224:TYR:HA | 40:WE:227:LEU:HB2 | 1.89 | 0.55 |
| 40:WH:235:VAL:HA | 40:WH:238:ILE:HG22 | 1.87 | 0.55 |
| 15:3E:235:SER:OG | 15:3E:239:LYS:NZ | 2.40 | 0.55 |
| 21:4E:309:PRO:HB3 | 41:CP:361:LEU:HG | 1.89 | 0.55 |
| 21:4F:170:ARG:HH21 | 21:4F:201:LEU:HB3 | 1.71 | 0.55 |
| 22:4I:642:CYS:HB3 | 22:4I:690:TYR:CZ | 2.42 | 0.55 |
| 22:4I:653:LEU:HD22 | 22:4I:654:PRO:HD2 | 1.88 | 0.55 |
| 22:4I:662:CYS:HA | 22:4I:667:LEU:HD23 | 1.89 | 0.55 |
| 22:4I:676:ALA:HB1 | 22:4I:680:LYS:HG2 | 1.89 | 0.55 |
| 40:AG:263:PRO:HG3 | 41:AO:396:HIS:CD2 | 2.41 | 0.55 |
| 41:AL:100:ASN:HB3 | 41:AL:103:LYS:HB2 | 1.88 | 0.55 |
| 41:AP:30:ILE:HD11 | 41:AP:47:ILE:HD11 | 1.88 | 0.55 |
| 41:BB:272:PRO:HD3 | 41:BB:364:SER:HA | 1.88 | 0.55 |
| 40:BI:272:TYR:HD2 | 40:BI:275:VAL:HG13 | 1.72 | 0.55 |
| 41:BM:271:ALA:HB1 | 41:BM:289:LEU:HB3 | 1.87 | 0.55 |
| 41:BP:138:SER:O | 41:BP:140:GLY:N | 2.40 | 0.55 |
| 41:CN:427:ALA:O | 41:CN:428:CYS:C | 2.44 | 0.55 |
| 40:DA:163:LYS:O | 40:DA:164:LYS:C | 2.45 | 0.55 |
| 40:DA:216:ASN:O | 40:DA:217:LEU:C | 2.45 | 0.55 |
| 41:DB:305:PRO:O | 41:DB:308:GLY:N | 2.39 | 0.55 |
| 40:DE:335:ILE:HG12 | 40:DE:336:LYS:N | 2.20 | 0.55 |
| 40:DI:111:GLY:O | 40:DI:112:LYS:C | 2.44 | 0.55 |
| 41:DL:226:ASN:CB | 43:DL:501:GDP:HN1 | 2.09 | 0.55 |
| 41:DM:144:GLY:O | 41:DM:145:SER:C | 2.45 | 0.55 |
| 40:EE:318:LEU:O | 40:EE:374:VAL:HA | 2.07 | 0.55 |
| 40:FA:144:GLY:O | 40:FA:145:THR:C | 2.44 | 0.55 |
| 40:FH:180:ALA:HB3 | 40:FH:183:GLU:HG3 | 1.88 | 0.55 |
| 41:FM:7:LEU:O | 41:FM:135:LEU:HA | 2.07 | 0.55 |
| 41:FN:263:LEU:HD11 | 41:FN:422:VAL:HG22 | 1.88 | 0.55 |
| 41:GO:226:ASN:HA | 41:GO:229:VAL:HG12 | 1.89 | 0.55 |
| 40:HE:335:ILE:HG23 | 40:HE:341:ILE:HD13 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HE:363:VAL:O | 40:HE:365:GLY:N | 2.40 | 0.55 |
| 40:HI:235:VAL:HA | 40:HI:238:ILE:HG22 | 1.86 | 0.55 |
| 40:HI:319:TYR:HB3 | 40:HI:323:VAL:HG21 | 1.87 | 0.55 |
| 40:IE:241:SER:OG | 40:IE:249:ASN:OD1 | 2.25 | 0.55 |
| 40:II:407:TYR:HB3 | 40:II:412:MET:HG3 | 1.89 | 0.55 |
| 41:JM:226:ASN:ND2 | 43:JM:501:GDP:HN1 | 2.05 | 0.55 |
| 40:KD:239:THR:O | 40:KD:243:ARG:NE | 2.40 | 0.55 |
| 41:KO:193:VAL:HG13 | 41:KO:194:GLU:HG2 | 1.87 | 0.55 |
| 40:LD:194:THR:O | 40:LD:198:SER:HB3 | 2.06 | 0.55 |
| 40:LD:322:ASP:O | 40:LD:372:ARG:NH1 | 2.38 | 0.55 |
| 40:LG:174:ALA:HB1 | 40:LG:177:VAL:HG23 | 1.88 | 0.55 |
| 41:LP:386:THR:O | 41:LP:390:ARG:HB2 | 2.06 | 0.55 |
| 41:MP:236:VAL:HG22 | 41:MP:368:ILE:HD11 | 1.88 | 0.55 |
| 41:NN:96:GLY:O | 41:NN:103:LYS:NZ | 2.31 | 0.55 |
| 41:OB:50:TYR:HE2 | 41:OB:241:ARG:HH21 | 1.54 | 0.55 |
| 40:OH:308:ARG:O | 40:OH:309:HIS:C | 2.45 | 0.55 |
| 41:QB:117:LEU:HD13 | 41:QB:154:LYS:HG2 | 1.89 | 0.55 |
| 40:QH:31:GLN:HG3 | 40:QH:37:PRO:HD3 | 1.88 | 0.55 |
| 40:QH:271:THR:HA | 40:QH:302:MET:HG2 | 1.89 | 0.55 |
| 40:QH:349:THR:O | 41:QP:179:VAL:HB | 2.07 | 0.55 |
| 41:QP:22:GLU:HG3 | 41:QP:23:VAL:N | 2.21 | 0.55 |
| 40:RF:436:MET:O | 41:RN:391:ARG:NH2 | 2.39 | 0.55 |
| 40:TG:362:VAL:HG13 | 40:TG:369:LYS:HZ2 | 1.71 | 0.55 |
| 40:TH:34:GLY:HA3 | 40:TH:60:LYS:HG3 | 1.89 | 0.55 |
| 40:TI:319:TYR:HB3 | 40:TI:323:VAL:HG21 | 1.87 | 0.55 |
| 40:UF:154:MET:HE1 | 40:UF:166:LYS:HB3 | 1.87 | 0.55 |
| 41:UM:230:SER:HA | 41:UM:233:MET:HB2 | 1.88 | 0.55 |
| 40:VH:328:VAL:HG11 | 40:VH:353:VAL:HG21 | 1.88 | 0.55 |
| 41:WN:391:ARG:O | 41:WN:392:LYS:C | 2.45 | 0.55 |
| 41:WO:180:VAL:HB | 41:WO:183:TYR:HB2 | 1.88 | 0.55 |
| 8:1W:508:ARG:NH2 | 8:1Y:186:GLU:OE2 | 2.40 | 0.55 |
| 13:2V:179:ALA:HA | 13:2V:182:LYS:HE2 | 1.89 | 0.55 |
| 17:3R:95:THR:O | 17:3R:96:PRO:C | 2.43 | 0.55 |
| 18:3T:313:ASP:HA | 18:3T:316:HIS:CE1 | 2.42 | 0.55 |
| 18:3T:328:GLU:HG3 | 18:3T:405:LEU:HD21 | 1.87 | 0.55 |
| 21:4D:352:ARG:HG3 | 21:4D:364:LEU:HD23 | 1.87 | 0.55 |
| 21:4F:246:TYR:HD2 | 21:4F:346:ASP:HB3 | 1.72 | 0.55 |
| 23:4M:92:PRO:HB2 | 40:AG:89:PRO:CB | 2.37 | 0.55 |
| 23:4N:184:MET:O | 23:4N:186:GLY:N | 2.39 | 0.55 |
| 23:4P:234:ARG:HG2 | 41:DN:41:ASP:HB3 | 1.87 | 0.55 |
| 41:AL:313:VAL:O | 41:AL:349:VAL:HA | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BG:326:LYS:NZ | 41:BO:225:LEU:HD21 | 2.21 | 0.55 |
| 41:BM:171:PRO:HB2 | 41:BM:381:ILE:HD11 | 1.89 | 0.55 |
| 41:BP:113:VAL:HA | 41:BP:116:VAL:HG12 | 1.87 | 0.55 |
| 40:CH:59:GLY:O | 40:CH:61:HIS:N | 2.39 | 0.55 |
| 41:DB:256:ASN:HD21 | 40:DG:101:ASN:HD21 | 1.54 | 0.55 |
| 40:EF:291:ILE:HG12 | 40:EF:374:VAL:HG12 | 1.89 | 0.55 |
| 40:EH:252:LEU:HA | 40:EH:255:PHE:CD2 | 2.42 | 0.55 |
| 40:EI:385:GLU:HA | 40:EI:388:ALA:HB3 | 1.88 | 0.55 |
| 41:EM:254:ALA:O | 41:EM:255:VAL:C | 2.44 | 0.55 |
| 41:EM:378:PHE:HB3 | 41:EM:415:MET:SD | 2.47 | 0.55 |
| 41:FB:285:THR:N | 41:FB:288:GLU:OE2 | 2.38 | 0.55 |
| 40:FE:53:PHE:HB3 | 40:FE:61:HIS:HB3 | 1.87 | 0.55 |
| 40:GA:16:ILE:HA | 40:GA:228:ASN:HD22 | 1.70 | 0.55 |
| 42:GB:502:GTP:O2B | 40:GG:145:THR:OG1 | 2.25 | 0.55 |
| 40:GE:348:PRO:HB2 | 41:GM:384:GLN:HE22 | 1.71 | 0.55 |
| 41:GM:230:SER:HA | 41:GM:233:MET:HG3 | 1.88 | 0.55 |
| 41:GP:207:LEU:HD13 | 41:GP:210:ILE:HD11 | 1.89 | 0.55 |
| 40:HA:260:VAL:HB | 41:HB:397:TRP:HH2 | 1.71 | 0.55 |
| 40:HI:242:LEU:HD21 | 40:HI:251:ASP:HA | 1.89 | 0.55 |
| 41:HO:318:ARG:HE | 41:HO:358:PRO:HD3 | 1.71 | 0.55 |
| 41:HP:95:SER:OG | 41:HP:96:GLY:N | 2.39 | 0.55 |
| 40:IG:103:TYR:HD1 | 40:IG:412:MET:HE1 | 1.71 | 0.55 |
| 40:KA:326:LYS:HD3 | 41:KB:220:PRO:HD2 | 1.89 | 0.55 |
| 40:KD:141:PHE:HB2 | 40:KD:173:PRO:HD3 | 1.89 | 0.55 |
| 40:ME:102:ASN:HB3 | 40:ME:105:ARG:HB3 | 1.89 | 0.55 |
| 40:MF:195:LEU:HD12 | 40:MF:266:HIS:NE2 | 2.22 | 0.55 |
| 41:ML:176:SER:OG | 41:ML:178:THR:O | 2.24 | 0.55 |
| 41:ML:248:ALA:HA | 41:ML:252:LYS:HD2 | 1.88 | 0.55 |
| 41:ML:392:LYS:HG3 | 41:ML:395:LEU:HD23 | 1.87 | 0.55 |
| 40:NH:89:PRO:HA | 40:NH:92:LEU:HD12 | 1.89 | 0.55 |
| 41:NP:253:LEU:O | 41:NP:257:MET:HB3 | 2.06 | 0.55 |
| 40:OD:70:LEU:HB2 | 40:OD:145:THR:HG22 | 1.87 | 0.55 |
| 40:OH:26:LEU:O | 40:OH:27:GLU:C | 2.45 | 0.55 |
| 40:PD:20:CYS:HA | 40:PD:232:SER:HB2 | 1.87 | 0.55 |
| 40:PF:141:PHE:HB2 | 40:PF:173:PRO:HD3 | 1.86 | 0.55 |
| 40:QA:269:LEU:HD21 | 40:QA:301:GLN:HB3 | 1.87 | 0.55 |
| 40:QA:320:ARG:HG2 | 40:QA:356:ASN:HB2 | 1.89 | 0.55 |
| 40:QF:189:LEU:HD11 | 40:QF:417:PHE:HE1 | 1.71 | 0.55 |
| 41:QM:135:LEU:O | 41:QM:166:THR:HA | 2.06 | 0.55 |
| 41:QN:236:VAL:HG22 | 41:QN:368:ILE:HD11 | 1.89 | 0.55 |
| 41:QO:182:PRO:HB3 | 41:QO:384:GLN:HB3 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QO:372:THR:OG1 | 41:QO:422:VAL:O | 2.23 | 0.55 |
| 41:QP:260:PHE:O | 41:QP:262:ARG:N | 2.36 | 0.55 |
| 41:RB:153:SER:OG | 41:RB:191:GLN:NE2 | 2.38 | 0.55 |
| 40:RE:416:GLU:HA | 40:RE:419:GLU:HB2 | 1.89 | 0.55 |
| 40:SF:222:PRO:HD2 | 41:SM:324:LYS:HB2 | 1.88 | 0.55 |
| 40:TE:258:ASN:HB3 | 40:TE:352:LYS:HG3 | 1.89 | 0.55 |
| 41:TM:149:THR:HG21 | 41:TM:188:SER:HA | 1.89 | 0.55 |
| 41:TM:289:LEU:O | 41:TM:293:MET:HB2 | 2.06 | 0.55 |
| 40:UG:336:LYS:NZ | 40:UG:348:PRO:O | 2.40 | 0.55 |
| 40:UH:3:GLU:N | 40:UH:3:GLU:OE1 | 2.40 | 0.55 |
| 41:UO:362:LYS:HD2 | 41:UO:363:MET:HG3 | 1.88 | 0.55 |
| 41:UP:100:ASN:O | 41:UP:101:TRP:C | 2.44 | 0.55 |
| 41:UP:238:THR:HG21 | 41:UP:318:ARG:HD2 | 1.88 | 0.55 |
| 40:WA:79:ARG:HH22 | 40:WA:94:THR:HG21 | 1.72 | 0.55 |
| 41:WB:46:ARG:NH1 | 40:WG:73:THR:OG1 | 2.37 | 0.55 |
| 41:WB:171:PRO:O | 41:WB:380:ARG:NH2 | 2.39 | 0.55 |
| 40:WE:278:ALA:H | 40:WE:368:ALA:HB2 | 1.72 | 0.55 |
| 40:WG:174:ALA:HB3 | 40:WG:178:SER:H | 1.71 | 0.55 |
| 41:WM:236:VAL:HG12 | 41:WM:250:LEU:HD22 | 1.88 | 0.55 |
| 41:WO:282:ARG:NH1 | 41:WO:288:GLU:OE2 | 2.40 | 0.55 |
| 7:1S:516:GLN:HG2 | 7:1S:530:GLU:HA | 1.87 | 0.55 |
| 7:1U:42:PRO:HB2 | 7:1U:67:VAL:HG11 | 1.89 | 0.55 |
| 11:2J:161:ARG:NH2 | 40:MF:398:TYR:O | 2.39 | 0.55 |
| 13:2V:115:LYS:HE2 | 13:2V:117:PHE:HB2 | 1.88 | 0.55 |
| 21:4F:461:ILE:O | 21:4F:462:ILE:C | 2.44 | 0.55 |
| 22:4I:439:LYS:HE3 | 22:4I:449:GLU:HB3 | 1.88 | 0.55 |
| 24:4O:201:SER:O | 24:4O:205:LEU:HG | 2.07 | 0.55 |
| 26:4V:128:LEU:HD23 | 26:4V:158:ILE:HD13 | 1.88 | 0.55 |
| 26:4V:298:GLU:HA | 26:4V:301:THR:HG22 | 1.89 | 0.55 |
| 40:BH:191:THR:HG21 | 40:BH:424:MET:SD | 2.47 | 0.55 |
| 41:BL:87:PRO:HG2 | 41:CL:277:GLY:O | 2.07 | 0.55 |
| 41:BP:189:VAL:HG11 | 41:BP:415:MET:HE3 | 1.89 | 0.55 |
| 40:CE:234:ILE:HD11 | 40:CE:272:TYR:HB2 | 1.89 | 0.55 |
| 40:CI:138:PHE:HZ | 40:CI:235:VAL:HG21 | 1.71 | 0.55 |
| 41:CL:240:LEU:HD21 | 41:CL:249:ASP:HB2 | 1.87 | 0.55 |
| 41:CM:172:SER:HA | 41:CM:380:ARG:HH12 | 1.70 | 0.55 |
| 41:CN:46:ARG:O | 41:CN:48:ASN:N | 2.39 | 0.55 |
| 41:CN:273:LEU:HB2 | 41:CN:292:GLN:HE22 | 1.70 | 0.55 |
| 41:DB:270:PHE:H | 41:DB:298:ASN:HD21 | 1.54 | 0.55 |
| 40:DE:213:CYS:SG | 40:DE:222:PRO:HG3 | 2.46 | 0.55 |
| 40:DI:214:ARG:HG2 | 40:DI:215:ARG:N | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DN:82:GLY:O | 41:DN:84:ILE:N | 2.33 | 0.55 |
| 41:DN:276:ARG:HA | 41:DN:279:GLN:HB2 | 1.87 | 0.55 |
| 41:DP:42:LEU:HD12 | 41:DP:43:GLN:HG3 | 1.88 | 0.55 |
| 40:EA:175:PRO:HB2 | 40:EA:389:ARG:HE | 1.72 | 0.55 |
| 40:EF:393:LYS:HD2 | 41:EM:346:PRO:HG3 | 1.89 | 0.55 |
| 40:FA:63:PRO:HD3 | 40:FA:86:LEU:HG | 1.89 | 0.55 |
| 41:FB:235:GLY:HA3 | 41:FB:366:THR:HG21 | 1.88 | 0.55 |
| 40:FE:298:PRO:HB3 | 40:FE:307:PRO:HD2 | 1.88 | 0.55 |
| 40:FF:97:GLU:OE2 | 41:FM:251:ARG:NH2 | 2.40 | 0.55 |
| 40:FG:141:PHE:HB2 | 40:FG:173:PRO:HD3 | 1.89 | 0.55 |
| 40:FH:20:CYS:HA | 40:FH:232:SER:HB2 | 1.88 | 0.55 |
| 41:FP:316:VAL:HG12 | 41:FP:352:ALA:HB3 | 1.86 | 0.55 |
| 41:HB:282:ARG:NH2 | 41:HB:292:GLN:OE1 | 2.36 | 0.55 |
| 40:HE:119:LEU:HA | 40:HE:122:ILE:HD13 | 1.88 | 0.55 |
| 40:HI:90:GLU:OE1 | 40:HI:121:ARG:NH2 | 2.39 | 0.55 |
| 41:HP:140:GLY:HA3 | 41:HP:181:GLU:HG3 | 1.89 | 0.55 |
| 40:IA:6:SER:O | 40:IA:65:ALA:HA | 2.06 | 0.55 |
| 40:IF:400:LYS:HZ1 | 41:IM:344:TRP:HB2 | 1.72 | 0.55 |
| 41:IQ:275:SER:O | 41:IQ:279:GLN:HB2 | 2.06 | 0.55 |
| 40:JD:269:LEU:HD21 | 40:JD:383:ILE:HD13 | 1.89 | 0.55 |
| 40:JE:70:LEU:HD22 | 40:JE:99:ALA:HB2 | 1.87 | 0.55 |
| 40:JH:171:ILE:HG21 | 42:JO:501:GTP:H1' | 1.89 | 0.55 |
| 41:JM:1:MET:O | 41:JM:2:ARG:C | 2.45 | 0.55 |
| 41:JM:392:LYS:HD2 | 41:JM:395:LEU:HD22 | 1.88 | 0.55 |
| 41:KN:173:PRO:HB3 | 41:KN:380:ARG:HD3 | 1.88 | 0.55 |
| 40:LA:50:ASN:O | 40:LA:64:ARG:NH1 | 2.40 | 0.55 |
| 41:LL:51:TYR:HB3 | 41:LL:59:TYR:HB3 | 1.89 | 0.55 |
| 41:LO:207:LEU:HB3 | 41:LO:225:LEU:HD22 | 1.87 | 0.55 |
| 40:MF:163:LYS:O | 40:MF:164:LYS:C | 2.44 | 0.55 |
| 41:ML:293:MET:HG3 | 41:ML:367:PHE:HB2 | 1.88 | 0.55 |
| 41:MP:263:LEU:HD21 | 41:MP:421:PRO:HB2 | 1.89 | 0.55 |
| 41:OB:35:THR:OG1 | 41:OB:58:LYS:NZ | 2.38 | 0.55 |
| 40:OH:320:ARG:HG2 | 40:OH:373:ALA:HB3 | 1.89 | 0.55 |
| 41:OL:271:ALA:HB1 | 41:OL:292:GLN:HG2 | 1.88 | 0.55 |
| 41:OP:236:VAL:HG13 | 41:OP:237:THR:HG23 | 1.89 | 0.55 |
| 40:PF:133:GLN:NE2 | 40:PF:251:ASP:OD1 | 2.28 | 0.55 |
| 40:PH:168:GLU:HB2 | 40:PH:201:ALA:HA | 1.88 | 0.55 |
| 40:RE:320:ARG:HG2 | 40:RE:356:ASN:HB2 | 1.89 | 0.55 |
| 40:SA:221:ARG:HD3 | 41:SN:322:SER:HB3 | 1.88 | 0.55 |
| 40:SE:154:MET:HG3 | 40:SE:194:THR:HG22 | 1.87 | 0.55 |
| 40:SF:332:ILE:HG23 | 40:SF:351:PHE:HD2 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SP:139:LEU:HD12 | 41:SP:170:VAL:HG12 | 1.87 | 0.55 |
| 40:TH:438:SER:HB2 | 41:TP:391:ARG:HD3 | 1.89 | 0.55 |
| 41:UB:259:PRO:HG2 | 41:UB:311:LEU:HD23 | 1.89 | 0.55 |
| 40:UF:261:PRO:HA | 41:UN:394:PHE:HE1 | 1.68 | 0.55 |
| 40:UG:167:LEU:HD23 | 40:UG:200:CYS:HB3 | 1.88 | 0.55 |
| 40:VG:224:TYR:O | 40:VG:228:ASN:ND2 | 2.40 | 0.55 |
| 40:VI:71:GLU:HB3 | 40:VI:98:ASP:HA | 1.89 | 0.55 |
| 41:VQ:95:SER:OG | 41:VQ:96:GLY:N | 2.40 | 0.55 |
| 41:WP:6:HIS:O | 41:WP:63:ALA:HA | 2.06 | 0.55 |
| 11:2I:88:VAL:HG11 | 41:LB:392:LYS:HG3 | 1.89 | 0.55 |
| 12:2N:146:ILE:HD13 | 12:2N:149:LEU:HD21 | 1.88 | 0.55 |
| 17:3R:330:VAL:HG12 | 17:3R:334:ASN:HD21 | 1.70 | 0.55 |
| 20:4A:198:GLN:HA | 20:4A:201:LYS:HD2 | 1.87 | 0.55 |
| 21:4D:30:THR:HG23 | 21:4D:31:LEU:HD12 | 1.87 | 0.55 |
| 21:4D:491:PHE:O | 21:4D:492:ILE:C | 2.45 | 0.55 |
| 21:4E:451:ILE:HG13 | 21:4E:467:LEU:HB2 | 1.89 | 0.55 |
| 21:4F:415:ASN:HA | 21:4F:418:LYS:HZ2 | 1.71 | 0.55 |
| 25:4T:323:GLN:OE1 | 40:JF:18:ASN:ND2 | 2.40 | 0.55 |
| 31:5I:333:THR:OG1 | 41:HN:56:GLY:HA2 | 2.07 | 0.55 |
| 32:5L:99:GLU:HG3 | 41:IP:362:LYS:HD2 | 1.89 | 0.55 |
| 36:5Y:179:PHE:O | 36:5Y:183:GLN:NE2 | 2.38 | 0.55 |
| 40:AG:109:THR:O | 40:AG:112:LYS:NZ | 2.40 | 0.55 |
| 40:AG:294:ALA:O | 40:AG:300:ASN:ND2 | 2.38 | 0.55 |
| 40:CA:182:VAL:HG23 | 40:CA:186:ASN:HD21 | 1.72 | 0.55 |
| 40:CA:260:VAL:HG13 | 40:CA:266:HIS:HB3 | 1.89 | 0.55 |
| 41:CB:240:LEU:HD12 | 41:CB:249:ASP:HB2 | 1.88 | 0.55 |
| 40:CI:64:ARG:NH2 | 40:CI:128:GLN:O | 2.39 | 0.55 |
| 41:CL:143:THR:O | 41:CL:144:GLY:C | 2.45 | 0.55 |
| 41:CP:57:GLY:O | 41:CP:59:TYR:N | 2.39 | 0.55 |
| 40:DG:15:GLN:NE2 | 42:DG:501:GTP:O6 | 2.35 | 0.55 |
| 40:DG:109:THR:HG21 | 40:DG:410:GLU:HG3 | 1.89 | 0.55 |
| 40:DH:101:ASN:N | 41:DO:252:LYS:HZ3 | 2.04 | 0.55 |
| 40:DH:102:ASN:HB3 | 40:DH:105:ARG:HG3 | 1.89 | 0.55 |
| 40:DI:1:GLN:HG3 | 40:DI:2:ARG:H | 1.70 | 0.55 |
| 41:EP:149:THR:HB | 41:EP:191:GLN:HG2 | 1.88 | 0.55 |
| 40:FA:276:ILE:HG22 | 40:FA:277:SER:H | 1.72 | 0.55 |
| 40:FA:286:LEU:HG | 40:FA:370:VAL:HG13 | 1.88 | 0.55 |
| 40:FG:51:THR:HG21 | 40:FG:242:LEU:HD13 | 1.88 | 0.55 |
| 40:FI:328:VAL:O | 40:FI:332:ILE:HB | 2.07 | 0.55 |
| 41:FP:314:ALA:HB3 | 41:FP:368:ILE:H | 1.72 | 0.55 |
| 40:GH:172:TYR:HB2 | 40:GH:203:MET:HG2 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GO:6:HIS:CE1 | 41:GO:8:GLN:HE21 | 2.25 | 0.55 |
| 40:HE:48:SER:O | 40:HE:49:PHE:C | 2.45 | 0.55 |
| 40:HE:72:PRO:O | 40:HE:74:VAL:N | 2.40 | 0.55 |
| 40:HE:254:GLU:O | 40:HE:255:PHE:C | 2.45 | 0.55 |
| 40:HF:254:GLU:O | 40:HF:258:ASN:ND2 | 2.39 | 0.55 |
| 41:HP:87:PRO:HA | 41:HP:90:PHE:HD2 | 1.72 | 0.55 |
| 41:HQ:19:LYS:HG3 | 41:HQ:226:ASN:HB2 | 1.89 | 0.55 |
| 40:JD:258:ASN:HD21 | 41:JL:99:ASN:HD22 | 1.52 | 0.55 |
| 40:JH:11:GLN:NE2 | 42:JO:501:GTP:O6 | 2.40 | 0.55 |
| 40:JH:204:VAL:HG21 | 40:JH:231:ILE:HD11 | 1.89 | 0.55 |
| 40:KA:210:TYR:HB3 | 41:KN:324:LYS:HZ3 | 1.72 | 0.55 |
| 40:KA:318:LEU:O | 40:KA:374:VAL:HA | 2.06 | 0.55 |
| 40:KF:269:LEU:HD21 | 40:KF:383:ILE:HD13 | 1.88 | 0.55 |
| 41:KO:107:THR:HG22 | 41:KO:108:GLU:H | 1.72 | 0.55 |
| 41:LB:2:ARG:HH12 | 40:LG:72:PRO:HD2 | 1.71 | 0.55 |
| 40:LE:223:THR:HG22 | 41:LL:322:SER:HA | 1.87 | 0.55 |
| 41:LL:31:ASP:OD2 | 41:LL:35:THR:OG1 | 2.24 | 0.55 |
| 40:MA:31:GLN:HG2 | 40:MA:37:PRO:HD3 | 1.87 | 0.55 |
| 40:MH:225:THR:HA | 40:MH:228:ASN:ND2 | 2.20 | 0.55 |
| 41:MM:11:GLN:HA | 41:MM:72:THR:HG21 | 1.89 | 0.55 |
| 41:MM:86:ARG:HG2 | 41:MM:88:ASP:H | 1.71 | 0.55 |
| 41:MM:421:PRO:HA | 41:MM:424:THR:HG22 | 1.88 | 0.55 |
| 41:MO:334:GLN:HE22 | 41:MO:348:ASN:H | 1.53 | 0.55 |
| 40:NG:105:ARG:HG2 | 40:NG:410:GLU:HG3 | 1.88 | 0.55 |
| 41:NO:7:LEU:HD13 | 41:NO:135:LEU:HD12 | 1.89 | 0.55 |
| 41:OB:236:VAL:HG23 | 41:OB:237:THR:HG23 | 1.87 | 0.55 |
| 41:OL:222:TYR:O | 41:OL:226:ASN:ND2 | 2.39 | 0.55 |
| 41:OM:334:GLN:HE22 | 41:OM:349:VAL:HG12 | 1.72 | 0.55 |
| 41:PB:407:GLU:HA | 41:PB:410:GLU:HB2 | 1.87 | 0.55 |
| 40:PE:206:ASN:OD1 | 42:PE:501:GTP:O2' | 2.22 | 0.55 |
| 41:PL:1:MET:HG3 | 41:PL:48:ASN:ND2 | 2.22 | 0.55 |
| 41:PO:100:ASN:HB3 | 41:PO:103:LYS:HB2 | 1.88 | 0.55 |
| 41:QB:121:ARG:O | 41:QB:125:GLU:HB2 | 2.07 | 0.55 |
| 41:QB:245:GLN:O | 41:QB:246:LEU:C | 2.45 | 0.55 |
| 41:QB:354:CYS:SG | 41:QB:355:ASP:N | 2.80 | 0.55 |
| 40:QE:426:ALA:HA | 40:QE:429:LYS:HG2 | 1.88 | 0.55 |
| 40:QG:180:ALA:HB3 | 40:QG:183:GLU:HG3 | 1.88 | 0.55 |
| 40:RA:6:SER:O | 40:RA:65:ALA:HA | 2.07 | 0.55 |
| 40:RA:181:VAL:HG22 | 41:RN:256:ASN:HD22 | 1.71 | 0.55 |
| 41:RB:276:ARG:HH12 | 41:RB:279:GLN:HG3 | 1.72 | 0.55 |
| 40:RF:88:HIS:CD2 | 40:SF:283:HIS:HB3 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RG:26:LEU:HD11 | 40:RG:363:VAL:HG22 | 1.89 | 0.55 |
| 40:RG:88:HIS:HB3 | 40:RG:91:GLN:HG2 | 1.89 | 0.55 |
| 41:RO:49:VAL:HB | 41:RO:241:ARG:HH12 | 1.71 | 0.55 |
| 41:SB:347:ASN:ND2 | 40:SG:178:SER:OG | 2.39 | 0.55 |
| 40:SF:315:CYS:HA | 40:SF:377:LEU:O | 2.06 | 0.55 |
| 41:SN:156:ARG:NH1 | 41:SN:162:ARG:O | 2.40 | 0.55 |
| 41:TN:163:ILE:HG21 | 41:TN:250:LEU:HB3 | 1.89 | 0.55 |
| 41:TP:288:GLU:O | 41:TP:292:GLN:HB2 | 2.05 | 0.55 |
| 40:UF:332:ILE:HG23 | 40:UF:351:PHE:HD2 | 1.72 | 0.55 |
| 40:VA:167:LEU:HD22 | 40:VA:200:CYS:HB3 | 1.89 | 0.55 |
| 40:VH:55:GLU:O | 40:WG:285:GLN:NE2 | 2.40 | 0.55 |
| 40:VJ:141:PHE:HB2 | 40:VJ:173:PRO:HD3 | 1.87 | 0.55 |
| 41:VN:354:CYS:SG | 41:VN:355:ASP:N | 2.80 | 0.55 |
| 41:VP:142:GLY:O | 41:VP:144:GLY:N | 2.40 | 0.55 |
| 40:WA:20:CYS:HA | 40:WA:232:SER:HB2 | 1.89 | 0.55 |
| 40:WF:260:VAL:HB | 41:WN:397:TRP:CZ3 | 2.42 | 0.55 |
| 12:2Q:154:LYS:HE2 | 41:AO:413:SER:HB3 | 1.89 | 0.55 |
| 12:2R:87:HIS:NE2 | 40:WI:126:ALA:O | 2.40 | 0.55 |
| 13:2U:135:ASN:HB3 | 13:2U:138:ASP:HB3 | 1.88 | 0.55 |
| 13:2W:2:PHE:O | 13:2W:7:GLN:NE2 | 2.39 | 0.55 |
| 13:2W:57:THR:HG23 | 13:2W:158:ALA:HB2 | 1.89 | 0.55 |
| 13:2X:78:MET:HB2 | 13:2X:80:ILE:HD11 | 1.88 | 0.55 |
| 15:3F:160:GLN:NE2 | 15:3F:164:ASN:OD1 | 2.38 | 0.55 |
| 21:4E:233:LYS:HZ2 | 40:BH:58:ALA:HB1 | 1.70 | 0.55 |
| 21:4F:433:ASP:HA | 21:4F:436:ARG:HG3 | 1.87 | 0.55 |
| 26:4V:292:VAL:HG21 | 32:5L:74:LEU:HD23 | 1.88 | 0.55 |
| 31:5I:367:LEU:HD21 | 40:IA:282:TYR:HE1 | 1.71 | 0.55 |
| 39:6H:122:ASP:HB3 | 39:6H:125:ASN:HB2 | 1.88 | 0.55 |
| 40:AA:179:THR:HG21 | 41:AN:246:LEU:HD21 | 1.88 | 0.55 |
| 40:AE:15:GLN:O | 40:AE:228:ASN:ND2 | 2.40 | 0.55 |
| 40:AH:226:ASN:ND2 | 40:AH:366:ASP:OD2 | 2.39 | 0.55 |
| 40:BA:141:PHE:HB2 | 40:BA:173:PRO:HD3 | 1.88 | 0.55 |
| 40:BI:406:TRP:CH2 | 41:BP:254:ALA:HB1 | 2.42 | 0.55 |
| 41:BM:375:GLN:HG2 | 41:BM:422:VAL:HG13 | 1.88 | 0.55 |
| 41:BN:61:PRO:HD3 | 41:BN:84:ILE:HG12 | 1.89 | 0.55 |
| 41:BP:107:THR:OG1 | 41:BP:108:GLU:N | 2.39 | 0.55 |
| 40:CH:228:ASN:OD1 | 42:CH:501:GTP:N2 | 2.36 | 0.55 |
| 41:CO:258:VAL:HG13 | 41:CO:266:PHE:HZ | 1.72 | 0.55 |
| 41:CP:425:ARG:O | 41:CP:426:GLY:C | 2.46 | 0.55 |
| 40:DA:36:MET:O | 40:DA:38:SER:N | 2.40 | 0.55 |
| 40:DG:71:GLU:HB3 | 40:DG:98:ASP:HA | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DI:315:CYS:HB3 | 40:DI:378:SER:HB2 | 1.89 | 0.55 |
| 41:DL:124:ALA:O | 41:DL:125:GLU:C | 2.45 | 0.55 |
| 41:DO:51:TYR:HB3 | 41:DO:59:TYR:HB3 | 1.89 | 0.55 |
| 40:EF:112:LYS:HA | 40:EF:115:ILE:HG22 | 1.89 | 0.55 |
| 41:EL:24:ILE:HG23 | 41:EL:241:ARG:NH2 | 2.22 | 0.55 |
| 41:EM:16:ILE:HA | 41:EM:226:ASN:ND2 | 2.22 | 0.55 |
| 40:FA:402:ALA:O | 40:FA:403:PHE:C | 2.44 | 0.55 |
| 40:GE:401:ARG:HD2 | 40:GE:404:VAL:HG21 | 1.89 | 0.55 |
| 40:GH:228:ASN:OD1 | 42:GH:501:GTP:N2 | 2.35 | 0.55 |
| 40:GI:210:TYR:OH | 41:GP:323:MET:HG3 | 2.06 | 0.55 |
| 40:HE:62:VAL:HG11 | 40:IE:283:HIS:HB3 | 1.87 | 0.55 |
| 40:HE:254:GLU:HG2 | 41:HM:98:GLY:HA2 | 1.89 | 0.55 |
| 41:HP:142:GLY:O | 41:HP:144:GLY:N | 2.40 | 0.55 |
| 40:IA:100:ALA:HA | 41:IN:252:LYS:HG3 | 1.88 | 0.55 |
| 40:IH:202:PHE:HE2 | 40:IH:238:ILE:HG12 | 1.71 | 0.55 |
| 41:IQ:49:VAL:HG21 | 41:IQ:241:ARG:HG2 | 1.87 | 0.55 |
| 40:LG:55:GLU:HG3 | 40:LG:57:GLY:H | 1.72 | 0.55 |
| 40:LG:273:ALA:O | 40:LG:274:PRO:C | 2.45 | 0.55 |
| 40:MD:207:GLU:OE2 | 40:MD:304:LYS:NZ | 2.37 | 0.55 |
| 40:MF:116:ASP:N | 40:MF:116:ASP:OD1 | 2.40 | 0.55 |
| 41:NB:211:CYS:HA | 41:NB:215:LEU:HD12 | 1.89 | 0.55 |
| 40:ND:352:LYS:HZ3 | 41:NL:99:ASN:HD22 | 1.53 | 0.55 |
| 41:NP:215:LEU:HD21 | 41:NP:273:LEU:HD12 | 1.87 | 0.55 |
| 40:OA:324:VAL:HG23 | 40:OA:327:ASP:HB2 | 1.88 | 0.55 |
| 40:OH:7:VAL:HG13 | 40:OH:66:VAL:HG13 | 1.89 | 0.55 |
| 40:OH:346:TRP:HB3 | 41:OP:391:ARG:HD2 | 1.89 | 0.55 |
| 40:OH:407:TYR:O | 40:OH:408:VAL:C | 2.44 | 0.55 |
| 41:OL:262:ARG:NH2 | 41:OL:414:ASN:OD1 | 2.39 | 0.55 |
| 40:PF:209:ILE:HD13 | 40:PF:212:ILE:HD12 | 1.87 | 0.55 |
| 41:PL:15:GLN:NE2 | 43:PL:501:GDP:O6 | 2.39 | 0.55 |
| 41:QB:308:GLY:HA3 | 41:QB:373:ALA:CA | 2.37 | 0.55 |
| 40:QG:296:PHE:CE1 | 40:QG:376:MET:HE1 | 2.42 | 0.55 |
| 40:QH:315:CYS:HA | 40:QH:377:LEU:O | 2.07 | 0.55 |
| 41:QM:51:TYR:HB3 | 41:QM:59:TYR:HB3 | 1.89 | 0.55 |
| 41:QP:48:ASN:O | 41:QP:49:VAL:C | 2.45 | 0.55 |
| 41:RB:32:PRO:HA | 41:RB:84:ILE:HD11 | 1.87 | 0.55 |
| 41:RB:135:LEU:HB3 | 41:RB:166:THR:HG22 | 1.88 | 0.55 |
| 40:RG:239:THR:O | 40:RG:243:ARG:NE | 2.39 | 0.55 |
| 40:RG:371:GLN:HG2 | 40:RG:372:ARG:HD2 | 1.89 | 0.55 |
| 40:RI:229:ARG:HH12 | 40:RI:365:GLY:HA3 | 1.72 | 0.55 |
| 41:RO:191:GLN:O | 41:RO:195:ASN:ND2 | 2.38 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:TG:318:LEU:O | 40:TG:374:VAL:HA | 2.06 | 0.55 |
| 41:TM:216:LYS:HE2 | 41:TM:275:SER:HB2 | 1.89 | 0.55 |
| 41:TP:172:SER:HB2 | 41:TP:205:GLU:HB2 | 1.89 | 0.55 |
| 41:VO:10:GLY:HA2 | 41:VO:143:THR:HG23 | 1.89 | 0.55 |
| 41:VQ:198:GLU:HG2 | 41:VQ:266:PHE:HE2 | 1.72 | 0.55 |
| 41:WN:323:MET:HA | 41:WN:326:VAL:HG23 | 1.88 | 0.55 |
| 7:1T:255:ALA:HB1 | 7:1T:296:ILE:HG13 | 1.89 | 0.55 |
| 14:3A:84:ARG:HH12 | 14:3A:92:LEU:HD12 | 1.72 | 0.55 |
| 14:3B:14:PHE:HD1 | 41:ML:174:LYS:HG3 | 1.71 | 0.55 |
| 15:3F:203:ASN:O | 15:3F:205:VAL:N | 2.40 | 0.55 |
| 17:3R:243:GLN:HE22 | 17:3R:317:ALA:HB1 | 1.72 | 0.55 |
| 19:3Y:318:ARG:NH1 | 41:LL:279:GLN:OE1 | 2.40 | 0.55 |
| 22:4J:651:LYS:HA | 22:4J:690:TYR:CE2 | 2.42 | 0.55 |
| 31:5I:573:ASP:HA | 31:5I:578:ARG:HD2 | 1.88 | 0.55 |
| 40:AG:142:GLY:HA2 | 40:AG:183:GLU:HG3 | 1.89 | 0.55 |
| 40:AG:318:LEU:O | 40:AG:374:VAL:HA | 2.07 | 0.55 |
| 40:AH:188:ILE:HG23 | 40:AH:424:MET:HG3 | 1.88 | 0.55 |
| 41:AN:31:ASP:OD2 | 41:AN:37:HIS:ND1 | 2.40 | 0.55 |
| 41:AP:173:PRO:HB3 | 41:AP:380:ARG:HD2 | 1.88 | 0.55 |
| 41:AP:273:LEU:O | 41:AP:292:GLN:NE2 | 2.34 | 0.55 |
| 40:BA:50:ASN:O | 40:BA:64:ARG:NH1 | 2.39 | 0.55 |
| 40:BE:157:LEU:HG | 40:BE:161:TYR:CD2 | 2.41 | 0.55 |
| 40:BF:213:CYS:HB3 | 40:BF:219:ILE:HB | 1.88 | 0.55 |
| 41:BO:358:PRO:HG3 | 41:BO:364:SER:CB | 2.34 | 0.55 |
| 41:BP:46:ARG:CB | 41:BP:241:ARG:HA | 2.36 | 0.55 |
| 41:BP:354:CYS:O | 41:BP:355:ASP:C | 2.44 | 0.55 |
| 40:CH:352:LYS:HA | 41:CP:177:ASP:O | 2.06 | 0.55 |
| 40:CI:180:ALA:HB1 | 41:CP:256:ASN:ND2 | 2.22 | 0.55 |
| 41:CM:3:GLU:HB2 | 41:CM:127:CYS:HB3 | 1.87 | 0.55 |
| 41:DL:181:GLU:N | 41:DL:182:PRO:HD2 | 2.22 | 0.55 |
| 41:DN:41:ASP:O | 41:DN:42:LEU:C | 2.45 | 0.55 |
| 41:EB:46:ARG:HH22 | 41:EB:243:PRO:HG3 | 1.71 | 0.55 |
| 41:EB:292:GLN:O | 41:EB:298:ASN:ND2 | 2.36 | 0.55 |
| 40:EG:73:THR:O | 40:EG:76:ASP:N | 2.39 | 0.55 |
| 41:EO:142:GLY:O | 41:EO:144:GLY:N | 2.39 | 0.55 |
| 41:EP:298:ASN:O | 41:EP:299:MET:C | 2.45 | 0.55 |
| 40:FA:72:PRO:HA | 40:FA:94:THR:HG21 | 1.89 | 0.55 |
| 41:FB:334:GLN:HE22 | 41:FB:347:ASN:HA | 1.72 | 0.55 |
| 40:FE:178:SER:OG | 40:FE:179:THR:N | 2.40 | 0.55 |
| 40:GI:109:THR:O | 40:GI:110:ILE:C | 2.46 | 0.55 |
| 41:GN:238:THR:HG21 | 41:GN:318:ARG:HE | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GP:86:ARG:NH1 | 41:HP:281:TYR:O | 2.40 | 0.55 |
| 40:HG:298:PRO:HG2 | 40:HG:308:ARG:HE | 1.72 | 0.55 |
| 41:HN:45:GLU:HG2 | 41:HN:46:ARG:HG2 | 1.88 | 0.55 |
| 41:HO:14:ASN:HD21 | 41:HO:67:ASP:HB3 | 1.72 | 0.55 |
| 41:HP:130:LEU:O | 41:HP:162:ARG:NH1 | 2.40 | 0.55 |
| 41:IQ:52:ASN:ND2 | 41:IQ:123:GLU:OE1 | 2.40 | 0.55 |
| 41:IQ:198:GLU:HA | 41:IQ:266:PHE:HE2 | 1.71 | 0.55 |
| 40:JA:247:ALA:HB3 | 40:JA:355:ILE:HD11 | 1.89 | 0.55 |
| 40:KD:79:ARG:NH2 | 40:KD:94:THR:OG1 | 2.39 | 0.55 |
| 40:KD:391:ASP:OD1 | 40:KD:421:ARG:NH2 | 2.40 | 0.55 |
| 40:KF:140:SER:OG | 42:KM:501:GTP:O2A | 2.25 | 0.55 |
| 42:LB:502:GTP:N2 | 40:LG:228:ASN:OD1 | 2.40 | 0.55 |
| 40:OA:180:ALA:HB3 | 40:OA:183:GLU:HG2 | 1.88 | 0.55 |
| 41:OP:202:ILE:HG23 | 41:OP:300:MET:HB3 | 1.89 | 0.55 |
| 40:PA:174:ALA:HB3 | 40:PA:177:VAL:HB | 1.89 | 0.55 |
| 40:PA:287:SER:OG | 40:PA:290:GLU:OE1 | 2.23 | 0.55 |
| 40:PF:177:VAL:HA | 41:PM:331:LEU:HD11 | 1.88 | 0.55 |
| 40:PH:167:LEU:HD21 | 40:PH:256:GLN:HE21 | 1.72 | 0.55 |
| 40:QA:21:TRP:HZ3 | 40:QA:52:PHE:HB3 | 1.72 | 0.55 |
| 40:QG:70:LEU:HD23 | 40:QG:114:LEU:HD12 | 1.89 | 0.55 |
| 41:RL:30:ILE:HD11 | 41:RL:47:ILE:HD11 | 1.87 | 0.55 |
| 41:RL:253:LEU:O | 41:RL:257:MET:CB | 2.55 | 0.55 |
| 41:RO:334:GLN:HA | 41:RO:341:PHE:HE2 | 1.72 | 0.55 |
| 40:SE:270:ALA:HA | 40:SE:376:MET:O | 2.07 | 0.55 |
| 40:SG:11:GLN:OE1 | 40:SG:15:GLN:NE2 | 2.40 | 0.55 |
| 40:SG:257:THR:HA | 41:SO:397:TRP:CZ2 | 2.42 | 0.55 |
| 40:SH:73:THR:HG23 | 41:SO:46:ARG:HH22 | 1.72 | 0.55 |
| 41:SL:32:PRO:HA | 41:SL:84:ILE:HD11 | 1.88 | 0.55 |
| 41:SO:319:GLY:O | 41:SO:320:ARG:C | 2.46 | 0.55 |
| 41:TM:63:ALA:O | 41:TM:89:ASN:ND2 | 2.40 | 0.55 |
| 41:TM:209:ASP:O | 41:TM:213:ARG:HB2 | 2.07 | 0.55 |
| 41:UB:8:GLN:HE21 | 41:UB:65:LEU:HD23 | 1.72 | 0.55 |
| 41:UN:10:GLY:O | 41:UN:14:ASN:HB2 | 2.07 | 0.55 |
| 41:UP:259:PRO:HG2 | 41:UP:311:LEU:HD23 | 1.89 | 0.55 |
| 40:WH:244:PHE:HB2 | 40:WH:356:ASN:HD21 | 1.72 | 0.55 |
| 40:WH:278:ALA:H | 40:WH:368:ALA:HB2 | 1.72 | 0.55 |
| 41:WM:248:ALA:HA | 41:WM:252:LYS:HE3 | 1.88 | 0.55 |
| 41:WM:314:ALA:HB3 | 41:WM:368:ILE:HB | 1.89 | 0.55 |
| 11:2J:219:ASP:HB2 | 40:VG:130:THR:HG21 | 1.89 | 0.54 |
| 12:2R:105:TYR:OH | 12:2R:137:HIS:O | 2.25 | 0.54 |
| 15:3F:343:GLU:O | 15:3F:347:ASN:ND2 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:3U:188:GLU:HB2 | 18:3U:192:ARG:NH1 | 2.21 | 0.54 |
| 18:3U:349:PRO:HA | 18:3U:352:VAL:HG22 | 1.89 | 0.54 |
| 21:4D:474:LYS:HD3 | 21:4D:497:GLU:HB2 | 1.88 | 0.54 |
| 22:4J:282:ARG:HH12 | 41:CN:80:PRO:HG3 | 1.72 | 0.54 |
| 23:4R:22:TYR:CZ | 23:4R:24:GLY:HA3 | 2.41 | 0.54 |
| 26:4V:9:PHE:HE1 | 26:4V:60:LEU:HB3 | 1.71 | 0.54 |
| 26:4V:193:ARG:HE | 26:4V:203:ASN:HD22 | 1.53 | 0.54 |
| 39:6F:146:VAL:HA | 39:6F:149:LEU:HD12 | 1.88 | 0.54 |
| 40:AH:11:GLN:HE22 | 41:AO:247:ASN:H | 1.55 | 0.54 |
| 40:BG:118:VAL:HG21 | 40:BG:149:PHE:HZ | 1.71 | 0.54 |
| 40:BI:140:SER:O | 40:BI:142:GLY:N | 2.33 | 0.54 |
| 40:BI:273:ALA:O | 40:BI:274:PRO:C | 2.44 | 0.54 |
| 41:BO:285:THR:HB | 41:BO:287:PRO:HD2 | 1.87 | 0.54 |
| 40:CA:319:TYR:HB3 | 40:CA:323:VAL:HG21 | 1.89 | 0.54 |
| 40:CE:133:GLN:NE2 | 40:CE:251:ASP:OD1 | 2.31 | 0.54 |
| 40:CH:100:ALA:O | 40:CH:101:ASN:C | 2.44 | 0.54 |
| 41:CO:226:ASN:CG | 43:CO:501:GDP:HN1 | 2.11 | 0.54 |
| 40:DE:88:HIS:CE1 | 40:DE:90:GLU:HB2 | 2.42 | 0.54 |
| 40:DI:99:ALA:HA | 40:DI:105:ARG:HH21 | 1.72 | 0.54 |
| 40:DI:167:LEU:HD11 | 40:DI:256:GLN:HE21 | 1.72 | 0.54 |
| 40:DI:273:ALA:CB | 40:DI:274:PRO:HD3 | 2.34 | 0.54 |
| 41:EB:8:GLN:HB2 | 41:EB:65:LEU:HA | 1.89 | 0.54 |
| 40:EI:400:LYS:O | 40:EI:401:ARG:C | 2.46 | 0.54 |
| 40:FA:277:SER:O | 40:FA:278:ALA:C | 2.45 | 0.54 |
| 41:FM:27:GLU:OE1 | 41:FM:241:ARG:NH2 | 2.40 | 0.54 |
| 41:FM:203:ASP:OD2 | 41:FM:302:ALA:N | 2.35 | 0.54 |
| 41:FP:226:ASN:N | 43:FP:501:GDP:HN21 | 2.05 | 0.54 |
| 40:GE:139:HIS:H | 40:GE:139:HIS:HD2 | 1.53 | 0.54 |
| 40:GI:366:ASP:O | 40:GI:367:LEU:C | 2.45 | 0.54 |
| 41:GN:397:TRP:CE3 | 41:GN:397:TRP:HA | 2.42 | 0.54 |
| 40:HA:294:ALA:O | 40:HA:300:ASN:ND2 | 2.40 | 0.54 |
| 41:HB:289:LEU:HD11 | 41:HB:363:MET:HG2 | 1.88 | 0.54 |
| 40:HE:263:PRO:HD3 | 41:HM:396:HIS:CD2 | 2.42 | 0.54 |
| 40:HH:101:ASN:HA | 40:HH:144:GLY:H | 1.71 | 0.54 |
| 41:HQ:309:ARG:NH1 | 41:HQ:343:GLU:OE1 | 2.39 | 0.54 |
| 41:IB:170:VAL:HG11 | 41:IB:377:LEU:HD21 | 1.89 | 0.54 |
| 40:IE:264:ARG:NH1 | 40:IE:430:ASP:OD2 | 2.39 | 0.54 |
| 40:II:217:LEU:HA | 40:II:277:SER:HB3 | 1.89 | 0.54 |
| 40:JD:291:ILE:HG12 | 40:JD:374:VAL:HG12 | 1.89 | 0.54 |
| 40:KG:98:ASP:O | 40:KG:105:ARG:NH1 | 2.41 | 0.54 |
| 40:KH:102:ASN:HB2 | 40:KH:105:ARG:HB2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LE:56:THR:HG22 | 40:LE:62:VAL:HG22 | 1.89 | 0.54 |
| 41:LL:248:ALA:HA | 41:LL:252:LYS:HD3 | 1.89 | 0.54 |
| 40:MA:255:PHE:HE1 | 40:MA:318:LEU:HD21 | 1.73 | 0.54 |
| 41:MM:330:MET:HB3 | 41:MM:349:VAL:HG11 | 1.89 | 0.54 |
| 41:MP:289:LEU:HD11 | 41:MP:363:MET:HG2 | 1.89 | 0.54 |
| 41:NP:31:ASP:OD2 | 41:NP:37:HIS:ND1 | 2.40 | 0.54 |
| 40:OD:318:LEU:O | 40:OD:374:VAL:HA | 2.07 | 0.54 |
| 41:OM:2:ARG:NH1 | 41:OM:240:LEU:O | 2.40 | 0.54 |
| 41:ON:271:ALA:HB1 | 41:ON:292:GLN:HG3 | 1.89 | 0.54 |
| 40:PA:437:ASP:HA | 41:PB:391:ARG:HH22 | 1.70 | 0.54 |
| 40:PF:137:ILE:HB | 40:PF:168:GLU:HG2 | 1.89 | 0.54 |
| 41:PO:287:PRO:HA | 41:PO:329:GLN:HG2 | 1.88 | 0.54 |
| 41:QB:55:THR:O | 41:QB:56:GLY:C | 2.44 | 0.54 |
| 41:QB:245:GLN:CD | 41:QB:246:LEU:H | 2.11 | 0.54 |
| 41:RB:22:GLU:HG3 | 41:RB:81:PHE:HD2 | 1.71 | 0.54 |
| 41:RB:139:LEU:HD12 | 41:RB:170:VAL:HG22 | 1.89 | 0.54 |
| 40:RF:274:PRO:HG2 | 40:RF:373:ALA:HA | 1.88 | 0.54 |
| 41:RL:248:ALA:HA | 41:RL:252:LYS:HG2 | 1.88 | 0.54 |
| 40:SA:112:LYS:HA | 40:SA:115:ILE:HG12 | 1.88 | 0.54 |
| 40:SG:324:VAL:HB | 40:SG:327:ASP:HB2 | 1.89 | 0.54 |
| 41:SO:3:GLU:HG3 | 41:SO:127:CYS:HB3 | 1.89 | 0.54 |
| 40:TH:226:ASN:ND2 | 40:TH:366:ASP:OD2 | 2.26 | 0.54 |
| 41:UB:52:ASN:OD1 | 41:UB:62:ARG:NH2 | 2.39 | 0.54 |
| 41:UP:82:GLY:O | 41:UP:84:ILE:N | 2.38 | 0.54 |
| 40:VA:262:TYR:HB2 | 40:VA:265:ILE:HG12 | 1.89 | 0.54 |
| 40:WF:210:TYR:CD1 | 41:WM:324:LYS:HE3 | 2.42 | 0.54 |
| 40:WG:318:LEU:O | 40:WG:374:VAL:HA | 2.07 | 0.54 |
| 40:WI:294:ALA:O | 40:WI:300:ASN:ND2 | 2.34 | 0.54 |
| 41:WM:30:ILE:HD11 | 41:WM:47:ILE:HD11 | 1.88 | 0.54 |
| 41:WN:163:ILE:HG23 | 41:WN:251:ARG:HH21 | 1.72 | 0.54 |
| 41:WP:68:LEU:HD23 | 41:WP:143:THR:HG23 | 1.89 | 0.54 |
| 41:WQ:98:GLY:HA3 | 41:WQ:103:LYS:HD2 | 1.88 | 0.54 |
| 7:1T:373:PRO:O | 7:1T:374:ASN:C | 2.45 | 0.54 |
| 12:2O:215:GLN:OE1 | 13:2W:38:THR:N | 2.35 | 0.54 |
| 15:3E:326:VAL:HG13 | 15:3E:327:GLU:HG3 | 1.89 | 0.54 |
| 16:3J:313:LEU:HA | 16:3L:199:ILE:HD11 | 1.89 | 0.54 |
| 22:4J:196:TYR:OH | 22:4J:200:ARG:NH2 | 2.40 | 0.54 |
| 22:4J:282:ARG:HH12 | 41:CN:80:PRO:CG | 2.20 | 0.54 |
| 22:4K:572:LYS:NZ | 22:4K:574:THR:OG1 | 2.40 | 0.54 |
| 38:6C:105:LYS:HD3 | 38:6C:115:GLY:HA3 | 1.89 | 0.54 |
| 40:AA:141:PHE:HB2 | 40:AA:173:PRO:HD3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AL:156:ARG:NH2 | 41:AL:197:ASP:OD1 | 2.39 | 0.54 |
| 40:BF:122:ILE:HG21 | 40:BF:157:LEU:HD21 | 1.89 | 0.54 |
| 40:BH:294:ALA:O | 40:BH:297:GLU:HB2 | 2.08 | 0.54 |
| 41:BN:7:LEU:HD22 | 41:BN:151:LEU:HD21 | 1.89 | 0.54 |
| 40:CE:181:VAL:HG12 | 41:CL:347:ASN:O | 2.06 | 0.54 |
| 41:CO:61:PRO:HD2 | 41:CO:84:ILE:O | 2.06 | 0.54 |
| 40:DG:128:GLN:OE1 | 40:EG:285:GLN:NE2 | 2.40 | 0.54 |
| 40:DG:246:GLY:HA3 | 40:DG:356:ASN:HA | 1.87 | 0.54 |
| 40:DI:437:ASP:O | 40:DI:438:SER:C | 2.44 | 0.54 |
| 41:DL:30:ILE:HD11 | 41:DL:84:ILE:HD13 | 1.89 | 0.54 |
| 41:DN:193:VAL:O | 41:DN:194:GLU:C | 2.45 | 0.54 |
| 40:EH:88:HIS:CD2 | 40:EH:89:PRO:HD2 | 2.41 | 0.54 |
| 41:EL:337:ASN:HB3 | 41:EL:340:TYR:HD2 | 1.72 | 0.54 |
| 41:EM:391:ARG:O | 41:EM:392:LYS:C | 2.45 | 0.54 |
| 40:GA:90:GLU:HB3 | 40:GA:121:ARG:HH22 | 1.70 | 0.54 |
| 40:GF:171:ILE:HG21 | 42:GF:501:GTP:H1' | 1.88 | 0.54 |
| 41:GM:174:LYS:HG3 | 41:GM:175:VAL:HG13 | 1.88 | 0.54 |
| 41:GP:412:GLU:OE2 | 41:GP:416:ASN:ND2 | 2.41 | 0.54 |
| 40:HA:195:LEU:HD21 | 40:HA:264:ARG:HH21 | 1.72 | 0.54 |
| 41:HQ:334:GLN:NE2 | 41:HQ:348:ASN:OD1 | 2.40 | 0.54 |
| 40:IA:70:LEU:HB2 | 40:IA:145:THR:HG22 | 1.88 | 0.54 |
| 41:IB:107:THR:HG22 | 41:IB:108:GLU:H | 1.72 | 0.54 |
| 40:IH:142:GLY:HA2 | 40:IH:183:GLU:HG3 | 1.88 | 0.54 |
| 40:KD:2:ARG:NH2 | 41:KL:70:PRO:O | 2.41 | 0.54 |
| 41:KP:213:ARG:HH12 | 41:KP:297:LYS:HD2 | 1.70 | 0.54 |
| 40:LA:311:LYS:H | 40:LA:381:THR:HG22 | 1.71 | 0.54 |
| 40:LG:167:LEU:HB3 | 40:LG:202:PHE:HE1 | 1.71 | 0.54 |
| 40:MG:137:ILE:HG21 | 40:MG:154:MET:HE3 | 1.90 | 0.54 |
| 40:ND:101:ASN:HA | 40:ND:144:GLY:CA | 2.36 | 0.54 |
| 40:NG:167:LEU:HA | 40:NG:200:CYS:O | 2.07 | 0.54 |
| 40:NH:370:VAL:HG12 | 40:NH:372:ARG:H | 1.72 | 0.54 |
| 40:OD:6:SER:O | 40:OD:65:ALA:HA | 2.07 | 0.54 |
| 40:OF:97:GLU:OE1 | 41:OM:251:ARG:NH2 | 2.30 | 0.54 |
| 41:PM:293:MET:HA | 41:PM:298:ASN:HD21 | 1.72 | 0.54 |
| 41:PN:36:TYR:OH | 41:PN:40:SER:O | 2.25 | 0.54 |
| 40:QE:100:ALA:HB2 | 41:QL:251:ARG:HB3 | 1.88 | 0.54 |
| 41:QL:5:VAL:HB | 41:QL:133:PHE:CD1 | 2.42 | 0.54 |
| 41:RB:189:VAL:HG21 | 41:RB:378:PHE:HE1 | 1.72 | 0.54 |
| 40:SF:6:SER:O | 40:SF:65:ALA:HA | 2.07 | 0.54 |
| 40:TE:16:ILE:HG13 | 40:TE:228:ASN:HB2 | 1.88 | 0.54 |
| 41:TP:238:THR:HG21 | 41:TP:318:ARG:HD3 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UB:49:VAL:HG21 | 41:UB:241:ARG:HG2 | 1.89 | 0.54 |
| 41:UP:3:GLU:H | 41:UP:130:LEU:HA | 1.72 | 0.54 |
| 40:VI:6:SER:O | 40:VI:65:ALA:HA | 2.08 | 0.54 |
| 41:WB:292:GLN:O | 41:WB:298:ASN:ND2 | 2.39 | 0.54 |
| 41:WN:137:HIS:HE1 | 41:WN:166:THR:HB | 1.70 | 0.54 |
| 7:1U:548:ILE:HD11 | 7:1U:562:THR:HB | 1.88 | 0.54 |
| 12:2N:191:ARG:HA | 12:2N:247:MET:SD | 2.48 | 0.54 |
| 16:3L:75:LYS:NZ | 16:3L:79:ASP:OD2 | 2.40 | 0.54 |
| 16:3L:96:LYS:O | 16:3L:100:GLU:CB | 2.55 | 0.54 |
| 18:3T:89:GLU:OE2 | 18:3W:346:LYS:NZ | 2.38 | 0.54 |
| 21:4D:461:ILE:O | 21:4D:462:ILE:C | 2.45 | 0.54 |
| 22:4H:232:PHE:HB2 | 22:4H:251:LEU:HB3 | 1.89 | 0.54 |
| 22:4J:656:LYS:O | 22:4J:660:ARG:HG2 | 2.08 | 0.54 |
| 23:4Q:190:TYR:O | 23:4Q:191:VAL:C | 2.45 | 0.54 |
| 23:4R:107:LYS:HG2 | 23:4R:111:GLN:CB | 2.37 | 0.54 |
| 28:5B:50:SER:HB2 | 28:5B:53:HIS:HB2 | 1.88 | 0.54 |
| 38:6C:100:PRO:HD2 | 41:UB:125:GLU:HG3 | 1.90 | 0.54 |
| 41:BL:73:MET:HB3 | 41:BL:90:PHE:CZ | 2.42 | 0.54 |
| 40:CA:195:LEU:HD11 | 40:CA:427:LEU:HD22 | 1.89 | 0.54 |
| 41:CL:206:ALA:O | 41:CL:210:ILE:HG13 | 2.07 | 0.54 |
| 41:CN:107:THR:O | 41:CN:110:ALA:N | 2.31 | 0.54 |
| 40:DA:25:CYS:HA | 40:DA:30:ILE:HB | 1.90 | 0.54 |
| 40:DA:402:ALA:C | 40:DA:404:VAL:H | 2.11 | 0.54 |
| 40:DF:261:PRO:HB3 | 40:DF:346:TRP:HH2 | 1.71 | 0.54 |
| 41:DL:14:ASN:HB3 | 41:DL:76:VAL:HG21 | 1.89 | 0.54 |
| 40:EE:207:GLU:HA | 40:EE:210:TYR:HB2 | 1.90 | 0.54 |
| 40:EH:429:LYS:HA | 40:EH:432:GLU:HB3 | 1.89 | 0.54 |
| 40:EI:140:SER:O | 40:EI:141:PHE:C | 2.44 | 0.54 |
| 41:EL:213:ARG:HH22 | 41:EL:297:LYS:HG3 | 1.71 | 0.54 |
| 41:EL:234:SER:O | 41:EL:238:THR:OG1 | 2.25 | 0.54 |
| 41:EP:417:ASP:O | 41:EP:418:LEU:C | 2.46 | 0.54 |
| 40:FA:48:SER:O | 40:FA:49:PHE:C | 2.44 | 0.54 |
| 40:FH:33:ASP:OD1 | 40:FH:34:GLY:N | 2.41 | 0.54 |
| 41:GN:377:LEU:HA | 41:GN:380:ARG:HD3 | 1.88 | 0.54 |
| 41:GO:156:ARG:NH1 | 41:GO:195:ASN:O | 2.40 | 0.54 |
| 41:GP:107:THR:HG22 | 41:GP:108:GLU:H | 1.73 | 0.54 |
| 41:HP:248:ALA:HA | 41:HP:252:LYS:HG2 | 1.89 | 0.54 |
| 40:IA:174:ALA:HB3 | 40:IA:178:SER:H | 1.71 | 0.54 |
| 40:II:328:VAL:O | 40:II:332:ILE:HG12 | 2.07 | 0.54 |
| 41:IP:314:ALA:HB3 | 41:IP:368:ILE:HB | 1.88 | 0.54 |
| 40:JA:329:ASN:HD22 | 41:JB:175:VAL:HG21 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JH:70:LEU:HD23 | 40:JH:114:LEU:HD22 | 1.90 | 0.54 |
| 41:KB:180:VAL:HG22 | 41:KB:183:TYR:HB2 | 1.90 | 0.54 |
| 40:KF:76:ASP:HA | 40:KF:79:ARG:HG2 | 1.88 | 0.54 |
| 40:KF:288:VAL:HA | 40:KF:291:ILE:HG12 | 1.90 | 0.54 |
| 41:KL:101:TRP:HD1 | 41:KL:145:SER:HB3 | 1.71 | 0.54 |
| 41:KM:51:TYR:HB3 | 41:KM:59:TYR:HB3 | 1.89 | 0.54 |
| 41:KM:117:LEU:HA | 41:KM:120:VAL:HG12 | 1.89 | 0.54 |
| 41:LB:313:VAL:HB | 41:LB:349:VAL:HG22 | 1.89 | 0.54 |
| 40:LE:228:ASN:HB3 | 40:LE:231:ILE:HD12 | 1.89 | 0.54 |
| 42:MB:502:GTP:HN21 | 40:MG:228:ASN:ND2 | 2.06 | 0.54 |
| 41:MN:221:THR:HG22 | 41:MN:223:GLY:H | 1.73 | 0.54 |
| 40:ND:109:THR:O | 40:ND:111:GLY:N | 2.40 | 0.54 |
| 41:NL:27:GLU:OE1 | 41:NL:318:ARG:NH2 | 2.39 | 0.54 |
| 41:NM:86:ARG:HA | 41:OM:281:TYR:HD2 | 1.73 | 0.54 |
| 40:OH:288:VAL:HA | 40:OH:291:ILE:HG12 | 1.89 | 0.54 |
| 40:PH:276:ILE:HG23 | 40:PH:280:LYS:HB3 | 1.88 | 0.54 |
| 41:QB:99:ASN:O | 41:QB:180:VAL:HG21 | 2.07 | 0.54 |
| 40:QE:12:ALA:HA | 40:QE:15:GLN:HE21 | 1.72 | 0.54 |
| 40:QF:246:GLY:HA3 | 40:QF:356:ASN:HA | 1.90 | 0.54 |
| 41:QL:77:ARG:HH21 | 41:QL:90:PHE:HZ | 1.55 | 0.54 |
| 41:QM:139:LEU:HD21 | 41:QM:192:LEU:HD11 | 1.88 | 0.54 |
| 41:QN:412:GLU:OE2 | 41:QN:416:ASN:ND2 | 2.40 | 0.54 |
| 41:QP:181:GLU:HA | 41:QP:184:ASN:HD21 | 1.71 | 0.54 |
| 40:RE:247:ALA:O | 41:RM:11:GLN:NE2 | 2.40 | 0.54 |
| 40:RG:433:GLU:O | 41:RO:391:ARG:NH2 | 2.41 | 0.54 |
| 40:RH:101:ASN:HD22 | 40:RH:143:GLY:HA2 | 1.71 | 0.54 |
| 41:SB:60:VAL:HG11 | 41:SB:86:ARG:HH21 | 1.73 | 0.54 |
| 40:SH:115:ILE:HD11 | 40:SH:156:ARG:HG3 | 1.89 | 0.54 |
| 41:SL:415:MET:HA | 41:SL:418:LEU:HD12 | 1.90 | 0.54 |
| 41:SO:405:GLU:HA | 41:SO:408:PHE:CD1 | 2.42 | 0.54 |
| 40:TE:248:LEU:H | 40:TE:355:ILE:HB | 1.73 | 0.54 |
| 40:TF:222:PRO:O | 41:TM:324:LYS:NZ | 2.41 | 0.54 |
| 40:TH:140:SER:OG | 42:TH:501:GTP:O2A | 2.25 | 0.54 |
| 41:TO:325:GLU:O | 41:TO:329:GLN:HG3 | 2.07 | 0.54 |
| 41:TO:380:ARG:HG3 | 41:TO:381:ILE:HD12 | 1.90 | 0.54 |
| 40:VI:98:ASP:O | 40:VI:105:ARG:NH1 | 2.38 | 0.54 |
| 41:VO:87:PRO:HD3 | 41:WN:281:TYR:HD2 | 1.72 | 0.54 |
| 40:WF:27:GLU:OE1 | 40:WF:243:ARG:NH2 | 2.40 | 0.54 |
| 12:2O:113:PHE:HB3 | 12:2O:152:PRO:HB2 | 1.89 | 0.54 |
| 13:2V:6:PHE:HB2 | 40:WI:117:LEU:HD13 | 1.88 | 0.54 |
| 13:2X:78:MET:HB3 | 13:2X:165:VAL:HG13 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2X:81:LYS:HD3 | 13:2X:161:ARG:HD3 | 1.87 | 0.54 |
| 16:3K:120:ARG:NH2 | 16:3K:134:GLU:OE2 | 2.37 | 0.54 |
| 18:3W:162:ARG:NH1 | 18:3W:166:ASP:O | 2.40 | 0.54 |
| 18:3W:172:VAL:HG23 | 18:3W:307:ARG:HG3 | 1.89 | 0.54 |
| 23:4M:106:ALA:HB2 | 40:BG:223:THR:HG23 | 1.90 | 0.54 |
| 23:4M:202:PHE:HB3 | 23:4M:203:PRO:HD3 | 1.90 | 0.54 |
| 23:4Q:257:PHE:HB3 | 41:EO:322:SER:HB3 | 1.89 | 0.54 |
| 23:4R:100:GLN:HA | 23:4R:103:PHE:CE2 | 2.40 | 0.54 |
| 23:4R:233:SER:N | 23:4R:246:TYR:HH | 2.06 | 0.54 |
| 26:4W:25:GLU:O | 26:4W:37:MET:HA | 2.06 | 0.54 |
| 33:5N:323:LEU:HD22 | 34:5Q:130:MET:HG3 | 1.88 | 0.54 |
| 41:AN:7:LEU:HD23 | 41:AN:64:VAL:HB | 1.89 | 0.54 |
| 41:AP:180:VAL:O | 41:AP:184:ASN:ND2 | 2.41 | 0.54 |
| 40:BE:313:MET:HA | 40:BE:344:VAL:HG22 | 1.89 | 0.54 |
| 40:BG:180:ALA:HB3 | 40:BG:183:GLU:HG3 | 1.89 | 0.54 |
| 40:CA:278:ALA:O | 40:CA:279:GLU:C | 2.44 | 0.54 |
| 40:CF:212:ILE:HD11 | 40:CF:300:ASN:HA | 1.89 | 0.54 |
| 41:CP:238:THR:O | 41:CP:239:CYS:C | 2.44 | 0.54 |
| 41:DB:327:ASP:O | 41:DB:328:GLU:C | 2.46 | 0.54 |
| 41:DB:395:LEU:HA | 41:DB:398:TYR:HB2 | 1.89 | 0.54 |
| 41:DN:171:PRO:HG3 | 41:DN:181:GLU:HG2 | 1.90 | 0.54 |
| 40:EH:324:VAL:O | 40:EH:326:LYS:N | 2.41 | 0.54 |
| 41:EO:134:GLN:HA | 41:EO:165:ASN:O | 2.07 | 0.54 |
| 40:GE:273:ALA:HB1 | 40:GE:291:ILE:HG22 | 1.89 | 0.54 |
| 40:GF:269:LEU:HD22 | 40:GF:303:VAL:HG21 | 1.89 | 0.54 |
| 41:GO:117:LEU:HB3 | 41:GO:121:ARG:HH22 | 1.71 | 0.54 |
| 40:HG:20:CYS:HB3 | 40:HG:24:TYR:HE2 | 1.72 | 0.54 |
| 40:HI:264:ARG:NH1 | 40:HI:430:ASP:OD2 | 2.40 | 0.54 |
| 41:HO:267:MET:HG3 | 41:HO:301:ALA:HB3 | 1.89 | 0.54 |
| 41:HQ:172:SER:OG | 41:HQ:175:VAL:O | 2.25 | 0.54 |
| 41:IB:209:ASP:OD2 | 41:IB:213:ARG:NH1 | 2.40 | 0.54 |
| 40:IE:208:ALA:HB2 | 40:IE:304:LYS:HZ1 | 1.72 | 0.54 |
| 40:IG:247:ALA:HB3 | 40:IG:355:ILE:HB | 1.90 | 0.54 |
| 41:IM:229:VAL:HA | 41:IM:300:MET:HE1 | 1.90 | 0.54 |
| 41:IO:222:TYR:O | 41:IO:226:ASN:ND2 | 2.40 | 0.54 |
| 41:JB:170:VAL:HG21 | 41:JB:377:LEU:HD11 | 1.88 | 0.54 |
| 40:JG:1:GLN:OE1 | 41:JO:94:GLN:NE2 | 2.37 | 0.54 |
| 40:JG:88:HIS:CE1 | 40:KG:280:LYS:HG3 | 2.42 | 0.54 |
| 41:JM:137:HIS:H | 41:JM:137:HIS:CD2 | 2.25 | 0.54 |
| 41:JM:143:THR:OG1 | 41:JM:144:GLY:N | 2.38 | 0.54 |
| 40:KE:328:VAL:HG11 | 40:KE:353:VAL:HG21 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KM:101:TRP:HE1 | 41:KM:188:SER:HG | 1.49 | 0.54 |
| 41:KO:132:GLY:CA | 41:KO:163:ILE:O | 2.55 | 0.54 |
| 40:LA:390:LEU:HD23 | 40:LA:393:LYS:HE3 | 1.90 | 0.54 |
| 40:LF:136:LEU:HD21 | 40:LF:252:LEU:HD11 | 1.90 | 0.54 |
| 40:LG:100:ALA:O | 40:LG:101:ASN:C | 2.45 | 0.54 |
| 41:MO:354:CYS:SG | 41:MO:355:ASP:N | 2.81 | 0.54 |
| 41:MP:178:THR:HB | 41:MP:181:GLU:HG3 | 1.89 | 0.54 |
| 40:NA:104:ALA:O | 40:NA:108:TYR:HB2 | 2.07 | 0.54 |
| 40:NG:188:ILE:HD12 | 40:NG:424:MET:HG3 | 1.89 | 0.54 |
| 41:NL:19:LYS:HG3 | 41:NL:226:ASN:HB2 | 1.89 | 0.54 |
| 41:NL:296:ALA:HB1 | 41:NL:305:PRO:HD2 | 1.89 | 0.54 |
| 40:OF:436:MET:O | 41:ON:391:ARG:NH2 | 2.40 | 0.54 |
| 40:OG:108:TYR:O | 40:OG:112:LYS:NZ | 2.41 | 0.54 |
| 40:OG:195:LEU:HD11 | 40:OG:427:LEU:HD13 | 1.89 | 0.54 |
| 40:OH:143:GLY:N | 42:OO:501:GTP:O2A | 2.40 | 0.54 |
| 40:PE:51:THR:HG21 | 40:PE:243:ARG:HG3 | 1.89 | 0.54 |
| 40:PE:189:LEU:HD11 | 40:PE:417:PHE:HE1 | 1.72 | 0.54 |
| 40:PE:235:VAL:HA | 40:PE:238:ILE:HG22 | 1.89 | 0.54 |
| 40:PH:239:THR:HG23 | 40:PH:243:ARG:HH12 | 1.73 | 0.54 |
| 41:PM:207:LEU:HB3 | 41:PM:225:LEU:HD22 | 1.90 | 0.54 |
| 41:PN:107:THR:O | 41:PN:110:ALA:N | 2.40 | 0.54 |
| 41:PO:325:GLU:O | 41:PO:329:GLN:NE2 | 2.40 | 0.54 |
| 40:RF:322:ASP:O | 40:RF:372:ARG:NH2 | 2.39 | 0.54 |
| 40:RF:326:LYS:HE3 | 41:RN:220:PRO:HG2 | 1.90 | 0.54 |
| 41:RP:273:LEU:O | 41:RP:292:GLN:NE2 | 2.36 | 0.54 |
| 40:SA:70:LEU:HD23 | 40:SA:114:LEU:HD12 | 1.89 | 0.54 |
| 41:SO:417:ASP:O | 41:SO:418:LEU:C | 2.45 | 0.54 |
| 40:TE:6:SER:O | 40:TE:65:ALA:HA | 2.07 | 0.54 |
| 40:TE:260:VAL:HG13 | 41:TM:397:TRP:HZ2 | 1.72 | 0.54 |
| 40:TI:213:CYS:HA | 40:TI:217:LEU:HB3 | 1.89 | 0.54 |
| 41:UB:124:ALA:HB1 | 41:UB:130:LEU:HD11 | 1.89 | 0.54 |
| 40:UE:168:GLU:HB2 | 40:UE:201:ALA:HA | 1.90 | 0.54 |
| 41:UP:100:ASN:O | 41:UP:102:ALA:N | 2.40 | 0.54 |
| 41:VB:284:LEU:HD11 | 41:VB:362:LYS:HD3 | 1.90 | 0.54 |
| 40:VF:27:GLU:HA | 40:VF:361:THR:HG21 | 1.90 | 0.54 |
| 40:VF:172:TYR:OH | 40:VF:386:ALA:O | 2.25 | 0.54 |
| 40:VH:60:LYS:NZ | 40:VH:85:GLN:O | 2.38 | 0.54 |
| 41:VO:87:PRO:HD3 | 41:WN:281:TYR:CD2 | 2.42 | 0.54 |
| 40:WA:96:LYS:HZ1 | 41:WN:1:MET:N | 2.06 | 0.54 |
| 41:WB:164:MET:HG2 | 41:WB:196:THR:HG22 | 1.89 | 0.54 |
| 7:1U:232:MET:HG2 | 7:1U:239:LEU:HA | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2T:119:CYS:O | 13:2T:120:THR:C | 2.45 | 0.54 |
| 16:3L:341:GLU:OE1 | 16:3M:60:ASN:ND2 | 2.40 | 0.54 |
| 17:3Q:359:ASN:HB2 | 17:3Q:360:LYS:HE3 | 1.89 | 0.54 |
| 17:3R:217:THR:O | 17:3R:218:GLU:C | 2.45 | 0.54 |
| 17:3R:232:ARG:HG3 | 17:3R:328:LEU:CD1 | 2.34 | 0.54 |
| 17:3R:253:GLU:HA | 17:3R:256:LYS:HE2 | 1.90 | 0.54 |
| 18:3U:193:THR:HG21 | 18:3U:285:ILE:HD11 | 1.88 | 0.54 |
| 18:3U:276:VAL:HA | 18:3U:279:ARG:HG3 | 1.90 | 0.54 |
| 19:3Y:276:ASP:HB2 | 41:LM:222:TYR:HB2 | 1.89 | 0.54 |
| 21:4D:498:VAL:O | 21:4D:499:PHE:C | 2.46 | 0.54 |
| 23:4M:249:TYR:CE2 | 23:4M:251:PRO:HA | 2.43 | 0.54 |
| 23:4R:98:VAL:HG21 | 23:4R:113:TRP:CD1 | 2.43 | 0.54 |
| 26:4V:87:LEU:HA | 26:4V:90:LYS:HG2 | 1.89 | 0.54 |
| 33:5N:465:LYS:NZ | 40:GE:39:ASP:OD1 | 2.41 | 0.54 |
| 38:6C:52:LYS:HD3 | 38:6C:59:ALA:HB1 | 1.88 | 0.54 |
| 40:AA:1:GLN:NE2 | 41:AB:94:GLN:OE1 | 2.39 | 0.54 |
| 41:AB:8:GLN:HE21 | 41:AB:65:LEU:HG | 1.72 | 0.54 |
| 40:BI:273:ALA:HB2 | 40:BI:374:VAL:HG12 | 1.90 | 0.54 |
| 41:BN:313:VAL:O | 41:BN:349:VAL:HA | 2.08 | 0.54 |
| 41:BP:61:PRO:HD3 | 41:BP:84:ILE:HG12 | 1.90 | 0.54 |
| 41:CB:156:ARG:NH1 | 41:CB:162:ARG:O | 2.40 | 0.54 |
| 40:CG:322:ASP:OD1 | 40:CG:372:ARG:NH1 | 2.39 | 0.54 |
| 41:CL:211:CYS:HB3 | 41:CL:220:PRO:HB3 | 1.89 | 0.54 |
| 40:DA:169:PHE:CE2 | 40:DA:238:ILE:HG21 | 2.43 | 0.54 |
| 40:DE:73:THR:O | 40:DE:74:VAL:C | 2.46 | 0.54 |
| 40:DE:253:THR:O | 40:DE:254:GLU:C | 2.44 | 0.54 |
| 40:DF:259:LEU:HA | 40:DF:314:ALA:O | 2.07 | 0.54 |
| 40:DG:316:CYS:HB3 | 40:DG:377:LEU:HB2 | 1.89 | 0.54 |
| 40:DI:143:GLY:HA3 | 42:DI:501:GTP:O3B | 2.07 | 0.54 |
| 41:DO:142:GLY:O | 41:DO:144:GLY:N | 2.41 | 0.54 |
| 41:DP:20:PHE:HZ | 41:DP:50:TYR:CE1 | 2.25 | 0.54 |
| 40:EA:258:ASN:HD22 | 40:EA:352:LYS:HB2 | 1.73 | 0.54 |
| 40:EE:116:ASP:N | 40:EE:116:ASP:OD1 | 2.40 | 0.54 |
| 40:EI:100:ALA:HB1 | 41:EP:252:LYS:HA | 1.90 | 0.54 |
| 41:EL:152:ILE:HA | 41:EL:155:ILE:HD12 | 1.89 | 0.54 |
| 41:EM:298:ASN:O | 41:EM:299:MET:C | 2.46 | 0.54 |
| 41:EM:377:LEU:O | 41:EM:381:ILE:HG23 | 2.08 | 0.54 |
| 40:FA:273:ALA:O | 40:FA:275:VAL:N | 2.40 | 0.54 |
| 40:FF:189:LEU:HD11 | 40:FF:417:PHE:HE2 | 1.71 | 0.54 |
| 40:FH:50:ASN:OD1 | 40:FH:64:ARG:NH2 | 2.41 | 0.54 |
| 41:GN:226:ASN:CG | 43:GN:501:GDP:HN1 | 2.11 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HG:26:LEU:HD21 | 40:HG:363:VAL:HG22 | 1.89 | 0.54 |
| 41:HO:118:ASP:OD2 | 41:IO:297:LYS:NZ | 2.36 | 0.54 |
| 41:HQ:125:GLU:OE2 | 41:IQ:291:GLN:NE2 | 2.39 | 0.54 |
| 40:IE:51:THR:HG21 | 40:IE:243:ARG:HG2 | 1.90 | 0.54 |
| 40:JA:313:MET:HE3 | 40:JA:346:TRP:HH2 | 1.72 | 0.54 |
| 41:JB:331:LEU:HD11 | 40:JG:177:VAL:HA | 1.90 | 0.54 |
| 40:JE:11:GLN:HG2 | 40:JE:15:GLN:HE21 | 1.73 | 0.54 |
| 41:JL:7:LEU:O | 41:JL:135:LEU:HA | 2.07 | 0.54 |
| 41:JM:222:TYR:HE2 | 43:JM:501:GDP:H2' | 1.72 | 0.54 |
| 40:KA:26:LEU:HD21 | 40:KA:363:VAL:HG23 | 1.89 | 0.54 |
| 40:KD:238:ILE:HD12 | 40:KD:377:LEU:HD11 | 1.89 | 0.54 |
| 40:KF:96:LYS:HD3 | 41:KM:129:CYS:HB2 | 1.89 | 0.54 |
| 41:KO:42:LEU:HD13 | 41:KO:356:ILE:HD11 | 1.90 | 0.54 |
| 40:LG:319:TYR:HB3 | 40:LG:323:VAL:HG21 | 1.88 | 0.54 |
| 40:MF:100:ALA:O | 40:MF:101:ASN:C | 2.44 | 0.54 |
| 41:MM:292:GLN:O | 41:MM:298:ASN:ND2 | 2.40 | 0.54 |
| 40:NG:215:ARG:NH2 | 40:NG:299:ALA:O | 2.40 | 0.54 |
| 41:PB:107:THR:HG22 | 41:PB:108:GLU:H | 1.71 | 0.54 |
| 40:PD:167:LEU:HA | 40:PD:200:CYS:O | 2.07 | 0.54 |
| 40:PF:251:ASP:OD1 | 40:PF:252:LEU:N | 2.40 | 0.54 |
| 40:QA:136:LEU:HD11 | 40:QA:169:PHE:HE1 | 1.72 | 0.54 |
| 40:QG:296:PHE:HE1 | 40:QG:376:MET:HE1 | 1.71 | 0.54 |
| 41:QL:163:ILE:HD11 | 41:QL:251:ARG:HG2 | 1.89 | 0.54 |
| 41:QP:151:LEU:O | 41:QP:152:ILE:C | 2.45 | 0.54 |
| 41:QP:222:TYR:O | 41:QP:223:GLY:C | 2.45 | 0.54 |
| 40:RA:298:PRO:HG2 | 40:RA:308:ARG:HE | 1.72 | 0.54 |
| 41:RN:74:ASP:OD1 | 41:RN:77:ARG:NH2 | 2.38 | 0.54 |
| 41:SL:222:TYR:HB3 | 43:SL:502:GDP:C6 | 2.42 | 0.54 |
| 41:SN:170:VAL:HG21 | 41:SN:377:LEU:HD21 | 1.88 | 0.54 |
| 41:SO:302:ALA:O | 41:SO:303:CYS:C | 2.46 | 0.54 |
| 41:TM:198:GLU:OE1 | 41:TM:200:TYR:OH | 2.22 | 0.54 |
| 41:TM:313:VAL:HG13 | 41:TM:367:PHE:HE2 | 1.72 | 0.54 |
| 40:UH:16:ILE:HD11 | 40:UH:138:PHE:HB3 | 1.89 | 0.54 |
| 40:UI:96:LYS:HG2 | 41:UP:129:CYS:SG | 2.48 | 0.54 |
| 41:UP:206:ALA:HB2 | 41:UP:302:ALA:N | 2.22 | 0.54 |
| 40:WA:274:PRO:HG3 | 40:WA:286:LEU:HD22 | 1.89 | 0.54 |
| 40:WE:294:ALA:O | 40:WE:300:ASN:ND2 | 2.36 | 0.54 |
| 40:WF:294:ALA:O | 40:WF:300:ASN:ND2 | 2.37 | 0.54 |
| 41:WO:350:LYS:NZ | 41:WO:351:THR:O | 2.39 | 0.54 |
| 41:WP:27:GLU:OE2 | 41:WP:318:ARG:NH2 | 2.33 | 0.54 |
| 7:1T:511:HIS:ND1 | 7:1T:513:GLU:HG3 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1U:261:THR:OG1 | 7:1U:262:GLY:N | 2.41 | 0.54 |
| 7:1U:524:ARG:HE | 7:1U:546:GLY:H | 1.56 | 0.54 |
| 8:1Y:101:ILE:CD1 | 11:2J:250:ILE:HA | 2.34 | 0.54 |
| 11:2K:207:VAL:HG11 | 11:2K:233:GLU:HB3 | 1.90 | 0.54 |
| 12:2O:47:MET:HG3 | 41:AM:336:LYS:HD3 | 1.89 | 0.54 |
| 14:3A:112:GLU:OE1 | 40:LF:163:LYS:HD3 | 2.07 | 0.54 |
| 16:3J:287:LEU:HD23 | 16:3J:370:LEU:HD21 | 1.90 | 0.54 |
| 16:3L:365:ALA:HB1 | 16:3M:31:GLN:HE21 | 1.73 | 0.54 |
| 22:4I:10:SER:HB2 | 41:MO:217:LEU:HD11 | 1.89 | 0.54 |
| 23:4M:20:PRO:HD2 | 40:BG:89:PRO:HB3 | 1.88 | 0.54 |
| 31:5I:322:THR:O | 41:IN:276:ARG:NH2 | 2.41 | 0.54 |
| 31:5I:627:ILE:HB | 31:5I:663:ILE:HB | 1.90 | 0.54 |
| 36:5X:96:GLU:OE1 | 41:OL:276:ARG:NH1 | 2.40 | 0.54 |
| 40:AE:132:LEU:HD23 | 40:AE:164:LYS:HZ2 | 1.72 | 0.54 |
| 40:AF:280:LYS:HB3 | 40:MF:88:HIS:CE1 | 2.39 | 0.54 |
| 40:AH:276:ILE:HD12 | 40:AH:281:ALA:HA | 1.90 | 0.54 |
| 40:BG:255:PHE:HZ | 40:BG:318:LEU:HD21 | 1.73 | 0.54 |
| 40:BG:318:LEU:O | 40:BG:374:VAL:HA | 2.08 | 0.54 |
| 40:CA:258:ASN:ND2 | 41:CB:180:VAL:HG22 | 2.21 | 0.54 |
| 40:CI:221:ARG:HG2 | 41:CP:322:SER:HB3 | 1.88 | 0.54 |
| 41:CL:1:MET:O | 41:CL:2:ARG:C | 2.46 | 0.54 |
| 41:CP:218:THR:O | 41:CP:220:PRO:HD3 | 2.06 | 0.54 |
| 40:DA:65:ALA:H | 40:DA:91:GLN:NE2 | 2.06 | 0.54 |
| 40:DA:137:ILE:HG23 | 40:DA:167:LEU:O | 2.08 | 0.54 |
| 40:DA:346:TRP:HB3 | 41:DB:391:ARG:HG3 | 1.89 | 0.54 |
| 40:DG:63:PRO:O | 40:DG:91:GLN:NE2 | 2.36 | 0.54 |
| 40:DH:191:THR:HA | 40:DH:194:THR:HG22 | 1.90 | 0.54 |
| 40:DI:73:THR:O | 40:DI:75:ILE:N | 2.41 | 0.54 |
| 40:DI:216:ASN:HB2 | 40:DI:275:VAL:O | 2.07 | 0.54 |
| 40:DI:258:ASN:CB | 40:DI:352:LYS:HG3 | 2.36 | 0.54 |
| 40:EA:76:ASP:HA | 40:EA:79:ARG:HG2 | 1.88 | 0.54 |
| 41:EM:9:ALA:HA | 41:EM:66:VAL:O | 2.07 | 0.54 |
| 41:EM:226:ASN:HA | 43:EM:501:GDP:HN21 | 1.72 | 0.54 |
| 41:EO:194:GLU:OE2 | 41:EO:262:ARG:NH1 | 2.41 | 0.54 |
| 40:FE:109:THR:OG1 | 40:FE:410:GLU:O | 2.25 | 0.54 |
| 40:FH:319:TYR:HB3 | 40:FH:323:VAL:HG21 | 1.88 | 0.54 |
| 40:FI:207:GLU:HA | 40:FI:210:TYR:HB2 | 1.90 | 0.54 |
| 40:FI:262:TYR:HB2 | 40:FI:265:ILE:HG12 | 1.88 | 0.54 |
| 41:FP:213:ARG:HH21 | 41:FP:297:LYS:HB3 | 1.72 | 0.54 |
| 41:FP:347:ASN:HD22 | 41:FP:347:ASN:C | 2.11 | 0.54 |
| 40:HA:73:THR:HA | 40:HA:76:ASP:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HE:239:THR:HG22 | 40:HE:252:LEU:HD21 | 1.89 | 0.54 |
| 40:HI:402:ALA:HA | 41:HP:260:PHE:HE1 | 1.73 | 0.54 |
| 40:IA:137:ILE:HB | 40:IA:168:GLU:HG2 | 1.88 | 0.54 |
| 40:IG:318:LEU:O | 40:IG:374:VAL:HA | 2.08 | 0.54 |
| 40:JA:235:VAL:HA | 40:JA:238:ILE:HG22 | 1.90 | 0.54 |
| 40:JA:294:ALA:O | 40:JA:300:ASN:ND2 | 2.41 | 0.54 |
| 41:JN:238:THR:HG21 | 41:JN:318:ARG:HD2 | 1.90 | 0.54 |
| 41:KB:234:SER:O | 41:KB:238:THR:HB | 2.08 | 0.54 |
| 41:KM:27:GLU:HA | 41:KM:359:ARG:HH12 | 1.72 | 0.54 |
| 41:KO:236:VAL:HG22 | 41:KO:368:ILE:HD11 | 1.89 | 0.54 |
| 41:LB:282:ARG:NH2 | 41:LB:288:GLU:OE2 | 2.41 | 0.54 |
| 40:LG:12:ALA:O | 40:LG:16:ILE:HG13 | 2.07 | 0.54 |
| 40:MA:317:LEU:HB3 | 40:MA:319:TYR:CE1 | 2.43 | 0.54 |
| 41:MB:404:ASP:N | 41:MB:404:ASP:OD2 | 2.41 | 0.54 |
| 40:ND:318:LEU:HD12 | 40:ND:354:GLY:HA3 | 1.87 | 0.54 |
| 40:NF:221:ARG:HH12 | 41:NM:325:GLU:H | 1.54 | 0.54 |
| 41:NM:167:PHE:CD2 | 41:NM:233:MET:HG2 | 2.43 | 0.54 |
| 41:PB:15:GLN:NE2 | 43:PB:501:GDP:O6 | 2.41 | 0.54 |
| 40:PE:228:ASN:HA | 40:PE:231:ILE:HD12 | 1.88 | 0.54 |
| 40:PF:21:TRP:HA | 40:PF:24:TYR:HD1 | 1.71 | 0.54 |
| 40:PG:128:GLN:HE21 | 40:QG:285:GLN:HG3 | 1.71 | 0.54 |
| 41:QL:178:THR:HB | 41:QL:181:GLU:HG3 | 1.90 | 0.54 |
| 41:QP:125:GLU:O | 41:QP:126:SER:C | 2.46 | 0.54 |
| 40:RF:97:GLU:OE2 | 40:RF:105:ARG:NH2 | 2.37 | 0.54 |
| 40:RG:185:TYR:HE2 | 40:RG:403:PHE:HB2 | 1.71 | 0.54 |
| 41:RO:179:VAL:HG23 | 41:RO:180:VAL:HG13 | 1.90 | 0.54 |
| 41:SM:216:LYS:HE2 | 41:SM:275:SER:HB3 | 1.89 | 0.54 |
| 41:SO:357:PRO:HB2 | 41:SO:361:LEU:O | 2.07 | 0.54 |
| 41:SP:51:TYR:HB3 | 41:SP:59:TYR:HB3 | 1.90 | 0.54 |
| 41:UB:372:THR:OG1 | 41:UB:422:VAL:O | 2.25 | 0.54 |
| 40:UF:291:ILE:HG12 | 40:UF:292:THR:N | 2.22 | 0.54 |
| 40:UH:326:LYS:HE3 | 41:UP:208:TYR:CB | 2.33 | 0.54 |
| 40:UI:277:SER:HA | 40:UI:368:ALA:HB2 | 1.89 | 0.54 |
| 40:UI:437:ASP:O | 40:UI:438:SER:C | 2.46 | 0.54 |
| 41:UM:178:THR:HB | 41:UM:181:GLU:HB3 | 1.90 | 0.54 |
| 41:UN:128:ASP:OD2 | 41:UN:129:CYS:N | 2.41 | 0.54 |
| 41:UP:282:ARG:HH11 | 41:UP:283:ALA:H | 1.56 | 0.54 |
| 41:VB:392:LYS:HE2 | 41:VB:395:LEU:HD22 | 1.90 | 0.54 |
| 40:VG:254:GLU:OE1 | 41:VO:99:ASN:ND2 | 2.41 | 0.54 |
| 41:VQ:285:THR:N | 41:VQ:288:GLU:OE2 | 2.41 | 0.54 |
| 40:WF:98:ASP:O | 40:WF:105:ARG:NH1 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1T:506:GLN:HG3 | 7:1T:549:ASN:HA | 1.90 | 0.54 |
| 9:2B:278:LYS:NZ | 40:TA:365:GLY:O | 2.36 | 0.54 |
| 11:2I:161:ARG:O | 11:2I:165:VAL:HG22 | 2.07 | 0.54 |
| 17:3O:470:GLN:HG3 | 17:3O:471:GLU:HG2 | 1.90 | 0.54 |
| 17:3P:164:LEU:HD13 | 17:3P:254:LEU:HB3 | 1.90 | 0.54 |
| 17:3P:212:HIS:CE1 | 17:3P:217:THR:HG22 | 2.43 | 0.54 |
| 22:4J:157:ASP:OD1 | 22:4J:166:LYS:NZ | 2.41 | 0.54 |
| 22:4K:439:LYS:O | 22:4K:521:LEU:N | 2.38 | 0.54 |
| 23:4N:233:SER:N | 23:4N:242:LEU:HD22 | 2.23 | 0.54 |
| 26:4W:12:GLU:OE2 | 26:4W:23:ARG:NH2 | 2.41 | 0.54 |
| 27:4Y:47:LYS:O | 27:4Y:51:LEU:HB2 | 2.08 | 0.54 |
| 31:5J:835:SER:OG | 31:5J:837:ASP:OD1 | 2.22 | 0.54 |
| 36:5Z:256:ARG:NH1 | 40:LD:433:GLU:OE2 | 2.41 | 0.54 |
| 41:BB:21:TRP:CZ2 | 41:BB:63:ALA:HB2 | 2.43 | 0.54 |
| 41:BB:358:PRO:CG | 41:BB:364:SER:HB3 | 2.31 | 0.54 |
| 41:BO:244:GLY:HA3 | 41:BO:354:CYS:HA | 1.90 | 0.54 |
| 40:CA:100:ALA:HB1 | 41:CN:252:LYS:HA | 1.90 | 0.54 |
| 40:CA:294:ALA:O | 40:CA:297:GLU:HB2 | 2.07 | 0.54 |
| 40:CE:294:ALA:O | 40:CE:300:ASN:ND2 | 2.40 | 0.54 |
| 40:CH:317:LEU:HD21 | 40:CH:332:ILE:HD11 | 1.89 | 0.54 |
| 40:CI:259:LEU:O | 40:CI:379:ASN:ND2 | 2.40 | 0.54 |
| 41:CL:309:ARG:HD3 | 41:CL:342:VAL:HA | 1.90 | 0.54 |
| 41:CM:13:GLY:HA3 | 41:CM:136:THR:O | 2.08 | 0.54 |
| 40:DA:213:CYS:HB3 | 40:DA:219:ILE:CG2 | 2.38 | 0.54 |
| 40:DF:291:ILE:HG12 | 40:DF:292:THR:N | 2.22 | 0.54 |
| 40:DH:86:LEU:O | 40:DH:87:PHE:C | 2.46 | 0.54 |
| 40:DI:31:GLN:HB2 | 40:DI:35:GLN:O | 2.08 | 0.54 |
| 41:DM:107:THR:OG1 | 41:DM:108:GLU:N | 2.40 | 0.54 |
| 41:EM:8:GLN:HE21 | 41:EM:17:GLY:HA2 | 1.73 | 0.54 |
| 41:EM:272:PRO:HG3 | 41:EM:364:SER:HB2 | 1.89 | 0.54 |
| 40:FA:144:GLY:O | 40:FA:147:SER:N | 2.37 | 0.54 |
| 40:FE:6:SER:O | 40:FE:65:ALA:HA | 2.08 | 0.54 |
| 40:FF:235:VAL:HA | 40:FF:238:ILE:HG22 | 1.90 | 0.54 |
| 40:FF:324:VAL:HG12 | 40:FF:326:LYS:H | 1.73 | 0.54 |
| 40:FG:297:GLU:OE2 | 40:FG:300:ASN:ND2 | 2.41 | 0.54 |
| 41:FP:122:LYS:NZ | 41:GP:291:GLN:O | 2.41 | 0.54 |
| 40:GA:294:ALA:O | 40:GA:300:ASN:ND2 | 2.39 | 0.54 |
| 40:GE:218:ASP:O | 40:GE:219:ILE:C | 2.45 | 0.54 |
| 41:GO:210:ILE:HD12 | 41:GO:298:ASN:HA | 1.89 | 0.54 |
| 40:HH:55:GLU:OE2 | 40:HH:61:HIS:NE2 | 2.40 | 0.54 |
| 41:HO:161:ASP:O | 41:HO:162:ARG:NH1 | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HO:222:TYR:O | 41:HO:226:ASN:ND2 | 2.41 | 0.54 |
| 40:JD:244:PHE:HD2 | 40:JD:356:ASN:HD21 | 1.55 | 0.54 |
| 40:JE:204:VAL:HA | 40:JE:302:MET:HG3 | 1.88 | 0.54 |
| 40:JH:204:VAL:HG23 | 40:JH:302:MET:HG2 | 1.88 | 0.54 |
| 41:JM:172:SER:HB2 | 41:JM:173:PRO:HD2 | 1.90 | 0.54 |
| 41:JN:83:GLN:O | 41:KN:281:TYR:OH | 2.26 | 0.54 |
| 41:JN:342:VAL:HG23 | 41:JN:345:ILE:HG22 | 1.90 | 0.54 |
| 40:KE:310:GLY:HA3 | 40:KE:382:ALA:HB2 | 1.89 | 0.54 |
| 40:KE:318:LEU:O | 40:KE:374:VAL:HA | 2.08 | 0.54 |
| 40:KE:436:MET:O | 41:KM:391:ARG:NH2 | 2.41 | 0.54 |
| 40:KG:274:PRO:HG3 | 40:KG:286:LEU:HD12 | 1.89 | 0.54 |
| 41:LB:295:ASP:OD2 | 41:LB:297:LYS:NZ | 2.40 | 0.54 |
| 40:LE:141:PHE:HB2 | 40:LE:173:PRO:HD3 | 1.89 | 0.54 |
| 40:MD:258:ASN:HD22 | 40:MD:352:LYS:HB2 | 1.71 | 0.54 |
| 40:MF:402:ALA:O | 40:MF:403:PHE:C | 2.46 | 0.54 |
| 41:ML:7:LEU:HD23 | 41:ML:64:VAL:HB | 1.89 | 0.54 |
| 41:MO:7:LEU:HB2 | 41:MO:135:LEU:HD12 | 1.88 | 0.54 |
| 40:NA:231:ILE:HD13 | 40:NA:234:ILE:HD12 | 1.90 | 0.54 |
| 40:OH:89:PRO:HD3 | 40:PH:283:HIS:ND1 | 2.23 | 0.54 |
| 41:ON:86:ARG:HG3 | 41:ON:88:ASP:H | 1.73 | 0.54 |
| 41:ON:236:VAL:HG13 | 41:ON:237:THR:HG23 | 1.90 | 0.54 |
| 41:OO:156:ARG:NH2 | 41:OO:162:ARG:O | 2.40 | 0.54 |
| 40:PA:163:LYS:HG3 | 40:PA:164:LYS:HD2 | 1.89 | 0.54 |
| 41:PB:7:LEU:HD12 | 41:PB:135:LEU:HB2 | 1.90 | 0.54 |
| 40:PG:247:ALA:O | 41:PO:11:GLN:NE2 | 2.41 | 0.54 |
| 41:PN:134:GLN:HA | 41:PN:165:ASN:O | 2.08 | 0.54 |
| 41:QP:386:THR:C | 41:QP:388:MET:H | 2.11 | 0.54 |
| 41:RO:209:ASP:HB3 | 41:RO:213:ARG:NH2 | 2.23 | 0.54 |
| 41:RP:52:ASN:OD1 | 41:RP:62:ARG:NH1 | 2.41 | 0.54 |
| 40:SG:254:GLU:HG2 | 41:SO:98:GLY:HA2 | 1.90 | 0.54 |
| 40:SH:51:THR:HG23 | 40:SH:52:PHE:HD1 | 1.72 | 0.54 |
| 41:SL:42:LEU:HD23 | 41:SL:243:PRO:HG3 | 1.89 | 0.54 |
| 41:SL:131:GLN:HG2 | 41:SL:163:ILE:HD12 | 1.90 | 0.54 |
| 41:TN:86:ARG:HG2 | 41:TN:88:ASP:H | 1.72 | 0.54 |
| 41:TP:325:GLU:HA | 41:TP:328:GLU:HB2 | 1.90 | 0.54 |
| 40:UI:207:GLU:HB2 | 40:UI:304:LYS:HG2 | 1.90 | 0.54 |
| 40:UI:312:TYR:CD1 | 40:UI:380:THR:HB | 2.43 | 0.54 |
| 41:UN:156:ARG:NH2 | 41:UN:197:ASP:OD2 | 2.41 | 0.54 |
| 41:VB:131:GLN:HE22 | 41:VB:240:LEU:HD22 | 1.72 | 0.54 |
| 41:VN:28:HIS:CE1 | 41:VN:47:ILE:HA | 2.43 | 0.54 |
| 41:VN:382:SER:OG | 41:VN:412:GLU:OE2 | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VO:275:SER:HB3 | 41:VO:278:SER:HB2 | 1.88 | 0.54 |
| 41:VQ:326:VAL:O | 41:VQ:330:MET:HG2 | 2.08 | 0.54 |
| 40:WA:329:ASN:HB2 | 41:WB:175:VAL:HG11 | 1.90 | 0.54 |
| 8:1W:310:GLN:NE2 | 40:UH:58:ALA:O | 2.38 | 0.54 |
| 8:1Z:512:ILE:HG22 | 8:1Z:516:LYS:HE3 | 1.90 | 0.54 |
| 10:2F:159:TYR:HE2 | 41:VB:46:ARG:HA | 1.73 | 0.54 |
| 16:3L:9:SER:OG | 16:3L:10:GLN:N | 2.40 | 0.54 |
| 16:3L:309:GLN:HA | 16:3L:312:LYS:HD3 | 1.89 | 0.54 |
| 34:5Q:183:GLN:HE22 | 40:GA:362:VAL:HG21 | 1.72 | 0.54 |
| 34:5R:418:GLU:O | 34:5R:422:ILE:HG23 | 2.08 | 0.54 |
| 40:AA:183:GLU:OE2 | 42:AA:501:GTP:O3' | 2.24 | 0.54 |
| 41:AB:207:LEU:HB3 | 41:AB:225:LEU:HD22 | 1.90 | 0.54 |
| 41:AN:67:ASP:OD2 | 41:AN:68:LEU:N | 2.41 | 0.54 |
| 41:AP:341:PHE:HB3 | 41:AP:348:ASN:HD21 | 1.72 | 0.54 |
| 40:BA:137:ILE:HD11 | 40:BA:168:GLU:HG2 | 1.88 | 0.54 |
| 40:BA:218:ASP:OD2 | 40:BA:280:LYS:NZ | 2.41 | 0.54 |
| 41:BB:27:GLU:HA | 41:BB:359:ARG:HE | 1.71 | 0.54 |
| 40:BE:172:TYR:HB2 | 40:BE:203:MET:HG2 | 1.89 | 0.54 |
| 40:BG:175:PRO:O | 40:BG:389:ARG:NH2 | 2.41 | 0.54 |
| 40:BI:115:ILE:HD13 | 40:BI:152:LEU:HG | 1.89 | 0.54 |
| 41:BO:311:LEU:HD13 | 41:BO:372:THR:HG23 | 1.88 | 0.54 |
| 41:CB:247:ASN:O | 41:CB:252:LYS:NZ | 2.40 | 0.54 |
| 40:CE:257:THR:HA | 41:CM:397:TRP:CE2 | 2.43 | 0.54 |
| 41:CO:103:LYS:HA | 41:CO:107:THR:CG2 | 2.37 | 0.54 |
| 40:DH:218:ASP:HB2 | 40:DH:277:SER:HB3 | 1.90 | 0.54 |
| 40:DH:252:LEU:HA | 40:DH:255:PHE:CD2 | 2.43 | 0.54 |
| 41:DL:333:VAL:HG22 | 41:DL:337:ASN:HD21 | 1.72 | 0.54 |
| 41:DM:193:VAL:O | 41:DM:195:ASN:N | 2.40 | 0.54 |
| 41:DM:417:ASP:O | 41:DM:418:LEU:C | 2.46 | 0.54 |
| 41:DP:180:VAL:O | 41:DP:181:GLU:C | 2.46 | 0.54 |
| 41:EB:318:ARG:HD3 | 41:EB:358:PRO:HD3 | 1.90 | 0.54 |
| 40:EH:176:GLN:O | 40:EH:177:VAL:C | 2.46 | 0.54 |
| 41:EP:3:GLU:HB2 | 41:EP:130:LEU:HD13 | 1.90 | 0.54 |
| 41:FN:290:THR:HG21 | 41:FN:329:GLN:HB3 | 1.89 | 0.54 |
| 40:GE:16:ILE:HD11 | 40:GE:138:PHE:HB3 | 1.90 | 0.54 |
| 40:GH:68:VAL:HG23 | 40:GH:93:ILE:HB | 1.90 | 0.54 |
| 41:HB:61:PRO:HD3 | 41:HB:84:ILE:HG12 | 1.90 | 0.54 |
| 41:HB:314:ALA:HB3 | 41:HB:368:ILE:HB | 1.89 | 0.54 |
| 40:HG:188:ILE:HG23 | 40:HG:424:MET:HG3 | 1.89 | 0.54 |
| 40:HH:60:LYS:NZ | 40:IH:283:HIS:HD2 | 2.05 | 0.54 |
| 41:IQ:103:LYS:HA | 41:IQ:107:THR:HB | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JD:136:LEU:HD23 | 40:JD:167:LEU:HB2 | 1.89 | 0.54 |
| 41:JN:323:MET:N | 41:JN:323:MET:SD | 2.81 | 0.54 |
| 40:KA:220:GLU:OE2 | 40:KA:221:ARG:NH1 | 2.41 | 0.54 |
| 40:KE:91:GLN:HG2 | 40:KE:121:ARG:HH21 | 1.72 | 0.54 |
| 40:KH:138:PHE:HZ | 40:KH:235:VAL:HG21 | 1.71 | 0.54 |
| 41:KM:204:ASN:OD1 | 43:KM:502:GDP:O2' | 2.23 | 0.54 |
| 41:LB:139:LEU:HD12 | 41:LB:170:VAL:HG22 | 1.90 | 0.54 |
| 40:LF:230:LEU:HD21 | 40:LF:275:VAL:HG12 | 1.88 | 0.54 |
| 40:LF:326:LYS:HG3 | 41:LN:220:PRO:HG2 | 1.89 | 0.54 |
| 41:LN:222:TYR:O | 41:LN:226:ASN:ND2 | 2.40 | 0.54 |
| 40:MG:325:PRO:HD2 | 41:MO:220:PRO:O | 2.08 | 0.54 |
| 40:ND:76:ASP:HA | 40:ND:79:ARG:HG2 | 1.89 | 0.54 |
| 40:ND:139:HIS:NE2 | 40:ND:168:GLU:HB3 | 2.22 | 0.54 |
| 41:NM:235:GLY:HA3 | 41:NM:366:THR:HG21 | 1.88 | 0.54 |
| 41:NN:237:THR:HG23 | 41:NN:240:LEU:HD21 | 1.89 | 0.54 |
| 41:OB:166:THR:HB | 41:OB:199:THR:HG22 | 1.90 | 0.54 |
| 40:PD:7:VAL:HG23 | 40:PD:66:VAL:HB | 1.90 | 0.54 |
| 41:PL:171:PRO:HG3 | 41:PL:181:GLU:HB3 | 1.88 | 0.54 |
| 41:PM:62:ARG:NH1 | 41:PM:127:CYS:SG | 2.81 | 0.54 |
| 40:QF:141:PHE:HB2 | 40:QF:173:PRO:HD3 | 1.89 | 0.54 |
| 40:RG:7:VAL:HG12 | 40:RG:66:VAL:HB | 1.90 | 0.54 |
| 40:RG:269:LEU:HD22 | 40:RG:383:ILE:HD11 | 1.89 | 0.54 |
| 40:RG:362:VAL:HG21 | 40:RG:369:LYS:HA | 1.89 | 0.54 |
| 41:RL:167:PHE:CE2 | 41:RL:233:MET:HB2 | 2.42 | 0.54 |
| 40:SF:70:LEU:HD12 | 40:SF:145:THR:HG22 | 1.89 | 0.54 |
| 40:SG:319:TYR:HB3 | 40:SG:323:VAL:HG21 | 1.89 | 0.54 |
| 41:SL:44:LEU:HA | 41:SL:47:ILE:HB | 1.89 | 0.54 |
| 41:SO:82:GLY:O | 41:SO:84:ILE:N | 2.33 | 0.54 |
| 41:SO:173:PRO:O | 41:SO:174:LYS:C | 2.46 | 0.54 |
| 41:SO:375:GLN:O | 41:SO:376:GLU:C | 2.46 | 0.54 |
| 41:TM:99:ASN:HA | 41:TM:142:GLY:HA3 | 1.90 | 0.54 |
| 41:TO:130:LEU:O | 41:TO:162:ARG:NH2 | 2.41 | 0.54 |
| 40:VA:251:ASP:H | 40:VA:254:GLU:HB2 | 1.71 | 0.54 |
| 41:VN:309:ARG:NH2 | 41:VN:343:GLU:OE1 | 2.40 | 0.54 |
| 41:VP:117:LEU:HA | 41:VP:120:VAL:HG12 | 1.89 | 0.54 |
| 40:WA:11:GLN:HE22 | 41:WN:247:ASN:H | 1.56 | 0.54 |
| 40:WH:254:GLU:OE1 | 41:WP:99:ASN:ND2 | 2.40 | 0.54 |
| 40:WH:318:LEU:O | 40:WH:374:VAL:HA | 2.07 | 0.54 |
| 40:WH:390:LEU:HA | 40:WH:393:LYS:HG3 | 1.90 | 0.54 |
| 41:WN:170:VAL:HG21 | 41:WN:377:LEU:HG | 1.90 | 0.54 |
| 7:1U:149:CYS:SG | 7:1U:150:GLY:N | 2.80 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1U:366:GLU:OE2 | 7:1U:369:ARG:NH2 | 2.39 | 0.54 |
| 7:1U:373:PRO:HG2 | 10:2G:137:LYS:HA | 1.89 | 0.54 |
| 9:2C:480:LEU:HA | 9:2C:483:LYS:HG2 | 1.89 | 0.54 |
| 12:2R:189:TYR:O | 12:2R:192:GLN:NE2 | 2.41 | 0.54 |
| 15:3G:310:ALA:HB2 | 15:3G:344:ILE:HG21 | 1.89 | 0.54 |
| 18:3T:315:ARG:HG2 | 18:3T:419:LYS:HB3 | 1.90 | 0.54 |
| 21:4F:133:VAL:HB | 21:4F:149:ILE:HB | 1.90 | 0.54 |
| 22:4I:489:PRO:HG3 | 22:4I:514:ASP:HB3 | 1.90 | 0.54 |
| 22:4J:630:HIS:O | 22:4J:631:ALA:C | 2.46 | 0.54 |
| 23:4N:91:ILE:CG2 | 40:AF:84:ARG:HB2 | 2.38 | 0.54 |
| 23:4N:254:LYS:HD2 | 41:DM:53:GLU:HB2 | 1.90 | 0.54 |
| 23:4P:184:MET:O | 23:4P:185:SER:C | 2.45 | 0.54 |
| 23:4P:233:SER:N | 23:4P:242:LEU:HD22 | 2.23 | 0.54 |
| 36:5Y:93:GLY:HA2 | 41:OO:217:LEU:HD11 | 1.90 | 0.54 |
| 37:6A:43:ARG:NE | 41:TO:45:GLU:OE2 | 2.41 | 0.54 |
| 39:6L:31:LEU:HD13 | 39:6L:68:LEU:HD11 | 1.90 | 0.54 |
| 40:AA:319:TYR:HB3 | 40:AA:323:VAL:HG21 | 1.90 | 0.54 |
| 41:AO:289:LEU:O | 41:AO:293:MET:HB2 | 2.08 | 0.54 |
| 41:BP:288:GLU:HG3 | 41:BP:289:LEU:N | 2.22 | 0.54 |
| 40:CH:241:SER:C | 40:CH:243:ARG:H | 2.10 | 0.54 |
| 41:CL:142:GLY:O | 41:CL:144:GLY:N | 2.41 | 0.54 |
| 41:CL:384:GLN:O | 41:CL:385:PHE:C | 2.45 | 0.54 |
| 41:CN:135:LEU:HD23 | 41:CN:166:THR:HG22 | 1.89 | 0.54 |
| 41:CN:240:LEU:HD21 | 41:CN:250:LEU:H | 1.73 | 0.54 |
| 41:DB:109:GLY:O | 41:DB:111:GLU:N | 2.41 | 0.54 |
| 41:DB:239:CYS:C | 41:DB:241:ARG:H | 2.11 | 0.54 |
| 41:DB:395:LEU:O | 41:DB:399:THR:N | 2.37 | 0.54 |
| 40:DF:351:PHE:N | 41:DN:179:VAL:HG12 | 2.23 | 0.54 |
| 41:DM:75:SER:O | 41:DM:76:VAL:C | 2.46 | 0.54 |
| 40:EF:108:TYR:O | 40:EF:112:LYS:NZ | 2.37 | 0.54 |
| 40:EF:158:SER:OG | 40:EF:166:LYS:NZ | 2.41 | 0.54 |
| 40:FA:35:GLN:O | 40:FA:36:MET:C | 2.46 | 0.54 |
| 41:FM:248:ALA:HA | 41:FM:252:LYS:HD3 | 1.89 | 0.54 |
| 40:GE:317:LEU:HB3 | 40:GE:319:TYR:HE1 | 1.71 | 0.54 |
| 40:GF:352:LYS:HD2 | 41:GN:179:VAL:H | 1.73 | 0.54 |
| 40:GI:278:ALA:O | 40:GI:279:GLU:C | 2.46 | 0.54 |
| 41:GM:99:ASN:HA | 41:GM:142:GLY:HA3 | 1.89 | 0.54 |
| 41:GN:206:ALA:HB2 | 41:GN:301:ALA:O | 2.08 | 0.54 |
| 40:HA:88:HIS:HB3 | 40:HA:91:GLN:HG2 | 1.89 | 0.54 |
| 41:HB:178:THR:HB | 41:HB:181:GLU:HB2 | 1.89 | 0.54 |
| 40:HH:180:ALA:HB3 | 40:HH:183:GLU:HG3 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IF:141:PHE:HB2 | 40:IF:173:PRO:HD3 | 1.90 | 0.54 |
| 41:IO:252:LYS:O | 41:IO:256:ASN:ND2 | 2.41 | 0.54 |
| 41:IQ:174:LYS:HD2 | 41:IQ:175:VAL:HG13 | 1.90 | 0.54 |
| 41:JB:348:ASN:HA | 40:JG:181:VAL:HG12 | 1.90 | 0.54 |
| 40:JE:100:ALA:HA | 41:JL:252:LYS:HD3 | 1.89 | 0.54 |
| 40:JF:217:LEU:HA | 40:JF:277:SER:HB2 | 1.90 | 0.54 |
| 41:JL:170:VAL:HG21 | 41:JL:377:LEU:HD11 | 1.90 | 0.54 |
| 40:KG:250:VAL:HG23 | 40:KG:254:GLU:HB2 | 1.90 | 0.54 |
| 40:KH:73:THR:HA | 40:KH:76:ASP:HB2 | 1.88 | 0.54 |
| 41:KO:256:ASN:HD22 | 41:KO:350:LYS:HE2 | 1.72 | 0.54 |
| 40:LA:101:ASN:HD22 | 40:LA:143:GLY:HA2 | 1.72 | 0.54 |
| 41:LB:142:GLY:O | 41:LB:144:GLY:N | 2.40 | 0.54 |
| 41:LN:318:ARG:HG2 | 41:LN:357:PRO:HA | 1.90 | 0.54 |
| 40:MA:11:GLN:HA | 40:MA:74:VAL:HG11 | 1.89 | 0.54 |
| 40:MH:104:ALA:HB2 | 40:MH:412:MET:HE3 | 1.90 | 0.54 |
| 40:MH:238:ILE:HG12 | 40:MH:377:LEU:HD11 | 1.88 | 0.54 |
| 41:MM:407:GLU:HA | 41:MM:410:GLU:HB2 | 1.90 | 0.54 |
| 40:NE:27:GLU:OE1 | 40:NE:243:ARG:NH2 | 2.40 | 0.54 |
| 40:NG:26:LEU:HG | 40:NG:363:VAL:HG12 | 1.89 | 0.54 |
| 40:OF:180:ALA:HB3 | 40:OF:183:GLU:HG2 | 1.90 | 0.54 |
| 40:OH:217:LEU:HA | 40:OH:277:SER:HB3 | 1.90 | 0.54 |
| 41:OP:395:LEU:HA | 41:OP:398:TYR:HD2 | 1.73 | 0.54 |
| 40:PA:100:ALA:HA | 41:PN:252:LYS:HG3 | 1.90 | 0.54 |
| 40:PA:276:ILE:HG23 | 40:PA:280:LYS:HG3 | 1.89 | 0.54 |
| 41:PP:22:GLU:HG3 | 41:PP:81:PHE:HD1 | 1.73 | 0.54 |
| 41:QM:130:LEU:HB3 | 41:QM:162:ARG:HE | 1.73 | 0.54 |
| 41:QN:169:VAL:HG22 | 41:QN:202:ILE:HD11 | 1.90 | 0.54 |
| 41:QO:19:LYS:NZ | 41:QO:223:GLY:O | 2.41 | 0.54 |
| 40:RA:107:HIS:HD2 | 40:RA:152:LEU:HB2 | 1.73 | 0.54 |
| 40:SA:252:LEU:HA | 40:SA:255:PHE:CD1 | 2.43 | 0.54 |
| 40:SE:108:TYR:O | 40:SE:112:LYS:NZ | 2.39 | 0.54 |
| 40:SE:177:VAL:HG12 | 41:SL:331:LEU:HB2 | 1.89 | 0.54 |
| 40:SI:172:TYR:N | 40:SI:204:VAL:O | 2.40 | 0.54 |
| 41:SM:142:GLY:O | 41:SM:144:GLY:N | 2.41 | 0.54 |
| 41:SP:27:GLU:HA | 41:SP:359:ARG:HH12 | 1.73 | 0.54 |
| 41:SP:45:GLU:OE2 | 41:SP:243:PRO:HD3 | 2.08 | 0.54 |
| 40:TF:175:PRO:HD2 | 40:TF:176:GLN:H | 1.73 | 0.54 |
| 41:TN:248:ALA:HA | 41:TN:252:LYS:HG2 | 1.89 | 0.54 |
| 40:UE:27:GLU:OE2 | 40:UE:361:THR:OG1 | 2.24 | 0.54 |
| 40:UF:35:GLN:O | 40:UF:36:MET:C | 2.46 | 0.54 |
| 40:UI:326:LYS:HA | 40:UI:329:ASN:HD21 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VP:52:ASN:OD1 | 41:VP:62:ARG:NH2 | 2.40 | 0.54 |
| 40:WF:400:LYS:HZ1 | 41:WM:344:TRP:HB2 | 1.72 | 0.54 |
| 40:WI:186:ASN:OD1 | 40:WI:407:TYR:OH | 2.26 | 0.54 |
| 41:WO:287:PRO:HA | 41:WO:329:GLN:HE22 | 1.72 | 0.54 |
| 41:WP:313:VAL:HB | 41:WP:349:VAL:HG22 | 1.90 | 0.54 |
| 11:2K:200:LEU:HB3 | 11:2K:241:ILE:HG22 | 1.90 | 0.54 |
| 17:3R:243:GLN:HB2 | 17:3R:321:LEU:HD23 | 1.90 | 0.54 |
| 17:3R:247:SER:HA | 17:3R:314:GLU:HG2 | 1.89 | 0.54 |
| 21:4D:41:ARG:O | 41:LN:77:ARG:NH1 | 2.41 | 0.54 |
| 22:4J:140:PRO:HB3 | 22:4J:143:GLU:HB3 | 1.88 | 0.54 |
| 22:4J:651:LYS:HA | 22:4J:690:TYR:CZ | 2.43 | 0.54 |
| 23:4N:183:PHE:O | 23:4N:184:MET:C | 2.45 | 0.54 |
| 23:4N:216:MET:O | 23:4N:217:LYS:C | 2.45 | 0.54 |
| 29:5D:24:THR:HG22 | 29:5D:70:VAL:HG23 | 1.90 | 0.54 |
| 31:5J:748:SER:OG | 40:IE:77:GLU:OE1 | 2.26 | 0.54 |
| 33:5N:483:LYS:HD3 | 40:GE:38:SER:HB3 | 1.89 | 0.54 |
| 34:5R:322:GLN:OE1 | 34:5R:326:ASP:OD1 | 2.26 | 0.54 |
| 36:5W:82:ASN:OD1 | 40:OF:369:LYS:NZ | 2.40 | 0.54 |
| 40:AA:255:PHE:HZ | 40:AA:318:LEU:HD21 | 1.72 | 0.54 |
| 40:BE:45:GLY:O | 40:BE:46:ASP:C | 2.46 | 0.54 |
| 40:BI:72:PRO:O | 40:BI:73:THR:C | 2.45 | 0.54 |
| 40:BI:193:THR:OG1 | 40:BI:194:THR:N | 2.41 | 0.54 |
| 41:BL:222:TYR:O | 41:BL:226:ASN:ND2 | 2.41 | 0.54 |
| 41:BO:12:CYS:CB | 41:BO:138:SER:HB3 | 2.37 | 0.54 |
| 41:BP:67:ASP:OD2 | 41:BP:73:MET:HG2 | 2.08 | 0.54 |
| 40:CH:7:VAL:HB | 40:CH:137:ILE:HG23 | 1.90 | 0.54 |
| 40:CH:39:ASP:O | 40:CH:40:LYS:HB2 | 2.08 | 0.54 |
| 40:CH:177:VAL:CG1 | 41:CO:327:ASP:HB3 | 2.38 | 0.54 |
| 40:CH:408:VAL:HA | 40:CH:412:MET:O | 2.08 | 0.54 |
| 41:CL:185:ALA:O | 41:CL:186:THR:C | 2.46 | 0.54 |
| 41:CM:326:VAL:HG13 | 41:CM:351:THR:HG21 | 1.90 | 0.54 |
| 41:CO:180:VAL:O | 41:CO:181:GLU:C | 2.46 | 0.54 |
| 40:DH:239:THR:HA | 40:DH:242:LEU:HD21 | 1.90 | 0.54 |
| 40:DI:19:ALA:O | 40:DI:22:GLU:HG3 | 2.08 | 0.54 |
| 40:DI:176:GLN:O | 40:DI:177:VAL:C | 2.47 | 0.54 |
| 40:DI:205:ASP:HB2 | 40:DI:303:VAL:HA | 1.89 | 0.54 |
| 41:DN:239:CYS:C | 41:DN:241:ARG:H | 2.11 | 0.54 |
| 41:DO:372:THR:OG1 | 41:DO:422:VAL:O | 2.25 | 0.54 |
| 41:DP:87:PRO:O | 41:DP:88:ASP:C | 2.45 | 0.54 |
| 41:EB:271:ALA:HB1 | 41:EB:292:GLN:HG3 | 1.89 | 0.54 |
| 40:EI:323:VAL:HA | 40:EI:372:ARG:HH11 | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EO:262:ARG:NH2 | 41:EO:414:ASN:OD1 | 2.41 | 0.54 |
| 41:FB:323:MET:HA | 41:FB:326:VAL:HB | 1.90 | 0.54 |
| 40:GE:281:ALA:O | 40:GE:282:TYR:C | 2.47 | 0.54 |
| 40:HA:99:ALA:HA | 40:HA:105:ARG:HG2 | 1.90 | 0.54 |
| 40:HE:200:CYS:HB2 | 40:HE:256:GLN:NE2 | 2.23 | 0.54 |
| 41:HN:398:TYR:HB3 | 41:HN:408:PHE:HZ | 1.73 | 0.54 |
| 41:HP:200:TYR:HE2 | 41:HP:368:ILE:HD12 | 1.73 | 0.54 |
| 41:HQ:1:MET:HG2 | 41:HQ:48:ASN:HD21 | 1.73 | 0.54 |
| 40:IH:252:LEU:HA | 40:IH:255:PHE:HD2 | 1.73 | 0.54 |
| 40:IH:262:TYR:HB2 | 40:IH:265:ILE:HG22 | 1.89 | 0.54 |
| 41:JM:48:ASN:O | 41:JM:49:VAL:C | 2.46 | 0.54 |
| 41:JM:218:THR:O | 41:JM:220:PRO:HD3 | 2.08 | 0.54 |
| 40:KA:262:TYR:OH | 41:KB:391:ARG:O | 2.22 | 0.54 |
| 40:LF:348:PRO:HB2 | 41:LN:384:GLN:OE1 | 2.08 | 0.54 |
| 40:LH:246:GLY:HA3 | 40:LH:356:ASN:HA | 1.90 | 0.54 |
| 41:LM:271:ALA:HB1 | 41:LM:292:GLN:HG2 | 1.90 | 0.54 |
| 41:LN:313:VAL:HB | 41:LN:349:VAL:HG22 | 1.90 | 0.54 |
| 40:MA:250:VAL:HG23 | 40:MA:254:GLU:HB3 | 1.90 | 0.54 |
| 42:MB:502:GTP:HN21 | 40:MG:228:ASN:HB3 | 1.73 | 0.54 |
| 41:MM:332:ASN:OD1 | 41:MM:336:LYS:NZ | 2.41 | 0.54 |
| 41:MN:313:VAL:O | 41:MN:349:VAL:HA | 2.08 | 0.54 |
| 40:NA:206:ASN:OD1 | 42:NN:501:GTP:O2' | 2.26 | 0.54 |
| 40:NH:73:THR:OG1 | 41:NO:46:ARG:NH1 | 2.39 | 0.54 |
| 41:ON:87:PRO:HD3 | 41:PN:281:TYR:CD2 | 2.43 | 0.54 |
| 40:PF:255:PHE:HE1 | 40:PF:318:LEU:HD11 | 1.71 | 0.54 |
| 41:PM:130:LEU:HB3 | 41:PM:162:ARG:NH1 | 2.22 | 0.54 |
| 41:PN:187:LEU:HD11 | 41:PN:408:PHE:HE1 | 1.73 | 0.54 |
| 40:QA:188:ILE:HG22 | 40:QA:420:ALA:HB1 | 1.90 | 0.54 |
| 41:QB:145:SER:O | 41:QB:146:GLY:C | 2.46 | 0.54 |
| 40:QE:116:ASP:N | 40:QE:116:ASP:OD1 | 2.41 | 0.54 |
| 41:SB:313:VAL:HB | 41:SB:349:VAL:HG22 | 1.89 | 0.54 |
| 40:SE:75:ILE:HG23 | 40:SE:92:LEU:HD12 | 1.89 | 0.54 |
| 40:SG:391:ASP:HB3 | 40:SG:421:ARG:HH22 | 1.73 | 0.54 |
| 41:SO:149:THR:O | 41:SO:150:LEU:C | 2.47 | 0.54 |
| 40:TF:217:LEU:HD12 | 40:TF:277:SER:HB3 | 1.89 | 0.54 |
| 40:TH:182:VAL:O | 40:TH:186:ASN:ND2 | 2.40 | 0.54 |
| 41:TL:118:ASP:OD1 | 41:TL:121:ARG:NH2 | 2.33 | 0.54 |
| 41:TO:170:VAL:HG21 | 41:TO:377:LEU:HD21 | 1.90 | 0.54 |
| 40:UF:99:ALA:HB3 | 40:UF:145:THR:HA | 1.89 | 0.54 |
| 40:UF:184:PRO:O | 40:UF:185:TYR:C | 2.47 | 0.54 |
| 40:UI:258:ASN:HB2 | 40:UI:352:LYS:HG3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VB:49:VAL:HG11 | 41:VB:241:ARG:HG2 | 1.89 | 0.54 |
| 41:VN:7:LEU:O | 41:VN:135:LEU:HA | 2.08 | 0.54 |
| 41:VP:215:LEU:HB3 | 41:VP:217:LEU:HD23 | 1.89 | 0.54 |
| 40:WA:269:LEU:HD23 | 40:WA:383:ILE:HD11 | 1.89 | 0.54 |
| 41:WB:258:VAL:HG13 | 40:WG:406:TRP:HE1 | 1.72 | 0.54 |
| 40:WI:188:ILE:HD12 | 40:WI:424:MET:HG3 | 1.90 | 0.54 |
| 41:WN:215:LEU:O | 41:WN:216:LYS:C | 2.45 | 0.54 |
| 7:1T:447:GLY:O | 7:1T:448:HIS:C | 2.45 | 0.53 |
| 7:1U:47:ILE:HD11 | 7:1U:81:SER:HB3 | 1.88 | 0.53 |
| 7:1U:380:ILE:HB | 7:1U:389:LEU:HD11 | 1.89 | 0.53 |
| 8:1X:99:SER:O | 8:1X:100:LEU:HB3 | 2.07 | 0.53 |
| 13:2U:88:THR:HG23 | 13:2U:157:HIS:HB2 | 1.88 | 0.53 |
| 15:3H:206:ARG:NH1 | 15:3H:207:ILE:O | 2.41 | 0.53 |
| 16:3J:325:PRO:HD2 | 16:3J:328:GLU:HB2 | 1.89 | 0.53 |
| 16:3M:36:HIS:HA | 16:3M:39:ARG:HH11 | 1.72 | 0.53 |
| 18:3U:447:GLN:OXT | 41:LM:37:HIS:ND1 | 2.42 | 0.53 |
| 19:3Y:144:GLN:NE2 | 41:LB:272:PRO:O | 2.41 | 0.53 |
| 23:4P:242:LEU:HD12 | 23:4P:261:TYR:CE2 | 2.43 | 0.53 |
| 39:6I:128:SER:HA | 40:OA:84:ARG:NH2 | 2.22 | 0.53 |
| 40:AA:221:ARG:NH1 | 41:AN:325:GLU:OE2 | 2.35 | 0.53 |
| 41:AB:163:ILE:HG21 | 41:AB:250:LEU:HB3 | 1.88 | 0.53 |
| 40:AE:178:SER:OG | 41:AL:347:ASN:ND2 | 2.41 | 0.53 |
| 40:BG:122:ILE:HD13 | 40:BG:157:LEU:HD11 | 1.90 | 0.53 |
| 41:BM:143:THR:O | 41:BM:144:GLY:C | 2.46 | 0.53 |
| 41:BM:310:TYR:CD1 | 41:BM:371:SER:HB2 | 2.43 | 0.53 |
| 41:CL:68:LEU:HD13 | 41:CL:97:ALA:HB2 | 1.90 | 0.53 |
| 41:CO:200:TYR:HE1 | 41:CO:266:PHE:HD2 | 1.56 | 0.53 |
| 40:DE:224:TYR:CE1 | 41:DL:323:MET:HB3 | 2.44 | 0.53 |
| 40:DE:241:SER:O | 40:DE:242:LEU:C | 2.47 | 0.53 |
| 40:EF:68:VAL:HG12 | 40:EF:93:ILE:HB | 1.91 | 0.53 |
| 40:EH:14:VAL:HG13 | 40:EH:67:PHE:HD2 | 1.71 | 0.53 |
| 41:FM:274:THR:OG1 | 41:FM:282:ARG:NH1 | 2.40 | 0.53 |
| 40:GG:34:GLY:HA3 | 40:GG:60:LYS:HD2 | 1.89 | 0.53 |
| 40:GH:328:VAL:HG21 | 40:GH:353:VAL:HG13 | 1.90 | 0.53 |
| 40:IE:255:PHE:O | 40:IE:259:LEU:HB2 | 2.09 | 0.53 |
| 41:IQ:234:SER:O | 41:IQ:238:THR:OG1 | 2.26 | 0.53 |
| 40:JA:262:TYR:OH | 41:JB:391:ARG:O | 2.23 | 0.53 |
| 40:JF:274:PRO:HG3 | 40:JF:286:LEU:HD11 | 1.91 | 0.53 |
| 41:JM:167:PHE:HZ | 41:JM:236:VAL:HG21 | 1.73 | 0.53 |
| 40:KA:205:ASP:HB2 | 40:KA:303:VAL:HG23 | 1.89 | 0.53 |
| 40:KG:217:LEU:HD23 | 40:KG:277:SER:HB2 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KM:253:LEU:HD22 | 41:KM:350:LYS:HZ1 | 1.73 | 0.53 |
| 40:LF:76:ASP:HA | 40:LF:79:ARG:HG2 | 1.90 | 0.53 |
| 40:MF:139:HIS:CE1 | 40:MF:170:SER:HB3 | 2.43 | 0.53 |
| 40:MF:239:THR:HA | 40:MF:242:LEU:HD21 | 1.90 | 0.53 |
| 40:MH:210:TYR:CG | 41:MO:324:LYS:HG2 | 2.42 | 0.53 |
| 40:NA:7:VAL:HG11 | 40:NA:153:LEU:HD21 | 1.90 | 0.53 |
| 40:ND:28:HIS:CD2 | 40:ND:49:PHE:HA | 2.43 | 0.53 |
| 40:ND:104:ALA:HB1 | 40:ND:410:GLU:HB3 | 1.89 | 0.53 |
| 40:NE:102:ASN:OD1 | 40:NE:105:ARG:N | 2.36 | 0.53 |
| 40:OA:20:CYS:HA | 40:OA:232:SER:HB2 | 1.91 | 0.53 |
| 40:OA:224:TYR:CZ | 41:ON:323:MET:HG2 | 2.42 | 0.53 |
| 40:OF:273:ALA:HB3 | 40:OF:374:VAL:H | 1.73 | 0.53 |
| 41:ON:226:ASN:ND2 | 43:ON:502:GDP:O6 | 2.39 | 0.53 |
| 41:PB:256:ASN:OD1 | 41:PB:350:LYS:HE2 | 2.08 | 0.53 |
| 40:PD:238:ILE:HG12 | 40:PD:377:LEU:HD11 | 1.90 | 0.53 |
| 40:PE:75:ILE:HG23 | 40:PE:92:LEU:HD12 | 1.90 | 0.53 |
| 41:PM:191:GLN:O | 41:PM:195:ASN:HB3 | 2.07 | 0.53 |
| 41:PP:223:GLY:O | 41:PP:227:HIS:HB2 | 2.08 | 0.53 |
| 40:QF:436:MET:O | 41:QN:391:ARG:NH2 | 2.42 | 0.53 |
| 41:SN:100:ASN:HB2 | 41:SN:103:LYS:HB2 | 1.90 | 0.53 |
| 41:SP:412:GLU:OE2 | 41:SP:416:ASN:ND2 | 2.41 | 0.53 |
| 40:TG:267:PHE:HE2 | 40:TG:427:LEU:HD21 | 1.73 | 0.53 |
| 40:TG:370:VAL:HG22 | 40:TG:372:ARG:H | 1.73 | 0.53 |
| 40:UE:269:LEU:HD21 | 40:UE:383:ILE:HD11 | 1.90 | 0.53 |
| 41:UP:65:LEU:HD11 | 41:UP:85:PHE:HB3 | 1.90 | 0.53 |
| 41:VB:95:SER:OG | 41:VB:96:GLY:N | 2.41 | 0.53 |
| 40:VF:370:VAL:HG22 | 40:VF:372:ARG:H | 1.73 | 0.53 |
| 40:VG:7:VAL:HB | 40:VG:137:ILE:HG12 | 1.90 | 0.53 |
| 41:VN:142:GLY:O | 41:VN:144:GLY:N | 2.41 | 0.53 |
| 41:WB:317:PHE:HB2 | 41:WB:353:VAL:HG12 | 1.89 | 0.53 |
| 40:WF:220:GLU:HG3 | 40:WF:221:ARG:HD2 | 1.90 | 0.53 |
| 41:WO:7:LEU:HG | 41:WO:64:VAL:HB | 1.90 | 0.53 |
| 7:1U:346:GLU:N | 7:1U:346:GLU:OE2 | 2.41 | 0.53 |
| 13:2X:13:ILE:HG12 | 13:2X:165:VAL:O | 2.08 | 0.53 |
| 17:3O:395:VAL:HG12 | 17:3O:399:ARG:HD2 | 1.88 | 0.53 |
| 17:3R:182:GLU:CG | 17:3R:237:LEU:HD21 | 2.38 | 0.53 |
| 17:3R:264:ALA:O | 17:3R:265:TYR:C | 2.46 | 0.53 |
| 22:4I:154:ILE:HG12 | 22:4I:185:LEU:HD12 | 1.90 | 0.53 |
| 23:4M:91:ILE:HB | 23:4M:92:PRO:HD2 | 1.90 | 0.53 |
| 23:4P:253:TYR:HE2 | 40:EA:220:GLU:OE1 | 1.91 | 0.53 |
| 23:4R:58:ARG:HH12 | 41:BP:43:GLN:HA | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:4V:64:ASN:OD1 | 26:4V:65:LYS:N | 2.39 | 0.53 |
| 26:4W:282:VAL:HG21 | 26:4W:304:TYR:HB3 | 1.91 | 0.53 |
| 34:5Q:162:GLU:OE2 | 41:GB:218:THR:OG1 | 2.25 | 0.53 |
| 39:6F:138:GLY:HA2 | 39:6F:141:SER:HB2 | 1.89 | 0.53 |
| 40:BE:332:ILE:HD13 | 40:BE:351:PHE:HB3 | 1.89 | 0.53 |
| 40:BI:264:ARG:O | 40:BI:265:ILE:C | 2.46 | 0.53 |
| 41:BM:272:PRO:HD3 | 41:BM:364:SER:HA | 1.89 | 0.53 |
| 41:CB:107:THR:O | 41:CB:110:ALA:N | 2.41 | 0.53 |
| 40:CH:45:GLY:O | 40:CH:47:ASP:N | 2.40 | 0.53 |
| 41:CM:141:GLY:HA3 | 43:CM:501:GDP:O1A | 2.08 | 0.53 |
| 41:CM:242:PHE:HB3 | 41:CM:356:ILE:HB | 1.90 | 0.53 |
| 41:CM:272:PRO:HG2 | 41:CM:361:LEU:HD13 | 1.90 | 0.53 |
| 40:DA:155:GLU:HA | 40:DA:197:HIS:CE1 | 2.43 | 0.53 |
| 41:DB:61:PRO:HD2 | 41:DB:84:ILE:O | 2.08 | 0.53 |
| 41:DL:237:THR:O | 41:DL:237:THR:OG1 | 2.25 | 0.53 |
| 41:DM:8:GLN:HE21 | 41:DM:17:GLY:HA3 | 1.73 | 0.53 |
| 41:EB:256:ASN:HD21 | 40:EG:101:ASN:HD22 | 1.56 | 0.53 |
| 40:EE:70:LEU:HD12 | 40:EE:145:THR:HG22 | 1.89 | 0.53 |
| 41:EN:318:ARG:HB3 | 41:EN:354:CYS:HB3 | 1.89 | 0.53 |
| 41:EP:288:GLU:O | 41:EP:291:GLN:HG3 | 2.07 | 0.53 |
| 41:FB:142:GLY:O | 41:FB:144:GLY:N | 2.41 | 0.53 |
| 41:FP:334:GLN:NE2 | 41:FP:348:ASN:OD1 | 2.41 | 0.53 |
| 40:GA:51:THR:HG21 | 40:GA:243:ARG:HA | 1.90 | 0.53 |
| 40:GA:271:THR:OG1 | 40:GA:300:ASN:O | 2.23 | 0.53 |
| 40:HE:6:SER:HB3 | 40:HE:138:PHE:HE1 | 1.72 | 0.53 |
| 40:HE:90:GLU:HB3 | 40:IE:280:LYS:HZ1 | 1.73 | 0.53 |
| 40:HF:191:THR:O | 40:HF:195:LEU:HB2 | 2.07 | 0.53 |
| 40:HH:224:TYR:HA | 40:HH:227:LEU:HB2 | 1.91 | 0.53 |
| 40:IE:319:TYR:HB3 | 40:IE:323:VAL:HG21 | 1.89 | 0.53 |
| 40:JD:20:CYS:HA | 40:JD:232:SER:HB2 | 1.90 | 0.53 |
| 40:JG:205:ASP:HB2 | 40:JG:303:VAL:HG23 | 1.91 | 0.53 |
| 40:JH:181:VAL:HG23 | 40:JH:182:VAL:HG13 | 1.90 | 0.53 |
| 41:JM:389:PHE:HZ | 41:JM:405:GLU:HG2 | 1.72 | 0.53 |
| 41:KB:180:VAL:HG13 | 41:KB:184:ASN:HD21 | 1.73 | 0.53 |
| 41:KB:324:LYS:NZ | 40:KG:222:PRO:HG2 | 2.23 | 0.53 |
| 40:KD:325:PRO:O | 40:KD:329:ASN:ND2 | 2.34 | 0.53 |
| 40:KE:141:PHE:HB2 | 40:KE:173:PRO:HD3 | 1.89 | 0.53 |
| 40:LF:102:ASN:O | 40:LF:103:TYR:C | 2.47 | 0.53 |
| 40:LH:16:ILE:HD11 | 40:LH:171:ILE:HD11 | 1.90 | 0.53 |
| 40:LH:394:PHE:HZ | 40:LH:417:PHE:HB3 | 1.72 | 0.53 |
| 40:MG:37:PRO:O | 40:MG:38:SER:C | 2.46 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MH:258:ASN:HD22 | 41:MP:179:VAL:H | 1.55 | 0.53 |
| 40:ND:139:HIS:CD2 | 40:ND:170:SER:HB2 | 2.44 | 0.53 |
| 40:ND:288:VAL:O | 40:ND:291:ILE:HG12 | 2.08 | 0.53 |
| 40:NH:406:TRP:HE1 | 41:NO:258:VAL:HB | 1.71 | 0.53 |
| 41:NL:263:LEU:HD11 | 41:NL:421:PRO:HB2 | 1.90 | 0.53 |
| 40:OF:49:PHE:O | 40:OF:53:PHE:HB2 | 2.08 | 0.53 |
| 40:OF:370:VAL:HG12 | 40:OF:372:ARG:H | 1.73 | 0.53 |
| 40:OH:174:ALA:HB3 | 40:OH:177:VAL:CG2 | 2.37 | 0.53 |
| 41:ON:322:SER:OG | 41:ON:325:GLU:OE2 | 2.21 | 0.53 |
| 40:PA:158:SER:OG | 40:PA:166:LYS:NZ | 2.39 | 0.53 |
| 41:PB:104:GLY:HA2 | 41:PB:109:GLY:HA3 | 1.90 | 0.53 |
| 40:PF:67:PHE:HB2 | 40:PF:92:LEU:HD13 | 1.90 | 0.53 |
| 40:PH:136:LEU:HD13 | 40:PH:167:LEU:HB2 | 1.89 | 0.53 |
| 41:PM:342:VAL:HG23 | 41:PM:345:ILE:HG22 | 1.90 | 0.53 |
| 41:PN:236:VAL:HG13 | 41:PN:237:THR:HG23 | 1.89 | 0.53 |
| 41:PP:133:PHE:O | 41:PP:164:MET:HA | 2.08 | 0.53 |
| 41:PP:379:LYS:O | 41:PP:382:SER:N | 2.40 | 0.53 |
| 41:RB:257:MET:HB3 | 41:RB:266:PHE:CZ | 2.43 | 0.53 |
| 41:RB:323:MET:HA | 41:RB:326:VAL:HB | 1.90 | 0.53 |
| 40:RG:175:PRO:HB3 | 40:RG:389:ARG:HH21 | 1.73 | 0.53 |
| 41:RP:45:GLU:HG2 | 41:RP:46:ARG:HG3 | 1.88 | 0.53 |
| 41:RP:314:ALA:HB3 | 41:RP:368:ILE:HB | 1.89 | 0.53 |
| 40:SA:246:GLY:HA2 | 40:SA:357:TYR:CD1 | 2.42 | 0.53 |
| 41:SO:7:LEU:HD22 | 41:SO:120:VAL:HG22 | 1.89 | 0.53 |
| 40:TA:239:THR:HG22 | 40:TA:252:LEU:HD21 | 1.91 | 0.53 |
| 40:TA:247:ALA:O | 41:TB:11:GLN:NE2 | 2.39 | 0.53 |
| 41:TB:156:ARG:HH21 | 41:TB:164:MET:HG2 | 1.73 | 0.53 |
| 40:TF:380:THR:O | 40:TF:431:TYR:OH | 2.26 | 0.53 |
| 41:TM:138:SER:O | 41:TM:145:SER:OG | 2.25 | 0.53 |
| 41:TO:267:MET:HE1 | 41:TO:373:ALA:HB3 | 1.90 | 0.53 |
| 40:VF:97:GLU:OE2 | 40:VF:105:ARG:NH2 | 2.41 | 0.53 |
| 40:VG:105:ARG:HG2 | 40:VG:410:GLU:HG2 | 1.90 | 0.53 |
| 40:WG:20:CYS:HA | 40:WG:232:SER:HB2 | 1.90 | 0.53 |
| 40:WG:138:PHE:HE2 | 40:WG:235:VAL:HG21 | 1.73 | 0.53 |
| 40:WI:405:HIS:HA | 40:WI:408:VAL:HG12 | 1.91 | 0.53 |
| 41:WO:49:VAL:O | 41:WO:62:ARG:NH1 | 2.41 | 0.53 |
| 41:WO:292:GLN:O | 41:WO:298:ASN:ND2 | 2.40 | 0.53 |
| 41:WP:51:TYR:HB3 | 41:WP:59:TYR:HB3 | 1.90 | 0.53 |
| 41:WQ:51:TYR:HB3 | 41:WQ:59:TYR:HB3 | 1.90 | 0.53 |
| 7:1S:585:GLY:O | 7:1S:586:HIS:C | 2.47 | 0.53 |
| 8:1W:371:ARG:N | 40:VH:369:LYS:HZ1 | 2.06 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:1Z:384:GLN:OE1 | 8:1Z:388:ARG:NH2 | 2.28 | 0.53 |
| 9:2B:318:HIS:HA | 9:2B:321:MET:HG3 | 1.89 | 0.53 |
| 13:2T:172:TYR:HB3 | 13:2T:176:GLU:HG3 | 1.89 | 0.53 |
| 16:3L:332:ASP:HA | 16:3M:215:LEU:HD21 | 1.89 | 0.53 |
| 19:3Y:46:ILE:HG12 | 40:KH:58:ALA:HB2 | 1.90 | 0.53 |
| 21:4F:350:PHE:N | 40:CE:39:ASP:OD1 | 2.40 | 0.53 |
| 22:4I:215:SER:OG | 22:4I:216:PHE:N | 2.39 | 0.53 |
| 23:4N:242:LEU:HD12 | 23:4N:261:TYR:CE2 | 2.43 | 0.53 |
| 33:5O:45:ASN:HD22 | 41:KL:218:THR:HA | 1.74 | 0.53 |
| 34:5R:424:GLU:HA | 34:5R:427:LYS:HD2 | 1.89 | 0.53 |
| 40:AF:254:GLU:OE2 | 41:AN:99:ASN:ND2 | 2.42 | 0.53 |
| 40:AG:76:ASP:HA | 40:AG:79:ARG:HG2 | 1.89 | 0.53 |
| 40:AH:260:VAL:HB | 41:AP:397:TRP:HH2 | 1.73 | 0.53 |
| 41:AP:318:ARG:HG2 | 41:AP:354:CYS:HB3 | 1.90 | 0.53 |
| 40:BG:73:THR:HA | 40:BG:76:ASP:HB3 | 1.91 | 0.53 |
| 40:CA:66:VAL:HG21 | 40:CA:122:ILE:HG13 | 1.90 | 0.53 |
| 40:CA:177:VAL:HG23 | 40:CA:178:SER:H | 1.73 | 0.53 |
| 40:DA:173:PRO:HG3 | 40:DA:183:GLU:HG2 | 1.89 | 0.53 |
| 40:DI:145:THR:HB | 42:DI:501:GTP:O2B | 2.08 | 0.53 |
| 40:DI:172:TYR:CD1 | 40:DI:173:PRO:HD2 | 2.43 | 0.53 |
| 41:DM:6:HIS:CE1 | 41:DM:8:GLN:HB3 | 2.43 | 0.53 |
| 40:EI:5:ILE:HD11 | 40:EI:129:CYS:SG | 2.49 | 0.53 |
| 40:FA:120:ASP:O | 40:FA:123:ARG:HB3 | 2.09 | 0.53 |
| 40:FF:270:ALA:HA | 40:FF:376:MET:O | 2.08 | 0.53 |
| 40:GE:99:ALA:HA | 40:GE:110:ILE:HD11 | 1.89 | 0.53 |
| 40:GI:429:LYS:NZ | 40:GI:432:GLU:HB2 | 2.23 | 0.53 |
| 41:GN:427:ALA:O | 41:GN:428:CYS:C | 2.46 | 0.53 |
| 40:HA:185:TYR:HE2 | 40:HA:403:PHE:HB2 | 1.74 | 0.53 |
| 40:HE:339:ARG:HA | 40:HE:339:ARG:HH21 | 1.72 | 0.53 |
| 41:HN:160:PRO:O | 41:HN:162:ARG:N | 2.41 | 0.53 |
| 41:HN:420:ASN:HB2 | 41:HN:421:PRO:HD3 | 1.90 | 0.53 |
| 40:IF:349:THR:OG1 | 41:IN:384:GLN:OE1 | 2.26 | 0.53 |
| 40:II:181:VAL:HG22 | 41:IP:256:ASN:HD22 | 1.72 | 0.53 |
| 41:IQ:11:GLN:HA | 41:IQ:72:THR:HG21 | 1.89 | 0.53 |
| 40:JA:298:PRO:HB3 | 40:JA:307:PRO:HD2 | 1.90 | 0.53 |
| 41:JB:236:VAL:HG22 | 41:JB:368:ILE:HD11 | 1.89 | 0.53 |
| 40:JD:262:TYR:HB2 | 40:JD:265:ILE:HG12 | 1.91 | 0.53 |
| 41:JO:259:PRO:HG2 | 41:JO:311:LEU:HD13 | 1.90 | 0.53 |
| 41:KL:305:PRO:O | 41:KL:306:ARG:C | 2.45 | 0.53 |
| 40:MA:224:TYR:HB3 | 42:MN:501:GTP:C2 | 2.43 | 0.53 |
| 41:MB:141:GLY:O | 41:MB:145:SER:OG | 2.26 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MF:182:VAL:HG22 | 41:MM:256:ASN:HD21 | 1.74 | 0.53 |
| 40:MH:174:ALA:HB1 | 40:MH:175:PRO:HD2 | 1.89 | 0.53 |
| 40:NA:278:ALA:H | 40:NA:368:ALA:HB2 | 1.73 | 0.53 |
| 41:NB:337:ASN:HB3 | 41:NB:340:TYR:HB2 | 1.91 | 0.53 |
| 40:OE:278:ALA:H | 40:OE:368:ALA:HB2 | 1.73 | 0.53 |
| 41:OM:215:LEU:HD21 | 41:OM:273:LEU:HD22 | 1.90 | 0.53 |
| 41:ON:19:LYS:HZ1 | 41:ON:227:HIS:HA | 1.72 | 0.53 |
| 40:PA:8:HIS:HB3 | 40:PA:138:PHE:CD1 | 2.44 | 0.53 |
| 40:PF:112:LYS:HA | 40:PF:115:ILE:HG22 | 1.89 | 0.53 |
| 41:PL:237:THR:HB | 41:PL:240:LEU:HD21 | 1.90 | 0.53 |
| 41:PM:222:TYR:O | 41:PM:226:ASN:ND2 | 2.41 | 0.53 |
| 41:RN:21:TRP:HA | 41:RN:24:ILE:HG12 | 1.89 | 0.53 |
| 40:SG:236:SER:O | 40:SG:240:ALA:HB2 | 2.08 | 0.53 |
| 41:SM:27:GLU:HA | 41:SM:359:ARG:HH22 | 1.73 | 0.53 |
| 41:SO:193:VAL:HA | 41:SO:264:HIS:CE1 | 2.43 | 0.53 |
| 41:SO:226:ASN:CG | 43:SO:501:GDP:HN1 | 2.12 | 0.53 |
| 40:UA:274:PRO:HD3 | 40:UA:291:ILE:HG23 | 1.91 | 0.53 |
| 41:UB:318:ARG:HB3 | 41:UB:364:SER:HB3 | 1.90 | 0.53 |
| 40:UF:271:THR:HG21 | 40:UF:295:CYS:HA | 1.89 | 0.53 |
| 40:UF:352:LYS:HZ2 | 41:UN:179:VAL:HA | 1.74 | 0.53 |
| 40:UF:402:ALA:HA | 41:UM:260:PHE:HE1 | 1.74 | 0.53 |
| 40:WA:95:GLY:HA2 | 40:WA:114:LEU:HD11 | 1.90 | 0.53 |
| 41:WB:316:VAL:HG12 | 41:WB:352:ALA:HB3 | 1.89 | 0.53 |
| 41:WO:113:VAL:HG21 | 41:WO:150:LEU:HD22 | 1.90 | 0.53 |
| 8:1W:495:PHE:O | 38:6D:300:LYS:NZ | 2.42 | 0.53 |
| 8:1X:263:MET:HG3 | 40:UF:282:TYR:HE2 | 1.72 | 0.53 |
| 10:2E:75:ARG:HB2 | 40:AE:298:PRO:HD3 | 1.90 | 0.53 |
| 12:2M:211:ILE:HG12 | 13:2U:36:ARG:HB3 | 1.91 | 0.53 |
| 12:2R:48:MET:HB2 | 12:2R:51:SER:HB3 | 1.89 | 0.53 |
| 14:3B:71:PRO:HG2 | 14:3B:74:VAL:HG12 | 1.91 | 0.53 |
| 15:3E:203:ASN:O | 15:3E:205:VAL:N | 2.42 | 0.53 |
| 17:3Q:410:GLU:O | 17:3Q:412:CYS:N | 2.41 | 0.53 |
| 22:4I:604:ARG:HA | 22:4I:607:ARG:HG3 | 1.91 | 0.53 |
| 22:4J:465:VAL:HG23 | 22:4J:480:PHE:HB3 | 1.90 | 0.53 |
| 26:4W:201:ILE:HG23 | 26:4W:202:ARG:HG3 | 1.91 | 0.53 |
| 30:5G:104:THR:HB | 41:HB:329:GLN:HE22 | 1.73 | 0.53 |
| 30:5G:108:ARG:HH22 | 41:GB:130:LEU:HD23 | 1.73 | 0.53 |
| 36:5Y:55:MET:HB2 | 36:5Y:61:ILE:HG21 | 1.91 | 0.53 |
| 37:6A:15:HIS:NE2 | 40:TG:127:ASP:O | 2.40 | 0.53 |
| 39:6K:31:LEU:HD23 | 39:6K:136:TYR:HE1 | 1.73 | 0.53 |
| 41:AB:347:ASN:HD22 | 40:AG:178:SER:HB3 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AE:100:ALA:HA | 41:AL:252:LYS:HG3 | 1.91 | 0.53 |
| 41:AM:341:PHE:HB3 | 41:AM:348:ASN:HD21 | 1.72 | 0.53 |
| 41:AO:271:ALA:HB3 | 41:AO:272:PRO:HD3 | 1.91 | 0.53 |
| 41:AP:236:VAL:HG22 | 41:AP:368:ILE:HD11 | 1.91 | 0.53 |
| 41:BB:116:VAL:HG11 | 41:BB:151:LEU:HD21 | 1.89 | 0.53 |
| 40:BI:273:ALA:HB1 | 40:BI:274:PRO:CD | 2.33 | 0.53 |
| 40:CA:400:LYS:O | 40:CA:401:ARG:C | 2.47 | 0.53 |
| 41:CB:13:GLY:HA2 | 41:CB:136:THR:HG22 | 1.89 | 0.53 |
| 40:CH:222:PRO:HD2 | 41:CO:324:LYS:HG2 | 1.91 | 0.53 |
| 40:CI:11:GLN:NE2 | 40:CI:71:GLU:OE2 | 2.42 | 0.53 |
| 41:CL:132:GLY:HA3 | 41:CL:163:ILE:HG22 | 1.91 | 0.53 |
| 40:DH:14:VAL:HG22 | 40:DH:67:PHE:HB3 | 1.90 | 0.53 |
| 41:DL:200:TYR:HE1 | 41:DL:368:ILE:HG23 | 1.74 | 0.53 |
| 41:DO:309:ARG:NH1 | 41:DO:339:SER:O | 2.40 | 0.53 |
| 41:EB:170:VAL:HG11 | 41:EB:377:LEU:HD23 | 1.90 | 0.53 |
| 40:EF:20:CYS:HA | 40:EF:232:SER:HB2 | 1.90 | 0.53 |
| 40:EH:188:ILE:HG13 | 40:EH:394:PHE:HB2 | 1.90 | 0.53 |
| 40:EH:274:PRO:HD2 | 40:EH:291:ILE:HB | 1.90 | 0.53 |
| 40:EI:288:VAL:HG11 | 40:EI:327:ASP:HB3 | 1.89 | 0.53 |
| 40:EI:383:ILE:HG23 | 40:EI:387:TRP:HE1 | 1.74 | 0.53 |
| 41:EL:202:ILE:HG23 | 41:EL:300:MET:HB2 | 1.89 | 0.53 |
| 41:EL:314:ALA:HB2 | 41:EL:350:LYS:HZ3 | 1.74 | 0.53 |
| 41:EN:169:VAL:HG22 | 41:EN:202:ILE:HD11 | 1.90 | 0.53 |
| 41:EN:248:ALA:HA | 41:EN:252:LYS:HD2 | 1.90 | 0.53 |
| 41:EO:372:THR:OG1 | 41:EO:422:VAL:O | 2.26 | 0.53 |
| 40:FA:63:PRO:HG3 | 40:FA:87:PHE:CD1 | 2.44 | 0.53 |
| 40:FA:273:ALA:O | 40:FA:274:PRO:C | 2.47 | 0.53 |
| 40:FA:352:LYS:HD2 | 41:FB:178:THR:CA | 2.38 | 0.53 |
| 40:FA:424:MET:HE1 | 40:FA:427:LEU:HD23 | 1.91 | 0.53 |
| 41:GB:217:LEU:HB3 | 41:GB:220:PRO:HG3 | 1.89 | 0.53 |
| 40:GG:391:ASP:HB3 | 40:GG:421:ARG:HH12 | 1.72 | 0.53 |
| 40:GH:102:ASN:O | 40:GH:103:TYR:C | 2.46 | 0.53 |
| 40:GI:205:ASP:HB2 | 40:GI:303:VAL:HA | 1.90 | 0.53 |
| 40:HE:278:ALA:O | 40:HE:279:GLU:C | 2.46 | 0.53 |
| 40:IF:407:TYR:HD1 | 40:IF:412:MET:HG3 | 1.72 | 0.53 |
| 40:IG:180:ALA:HB3 | 40:IG:183:GLU:HG3 | 1.89 | 0.53 |
| 40:IH:6:SER:O | 40:IH:65:ALA:HA | 2.08 | 0.53 |
| 40:IH:20:CYS:HA | 40:IH:232:SER:HB2 | 1.91 | 0.53 |
| 40:IH:101:ASN:HD21 | 40:IH:180:ALA:HB1 | 1.72 | 0.53 |
| 40:IH:318:LEU:O | 40:IH:374:VAL:HA | 2.08 | 0.53 |
| 40:II:289:ALA:O | 40:II:293:ASN:ND2 | 2.40 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KB:100:ASN:HB3 | 41:KB:103:LYS:HB2 | 1.90 | 0.53 |
| 40:KH:51:THR:HG21 | 40:KH:243:ARG:HG2 | 1.90 | 0.53 |
| 41:KN:293:MET:HG3 | 41:KN:367:PHE:HB2 | 1.91 | 0.53 |
| 40:LG:112:LYS:HG2 | 40:LG:152:LEU:HD22 | 1.89 | 0.53 |
| 40:MG:287:SER:O | 40:MG:291:ILE:HG23 | 2.08 | 0.53 |
| 40:NF:76:ASP:OD2 | 41:NM:46:ARG:NH2 | 2.41 | 0.53 |
| 40:OH:349:THR:HB | 41:OP:176:SER:CB | 2.38 | 0.53 |
| 41:OM:132:GLY:HA2 | 41:OM:163:ILE:O | 2.08 | 0.53 |
| 41:PL:319:GLY:HA2 | 41:PL:357:PRO:HD3 | 1.89 | 0.53 |
| 41:PN:271:ALA:O | 41:PN:292:GLN:NE2 | 2.41 | 0.53 |
| 41:PP:235:GLY:HA3 | 41:PP:366:THR:HG21 | 1.91 | 0.53 |
| 41:QB:107:THR:O | 41:QB:108:GLU:C | 2.46 | 0.53 |
| 41:QB:296:ALA:O | 41:QB:298:ASN:N | 2.41 | 0.53 |
| 40:QF:144:GLY:N | 42:QF:501:GTP:O2G | 2.41 | 0.53 |
| 40:QG:269:LEU:HD11 | 40:QG:301:GLN:HB3 | 1.89 | 0.53 |
| 41:QP:68:LEU:HD13 | 41:QP:97:ALA:HA | 1.90 | 0.53 |
| 41:QP:137:HIS:N | 41:QP:168:SER:HB2 | 2.24 | 0.53 |
| 41:RB:139:LEU:HG | 41:RB:168:SER:HB3 | 1.90 | 0.53 |
| 40:RG:371:GLN:N | 40:RG:371:GLN:OE1 | 2.38 | 0.53 |
| 40:RH:238:ILE:HD13 | 40:RH:377:LEU:HD11 | 1.91 | 0.53 |
| 41:RN:54:ALA:HB3 | 41:RN:58:LYS:O | 2.08 | 0.53 |
| 40:SF:406:TRP:CH2 | 41:SM:258:VAL:HB | 2.43 | 0.53 |
| 41:SM:103:LYS:HG2 | 41:SM:107:THR:HG21 | 1.89 | 0.53 |
| 41:SO:189:VAL:HA | 41:SO:192:LEU:HB2 | 1.91 | 0.53 |
| 40:TE:26:LEU:HD21 | 40:TE:363:VAL:HG22 | 1.89 | 0.53 |
| 40:TF:223:THR:HG22 | 41:TM:322:SER:HA | 1.88 | 0.53 |
| 41:TM:407:GLU:HA | 41:TM:410:GLU:OE1 | 2.08 | 0.53 |
| 41:TN:172:SER:HB2 | 41:TN:205:GLU:HG2 | 1.89 | 0.53 |
| 41:TN:207:LEU:HB3 | 41:TN:225:LEU:HD22 | 1.91 | 0.53 |
| 41:UB:309:ARG:NH1 | 41:UB:339:SER:O | 2.41 | 0.53 |
| 40:UE:188:ILE:HG22 | 40:UE:420:ALA:HB1 | 1.91 | 0.53 |
| 40:UI:50:ASN:O | 40:UI:51:THR:C | 2.46 | 0.53 |
| 41:UO:313:VAL:O | 41:UO:349:VAL:HA | 2.09 | 0.53 |
| 41:UP:292:GLN:HA | 41:UP:295:ASP:HB3 | 1.90 | 0.53 |
| 41:UP:416:ASN:C | 41:UP:418:LEU:H | 2.12 | 0.53 |
| 41:VB:309:ARG:NH1 | 41:VB:426:GLY:O | 2.42 | 0.53 |
| 41:VO:61:PRO:HD3 | 41:VO:84:ILE:HG12 | 1.90 | 0.53 |
| 41:VP:396:HIS:HA | 41:VP:399:THR:HG22 | 1.89 | 0.53 |
| 40:WE:298:PRO:HB3 | 40:WE:307:PRO:HD2 | 1.91 | 0.53 |
| 40:WI:181:VAL:HG22 | 41:WP:348:ASN:HA | 1.89 | 0.53 |
| 41:WM:100:ASN:O | 41:WM:102:ALA:N | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WO:10:GLY:O | 41:WO:14:ASN:HB2 | 2.08 | 0.53 |
| 7:1U:157:ASN:ND2 | 40:WH:322:ASP:OD1 | 2.42 | 0.53 |
| 8:1W:317:ASN:HD22 | 40:VI:282:TYR:HE1 | 1.57 | 0.53 |
| 8:1Y:107:PHE:CG | 11:2J:252:ILE:HG21 | 2.43 | 0.53 |
| 9:2B:303:LYS:HG2 | 41:TN:359:ARG:HH21 | 1.74 | 0.53 |
| 13:2T:139:PHE:HA | 13:2T:142:ARG:HE | 1.73 | 0.53 |
| 21:4F:242:VAL:HG23 | 40:CE:41:THR:HG23 | 1.91 | 0.53 |
| 22:4I:76:LYS:HD2 | 40:AG:42:ILE:HD11 | 1.90 | 0.53 |
| 22:4J:92:LYS:HG3 | 22:4J:94:GLN:N | 2.24 | 0.53 |
| 22:4J:354:CYS:HA | 22:4J:376:ILE:HG12 | 1.90 | 0.53 |
| 22:4K:616:THR:O | 22:4K:617:CYS:C | 2.47 | 0.53 |
| 23:4P:197:LEU:HD23 | 23:4P:205:LEU:HG | 1.89 | 0.53 |
| 23:4Q:181:LYS:HE3 | 23:4Q:211:GLN:HG3 | 1.89 | 0.53 |
| 26:4W:101:ASP:OD2 | 26:4W:102:ALA:N | 2.41 | 0.53 |
| 39:6I:129:CYS:SG | 40:OA:85:GLN:NE2 | 2.82 | 0.53 |
| 40:AH:98:ASP:O | 40:AH:105:ARG:NH1 | 2.41 | 0.53 |
| 41:AN:95:SER:OG | 41:AN:96:GLY:N | 2.41 | 0.53 |
| 41:AO:192:LEU:HA | 41:AO:196:THR:HG23 | 1.89 | 0.53 |
| 41:BB:211:CYS:HA | 41:BB:215:LEU:HB2 | 1.89 | 0.53 |
| 40:BI:234:ILE:O | 40:BI:238:ILE:HG12 | 2.08 | 0.53 |
| 41:BM:107:THR:O | 41:BM:108:GLU:C | 2.45 | 0.53 |
| 41:BN:216:LYS:HB2 | 41:BN:276:ARG:HB2 | 1.91 | 0.53 |
| 41:BO:98:GLY:O | 41:BO:99:ASN:C | 2.47 | 0.53 |
| 41:BO:272:PRO:HD3 | 41:BO:364:SER:HA | 1.89 | 0.53 |
| 40:CG:67:PHE:HB2 | 40:CG:92:LEU:HD13 | 1.89 | 0.53 |
| 40:CG:109:THR:OG1 | 40:CG:410:GLU:O | 2.26 | 0.53 |
| 40:CG:273:ALA:HB3 | 40:CG:374:VAL:HG22 | 1.91 | 0.53 |
| 40:CG:335:ILE:HD13 | 40:CG:338:LYS:HZ3 | 1.72 | 0.53 |
| 40:CH:363:VAL:O | 40:CH:365:GLY:N | 2.42 | 0.53 |
| 41:CL:323:MET:HE1 | 41:CL:353:VAL:HG21 | 1.91 | 0.53 |
| 41:CM:98:GLY:O | 41:CM:99:ASN:C | 2.47 | 0.53 |
| 41:CP:180:VAL:O | 41:CP:181:GLU:C | 2.46 | 0.53 |
| 40:DA:10:GLY:HA2 | 40:DA:145:THR:HB | 1.91 | 0.53 |
| 40:DA:58:ALA:HB3 | 40:DA:60:LYS:HG2 | 1.91 | 0.53 |
| 40:DA:276:ILE:HG23 | 40:DA:281:ALA:HB2 | 1.89 | 0.53 |
| 40:DG:3:GLU:HG3 | 40:DG:51:THR:HA | 1.90 | 0.53 |
| 40:DG:142:GLY:HA3 | 42:DG:501:GTP:H5' | 1.90 | 0.53 |
| 41:DL:319:GLY:O | 41:DL:321:MET:N | 2.42 | 0.53 |
| 41:DM:266:PHE:HB3 | 41:DM:369:GLY:C | 2.29 | 0.53 |
| 41:DN:5:VAL:HG22 | 41:DN:62:ARG:HE | 1.73 | 0.53 |
| 40:EA:75:ILE:HD11 | 40:EA:92:LEU:HB3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EG:208:ALA:HB2 | 40:EG:304:LYS:HG3 | 1.90 | 0.53 |
| 40:EH:433:GLU:C | 40:EH:435:GLY:H | 2.12 | 0.53 |
| 40:EI:171:ILE:HG23 | 40:EI:204:VAL:HG23 | 1.90 | 0.53 |
| 40:FA:181:VAL:HG22 | 41:FN:256:ASN:HD22 | 1.73 | 0.53 |
| 40:FA:363:VAL:O | 40:FA:365:GLY:N | 2.42 | 0.53 |
| 40:FH:255:PHE:HZ | 40:FH:318:LEU:HD21 | 1.73 | 0.53 |
| 41:GB:13:GLY:HA2 | 41:GB:136:THR:HG22 | 1.89 | 0.53 |
| 41:GB:256:ASN:OD1 | 40:GG:181:VAL:HG22 | 2.08 | 0.53 |
| 40:GI:261:PRO:HD2 | 40:GI:265:ILE:HB | 1.90 | 0.53 |
| 40:GI:278:ALA:CA | 40:GI:368:ALA:HB2 | 2.38 | 0.53 |
| 40:HG:2:ARG:NH2 | 41:HO:69:GLU:OE1 | 2.39 | 0.53 |
| 40:HH:102:ASN:H | 40:HH:144:GLY:HA3 | 1.73 | 0.53 |
| 40:IA:395:ASP:OD2 | 40:IA:421:ARG:NE | 2.38 | 0.53 |
| 40:II:225:THR:OG1 | 40:II:229:ARG:NH2 | 2.41 | 0.53 |
| 41:IM:45:GLU:HG3 | 41:IM:46:ARG:HG2 | 1.91 | 0.53 |
| 40:JA:241:SER:OG | 40:JA:250:VAL:O | 2.25 | 0.53 |
| 40:JE:217:LEU:HD11 | 40:JE:366:ASP:HB2 | 1.90 | 0.53 |
| 41:JO:8:GLN:HE22 | 41:JO:65:LEU:HD22 | 1.73 | 0.53 |
| 40:KF:71:GLU:HB2 | 41:KM:2:ARG:HH12 | 1.72 | 0.53 |
| 40:KF:297:GLU:CA | 40:KF:298:PRO:HG2 | 2.39 | 0.53 |
| 40:KG:225:THR:OG1 | 40:KG:229:ARG:NH2 | 2.42 | 0.53 |
| 40:LA:215:ARG:NH2 | 40:LA:299:ALA:O | 2.41 | 0.53 |
| 40:LD:206:ASN:ND2 | 42:LD:501:GTP:O2' | 2.42 | 0.53 |
| 40:LE:224:TYR:HA | 40:LE:227:LEU:HB2 | 1.90 | 0.53 |
| 40:LG:188:ILE:HD11 | 40:LG:390:LEU:HB3 | 1.91 | 0.53 |
| 40:LH:397:MET:HG3 | 41:LO:346:PRO:HD2 | 1.91 | 0.53 |
| 41:LL:36:TYR:OH | 41:LL:40:SER:O | 2.26 | 0.53 |
| 41:LN:341:PHE:HB3 | 41:LN:348:ASN:HD21 | 1.73 | 0.53 |
| 40:MA:21:TRP:CZ2 | 40:MA:65:ALA:HB2 | 2.44 | 0.53 |
| 40:MG:352:LYS:HZ2 | 41:MO:179:VAL:N | 2.06 | 0.53 |
| 40:NA:88:HIS:HB3 | 40:NA:91:GLN:OE1 | 2.09 | 0.53 |
| 40:NE:171:ILE:HA | 40:NE:204:VAL:O | 2.08 | 0.53 |
| 40:NG:228:ASN:HD21 | 42:NG:501:GTP:HN1 | 1.57 | 0.53 |
| 41:NN:121:ARG:NH1 | 41:NN:158:GLU:OE2 | 2.42 | 0.53 |
| 41:NP:51:TYR:HA | 41:NP:60:VAL:O | 2.08 | 0.53 |
| 40:OH:414:GLU:O | 40:OH:415:GLY:C | 2.47 | 0.53 |
| 41:OL:137:HIS:O | 41:OL:168:SER:HA | 2.08 | 0.53 |
| 40:PE:318:LEU:O | 40:PE:374:VAL:HA | 2.08 | 0.53 |
| 41:PL:291:GLN:O | 41:PL:295:ASP:HB2 | 2.08 | 0.53 |
| 41:QB:68:LEU:HD13 | 41:QB:97:ALA:HB2 | 1.89 | 0.53 |
| 41:QN:51:TYR:HB3 | 41:QN:59:TYR:HB3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QP:9:ALA:HA | 41:QP:66:VAL:O | 2.08 | 0.53 |
| 40:RG:20:CYS:HA | 40:RG:232:SER:HB2 | 1.89 | 0.53 |
| 40:RI:74:VAL:HG23 | 40:RI:75:ILE:HD12 | 1.89 | 0.53 |
| 40:RI:136:LEU:HD22 | 40:RI:169:PHE:HE2 | 1.74 | 0.53 |
| 41:RP:289:LEU:HB3 | 41:RP:317:PHE:HE2 | 1.73 | 0.53 |
| 40:SA:191:THR:O | 40:SA:195:LEU:HB2 | 2.09 | 0.53 |
| 41:SP:36:TYR:OH | 41:SP:43:GLN:NE2 | 2.41 | 0.53 |
| 41:TB:421:PRO:HA | 41:TB:424:THR:HG22 | 1.91 | 0.53 |
| 40:TF:100:ALA:HA | 41:TM:252:LYS:HB3 | 1.88 | 0.53 |
| 40:TG:121:ARG:NH1 | 40:TG:124:LYS:HE2 | 2.24 | 0.53 |
| 40:TH:224:TYR:HE2 | 41:TO:246:LEU:HD22 | 1.72 | 0.53 |
| 41:TM:376:GLU:OE2 | 41:TM:380:ARG:NH2 | 2.41 | 0.53 |
| 41:TN:239:CYS:HB3 | 41:TN:248:ALA:H | 1.73 | 0.53 |
| 41:UB:62:ARG:NH1 | 41:UB:127:CYS:SG | 2.80 | 0.53 |
| 40:UH:70:LEU:HB2 | 40:UH:145:THR:HG22 | 1.90 | 0.53 |
| 40:VA:391:ASP:HB3 | 40:VA:421:ARG:HH22 | 1.73 | 0.53 |
| 41:VB:3:GLU:HG2 | 41:VB:62:ARG:HH12 | 1.73 | 0.53 |
| 40:VI:370:VAL:HG12 | 40:VI:372:ARG:H | 1.73 | 0.53 |
| 41:VO:424:THR:OG1 | 41:VO:425:ARG:NH1 | 2.42 | 0.53 |
| 40:WF:240:ALA:HB1 | 40:WF:356:ASN:HD22 | 1.73 | 0.53 |
| 40:WG:269:LEU:HD23 | 40:WG:303:VAL:HB | 1.89 | 0.53 |
| 40:WI:335:ILE:HD13 | 40:WI:338:LYS:HZ1 | 1.74 | 0.53 |
| 41:WP:52:ASN:OD1 | 41:WP:62:ARG:NH2 | 2.42 | 0.53 |
| 41:WP:95:SER:OG | 41:WP:96:GLY:N | 2.42 | 0.53 |
| 7:1T:74:LYS:HG3 | 7:1T:121:PRO:HA | 1.89 | 0.53 |
| 7:1T:259:LEU:HD11 | 7:1T:265:LEU:HG | 1.91 | 0.53 |
| 11:2I:220:SER:O | 11:2I:221:ILE:C | 2.46 | 0.53 |
| 11:2K:204:TRP:HA | 11:2K:237:LEU:HD13 | 1.91 | 0.53 |
| 12:2O:104:ASP:C | 12:2O:106:HIS:H | 2.12 | 0.53 |
| 12:2P:105:TYR:OH | 12:2P:137:HIS:O | 2.26 | 0.53 |
| 17:3P:270:LYS:HD2 | 17:3Q:402:GLU:HG2 | 1.90 | 0.53 |
| 17:3R:201:HIS:HA | 17:3R:204:LYS:HD3 | 1.90 | 0.53 |
| 20:4B:345:GLN:HA | 20:4B:348:LYS:HD2 | 1.89 | 0.53 |
| 22:4I:653:LEU:HB2 | 22:4I:690:TYR:CE2 | 2.43 | 0.53 |
| 23:4M:103:PHE:HD2 | 23:4M:104:ILE:HG12 | 1.74 | 0.53 |
| 26:4W:335:ARG:NE | 26:4W:344:ALA:O | 2.42 | 0.53 |
| 40:AF:188:ILE:HD12 | 40:AF:424:MET:HG2 | 1.91 | 0.53 |
| 41:BB:252:LYS:HE3 | 41:BB:350:LYS:HZ1 | 1.74 | 0.53 |
| 40:BE:182:VAL:O | 40:BE:183:GLU:C | 2.47 | 0.53 |
| 40:BH:20:CYS:HA | 40:BH:232:SER:HB2 | 1.91 | 0.53 |
| 40:BI:291:ILE:HG12 | 40:BI:292:THR:N | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BL:87:PRO:HD3 | 41:CL:281:TYR:CD2 | 2.42 | 0.53 |
| 41:BM:310:TYR:N | 41:BM:340:TYR:O | 2.42 | 0.53 |
| 41:BO:93:GLY:O | 41:BO:94:GLN:C | 2.47 | 0.53 |
| 40:CA:106:GLY:HA3 | 40:CA:148:GLY:CA | 2.37 | 0.53 |
| 40:CG:116:ASP:OD1 | 40:CG:117:LEU:N | 2.42 | 0.53 |
| 41:CL:20:PHE:HA | 41:CL:230:SER:HB2 | 1.89 | 0.53 |
| 41:CN:21:TRP:CZ3 | 41:CN:61:PRO:HB3 | 2.43 | 0.53 |
| 41:CO:98:GLY:O | 41:CO:99:ASN:C | 2.46 | 0.53 |
| 41:CO:107:THR:O | 41:CO:110:ALA:N | 2.42 | 0.53 |
| 40:DA:49:PHE:HD2 | 40:DA:53:PHE:HB2 | 1.73 | 0.53 |
| 41:DB:313:VAL:HG22 | 41:DB:367:PHE:HE1 | 1.73 | 0.53 |
| 40:DE:181:VAL:HG12 | 41:DL:349:VAL:N | 2.24 | 0.53 |
| 40:DH:241:SER:HA | 40:DH:356:ASN:HB3 | 1.90 | 0.53 |
| 40:DI:105:ARG:HG2 | 40:DI:410:GLU:HG2 | 1.91 | 0.53 |
| 40:DI:383:ILE:HG13 | 40:DI:387:TRP:NE1 | 2.24 | 0.53 |
| 41:DL:143:THR:O | 41:DL:144:GLY:C | 2.47 | 0.53 |
| 41:DN:113:VAL:HG11 | 41:DN:150:LEU:HD13 | 1.91 | 0.53 |
| 41:DO:176:SER:OG | 41:DO:181:GLU:OE1 | 2.25 | 0.53 |
| 40:EG:71:GLU:OE1 | 40:EG:71:GLU:N | 2.42 | 0.53 |
| 40:EH:276:ILE:HG22 | 40:EH:280:LYS:HD3 | 1.89 | 0.53 |
| 41:EM:310:TYR:O | 41:EM:311:LEU:C | 2.47 | 0.53 |
| 41:FN:318:ARG:HD3 | 41:FN:358:PRO:HD3 | 1.90 | 0.53 |
| 41:FP:99:ASN:HA | 41:FP:142:GLY:H | 1.73 | 0.53 |
| 40:GH:93:ILE:HD12 | 40:GH:118:VAL:HA | 1.91 | 0.53 |
| 40:GH:250:VAL:HB | 40:GH:255:PHE:CE1 | 2.43 | 0.53 |
| 41:HN:193:VAL:HG12 | 41:HN:265:PHE:CE2 | 2.43 | 0.53 |
| 41:HP:117:LEU:HD11 | 41:HP:154:LYS:HB3 | 1.91 | 0.53 |
| 40:JA:287:SER:O | 40:JA:291:ILE:HG12 | 2.09 | 0.53 |
| 41:LB:156:ARG:NH2 | 41:LB:197:ASP:OD2 | 2.42 | 0.53 |
| 40:MA:288:VAL:HA | 40:MA:291:ILE:HG12 | 1.90 | 0.53 |
| 40:MA:348:PRO:HD2 | 41:MB:388:MET:HG3 | 1.90 | 0.53 |
| 41:ML:313:VAL:HG12 | 41:ML:349:VAL:HG13 | 1.90 | 0.53 |
| 41:MM:16:ILE:HA | 41:MM:226:ASN:HB3 | 1.90 | 0.53 |
| 41:MP:309:ARG:N | 41:MP:372:THR:OG1 | 2.40 | 0.53 |
| 40:NA:195:LEU:HD11 | 40:NA:427:LEU:HD13 | 1.90 | 0.53 |
| 41:NB:8:GLN:HG2 | 41:NB:17:GLY:HA3 | 1.90 | 0.53 |
| 40:OF:175:PRO:HD2 | 40:OF:207:GLU:HG3 | 1.91 | 0.53 |
| 40:OF:206:ASN:OD1 | 42:OM:501:GTP:O2' | 2.20 | 0.53 |
| 41:OP:383:GLU:HA | 41:OP:386:THR:HG22 | 1.89 | 0.53 |
| 40:PA:75:ILE:HG23 | 40:PA:92:LEU:HD12 | 1.90 | 0.53 |
| 40:PA:316:CYS:HA | 40:PA:352:LYS:HB2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PB:178:THR:HB | 41:PB:181:GLU:HG3 | 1.91 | 0.53 |
| 41:PB:238:THR:HA | 41:PB:241:ARG:NH1 | 2.23 | 0.53 |
| 40:PE:311:LYS:HE3 | 40:PE:344:VAL:HA | 1.90 | 0.53 |
| 40:PG:288:VAL:HA | 40:PG:291:ILE:HG12 | 1.89 | 0.53 |
| 41:QB:308:GLY:HA3 | 41:QB:373:ALA:CB | 2.38 | 0.53 |
| 41:QL:237:THR:OG1 | 41:QL:241:ARG:NH2 | 2.42 | 0.53 |
| 41:QP:35:THR:O | 41:QP:37:HIS:N | 2.39 | 0.53 |
| 41:QP:99:ASN:CG | 41:QP:178:THR:HG21 | 2.29 | 0.53 |
| 41:QP:192:LEU:O | 41:QP:196:THR:N | 2.34 | 0.53 |
| 40:RA:105:ARG:HG3 | 40:RA:410:GLU:HG2 | 1.90 | 0.53 |
| 40:RI:206:ASN:OD1 | 42:RP:501:GTP:O2' | 2.23 | 0.53 |
| 41:RL:316:VAL:HA | 41:RL:352:ALA:HB3 | 1.89 | 0.53 |
| 41:RP:279:GLN:O | 41:RP:282:ARG:NH1 | 2.42 | 0.53 |
| 40:SG:352:LYS:HD2 | 41:SO:179:VAL:HG13 | 1.91 | 0.53 |
| 41:UN:375:GLN:NE2 | 41:UN:422:VAL:O | 2.41 | 0.53 |
| 40:VF:141:PHE:HB2 | 40:VF:173:PRO:HD3 | 1.90 | 0.53 |
| 40:VI:100:ALA:HA | 41:VP:252:LYS:HB2 | 1.89 | 0.53 |
| 41:VO:167:PHE:CZ | 41:VO:233:MET:HG2 | 2.43 | 0.53 |
| 40:WG:109:THR:OG1 | 40:WG:410:GLU:O | 2.25 | 0.53 |
| 41:WN:132:GLY:HA3 | 41:WN:163:ILE:HG13 | 1.91 | 0.53 |
| 11:2I:119:LYS:HZ1 | 40:LG:409:GLY:C | 2.11 | 0.53 |
| 12:2N:105:TYR:OH | 12:2N:137:HIS:O | 2.26 | 0.53 |
| 15:3H:81:LEU:HD13 | 15:3H:171:LEU:HD23 | 1.91 | 0.53 |
| 17:3R:182:GLU:HG2 | 17:3R:237:LEU:HD11 | 1.90 | 0.53 |
| 17:3R:207:GLY:C | 17:3R:209:ASP:H | 2.10 | 0.53 |
| 18:3T:405:LEU:HD11 | 18:3U:74:SER:HB3 | 1.91 | 0.53 |
| 20:4A:181:ALA:HA | 20:4A:184:LEU:HB2 | 1.90 | 0.53 |
| 21:4D:122:ILE:HG12 | 21:4D:133:VAL:HG22 | 1.90 | 0.53 |
| 22:4J:551:LYS:NZ | 22:4J:594:LEU:HB3 | 2.24 | 0.53 |
| 22:4K:435:ARG:HH22 | 40:EI:38:SER:C | 2.12 | 0.53 |
| 22:4K:670:ASN:O | 22:4K:671:ASP:C | 2.47 | 0.53 |
| 33:5O:118:SER:HB3 | 33:5O:121:LEU:HB2 | 1.89 | 0.53 |
| 39:6G:99:LEU:HG | 39:6G:103:LYS:HE2 | 1.91 | 0.53 |
| 40:BA:172:TYR:OH | 40:BA:386:ALA:O | 2.26 | 0.53 |
| 40:BH:402:ALA:O | 40:BH:403:PHE:C | 2.47 | 0.53 |
| 41:BP:42:LEU:O | 41:BP:45:GLU:N | 2.41 | 0.53 |
| 41:BP:56:GLY:O | 41:BP:57:GLY:C | 2.47 | 0.53 |
| 40:CF:401:ARG:NH1 | 40:CF:414:GLU:OE2 | 2.41 | 0.53 |
| 40:CH:277:SER:O | 40:CH:279:GLU:HG2 | 2.09 | 0.53 |
| 41:CL:44:LEU:HA | 41:CL:47:ILE:HG23 | 1.90 | 0.53 |
| 41:CM:7:LEU:HD22 | 41:CM:151:LEU:HD21 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DA:21:TRP:CZ3 | 40:DA:63:PRO:HB3 | 2.43 | 0.53 |
| 41:DB:60:VAL:HG12 | 41:EB:281:TYR:HD2 | 1.74 | 0.53 |
| 40:DG:298:PRO:HB3 | 40:DG:307:PRO:HD2 | 1.91 | 0.53 |
| 41:DL:391:ARG:HG3 | 41:DL:393:ALA:HB2 | 1.91 | 0.53 |
| 41:DN:335:ASN:O | 41:DN:336:LYS:C | 2.47 | 0.53 |
| 41:DN:385:PHE:HE2 | 41:DN:389:PHE:HB2 | 1.71 | 0.53 |
| 40:EF:107:HIS:CD2 | 40:EF:152:LEU:HB2 | 2.44 | 0.53 |
| 40:EI:278:ALA:O | 40:EI:279:GLU:C | 2.47 | 0.53 |
| 41:EN:193:VAL:HA | 41:EN:264:HIS:HE1 | 1.72 | 0.53 |
| 40:FA:101:ASN:H | 41:FN:252:LYS:HE2 | 1.72 | 0.53 |
| 40:FA:106:GLY:O | 40:FA:108:TYR:N | 2.42 | 0.53 |
| 40:GF:352:LYS:HD2 | 41:GN:179:VAL:N | 2.24 | 0.53 |
| 41:GP:226:ASN:N | 43:GP:502:GDP:HN21 | 2.06 | 0.53 |
| 41:HN:313:VAL:HA | 41:HN:369:GLY:HA2 | 1.90 | 0.53 |
| 40:IF:102:ASN:HB3 | 40:IF:105:ARG:HG3 | 1.90 | 0.53 |
| 41:IP:163:ILE:HD11 | 41:IP:251:ARG:HD3 | 1.90 | 0.53 |
| 41:IQ:334:GLN:NE2 | 41:IQ:348:ASN:OD1 | 2.42 | 0.53 |
| 41:JM:192:LEU:HD13 | 41:JM:196:THR:HG21 | 1.91 | 0.53 |
| 40:KD:76:ASP:HA | 40:KD:79:ARG:HG2 | 1.90 | 0.53 |
| 41:KL:163:ILE:HD11 | 41:KL:251:ARG:HB3 | 1.91 | 0.53 |
| 41:KM:27:GLU:OE1 | 41:KM:241:ARG:NH2 | 2.38 | 0.53 |
| 41:KM:107:THR:O | 41:KM:110:ALA:N | 2.38 | 0.53 |
| 41:KO:372:THR:OG1 | 41:KO:422:VAL:O | 2.24 | 0.53 |
| 40:LG:271:THR:HA | 40:LG:302:MET:HG3 | 1.91 | 0.53 |
| 40:LG:352:LYS:HE3 | 41:LO:179:VAL:CA | 2.39 | 0.53 |
| 40:MH:305:CYS:O | 40:MH:305:CYS:SG | 2.67 | 0.53 |
| 41:MP:237:THR:O | 41:MP:241:ARG:NH1 | 2.42 | 0.53 |
| 41:NB:7:LEU:HG | 41:NB:64:VAL:HB | 1.91 | 0.53 |
| 40:ND:112:LYS:HD2 | 40:ND:112:LYS:N | 2.24 | 0.53 |
| 40:OG:88:HIS:CE1 | 40:OG:90:GLU:HB2 | 2.44 | 0.53 |
| 41:OP:142:GLY:O | 41:OP:144:GLY:N | 2.41 | 0.53 |
| 40:PE:329:ASN:HD22 | 41:PM:175:VAL:HG21 | 1.73 | 0.53 |
| 40:PF:20:CYS:HA | 40:PF:232:SER:HB2 | 1.91 | 0.53 |
| 41:PL:63:ALA:O | 41:PL:89:ASN:ND2 | 2.41 | 0.53 |
| 41:PM:421:PRO:HA | 41:PM:424:THR:HG22 | 1.91 | 0.53 |
| 41:PN:252:LYS:O | 41:PN:256:ASN:HB2 | 2.09 | 0.53 |
| 41:PO:328:GLU:OE2 | 41:PO:332:ASN:ND2 | 2.42 | 0.53 |
| 40:QA:107:HIS:HD1 | 40:QA:151:SER:HG | 1.56 | 0.53 |
| 40:QA:276:ILE:HG23 | 40:QA:280:LYS:HG2 | 1.91 | 0.53 |
| 41:RN:103:LYS:O | 41:RN:107:THR:OG1 | 2.27 | 0.53 |
| 41:RO:165:ASN:ND2 | 41:RO:198:GLU:OE1 | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RP:132:GLY:HA3 | 41:RP:163:ILE:O | 2.07 | 0.53 |
| 40:SG:88:HIS:HB3 | 40:SG:91:GLN:HB2 | 1.91 | 0.53 |
| 40:SH:221:ARG:HH12 | 41:SO:325:GLU:HB2 | 1.73 | 0.53 |
| 41:SM:309:ARG:NH1 | 41:SM:339:SER:O | 2.42 | 0.53 |
| 41:SP:66:VAL:HG11 | 41:SP:147:MET:HE2 | 1.91 | 0.53 |
| 40:TE:139:HIS:CD2 | 40:TE:150:THR:HG21 | 2.43 | 0.53 |
| 40:TH:181:VAL:HG12 | 41:TO:348:ASN:HA | 1.91 | 0.53 |
| 41:TM:260:PHE:HE2 | 41:TM:425:ARG:HH11 | 1.55 | 0.53 |
| 41:TP:113:VAL:HA | 41:TP:116:VAL:HG12 | 1.91 | 0.53 |
| 40:UA:217:LEU:HA | 40:UA:277:SER:HB2 | 1.89 | 0.53 |
| 40:UI:353:VAL:HG12 | 40:UI:354:GLY:H | 1.73 | 0.53 |
| 41:UP:61:PRO:HD3 | 41:UP:84:ILE:HG13 | 1.91 | 0.53 |
| 41:VO:52:ASN:OD1 | 41:VO:62:ARG:NH2 | 2.42 | 0.53 |
| 40:WF:20:CYS:HA | 40:WF:232:SER:HB2 | 1.90 | 0.53 |
| 40:WH:255:PHE:O | 40:WH:259:LEU:HB2 | 2.09 | 0.53 |
| 41:WN:248:ALA:HA | 41:WN:252:LYS:CE | 2.39 | 0.53 |
| 8:1Z:371:ARG:HB3 | 40:UI:282:TYR:CE1 | 2.43 | 0.53 |
| 10:2F:157:ARG:NH2 | 41:VB:51:TYR:HB3 | 2.24 | 0.53 |
| 11:2K:186:LYS:HB2 | 11:2K:252:ILE:HG22 | 1.91 | 0.53 |
| 13:2W:97:LYS:HB3 | 41:AN:392:LYS:NZ | 2.23 | 0.53 |
| 21:4D:520:PRO:O | 21:4D:521:ALA:C | 2.47 | 0.53 |
| 23:4M:92:PRO:CB | 40:AG:89:PRO:HB3 | 2.34 | 0.53 |
| 23:4P:260:THR:O | 23:4P:262:GLY:N | 2.37 | 0.53 |
| 27:4Z:65:HIS:HA | 27:4Z:140:VAL:HA | 1.91 | 0.53 |
| 35:5T:188:ARG:NH1 | 40:KE:47:ASP:OD2 | 2.42 | 0.53 |
| 41:AB:198:GLU:OE2 | 41:AB:200:TYR:OH | 2.22 | 0.53 |
| 40:CI:286:LEU:O | 40:CI:372:ARG:NH1 | 2.41 | 0.53 |
| 41:CN:326:VAL:O | 41:CN:330:MET:HG2 | 2.09 | 0.53 |
| 40:DF:195:LEU:HG | 40:DF:267:PHE:CZ | 2.42 | 0.53 |
| 40:DH:119:LEU:HA | 40:DH:122:ILE:HD12 | 1.90 | 0.53 |
| 40:DH:303:VAL:O | 40:DH:304:LYS:C | 2.47 | 0.53 |
| 41:DL:138:SER:HA | 41:DL:169:VAL:HG23 | 1.90 | 0.53 |
| 41:DN:12:CYS:HB2 | 43:DN:501:GDP:C8 | 2.43 | 0.53 |
| 41:DN:34:GLY:HA3 | 41:DN:58:LYS:HD2 | 1.90 | 0.53 |
| 41:DO:412:GLU:O | 41:DO:416:ASN:ND2 | 2.42 | 0.53 |
| 41:DP:144:GLY:O | 41:DP:148:GLY:HA3 | 2.09 | 0.53 |
| 41:DP:199:THR:HG23 | 41:DP:264:HIS:CD2 | 2.43 | 0.53 |
| 41:EB:358:PRO:HG2 | 41:EB:361:LEU:HD12 | 1.89 | 0.53 |
| 40:EI:212:ILE:HG13 | 40:EI:213:CYS:N | 2.23 | 0.53 |
| 41:EM:268:PRO:O | 41:EM:300:MET:HB2 | 2.09 | 0.53 |
| 41:EP:303:CYS:O | 41:EP:304:ASP:C | 2.45 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FA:11:GLN:HG3 | 40:FA:15:GLN:HG3 | 1.91 | 0.53 |
| 40:FA:72:PRO:O | 40:FA:73:THR:C | 2.46 | 0.53 |
| 40:FH:171:ILE:HG21 | 42:FO:501:GTP:H1' | 1.90 | 0.53 |
| 40:FI:175:PRO:O | 40:FI:389:ARG:NH2 | 2.42 | 0.53 |
| 41:GB:139:LEU:HG | 41:GB:168:SER:HB3 | 1.91 | 0.53 |
| 40:GE:293:ASN:HA | 40:GE:335:ILE:HD11 | 1.91 | 0.53 |
| 40:GF:133:GLN:NE2 | 40:GF:251:ASP:OD2 | 2.42 | 0.53 |
| 41:GN:244:GLY:HA2 | 41:GN:355:ASP:HB2 | 1.91 | 0.53 |
| 40:HE:109:THR:O | 40:HE:110:ILE:C | 2.47 | 0.53 |
| 40:HH:53:PHE:O | 40:HH:64:ARG:NH1 | 2.42 | 0.53 |
| 41:HN:6:HIS:CD2 | 41:HN:134:GLN:HE21 | 2.26 | 0.53 |
| 41:HN:235:GLY:O | 41:HN:238:THR:HG22 | 2.09 | 0.53 |
| 41:HN:292:GLN:O | 41:HN:293:MET:C | 2.47 | 0.53 |
| 41:IB:87:PRO:HG2 | 40:JF:280:LYS:HG2 | 1.89 | 0.53 |
| 41:IB:215:LEU:HD21 | 41:IB:273:LEU:HD22 | 1.90 | 0.53 |
| 40:IG:2:ARG:HH12 | 40:IG:249:ASN:HD21 | 1.55 | 0.53 |
| 41:IO:139:LEU:HD12 | 41:IO:170:VAL:HG12 | 1.91 | 0.53 |
| 40:JH:76:ASP:OD2 | 41:JO:46:ARG:NH2 | 2.36 | 0.53 |
| 40:KD:2:ARG:HD3 | 40:KD:242:LEU:HB2 | 1.89 | 0.53 |
| 40:KE:217:LEU:HA | 40:KE:277:SER:HB2 | 1.89 | 0.53 |
| 40:KF:248:LEU:HB2 | 40:KF:355:ILE:H | 1.72 | 0.53 |
| 40:KH:50:ASN:O | 40:KH:64:ARG:NH1 | 2.41 | 0.53 |
| 40:KH:210:TYR:HE2 | 40:KH:227:LEU:HD11 | 1.74 | 0.53 |
| 40:KH:329:ASN:HB3 | 41:KP:175:VAL:HG11 | 1.88 | 0.53 |
| 40:LA:226:ASN:ND2 | 40:LA:366:ASP:OD2 | 2.42 | 0.53 |
| 40:LA:273:ALA:HB3 | 40:LA:374:VAL:H | 1.74 | 0.53 |
| 41:LB:77:ARG:HH12 | 41:LB:83:GLN:HA | 1.74 | 0.53 |
| 40:LG:209:ILE:HB | 40:LG:227:LEU:HG | 1.91 | 0.53 |
| 40:NA:66:VAL:HG12 | 40:NA:91:GLN:HB2 | 1.90 | 0.53 |
| 40:ND:101:ASN:HA | 40:ND:144:GLY:H | 1.73 | 0.53 |
| 41:NL:17:GLY:HA2 | 41:NL:20:PHE:CD2 | 2.44 | 0.53 |
| 41:NL:64:VAL:HG12 | 41:NL:89:ASN:HB3 | 1.89 | 0.53 |
| 41:NP:309:ARG:NH2 | 41:NP:343:GLU:OE1 | 2.41 | 0.53 |
| 40:OD:143:GLY:N | 42:OD:501:GTP:O2A | 2.36 | 0.53 |
| 41:OM:52:ASN:HD21 | 41:OM:86:ARG:HH22 | 1.54 | 0.53 |
| 41:OP:222:TYR:O | 41:OP:226:ASN:ND2 | 2.41 | 0.53 |
| 41:PB:236:VAL:HG13 | 41:PB:237:THR:HG23 | 1.91 | 0.53 |
| 41:QB:23:VAL:HG22 | 41:QB:227:HIS:CE1 | 2.44 | 0.53 |
| 41:QB:218:THR:O | 41:QB:220:PRO:HD3 | 2.09 | 0.53 |
| 41:QN:289:LEU:HD11 | 41:QN:363:MET:HG3 | 1.90 | 0.53 |
| 41:QP:375:GLN:O | 41:QP:379:LYS:HB2 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RB:331:LEU:HD11 | 40:RG:177:VAL:HA | 1.89 | 0.53 |
| 40:RE:175:PRO:O | 40:RE:393:LYS:NZ | 2.36 | 0.53 |
| 41:RN:216:LYS:HB2 | 41:RN:275:SER:HB3 | 1.91 | 0.53 |
| 40:SA:90:GLU:HB2 | 40:SA:121:ARG:HH22 | 1.74 | 0.53 |
| 40:SH:2:ARG:NH2 | 41:SP:69:GLU:OE2 | 2.42 | 0.53 |
| 40:SI:101:ASN:HD22 | 41:SP:256:ASN:HD21 | 1.57 | 0.53 |
| 40:SI:137:ILE:HB | 40:SI:168:GLU:HG3 | 1.91 | 0.53 |
| 40:TH:319:TYR:HB3 | 40:TH:323:VAL:HG21 | 1.90 | 0.53 |
| 41:TO:329:GLN:HA | 41:TO:332:ASN:HB3 | 1.91 | 0.53 |
| 40:UF:235:VAL:HA | 40:UF:238:ILE:HG22 | 1.89 | 0.53 |
| 41:UM:237:THR:HG22 | 41:UM:250:LEU:HD21 | 1.91 | 0.53 |
| 41:UO:132:GLY:HA2 | 41:UO:162:ARG:HB3 | 1.90 | 0.53 |
| 41:VB:194:GLU:OE2 | 41:VB:262:ARG:NH1 | 2.42 | 0.53 |
| 40:VG:316:CYS:HA | 40:VG:352:LYS:HB3 | 1.91 | 0.53 |
| 40:VH:175:PRO:HB2 | 40:VH:389:ARG:HH11 | 1.74 | 0.53 |
| 40:WE:108:TYR:O | 40:WE:112:LYS:NZ | 2.42 | 0.53 |
| 41:WM:66:VAL:HG13 | 41:WM:147:MET:HE1 | 1.90 | 0.53 |
| 41:WP:165:ASN:ND2 | 41:WP:198:GLU:OE1 | 2.42 | 0.53 |
| 10:2F:151:HIS:HB3 | 10:2F:157:ARG:H | 1.74 | 0.53 |
| 11:2J:105:PHE:HA | 11:2J:108:THR:HB | 1.91 | 0.53 |
| 11:2J:188:LEU:HD12 | 11:2J:250:ILE:HB | 1.91 | 0.53 |
| 15:3E:311:LYS:HB3 | 15:3H:198:ILE:HG22 | 1.90 | 0.53 |
| 17:3O:211:VAL:HG12 | 17:3R:94:TYR:HB2 | 1.90 | 0.53 |
| 21:4D:96:VAL:HG12 | 21:4D:125:TYR:HA | 1.91 | 0.53 |
| 21:4E:442:TYR:CD2 | 21:4E:449:ILE:HG13 | 2.44 | 0.53 |
| 22:4I:583:ARG:HH12 | 22:4I:596:ASP:HA | 1.73 | 0.53 |
| 23:4N:205:LEU:O | 23:4N:206:SER:C | 2.47 | 0.53 |
| 23:4Q:240:LEU:HB3 | 23:4Q:266:HIS:HB3 | 1.91 | 0.53 |
| 23:4R:59:THR:CG2 | 41:BP:42:LEU:HD22 | 2.39 | 0.53 |
| 23:4R:91:ILE:HB | 23:4R:92:PRO:HD2 | 1.91 | 0.53 |
| 23:4R:257:PHE:HB3 | 40:EI:221:ARG:CD | 2.37 | 0.53 |
| 33:5O:68:ASP:OD2 | 35:5T:69:TYR:OH | 2.27 | 0.53 |
| 38:6C:45:GLN:OE1 | 41:VO:306:ARG:NH1 | 2.42 | 0.53 |
| 40:AA:313:MET:HB2 | 40:AA:379:ASN:HB3 | 1.90 | 0.53 |
| 40:AA:360:PRO:O | 40:AA:369:LYS:NZ | 2.41 | 0.53 |
| 41:BB:28:HIS:HB3 | 41:BB:47:ILE:HD11 | 1.91 | 0.53 |
| 40:BI:411:GLY:O | 40:BI:412:MET:C | 2.47 | 0.53 |
| 41:BM:22:GLU:HG2 | 41:BM:81:PHE:HB2 | 1.91 | 0.53 |
| 41:BM:28:HIS:O | 41:BM:43:GLN:HB3 | 2.09 | 0.53 |
| 41:BM:354:CYS:O | 41:BM:355:ASP:C | 2.47 | 0.53 |
| 41:BO:113:VAL:HA | 41:BO:116:VAL:HG22 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CB:49:VAL:O | 41:CB:62:ARG:NH1 | 2.42 | 0.53 |
| 40:CE:177:VAL:HG23 | 41:CL:331:LEU:HB2 | 1.90 | 0.53 |
| 40:CH:209:ILE:HB | 40:CH:227:LEU:HD13 | 1.91 | 0.53 |
| 40:CH:274:PRO:HB2 | 40:CH:370:VAL:HG21 | 1.90 | 0.53 |
| 41:CO:266:PHE:CE1 | 41:CO:370:ASN:HB2 | 2.43 | 0.53 |
| 41:CP:172:SER:HB2 | 41:CP:175:VAL:HG23 | 1.90 | 0.53 |
| 41:CP:424:THR:OG1 | 41:CP:425:ARG:N | 2.42 | 0.53 |
| 40:DA:137:ILE:HD11 | 40:DA:139:HIS:CD2 | 2.43 | 0.53 |
| 41:DB:170:VAL:HB | 41:DB:171:PRO:HD2 | 1.90 | 0.53 |
| 40:DE:404:VAL:O | 40:DE:405:HIS:C | 2.46 | 0.53 |
| 41:DM:420:ASN:HB2 | 41:DM:421:PRO:CD | 2.39 | 0.53 |
| 41:DP:257:MET:CE | 41:DP:314:ALA:HB2 | 2.39 | 0.53 |
| 41:EM:109:GLY:O | 41:EM:110:ALA:C | 2.47 | 0.53 |
| 40:FA:106:GLY:HA3 | 40:FA:148:GLY:CA | 2.37 | 0.53 |
| 40:FG:147:SER:HB2 | 40:FG:190:THR:HG21 | 1.91 | 0.53 |
| 41:FM:290:THR:HG21 | 41:FM:329:GLN:HB3 | 1.90 | 0.53 |
| 41:FP:89:ASN:ND2 | 41:FP:123:GLU:OE2 | 2.42 | 0.53 |
| 40:GF:105:ARG:HH21 | 40:GF:110:ILE:HD13 | 1.74 | 0.53 |
| 40:GH:278:ALA:CA | 40:GH:368:ALA:HB2 | 2.36 | 0.53 |
| 40:GH:370:VAL:HG22 | 40:GH:372:ARG:H | 1.74 | 0.53 |
| 40:GI:326:LYS:HA | 40:GI:329:ASN:HD21 | 1.74 | 0.53 |
| 41:GO:33:THR:O | 41:GO:58:LYS:NZ | 2.36 | 0.53 |
| 41:HB:317:PHE:HB2 | 41:HB:353:VAL:HG12 | 1.90 | 0.53 |
| 40:HF:316:CYS:HB3 | 40:HF:377:LEU:HB2 | 1.91 | 0.53 |
| 40:HI:73:THR:HA | 40:HI:76:ASP:HB2 | 1.91 | 0.53 |
| 41:HN:21:TRP:CE3 | 41:HN:24:ILE:HD11 | 2.43 | 0.53 |
| 41:HQ:414:ASN:HA | 41:HQ:417:ASP:HB2 | 1.90 | 0.53 |
| 40:IE:7:VAL:HB | 40:IE:137:ILE:HG22 | 1.91 | 0.53 |
| 40:IH:73:THR:HA | 40:IH:76:ASP:HB2 | 1.90 | 0.53 |
| 40:IH:226:ASN:ND2 | 40:IH:366:ASP:OD2 | 2.41 | 0.53 |
| 41:IO:86:ARG:NH1 | 41:IO:123:GLU:OE2 | 2.42 | 0.53 |
| 41:IP:134:GLN:HA | 41:IP:165:ASN:O | 2.08 | 0.53 |
| 41:IQ:107:THR:HG22 | 41:IQ:108:GLU:H | 1.74 | 0.53 |
| 41:IQ:317:PHE:HB2 | 41:IQ:353:VAL:HG12 | 1.91 | 0.53 |
| 40:JE:177:VAL:HG12 | 41:JL:331:LEU:HD22 | 1.91 | 0.53 |
| 40:JH:324:VAL:HG13 | 40:JH:327:ASP:H | 1.74 | 0.53 |
| 41:JN:98:GLY:C | 41:JN:99:ASN:HD22 | 2.11 | 0.53 |
| 41:JN:191:GLN:O | 41:JN:195:ASN:ND2 | 2.38 | 0.53 |
| 40:KA:204:VAL:HG23 | 40:KA:302:MET:HG2 | 1.90 | 0.53 |
| 40:KA:329:ASN:HB3 | 41:KB:175:VAL:HG11 | 1.91 | 0.53 |
| 41:KB:286:VAL:HG21 | 41:KB:325:GLU:HB3 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KE:308:ARG:HD3 | 40:NE:282:TYR:HE2 | 1.74 | 0.53 |
| 41:KO:199:THR:OG1 | 41:KO:264:HIS:O | 2.23 | 0.53 |
| 41:ML:178:THR:HG22 | 41:ML:180:VAL:H | 1.72 | 0.53 |
| 41:MM:328:GLU:O | 41:MM:332:ASN:HB2 | 2.09 | 0.53 |
| 40:ND:131:GLY:O | 40:ND:132:LEU:C | 2.48 | 0.53 |
| 40:NF:6:SER:O | 40:NF:65:ALA:HA | 2.07 | 0.53 |
| 41:NL:164:MET:O | 41:NL:196:THR:OG1 | 2.27 | 0.53 |
| 41:OB:347:ASN:ND2 | 40:OG:177:VAL:O | 2.42 | 0.53 |
| 40:OF:294:ALA:O | 40:OF:300:ASN:ND2 | 2.39 | 0.53 |
| 40:OH:354:GLY:O | 40:OH:355:ILE:C | 2.47 | 0.53 |
| 40:OH:403:PHE:CE1 | 41:OO:345:ILE:HD13 | 2.44 | 0.53 |
| 41:ON:263:LEU:HD21 | 41:ON:421:PRO:HB2 | 1.91 | 0.53 |
| 40:PD:288:VAL:HG11 | 40:PD:323:VAL:HG23 | 1.91 | 0.53 |
| 40:PD:359:PRO:HB3 | 40:PD:371:GLN:HA | 1.89 | 0.53 |
| 41:PM:101:TRP:CD1 | 41:PM:105:HIS:HB2 | 2.43 | 0.53 |
| 41:QB:108:GLU:O | 41:QB:109:GLY:C | 2.47 | 0.53 |
| 40:QF:273:ALA:HB3 | 40:QF:374:VAL:H | 1.73 | 0.53 |
| 40:QH:241:SER:OG | 40:QH:249:ASN:OD1 | 2.26 | 0.53 |
| 41:QL:22:GLU:HG2 | 41:QL:81:PHE:HB2 | 1.91 | 0.53 |
| 41:QO:142:GLY:O | 41:QO:144:GLY:N | 2.42 | 0.53 |
| 41:QP:167:PHE:HB3 | 41:QP:200:TYR:HB2 | 1.91 | 0.53 |
| 41:QP:311:LEU:HB3 | 41:QP:370:ASN:CB | 2.30 | 0.53 |
| 40:RF:71:GLU:HB3 | 40:RF:98:ASP:HA | 1.91 | 0.53 |
| 40:RF:209:ILE:HA | 40:RF:212:ILE:HG22 | 1.90 | 0.53 |
| 41:RP:253:LEU:O | 41:RP:257:MET:HB2 | 2.09 | 0.53 |
| 40:SA:88:HIS:HD2 | 40:TA:283:HIS:HB2 | 1.74 | 0.53 |
| 41:SB:89:ASN:ND2 | 41:SB:123:GLU:OE2 | 2.40 | 0.53 |
| 41:SL:330:MET:HB3 | 41:SL:349:VAL:HG11 | 1.90 | 0.53 |
| 41:SN:4:ILE:HD11 | 41:SN:131:GLN:HE21 | 1.74 | 0.53 |
| 40:TA:226:ASN:ND2 | 40:TA:366:ASP:OD2 | 2.42 | 0.53 |
| 40:TH:60:LYS:HD3 | 40:UH:282:TYR:HB3 | 1.91 | 0.53 |
| 41:UB:413:SER:O | 41:UB:417:ASP:HB2 | 2.08 | 0.53 |
| 40:UF:109:THR:OG1 | 40:UF:110:ILE:N | 2.42 | 0.53 |
| 40:UI:413:GLU:O | 40:UI:414:GLU:C | 2.47 | 0.53 |
| 41:UM:165:ASN:ND2 | 41:UM:250:LEU:HD13 | 2.21 | 0.53 |
| 41:UN:36:TYR:HB2 | 41:UN:59:TYR:HE2 | 1.74 | 0.53 |
| 41:UP:244:GLY:HA3 | 41:UP:355:ASP:H | 1.73 | 0.53 |
| 40:VG:71:GLU:HB3 | 40:VG:98:ASP:HA | 1.91 | 0.53 |
| 40:WE:274:PRO:HG3 | 40:WE:286:LEU:HD12 | 1.90 | 0.53 |
| 40:WF:274:PRO:HB3 | 40:WF:370:VAL:HG11 | 1.91 | 0.53 |
| 8:1X:100:LEU:HD21 | 11:2I:251:TYR:CD2 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:1Y:159:LYS:NZ | 8:1Y:161:SER:OG | 2.41 | 0.53 |
| 11:2I:128:LYS:HD2 | 40:MG:214:ARG:HG2 | 1.91 | 0.53 |
| 11:2J:161:ARG:HA | 11:2J:164:GLU:HG3 | 1.91 | 0.53 |
| 12:2M:199:ILE:HG12 | 41:AB:424:THR:HG21 | 1.90 | 0.53 |
| 12:2O:56:PRO:HG2 | 41:AM:309:ARG:HD3 | 1.91 | 0.53 |
| 16:3J:31:GLN:HE22 | 16:3K:366:LEU:HA | 1.74 | 0.53 |
| 21:4F:430:ILE:HD13 | 41:FM:280:GLN:HG2 | 1.91 | 0.53 |
| 22:4J:69:PRO:HG3 | 40:MF:58:ALA:HA | 1.89 | 0.53 |
| 23:4N:260:THR:O | 23:4N:262:GLY:N | 2.37 | 0.53 |
| 24:4O:173:SER:CB | 24:4O:181:LYS:HA | 2.37 | 0.53 |
| 33:5N:451:LEU:HD23 | 33:5O:124:LEU:HD23 | 1.90 | 0.53 |
| 41:AL:51:TYR:O | 41:AL:62:ARG:NH2 | 2.42 | 0.53 |
| 41:AO:22:GLU:HG2 | 41:AO:81:PHE:HB2 | 1.91 | 0.53 |
| 40:BE:8:HIS:ND1 | 40:BE:17:GLY:HA3 | 2.23 | 0.53 |
| 40:BF:96:LYS:HB3 | 41:BM:129:CYS:SG | 2.49 | 0.53 |
| 40:CF:262:TYR:HE1 | 41:CN:393:ALA:HA | 1.74 | 0.53 |
| 40:CH:208:ALA:O | 40:CH:212:ILE:HG13 | 2.08 | 0.53 |
| 41:CM:149:THR:HA | 41:CM:152:ILE:HB | 1.91 | 0.53 |
| 41:CN:268:PRO:HG2 | 41:CN:300:MET:HB2 | 1.91 | 0.53 |
| 41:DB:198:GLU:HG2 | 41:DB:266:PHE:CZ | 2.44 | 0.53 |
| 40:DE:76:ASP:HA | 40:DE:79:ARG:HB2 | 1.91 | 0.53 |
| 40:DH:140:SER:OG | 40:DH:141:PHE:N | 2.42 | 0.53 |
| 40:DI:224:TYR:N | 41:DP:323:MET:SD | 2.82 | 0.53 |
| 41:DO:378:PHE:HA | 41:DO:381:ILE:HG22 | 1.89 | 0.53 |
| 41:DP:104:GLY:CA | 41:DP:109:GLY:HA3 | 2.38 | 0.53 |
| 40:EG:239:THR:HG23 | 40:EG:242:LEU:HD21 | 1.91 | 0.53 |
| 40:EG:265:ILE:HD11 | 40:EG:430:ASP:HB3 | 1.91 | 0.53 |
| 41:EL:167:PHE:CE1 | 41:EL:233:MET:HG2 | 2.43 | 0.53 |
| 41:EN:172:SER:OG | 41:EN:175:VAL:O | 2.22 | 0.53 |
| 41:EP:222:TYR:CD1 | 41:EP:225:LEU:HD12 | 2.44 | 0.53 |
| 41:FM:49:VAL:HG13 | 41:FM:50:TYR:HD1 | 1.73 | 0.53 |
| 41:FM:257:MET:HE3 | 41:FM:368:ILE:HG23 | 1.91 | 0.53 |
| 41:FN:240:LEU:HB3 | 41:FN:249:ASP:HB3 | 1.91 | 0.53 |
| 40:GF:181:VAL:HG12 | 41:GM:348:ASN:HA | 1.91 | 0.53 |
| 41:GN:393:ALA:O | 41:GN:394:PHE:C | 2.47 | 0.53 |
| 41:GP:103:LYS:HA | 41:GP:107:THR:HB | 1.91 | 0.53 |
| 40:HA:268:PRO:HB2 | 40:HA:377:LEU:HD12 | 1.90 | 0.53 |
| 41:HB:141:GLY:O | 41:HB:184:ASN:ND2 | 2.42 | 0.53 |
| 40:HE:114:LEU:HB3 | 40:HE:149:PHE:HZ | 1.74 | 0.53 |
| 41:HN:393:ALA:O | 41:HN:394:PHE:C | 2.46 | 0.53 |
| 40:IG:242:LEU:HD11 | 40:IG:252:LEU:HG | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IQ:173:PRO:HB3 | 41:IQ:384:GLN:HE22 | 1.73 | 0.53 |
| 40:JD:313:MET:SD | 40:JD:379:ASN:ND2 | 2.82 | 0.53 |
| 40:JE:316:CYS:HA | 40:JE:352:LYS:HB2 | 1.91 | 0.53 |
| 40:JH:193:THR:O | 40:JH:197:HIS:ND1 | 2.40 | 0.53 |
| 41:JL:213:ARG:HE | 41:JL:297:LYS:NZ | 2.06 | 0.53 |
| 40:KA:165:SER:HB3 | 40:KA:256:GLN:HE22 | 1.74 | 0.53 |
| 40:KD:228:ASN:ND2 | 42:KD:501:GTP:HN1 | 2.01 | 0.53 |
| 40:KE:265:ILE:HG23 | 40:KE:431:TYR:HE2 | 1.74 | 0.53 |
| 41:KM:120:VAL:HG11 | 41:KM:155:ILE:HD11 | 1.91 | 0.53 |
| 40:LA:174:ALA:HB3 | 40:LA:178:SER:H | 1.73 | 0.53 |
| 41:LL:7:LEU:O | 41:LL:135:LEU:HA | 2.09 | 0.53 |
| 41:MB:3:GLU:HA | 41:MB:49:VAL:HG13 | 1.91 | 0.53 |
| 40:MD:326:LYS:HE2 | 41:ML:208:TYR:HB3 | 1.91 | 0.53 |
| 40:NA:256:GLN:HG2 | 41:NB:397:TRP:CZ2 | 2.44 | 0.53 |
| 40:ND:141:PHE:HE2 | 40:ND:203:MET:HB3 | 1.74 | 0.53 |
| 40:NG:143:GLY:N | 42:NG:501:GTP:O2A | 2.42 | 0.53 |
| 41:OB:42:LEU:HD22 | 41:OB:243:PRO:HG3 | 1.90 | 0.53 |
| 40:OD:244:PHE:HB2 | 40:OD:356:ASN:HD21 | 1.72 | 0.53 |
| 41:PB:263:LEU:HD22 | 41:PB:422:VAL:HB | 1.91 | 0.53 |
| 40:PD:30:ILE:HG13 | 40:PD:36:MET:HB2 | 1.91 | 0.53 |
| 40:PD:180:ALA:HB3 | 40:PD:183:GLU:HG3 | 1.90 | 0.53 |
| 41:PP:271:ALA:HB1 | 41:PP:292:GLN:HG2 | 1.91 | 0.53 |
| 40:QF:316:CYS:HB3 | 40:QF:377:LEU:HB2 | 1.89 | 0.53 |
| 41:QP:116:VAL:HG11 | 41:QP:151:LEU:HD21 | 1.89 | 0.53 |
| 41:RM:11:GLN:HA | 41:RM:72:THR:HG21 | 1.91 | 0.53 |
| 41:RP:89:ASN:ND2 | 41:RP:123:GLU:OE2 | 2.42 | 0.53 |
| 40:SA:91:GLN:OE1 | 40:SA:121:ARG:NH1 | 2.42 | 0.53 |
| 40:SE:231:ILE:HA | 40:SE:234:ILE:HD12 | 1.91 | 0.53 |
| 40:SF:326:LYS:NZ | 41:SN:225:LEU:HD21 | 2.24 | 0.53 |
| 40:SG:329:ASN:HA | 40:SG:332:ILE:HG12 | 1.90 | 0.53 |
| 41:SO:81:PHE:C | 41:SO:84:ILE:HD13 | 2.29 | 0.53 |
| 41:SO:302:ALA:O | 41:SO:304:ASP:N | 2.42 | 0.53 |
| 41:SP:252:LYS:O | 41:SP:256:ASN:ND2 | 2.42 | 0.53 |
| 40:TG:252:LEU:HA | 40:TG:255:PHE:HD2 | 1.73 | 0.53 |
| 40:TI:168:GLU:HB2 | 40:TI:201:ALA:HA | 1.91 | 0.53 |
| 41:TP:27:GLU:OE2 | 41:TP:318:ARG:NH2 | 2.42 | 0.53 |
| 40:UA:101:ASN:HA | 40:UA:144:GLY:H | 1.73 | 0.53 |
| 41:UB:170:VAL:HG21 | 41:UB:377:LEU:HD11 | 1.90 | 0.53 |
| 40:UF:261:PRO:HA | 41:UN:394:PHE:CD1 | 2.44 | 0.53 |
| 41:UO:165:ASN:HA | 41:UO:198:GLU:O | 2.08 | 0.53 |
| 41:UP:97:ALA:O | 41:UP:99:ASN:N | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UP:322:SER:O | 41:UP:324:LYS:N | 2.42 | 0.53 |
| 41:WM:98:GLY:O | 41:WM:99:ASN:C | 2.46 | 0.53 |
| 41:WQ:7:LEU:HD22 | 41:WQ:151:LEU:HD21 | 1.90 | 0.53 |
| 4:1H:161:ARG:HH22 | 41:GO:121:ARG:NH2 | 2.05 | 0.52 |
| 5:1N:161:LYS:HD2 | 41:HQ:336:LYS:NZ | 2.22 | 0.52 |
| 8:1X:254:ARG:HD2 | 8:1X:258:HIS:CE1 | 2.45 | 0.52 |
| 11:2J:187:ARG:HA | 11:2J:251:TYR:HB3 | 1.90 | 0.52 |
| 13:2X:171:LEU:O | 13:2X:172:TYR:C | 2.47 | 0.52 |
| 22:4J:627:LEU:HD13 | 22:4J:697:LEU:HD21 | 1.92 | 0.52 |
| 23:4N:234:ARG:HG2 | 41:DM:41:ASP:CG | 2.29 | 0.52 |
| 24:4O:194:ALA:HB2 | 24:4O:209:ALA:HB1 | 1.92 | 0.52 |
| 23:4R:19:ILE:HG13 | 40:BI:79:ARG:HB3 | 1.90 | 0.52 |
| 39:6J:131:GLU:HA | 39:6J:135:HIS:HB2 | 1.89 | 0.52 |
| 40:AA:107:HIS:HD2 | 40:AA:152:LEU:HB2 | 1.73 | 0.52 |
| 41:BB:3:GLU:HG3 | 41:BB:127:CYS:HB3 | 1.91 | 0.52 |
| 40:BI:11:GLN:HA | 40:BI:74:VAL:HG21 | 1.91 | 0.52 |
| 41:BM:221:THR:OG1 | 41:BM:222:TYR:N | 2.43 | 0.52 |
| 41:BP:101:TRP:CD1 | 41:BP:145:SER:HB2 | 2.44 | 0.52 |
| 40:CA:219:ILE:O | 40:CA:220:GLU:C | 2.47 | 0.52 |
| 40:CE:400:LYS:HD2 | 41:CL:344:TRP:HB2 | 1.91 | 0.52 |
| 40:CH:8:HIS:CD2 | 40:CH:17:GLY:HA3 | 2.44 | 0.52 |
| 40:CH:259:LEU:HD11 | 40:CH:377:LEU:HB2 | 1.92 | 0.52 |
| 40:CH:328:VAL:HG11 | 40:CH:353:VAL:HG11 | 1.89 | 0.52 |
| 41:CO:212:PHE:O | 41:CO:216:LYS:HA | 2.09 | 0.52 |
| 41:CO:271:ALA:CB | 41:CO:365:ALA:HB3 | 2.39 | 0.52 |
| 41:CP:88:ASP:C | 41:CP:90:PHE:H | 2.12 | 0.52 |
| 40:DE:409:GLY:O | 40:DE:410:GLU:C | 2.48 | 0.52 |
| 40:DF:76:ASP:O | 40:DF:79:ARG:HB2 | 2.09 | 0.52 |
| 40:DI:153:LEU:O | 40:DI:154:MET:C | 2.47 | 0.52 |
| 40:DI:183:GLU:HB2 | 40:DI:184:PRO:HD3 | 1.90 | 0.52 |
| 41:DL:171:PRO:HB3 | 41:DL:181:GLU:HG2 | 1.91 | 0.52 |
| 41:DM:56:GLY:O | 41:DM:57:GLY:C | 2.47 | 0.52 |
| 41:DP:3:GLU:HA | 41:DP:49:VAL:HA | 1.91 | 0.52 |
| 41:DP:31:ASP:OD1 | 41:DP:34:GLY:N | 2.41 | 0.52 |
| 41:DP:113:VAL:HG23 | 41:DP:151:LEU:HD22 | 1.91 | 0.52 |
| 41:DP:266:PHE:HA | 41:DP:370:ASN:HA | 1.90 | 0.52 |
| 40:EG:436:MET:O | 41:EO:391:ARG:NH2 | 2.33 | 0.52 |
| 41:EM:286:VAL:HB | 41:EM:325:GLU:HG2 | 1.90 | 0.52 |
| 40:FA:252:LEU:HA | 40:FA:255:PHE:CD2 | 2.44 | 0.52 |
| 40:FE:224:TYR:HA | 40:FE:227:LEU:HD12 | 1.91 | 0.52 |
| 40:GE:203:MET:HG3 | 40:GE:204:VAL:N | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GH:212:ILE:HG23 | 40:GH:216:ASN:HD21 | 1.73 | 0.52 |
| 41:GN:222:TYR:HA | 41:GN:225:LEU:HD12 | 1.91 | 0.52 |
| 41:GP:203:ASP:OD2 | 41:GP:302:ALA:N | 2.39 | 0.52 |
| 40:HH:401:ARG:NH1 | 40:HH:414:GLU:OE2 | 2.42 | 0.52 |
| 41:HM:170:VAL:HG11 | 41:HM:377:LEU:HD21 | 1.90 | 0.52 |
| 41:HN:103:LYS:HA | 41:HN:107:THR:OG1 | 2.08 | 0.52 |
| 41:HN:335:ASN:O | 41:HN:336:LYS:C | 2.48 | 0.52 |
| 41:HN:361:LEU:O | 41:HN:362:LYS:C | 2.47 | 0.52 |
| 41:HO:191:GLN:O | 41:HO:195:ASN:ND2 | 2.42 | 0.52 |
| 41:IP:268:PRO:HG2 | 41:IP:300:MET:HB2 | 1.90 | 0.52 |
| 40:JA:101:ASN:HD22 | 41:JN:256:ASN:HD21 | 1.56 | 0.52 |
| 40:JE:16:ILE:HA | 40:JE:228:ASN:HB3 | 1.90 | 0.52 |
| 40:JE:405:HIS:HA | 40:JE:408:VAL:HG12 | 1.91 | 0.52 |
| 40:JG:228:ASN:HB3 | 40:JG:231:ILE:HD12 | 1.90 | 0.52 |
| 40:KA:71:GLU:HB3 | 40:KA:98:ASP:HA | 1.90 | 0.52 |
| 41:KB:60:VAL:HG11 | 41:KB:86:ARG:HG2 | 1.91 | 0.52 |
| 40:KH:236:SER:HA | 40:KH:243:ARG:HH12 | 1.73 | 0.52 |
| 40:LE:264:ARG:NH1 | 40:LE:430:ASP:OD2 | 2.42 | 0.52 |
| 40:LF:136:LEU:HD22 | 40:LF:169:PHE:HE2 | 1.75 | 0.52 |
| 40:MA:99:ALA:HB3 | 40:MA:144:GLY:HA3 | 1.91 | 0.52 |
| 41:MB:130:LEU:O | 41:MB:162:ARG:NH1 | 2.41 | 0.52 |
| 40:NE:11:GLN:HA | 40:NE:74:VAL:HG11 | 1.91 | 0.52 |
| 40:NE:207:GLU:HB3 | 40:NE:304:LYS:HZ1 | 1.74 | 0.52 |
| 40:NF:122:ILE:HG21 | 40:NF:157:LEU:HD21 | 1.91 | 0.52 |
| 41:NM:159:TYR:HB3 | 41:NM:162:ARG:HD3 | 1.91 | 0.52 |
| 41:NP:15:GLN:OE1 | 41:NP:19:LYS:NZ | 2.42 | 0.52 |
| 40:OD:135:PHE:HD2 | 40:OD:166:LYS:HB3 | 1.73 | 0.52 |
| 40:OE:75:ILE:HG23 | 40:OE:92:LEU:HD12 | 1.91 | 0.52 |
| 40:OF:195:LEU:HD12 | 40:OF:266:HIS:HE1 | 1.74 | 0.52 |
| 41:ON:137:HIS:O | 41:ON:168:SER:HA | 2.09 | 0.52 |
| 40:PD:182:VAL:O | 40:PD:186:ASN:ND2 | 2.41 | 0.52 |
| 41:PL:271:ALA:O | 41:PL:292:GLN:NE2 | 2.42 | 0.52 |
| 41:PO:249:ASP:H | 41:PO:252:LYS:HB3 | 1.74 | 0.52 |
| 40:QA:20:CYS:HA | 40:QA:232:SER:HB2 | 1.91 | 0.52 |
| 40:QA:157:LEU:HB3 | 40:QA:166:LYS:HE2 | 1.91 | 0.52 |
| 40:QA:210:TYR:CD1 | 41:QN:324:LYS:HE3 | 2.44 | 0.52 |
| 41:QB:56:GLY:O | 41:QB:57:GLY:C | 2.46 | 0.52 |
| 40:QE:112:LYS:HA | 40:QE:115:ILE:HG12 | 1.90 | 0.52 |
| 41:QN:63:ALA:O | 41:QN:89:ASN:ND2 | 2.42 | 0.52 |
| 41:QP:397:TRP:O | 41:QP:398:TYR:C | 2.47 | 0.52 |
| 40:RA:254:GLU:O | 40:RA:258:ASN:ND2 | 2.34 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SO:87:PRO:O | 41:SO:88:ASP:C | 2.46 | 0.52 |
| 41:SO:341:PHE:O | 41:SO:342:VAL:C | 2.46 | 0.52 |
| 40:TA:51:THR:HG23 | 40:TA:52:PHE:HD1 | 1.73 | 0.52 |
| 40:TA:318:LEU:O | 40:TA:374:VAL:HA | 2.10 | 0.52 |
| 40:TG:259:LEU:O | 40:TG:379:ASN:ND2 | 2.42 | 0.52 |
| 41:UB:86:ARG:NH1 | 41:VB:281:TYR:O | 2.42 | 0.52 |
| 40:UG:217:LEU:HB3 | 40:UG:219:ILE:HG12 | 1.91 | 0.52 |
| 40:UI:13:GLY:O | 40:UI:16:ILE:HG12 | 2.08 | 0.52 |
| 40:UI:190:THR:OG1 | 40:UI:191:THR:N | 2.43 | 0.52 |
| 41:UN:22:GLU:HG2 | 41:UN:81:PHE:CD2 | 2.44 | 0.52 |
| 41:UO:424:THR:OG1 | 41:UO:425:ARG:NH1 | 2.42 | 0.52 |
| 41:VN:7:LEU:HD13 | 41:VN:151:LEU:HD13 | 1.90 | 0.52 |
| 40:WE:51:THR:HG23 | 40:WE:52:PHE:HD1 | 1.72 | 0.52 |
| 41:WM:256:ASN:HB2 | 41:WM:257:MET:HE1 | 1.91 | 0.52 |
| 41:WN:186:THR:HG21 | 41:WN:385:PHE:HB2 | 1.91 | 0.52 |
| 41:WN:326:VAL:O | 41:WN:327:ASP:C | 2.47 | 0.52 |
| 41:WO:105:HIS:CD2 | 41:WO:150:LEU:HB2 | 2.44 | 0.52 |
| 7:1U:507:CYS:SG | 7:1U:520:SER:OG | 2.62 | 0.52 |
| 15:3E:309:PRO:HA | 15:3E:312:VAL:HG12 | 1.92 | 0.52 |
| 16:3J:301:GLU:HB3 | 16:3J:305:ARG:HH12 | 1.73 | 0.52 |
| 16:3L:262:GLU:OE2 | 16:3L:394:ARG:NH1 | 2.41 | 0.52 |
| 18:3T:367:GLU:HG3 | 18:3U:257:TRP:HE1 | 1.75 | 0.52 |
| 18:3W:313:ASP:HA | 18:3W:316:HIS:CE1 | 2.44 | 0.52 |
| 20:4A:39:GLY:HA3 | 40:MA:372:ARG:HH22 | 1.74 | 0.52 |
| 21:4F:473:VAL:HB | 21:4F:482:PRO:HB2 | 1.91 | 0.52 |
| 22:4H:125:LEU:HD13 | 41:BL:277:GLY:HA2 | 1.91 | 0.52 |
| 22:4I:109:GLU:OE2 | 22:4I:133:ARG:NH2 | 2.42 | 0.52 |
| 23:4N:194:ALA:O | 23:4N:197:LEU:N | 2.43 | 0.52 |
| 26:4V:265:ALA:O | 26:4V:317:ASN:ND2 | 2.26 | 0.52 |
| 26:4V:342:LEU:HD13 | 26:4V:355:VAL:HG11 | 1.90 | 0.52 |
| 31:5I:432:PHE:CE2 | 40:IG:368:ALA:HB1 | 2.44 | 0.52 |
| 38:6C:137:PRO:HB2 | 41:VP:306:ARG:HH11 | 1.74 | 0.52 |
| 40:AA:258:ASN:HB2 | 40:AA:352:LYS:HD2 | 1.91 | 0.52 |
| 40:AA:280:LYS:HB3 | 40:MA:88:HIS:CE1 | 2.41 | 0.52 |
| 41:AB:281:TYR:HD2 | 41:MB:87:PRO:HD3 | 1.74 | 0.52 |
| 40:AG:226:ASN:ND2 | 40:AG:366:ASP:OD2 | 2.41 | 0.52 |
| 41:AL:101:TRP:HB2 | 41:AL:184:ASN:HD22 | 1.74 | 0.52 |
| 41:AO:100:ASN:HD22 | 41:AO:102:ALA:HB3 | 1.74 | 0.52 |
| 40:BE:3:GLU:HG3 | 40:BE:129:CYS:HB2 | 1.92 | 0.52 |
| 40:BH:254:GLU:O | 40:BH:255:PHE:C | 2.47 | 0.52 |
| 40:BI:147:SER:HB2 | 40:BI:190:THR:OG1 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CA:328:VAL:HG11 | 40:CA:353:VAL:CG1 | 2.38 | 0.52 |
| 40:CE:63:PRO:HD3 | 40:CE:86:LEU:HG | 1.91 | 0.52 |
| 40:CF:119:LEU:HG | 40:CF:156:ARG:HD2 | 1.91 | 0.52 |
| 40:CF:248:LEU:HD21 | 41:CN:222:TYR:CE2 | 2.44 | 0.52 |
| 41:CM:60:VAL:HG21 | 41:DM:281:TYR:O | 2.09 | 0.52 |
| 41:CN:44:LEU:HA | 41:CN:47:ILE:HG12 | 1.91 | 0.52 |
| 40:DF:328:VAL:HG11 | 40:DF:353:VAL:HG11 | 1.91 | 0.52 |
| 40:DI:303:VAL:O | 40:DI:304:LYS:C | 2.46 | 0.52 |
| 41:DM:259:PRO:CG | 41:DM:311:LEU:HD21 | 2.39 | 0.52 |
| 41:DP:6:HIS:CE1 | 41:DP:8:GLN:HB3 | 2.45 | 0.52 |
| 40:EE:269:LEU:HD22 | 40:EE:303:VAL:HG21 | 1.90 | 0.52 |
| 40:EF:91:GLN:HE22 | 40:EF:125:LEU:HD21 | 1.74 | 0.52 |
| 40:EF:141:PHE:HB2 | 40:EF:173:PRO:HD3 | 1.90 | 0.52 |
| 41:EL:165:ASN:HB3 | 41:EL:167:PHE:CE2 | 2.44 | 0.52 |
| 41:EM:98:GLY:O | 41:EM:100:ASN:N | 2.43 | 0.52 |
| 41:EM:103:LYS:HA | 41:EM:107:THR:CG2 | 2.39 | 0.52 |
| 40:FA:415:GLY:O | 40:FA:416:GLU:C | 2.47 | 0.52 |
| 40:FF:97:GLU:HG2 | 40:FF:110:ILE:HG13 | 1.91 | 0.52 |
| 40:FI:271:THR:HA | 40:FI:302:MET:HG2 | 1.91 | 0.52 |
| 41:GB:253:LEU:O | 41:GB:257:MET:CB | 2.56 | 0.52 |
| 40:GF:326:LYS:NZ | 41:GN:208:TYR:HB2 | 2.24 | 0.52 |
| 40:HE:5:ILE:HD12 | 40:HE:125:LEU:HB3 | 1.91 | 0.52 |
| 40:HF:133:GLN:O | 40:HF:165:SER:OG | 2.24 | 0.52 |
| 40:HF:352:LYS:HD2 | 41:HN:177:ASP:O | 2.09 | 0.52 |
| 40:HI:119:LEU:HA | 40:HI:122:ILE:HG22 | 1.91 | 0.52 |
| 41:HN:301:ALA:O | 41:HN:303:CYS:N | 2.42 | 0.52 |
| 41:HQ:87:PRO:HA | 41:HQ:90:PHE:HD2 | 1.74 | 0.52 |
| 41:IB:248:ALA:HA | 41:IB:252:LYS:HE3 | 1.90 | 0.52 |
| 40:IG:209:ILE:HA | 40:IG:212:ILE:HG22 | 1.91 | 0.52 |
| 40:IH:65:ALA:O | 40:IH:91:GLN:NE2 | 2.42 | 0.52 |
| 40:KA:206:ASN:OD1 | 42:KN:501:GTP:O2' | 2.28 | 0.52 |
| 41:LB:172:SER:HB2 | 41:LB:205:GLU:HG2 | 1.91 | 0.52 |
| 40:LE:246:GLY:HA3 | 40:LE:356:ASN:HA | 1.92 | 0.52 |
| 41:LO:248:ALA:HA | 41:LO:252:LYS:HD2 | 1.91 | 0.52 |
| 40:MF:162:GLY:O | 40:MF:163:LYS:C | 2.48 | 0.52 |
| 40:MG:132:LEU:HB3 | 40:MG:164:LYS:HE2 | 1.91 | 0.52 |
| 40:MG:260:VAL:HB | 41:MO:397:TRP:CZ3 | 2.43 | 0.52 |
| 40:MH:258:ASN:HD21 | 41:MP:178:THR:HG23 | 1.72 | 0.52 |
| 41:MM:237:THR:HG22 | 41:MM:250:LEU:HD21 | 1.91 | 0.52 |
| 40:NF:311:LYS:NZ | 40:NF:437:ASP:OD1 | 2.33 | 0.52 |
| 40:NG:405:HIS:HA | 40:NG:408:VAL:HG12 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OD:265:ILE:HG22 | 40:OD:379:ASN:HD21 | 1.74 | 0.52 |
| 40:OF:68:VAL:HA | 40:OF:93:ILE:O | 2.09 | 0.52 |
| 40:OH:221:ARG:N | 41:OO:324:LYS:HZ2 | 2.07 | 0.52 |
| 41:OO:215:LEU:HD21 | 41:OO:273:LEU:HD22 | 1.91 | 0.52 |
| 41:PB:286:VAL:HG12 | 41:PB:289:LEU:HD12 | 1.91 | 0.52 |
| 41:PN:149:THR:HA | 41:PN:152:ILE:HD12 | 1.92 | 0.52 |
| 41:QB:104:GLY:C | 41:QB:109:GLY:HA3 | 2.25 | 0.52 |
| 41:QN:22:GLU:HG2 | 41:QN:81:PHE:HD2 | 1.73 | 0.52 |
| 40:RA:177:VAL:HA | 41:RN:331:LEU:HD11 | 1.89 | 0.52 |
| 41:RB:67:ASP:HA | 41:RB:143:THR:HG21 | 1.90 | 0.52 |
| 41:RB:323:MET:HG2 | 41:RB:353:VAL:HG21 | 1.91 | 0.52 |
| 40:RE:178:SER:OG | 40:RE:183:GLU:OE1 | 2.26 | 0.52 |
| 40:RH:6:SER:O | 40:RH:65:ALA:HA | 2.09 | 0.52 |
| 41:SB:152:ILE:HA | 41:SB:155:ILE:HG22 | 1.91 | 0.52 |
| 40:SE:76:ASP:OD2 | 41:SL:46:ARG:NH2 | 2.36 | 0.52 |
| 40:SF:151:SER:HB3 | 40:SF:193:THR:HG21 | 1.91 | 0.52 |
| 40:SF:167:LEU:HD22 | 40:SF:200:CYS:HB3 | 1.91 | 0.52 |
| 40:SG:223:THR:OG1 | 40:SG:225:THR:OG1 | 2.25 | 0.52 |
| 41:TP:1:MET:SD | 41:TP:46:ARG:NH2 | 2.82 | 0.52 |
| 40:UG:2:ARG:HG3 | 40:UG:242:LEU:HB2 | 1.90 | 0.52 |
| 41:UP:212:PHE:HB3 | 41:UP:213:ARG:HH11 | 1.73 | 0.52 |
| 41:VN:269:GLY:O | 41:VN:367:PHE:N | 2.41 | 0.52 |
| 40:WE:88:HIS:HB2 | 40:WE:91:GLN:HG3 | 1.91 | 0.52 |
| 40:WE:112:LYS:HA | 40:WE:115:ILE:HG22 | 1.89 | 0.52 |
| 40:WI:276:ILE:HG23 | 40:WI:280:LYS:HB2 | 1.90 | 0.52 |
| 41:WQ:105:HIS:HD2 | 41:WQ:150:LEU:HB2 | 1.74 | 0.52 |
| 7:1T:440:GLU:HG2 | 7:1T:442:ARG:HD2 | 1.91 | 0.52 |
| 8:1Z:357:GLU:HA | 8:1Z:360:ARG:HB2 | 1.90 | 0.52 |
| 13:2T:6:PHE:HB2 | 40:WG:117:LEU:HD13 | 1.91 | 0.52 |
| 13:2W:174:GLU:O | 13:2W:175:ASP:C | 2.48 | 0.52 |
| 14:3A:109:LEU:HD13 | 40:LF:159:VAL:HG22 | 1.91 | 0.52 |
| 17:3P:379:ILE:HG12 | 17:3P:441:ALA:HB1 | 1.91 | 0.52 |
| 19:3Y:167:TRP:HZ2 | 25:4T:399:GLU:HG2 | 1.75 | 0.52 |
| 20:4A:84:GLN:HA | 20:4A:87:ARG:HE | 1.73 | 0.52 |
| 20:4A:232:GLU:O | 20:4A:235:CYS:HB2 | 2.10 | 0.52 |
| 21:4D:283:ASP:O | 21:4D:285:ARG:NH1 | 2.42 | 0.52 |
| 23:4Q:241:GLY:O | 23:4Q:242:LEU:C | 2.48 | 0.52 |
| 26:4W:268:GLU:HB3 | 26:4W:314:GLN:HB2 | 1.90 | 0.52 |
| 27:4Z:72:LEU:HD11 | 27:4Z:149:LEU:HD13 | 1.90 | 0.52 |
| 40:AH:188:ILE:HD12 | 40:AH:424:MET:HG3 | 1.91 | 0.52 |
| 41:AM:253:LEU:O | 41:AM:257:MET:CB | 2.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AN:311:LEU:HD21 | 41:AN:425:ARG:HB3 | 1.90 | 0.52 |
| 40:BA:205:ASP:HB2 | 40:BA:303:VAL:HG23 | 1.92 | 0.52 |
| 41:BB:193:VAL:HG12 | 41:BB:262:ARG:HG2 | 1.91 | 0.52 |
| 40:BF:238:ILE:HG23 | 40:BF:255:PHE:CE2 | 2.41 | 0.52 |
| 40:BI:301:GLN:HG3 | 40:BI:307:PRO:HG2 | 1.91 | 0.52 |
| 41:BP:242:PHE:HB3 | 41:BP:243:PRO:HD2 | 1.90 | 0.52 |
| 40:CE:271:THR:HG22 | 40:CE:376:MET:HB3 | 1.91 | 0.52 |
| 40:CF:167:LEU:HD22 | 40:CF:200:CYS:HB3 | 1.90 | 0.52 |
| 40:CG:9:VAL:HG12 | 40:CG:68:VAL:HB | 1.91 | 0.52 |
| 40:CH:174:ALA:HB1 | 40:CH:175:PRO:HD2 | 1.92 | 0.52 |
| 41:CL:232:THR:HG21 | 41:CL:268:PRO:HB3 | 1.90 | 0.52 |
| 41:CM:331:LEU:HG | 41:CM:335:ASN:HD21 | 1.73 | 0.52 |
| 40:DA:73:THR:O | 40:DA:74:VAL:C | 2.47 | 0.52 |
| 40:DA:258:ASN:OD1 | 41:DB:180:VAL:HG22 | 2.10 | 0.52 |
| 40:DG:270:ALA:HA | 40:DG:376:MET:O | 2.09 | 0.52 |
| 41:DN:41:ASP:O | 41:DN:43:GLN:N | 2.42 | 0.52 |
| 41:DN:199:THR:HG23 | 41:DN:264:HIS:HD2 | 1.74 | 0.52 |
| 40:EH:273:ALA:HB1 | 40:EH:274:PRO:CD | 2.33 | 0.52 |
| 40:EH:273:ALA:O | 40:EH:275:VAL:N | 2.43 | 0.52 |
| 40:EH:307:PRO:HB2 | 40:EH:312:TYR:CE2 | 2.38 | 0.52 |
| 41:EP:215:LEU:O | 41:EP:216:LYS:C | 2.48 | 0.52 |
| 40:FA:139:HIS:CE1 | 40:FA:150:THR:HG21 | 2.43 | 0.52 |
| 40:FF:6:SER:O | 40:FF:65:ALA:HA | 2.08 | 0.52 |
| 40:GE:329:ASN:HB3 | 41:GM:175:VAL:HG11 | 1.91 | 0.52 |
| 41:GM:68:LEU:HD22 | 41:GM:97:ALA:HA | 1.90 | 0.52 |
| 41:HB:139:LEU:HD12 | 41:HB:170:VAL:HG22 | 1.90 | 0.52 |
| 40:HI:223:THR:OG1 | 40:HI:224:TYR:N | 2.42 | 0.52 |
| 41:HM:7:LEU:O | 41:HM:135:LEU:HA | 2.09 | 0.52 |
| 41:HO:333:VAL:HA | 41:HO:336:LYS:HB2 | 1.92 | 0.52 |
| 41:IO:63:ALA:O | 41:IO:89:ASN:ND2 | 2.42 | 0.52 |
| 41:IP:172:SER:OG | 41:IP:175:VAL:O | 2.27 | 0.52 |
| 40:JE:128:GLN:NE2 | 40:KE:290:GLU:OE1 | 2.43 | 0.52 |
| 40:JE:352:LYS:CD | 41:JM:179:VAL:HG13 | 2.39 | 0.52 |
| 41:JM:18:ALA:O | 41:JM:22:GLU:HG2 | 2.10 | 0.52 |
| 41:JN:167:PHE:HD2 | 41:JN:202:ILE:HD11 | 1.74 | 0.52 |
| 40:KA:338:LYS:NZ | 40:KA:340:SER:OG | 2.35 | 0.52 |
| 40:KG:241:SER:HB2 | 40:KG:250:VAL:H | 1.74 | 0.52 |
| 40:KH:26:LEU:HD13 | 40:KH:363:VAL:HG12 | 1.90 | 0.52 |
| 41:KN:318:ARG:HG2 | 41:KN:354:CYS:HB3 | 1.92 | 0.52 |
| 40:LE:235:VAL:HA | 40:LE:238:ILE:HG22 | 1.92 | 0.52 |
| 40:LE:274:PRO:HG3 | 40:LE:286:LEU:HD22 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:ME:73:THR:HA | 40:ME:76:ASP:HB3 | 1.90 | 0.52 |
| 40:ME:205:ASP:HB3 | 40:ME:303:VAL:HA | 1.91 | 0.52 |
| 40:MG:109:THR:O | 40:MG:111:GLY:N | 2.42 | 0.52 |
| 41:ML:170:VAL:HG21 | 41:ML:377:LEU:HD11 | 1.91 | 0.52 |
| 41:ML:214:THR:O | 41:ML:275:SER:OG | 2.25 | 0.52 |
| 40:ND:21:TRP:CZ2 | 40:ND:65:ALA:HB2 | 2.44 | 0.52 |
| 40:NG:286:LEU:O | 40:NG:372:ARG:NH2 | 2.42 | 0.52 |
| 41:NM:113:VAL:HA | 41:NM:116:VAL:HG12 | 1.91 | 0.52 |
| 41:NN:182:PRO:HG3 | 41:NN:384:GLN:HG2 | 1.91 | 0.52 |
| 41:NP:392:LYS:HG3 | 41:NP:395:LEU:HD23 | 1.91 | 0.52 |
| 41:OB:392:LYS:HB3 | 41:OB:395:LEU:HD23 | 1.90 | 0.52 |
| 40:OE:265:ILE:HG22 | 40:OE:379:ASN:HD21 | 1.74 | 0.52 |
| 40:OH:174:ALA:HB1 | 40:OH:175:PRO:HD2 | 1.89 | 0.52 |
| 40:OH:219:ILE:HG12 | 40:OH:221:ARG:H | 1.74 | 0.52 |
| 41:PB:19:LYS:HE3 | 41:PB:226:ASN:HB2 | 1.90 | 0.52 |
| 41:PB:262:ARG:HG3 | 41:PB:263:LEU:HD23 | 1.91 | 0.52 |
| 40:PG:141:PHE:HB2 | 40:PG:173:PRO:HD3 | 1.90 | 0.52 |
| 40:QF:256:GLN:HA | 40:QF:259:LEU:HB2 | 1.91 | 0.52 |
| 40:QH:421:ARG:O | 40:QH:421:ARG:NH1 | 2.41 | 0.52 |
| 41:QN:34:GLY:HA3 | 41:QN:58:LYS:HG3 | 1.91 | 0.52 |
| 41:QN:271:ALA:O | 41:QN:292:GLN:NE2 | 2.43 | 0.52 |
| 41:QP:323:MET:O | 41:QP:324:LYS:C | 2.47 | 0.52 |
| 40:RG:276:ILE:HG22 | 40:RG:280:LYS:HB3 | 1.92 | 0.52 |
| 41:RP:226:ASN:ND2 | 43:RP:502:GDP:O6 | 2.42 | 0.52 |
| 40:SI:168:GLU:OE2 | 40:SI:198:SER:OG | 2.23 | 0.52 |
| 41:SM:309:ARG:H | 41:SM:372:THR:HG1 | 1.56 | 0.52 |
| 40:TA:70:LEU:HD23 | 40:TA:114:LEU:HD12 | 1.90 | 0.52 |
| 40:TE:70:LEU:HD13 | 40:TE:145:THR:HG23 | 1.90 | 0.52 |
| 40:TE:312:TYR:HA | 40:TE:380:THR:HG22 | 1.91 | 0.52 |
| 40:TG:254:GLU:OE2 | 40:TG:254:GLU:N | 2.37 | 0.52 |
| 41:TP:6:HIS:O | 41:TP:63:ALA:HA | 2.09 | 0.52 |
| 40:UG:391:ASP:HB3 | 40:UG:421:ARG:HH22 | 1.74 | 0.52 |
| 41:UN:68:LEU:HD23 | 41:UN:143:THR:HG23 | 1.90 | 0.52 |
| 40:VH:353:VAL:HG12 | 41:VP:177:ASP:HA | 1.91 | 0.52 |
| 41:WB:252:LYS:NZ | 42:WG:501:GTP:O1G | 2.36 | 0.52 |
| 40:WG:271:THR:HG22 | 40:WG:301:GLN:HA | 1.92 | 0.52 |
| 40:WG:294:ALA:O | 40:WG:300:ASN:ND2 | 2.42 | 0.52 |
| 7:1T:459:GLU:O | 7:1T:460:HIS:C | 2.48 | 0.52 |
| 7:1U:561:VAL:HG23 | 7:1U:571:VAL:HG22 | 1.91 | 0.52 |
| 11:2K:68:LYS:HB2 | 41:LO:194:GLU:HB2 | 1.91 | 0.52 |
| 12:2R:59:ALA:HB3 | 41:AP:427:ALA:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2T:74:PRO:HD2 | 13:2T:169:ASP:HA | 1.90 | 0.52 |
| 15:3E:250:ALA:O | 15:3E:400:ARG:NH1 | 2.43 | 0.52 |
| 16:3K:169:ARG:NH1 | 16:3K:173:ASN:OD1 | 2.43 | 0.52 |
| 20:4B:297:GLU:HA | 20:4B:300:ARG:HE | 1.73 | 0.52 |
| 21:4E:429:PRO:HB3 | 22:4K:644:TYR:HB2 | 1.91 | 0.52 |
| 21:4F:35:ASN:HD22 | 40:MD:326:LYS:HG3 | 1.75 | 0.52 |
| 21:4F:451:ILE:HD12 | 21:4F:467:LEU:HB3 | 1.92 | 0.52 |
| 22:4H:35:LEU:O | 22:4H:37:SER:N | 2.42 | 0.52 |
| 22:4J:34:MET:HG3 | 22:4J:36:VAL:H | 1.74 | 0.52 |
| 22:4K:662:CYS:HB3 | 22:4K:667:LEU:HD22 | 1.91 | 0.52 |
| 23:4M:173:SER:HB2 | 23:4M:181:LYS:HA | 1.91 | 0.52 |
| 23:4N:33:MET:HG2 | 41:CM:320:ARG:NH1 | 2.22 | 0.52 |
| 23:4N:33:MET:SD | 41:CM:320:ARG:NH2 | 2.81 | 0.52 |
| 23:4P:240:LEU:HB2 | 23:4P:266:HIS:HA | 1.91 | 0.52 |
| 23:4P:259:ARG:HH21 | 40:EA:365:GLY:CA | 2.13 | 0.52 |
| 27:4Z:142:ARG:HH12 | 27:4Z:210:PRO:HD3 | 1.74 | 0.52 |
| 29:5E:107:ILE:HG22 | 29:5E:108:VAL:H | 1.74 | 0.52 |
| 31:5I:469:SER:OG | 31:5I:470:HIS:N | 2.40 | 0.52 |
| 34:5Q:183:GLN:NE2 | 40:GA:367:LEU:O | 2.41 | 0.52 |
| 39:6J:129:CYS:SG | 39:6J:133:ARG:NH2 | 2.81 | 0.52 |
| 40:AA:26:LEU:HD21 | 40:AA:363:VAL:HG12 | 1.91 | 0.52 |
| 41:AO:237:THR:HA | 41:AO:240:LEU:HD21 | 1.90 | 0.52 |
| 40:BF:2:ARG:HH22 | 41:BN:69:GLU:HB2 | 1.74 | 0.52 |
| 40:BH:51:THR:HG21 | 40:BH:243:ARG:HB2 | 1.92 | 0.52 |
| 40:CA:41:THR:OG1 | 40:CA:42:ILE:N | 2.42 | 0.52 |
| 40:CA:49:PHE:CE2 | 40:CA:55:GLU:HB2 | 2.40 | 0.52 |
| 41:CL:56:GLY:O | 41:CL:58:LYS:N | 2.43 | 0.52 |
| 41:CL:267:MET:HE3 | 41:CL:301:ALA:HB3 | 1.90 | 0.52 |
| 41:CM:105:HIS:HA | 41:CM:150:LEU:HD22 | 1.90 | 0.52 |
| 41:DB:104:GLY:HA3 | 41:DB:146:GLY:CA | 2.39 | 0.52 |
| 40:DF:141:PHE:HD2 | 40:DF:172:TYR:HA | 1.74 | 0.52 |
| 40:DH:73:THR:O | 40:DH:75:ILE:N | 2.42 | 0.52 |
| 41:DL:157:GLU:O | 41:DL:158:GLU:C | 2.48 | 0.52 |
| 41:DM:345:ILE:HD13 | 41:DM:348:ASN:HB3 | 1.91 | 0.52 |
| 41:DP:21:TRP:CZ2 | 41:DP:63:ALA:HB2 | 2.44 | 0.52 |
| 40:EI:188:ILE:HG13 | 40:EI:394:PHE:HB2 | 1.91 | 0.52 |
| 41:FB:222:TYR:HD1 | 41:FB:225:LEU:HD12 | 1.75 | 0.52 |
| 40:FE:318:LEU:O | 40:FE:374:VAL:HA | 2.08 | 0.52 |
| 40:FH:70:LEU:HD23 | 40:FH:114:LEU:HD12 | 1.90 | 0.52 |
| 40:FI:213:CYS:HA | 40:FI:217:LEU:HD13 | 1.91 | 0.52 |
| 40:GA:224:TYR:HE2 | 41:GN:323:MET:HG2 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GH:104:ALA:HA | 40:GH:108:TYR:HD2 | 1.75 | 0.52 |
| 40:GI:79:ARG:HG3 | 40:GI:92:LEU:HD12 | 1.91 | 0.52 |
| 40:GI:114:LEU:HB2 | 40:GI:149:PHE:HZ | 1.74 | 0.52 |
| 41:GO:330:MET:HB3 | 41:GO:349:VAL:HG21 | 1.90 | 0.52 |
| 41:HB:342:VAL:HG23 | 41:HB:345:ILE:HG22 | 1.90 | 0.52 |
| 40:HE:17:GLY:O | 40:HE:18:ASN:C | 2.47 | 0.52 |
| 40:IA:175:PRO:HG3 | 40:IA:304:LYS:HB2 | 1.91 | 0.52 |
| 40:IF:107:HIS:CD2 | 40:IF:152:LEU:HB2 | 2.45 | 0.52 |
| 41:IO:286:VAL:HG11 | 41:IO:326:VAL:HG22 | 1.91 | 0.52 |
| 41:JB:136:THR:HG22 | 41:JB:167:PHE:HB2 | 1.92 | 0.52 |
| 41:JB:207:LEU:HD13 | 41:JB:225:LEU:HB3 | 1.91 | 0.52 |
| 41:JN:131:GLN:HE22 | 41:JN:249:ASP:HB2 | 1.74 | 0.52 |
| 40:KH:217:LEU:HA | 40:KH:277:SER:HB3 | 1.91 | 0.52 |
| 41:KO:135:LEU:O | 41:KO:166:THR:HA | 2.09 | 0.52 |
| 40:LF:51:THR:HG21 | 40:LF:243:ARG:HB3 | 1.90 | 0.52 |
| 41:LN:248:ALA:HA | 41:LN:252:LYS:HD2 | 1.91 | 0.52 |
| 41:LP:142:GLY:O | 41:LP:144:GLY:N | 2.43 | 0.52 |
| 40:MA:141:PHE:CZ | 40:MA:194:THR:HG21 | 2.44 | 0.52 |
| 40:MH:273:ALA:HB1 | 40:MH:291:ILE:HB | 1.91 | 0.52 |
| 41:MO:135:LEU:HD22 | 41:MO:152:ILE:HD11 | 1.92 | 0.52 |
| 41:MP:248:ALA:HA | 41:MP:252:LYS:HE2 | 1.92 | 0.52 |
| 40:NA:7:VAL:HG13 | 40:NA:66:VAL:HG23 | 1.91 | 0.52 |
| 41:OB:143:THR:OG1 | 43:OB:501:GDP:O1B | 2.26 | 0.52 |
| 40:OD:104:ALA:HB2 | 40:OD:412:MET:HB2 | 1.92 | 0.52 |
| 40:PA:171:ILE:HG21 | 42:PN:501:GTP:H1' | 1.92 | 0.52 |
| 41:PB:2:ARG:NH2 | 41:PB:249:ASP:OD2 | 2.39 | 0.52 |
| 41:PM:237:THR:O | 41:PM:241:ARG:NH2 | 2.40 | 0.52 |
| 40:QE:16:ILE:HG13 | 40:QE:228:ASN:ND2 | 2.24 | 0.52 |
| 41:QP:44:LEU:O | 41:QP:48:ASN:N | 2.42 | 0.52 |
| 40:RA:305:CYS:HB3 | 40:RA:386:ALA:HB2 | 1.91 | 0.52 |
| 41:RN:242:PHE:HD2 | 41:RN:356:ILE:HB | 1.75 | 0.52 |
| 40:SA:176:GLN:OE1 | 40:SA:389:ARG:NH2 | 2.42 | 0.52 |
| 41:SB:331:LEU:HD11 | 40:SG:177:VAL:HG12 | 1.91 | 0.52 |
| 40:SF:20:CYS:HA | 40:SF:232:SER:HB2 | 1.92 | 0.52 |
| 40:SG:70:LEU:HD23 | 40:SG:114:LEU:HD12 | 1.91 | 0.52 |
| 40:SG:326:LYS:HD3 | 41:SO:208:TYR:CG | 2.44 | 0.52 |
| 40:SI:224:TYR:HB3 | 42:SP:501:GTP:N1 | 2.25 | 0.52 |
| 41:SO:309:ARG:HE | 41:SO:427:ALA:HA | 1.74 | 0.52 |
| 41:TB:49:VAL:HG21 | 41:TB:241:ARG:HG2 | 1.92 | 0.52 |
| 41:TB:107:THR:O | 41:TB:110:ALA:N | 2.34 | 0.52 |
| 41:TP:262:ARG:NH2 | 41:TP:417:ASP:O | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UB:282:ARG:NH2 | 41:UB:292:GLN:OE1 | 2.43 | 0.52 |
| 40:UE:167:LEU:HD22 | 40:UE:200:CYS:HB3 | 1.91 | 0.52 |
| 41:UN:52:ASN:OD1 | 41:UN:62:ARG:NH1 | 2.43 | 0.52 |
| 41:UP:141:GLY:HA3 | 43:UP:501:GDP:O1A | 2.09 | 0.52 |
| 40:VF:273:ALA:HB3 | 40:VF:374:VAL:H | 1.74 | 0.52 |
| 41:VN:87:PRO:HD3 | 41:WM:281:TYR:CD2 | 2.40 | 0.52 |
| 41:VP:87:PRO:HD3 | 41:WO:281:TYR:HD2 | 1.75 | 0.52 |
| 40:WG:107:HIS:ND1 | 40:WG:151:SER:OG | 2.40 | 0.52 |
| 41:WN:372:THR:HG22 | 41:WN:422:VAL:HG13 | 1.90 | 0.52 |
| 41:WP:173:PRO:HB3 | 41:WP:380:ARG:HD3 | 1.90 | 0.52 |
| 8:1X:143:ARG:HA | 8:1X:146:ILE:HD12 | 1.90 | 0.52 |
| 8:1Z:499:GLN:NE2 | 8:1Z:503:GLU:OE2 | 2.43 | 0.52 |
| 12:2P:146:ILE:HD13 | 12:2P:149:LEU:HD21 | 1.92 | 0.52 |
| 16:3J:372:ARG:HG2 | 16:3L:24:LEU:HD11 | 1.92 | 0.52 |
| 17:3Q:383:LYS:HG2 | 17:3Q:438:LEU:HD21 | 1.90 | 0.52 |
| 17:3Q:403:ARG:HG2 | 17:3Q:406:ARG:HD3 | 1.90 | 0.52 |
| 20:4A:149:ARG:CZ | 20:4A:150:SER:CA | 2.88 | 0.52 |
| 22:4K:701:ALA:O | 22:4K:702:ASN:C | 2.48 | 0.52 |
| 23:4M:170:SER:N | 41:CB:45:GLU:OE2 | 2.42 | 0.52 |
| 23:4N:240:LEU:HB2 | 23:4N:266:HIS:HA | 1.91 | 0.52 |
| 27:4Z:132:ALA:HA | 27:4Z:148:ARG:HD3 | 1.91 | 0.52 |
| 31:5I:628:ASP:H | 31:5I:631:GLU:HG3 | 1.73 | 0.52 |
| 36:5W:116:ARG:NH2 | 36:5W:118:TYR:OH | 2.39 | 0.52 |
| 40:AE:7:VAL:HB | 40:AE:137:ILE:HG22 | 1.92 | 0.52 |
| 40:AG:200:CYS:HA | 40:AG:266:HIS:HB2 | 1.91 | 0.52 |
| 41:AL:316:VAL:HG12 | 41:AL:352:ALA:HB3 | 1.91 | 0.52 |
| 40:BH:273:ALA:HB3 | 40:BH:274:PRO:HD3 | 1.92 | 0.52 |
| 40:CA:69:ASP:H | 40:CA:75:ILE:HD11 | 1.74 | 0.52 |
| 40:CA:211:ASP:HA | 40:CA:214:ARG:HD3 | 1.90 | 0.52 |
| 41:CB:66:VAL:HG12 | 41:CB:91:VAL:HB | 1.91 | 0.52 |
| 41:CM:354:CYS:SG | 41:CM:355:ASP:N | 2.83 | 0.52 |
| 41:DB:183:TYR:O | 41:DB:184:ASN:C | 2.48 | 0.52 |
| 40:DH:156:ARG:HB3 | 40:DH:156:ARG:HH11 | 1.74 | 0.52 |
| 41:DO:139:LEU:HD12 | 41:DO:170:VAL:HG12 | 1.90 | 0.52 |
| 40:EF:322:ASP:O | 40:EF:372:ARG:NH1 | 2.41 | 0.52 |
| 40:EH:291:ILE:HG13 | 40:EH:374:VAL:CG1 | 2.40 | 0.52 |
| 41:EM:100:ASN:O | 41:EM:103:LYS:N | 2.41 | 0.52 |
| 41:EN:207:LEU:HB3 | 41:EN:225:LEU:HD11 | 1.91 | 0.52 |
| 41:EP:54:ALA:HB3 | 41:EP:58:LYS:HB3 | 1.91 | 0.52 |
| 40:HE:56:THR:OG1 | 40:HE:57:GLY:N | 2.42 | 0.52 |
| 40:IH:404:VAL:HG13 | 40:IH:417:PHE:HE2 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IN:314:ALA:HB3 | 41:IN:368:ILE:HB | 1.91 | 0.52 |
| 40:JG:311:LYS:HE3 | 40:JG:344:VAL:HG12 | 1.91 | 0.52 |
| 41:JN:204:ASN:HD22 | 41:JN:207:LEU:HD12 | 1.73 | 0.52 |
| 40:KH:406:TRP:HE1 | 41:KO:258:VAL:HG23 | 1.75 | 0.52 |
| 40:LH:70:LEU:HD23 | 40:LH:114:LEU:HD12 | 1.91 | 0.52 |
| 40:MA:274:PRO:HG2 | 40:MA:373:ALA:HA | 1.90 | 0.52 |
| 40:MA:277:SER:O | 40:MA:278:ALA:C | 2.48 | 0.52 |
| 40:MF:174:ALA:CB | 40:MF:177:VAL:HG23 | 2.39 | 0.52 |
| 40:MF:305:CYS:O | 40:MF:305:CYS:SG | 2.67 | 0.52 |
| 40:MF:433:GLU:HA | 40:MF:436:MET:HE3 | 1.91 | 0.52 |
| 40:MH:73:THR:O | 40:MH:74:VAL:C | 2.48 | 0.52 |
| 40:MH:259:LEU:HD23 | 40:MH:379:ASN:HB2 | 1.91 | 0.52 |
| 40:NE:252:LEU:HA | 40:NE:255:PHE:HD2 | 1.75 | 0.52 |
| 40:NG:371:GLN:HG3 | 40:NG:372:ARG:HD3 | 1.91 | 0.52 |
| 41:NL:28:HIS:HD1 | 41:NL:47:ILE:HG13 | 1.75 | 0.52 |
| 41:NP:83:GLN:O | 41:OP:281:TYR:OH | 2.27 | 0.52 |
| 40:OA:206:ASN:OD1 | 42:ON:501:GTP:O2' | 2.28 | 0.52 |
| 40:OH:261:PRO:HB2 | 40:OH:346:TRP:HZ3 | 1.74 | 0.52 |
| 41:PB:6:HIS:CE1 | 41:PB:8:GLN:HE21 | 2.27 | 0.52 |
| 40:QA:31:GLN:HG3 | 40:QA:34:GLY:H | 1.75 | 0.52 |
| 40:QH:260:VAL:HB | 41:QP:397:TRP:CH2 | 2.45 | 0.52 |
| 41:QP:109:GLY:O | 41:QP:112:LEU:HB3 | 2.09 | 0.52 |
| 41:QP:292:GLN:O | 41:QP:295:ASP:HB3 | 2.10 | 0.52 |
| 40:RE:93:ILE:HG13 | 40:RE:118:VAL:HG22 | 1.91 | 0.52 |
| 40:RI:64:ARG:NH1 | 40:RI:129:CYS:SG | 2.83 | 0.52 |
| 41:RL:306:ARG:HA | 41:RL:340:TYR:CE2 | 2.44 | 0.52 |
| 41:RN:190:HIS:CE1 | 41:RN:414:ASN:HD22 | 2.28 | 0.52 |
| 40:SG:240:ALA:HA | 40:SG:243:ARG:HG3 | 1.92 | 0.52 |
| 41:SM:287:PRO:HD3 | 41:SM:329:GLN:HE22 | 1.75 | 0.52 |
| 41:SO:288:GLU:O | 41:SO:291:GLN:HG3 | 2.08 | 0.52 |
| 41:SP:100:ASN:HB2 | 41:SP:103:LYS:HB2 | 1.92 | 0.52 |
| 41:TO:273:LEU:N | 41:TO:292:GLN:OE1 | 2.42 | 0.52 |
| 41:TP:134:GLN:HA | 41:TP:165:ASN:O | 2.09 | 0.52 |
| 40:UE:306:ASP:HB3 | 40:UE:309:HIS:HB2 | 1.91 | 0.52 |
| 40:UF:335:ILE:HG23 | 40:UF:341:ILE:HD13 | 1.92 | 0.52 |
| 40:UG:346:TRP:HB2 | 41:UO:391:ARG:HD3 | 1.91 | 0.52 |
| 40:VG:112:LYS:HA | 40:VG:115:ILE:HG22 | 1.90 | 0.52 |
| 40:WA:16:ILE:HA | 40:WA:228:ASN:HB3 | 1.92 | 0.52 |
| 40:WE:325:PRO:HB2 | 40:WE:326:LYS:HE2 | 1.90 | 0.52 |
| 40:WG:235:VAL:HA | 40:WG:238:ILE:HG22 | 1.91 | 0.52 |
| 41:WQ:189:VAL:HA | 41:WQ:192:LEU:HB2 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:2J:43:LYS:NZ | 41:ML:335:ASN:OD1 | 2.42 | 0.52 |
| 11:2K:189:SER:O | 11:2K:190:ASP:C | 2.47 | 0.52 |
| 17:3R:243:GLN:NE2 | 17:3R:317:ALA:HB1 | 2.25 | 0.52 |
| 18:3T:197:ALA:HA | 18:3T:278:LEU:HD21 | 1.92 | 0.52 |
| 22:4J:327:ASN:H | 41:CN:276:ARG:HD2 | 1.75 | 0.52 |
| 22:4J:572:LYS:HG3 | 22:4J:573:HIS:H | 1.75 | 0.52 |
| 23:4P:192:PRO:HG3 | 41:CN:44:LEU:CD2 | 2.39 | 0.52 |
| 23:4R:108:ASN:HD22 | 23:4R:111:GLN:HG3 | 1.73 | 0.52 |
| 31:5I:494:TYR:CE1 | 40:IH:282:TYR:HE1 | 2.28 | 0.52 |
| 34:5R:320:ASN:O | 34:5R:324:GLU:HG2 | 2.09 | 0.52 |
| 40:BE:239:THR:O | 40:BE:243:ARG:NE | 2.41 | 0.52 |
| 40:BF:318:LEU:O | 40:BF:374:VAL:HA | 2.10 | 0.52 |
| 40:BF:433:GLU:HA | 40:BF:436:MET:HG2 | 1.92 | 0.52 |
| 40:BG:128:GLN:OE1 | 40:CG:285:GLN:NE2 | 2.41 | 0.52 |
| 40:BH:411:GLY:O | 40:BH:412:MET:C | 2.46 | 0.52 |
| 41:BM:273:LEU:HB2 | 41:BM:292:GLN:HE22 | 1.75 | 0.52 |
| 41:CO:263:LEU:HD22 | 41:CO:422:VAL:HG13 | 1.91 | 0.52 |
| 40:DE:234:ILE:O | 40:DE:238:ILE:HG12 | 2.10 | 0.52 |
| 40:DE:424:MET:HE1 | 40:DE:427:LEU:HD23 | 1.92 | 0.52 |
| 40:DF:90:GLU:O | 40:DF:91:GLN:C | 2.47 | 0.52 |
| 40:DI:11:GLN:HB2 | 40:DI:74:VAL:HG21 | 1.92 | 0.52 |
| 40:DI:114:LEU:HB3 | 40:DI:149:PHE:CE2 | 2.44 | 0.52 |
| 41:DN:199:THR:HG23 | 41:DN:264:HIS:CD2 | 2.45 | 0.52 |
| 40:EH:60:LYS:HG2 | 40:FH:283:HIS:HA | 1.91 | 0.52 |
| 40:EI:100:ALA:O | 41:EP:255:VAL:HG11 | 2.09 | 0.52 |
| 41:EM:50:TYR:HE1 | 41:EM:237:THR:HG21 | 1.75 | 0.52 |
| 41:EM:397:TRP:O | 41:EM:398:TYR:C | 2.47 | 0.52 |
| 40:FA:101:ASN:OD1 | 41:FN:252:LYS:NZ | 2.43 | 0.52 |
| 40:FH:132:LEU:HB3 | 40:FH:164:LYS:HE2 | 1.90 | 0.52 |
| 41:FP:325:GLU:HA | 41:FP:328:GLU:HG3 | 1.90 | 0.52 |
| 40:GA:397:MET:HG3 | 41:GN:346:PRO:HD2 | 1.90 | 0.52 |
| 40:GE:382:ALA:O | 40:GE:385:GLU:N | 2.41 | 0.52 |
| 40:GH:105:ARG:HH21 | 40:GH:110:ILE:HG12 | 1.73 | 0.52 |
| 40:GH:315:CYS:SG | 40:GH:316:CYS:N | 2.82 | 0.52 |
| 40:GI:273:ALA:HB1 | 40:GI:274:PRO:CD | 2.27 | 0.52 |
| 40:GI:273:ALA:CB | 40:GI:374:VAL:H | 2.22 | 0.52 |
| 41:GM:139:LEU:HD23 | 41:GM:170:VAL:HG23 | 1.92 | 0.52 |
| 41:GN:183:TYR:CZ | 41:GN:388:MET:HB3 | 2.45 | 0.52 |
| 41:GP:253:LEU:O | 41:GP:257:MET:HB2 | 2.08 | 0.52 |
| 41:HB:314:ALA:HA | 41:HB:350:LYS:HB2 | 1.92 | 0.52 |
| 40:HE:380:THR:O | 40:HE:382:ALA:N | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HG:191:THR:O | 40:HG:195:LEU:HB2 | 2.09 | 0.52 |
| 41:HN:13:GLY:O | 41:HN:16:ILE:HG22 | 2.10 | 0.52 |
| 41:IB:331:LEU:HB2 | 40:IG:177:VAL:HG12 | 1.90 | 0.52 |
| 41:IN:61:PRO:HD3 | 41:IN:84:ILE:HG12 | 1.92 | 0.52 |
| 41:JB:396:HIS:HA | 41:JB:399:THR:HG22 | 1.92 | 0.52 |
| 40:JE:145:THR:OG1 | 42:JE:501:GTP:O2B | 2.28 | 0.52 |
| 40:JF:337:THR:O | 40:JF:339:ARG:NH1 | 2.43 | 0.52 |
| 41:JL:55:THR:HG23 | 41:KL:283:ALA:HA | 1.92 | 0.52 |
| 41:JM:137:HIS:CE1 | 41:JM:192:LEU:HD11 | 2.45 | 0.52 |
| 40:KF:328:VAL:HG21 | 40:KF:355:ILE:HD11 | 1.91 | 0.52 |
| 41:KO:173:PRO:HB3 | 41:KO:380:ARG:HD2 | 1.91 | 0.52 |
| 42:LB:502:GTP:HN21 | 40:LG:228:ASN:CG | 2.13 | 0.52 |
| 41:LN:314:ALA:HB3 | 41:LN:368:ILE:HB | 1.92 | 0.52 |
| 41:LO:207:LEU:HD23 | 41:LO:210:ILE:HD11 | 1.92 | 0.52 |
| 41:LP:232:THR:HG21 | 41:LP:268:PRO:HB2 | 1.89 | 0.52 |
| 41:MB:202:ILE:HG21 | 41:MB:229:VAL:HG22 | 1.92 | 0.52 |
| 41:MO:141:GLY:HA3 | 43:MO:501:GDP:O1A | 2.09 | 0.52 |
| 41:MO:344:TRP:CZ2 | 41:MO:425:ARG:HB3 | 2.45 | 0.52 |
| 40:NA:188:ILE:HG23 | 40:NA:424:MET:HG3 | 1.92 | 0.52 |
| 40:NF:202:PHE:HE2 | 40:NF:238:ILE:HG12 | 1.73 | 0.52 |
| 40:NG:8:HIS:HE1 | 40:NG:21:TRP:HE1 | 1.57 | 0.52 |
| 40:NH:118:VAL:HG21 | 40:NH:149:PHE:HZ | 1.75 | 0.52 |
| 41:NL:26:ASP:HB3 | 41:NL:359:ARG:HH22 | 1.73 | 0.52 |
| 41:NM:306:ARG:HG2 | 41:NM:340:TYR:HE1 | 1.74 | 0.52 |
| 40:OA:315:CYS:HA | 40:OA:377:LEU:O | 2.10 | 0.52 |
| 41:OB:130:LEU:O | 41:OB:162:ARG:NH1 | 2.43 | 0.52 |
| 40:OF:278:ALA:HB2 | 40:OF:368:ALA:HA | 1.92 | 0.52 |
| 40:PA:362:VAL:HG21 | 40:PA:369:LYS:HA | 1.90 | 0.52 |
| 41:PB:344:TRP:HE3 | 41:PB:425:ARG:HH21 | 1.57 | 0.52 |
| 40:PG:385:GLU:OE1 | 40:PG:389:ARG:NH1 | 2.42 | 0.52 |
| 40:PH:240:ALA:O | 40:PH:356:ASN:ND2 | 2.43 | 0.52 |
| 41:PL:53:GLU:HG2 | 41:PL:59:TYR:HE1 | 1.73 | 0.52 |
| 41:PL:137:HIS:CE1 | 41:PL:168:SER:HG | 2.27 | 0.52 |
| 40:RG:255:PHE:O | 40:RG:259:LEU:HB2 | 2.10 | 0.52 |
| 40:SE:271:THR:HB | 40:SE:376:MET:HB3 | 1.91 | 0.52 |
| 40:SF:2:ARG:HG3 | 40:SF:51:THR:HG22 | 1.92 | 0.52 |
| 40:SF:391:ASP:HA | 40:SF:421:ARG:HH12 | 1.74 | 0.52 |
| 40:SH:336:LYS:HG2 | 40:SH:351:PHE:HE2 | 1.73 | 0.52 |
| 40:TA:16:ILE:HA | 40:TA:228:ASN:HD22 | 1.74 | 0.52 |
| 40:TA:31:GLN:HE22 | 40:TA:37:PRO:HG3 | 1.74 | 0.52 |
| 40:TI:274:PRO:HA | 40:TI:276:ILE:HD12 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TM:180:VAL:HG23 | 41:TM:184:ASN:HD21 | 1.73 | 0.52 |
| 41:TM:331:LEU:O | 41:TM:335:ASN:ND2 | 2.43 | 0.52 |
| 41:TO:310:TYR:HD1 | 41:TO:371:SER:HB2 | 1.74 | 0.52 |
| 40:UF:288:VAL:HA | 40:UF:291:ILE:HD13 | 1.92 | 0.52 |
| 40:UF:352:LYS:NZ | 41:UN:179:VAL:HA | 2.24 | 0.52 |
| 41:UM:385:PHE:O | 41:UM:389:PHE:HB3 | 2.09 | 0.52 |
| 40:VG:73:THR:HA | 40:VG:76:ASP:HB2 | 1.91 | 0.52 |
| 40:VJ:281:ALA:HB1 | 40:VJ:286:LEU:HD11 | 1.92 | 0.52 |
| 41:VP:317:PHE:HB2 | 41:VP:353:VAL:HG12 | 1.92 | 0.52 |
| 41:WB:43:GLN:O | 41:WB:47:ILE:HB | 2.10 | 0.52 |
| 40:WG:90:GLU:N | 40:WG:90:GLU:OE1 | 2.43 | 0.52 |
| 9:2B:401:GLN:OE1 | 41:TL:362:LYS:NZ | 2.43 | 0.52 |
| 16:3J:301:GLU:HB3 | 16:3J:305:ARG:NH1 | 2.24 | 0.52 |
| 16:3K:134:GLU:O | 16:3K:138:HIS:ND1 | 2.41 | 0.52 |
| 21:4D:210:ASP:HB3 | 21:4D:213:THR:HG22 | 1.91 | 0.52 |
| 21:4D:457:ARG:O | 21:4D:458:ASN:C | 2.48 | 0.52 |
| 22:4I:559:SER:HB2 | 22:4I:562:LEU:HD23 | 1.90 | 0.52 |
| 23:4M:103:PHE:O | 23:4M:104:ILE:C | 2.48 | 0.52 |
| 35:5T:71:LYS:NZ | 35:5T:75:GLU:OE1 | 2.34 | 0.52 |
| 39:6I:115:LEU:HD11 | 39:6I:145:VAL:HG21 | 1.92 | 0.52 |
| 40:BA:324:VAL:HB | 40:BA:327:ASP:HB2 | 1.92 | 0.52 |
| 40:BE:160:ASP:O | 40:BE:162:GLY:N | 2.43 | 0.52 |
| 40:BG:380:THR:HG22 | 40:BG:382:ALA:H | 1.74 | 0.52 |
| 40:BI:184:PRO:HG2 | 40:BI:397:MET:HE1 | 1.92 | 0.52 |
| 41:BO:44:LEU:O | 41:BO:45:GLU:C | 2.48 | 0.52 |
| 41:BO:138:SER:O | 41:BO:139:LEU:C | 2.48 | 0.52 |
| 41:BO:142:GLY:O | 41:BO:144:GLY:N | 2.42 | 0.52 |
| 41:BO:285:THR:H | 41:BO:288:GLU:HG2 | 1.75 | 0.52 |
| 40:CI:109:THR:OG1 | 40:CI:410:GLU:O | 2.28 | 0.52 |
| 41:CN:359:ARG:NH2 | 41:CN:359:ARG:HB2 | 2.24 | 0.52 |
| 40:DA:100:ALA:O | 40:DA:101:ASN:C | 2.48 | 0.52 |
| 40:DA:216:ASN:O | 40:DA:218:ASP:N | 2.43 | 0.52 |
| 41:DB:66:VAL:HB | 41:DB:91:VAL:HG22 | 1.91 | 0.52 |
| 41:DB:251:ARG:O | 41:DB:255:VAL:HG23 | 2.09 | 0.52 |
| 40:DE:93:ILE:HD13 | 40:DE:118:VAL:HG22 | 1.92 | 0.52 |
| 40:DE:247:ALA:O | 40:DE:248:LEU:C | 2.48 | 0.52 |
| 40:DI:362:VAL:HG22 | 40:DI:363:VAL:H | 1.75 | 0.52 |
| 40:EG:11:GLN:HB2 | 40:EG:74:VAL:HG11 | 1.92 | 0.52 |
| 41:EP:200:TYR:HE1 | 41:EP:236:VAL:HG21 | 1.75 | 0.52 |
| 40:FA:69:ASP:HB3 | 40:FA:75:ILE:HD11 | 1.91 | 0.52 |
| 40:FF:70:LEU:HB2 | 40:FF:145:THR:HG22 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FP:274:THR:OG1 | 41:FP:282:ARG:NH1 | 2.43 | 0.52 |
| 40:GA:101:ASN:HD22 | 41:GN:256:ASN:HD21 | 1.57 | 0.52 |
| 41:GP:266:PHE:HE1 | 41:GP:370:ASN:HD22 | 1.58 | 0.52 |
| 40:HE:325:PRO:HG2 | 41:HM:221:THR:HA | 1.92 | 0.52 |
| 40:HI:17:GLY:HA2 | 40:HI:20:CYS:HB2 | 1.90 | 0.52 |
| 41:HN:40:SER:O | 41:HN:43:GLN:HB2 | 2.09 | 0.52 |
| 41:HN:215:LEU:O | 41:HN:216:LYS:C | 2.47 | 0.52 |
| 41:HP:257:MET:HA | 41:HP:312:THR:HG21 | 1.91 | 0.52 |
| 41:HQ:100:ASN:HB3 | 41:HQ:103:LYS:HB3 | 1.92 | 0.52 |
| 40:IF:5:ILE:HD13 | 40:IF:64:ARG:HB3 | 1.92 | 0.52 |
| 40:II:205:ASP:HB2 | 40:II:303:VAL:HG12 | 1.90 | 0.52 |
| 40:JD:274:PRO:HB3 | 40:JD:370:VAL:HG11 | 1.92 | 0.52 |
| 40:JE:70:LEU:HB2 | 40:JE:145:THR:HG22 | 1.90 | 0.52 |
| 40:KD:268:PRO:HG3 | 40:KD:379:ASN:HD22 | 1.74 | 0.52 |
| 40:KE:70:LEU:HD23 | 40:KE:114:LEU:HD22 | 1.90 | 0.52 |
| 40:KG:90:GLU:HG3 | 40:KG:121:ARG:NH1 | 2.24 | 0.52 |
| 41:KL:141:GLY:O | 41:KL:145:SER:HB2 | 2.09 | 0.52 |
| 41:KN:6:HIS:O | 41:KN:63:ALA:HA | 2.09 | 0.52 |
| 41:KO:193:VAL:HG21 | 41:KO:418:LEU:HD11 | 1.90 | 0.52 |
| 40:LE:209:ILE:HG21 | 40:LE:227:LEU:HA | 1.92 | 0.52 |
| 41:LL:176:SER:OG | 41:LL:178:THR:O | 2.28 | 0.52 |
| 41:LO:139:LEU:HD12 | 41:LO:170:VAL:HG12 | 1.92 | 0.52 |
| 41:MN:269:GLY:O | 41:MN:367:PHE:N | 2.42 | 0.52 |
| 41:MP:27:GLU:OE2 | 41:MP:318:ARG:NH2 | 2.36 | 0.52 |
| 41:OB:322:SER:OG | 41:OB:323:MET:N | 2.42 | 0.52 |
| 40:OG:315:CYS:HA | 40:OG:377:LEU:O | 2.10 | 0.52 |
| 41:OM:19:LYS:NZ | 41:OM:223:GLY:O | 2.43 | 0.52 |
| 41:PM:10:GLY:O | 41:PM:14:ASN:ND2 | 2.43 | 0.52 |
| 40:QA:200:CYS:HA | 40:QA:266:HIS:HB2 | 1.92 | 0.52 |
| 41:QB:142:GLY:O | 41:QB:143:THR:C | 2.48 | 0.52 |
| 40:QE:264:ARG:HG3 | 40:QE:265:ILE:HD12 | 1.92 | 0.52 |
| 40:QF:20:CYS:HA | 40:QF:232:SER:HB2 | 1.92 | 0.52 |
| 41:QM:222:TYR:HD1 | 41:QM:225:LEU:HD12 | 1.74 | 0.52 |
| 40:RG:332:ILE:HG23 | 40:RG:351:PHE:HD2 | 1.74 | 0.52 |
| 40:RH:228:ASN:HD21 | 42:RO:501:GTP:HN1 | 1.58 | 0.52 |
| 40:SH:406:TRP:CZ3 | 41:SO:255:VAL:HA | 2.45 | 0.52 |
| 40:TI:70:LEU:HB2 | 40:TI:145:THR:HG22 | 1.91 | 0.52 |
| 40:TI:154:MET:HG3 | 40:TI:194:THR:HG22 | 1.91 | 0.52 |
| 41:TO:318:ARG:HG2 | 41:TO:354:CYS:HB3 | 1.91 | 0.52 |
| 41:UM:375:GLN:NE2 | 41:UM:419:GLY:O | 2.43 | 0.52 |
| 41:UP:212:PHE:HB3 | 41:UP:213:ARG:NH1 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VA:254:GLU:OE1 | 41:VB:99:ASN:ND2 | 2.43 | 0.52 |
| 41:VB:8:GLN:NE2 | 41:VB:17:GLY:HA3 | 2.25 | 0.52 |
| 41:VB:42:LEU:HA | 41:VB:45:GLU:HB2 | 1.92 | 0.52 |
| 40:VJ:122:ILE:HG21 | 40:VJ:157:LEU:HD21 | 1.92 | 0.52 |
| 41:VN:341:PHE:HB3 | 41:VN:348:ASN:HD21 | 1.73 | 0.52 |
| 41:VP:113:VAL:HA | 41:VP:116:VAL:HG12 | 1.91 | 0.52 |
| 41:VP:209:ASP:O | 41:VP:213:ARG:HB3 | 2.10 | 0.52 |
| 41:VQ:22:GLU:HG3 | 41:VQ:81:PHE:CG | 2.45 | 0.52 |
| 41:VQ:107:THR:O | 41:VQ:110:ALA:N | 2.42 | 0.52 |
| 40:WA:96:LYS:NZ | 41:WN:1:MET:N | 2.58 | 0.52 |
| 41:WB:421:PRO:HA | 41:WB:424:THR:HG22 | 1.92 | 0.52 |
| 40:WE:138:PHE:HZ | 40:WE:235:VAL:HG11 | 1.75 | 0.52 |
| 40:WF:217:LEU:HD12 | 40:WF:277:SER:HB3 | 1.92 | 0.52 |
| 40:WH:217:LEU:HA | 40:WH:277:SER:HB2 | 1.91 | 0.52 |
| 41:WM:393:ALA:O | 41:WM:394:PHE:C | 2.47 | 0.52 |
| 7:1U:68:SER:HB2 | 7:1U:84:VAL:HG22 | 1.92 | 0.52 |
| 8:1Y:186:GLU:OE1 | 8:1Y:188:GLU:N | 2.43 | 0.52 |
| 10:2F:147:ILE:HD11 | 41:WB:322:SER:HB2 | 1.92 | 0.52 |
| 12:2O:145:VAL:O | 12:2O:146:ILE:C | 2.48 | 0.52 |
| 14:3C:44:ASN:HD21 | 14:3C:48:HIS:HB2 | 1.75 | 0.52 |
| 17:3P:380:ASP:HA | 17:3P:383:LYS:HD2 | 1.91 | 0.52 |
| 17:3R:328:LEU:HD23 | 17:3R:329:LEU:HG | 1.92 | 0.52 |
| 20:4A:23:GLU:HA | 20:4A:26:ARG:HG3 | 1.91 | 0.52 |
| 21:4D:516:MET:SD | 21:4D:531:ILE:HG13 | 2.50 | 0.52 |
| 23:4P:186:GLY:O | 23:4P:188:THR:N | 2.43 | 0.52 |
| 23:4Q:236:TYR:O | 23:4Q:267:ASP:HA | 2.09 | 0.52 |
| 23:4Q:259:ARG:NH2 | 40:EH:366:ASP:H | 2.06 | 0.52 |
| 25:4T:403:THR:H | 25:4T:406:ILE:HG22 | 1.74 | 0.52 |
| 30:5G:113:ASP:OD2 | 40:GG:96:LYS:NZ | 2.43 | 0.52 |
| 36:5W:101:TRP:HB2 | 41:ON:361:LEU:HD23 | 1.92 | 0.52 |
| 36:5X:188:GLN:HA | 36:5X:191:VAL:HG22 | 1.92 | 0.52 |
| 40:AH:255:PHE:O | 40:AH:259:LEU:HB2 | 2.09 | 0.52 |
| 41:AM:257:MET:HA | 41:AM:312:THR:HG21 | 1.90 | 0.52 |
| 41:AN:237:THR:HG23 | 41:AN:241:ARG:HH11 | 1.74 | 0.52 |
| 40:BA:224:TYR:HD1 | 40:BA:227:LEU:HD22 | 1.75 | 0.52 |
| 40:BH:8:HIS:ND1 | 40:BH:17:GLY:HA3 | 2.24 | 0.52 |
| 40:BI:109:THR:C | 40:BI:111:GLY:H | 2.13 | 0.52 |
| 41:BM:260:PHE:HB3 | 41:BM:261:PRO:CD | 2.40 | 0.52 |
| 40:CE:349:THR:OG1 | 41:CM:176:SER:HB3 | 2.09 | 0.52 |
| 40:CI:239:THR:O | 40:CI:243:ARG:NE | 2.38 | 0.52 |
| 41:CL:142:GLY:O | 41:CL:143:THR:C | 2.47 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CL:305:PRO:HB3 | 41:CL:310:TYR:HE1 | 1.74 | 0.52 |
| 41:CP:224:ASP:C | 41:CP:226:ASN:H | 2.13 | 0.52 |
| 40:DA:252:LEU:O | 40:DA:253:THR:C | 2.48 | 0.52 |
| 40:DA:273:ALA:HB3 | 40:DA:274:PRO:HD3 | 1.90 | 0.52 |
| 41:DB:21:TRP:O | 41:DB:25:SER:HB3 | 2.09 | 0.52 |
| 40:DH:103:TYR:O | 40:DH:104:ALA:C | 2.48 | 0.52 |
| 41:DL:346:PRO:O | 41:DL:347:ASN:C | 2.47 | 0.52 |
| 40:EI:73:THR:OG1 | 40:EI:74:VAL:N | 2.43 | 0.52 |
| 40:EI:277:SER:O | 40:EI:278:ALA:C | 2.48 | 0.52 |
| 41:EL:89:ASN:ND2 | 41:EL:123:GLU:OE2 | 2.37 | 0.52 |
| 41:EM:186:THR:HG22 | 41:EM:411:ALA:HB1 | 1.91 | 0.52 |
| 41:EP:8:GLN:HG3 | 41:EP:65:LEU:HA | 1.92 | 0.52 |
| 40:FF:139:HIS:ND1 | 40:FF:168:GLU:OE2 | 2.43 | 0.52 |
| 41:FP:26:ASP:O | 41:FP:359:ARG:NH1 | 2.42 | 0.52 |
| 41:FP:156:ARG:NH1 | 41:FP:195:ASN:O | 2.43 | 0.52 |
| 40:GE:70:LEU:HG | 40:GE:110:ILE:HD13 | 1.92 | 0.52 |
| 40:GE:217:LEU:CA | 40:GE:277:SER:HB2 | 2.37 | 0.52 |
| 40:GI:121:ARG:HA | 40:GI:124:LYS:HD2 | 1.91 | 0.52 |
| 41:GN:274:THR:OG1 | 41:GN:275:SER:N | 2.41 | 0.52 |
| 41:GO:107:THR:O | 41:GO:110:ALA:N | 2.40 | 0.52 |
| 41:GP:325:GLU:O | 41:GP:329:GLN:NE2 | 2.43 | 0.52 |
| 40:HI:242:LEU:HD11 | 40:HI:252:LEU:HG | 1.92 | 0.52 |
| 41:HO:290:THR:HA | 41:HO:293:MET:HE3 | 1.91 | 0.52 |
| 40:IG:286:LEU:HD13 | 40:IG:370:VAL:HG13 | 1.91 | 0.52 |
| 41:IQ:113:VAL:HA | 41:IQ:116:VAL:HG12 | 1.91 | 0.52 |
| 40:JA:169:PHE:HZ | 40:JA:238:ILE:HG21 | 1.75 | 0.52 |
| 40:KG:254:GLU:HG2 | 41:KO:98:GLY:HA2 | 1.91 | 0.52 |
| 40:KH:27:GLU:HG2 | 40:KH:28:HIS:HD2 | 1.75 | 0.52 |
| 41:KP:198:GLU:HG2 | 41:KP:266:PHE:HE2 | 1.74 | 0.52 |
| 41:LB:27:GLU:O | 41:LB:43:GLN:NE2 | 2.42 | 0.52 |
| 40:LF:205:ASP:O | 40:LF:209:ILE:HG13 | 2.09 | 0.52 |
| 41:LO:142:GLY:O | 41:LO:144:GLY:N | 2.43 | 0.52 |
| 41:LP:236:VAL:HG22 | 41:LP:368:ILE:HD11 | 1.92 | 0.52 |
| 42:MB:502:GTP:C2 | 40:MG:224:TYR:HB3 | 2.45 | 0.52 |
| 40:MD:206:ASN:OD1 | 42:MD:501:GTP:O2' | 2.27 | 0.52 |
| 41:MO:316:VAL:HG13 | 41:MO:352:ALA:HB3 | 1.91 | 0.52 |
| 40:ND:32:PRO:O | 40:ND:33:ASP:C | 2.48 | 0.52 |
| 40:ND:140:SER:O | 40:ND:142:GLY:N | 2.37 | 0.52 |
| 40:NE:101:ASN:OD1 | 41:NL:256:ASN:ND2 | 2.41 | 0.52 |
| 40:NH:298:PRO:HB3 | 40:NH:307:PRO:HD2 | 1.90 | 0.52 |
| 41:NL:7:LEU:HG | 41:NL:135:LEU:HD13 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:NL:222:TYR:O | 41:NL:226:ASN:ND2 | 2.42 | 0.52 |
| 41:NO:171:PRO:O | 41:NO:380:ARG:NH2 | 2.41 | 0.52 |
| 41:NP:316:VAL:HB | 41:NP:366:THR:HB | 1.91 | 0.52 |
| 40:OA:76:ASP:HA | 40:OA:79:ARG:HG2 | 1.91 | 0.52 |
| 40:OD:108:TYR:O | 40:OD:112:LYS:NZ | 2.42 | 0.52 |
| 40:OH:258:ASN:O | 41:OP:394:PHE:HE1 | 1.92 | 0.52 |
| 40:PA:67:PHE:HB2 | 40:PA:92:LEU:HA | 1.92 | 0.52 |
| 40:PH:278:ALA:HB2 | 40:PH:368:ALA:HB2 | 1.91 | 0.52 |
| 41:PL:211:CYS:HA | 41:PL:215:LEU:HB2 | 1.92 | 0.52 |
| 41:PM:289:LEU:HD11 | 41:PM:363:MET:HB3 | 1.91 | 0.52 |
| 41:PP:343:GLU:OE1 | 41:PP:343:GLU:N | 2.43 | 0.52 |
| 40:QF:101:ASN:N | 41:QM:252:LYS:HZ3 | 2.08 | 0.52 |
| 41:QM:63:ALA:O | 41:QM:89:ASN:ND2 | 2.43 | 0.52 |
| 40:RA:16:ILE:HD11 | 40:RA:138:PHE:HB3 | 1.91 | 0.52 |
| 41:RB:136:THR:HG22 | 41:RB:167:PHE:HB2 | 1.91 | 0.52 |
| 41:RL:171:PRO:HG3 | 41:RL:181:GLU:HB3 | 1.92 | 0.52 |
| 41:RN:323:MET:SD | 41:RN:323:MET:N | 2.83 | 0.52 |
| 40:SA:265:ILE:HA | 40:SA:431:TYR:OH | 2.10 | 0.52 |
| 40:SH:182:VAL:O | 40:SH:186:ASN:ND2 | 2.42 | 0.52 |
| 41:SO:193:VAL:HA | 41:SO:264:HIS:NE2 | 2.25 | 0.52 |
| 41:SO:236:VAL:HG12 | 41:SO:237:THR:HG23 | 1.92 | 0.52 |
| 41:SP:191:GLN:O | 41:SP:195:ASN:ND2 | 2.40 | 0.52 |
| 41:SP:309:ARG:NH1 | 41:SP:339:SER:O | 2.43 | 0.52 |
| 40:TG:320:ARG:HB3 | 40:TG:356:ASN:HB2 | 1.91 | 0.52 |
| 40:TG:352:LYS:HD2 | 41:TO:179:VAL:HG13 | 1.92 | 0.52 |
| 41:TN:178:THR:HB | 41:TN:181:GLU:HG3 | 1.90 | 0.52 |
| 41:UB:143:THR:OG1 | 43:UB:501:GDP:O1B | 2.26 | 0.52 |
| 40:UF:326:LYS:HE3 | 41:UN:208:TYR:CD1 | 2.45 | 0.52 |
| 40:UH:211:ASP:HB3 | 40:UH:215:ARG:HH21 | 1.74 | 0.52 |
| 41:UO:87:PRO:HD3 | 41:VP:281:TYR:HD2 | 1.73 | 0.52 |
| 40:VG:7:VAL:HG13 | 40:VG:66:VAL:HG23 | 1.91 | 0.52 |
| 40:VI:323:VAL:HG22 | 40:VI:372:ARG:HG2 | 1.91 | 0.52 |
| 41:VO:178:THR:HB | 41:VO:181:GLU:HG3 | 1.91 | 0.52 |
| 41:VP:33:THR:O | 41:VP:58:LYS:NZ | 2.41 | 0.52 |
| 40:WG:175:PRO:HG3 | 40:WG:304:LYS:HB3 | 1.91 | 0.52 |
| 7:1S:507:CYS:SG | 7:1S:520:SER:OG | 2.59 | 0.52 |
| 7:1T:503:THR:HB | 7:1T:523:ASP:HB2 | 1.92 | 0.52 |
| 8:1W:304:GLN:OE1 | 8:1W:308:LYS:NZ | 2.40 | 0.52 |
| 12:2O:45:LYS:HA | 12:2O:48:MET:HG2 | 1.92 | 0.52 |
| 14:3B:81:LEU:HD23 | 14:3B:84:ARG:HH11 | 1.75 | 0.52 |
| 21:4F:407:LYS:HZ3 | 21:4F:410:ILE:CD1 | 2.16 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4I:658:ILE:HG23 | 22:4I:690:TYR:HE1 | 1.75 | 0.52 |
| 23:4N:37:TYR:CD2 | 23:4N:41:THR:HG21 | 2.44 | 0.52 |
| 23:4Q:183:PHE:HE2 | 40:CH:80:THR:HG22 | 1.75 | 0.52 |
| 23:4R:241:GLY:N | 23:4R:265:THR:O | 2.40 | 0.52 |
| 28:5B:55:ARG:HH21 | 40:IH:84:ARG:HH11 | 1.56 | 0.52 |
| 34:5R:502:HIS:H | 34:5R:502:HIS:CD2 | 2.27 | 0.52 |
| 35:5T:103:ASN:ND2 | 40:JE:82:THR:OG1 | 2.39 | 0.52 |
| 37:6A:113:ARG:NH1 | 40:TH:244:PHE:O | 2.40 | 0.52 |
| 39:6L:25:PHE:HE2 | 40:OD:80:THR:HG1 | 1.57 | 0.52 |
| 40:AE:206:ASN:OD1 | 42:AE:501:GTP:O2' | 2.27 | 0.52 |
| 40:AF:318:LEU:O | 40:AF:374:VAL:HA | 2.10 | 0.52 |
| 41:BB:354:CYS:O | 41:BB:355:ASP:C | 2.48 | 0.52 |
| 41:BP:294:PHE:CD1 | 41:BP:333:VAL:HG11 | 2.45 | 0.52 |
| 40:CE:154:MET:HG3 | 40:CE:194:THR:HG22 | 1.90 | 0.52 |
| 40:CI:73:THR:HA | 40:CI:76:ASP:HB2 | 1.90 | 0.52 |
| 41:CP:323:MET:SD | 41:CP:353:VAL:HG21 | 2.50 | 0.52 |
| 40:DA:31:GLN:C | 40:DA:33:ASP:H | 2.14 | 0.52 |
| 40:DA:58:ALA:C | 40:DA:60:LYS:H | 2.13 | 0.52 |
| 40:DF:133:GLN:HB3 | 40:DF:252:LEU:HD12 | 1.92 | 0.52 |
| 40:DF:185:TYR:O | 40:DF:186:ASN:C | 2.48 | 0.52 |
| 40:DH:232:SER:O | 40:DH:235:VAL:HG12 | 2.10 | 0.52 |
| 41:DN:102:ALA:O | 41:DN:103:LYS:C | 2.49 | 0.52 |
| 41:DO:22:GLU:HG3 | 41:DO:81:PHE:CD1 | 2.45 | 0.52 |
| 41:DP:99:ASN:HB2 | 41:DP:180:VAL:HG21 | 1.92 | 0.52 |
| 40:EH:401:ARG:HG2 | 40:EH:404:VAL:HG21 | 1.92 | 0.52 |
| 40:EI:85:GLN:O | 40:EI:86:LEU:C | 2.47 | 0.52 |
| 40:EI:278:ALA:HB2 | 40:EI:368:ALA:HB2 | 1.92 | 0.52 |
| 41:EL:132:GLY:CA | 41:EL:163:ILE:O | 2.58 | 0.52 |
| 41:EN:293:MET:HG3 | 41:EN:367:PHE:HB2 | 1.92 | 0.52 |
| 41:EO:204:ASN:HA | 41:EO:207:LEU:HD12 | 1.92 | 0.52 |
| 41:EP:228:LEU:HA | 41:EP:270:PHE:HE2 | 1.74 | 0.52 |
| 40:FE:231:ILE:HA | 40:FE:234:ILE:HD12 | 1.92 | 0.52 |
| 41:FN:313:VAL:HG13 | 41:FN:349:VAL:HG23 | 1.91 | 0.52 |
| 41:FO:207:LEU:HB3 | 41:FO:225:LEU:HD22 | 1.92 | 0.52 |
| 40:GA:397:MET:CG | 41:GN:346:PRO:HD2 | 2.40 | 0.52 |
| 40:GF:298:PRO:HB3 | 40:GF:307:PRO:HD2 | 1.92 | 0.52 |
| 40:GH:140:SER:O | 40:GH:141:PHE:C | 2.47 | 0.52 |
| 40:GH:370:VAL:C | 40:GH:372:ARG:H | 2.13 | 0.52 |
| 40:GI:228:ASN:HD22 | 42:GP:501:GTP:N2 | 2.04 | 0.52 |
| 40:GI:293:ASN:HA | 40:GI:335:ILE:HD11 | 1.91 | 0.52 |
| 41:GN:218:THR:O | 41:GN:220:PRO:HD3 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HA:224:TYR:HA | 40:HA:227:LEU:HB2 | 1.92 | 0.52 |
| 40:HE:205:ASP:HB2 | 40:HE:302:MET:O | 2.09 | 0.52 |
| 40:HE:325:PRO:HB3 | 41:HM:222:TYR:CE2 | 2.44 | 0.52 |
| 41:HN:285:THR:O | 41:HN:286:VAL:C | 2.47 | 0.52 |
| 41:IM:27:GLU:HG2 | 41:IM:241:ARG:HH21 | 1.75 | 0.52 |
| 41:IO:105:HIS:CD2 | 41:IO:150:LEU:HB2 | 2.44 | 0.52 |
| 40:JD:142:GLY:O | 40:JD:186:ASN:ND2 | 2.43 | 0.52 |
| 40:JE:349:THR:O | 41:JM:179:VAL:HG12 | 2.10 | 0.52 |
| 41:JO:52:ASN:OD1 | 41:JO:62:ARG:NH1 | 2.42 | 0.52 |
| 40:KE:31:GLN:HE21 | 40:KE:37:PRO:HG2 | 1.75 | 0.52 |
| 41:KM:100:ASN:HB3 | 41:KM:103:LYS:HB2 | 1.91 | 0.52 |
| 41:KO:39:ASP:N | 41:KO:39:ASP:OD1 | 2.43 | 0.52 |
| 41:KO:316:VAL:HB | 41:KO:366:THR:HG22 | 1.91 | 0.52 |
| 41:LB:375:GLN:HE22 | 41:LB:423:VAL:HA | 1.74 | 0.52 |
| 40:LD:260:VAL:HG13 | 41:LL:397:TRP:CH2 | 2.43 | 0.52 |
| 40:LG:88:HIS:HE1 | 40:MG:280:LYS:HG2 | 1.74 | 0.52 |
| 40:LG:232:SER:O | 40:LG:235:VAL:HG12 | 2.10 | 0.52 |
| 41:LM:101:TRP:HB2 | 41:LM:184:ASN:HD22 | 1.75 | 0.52 |
| 41:MB:214:THR:OG1 | 41:MB:297:LYS:NZ | 2.43 | 0.52 |
| 40:MF:328:VAL:HG11 | 40:MF:353:VAL:HG11 | 1.91 | 0.52 |
| 40:MG:108:TYR:HA | 40:MG:112:LYS:HZ2 | 1.75 | 0.52 |
| 40:MH:214:ARG:NH2 | 41:MO:324:LYS:HG3 | 2.15 | 0.52 |
| 41:ML:269:GLY:O | 41:ML:367:PHE:N | 2.42 | 0.52 |
| 41:MN:268:PRO:HG2 | 41:MN:300:MET:HB2 | 1.91 | 0.52 |
| 40:NA:70:LEU:HD12 | 40:NA:145:THR:HG22 | 1.91 | 0.52 |
| 41:NB:86:ARG:NH2 | 41:OB:281:TYR:O | 2.43 | 0.52 |
| 41:NB:329:GLN:OE1 | 41:NB:332:ASN:ND2 | 2.43 | 0.52 |
| 40:NF:168:GLU:HB3 | 40:NF:201:ALA:HA | 1.92 | 0.52 |
| 40:NH:174:ALA:HB3 | 40:NH:178:SER:H | 1.75 | 0.52 |
| 41:NL:60:VAL:HG21 | 41:NL:86:ARG:HG3 | 1.91 | 0.52 |
| 40:OD:28:HIS:CE1 | 40:OD:243:ARG:HD3 | 2.45 | 0.52 |
| 40:OD:34:GLY:HA2 | 40:OD:86:LEU:HD12 | 1.92 | 0.52 |
| 41:OM:222:TYR:O | 41:OM:226:ASN:ND2 | 2.43 | 0.52 |
| 41:OP:138:SER:HA | 41:OP:169:VAL:HG12 | 1.92 | 0.52 |
| 40:PF:56:THR:HG22 | 40:QF:285:GLN:HA | 1.91 | 0.52 |
| 41:PM:210:ILE:O | 41:PM:214:THR:OG1 | 2.26 | 0.52 |
| 41:PP:101:TRP:CD1 | 41:PP:105:HIS:HB2 | 2.45 | 0.52 |
| 40:QA:265:ILE:HG23 | 40:QA:431:TYR:HE1 | 1.75 | 0.52 |
| 41:QB:325:GLU:O | 41:QB:326:VAL:C | 2.48 | 0.52 |
| 40:QH:76:ASP:HA | 40:QH:79:ARG:HG2 | 1.92 | 0.52 |
| 41:QL:31:ASP:OD1 | 41:QL:35:THR:N | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RH:90:GLU:HB3 | 40:RH:121:ARG:HH12 | 1.75 | 0.52 |
| 41:RL:320:ARG:NH1 | 41:RL:355:ASP:OD1 | 2.43 | 0.52 |
| 41:RO:149:THR:HB | 41:RO:191:GLN:HG2 | 1.92 | 0.52 |
| 40:SA:65:ALA:O | 40:SA:91:GLN:NE2 | 2.43 | 0.52 |
| 40:SH:204:VAL:HG13 | 40:SH:302:MET:HB3 | 1.92 | 0.52 |
| 40:SH:209:ILE:HA | 40:SH:212:ILE:HG12 | 1.92 | 0.52 |
| 41:SO:31:ASP:O | 41:SO:34:GLY:N | 2.42 | 0.52 |
| 40:TE:224:TYR:HA | 40:TE:227:LEU:HB2 | 1.92 | 0.52 |
| 40:TF:141:PHE:HB2 | 40:TF:173:PRO:HD3 | 1.92 | 0.52 |
| 40:TG:107:HIS:CD2 | 40:TG:152:LEU:HB2 | 2.45 | 0.52 |
| 40:TI:7:VAL:O | 40:TI:137:ILE:HA | 2.10 | 0.52 |
| 41:TM:105:HIS:HA | 41:TM:150:LEU:HD23 | 1.92 | 0.52 |
| 40:UF:7:VAL:HG11 | 40:UF:153:LEU:HD21 | 1.92 | 0.52 |
| 40:UF:363:VAL:O | 40:UF:365:GLY:N | 2.43 | 0.52 |
| 40:UH:93:ILE:HD11 | 40:UH:121:ARG:HG3 | 1.91 | 0.52 |
| 41:UM:49:VAL:HG11 | 41:UM:241:ARG:HG2 | 1.91 | 0.52 |
| 41:UM:105:HIS:CD2 | 41:UM:150:LEU:HB2 | 2.45 | 0.52 |
| 41:UN:87:PRO:HD3 | 41:VO:281:TYR:HD2 | 1.75 | 0.52 |
| 40:VG:238:ILE:HG23 | 40:VG:255:PHE:HE2 | 1.74 | 0.52 |
| 40:VH:167:LEU:HD22 | 40:VH:200:CYS:HB3 | 1.92 | 0.52 |
| 40:VJ:76:ASP:OD2 | 41:VQ:46:ARG:NH2 | 2.43 | 0.52 |
| 40:VJ:98:ASP:O | 40:VJ:105:ARG:NH1 | 2.43 | 0.52 |
| 40:WE:257:THR:HA | 41:WM:397:TRP:CE2 | 2.44 | 0.52 |
| 41:WM:337:ASN:HB3 | 41:WM:340:TYR:HD2 | 1.75 | 0.52 |
| 41:WQ:318:ARG:HG2 | 41:WQ:358:PRO:HD3 | 1.92 | 0.52 |
| 11:2J:186:LYS:O | 11:2J:251:TYR:HB2 | 2.09 | 0.52 |
| 12:2R:161:ASN:HB3 | 12:2R:164:VAL:HG12 | 1.91 | 0.52 |
| 14:3C:105:ALA:O | 14:3C:110:ARG:NH2 | 2.43 | 0.52 |
| 17:3P:185:LEU:HD11 | 17:3P:234:LYS:HA | 1.91 | 0.52 |
| 17:3P:222:GLU:HA | 17:3P:339:GLN:HG2 | 1.92 | 0.52 |
| 20:4A:29:ARG:HH12 | 20:4A:36:ARG:HA | 1.74 | 0.52 |
| 20:4A:176:ILE:O | 20:4A:177:ASP:C | 2.49 | 0.52 |
| 21:4D:426:LEU:HB2 | 21:4D:438:PHE:HE2 | 1.75 | 0.52 |
| 21:4E:513:LEU:HD12 | 21:4E:513:LEU:H | 1.75 | 0.52 |
| 22:4I:98:ARG:HH21 | 41:BO:279:GLN:HE21 | 1.55 | 0.52 |
| 22:4J:92:LYS:HA | 41:BN:280:GLN:HB3 | 1.91 | 0.52 |
| 23:4R:184:MET:O | 23:4R:186:GLY:N | 2.43 | 0.52 |
| 27:4Y:74:ASN:ND2 | 27:4Y:263:HIS:O | 2.42 | 0.52 |
| 28:5B:215:LEU:HA | 28:5B:218:LYS:HZ3 | 1.75 | 0.52 |
| 34:5Q:62:LEU:HD13 | 41:JN:94:GLN:HG3 | 1.92 | 0.52 |
| 36:5W:186:TYR:HB2 | 41:OB:276:ARG:NH1 | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AA:118:VAL:HG11 | 40:AA:149:PHE:HZ | 1.75 | 0.52 |
| 40:AG:255:PHE:HZ | 40:AG:318:LEU:HD21 | 1.75 | 0.52 |
| 40:AG:405:HIS:HA | 40:AG:408:VAL:HG22 | 1.92 | 0.52 |
| 40:BE:210:TYR:CE2 | 40:BE:227:LEU:HD11 | 2.45 | 0.52 |
| 40:BH:105:ARG:HA | 40:BH:109:THR:CG2 | 2.39 | 0.52 |
| 41:BM:228:LEU:HB3 | 41:BM:300:MET:SD | 2.50 | 0.52 |
| 40:CF:16:ILE:HA | 40:CF:228:ASN:HB3 | 1.92 | 0.52 |
| 41:CL:145:SER:O | 41:CL:146:GLY:C | 2.48 | 0.52 |
| 41:CN:212:PHE:HD2 | 41:CN:213:ARG:HG2 | 1.75 | 0.52 |
| 41:CO:12:CYS:HB3 | 41:CO:138:SER:HB3 | 1.91 | 0.52 |
| 41:CO:309:ARG:HH21 | 41:CO:342:VAL:HA | 1.75 | 0.52 |
| 40:DH:250:VAL:CG1 | 40:DH:354:GLY:HA3 | 2.39 | 0.52 |
| 40:DI:31:GLN:C | 40:DI:33:ASP:H | 2.14 | 0.52 |
| 41:DP:101:TRP:HB2 | 41:DP:184:ASN:OD1 | 2.10 | 0.52 |
| 41:DP:102:ALA:O | 41:DP:103:LYS:C | 2.49 | 0.52 |
| 41:DP:218:THR:O | 41:DP:220:PRO:HD3 | 2.10 | 0.52 |
| 40:EE:76:ASP:HA | 40:EE:79:ARG:HG2 | 1.92 | 0.52 |
| 41:EM:69:GLU:O | 41:EM:71:GLY:N | 2.36 | 0.52 |
| 41:EO:156:ARG:HD3 | 41:EO:164:MET:HB2 | 1.91 | 0.52 |
| 41:EP:65:LEU:HD12 | 41:EP:65:LEU:H | 1.74 | 0.52 |
| 41:EP:305:PRO:O | 41:EP:308:GLY:N | 2.41 | 0.52 |
| 40:FA:56:THR:OG1 | 40:FA:57:GLY:N | 2.43 | 0.52 |
| 40:FH:73:THR:HA | 40:FH:76:ASP:HB2 | 1.92 | 0.52 |
| 40:GH:104:ALA:CB | 40:GH:410:GLU:HB3 | 2.40 | 0.52 |
| 41:GM:39:ASP:OD1 | 41:GM:43:GLN:NE2 | 2.43 | 0.52 |
| 41:GN:188:SER:O | 41:GN:189:VAL:C | 2.49 | 0.52 |
| 40:HE:122:ILE:HD11 | 40:HE:161:TYR:HE2 | 1.75 | 0.52 |
| 40:HH:27:GLU:OE2 | 40:HH:243:ARG:NH2 | 2.42 | 0.52 |
| 41:HO:87:PRO:HD3 | 41:IO:281:TYR:HD2 | 1.75 | 0.52 |
| 40:IH:139:HIS:O | 40:IH:170:SER:HA | 2.09 | 0.52 |
| 40:II:170:SER:OG | 40:II:203:MET:SD | 2.68 | 0.52 |
| 40:II:206:ASN:OD1 | 42:II:501:GTP:O2' | 2.27 | 0.52 |
| 41:IN:178:THR:HB | 41:IN:181:GLU:HG3 | 1.92 | 0.52 |
| 40:JA:348:PRO:HB2 | 41:JB:384:GLN:HE22 | 1.75 | 0.52 |
| 41:JO:165:ASN:ND2 | 41:JO:198:GLU:OE1 | 2.42 | 0.52 |
| 40:KF:76:ASP:OD1 | 41:KM:46:ARG:NH2 | 2.42 | 0.52 |
| 41:KM:341:PHE:HB3 | 41:KM:348:ASN:HD21 | 1.75 | 0.52 |
| 41:KN:311:LEU:HD23 | 41:KN:342:VAL:HG11 | 1.91 | 0.52 |
| 40:LE:286:LEU:HD13 | 40:LE:370:VAL:HG23 | 1.91 | 0.52 |
| 41:MB:237:THR:HG23 | 41:MB:241:ARG:HH11 | 1.75 | 0.52 |
| 42:MB:502:GTP:C6 | 40:MG:224:TYR:HB3 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:ME:231:ILE:HA | 40:ME:234:ILE:HD12 | 1.92 | 0.52 |
| 40:MH:258:ASN:HA | 41:MP:179:VAL:CG2 | 2.40 | 0.52 |
| 40:MH:273:ALA:HB3 | 40:MH:274:PRO:CD | 2.38 | 0.52 |
| 41:MO:171:PRO:HG3 | 41:MO:185:ALA:HB2 | 1.92 | 0.52 |
| 41:MP:234:SER:O | 41:MP:238:THR:OG1 | 2.27 | 0.52 |
| 40:NG:22:GLU:OE2 | 40:NG:83:TYR:OH | 2.28 | 0.52 |
| 40:NH:167:LEU:HD23 | 40:NH:200:CYS:HB3 | 1.92 | 0.52 |
| 40:NH:178:SER:OG | 41:NO:347:ASN:ND2 | 2.28 | 0.52 |
| 41:NM:309:ARG:NH2 | 41:NM:341:PHE:O | 2.43 | 0.52 |
| 41:NP:44:LEU:HA | 41:NP:47:ILE:HB | 1.91 | 0.52 |
| 41:OB:207:LEU:HB3 | 41:OB:225:LEU:HD12 | 1.91 | 0.52 |
| 41:OO:165:ASN:HA | 41:OO:198:GLU:O | 2.10 | 0.52 |
| 41:PL:36:TYR:CD2 | 41:PL:44:LEU:HD13 | 2.45 | 0.52 |
| 41:PM:33:THR:O | 41:PM:58:LYS:NZ | 2.43 | 0.52 |
| 41:PN:173:PRO:HB3 | 41:PN:380:ARG:HD2 | 1.91 | 0.52 |
| 40:QA:288:VAL:HA | 40:QA:291:ILE:HG12 | 1.91 | 0.52 |
| 41:QB:72:THR:O | 41:QB:76:VAL:HG23 | 2.10 | 0.52 |
| 40:QG:11:GLN:HG3 | 40:QG:74:VAL:HG21 | 1.92 | 0.52 |
| 40:SA:76:ASP:OD2 | 41:SN:46:ARG:NH2 | 2.38 | 0.52 |
| 40:SE:204:VAL:HG13 | 40:SE:302:MET:HB3 | 1.91 | 0.52 |
| 41:SM:171:PRO:O | 41:SM:380:ARG:NH2 | 2.37 | 0.52 |
| 41:SN:54:ALA:HA | 41:TN:283:ALA:HB2 | 1.91 | 0.52 |
| 41:SO:101:TRP:HB3 | 41:SO:398:TYR:HE1 | 1.75 | 0.52 |
| 41:SP:282:ARG:HE | 41:SP:283:ALA:H | 1.58 | 0.52 |
| 40:TI:171:ILE:HG21 | 42:TI:501:GTP:H1' | 1.92 | 0.52 |
| 41:TN:103:LYS:HG2 | 41:TN:107:THR:HG21 | 1.91 | 0.52 |
| 40:UA:217:LEU:HD21 | 40:UA:367:LEU:HD23 | 1.91 | 0.52 |
| 40:UG:251:ASP:HB3 | 40:UG:254:GLU:HG3 | 1.92 | 0.52 |
| 40:VJ:190:THR:O | 40:VJ:194:THR:OG1 | 2.20 | 0.52 |
| 40:WE:239:THR:O | 40:WE:243:ARG:NE | 2.26 | 0.52 |
| 40:WI:97:GLU:OE1 | 41:WP:251:ARG:NH1 | 2.43 | 0.52 |
| 7:1U:392:ALA:HB2 | 7:1U:423:VAL:HG13 | 1.92 | 0.51 |
| 11:2K:7:SER:OG | 11:2K:8:GLU:N | 2.42 | 0.51 |
| 11:2K:132:ASP:N | 11:2K:132:ASP:OD1 | 2.43 | 0.51 |
| 13:2T:97:LYS:O | 13:2T:98:ASN:C | 2.47 | 0.51 |
| 13:2U:108:TYR:CE1 | 40:AG:418:SER:HB3 | 2.45 | 0.51 |
| 13:2X:69:LEU:O | 13:2X:71:ILE:N | 2.42 | 0.51 |
| 14:3A:85:THR:HG23 | 14:3A:88:GLY:H | 1.75 | 0.51 |
| 16:3J:120:ARG:NH2 | 16:3J:131:ASP:OD2 | 2.33 | 0.51 |
| 17:3R:163:GLU:O | 17:3R:164:LEU:C | 2.49 | 0.51 |
| 18:3U:116:GLU:O | 18:3U:120:HIS:ND1 | 2.31 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4D:246:TYR:HB2 | 21:4D:346:ASP:HB3 | 1.93 | 0.51 |
| 23:4R:107:LYS:H | 40:BI:219:ILE:HG22 | 1.75 | 0.51 |
| 26:4W:332:GLU:OE2 | 31:5I:396:LYS:NZ | 2.37 | 0.51 |
| 31:5I:603:LYS:HE2 | 31:5I:674:TRP:HH2 | 1.75 | 0.51 |
| 31:5I:745:LYS:HG3 | 41:IQ:320:ARG:HH22 | 1.75 | 0.51 |
| 40:BA:31:GLN:OE1 | 40:BA:32:PRO:HD2 | 2.10 | 0.51 |
| 41:BB:202:ILE:HD13 | 41:BB:229:VAL:HG13 | 1.92 | 0.51 |
| 41:BB:319:GLY:HA2 | 41:BB:357:PRO:HB3 | 1.90 | 0.51 |
| 41:BB:394:PHE:HA | 41:BB:397:TRP:CZ3 | 2.45 | 0.51 |
| 40:BE:273:ALA:CB | 40:BE:374:VAL:HG13 | 2.40 | 0.51 |
| 40:BE:298:PRO:HG3 | 40:BE:308:ARG:NE | 2.25 | 0.51 |
| 41:BM:135:LEU:HB3 | 41:BM:166:THR:HG22 | 1.92 | 0.51 |
| 41:BO:67:ASP:OD2 | 41:BO:73:MET:HG2 | 2.09 | 0.51 |
| 41:CL:44:LEU:O | 41:CL:45:GLU:C | 2.48 | 0.51 |
| 40:DA:400:LYS:O | 40:DA:401:ARG:C | 2.49 | 0.51 |
| 41:DB:348:ASN:HA | 40:DG:181:VAL:CG1 | 2.40 | 0.51 |
| 40:DE:31:GLN:HB2 | 40:DE:35:GLN:O | 2.10 | 0.51 |
| 40:DF:307:PRO:O | 40:DF:310:GLY:N | 2.40 | 0.51 |
| 40:DI:336:LYS:HA | 40:DI:343:PHE:HE2 | 1.75 | 0.51 |
| 41:DL:222:TYR:HA | 41:DL:225:LEU:HD12 | 1.92 | 0.51 |
| 41:DM:97:ALA:HB1 | 41:DM:100:ASN:HD21 | 1.73 | 0.51 |
| 41:DO:100:ASN:HD22 | 41:DO:103:LYS:HE2 | 1.75 | 0.51 |
| 41:DP:372:THR:HA | 41:DP:422:VAL:HG12 | 1.92 | 0.51 |
| 41:EB:46:ARG:NH2 | 41:EB:243:PRO:HG3 | 2.25 | 0.51 |
| 40:EG:90:GLU:HB2 | 40:EG:121:ARG:HH21 | 1.75 | 0.51 |
| 40:FF:176:GLN:HB3 | 41:FM:331:LEU:HD11 | 1.91 | 0.51 |
| 41:FO:289:LEU:O | 41:FO:293:MET:HB2 | 2.10 | 0.51 |
| 40:GE:115:ILE:HG12 | 40:GE:152:LEU:HG | 1.92 | 0.51 |
| 40:GF:234:ILE:HD11 | 40:GF:272:TYR:HB2 | 1.93 | 0.51 |
| 40:GG:191:THR:HA | 40:GG:194:THR:HG22 | 1.91 | 0.51 |
| 40:GI:278:ALA:HA | 40:GI:368:ALA:HB2 | 1.92 | 0.51 |
| 41:HB:274:THR:OG1 | 41:HB:279:GLN:OE1 | 2.28 | 0.51 |
| 40:HE:79:ARG:HG2 | 40:HE:92:LEU:HD13 | 1.92 | 0.51 |
| 41:IB:155:ILE:HA | 41:IB:158:GLU:HG2 | 1.92 | 0.51 |
| 40:II:6:SER:HA | 40:II:136:LEU:O | 2.10 | 0.51 |
| 41:IP:42:LEU:HD22 | 41:IP:356:ILE:HD12 | 1.91 | 0.51 |
| 41:IQ:203:ASP:OD2 | 41:IQ:302:ALA:N | 2.40 | 0.51 |
| 40:JF:269:LEU:HD21 | 40:JF:383:ILE:HD13 | 1.91 | 0.51 |
| 41:JN:204:ASN:OD1 | 43:JN:501:GDP:O2' | 2.27 | 0.51 |
| 40:KH:165:SER:HB3 | 40:KH:256:GLN:HE22 | 1.73 | 0.51 |
| 41:KN:15:GLN:NE2 | 43:KN:502:GDP:O6 | 2.42 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LA:236:SER:OG | 40:LA:243:ARG:NH2 | 2.42 | 0.51 |
| 40:LA:247:ALA:O | 41:LB:11:GLN:NE2 | 2.41 | 0.51 |
| 40:LF:104:ALA:HB1 | 40:LF:410:GLU:CD | 2.29 | 0.51 |
| 40:LG:413:GLU:O | 40:LG:414:GLU:C | 2.48 | 0.51 |
| 41:LM:313:VAL:HB | 41:LM:349:VAL:HG22 | 1.91 | 0.51 |
| 41:LN:114:ASP:N | 41:LN:114:ASP:OD1 | 2.43 | 0.51 |
| 41:LN:165:ASN:HD21 | 41:LN:250:LEU:HD22 | 1.75 | 0.51 |
| 40:NH:130:THR:OG1 | 40:NH:131:GLY:N | 2.43 | 0.51 |
| 41:NL:215:LEU:HD21 | 41:NL:273:LEU:HD12 | 1.92 | 0.51 |
| 41:NP:62:ARG:NE | 41:NP:127:CYS:SG | 2.83 | 0.51 |
| 40:OD:262:TYR:HB2 | 40:OD:265:ILE:HG12 | 1.91 | 0.51 |
| 40:PF:108:TYR:O | 40:PF:112:LYS:NZ | 2.43 | 0.51 |
| 40:QH:404:VAL:HG12 | 40:QH:417:PHE:HE2 | 1.75 | 0.51 |
| 41:QM:67:ASP:HA | 41:QM:143:THR:HG21 | 1.92 | 0.51 |
| 41:QP:169:VAL:HG12 | 41:QP:170:VAL:H | 1.74 | 0.51 |
| 40:RA:70:LEU:HD23 | 40:RA:114:LEU:HD12 | 1.91 | 0.51 |
| 40:RA:248:LEU:HD23 | 40:RA:355:ILE:HD12 | 1.91 | 0.51 |
| 40:RE:219:ILE:HG12 | 40:RE:222:PRO:HD3 | 1.92 | 0.51 |
| 40:RF:1:GLN:HG3 | 40:RF:2:ARG:HD3 | 1.91 | 0.51 |
| 40:RG:180:ALA:HB3 | 40:RG:183:GLU:HG3 | 1.91 | 0.51 |
| 40:RH:91:GLN:HE22 | 40:RH:125:LEU:HD11 | 1.76 | 0.51 |
| 40:SA:185:TYR:HE2 | 40:SA:403:PHE:HB2 | 1.75 | 0.51 |
| 41:SB:288:GLU:HA | 41:SB:291:GLN:HG3 | 1.91 | 0.51 |
| 40:SE:288:VAL:HA | 40:SE:291:ILE:HG12 | 1.91 | 0.51 |
| 40:SF:56:THR:OG1 | 40:SF:57:GLY:N | 2.41 | 0.51 |
| 40:SF:175:PRO:HB3 | 40:SF:389:ARG:CZ | 2.41 | 0.51 |
| 40:SF:370:VAL:HG12 | 40:SF:372:ARG:H | 1.75 | 0.51 |
| 40:SH:402:ALA:HB2 | 41:SO:344:TRP:HZ3 | 1.75 | 0.51 |
| 41:SL:286:VAL:HG21 | 41:SL:326:VAL:HG22 | 1.91 | 0.51 |
| 41:SO:181:GLU:HB3 | 41:SO:182:PRO:HD3 | 1.91 | 0.51 |
| 40:TE:276:ILE:HD13 | 40:TE:286:LEU:HD11 | 1.91 | 0.51 |
| 41:TL:164:MET:O | 41:TL:196:THR:OG1 | 2.27 | 0.51 |
| 40:UA:225:THR:O | 40:UA:229:ARG:HB2 | 2.09 | 0.51 |
| 41:UB:271:ALA:HB1 | 41:UB:292:GLN:HB3 | 1.92 | 0.51 |
| 40:UE:6:SER:O | 40:UE:65:ALA:HA | 2.09 | 0.51 |
| 40:VG:306:ASP:OD1 | 40:VG:309:HIS:ND1 | 2.43 | 0.51 |
| 40:VI:213:CYS:HA | 40:VI:217:LEU:HD23 | 1.92 | 0.51 |
| 41:VQ:341:PHE:HB3 | 41:VQ:348:ASN:HD21 | 1.74 | 0.51 |
| 41:WB:7:LEU:O | 41:WB:135:LEU:HA | 2.10 | 0.51 |
| 40:WH:150:THR:O | 40:WH:154:MET:HG2 | 2.10 | 0.51 |
| 40:WI:101:ASN:HD22 | 41:WP:256:ASN:HD22 | 1.58 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WN:138:SER:O | 41:WN:139:LEU:C | 2.49 | 0.51 |
| 7:1T:507:CYS:HB2 | 7:1T:551:MET:HE2 | 1.92 | 0.51 |
| 7:1U:341:PRO:HG2 | 11:2K:10:ILE:HG21 | 1.93 | 0.51 |
| 14:3C:24:LEU:HD13 | 40:LG:160:ASP:O | 2.11 | 0.51 |
| 16:3L:109:PRO:HG2 | 16:3L:254:LEU:HD21 | 1.91 | 0.51 |
| 18:3T:356:ARG:NH2 | 18:3U:231:TYR:O | 2.43 | 0.51 |
| 21:4E:169:ASN:H | 21:4E:172:ILE:HD13 | 1.75 | 0.51 |
| 21:4F:96:VAL:HG23 | 40:AE:41:THR:HG23 | 1.93 | 0.51 |
| 22:4J:486:VAL:HG11 | 22:4J:515:VAL:HG12 | 1.91 | 0.51 |
| 22:4K:562:LEU:HD11 | 22:4K:589:LEU:HD21 | 1.92 | 0.51 |
| 23:4N:33:MET:SD | 23:4N:33:MET:N | 2.83 | 0.51 |
| 34:5R:410:LYS:HZ2 | 34:5R:414:GLU:HB2 | 1.74 | 0.51 |
| 37:6A:46:HIS:CD2 | 40:UH:221:ARG:HG2 | 2.45 | 0.51 |
| 39:6F:66:ARG:NH2 | 41:OO:38:GLY:O | 2.44 | 0.51 |
| 40:AG:98:ASP:O | 40:AG:105:ARG:NH2 | 2.32 | 0.51 |
| 41:AL:248:ALA:HA | 41:AL:252:LYS:HD3 | 1.93 | 0.51 |
| 40:BA:248:LEU:HD13 | 40:BA:355:ILE:HD12 | 1.91 | 0.51 |
| 40:BF:292:THR:OG1 | 40:BF:319:TYR:OH | 2.27 | 0.51 |
| 40:BH:274:PRO:HD3 | 40:BH:373:ALA:HA | 1.92 | 0.51 |
| 40:BI:4:CYS:SG | 40:BI:133:GLN:NE2 | 2.83 | 0.51 |
| 41:BL:170:VAL:HG21 | 41:BL:377:LEU:HD21 | 1.91 | 0.51 |
| 41:BO:213:ARG:HH22 | 41:BO:297:LYS:HB3 | 1.75 | 0.51 |
| 41:BP:360:GLY:O | 41:BP:362:LYS:N | 2.43 | 0.51 |
| 40:CA:217:LEU:HD12 | 40:CA:277:SER:HB3 | 1.93 | 0.51 |
| 41:CL:268:PRO:HG2 | 41:CL:300:MET:HB2 | 1.92 | 0.51 |
| 41:CM:61:PRO:HG3 | 41:CM:84:ILE:HG23 | 1.91 | 0.51 |
| 41:DB:139:LEU:HD22 | 41:DB:188:SER:HB2 | 1.92 | 0.51 |
| 41:DB:183:TYR:HE1 | 41:DB:388:MET:HB3 | 1.75 | 0.51 |
| 40:DE:66:VAL:HG12 | 40:DE:93:ILE:HD11 | 1.91 | 0.51 |
| 40:DE:305:CYS:O | 40:DE:306:ASP:C | 2.48 | 0.51 |
| 40:DG:209:ILE:HA | 40:DG:212:ILE:HG22 | 1.92 | 0.51 |
| 41:DM:130:LEU:HD23 | 41:DM:162:ARG:HG3 | 1.93 | 0.51 |
| 41:EB:45:GLU:OE2 | 41:EB:46:ARG:NH2 | 2.43 | 0.51 |
| 40:EI:272:TYR:CD1 | 40:EI:375:CYS:HB2 | 2.46 | 0.51 |
| 41:EM:2:ARG:HA | 41:EM:129:CYS:O | 2.10 | 0.51 |
| 41:EM:95:SER:OG | 41:EM:96:GLY:N | 2.43 | 0.51 |
| 41:EM:108:GLU:O | 41:EM:111:GLU:HG2 | 2.10 | 0.51 |
| 41:EN:237:THR:O | 41:EN:241:ARG:NH1 | 2.39 | 0.51 |
| 41:EP:96:GLY:O | 41:EP:97:ALA:C | 2.48 | 0.51 |
| 40:FA:328:VAL:HG21 | 40:FA:353:VAL:CG2 | 2.41 | 0.51 |
| 40:FF:205:ASP:HB3 | 40:FF:303:VAL:HA | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FP:142:GLY:O | 41:FP:144:GLY:N | 2.42 | 0.51 |
| 40:GA:228:ASN:HB3 | 40:GA:231:ILE:HD12 | 1.91 | 0.51 |
| 41:GB:244:GLY:O | 41:GB:247:ASN:ND2 | 2.43 | 0.51 |
| 40:GI:211:ASP:O | 40:GI:212:ILE:C | 2.47 | 0.51 |
| 40:GI:225:THR:HA | 40:GI:228:ASN:ND2 | 2.25 | 0.51 |
| 40:GI:274:PRO:HB2 | 40:GI:370:VAL:HG21 | 1.91 | 0.51 |
| 41:GO:177:ASP:N | 41:GO:181:GLU:OE2 | 2.42 | 0.51 |
| 41:GP:314:ALA:HB3 | 41:GP:368:ILE:HB | 1.92 | 0.51 |
| 41:HM:7:LEU:HD23 | 41:HM:64:VAL:HB | 1.92 | 0.51 |
| 41:HN:226:ASN:CG | 43:HN:501:GDP:HN1 | 2.14 | 0.51 |
| 41:HQ:143:THR:OG1 | 41:HQ:144:GLY:N | 2.42 | 0.51 |
| 41:HQ:334:GLN:HE22 | 41:HQ:347:ASN:HA | 1.75 | 0.51 |
| 40:IE:75:ILE:HD11 | 40:IE:92:LEU:HD22 | 1.91 | 0.51 |
| 41:JB:2:ARG:HB3 | 41:JB:131:GLN:HG2 | 1.92 | 0.51 |
| 40:JE:241:SER:OG | 40:JE:249:ASN:OD1 | 2.28 | 0.51 |
| 40:JE:352:LYS:HD3 | 41:JM:178:THR:HA | 1.91 | 0.51 |
| 41:JM:144:GLY:O | 41:JM:145:SER:C | 2.49 | 0.51 |
| 40:KA:215:ARG:NH2 | 40:KA:300:ASN:OD1 | 2.42 | 0.51 |
| 40:KE:64:ARG:HH12 | 40:KE:128:GLN:HG3 | 1.74 | 0.51 |
| 40:KE:191:THR:HG21 | 40:KE:387:TRP:HH2 | 1.75 | 0.51 |
| 40:KE:311:LYS:NZ | 40:KE:435:GLY:O | 2.43 | 0.51 |
| 41:LB:54:ALA:HA | 41:MB:283:ALA:HB2 | 1.93 | 0.51 |
| 41:LB:252:LYS:O | 41:LB:256:ASN:ND2 | 2.38 | 0.51 |
| 40:MA:380:THR:HG23 | 40:MA:382:ALA:N | 2.25 | 0.51 |
| 41:MB:246:LEU:HD11 | 40:MG:179:THR:HG21 | 1.92 | 0.51 |
| 40:NE:179:THR:HG21 | 41:NL:246:LEU:HD11 | 1.92 | 0.51 |
| 41:NL:342:VAL:HG21 | 41:NL:345:ILE:HD12 | 1.92 | 0.51 |
| 41:NM:40:SER:HB3 | 41:NM:43:GLN:HB2 | 1.92 | 0.51 |
| 41:NO:49:VAL:HG11 | 41:NO:240:LEU:HD13 | 1.91 | 0.51 |
| 41:NO:286:VAL:HG22 | 41:NO:363:MET:HE1 | 1.92 | 0.51 |
| 40:OD:71:GLU:HB3 | 40:OD:98:ASP:HA | 1.92 | 0.51 |
| 40:OE:217:LEU:HA | 40:OE:277:SER:HB2 | 1.92 | 0.51 |
| 40:OG:306:ASP:OD1 | 40:OG:309:HIS:ND1 | 2.43 | 0.51 |
| 41:ON:341:PHE:HB3 | 41:ON:348:ASN:HD21 | 1.75 | 0.51 |
| 40:PA:231:ILE:O | 40:PA:235:VAL:HG23 | 2.10 | 0.51 |
| 41:PB:120:VAL:HG11 | 41:PB:155:ILE:HD13 | 1.92 | 0.51 |
| 40:PD:229:ARG:HH22 | 40:PD:363:VAL:HG11 | 1.72 | 0.51 |
| 40:PD:324:VAL:HG22 | 40:PD:326:LYS:H | 1.75 | 0.51 |
| 40:PF:202:PHE:CD1 | 40:PF:377:LEU:HD12 | 2.45 | 0.51 |
| 40:PG:254:GLU:OE1 | 41:PO:99:ASN:ND2 | 2.43 | 0.51 |
| 41:PL:249:ASP:OD1 | 41:PL:252:LYS:N | 2.34 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PN:165:ASN:HB3 | 41:PN:200:TYR:HE2 | 1.74 | 0.51 |
| 41:PO:142:GLY:O | 41:PO:144:GLY:N | 2.44 | 0.51 |
| 41:QB:65:LEU:H | 41:QB:65:LEU:HD22 | 1.75 | 0.51 |
| 40:QG:319:TYR:HB2 | 40:QG:355:ILE:HG12 | 1.92 | 0.51 |
| 41:QM:161:ASP:OD1 | 41:QM:162:ARG:NH1 | 2.43 | 0.51 |
| 41:QO:221:THR:HG23 | 41:QO:223:GLY:H | 1.75 | 0.51 |
| 41:QP:250:LEU:HA | 41:QP:253:LEU:HB2 | 1.92 | 0.51 |
| 40:RA:68:VAL:HA | 40:RA:93:ILE:HB | 1.92 | 0.51 |
| 40:RA:239:THR:HG22 | 40:RA:252:LEU:HD21 | 1.91 | 0.51 |
| 41:RB:117:LEU:HA | 41:RB:120:VAL:HG22 | 1.91 | 0.51 |
| 40:RE:5:ILE:O | 40:RE:135:PHE:HA | 2.11 | 0.51 |
| 40:RE:160:ASP:OD1 | 40:RE:161:TYR:N | 2.42 | 0.51 |
| 40:RH:179:THR:OG1 | 40:RH:183:GLU:OE2 | 2.28 | 0.51 |
| 40:RH:235:VAL:HA | 40:RH:238:ILE:HG22 | 1.93 | 0.51 |
| 41:RM:133:PHE:HD2 | 41:RM:155:ILE:HD12 | 1.75 | 0.51 |
| 41:SB:5:VAL:HG23 | 41:SB:62:ARG:HB2 | 1.91 | 0.51 |
| 40:SI:97:GLU:OE2 | 41:SP:162:ARG:NH1 | 2.41 | 0.51 |
| 41:SL:12:CYS:O | 41:SL:16:ILE:HD12 | 2.11 | 0.51 |
| 41:TB:271:ALA:HB1 | 41:TB:292:GLN:HG3 | 1.91 | 0.51 |
| 41:TM:163:ILE:HD11 | 41:TM:251:ARG:HG3 | 1.90 | 0.51 |
| 41:TO:152:ILE:HG21 | 41:TO:196:THR:HG22 | 1.92 | 0.51 |
| 41:UN:141:GLY:O | 41:UN:184:ASN:ND2 | 2.41 | 0.51 |
| 40:VH:256:GLN:HE21 | 41:VP:397:TRP:HZ2 | 1.56 | 0.51 |
| 41:WB:309:ARG:NH1 | 41:WB:339:SER:O | 2.43 | 0.51 |
| 40:WF:88:HIS:HB3 | 40:WF:91:GLN:HG3 | 1.90 | 0.51 |
| 40:WG:70:LEU:HD22 | 40:WG:110:ILE:HG22 | 1.91 | 0.51 |
| 40:WI:100:ALA:HA | 41:WP:252:LYS:HB2 | 1.92 | 0.51 |
| 41:WQ:100:ASN:HB3 | 41:WQ:103:LYS:HB3 | 1.92 | 0.51 |
| 8:1X:168:LYS:O | 8:1X:171:ALA:HB3 | 2.11 | 0.51 |
| 11:2J:193:ARG:HH22 | 11:2J:248:LYS:HZ2 | 1.57 | 0.51 |
| 11:2J:251:TYR:O | 11:2J:252:ILE:HG23 | 2.10 | 0.51 |
| 12:2O:85:LEU:HD23 | 12:2O:87:HIS:H | 1.73 | 0.51 |
| 13:2W:139:PHE:HA | 13:2W:142:ARG:HG3 | 1.92 | 0.51 |
| 17:3O:99:TRP:HD1 | 17:3P:208:ILE:HG13 | 1.76 | 0.51 |
| 17:3O:160:ILE:HD11 | 17:3O:304:THR:HG23 | 1.93 | 0.51 |
| 17:3O:426:GLU:HG3 | 17:3O:427:VAL:N | 2.25 | 0.51 |
| 21:4D:477:SER:HB3 | 21:4D:482:PRO:HA | 1.93 | 0.51 |
| 21:4F:309:PRO:HB3 | 41:CM:361:LEU:HG | 1.93 | 0.51 |
| 22:4J:526:ASP:O | 22:4J:529:THR:OG1 | 2.25 | 0.51 |
| 31:5I:516:GLU:O | 31:5I:520:LYS:HG2 | 2.09 | 0.51 |
| 36:5Y:222:LEU:HD23 | 41:KP:160:PRO:HB3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AN:173:PRO:HB3 | 41:AN:380:ARG:HD3 | 1.92 | 0.51 |
| 41:AP:268:PRO:HG2 | 41:AP:300:MET:HB2 | 1.91 | 0.51 |
| 40:BA:210:TYR:CD1 | 41:BN:324:LYS:HE3 | 2.45 | 0.51 |
| 40:BA:298:PRO:HA | 40:BA:301:GLN:HE22 | 1.74 | 0.51 |
| 40:BF:15:GLN:HA | 40:BF:18:ASN:HD22 | 1.76 | 0.51 |
| 40:BI:64:ARG:HG3 | 40:BI:125:LEU:HD22 | 1.92 | 0.51 |
| 41:BM:289:LEU:O | 41:BM:293:MET:HB2 | 2.10 | 0.51 |
| 40:CA:420:ALA:O | 40:CA:424:MET:HE2 | 2.10 | 0.51 |
| 40:CE:20:CYS:HA | 40:CE:232:SER:HB2 | 1.92 | 0.51 |
| 40:CE:95:GLY:HA2 | 40:CE:114:LEU:HD11 | 1.92 | 0.51 |
| 40:CH:109:THR:HG21 | 40:CH:410:GLU:HG3 | 1.92 | 0.51 |
| 41:CL:386:THR:O | 41:CL:387:ALA:C | 2.48 | 0.51 |
| 40:DA:141:PHE:HB2 | 40:DA:173:PRO:HD3 | 1.92 | 0.51 |
| 40:DA:414:GLU:O | 40:DA:415:GLY:C | 2.49 | 0.51 |
| 41:DB:112:LEU:HD23 | 41:DB:147:MET:HE1 | 1.92 | 0.51 |
| 41:DB:322:SER:OG | 41:DB:323:MET:N | 2.42 | 0.51 |
| 40:DF:12:ALA:HB2 | 42:DF:501:GTP:C8 | 2.46 | 0.51 |
| 40:DF:16:ILE:HD11 | 40:DF:138:PHE:HB2 | 1.92 | 0.51 |
| 40:DG:329:ASN:HB2 | 41:DO:175:VAL:HG11 | 1.92 | 0.51 |
| 40:DH:183:GLU:O | 40:DH:184:PRO:C | 2.49 | 0.51 |
| 41:DL:7:LEU:HB2 | 41:DL:135:LEU:HA | 1.92 | 0.51 |
| 41:DP:260:PHE:HB2 | 41:DP:263:LEU:HD12 | 1.91 | 0.51 |
| 40:EE:406:TRP:HE1 | 41:EL:258:VAL:HB | 1.76 | 0.51 |
| 41:EO:383:GLU:HA | 41:EO:386:THR:HG22 | 1.92 | 0.51 |
| 40:FA:101:ASN:HA | 40:FA:144:GLY:H | 1.75 | 0.51 |
| 40:FE:398:TYR:O | 40:FE:401:ARG:NH1 | 2.43 | 0.51 |
| 41:FM:172:SER:OG | 41:FM:175:VAL:O | 2.28 | 0.51 |
| 40:GI:88:HIS:CD2 | 40:GI:89:PRO:HD2 | 2.46 | 0.51 |
| 40:GI:100:ALA:O | 40:GI:101:ASN:C | 2.49 | 0.51 |
| 40:GI:162:GLY:O | 40:GI:163:LYS:C | 2.49 | 0.51 |
| 40:GI:222:PRO:HD2 | 41:GP:324:LYS:HZ1 | 1.75 | 0.51 |
| 40:GI:287:SER:O | 40:GI:291:ILE:HG23 | 2.09 | 0.51 |
| 41:GM:8:GLN:HE21 | 41:GM:14:ASN:HA | 1.75 | 0.51 |
| 41:GN:355:ASP:O | 41:GN:356:ILE:C | 2.48 | 0.51 |
| 41:GO:105:HIS:CD2 | 41:GO:150:LEU:HB2 | 2.45 | 0.51 |
| 41:GP:248:ALA:HA | 41:GP:252:LYS:HD3 | 1.92 | 0.51 |
| 40:HA:196:GLU:OE1 | 40:HA:196:GLU:N | 2.40 | 0.51 |
| 40:HE:81:GLY:O | 40:HE:84:ARG:HB3 | 2.11 | 0.51 |
| 40:HE:290:GLU:O | 40:HE:291:ILE:C | 2.49 | 0.51 |
| 40:HE:381:THR:O | 40:HE:382:ALA:C | 2.49 | 0.51 |
| 41:HN:36:TYR:CZ | 41:HN:44:LEU:HD22 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HQ:171:PRO:HB3 | 41:HQ:181:GLU:HB3 | 1.92 | 0.51 |
| 40:II:141:PHE:HB2 | 40:II:173:PRO:HD3 | 1.93 | 0.51 |
| 41:JN:6:HIS:O | 41:JN:63:ALA:HA | 2.11 | 0.51 |
| 41:JN:236:VAL:HG22 | 41:JN:368:ILE:HD11 | 1.91 | 0.51 |
| 40:KA:6:SER:O | 40:KA:65:ALA:HA | 2.11 | 0.51 |
| 40:KA:53:PHE:HB3 | 40:KA:61:HIS:HB3 | 1.92 | 0.51 |
| 41:KB:27:GLU:OE1 | 41:KB:318:ARG:NH2 | 2.42 | 0.51 |
| 40:KH:238:ILE:HD13 | 40:KH:377:LEU:HD11 | 1.91 | 0.51 |
| 41:KM:318:ARG:HG3 | 41:KM:354:CYS:HB3 | 1.92 | 0.51 |
| 42:LB:502:GTP:HN1 | 40:LG:228:ASN:HD21 | 1.56 | 0.51 |
| 40:LD:88:HIS:CD2 | 40:LD:90:GLU:H | 2.28 | 0.51 |
| 40:LG:363:VAL:O | 40:LG:365:GLY:N | 2.43 | 0.51 |
| 41:LL:178:THR:HB | 41:LL:181:GLU:HB3 | 1.92 | 0.51 |
| 40:MF:15:GLN:HB3 | 42:MM:501:GTP:C6 | 2.46 | 0.51 |
| 41:MN:342:VAL:HG23 | 41:MN:345:ILE:HG22 | 1.91 | 0.51 |
| 40:NH:123:ARG:HH22 | 40:OH:338:LYS:HZ2 | 1.58 | 0.51 |
| 41:OB:2:ARG:HD2 | 41:OB:240:LEU:HB3 | 1.92 | 0.51 |
| 40:OE:102:ASN:HB3 | 40:OE:105:ARG:HB3 | 1.93 | 0.51 |
| 41:OO:21:TRP:O | 41:OO:25:SER:OG | 2.25 | 0.51 |
| 40:PA:437:ASP:OD1 | 40:PA:437:ASP:N | 2.43 | 0.51 |
| 41:PB:87:PRO:HA | 41:PB:90:PHE:HD2 | 1.74 | 0.51 |
| 41:PL:31:ASP:HB3 | 41:PL:34:GLY:H | 1.75 | 0.51 |
| 41:PN:105:HIS:CD2 | 41:PN:150:LEU:HB2 | 2.45 | 0.51 |
| 41:PP:73:MET:HA | 41:PP:76:VAL:HG12 | 1.92 | 0.51 |
| 41:QB:73:MET:HB3 | 41:QB:77:ARG:HH22 | 1.76 | 0.51 |
| 41:QB:192:LEU:O | 41:QB:193:VAL:C | 2.49 | 0.51 |
| 40:QE:80:THR:HA | 40:QE:84:ARG:HH11 | 1.76 | 0.51 |
| 40:QH:325:PRO:HA | 40:QH:328:VAL:HG22 | 1.93 | 0.51 |
| 41:QM:101:TRP:N | 41:QM:184:ASN:OD1 | 2.43 | 0.51 |
| 41:QP:192:LEU:CB | 41:QP:196:THR:HB | 2.40 | 0.51 |
| 41:RO:310:TYR:HA | 41:RO:371:SER:HA | 1.92 | 0.51 |
| 41:SO:101:TRP:CD1 | 41:SO:146:GLY:HA2 | 2.45 | 0.51 |
| 41:SO:412:GLU:HG3 | 41:SO:416:ASN:HD21 | 1.76 | 0.51 |
| 40:TG:209:ILE:HA | 40:TG:212:ILE:HG22 | 1.93 | 0.51 |
| 41:TN:222:TYR:O | 41:TN:226:ASN:ND2 | 2.43 | 0.51 |
| 40:UA:320:ARG:HD3 | 40:UA:358:GLN:HG3 | 1.92 | 0.51 |
| 40:UE:205:ASP:HB3 | 40:UE:303:VAL:HA | 1.91 | 0.51 |
| 40:UH:217:LEU:HA | 40:UH:277:SER:HB2 | 1.93 | 0.51 |
| 41:VB:245:GLN:N | 41:VB:245:GLN:OE1 | 2.43 | 0.51 |
| 40:WA:251:ASP:H | 40:WA:254:GLU:HB2 | 1.75 | 0.51 |
| 41:WB:311:LEU:HD12 | 41:WB:342:VAL:HG11 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:WE:386:ALA:HA | 40:WE:389:ARG:HD2 | 1.91 | 0.51 |
| 40:WH:319:TYR:HB2 | 40:WH:355:ILE:HG22 | 1.93 | 0.51 |
| 40:WI:210:TYR:O | 41:WP:324:LYS:NZ | 2.44 | 0.51 |
| 40:WI:406:TRP:HE1 | 41:WP:258:VAL:HG23 | 1.76 | 0.51 |
| 41:WM:142:GLY:O | 41:WM:143:THR:C | 2.49 | 0.51 |
| 41:WM:254:ALA:O | 41:WM:258:VAL:HG22 | 2.09 | 0.51 |
| 13:2T:38:THR:HA | 13:2T:44:SER:O | 2.11 | 0.51 |
| 13:2X:151:THR:HG21 | 13:2X:167:PHE:CZ | 2.45 | 0.51 |
| 17:3O:107:TYR:O | 17:3O:111:ASN:ND2 | 2.43 | 0.51 |
| 17:3R:222:GLU:OE1 | 17:3R:343:VAL:HG21 | 2.10 | 0.51 |
| 21:4D:43:PRO:HG2 | 41:LN:83:GLN:HE22 | 1.74 | 0.51 |
| 22:4I:99:ILE:HB | 22:4I:194:ASP:HB3 | 1.91 | 0.51 |
| 22:4I:509:VAL:HB | 22:4I:597:GLN:HG2 | 1.93 | 0.51 |
| 22:4I:677:LEU:O | 22:4I:678:LEU:C | 2.48 | 0.51 |
| 22:4J:662:CYS:HA | 22:4J:667:LEU:HD13 | 1.93 | 0.51 |
| 22:4K:654:PRO:HA | 22:4K:686:LYS:O | 2.11 | 0.51 |
| 22:4K:669:PHE:HB3 | 22:4K:673:LEU:HB3 | 1.92 | 0.51 |
| 23:4R:240:LEU:CA | 23:4R:266:HIS:HA | 2.37 | 0.51 |
| 26:4V:64:ASN:HB3 | 26:4V:75:LEU:HD13 | 1.91 | 0.51 |
| 31:5I:325:THR:O | 41:IN:276:ARG:NH2 | 2.43 | 0.51 |
| 31:5I:502:ASN:HA | 41:IP:221:THR:HG21 | 1.91 | 0.51 |
| 41:AL:273:LEU:O | 41:AL:292:GLN:NE2 | 2.43 | 0.51 |
| 41:AM:36:TYR:OH | 41:AM:40:SER:O | 2.29 | 0.51 |
| 41:AP:172:SER:OG | 41:AP:175:VAL:O | 2.29 | 0.51 |
| 41:BB:245:GLN:HE21 | 41:BB:353:VAL:HG11 | 1.74 | 0.51 |
| 40:BF:27:GLU:HA | 40:BF:361:THR:HG21 | 1.93 | 0.51 |
| 40:BF:217:LEU:HB3 | 40:BF:219:ILE:HG12 | 1.90 | 0.51 |
| 41:BM:215:LEU:O | 41:BM:216:LYS:C | 2.49 | 0.51 |
| 41:DB:372:THR:HA | 41:DB:422:VAL:HG22 | 1.93 | 0.51 |
| 40:DE:21:TRP:CZ2 | 40:DE:65:ALA:HB2 | 2.45 | 0.51 |
| 40:DE:201:ALA:O | 40:DE:203:MET:N | 2.43 | 0.51 |
| 40:DG:213:CYS:HA | 40:DG:217:LEU:HD23 | 1.92 | 0.51 |
| 40:DH:125:LEU:O | 40:DH:126:ALA:C | 2.49 | 0.51 |
| 40:DI:273:ALA:HB3 | 40:DI:274:PRO:CD | 2.37 | 0.51 |
| 41:DN:188:SER:O | 41:DN:192:LEU:N | 2.43 | 0.51 |
| 41:EB:11:GLN:NE2 | 41:EB:15:GLN:OE1 | 2.43 | 0.51 |
| 40:EI:416:GLU:O | 40:EI:417:PHE:C | 2.49 | 0.51 |
| 41:EO:95:SER:OG | 41:EO:96:GLY:N | 2.43 | 0.51 |
| 40:FA:31:GLN:HB2 | 40:FA:37:PRO:HD3 | 1.93 | 0.51 |
| 40:FA:109:THR:OG1 | 40:FA:110:ILE:N | 2.43 | 0.51 |
| 40:FE:8:HIS:CD2 | 40:FE:17:GLY:HA3 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FG:138:PHE:HE2 | 40:FG:235:VAL:HG21 | 1.75 | 0.51 |
| 41:FO:54:ALA:HB3 | 41:FO:58:LYS:HB3 | 1.93 | 0.51 |
| 40:GA:16:ILE:CA | 40:GA:228:ASN:HD22 | 2.24 | 0.51 |
| 41:GB:25:SER:OG | 41:GB:51:TYR:OH | 2.28 | 0.51 |
| 40:GF:406:TRP:HE1 | 41:GM:258:VAL:HG23 | 1.75 | 0.51 |
| 40:GH:188:ILE:HD12 | 40:GH:424:MET:HG3 | 1.91 | 0.51 |
| 41:HO:272:PRO:HG3 | 41:HO:364:SER:HA | 1.92 | 0.51 |
| 40:IA:402:ALA:HA | 41:IN:260:PHE:HE2 | 1.75 | 0.51 |
| 40:IE:139:HIS:NE2 | 40:IE:168:GLU:OE2 | 2.36 | 0.51 |
| 40:II:371:GLN:HB2 | 40:II:372:ARG:HD2 | 1.92 | 0.51 |
| 41:IP:6:HIS:O | 41:IP:63:ALA:HA | 2.10 | 0.51 |
| 41:IP:207:LEU:HG | 41:IP:225:LEU:HD22 | 1.92 | 0.51 |
| 40:JD:211:ASP:O | 40:JD:215:ARG:HG3 | 2.10 | 0.51 |
| 40:JD:356:ASN:OD1 | 40:JD:357:TYR:N | 2.43 | 0.51 |
| 40:JE:141:PHE:HB2 | 40:JE:173:PRO:HD3 | 1.92 | 0.51 |
| 40:JG:141:PHE:HB2 | 40:JG:173:PRO:HD3 | 1.92 | 0.51 |
| 41:JO:248:ALA:HA | 41:JO:252:LYS:HG2 | 1.92 | 0.51 |
| 40:KD:252:LEU:HA | 40:KD:255:PHE:HD2 | 1.75 | 0.51 |
| 40:KG:241:SER:HA | 40:KG:356:ASN:HD21 | 1.75 | 0.51 |
| 40:KH:254:GLU:HA | 40:KH:257:THR:HG22 | 1.91 | 0.51 |
| 41:KP:39:ASP:OD1 | 41:KP:39:ASP:N | 2.43 | 0.51 |
| 40:MH:252:LEU:HA | 40:MH:255:PHE:CD2 | 2.45 | 0.51 |
| 41:MO:334:GLN:NE2 | 41:MO:349:VAL:HG23 | 2.26 | 0.51 |
| 40:NF:208:ALA:HB2 | 40:NF:304:LYS:HG2 | 1.92 | 0.51 |
| 40:NG:67:PHE:HB3 | 40:NG:75:ILE:HD12 | 1.91 | 0.51 |
| 40:OA:235:VAL:HA | 40:OA:238:ILE:HG22 | 1.93 | 0.51 |
| 40:OE:407:TYR:HD2 | 40:OE:417:PHE:HZ | 1.58 | 0.51 |
| 40:OF:296:PHE:HD2 | 40:OF:341:ILE:HD13 | 1.74 | 0.51 |
| 40:OH:163:LYS:HB2 | 40:OH:164:LYS:HE2 | 1.93 | 0.51 |
| 41:ON:6:HIS:HA | 41:ON:134:GLN:HB2 | 1.93 | 0.51 |
| 41:ON:153:SER:HA | 41:ON:195:ASN:HD21 | 1.76 | 0.51 |
| 41:ON:304:ASP:HB3 | 41:ON:307:HIS:HB2 | 1.92 | 0.51 |
| 41:PB:271:ALA:HB1 | 41:PB:292:GLN:HG2 | 1.92 | 0.51 |
| 40:PD:319:TYR:CE2 | 40:PD:328:VAL:HG22 | 2.46 | 0.51 |
| 40:PE:356:ASN:OD1 | 40:PE:357:TYR:N | 2.44 | 0.51 |
| 40:PG:169:PHE:HE1 | 40:PG:202:PHE:HD2 | 1.57 | 0.51 |
| 40:QE:224:TYR:HB3 | 42:QL:501:GTP:N1 | 2.26 | 0.51 |
| 40:QH:179:THR:OG1 | 40:QH:183:GLU:OE2 | 2.25 | 0.51 |
| 40:RA:288:VAL:HA | 40:RA:291:ILE:HG12 | 1.93 | 0.51 |
| 40:RF:315:CYS:HA | 40:RF:377:LEU:O | 2.09 | 0.51 |
| 41:RM:91:VAL:HG11 | 41:RM:116:VAL:HG22 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RN:292:GLN:O | 41:RN:298:ASN:ND2 | 2.37 | 0.51 |
| 41:RP:7:LEU:HD23 | 41:RP:64:VAL:HB | 1.92 | 0.51 |
| 40:SA:20:CYS:HA | 40:SA:232:SER:HB2 | 1.92 | 0.51 |
| 40:SE:329:ASN:HB3 | 41:SM:175:VAL:HG11 | 1.93 | 0.51 |
| 40:TE:2:ARG:HD3 | 40:TE:242:LEU:HB2 | 1.91 | 0.51 |
| 40:TE:47:ASP:O | 40:TE:50:ASN:ND2 | 2.24 | 0.51 |
| 40:TH:259:LEU:O | 40:TH:379:ASN:ND2 | 2.43 | 0.51 |
| 41:TM:262:ARG:NH1 | 41:TM:417:ASP:OD2 | 2.36 | 0.51 |
| 41:UB:316:VAL:HG23 | 41:UB:366:THR:HB | 1.92 | 0.51 |
| 40:UF:146:GLY:O | 40:UF:147:SER:C | 2.48 | 0.51 |
| 40:UI:73:THR:O | 40:UI:74:VAL:C | 2.49 | 0.51 |
| 40:UI:312:TYR:HD1 | 40:UI:380:THR:HB | 1.76 | 0.51 |
| 41:UN:372:THR:HA | 41:UN:375:GLN:HE22 | 1.74 | 0.51 |
| 41:VQ:7:LEU:HD23 | 41:VQ:64:VAL:HB | 1.92 | 0.51 |
| 41:WM:12:CYS:HB3 | 41:WM:138:SER:HB2 | 1.91 | 0.51 |
| 41:WM:47:ILE:HG13 | 41:WM:51:TYR:HB2 | 1.92 | 0.51 |
| 41:WN:244:GLY:HA2 | 41:WN:355:ASP:HB3 | 1.91 | 0.51 |
| 41:WP:194:GLU:O | 41:WP:195:ASN:ND2 | 2.44 | 0.51 |
| 41:WQ:253:LEU:O | 41:WQ:257:MET:HB2 | 2.09 | 0.51 |
| 7:1S:371:THR:HB | 10:2F:133:ILE:HG13 | 1.90 | 0.51 |
| 7:1U:530:GLU:HB2 | 7:1U:537:ILE:HD11 | 1.91 | 0.51 |
| 8:1W:499:GLN:NE2 | 8:1W:503:GLU:OE2 | 2.41 | 0.51 |
| 8:1X:321:GLN:HA | 8:1X:324:LYS:HG2 | 1.93 | 0.51 |
| 12:2O:87:HIS:NE2 | 40:WF:126:ALA:O | 2.43 | 0.51 |
| 12:2R:109:LEU:HD23 | 12:2R:145:VAL:HG11 | 1.92 | 0.51 |
| 13:2X:42:ILE:HD12 | 13:2X:183:LEU:HG | 1.93 | 0.51 |
| 17:3P:181:LEU:HG | 17:3P:237:LEU:HD12 | 1.93 | 0.51 |
| 17:3R:205:ARG:HB3 | 17:3R:209:ASP:CG | 2.31 | 0.51 |
| 17:3R:327:ASN:O | 17:3R:330:VAL:N | 2.43 | 0.51 |
| 21:4E:498:VAL:O | 21:4E:499:PHE:C | 2.48 | 0.51 |
| 22:4J:530:LEU:HD13 | 22:4J:604:ARG:HD2 | 1.92 | 0.51 |
| 22:4K:678:LEU:O | 22:4K:688:ILE:HD11 | 2.11 | 0.51 |
| 23:4M:116:ALA:O | 23:4M:117:LEU:C | 2.48 | 0.51 |
| 23:4N:195:ARG:C | 23:4N:197:LEU:H | 2.14 | 0.51 |
| 26:4W:176:LEU:HD13 | 26:4W:193:ARG:HH22 | 1.74 | 0.51 |
| 31:5I:340:PHE:CE2 | 41:HN:44:LEU:HG | 2.46 | 0.51 |
| 40:AA:229:ARG:HD3 | 40:AA:363:VAL:HG21 | 1.92 | 0.51 |
| 40:AF:188:ILE:HG22 | 40:AF:420:ALA:HB1 | 1.91 | 0.51 |
| 41:AN:267:MET:HG2 | 41:AN:301:ALA:HB3 | 1.92 | 0.51 |
| 41:AO:262:ARG:O | 41:AO:263:LEU:C | 2.48 | 0.51 |
| 40:BE:99:ALA:HB3 | 40:BE:145:THR:HG22 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BF:247:ALA:HB3 | 40:BF:355:ILE:HB | 1.92 | 0.51 |
| 40:BG:168:GLU:HB2 | 40:BG:201:ALA:HA | 1.93 | 0.51 |
| 40:BH:26:LEU:HD22 | 40:BH:363:VAL:HG13 | 1.93 | 0.51 |
| 40:BI:396:LEU:HD13 | 41:BP:346:PRO:HD3 | 1.93 | 0.51 |
| 40:CE:171:ILE:HG21 | 42:CE:501:GTP:H1' | 1.91 | 0.51 |
| 40:CH:288:VAL:HA | 40:CH:291:ILE:HG12 | 1.93 | 0.51 |
| 40:CI:11:GLN:N | 42:CI:501:GTP:O1B | 2.39 | 0.51 |
| 41:CL:3:GLU:HB3 | 41:CL:62:ARG:CZ | 2.40 | 0.51 |
| 41:CL:118:ASP:OD1 | 41:CL:119:VAL:N | 2.43 | 0.51 |
| 41:CL:188:SER:O | 41:CL:189:VAL:C | 2.48 | 0.51 |
| 41:CL:240:LEU:HD11 | 41:CL:250:LEU:H | 1.76 | 0.51 |
| 41:CM:263:LEU:HD11 | 41:CM:425:ARG:HH11 | 1.75 | 0.51 |
| 40:DH:12:ALA:HA | 40:DH:15:GLN:HE21 | 1.73 | 0.51 |
| 41:EB:313:VAL:HB | 41:EB:349:VAL:HG22 | 1.93 | 0.51 |
| 40:EE:108:TYR:O | 40:EE:112:LYS:NZ | 2.37 | 0.51 |
| 40:EH:191:THR:O | 40:EH:192:HIS:C | 2.47 | 0.51 |
| 41:EN:256:ASN:HB2 | 41:EN:350:LYS:HD2 | 1.93 | 0.51 |
| 41:EO:16:ILE:HD11 | 41:EO:136:THR:HB | 1.91 | 0.51 |
| 41:EP:323:MET:SD | 41:EP:323:MET:N | 2.84 | 0.51 |
| 40:FG:180:ALA:HB3 | 40:FG:183:GLU:HG3 | 1.92 | 0.51 |
| 41:FM:61:PRO:HD3 | 41:FM:84:ILE:HG12 | 1.92 | 0.51 |
| 41:FP:6:HIS:O | 41:FP:63:ALA:HA | 2.11 | 0.51 |
| 40:GA:23:LEU:HD11 | 40:GA:233:GLN:NE2 | 2.26 | 0.51 |
| 41:GN:293:MET:HG3 | 41:GN:367:PHE:HB2 | 1.93 | 0.51 |
| 41:GP:323:MET:O | 41:GP:327:ASP:HB2 | 2.10 | 0.51 |
| 41:IN:392:LYS:HD2 | 41:IN:395:LEU:HD23 | 1.92 | 0.51 |
| 41:IP:141:GLY:O | 41:IP:145:SER:OG | 2.24 | 0.51 |
| 40:JG:27:GLU:OE2 | 40:JG:320:ARG:NH2 | 2.41 | 0.51 |
| 41:JL:382:SER:OG | 41:JL:412:GLU:OE1 | 2.27 | 0.51 |
| 40:KH:124:LYS:NZ | 40:LH:297:GLU:OE1 | 2.43 | 0.51 |
| 41:KO:237:THR:HG22 | 41:KO:250:LEU:HD21 | 1.91 | 0.51 |
| 41:KP:54:ALA:HB3 | 41:KP:58:LYS:HB2 | 1.91 | 0.51 |
| 41:LB:103:LYS:O | 41:LB:107:THR:OG1 | 2.29 | 0.51 |
| 41:LL:313:VAL:HB | 41:LL:349:VAL:HG22 | 1.90 | 0.51 |
| 40:MH:214:ARG:HH12 | 41:MO:324:LYS:HB3 | 1.76 | 0.51 |
| 41:MP:31:ASP:OD2 | 41:MP:35:THR:OG1 | 2.23 | 0.51 |
| 40:ND:281:ALA:O | 40:ND:282:TYR:C | 2.49 | 0.51 |
| 40:OD:51:THR:HG21 | 40:OD:243:ARG:HG3 | 1.93 | 0.51 |
| 40:OD:276:ILE:HD11 | 40:OD:280:LYS:HG3 | 1.91 | 0.51 |
| 40:OE:206:ASN:OD1 | 42:OL:501:GTP:O2' | 2.26 | 0.51 |
| 40:OG:141:PHE:HB2 | 40:OG:173:PRO:HD3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OL:132:GLY:CA | 41:OL:163:ILE:O | 2.53 | 0.51 |
| 40:PE:70:LEU:HD23 | 40:PE:114:LEU:HD12 | 1.93 | 0.51 |
| 40:PG:285:GLN:HG3 | 40:PG:287:SER:HB3 | 1.91 | 0.51 |
| 40:PH:88:HIS:CE1 | 40:PH:90:GLU:HB2 | 2.45 | 0.51 |
| 41:PN:237:THR:HG22 | 41:PN:250:LEU:HD21 | 1.91 | 0.51 |
| 40:QA:324:VAL:HG11 | 41:QB:219:THR:HB | 1.93 | 0.51 |
| 41:QB:222:TYR:O | 41:QB:223:GLY:C | 2.48 | 0.51 |
| 40:QF:68:VAL:HG12 | 40:QF:93:ILE:HB | 1.91 | 0.51 |
| 40:QH:180:ALA:HB3 | 40:QH:183:GLU:HG3 | 1.90 | 0.51 |
| 40:QH:224:TYR:HD1 | 40:QH:227:LEU:HD12 | 1.75 | 0.51 |
| 41:QL:323:MET:SD | 41:QL:323:MET:N | 2.69 | 0.51 |
| 41:QP:181:GLU:O | 41:QP:182:PRO:C | 2.49 | 0.51 |
| 41:QP:188:SER:O | 41:QP:189:VAL:C | 2.49 | 0.51 |
| 41:QP:269:GLY:O | 41:QP:270:PHE:HB2 | 2.10 | 0.51 |
| 40:RE:191:THR:HG21 | 40:RE:387:TRP:HZ3 | 1.75 | 0.51 |
| 40:RG:207:GLU:HA | 40:RG:210:TYR:HB2 | 1.92 | 0.51 |
| 40:SG:21:TRP:HZ3 | 40:SG:63:PRO:HB3 | 1.75 | 0.51 |
| 40:SH:284:GLU:HB2 | 40:SH:286:LEU:HD22 | 1.92 | 0.51 |
| 41:SO:386:THR:O | 41:SO:387:ALA:C | 2.48 | 0.51 |
| 40:TA:133:GLN:O | 40:TA:165:SER:OG | 2.21 | 0.51 |
| 40:TF:70:LEU:HD23 | 40:TF:114:LEU:HD12 | 1.92 | 0.51 |
| 40:TF:212:ILE:HD13 | 40:TF:300:ASN:HA | 1.92 | 0.51 |
| 41:UB:28:HIS:O | 41:UB:43:GLN:NE2 | 2.43 | 0.51 |
| 40:UH:169:PHE:HZ | 40:UH:238:ILE:HG21 | 1.75 | 0.51 |
| 41:UN:323:MET:HB2 | 41:UN:326:VAL:HB | 1.93 | 0.51 |
| 41:UO:86:ARG:HH11 | 41:VP:282:ARG:HH21 | 1.58 | 0.51 |
| 41:VB:31:ASP:OD1 | 41:VB:35:THR:N | 2.43 | 0.51 |
| 40:VJ:251:ASP:H | 40:VJ:254:GLU:HB2 | 1.76 | 0.51 |
| 41:VO:16:ILE:HD11 | 41:VO:229:VAL:HG11 | 1.93 | 0.51 |
| 40:WG:312:TYR:HA | 40:WG:380:THR:HG22 | 1.93 | 0.51 |
| 40:WH:405:HIS:CD2 | 41:WO:261:PRO:HD3 | 2.45 | 0.51 |
| 41:WM:70:PRO:HB3 | 41:WM:92:PHE:HE2 | 1.76 | 0.51 |
| 41:WN:331:LEU:HG | 41:WN:332:ASN:N | 2.25 | 0.51 |
| 41:WO:202:ILE:HG21 | 41:WO:229:VAL:HG22 | 1.92 | 0.51 |
| 7:1T:568:LEU:HD11 | 7:1T:584:VAL:HG12 | 1.92 | 0.51 |
| 12:2O:216:GLN:HE21 | 41:WN:118:ASP:CG | 2.14 | 0.51 |
| 13:2V:97:LYS:O | 13:2V:98:ASN:C | 2.48 | 0.51 |
| 18:3U:335:ASN:ND2 | 18:3V:81:SER:OG | 2.44 | 0.51 |
| 21:4D:176:ILE:HB | 21:4D:181:PHE:HE2 | 1.76 | 0.51 |
| 21:4D:420:LEU:HD11 | 21:4D:515:TYR:HD2 | 1.74 | 0.51 |
| 21:4E:442:TYR:HD2 | 21:4E:449:ILE:HG13 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4E:491:PHE:O | 21:4E:492:ILE:C | 2.49 | 0.51 |
| 22:4J:457:PHE:HB2 | 22:4J:462:THR:HB | 1.90 | 0.51 |
| 31:5I:685:GLU:O | 31:5I:712:LEU:HB2 | 2.11 | 0.51 |
| 40:AA:168:GLU:HB2 | 40:AA:201:ALA:HA | 1.91 | 0.51 |
| 40:AF:208:ALA:HB2 | 40:AF:304:LYS:HG2 | 1.91 | 0.51 |
| 41:BB:224:ASP:C | 41:BB:226:ASN:H | 2.14 | 0.51 |
| 41:BB:371:SER:C | 41:BB:373:ALA:H | 2.14 | 0.51 |
| 40:BE:271:THR:HG23 | 40:BE:301:GLN:HA | 1.92 | 0.51 |
| 40:BI:5:ILE:HG13 | 40:BI:132:LEU:HD13 | 1.92 | 0.51 |
| 40:BI:435:GLY:O | 40:BI:436:MET:C | 2.48 | 0.51 |
| 41:BO:70:PRO:HD3 | 41:BO:94:GLN:HA | 1.91 | 0.51 |
| 41:BP:294:PHE:CE1 | 41:BP:313:VAL:HG11 | 2.45 | 0.51 |
| 41:BP:334:GLN:HE22 | 41:BP:347:ASN:HA | 1.76 | 0.51 |
| 41:CB:238:THR:HG23 | 41:CB:318:ARG:HD3 | 1.93 | 0.51 |
| 40:CI:342:GLN:NE2 | 40:CI:343:PHE:O | 2.44 | 0.51 |
| 41:CL:108:GLU:O | 41:CL:109:GLY:C | 2.49 | 0.51 |
| 41:CN:139:LEU:O | 41:CN:141:GLY:N | 2.44 | 0.51 |
| 41:CN:284:LEU:HD23 | 41:CN:363:MET:HB2 | 1.91 | 0.51 |
| 41:DB:119:VAL:O | 41:DB:120:VAL:C | 2.49 | 0.51 |
| 40:DE:259:LEU:HD21 | 40:DE:316:CYS:N | 2.26 | 0.51 |
| 40:DG:204:VAL:HG23 | 40:DG:302:MET:HB3 | 1.92 | 0.51 |
| 41:DN:21:TRP:HZ3 | 41:DN:50:TYR:HB3 | 1.76 | 0.51 |
| 41:DN:303:CYS:O | 41:DN:303:CYS:SG | 2.68 | 0.51 |
| 40:EE:169:PHE:HE1 | 40:EE:235:VAL:HG22 | 1.76 | 0.51 |
| 40:EH:99:ALA:HA | 40:EH:110:ILE:CD1 | 2.41 | 0.51 |
| 40:EI:123:ARG:HA | 40:EI:161:TYR:HE2 | 1.76 | 0.51 |
| 40:EI:400:LYS:HE2 | 41:EP:260:PHE:CZ | 2.46 | 0.51 |
| 41:EN:10:GLY:O | 41:EN:14:ASN:ND2 | 2.33 | 0.51 |
| 40:FA:288:VAL:O | 40:FA:291:ILE:HG12 | 2.11 | 0.51 |
| 40:FI:223:THR:HG23 | 40:FI:225:THR:H | 1.76 | 0.51 |
| 40:GA:21:TRP:CZ2 | 40:GA:65:ALA:HB2 | 2.45 | 0.51 |
| 41:GB:257:MET:HG3 | 41:GB:266:PHE:CE1 | 2.46 | 0.51 |
| 40:GE:296:PHE:HE2 | 40:GE:335:ILE:HG13 | 1.75 | 0.51 |
| 41:GO:139:LEU:HD12 | 41:GO:170:VAL:HG12 | 1.93 | 0.51 |
| 40:HF:224:TYR:O | 40:HF:228:ASN:ND2 | 2.44 | 0.51 |
| 40:HG:241:SER:OG | 40:HG:249:ASN:OD1 | 2.25 | 0.51 |
| 40:IA:210:TYR:CD2 | 41:IN:324:LYS:HE3 | 2.40 | 0.51 |
| 40:IH:97:GLU:OE2 | 41:IO:251:ARG:NH2 | 2.35 | 0.51 |
| 40:II:20:CYS:HA | 40:II:232:SER:HB2 | 1.93 | 0.51 |
| 40:JF:88:HIS:HB3 | 40:JF:91:GLN:HB2 | 1.91 | 0.51 |
| 41:JM:388:MET:O | 41:JM:389:PHE:C | 2.48 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KF:319:TYR:HB3 | 40:KF:323:VAL:HG11 | 1.92 | 0.51 |
| 40:KG:235:VAL:HA | 40:KG:238:ILE:HG22 | 1.91 | 0.51 |
| 41:KL:98:GLY:O | 41:KL:99:ASN:C | 2.48 | 0.51 |
| 41:KO:171:PRO:HB3 | 41:KO:181:GLU:HG3 | 1.92 | 0.51 |
| 41:KP:6:HIS:O | 41:KP:63:ALA:HA | 2.09 | 0.51 |
| 40:ME:141:PHE:HB2 | 40:ME:173:PRO:HD3 | 1.92 | 0.51 |
| 40:MH:140:SER:O | 40:MH:141:PHE:C | 2.48 | 0.51 |
| 40:MH:210:TYR:CE1 | 40:MH:222:PRO:HB2 | 2.45 | 0.51 |
| 41:MO:171:PRO:HB3 | 41:MO:181:GLU:HG3 | 1.92 | 0.51 |
| 41:NB:318:ARG:HB3 | 41:NB:357:PRO:HA | 1.93 | 0.51 |
| 40:NE:228:ASN:ND2 | 42:NE:501:GTP:HN1 | 2.08 | 0.51 |
| 40:OA:269:LEU:HD22 | 40:OA:303:VAL:HG21 | 1.92 | 0.51 |
| 40:OD:84:ARG:HG3 | 40:OD:85:GLN:H | 1.75 | 0.51 |
| 40:OF:177:VAL:HG22 | 41:OM:331:LEU:HB2 | 1.93 | 0.51 |
| 40:OH:194:THR:C | 40:OH:196:GLU:H | 2.13 | 0.51 |
| 40:PF:70:LEU:HD23 | 40:PF:114:LEU:HD12 | 1.93 | 0.51 |
| 41:PN:193:VAL:HG22 | 41:PN:418:LEU:HD22 | 1.91 | 0.51 |
| 41:PO:11:GLN:HA | 41:PO:72:THR:HG21 | 1.92 | 0.51 |
| 40:QA:182:VAL:O | 40:QA:186:ASN:ND2 | 2.43 | 0.51 |
| 40:QG:210:TYR:HE1 | 40:QG:227:LEU:HD11 | 1.74 | 0.51 |
| 40:QH:158:SER:OG | 40:QH:166:LYS:NZ | 2.44 | 0.51 |
| 40:QH:217:LEU:HD21 | 40:QH:275:VAL:HG22 | 1.92 | 0.51 |
| 41:QM:24:ILE:HG21 | 41:QM:50:TYR:HD2 | 1.76 | 0.51 |
| 41:QO:44:LEU:HA | 41:QO:47:ILE:HG23 | 1.91 | 0.51 |
| 40:RG:31:GLN:HG2 | 40:RG:33:ASP:H | 1.75 | 0.51 |
| 41:RM:143:THR:OG1 | 43:RM:501:GDP:O1B | 2.27 | 0.51 |
| 41:RM:310:TYR:HA | 41:RM:371:SER:HA | 1.93 | 0.51 |
| 41:RN:83:GLN:O | 41:SN:281:TYR:OH | 2.25 | 0.51 |
| 40:SE:73:THR:HA | 40:SE:76:ASP:HB2 | 1.91 | 0.51 |
| 41:SM:211:CYS:HA | 41:SM:215:LEU:HB2 | 1.92 | 0.51 |
| 41:SO:409:THR:HA | 41:SO:412:GLU:HB3 | 1.92 | 0.51 |
| 41:SP:137:HIS:O | 41:SP:168:SER:HA | 2.11 | 0.51 |
| 40:TA:370:VAL:HG22 | 40:TA:372:ARG:H | 1.76 | 0.51 |
| 40:TG:196:GLU:OE1 | 40:TG:196:GLU:N | 2.37 | 0.51 |
| 40:TG:326:LYS:NZ | 41:TO:219:THR:HA | 2.25 | 0.51 |
| 41:TL:274:THR:HG21 | 41:TL:282:ARG:HD2 | 1.93 | 0.51 |
| 41:TM:55:THR:OG1 | 41:UM:284:LEU:N | 2.44 | 0.51 |
| 41:TM:139:LEU:HD12 | 41:TM:170:VAL:HG12 | 1.93 | 0.51 |
| 41:TN:105:HIS:CD2 | 41:TN:150:LEU:HD12 | 2.44 | 0.51 |
| 41:TP:330:MET:HB3 | 41:TP:349:VAL:HG11 | 1.92 | 0.51 |
| 40:UE:225:THR:O | 40:UE:229:ARG:HG2 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UF:16:ILE:HG12 | 40:UF:228:ASN:HD21 | 1.75 | 0.51 |
| 41:VB:142:GLY:O | 41:VB:144:GLY:N | 2.44 | 0.51 |
| 40:VF:208:ALA:HB2 | 40:VF:304:LYS:HD2 | 1.92 | 0.51 |
| 40:WG:47:ASP:O | 40:WG:50:ASN:HB3 | 2.11 | 0.51 |
| 40:WH:247:ALA:HB3 | 40:WH:355:ILE:HD11 | 1.93 | 0.51 |
| 41:WM:271:ALA:HB3 | 41:WM:272:PRO:CD | 2.41 | 0.51 |
| 41:WN:34:GLY:O | 41:WN:35:THR:C | 2.48 | 0.51 |
| 41:WO:375:GLN:O | 41:WO:379:LYS:NZ | 2.43 | 0.51 |
| 41:WQ:7:LEU:HD23 | 41:WQ:64:VAL:HB | 1.92 | 0.51 |
| 17:3O:218:GLU:HB3 | 17:3O:343:VAL:HG22 | 1.93 | 0.51 |
| 18:3U:168:VAL:HG12 | 18:3V:51:TYR:HB2 | 1.92 | 0.51 |
| 18:3W:360:ARG:NH2 | 18:3W:374:GLN:OE1 | 2.42 | 0.51 |
| 20:4B:357:LEU:HG | 20:4B:358:ASN:N | 2.24 | 0.51 |
| 21:4E:94:LYS:HZ1 | 40:AH:361:THR:HG22 | 1.76 | 0.51 |
| 22:4I:319:LEU:HD12 | 41:BO:92:PHE:CG | 2.46 | 0.51 |
| 22:4I:462:THR:HG21 | 22:4I:483:ARG:HG3 | 1.92 | 0.51 |
| 23:4M:235:THR:OG1 | 23:4M:240:LEU:HA | 2.11 | 0.51 |
| 26:4W:245:VAL:HG21 | 26:4W:255:LEU:HD13 | 1.92 | 0.51 |
| 28:5B:56:GLU:HG2 | 41:JB:277:GLY:HA3 | 1.93 | 0.51 |
| 36:5X:179:PHE:HZ | 41:OM:22:GLU:HG3 | 1.76 | 0.51 |
| 39:6K:61:ASN:OD1 | 39:6K:63:THR:OG1 | 2.26 | 0.51 |
| 41:AB:180:VAL:HG23 | 41:AB:184:ASN:HD21 | 1.75 | 0.51 |
| 40:AF:221:ARG:NH1 | 41:AM:325:GLU:OE2 | 2.38 | 0.51 |
| 41:AN:100:ASN:HB3 | 41:AN:103:LYS:HB2 | 1.93 | 0.51 |
| 41:AO:360:GLY:O | 41:AO:361:LEU:C | 2.47 | 0.51 |
| 41:BB:82:GLY:O | 41:BB:84:ILE:N | 2.41 | 0.51 |
| 40:BE:274:PRO:CG | 40:BE:373:ALA:HA | 2.40 | 0.51 |
| 40:BF:11:GLN:HG3 | 40:BF:74:VAL:HG21 | 1.91 | 0.51 |
| 41:BO:193:VAL:HA | 41:BO:264:HIS:NE2 | 2.26 | 0.51 |
| 40:CA:407:TYR:O | 40:CA:408:VAL:C | 2.49 | 0.51 |
| 41:CO:10:GLY:O | 41:CO:14:ASN:HB2 | 2.10 | 0.51 |
| 41:CO:192:LEU:HD13 | 41:CO:196:THR:HG21 | 1.93 | 0.51 |
| 40:DF:1:GLN:HE21 | 41:DN:70:PRO:HG2 | 1.76 | 0.51 |
| 40:DF:192:HIS:CE1 | 40:DF:419:GLU:HG3 | 2.45 | 0.51 |
| 40:DI:363:VAL:O | 40:DI:365:GLY:N | 2.44 | 0.51 |
| 41:DL:135:LEU:HD23 | 41:DL:152:ILE:HG12 | 1.92 | 0.51 |
| 41:DN:142:GLY:O | 41:DN:143:THR:C | 2.49 | 0.51 |
| 41:DP:181:GLU:O | 41:DP:182:PRO:C | 2.48 | 0.51 |
| 40:EF:405:HIS:HA | 40:EF:408:VAL:HG12 | 1.91 | 0.51 |
| 40:EI:217:LEU:O | 40:EI:219:ILE:N | 2.44 | 0.51 |
| 41:EM:178:THR:O | 41:EM:179:VAL:C | 2.48 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FG:136:LEU:HD12 | 40:FG:167:LEU:HB2 | 1.92 | 0.51 |
| 40:FG:326:LYS:NZ | 41:FO:212:PHE:HB2 | 2.25 | 0.51 |
| 41:FO:242:PHE:HB3 | 41:FO:356:ILE:HD13 | 1.93 | 0.51 |
| 41:FP:31:ASP:OD1 | 41:FP:35:THR:OG1 | 2.21 | 0.51 |
| 40:GF:239:THR:O | 40:GF:243:ARG:NH1 | 2.43 | 0.51 |
| 40:HA:27:GLU:OE2 | 40:HA:236:SER:OG | 2.26 | 0.51 |
| 40:HE:413:GLU:O | 40:HE:414:GLU:C | 2.49 | 0.51 |
| 40:HI:175:PRO:HG3 | 40:HI:304:LYS:HB2 | 1.93 | 0.51 |
| 40:HI:298:PRO:HB3 | 40:HI:307:PRO:HD2 | 1.92 | 0.51 |
| 40:IA:407:TYR:HD2 | 40:IA:417:PHE:HZ | 1.59 | 0.51 |
| 41:IB:113:VAL:HA | 41:IB:116:VAL:HG12 | 1.92 | 0.51 |
| 40:IE:6:SER:HA | 40:IE:136:LEU:O | 2.11 | 0.51 |
| 40:IE:140:SER:OG | 42:IE:501:GTP:O2A | 2.27 | 0.51 |
| 41:IN:5:VAL:HB | 41:IN:133:PHE:HD1 | 1.75 | 0.51 |
| 41:JB:311:LEU:HD12 | 41:JB:342:VAL:HG21 | 1.93 | 0.51 |
| 40:JD:213:CYS:HA | 40:JD:217:LEU:HD23 | 1.92 | 0.51 |
| 40:JG:142:GLY:HA2 | 40:JG:183:GLU:HG2 | 1.93 | 0.51 |
| 40:LH:206:ASN:OD1 | 42:LO:501:GTP:O2' | 2.26 | 0.51 |
| 41:LL:213:ARG:HH21 | 41:LL:297:LYS:HG2 | 1.76 | 0.51 |
| 40:MF:26:LEU:HD21 | 40:MF:363:VAL:HG12 | 1.92 | 0.51 |
| 40:MG:46:ASP:O | 40:MG:48:SER:N | 2.44 | 0.51 |
| 40:MG:260:VAL:HB | 41:MO:397:TRP:HZ3 | 1.75 | 0.51 |
| 41:ML:263:LEU:O | 41:ML:370:ASN:ND2 | 2.43 | 0.51 |
| 40:NA:27:GLU:HA | 40:NA:361:THR:HG21 | 1.93 | 0.51 |
| 41:NB:282:ARG:NH2 | 41:NB:288:GLU:OE1 | 2.44 | 0.51 |
| 40:NE:4:CYS:SG | 40:NE:133:GLN:NE2 | 2.84 | 0.51 |
| 40:NE:235:VAL:HA | 40:NE:238:ILE:HG22 | 1.92 | 0.51 |
| 40:NE:250:VAL:HG23 | 40:NE:254:GLU:HB2 | 1.92 | 0.51 |
| 41:NL:119:VAL:HG23 | 41:NL:122:LYS:HE2 | 1.92 | 0.51 |
| 40:OA:180:ALA:O | 41:ON:347:ASN:ND2 | 2.44 | 0.51 |
| 40:OF:79:ARG:O | 40:OF:84:ARG:NH1 | 2.39 | 0.51 |
| 40:OF:247:ALA:HB3 | 40:OF:355:ILE:HB | 1.92 | 0.51 |
| 40:OH:28:HIS:O | 40:OH:30:ILE:HG12 | 2.11 | 0.51 |
| 40:OH:63:PRO:HG3 | 40:OH:87:PHE:CD1 | 2.46 | 0.51 |
| 40:OH:345:ASP:N | 40:OH:345:ASP:OD1 | 2.44 | 0.51 |
| 41:OO:276:ARG:NH2 | 41:OO:279:GLN:OE1 | 2.43 | 0.51 |
| 41:OP:190:HIS:HA | 41:OP:414:ASN:HD21 | 1.75 | 0.51 |
| 40:PD:192:HIS:NE2 | 40:PD:424:MET:HG2 | 2.26 | 0.51 |
| 40:PE:141:PHE:HB2 | 40:PE:173:PRO:HD3 | 1.93 | 0.51 |
| 41:PL:392:LYS:HG3 | 41:PL:395:LEU:HD11 | 1.92 | 0.51 |
| 41:PM:104:GLY:HA2 | 41:PM:109:GLY:HA3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PP:236:VAL:HG13 | 41:PP:237:THR:HG23 | 1.93 | 0.51 |
| 40:QE:206:ASN:OD1 | 42:QL:501:GTP:O2' | 2.21 | 0.51 |
| 40:QE:362:VAL:HG21 | 40:QE:369:LYS:HA | 1.92 | 0.51 |
| 40:QG:181:VAL:HG23 | 40:QG:182:VAL:HG13 | 1.91 | 0.51 |
| 41:QM:99:ASN:O | 41:QM:184:ASN:ND2 | 2.42 | 0.51 |
| 41:QP:5:VAL:HG12 | 41:QP:6:HIS:H | 1.74 | 0.51 |
| 41:QP:215:LEU:HB3 | 41:QP:217:LEU:HG | 1.93 | 0.51 |
| 40:RA:394:PHE:CD1 | 40:RA:421:ARG:HD3 | 2.46 | 0.51 |
| 40:RE:398:TYR:O | 40:RE:401:ARG:NH1 | 2.44 | 0.51 |
| 40:RH:284:GLU:OE2 | 40:RH:284:GLU:N | 2.44 | 0.51 |
| 41:RP:172:SER:OG | 41:RP:175:VAL:O | 2.25 | 0.51 |
| 41:SB:202:ILE:HG23 | 41:SB:300:MET:HB3 | 1.92 | 0.51 |
| 40:SE:205:ASP:HB2 | 40:SE:303:VAL:HG22 | 1.92 | 0.51 |
| 40:SE:352:LYS:HD2 | 41:SM:179:VAL:HG13 | 1.91 | 0.51 |
| 40:TE:326:LYS:HA | 40:TE:329:ASN:HB2 | 1.93 | 0.51 |
| 40:TI:297:GLU:OE2 | 40:TI:300:ASN:ND2 | 2.44 | 0.51 |
| 41:TO:137:HIS:HE1 | 41:TO:166:THR:HB | 1.75 | 0.51 |
| 41:TP:137:HIS:CE1 | 41:TP:168:SER:HG | 2.29 | 0.51 |
| 40:UG:79:ARG:NH1 | 40:UG:92:LEU:O | 2.42 | 0.51 |
| 41:UP:44:LEU:O | 41:UP:45:GLU:C | 2.49 | 0.51 |
| 41:UP:275:SER:O | 41:UP:276:ARG:NH2 | 2.44 | 0.51 |
| 40:VA:96:LYS:HD3 | 41:VO:129:CYS:HB2 | 1.93 | 0.51 |
| 40:VH:217:LEU:HA | 40:VH:277:SER:HB3 | 1.92 | 0.51 |
| 40:VJ:185:TYR:OH | 40:VJ:397:MET:O | 2.27 | 0.51 |
| 41:VN:173:PRO:HB3 | 41:VN:380:ARG:HD3 | 1.93 | 0.51 |
| 40:WE:405:HIS:HA | 40:WE:408:VAL:HG12 | 1.91 | 0.51 |
| 7:1U:164:VAL:HG23 | 7:1U:176:THR:HG22 | 1.93 | 0.51 |
| 11:2J:211:PHE:HD2 | 11:2J:230:LEU:HD22 | 1.75 | 0.51 |
| 12:2M:41:GLY:HA3 | 41:AB:306:ARG:HD3 | 1.93 | 0.51 |
| 13:2X:115:LYS:HB2 | 13:2X:116:PRO:HD2 | 1.91 | 0.51 |
| 18:3U:156:LEU:O | 18:3U:160:GLU:HG3 | 2.11 | 0.51 |
| 18:3U:328:GLU:HG3 | 18:3U:405:LEU:HD21 | 1.92 | 0.51 |
| 22:4J:511:ALA:HB3 | 22:4J:522:LEU:HD13 | 1.92 | 0.51 |
| 24:4O:173:SER:CB | 24:4O:181:LYS:HG3 | 2.38 | 0.51 |
| 24:4O:186:GLY:O | 24:4O:188:THR:N | 2.44 | 0.51 |
| 38:6C:63:ASP:O | 38:6C:65:HIS:N | 2.44 | 0.51 |
| 38:6C:69:ILE:HB | 40:VA:298:PRO:HD3 | 1.93 | 0.51 |
| 40:AA:205:ASP:HB2 | 40:AA:303:VAL:HG23 | 1.92 | 0.51 |
| 40:AA:258:ASN:HD22 | 40:AA:352:LYS:HD2 | 1.76 | 0.51 |
| 40:AF:328:VAL:O | 40:AF:332:ILE:HG12 | 2.11 | 0.51 |
| 41:AN:242:PHE:HB3 | 41:AN:356:ILE:HD13 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AO:318:ARG:HH21 | 41:AO:356:ILE:HG22 | 1.76 | 0.51 |
| 41:BB:215:LEU:HD21 | 41:BB:273:LEU:HD22 | 1.93 | 0.51 |
| 40:BE:157:LEU:HG | 40:BE:161:TYR:HD2 | 1.75 | 0.51 |
| 40:BF:93:ILE:HD11 | 40:BF:121:ARG:HG3 | 1.92 | 0.51 |
| 40:BF:177:VAL:HG21 | 40:BF:207:GLU:HG3 | 1.92 | 0.51 |
| 40:BI:151:SER:HB3 | 40:BI:193:THR:HG21 | 1.92 | 0.51 |
| 41:BL:7:LEU:HD22 | 41:BL:151:LEU:HD21 | 1.92 | 0.51 |
| 41:BM:98:GLY:O | 41:BM:100:ASN:N | 2.44 | 0.51 |
| 41:BM:420:ASN:HB2 | 41:BM:421:PRO:HD3 | 1.93 | 0.51 |
| 41:BN:194:GLU:OE2 | 41:BN:262:ARG:NH1 | 2.43 | 0.51 |
| 41:BP:226:ASN:ND2 | 43:BP:501:GDP:HN1 | 2.08 | 0.51 |
| 40:CG:188:ILE:HD12 | 40:CG:424:MET:HG3 | 1.92 | 0.51 |
| 40:CI:311:LYS:HE3 | 40:CI:344:VAL:HA | 1.92 | 0.51 |
| 41:CN:197:ASP:O | 41:CN:264:HIS:HB2 | 2.10 | 0.51 |
| 41:CP:371:SER:C | 41:CP:373:ALA:H | 2.13 | 0.51 |
| 40:DA:186:ASN:O | 40:DA:190:THR:HG23 | 2.11 | 0.51 |
| 41:DB:50:TYR:HA | 41:DB:62:ARG:HD2 | 1.92 | 0.51 |
| 40:DF:119:LEU:HD22 | 40:DF:156:ARG:HH21 | 1.75 | 0.51 |
| 40:DH:87:PHE:HB3 | 40:DH:92:LEU:HD21 | 1.92 | 0.51 |
| 41:DM:309:ARG:HG2 | 41:DM:342:VAL:HG13 | 1.91 | 0.51 |
| 41:DO:107:THR:O | 41:DO:110:ALA:N | 2.37 | 0.51 |
| 41:DP:68:LEU:HD13 | 41:DP:97:ALA:HB2 | 1.93 | 0.51 |
| 41:DP:238:THR:O | 41:DP:241:ARG:N | 2.44 | 0.51 |
| 40:EH:190:THR:O | 40:EH:192:HIS:N | 2.43 | 0.51 |
| 41:EM:27:GLU:O | 41:EM:28:HIS:C | 2.49 | 0.51 |
| 41:EM:108:GLU:O | 41:EM:109:GLY:C | 2.49 | 0.51 |
| 41:EM:143:THR:OG1 | 41:EM:144:GLY:N | 2.44 | 0.51 |
| 41:EP:16:ILE:HG13 | 41:EP:136:THR:HB | 1.93 | 0.51 |
| 41:EP:164:MET:O | 41:EP:166:THR:HG22 | 2.11 | 0.51 |
| 41:EP:310:TYR:HA | 41:EP:371:SER:HA | 1.92 | 0.51 |
| 41:EP:344:TRP:CZ2 | 41:EP:425:ARG:HG2 | 2.45 | 0.51 |
| 40:FH:213:CYS:HA | 40:FH:217:LEU:HD13 | 1.91 | 0.51 |
| 41:GB:137:HIS:HE1 | 41:GB:166:THR:HB | 1.74 | 0.51 |
| 40:GE:276:ILE:HG21 | 40:GE:281:ALA:HB2 | 1.93 | 0.51 |
| 40:GI:217:LEU:CA | 40:GI:277:SER:HB2 | 2.41 | 0.51 |
| 42:HA:501:GTP:O1G | 41:HN:252:LYS:HD2 | 2.10 | 0.51 |
| 40:HE:415:GLY:O | 40:HE:416:GLU:C | 2.49 | 0.51 |
| 40:HG:174:ALA:HB3 | 40:HG:178:SER:H | 1.75 | 0.51 |
| 41:HN:10:GLY:HA2 | 41:HN:143:THR:OG1 | 2.11 | 0.51 |
| 41:HN:283:ALA:O | 41:HN:285:THR:N | 2.44 | 0.51 |
| 41:HO:95:SER:OG | 41:HO:96:GLY:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HQ:179:VAL:HG23 | 41:HQ:180:VAL:HG13 | 1.91 | 0.51 |
| 41:HQ:268:PRO:HG2 | 41:HQ:300:MET:HG3 | 1.92 | 0.51 |
| 40:IE:136:LEU:HD13 | 40:IE:167:LEU:HB2 | 1.92 | 0.51 |
| 40:II:178:SER:OG | 41:IP:347:ASN:ND2 | 2.37 | 0.51 |
| 41:IM:289:LEU:O | 41:IM:293:MET:HG3 | 2.10 | 0.51 |
| 40:JA:20:CYS:HA | 40:JA:232:SER:HB2 | 1.93 | 0.51 |
| 40:JD:395:ASP:OD2 | 40:JD:421:ARG:NH2 | 2.38 | 0.51 |
| 40:JE:168:GLU:HB2 | 40:JE:201:ALA:HA | 1.93 | 0.51 |
| 40:JE:222:PRO:O | 41:JL:322:SER:OG | 2.27 | 0.51 |
| 40:JE:257:THR:HA | 41:JM:397:TRP:CH2 | 2.46 | 0.51 |
| 40:JG:319:TYR:HB3 | 40:JG:323:VAL:HG11 | 1.92 | 0.51 |
| 40:LG:174:ALA:CB | 40:LG:177:VAL:HG23 | 2.41 | 0.51 |
| 40:LG:200:CYS:SG | 40:LG:268:PRO:HG2 | 2.50 | 0.51 |
| 40:LG:316:CYS:SG | 40:LG:316:CYS:O | 2.69 | 0.51 |
| 41:LO:13:GLY:HA2 | 41:LO:136:THR:HG22 | 1.93 | 0.51 |
| 41:LO:313:VAL:HG12 | 41:LO:349:VAL:HG23 | 1.93 | 0.51 |
| 40:MA:224:TYR:CZ | 42:MN:501:GTP:H2' | 2.46 | 0.51 |
| 40:MA:246:GLY:HA2 | 40:MA:357:TYR:CD2 | 2.46 | 0.51 |
| 40:ME:221:ARG:NE | 41:ML:325:GLU:OE2 | 2.43 | 0.51 |
| 40:MF:174:ALA:HB1 | 40:MF:177:VAL:HG23 | 1.93 | 0.51 |
| 41:MN:240:LEU:HD12 | 41:MN:241:ARG:HG3 | 1.92 | 0.51 |
| 41:MN:263:LEU:O | 41:MN:370:ASN:ND2 | 2.44 | 0.51 |
| 41:MO:334:GLN:HE22 | 41:MO:348:ASN:N | 2.09 | 0.51 |
| 41:MP:107:THR:HG22 | 41:MP:108:GLU:H | 1.76 | 0.51 |
| 40:NA:406:TRP:HE1 | 41:NN:258:VAL:HG23 | 1.75 | 0.51 |
| 40:ND:281:ALA:O | 40:ND:284:GLU:N | 2.44 | 0.51 |
| 40:NE:7:VAL:O | 40:NE:137:ILE:HA | 2.10 | 0.51 |
| 41:NM:139:LEU:HG | 41:NM:168:SER:HB2 | 1.92 | 0.51 |
| 41:NN:8:GLN:HE21 | 41:NN:65:LEU:HD22 | 1.76 | 0.51 |
| 41:NP:392:LYS:NZ | 41:NP:405:GLU:OE2 | 2.41 | 0.51 |
| 40:OG:6:SER:O | 40:OG:65:ALA:HA | 2.10 | 0.51 |
| 40:OG:296:PHE:HD2 | 40:OG:341:ILE:HD13 | 1.76 | 0.51 |
| 40:OH:89:PRO:HG2 | 40:PH:279:GLU:O | 2.11 | 0.51 |
| 41:ON:202:ILE:HG21 | 41:ON:229:VAL:HG22 | 1.92 | 0.51 |
| 41:PB:139:LEU:HG | 41:PB:168:SER:HB2 | 1.93 | 0.51 |
| 41:PO:7:LEU:O | 41:PO:8:GLN:NE2 | 2.44 | 0.51 |
| 41:QB:125:GLU:O | 41:QB:127:CYS:N | 2.43 | 0.51 |
| 40:QF:273:ALA:HB1 | 40:QF:291:ILE:HB | 1.92 | 0.51 |
| 41:QN:31:ASP:OD2 | 41:QN:35:THR:OG1 | 2.29 | 0.51 |
| 41:QP:372:THR:O | 41:QP:372:THR:OG1 | 2.29 | 0.51 |
| 40:RH:101:ASN:HA | 40:RH:144:GLY:H | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RO:4:ILE:HA | 41:RO:132:GLY:O | 2.10 | 0.51 |
| 41:RO:139:LEU:HD12 | 41:RO:170:VAL:HG12 | 1.91 | 0.51 |
| 41:RO:193:VAL:HG11 | 41:RO:418:LEU:HG | 1.92 | 0.51 |
| 41:SN:375:GLN:NE2 | 41:SN:419:GLY:O | 2.40 | 0.51 |
| 41:SO:103:LYS:HA | 41:SO:107:THR:OG1 | 2.11 | 0.51 |
| 41:SP:142:GLY:O | 41:SP:144:GLY:N | 2.44 | 0.51 |
| 41:SP:292:GLN:O | 41:SP:298:ASN:ND2 | 2.41 | 0.51 |
| 41:TB:42:LEU:HD11 | 41:TB:243:PRO:HG3 | 1.93 | 0.51 |
| 41:TB:86:ARG:HD3 | 41:TB:88:ASP:HB3 | 1.92 | 0.51 |
| 40:TI:235:VAL:HA | 40:TI:238:ILE:HG12 | 1.92 | 0.51 |
| 41:TM:309:ARG:NH1 | 41:TM:339:SER:O | 2.44 | 0.51 |
| 41:TO:73:MET:HA | 41:TO:76:VAL:HG12 | 1.91 | 0.51 |
| 40:UF:219:ILE:O | 40:UF:220:GLU:C | 2.49 | 0.51 |
| 40:UG:133:GLN:O | 40:UG:165:SER:OG | 2.29 | 0.51 |
| 40:UH:320:ARG:HH21 | 40:UH:360:PRO:HA | 1.76 | 0.51 |
| 41:UO:100:ASN:HB3 | 41:UO:103:LYS:HB2 | 1.93 | 0.51 |
| 41:VP:271:ALA:HB1 | 41:VP:292:GLN:HB3 | 1.92 | 0.51 |
| 40:WF:402:ALA:HB2 | 41:WM:344:TRP:HZ3 | 1.76 | 0.51 |
| 40:WI:27:GLU:HG2 | 40:WI:243:ARG:HH22 | 1.76 | 0.51 |
| 41:WM:391:ARG:O | 41:WM:392:LYS:C | 2.50 | 0.51 |
| 41:WN:222:TYR:O | 41:WN:223:GLY:C | 2.49 | 0.51 |
| 8:1X:100:LEU:HD21 | 11:2I:251:TYR:CG | 2.46 | 0.51 |
| 11:2I:118:ALA:C | 11:2I:119:LYS:HD2 | 2.32 | 0.51 |
| 11:2J:207:VAL:HA | 11:2J:210:GLU:HG2 | 1.93 | 0.51 |
| 13:2U:88:THR:HG23 | 13:2U:157:HIS:CB | 2.41 | 0.51 |
| 15:3E:338:ILE:HG12 | 15:3H:205:VAL:HG23 | 1.93 | 0.51 |
| 17:3R:184:ALA:O | 17:3R:187:GLU:HG3 | 2.11 | 0.51 |
| 18:3U:315:ARG:HH21 | 18:3U:423:LEU:HD12 | 1.76 | 0.51 |
| 22:4J:89:VAL:O | 41:BN:282:ARG:N | 2.36 | 0.51 |
| 24:4O:191:VAL:O | 24:4O:192:PRO:C | 2.49 | 0.51 |
| 23:4R:100:GLN:O | 23:4R:116:ALA:HB1 | 2.11 | 0.51 |
| 23:4R:107:LYS:HZ2 | 23:4R:112:VAL:HA | 1.76 | 0.51 |
| 23:4R:198:PHE:HB3 | 40:DI:221:ARG:HB2 | 1.93 | 0.51 |
| 26:4W:113:ILE:HG23 | 26:4W:118:PHE:HB2 | 1.92 | 0.51 |
| 27:4Y:94:MET:HG2 | 27:4Y:96:PRO:HD3 | 1.93 | 0.51 |
| 36:5X:188:GLN:O | 36:5X:192:GLN:NE2 | 2.44 | 0.51 |
| 39:6H:13:VAL:HG22 | 39:6H:77:GLU:HG3 | 1.93 | 0.51 |
| 39:6I:31:LEU:HD21 | 39:6I:45:ILE:HG13 | 1.91 | 0.51 |
| 40:AA:177:VAL:HG12 | 41:AN:331:LEU:HB2 | 1.93 | 0.51 |
| 41:AB:385:PHE:HZ | 41:AB:408:PHE:HB3 | 1.76 | 0.51 |
| 40:AF:181:VAL:HG12 | 41:AM:348:ASN:HA | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AO:170:VAL:HG12 | 41:AO:171:PRO:HD2 | 1.93 | 0.51 |
| 41:AO:216:LYS:HG3 | 41:AO:275:SER:HB3 | 1.92 | 0.51 |
| 40:BF:134:GLY:HA2 | 40:BF:165:SER:O | 2.11 | 0.51 |
| 41:BL:105:HIS:CD2 | 41:BL:150:LEU:HB2 | 2.46 | 0.51 |
| 41:BO:286:VAL:HB | 41:BO:287:PRO:HD3 | 1.93 | 0.51 |
| 40:CA:34:GLY:O | 40:CA:60:LYS:HA | 2.11 | 0.51 |
| 40:CH:99:ALA:O | 40:CH:100:ALA:C | 2.48 | 0.51 |
| 41:CL:192:LEU:O | 41:CL:193:VAL:C | 2.49 | 0.51 |
| 40:DA:420:ALA:O | 40:DA:421:ARG:C | 2.49 | 0.51 |
| 40:DE:90:GLU:O | 40:DE:91:GLN:C | 2.49 | 0.51 |
| 40:DE:97:GLU:HB3 | 40:DE:110:ILE:HD13 | 1.93 | 0.51 |
| 40:DH:268:PRO:HA | 40:DH:379:ASN:HA | 1.93 | 0.51 |
| 40:DI:256:GLN:HA | 40:DI:260:VAL:HB | 1.93 | 0.51 |
| 41:DL:183:TYR:O | 41:DL:184:ASN:C | 2.48 | 0.51 |
| 41:DN:100:ASN:O | 41:DN:101:TRP:C | 2.49 | 0.51 |
| 41:DN:181:GLU:O | 41:DN:182:PRO:C | 2.49 | 0.51 |
| 41:DN:271:ALA:HB3 | 41:DN:272:PRO:HD3 | 1.93 | 0.51 |
| 40:EA:271:THR:HA | 40:EA:302:MET:HG2 | 1.93 | 0.51 |
| 40:EI:32:PRO:O | 40:EI:33:ASP:C | 2.48 | 0.51 |
| 40:EI:63:PRO:CG | 40:EI:86:LEU:HG | 2.40 | 0.51 |
| 41:EM:100:ASN:O | 41:EM:101:TRP:C | 2.49 | 0.51 |
| 41:EM:182:PRO:O | 41:EM:183:TYR:C | 2.49 | 0.51 |
| 41:FB:2:ARG:HE | 41:FB:240:LEU:HB2 | 1.76 | 0.51 |
| 40:FF:342:GLN:NE2 | 40:FF:343:PHE:O | 2.44 | 0.51 |
| 41:FN:42:LEU:HD22 | 41:FN:243:PRO:HG3 | 1.93 | 0.51 |
| 41:FN:317:PHE:HB2 | 41:FN:353:VAL:HG12 | 1.93 | 0.51 |
| 41:FO:139:LEU:HD12 | 41:FO:170:VAL:HG12 | 1.93 | 0.51 |
| 41:FO:148:GLY:O | 41:FO:152:ILE:HG12 | 2.10 | 0.51 |
| 41:GB:77:ARG:NH1 | 41:GB:82:GLY:O | 2.44 | 0.51 |
| 40:GE:21:TRP:CZ2 | 40:GE:65:ALA:HB2 | 2.45 | 0.51 |
| 40:GH:256:GLN:O | 40:GH:260:VAL:HG22 | 2.11 | 0.51 |
| 40:GI:100:ALA:HA | 41:GP:252:LYS:CB | 2.36 | 0.51 |
| 41:GN:12:CYS:SG | 41:GN:138:SER:HB3 | 2.51 | 0.51 |
| 40:HG:9:VAL:HG12 | 40:HG:68:VAL:HB | 1.91 | 0.51 |
| 40:HH:205:ASP:HB3 | 40:HH:303:VAL:HA | 1.93 | 0.51 |
| 41:HN:222:TYR:HA | 41:HN:225:LEU:HD12 | 1.91 | 0.51 |
| 41:IP:61:PRO:HD3 | 41:IP:84:ILE:HG12 | 1.93 | 0.51 |
| 41:JN:317:PHE:HB2 | 41:JN:353:VAL:HG12 | 1.92 | 0.51 |
| 40:KA:396:LEU:HD23 | 41:KN:346:PRO:HD3 | 1.92 | 0.51 |
| 41:KN:139:LEU:HD12 | 41:KN:170:VAL:HG12 | 1.93 | 0.51 |
| 40:LE:76:ASP:HA | 40:LE:79:ARG:HG2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LF:236:SER:O | 40:LF:240:ALA:HB2 | 2.11 | 0.51 |
| 41:LO:180:VAL:HG23 | 41:LO:184:ASN:HD21 | 1.76 | 0.51 |
| 41:MB:140:GLY:HA3 | 41:MB:181:GLU:HG3 | 1.93 | 0.51 |
| 41:MB:232:THR:HG21 | 41:MB:268:PRO:HB2 | 1.93 | 0.51 |
| 41:MB:252:LYS:HB2 | 40:MG:100:ALA:CA | 2.41 | 0.51 |
| 40:MG:104:ALA:HA | 40:MG:108:TYR:HD2 | 1.75 | 0.51 |
| 40:MG:249:ASN:H | 41:MO:11:GLN:HE22 | 1.58 | 0.51 |
| 41:MP:73:MET:HB3 | 41:MP:90:PHE:CE1 | 2.44 | 0.51 |
| 40:NH:2:ARG:NH2 | 41:NP:70:PRO:O | 2.44 | 0.51 |
| 41:NL:248:ALA:HA | 41:NL:252:LYS:HG2 | 1.92 | 0.51 |
| 41:NL:326:VAL:O | 41:NL:330:MET:HG2 | 2.11 | 0.51 |
| 41:NN:107:THR:O | 41:NN:110:ALA:N | 2.43 | 0.51 |
| 41:NO:289:LEU:O | 41:NO:293:MET:HB2 | 2.10 | 0.51 |
| 40:OA:108:TYR:O | 40:OA:112:LYS:NZ | 2.44 | 0.51 |
| 40:OE:32:PRO:HB3 | 40:OE:83:TYR:HE1 | 1.76 | 0.51 |
| 40:OG:51:THR:HG21 | 40:OG:243:ARG:HG2 | 1.92 | 0.51 |
| 41:ON:156:ARG:NH2 | 41:ON:162:ARG:O | 2.44 | 0.51 |
| 41:OO:16:ILE:HA | 41:OO:226:ASN:HB3 | 1.93 | 0.51 |
| 40:PD:322:ASP:O | 40:PD:372:ARG:NH1 | 2.44 | 0.51 |
| 40:PG:70:LEU:HD23 | 40:PG:114:LEU:HD12 | 1.93 | 0.51 |
| 40:QA:88:HIS:ND1 | 40:QA:91:GLN:OE1 | 2.43 | 0.51 |
| 40:QE:289:ALA:O | 40:QE:292:THR:OG1 | 2.26 | 0.51 |
| 41:QO:179:VAL:HG23 | 41:QO:180:VAL:HG13 | 1.93 | 0.51 |
| 41:QP:5:VAL:HG23 | 41:QP:130:LEU:HD11 | 1.92 | 0.51 |
| 40:RA:71:GLU:HB3 | 40:RA:98:ASP:HA | 1.92 | 0.51 |
| 40:RF:213:CYS:HA | 40:RF:217:LEU:HD13 | 1.92 | 0.51 |
| 41:RL:180:VAL:O | 41:RL:184:ASN:ND2 | 2.44 | 0.51 |
| 41:RM:6:HIS:O | 41:RM:63:ALA:HA | 2.10 | 0.51 |
| 40:SG:191:THR:HA | 40:SG:194:THR:HG22 | 1.92 | 0.51 |
| 41:SN:288:GLU:HA | 41:SN:291:GLN:HB3 | 1.93 | 0.51 |
| 40:TE:274:PRO:HG3 | 40:TE:286:LEU:HD12 | 1.93 | 0.51 |
| 40:TF:180:ALA:N | 40:TF:183:GLU:OE2 | 2.42 | 0.51 |
| 40:TG:51:THR:HG21 | 40:TG:243:ARG:HA | 1.93 | 0.51 |
| 40:TH:274:PRO:HG3 | 40:TH:286:LEU:HD12 | 1.93 | 0.51 |
| 41:TL:139:LEU:HG | 41:TL:168:SER:HB3 | 1.92 | 0.51 |
| 40:UF:129:CYS:SG | 40:UF:132:LEU:HB2 | 2.50 | 0.51 |
| 40:UF:352:LYS:CG | 41:UN:179:VAL:HG23 | 2.36 | 0.51 |
| 40:UI:301:GLN:HG3 | 40:UI:307:PRO:HD3 | 1.93 | 0.51 |
| 41:UM:323:MET:HG3 | 41:UM:326:VAL:HB | 1.93 | 0.51 |
| 41:UO:143:THR:OG1 | 43:UO:502:GDP:O1B | 2.29 | 0.51 |
| 41:UP:41:ASP:O | 41:UP:44:LEU:N | 2.42 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UP:310:TYR:CD1 | 41:UP:371:SER:HB2 | 2.46 | 0.51 |
| 41:UP:380:ARG:O | 41:UP:384:GLN:HG2 | 2.11 | 0.51 |
| 41:VB:334:GLN:HE21 | 41:VB:349:VAL:HG23 | 1.76 | 0.51 |
| 40:VF:262:TYR:OH | 41:VN:391:ARG:O | 2.20 | 0.51 |
| 40:VH:108:TYR:O | 40:VH:112:LYS:NZ | 2.41 | 0.51 |
| 40:VH:247:ALA:HB3 | 40:VH:355:ILE:HB | 1.93 | 0.51 |
| 41:VP:122:LYS:NZ | 41:WO:291:GLN:OE1 | 2.32 | 0.51 |
| 41:WB:51:TYR:HB3 | 41:WB:59:TYR:HB3 | 1.93 | 0.51 |
| 41:WB:105:HIS:CD2 | 41:WB:150:LEU:HB2 | 2.44 | 0.51 |
| 41:WB:139:LEU:HD12 | 41:WB:170:VAL:HG12 | 1.91 | 0.51 |
| 41:WB:256:ASN:HD22 | 41:WB:350:LYS:HD3 | 1.76 | 0.51 |
| 40:WE:3:GLU:OE2 | 40:WE:3:GLU:N | 2.44 | 0.51 |
| 40:WE:269:LEU:HD23 | 40:WE:383:ILE:HD11 | 1.92 | 0.51 |
| 40:WF:11:GLN:HG3 | 40:WF:74:VAL:HG11 | 1.93 | 0.51 |
| 40:WG:70:LEU:HD23 | 40:WG:114:LEU:HD12 | 1.93 | 0.51 |
| 41:WM:171:PRO:O | 41:WM:380:ARG:NH2 | 2.44 | 0.51 |
| 8:1W:531:LYS:HA | 8:1W:534:ILE:HG22 | 1.93 | 0.51 |
| 8:1Y:134:GLU:HA | 8:1Y:137:VAL:HG12 | 1.92 | 0.51 |
| 12:2Q:170:LYS:HE2 | 12:2Q:218:ARG:HE | 1.76 | 0.51 |
| 13:2U:51:GLY:HA3 | 13:2U:57:THR:HG21 | 1.92 | 0.51 |
| 13:2W:61:CYS:HB3 | 13:2W:62:PRO:HD3 | 1.93 | 0.51 |
| 15:3H:194:ASN:HD22 | 17:3P:168:ILE:HG12 | 1.76 | 0.51 |
| 21:4D:148:LEU:HD23 | 21:4D:149:ILE:HG13 | 1.93 | 0.51 |
| 21:4F:245:PHE:HB2 | 21:4F:264:ILE:HG23 | 1.93 | 0.51 |
| 22:4J:679:SER:HA | 22:4J:683:ASP:HB2 | 1.93 | 0.51 |
| 22:4K:638:LEU:HD21 | 22:4K:662:CYS:HA | 1.93 | 0.51 |
| 23:4R:59:THR:O | 23:4R:60:LEU:C | 2.48 | 0.51 |
| 23:4R:259:ARG:NH2 | 40:EI:365:GLY:HA2 | 2.26 | 0.51 |
| 36:5W:73:SER:O | 40:NF:84:ARG:NH1 | 2.44 | 0.51 |
| 41:AB:55:THR:HG23 | 41:BB:283:ALA:HA | 1.92 | 0.51 |
| 41:AB:202:ILE:HG23 | 41:AB:300:MET:HB3 | 1.92 | 0.51 |
| 40:BH:109:THR:O | 40:BH:111:GLY:N | 2.44 | 0.51 |
| 40:BH:132:LEU:HG | 40:BH:164:LYS:HE2 | 1.93 | 0.51 |
| 40:BH:261:PRO:HB3 | 40:BH:346:TRP:CH2 | 2.46 | 0.51 |
| 40:BH:325:PRO:HB2 | 41:BP:208:TYR:OH | 2.10 | 0.51 |
| 41:BL:213:ARG:HH22 | 41:BL:297:LYS:HG2 | 1.75 | 0.51 |
| 41:BM:274:THR:HG22 | 41:BM:282:ARG:HD3 | 1.93 | 0.51 |
| 41:BO:54:ALA:HB2 | 41:BO:60:VAL:HG12 | 1.92 | 0.51 |
| 40:CI:236:SER:O | 40:CI:243:ARG:NH2 | 2.39 | 0.51 |
| 41:CP:393:ALA:O | 41:CP:394:PHE:C | 2.48 | 0.51 |
| 40:DA:90:GLU:O | 40:DA:91:GLN:C | 2.49 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DF:88:HIS:HE2 | 40:EF:280:LYS:HB3 | 1.75 | 0.51 |
| 40:DF:252:LEU:HA | 40:DF:255:PHE:CE2 | 2.46 | 0.51 |
| 41:DL:102:ALA:HB2 | 41:DL:403:MET:HG3 | 1.93 | 0.51 |
| 41:DL:189:VAL:O | 41:DL:193:VAL:HG23 | 2.11 | 0.51 |
| 41:DN:256:ASN:ND2 | 41:DN:350:LYS:HG2 | 2.26 | 0.51 |
| 41:DP:137:HIS:HE1 | 41:DP:166:THR:HB | 1.74 | 0.51 |
| 41:DP:412:GLU:HG3 | 41:DP:416:ASN:HD21 | 1.76 | 0.51 |
| 40:EA:204:VAL:HG13 | 40:EA:302:MET:HB3 | 1.93 | 0.51 |
| 40:EG:132:LEU:HB3 | 40:EG:164:LYS:HE2 | 1.93 | 0.51 |
| 40:EI:130:THR:OG1 | 40:EI:131:GLY:N | 2.42 | 0.51 |
| 40:FA:287:SER:O | 40:FA:291:ILE:HG23 | 2.11 | 0.51 |
| 41:FO:135:LEU:HB3 | 41:FO:166:THR:HG22 | 1.92 | 0.51 |
| 40:GA:251:ASP:OD2 | 40:GA:252:LEU:N | 2.44 | 0.51 |
| 40:GF:209:ILE:HA | 40:GF:212:ILE:HG22 | 1.92 | 0.51 |
| 40:GG:276:ILE:CG2 | 40:GG:281:ALA:HB2 | 2.32 | 0.51 |
| 41:GM:285:THR:HG23 | 41:GM:287:PRO:HD2 | 1.92 | 0.51 |
| 41:GM:424:THR:OG1 | 41:GM:425:ARG:NH1 | 2.43 | 0.51 |
| 41:GN:390:ARG:C | 41:GN:392:LYS:H | 2.15 | 0.51 |
| 40:HE:99:ALA:O | 40:HE:100:ALA:C | 2.48 | 0.51 |
| 40:HG:332:ILE:HG23 | 40:HG:351:PHE:HD2 | 1.76 | 0.51 |
| 40:HI:177:VAL:HG23 | 41:HP:331:LEU:HB2 | 1.92 | 0.51 |
| 40:IA:269:LEU:HD22 | 40:IA:303:VAL:HG22 | 1.93 | 0.51 |
| 41:IB:194:GLU:OE2 | 41:IB:262:ARG:NH1 | 2.40 | 0.51 |
| 40:IE:260:VAL:HG23 | 41:IM:397:TRP:HH2 | 1.76 | 0.51 |
| 40:IH:167:LEU:HD22 | 40:IH:200:CYS:HB3 | 1.93 | 0.51 |
| 40:IH:405:HIS:HA | 40:IH:408:VAL:HG12 | 1.93 | 0.51 |
| 41:IN:284:LEU:HD21 | 41:IN:363:MET:HB2 | 1.93 | 0.51 |
| 41:IP:248:ALA:HA | 41:IP:252:LYS:HD2 | 1.93 | 0.51 |
| 41:IQ:5:VAL:HA | 41:IQ:62:ARG:HD2 | 1.92 | 0.51 |
| 41:JB:187:LEU:HD11 | 41:JB:408:PHE:HE2 | 1.77 | 0.51 |
| 41:JM:293:MET:C | 41:JM:295:ASP:H | 2.14 | 0.51 |
| 41:JN:247:ASN:O | 41:JN:252:LYS:NZ | 2.38 | 0.51 |
| 41:KL:420:ASN:O | 41:KL:423:VAL:N | 2.39 | 0.51 |
| 41:KM:385:PHE:HZ | 41:KM:408:PHE:HB3 | 1.74 | 0.51 |
| 40:LA:182:VAL:O | 40:LA:186:ASN:ND2 | 2.44 | 0.51 |
| 41:LB:11:GLN:HA | 41:LB:72:THR:HG21 | 1.93 | 0.51 |
| 40:LF:31:GLN:HG2 | 40:LF:32:PRO:HD2 | 1.93 | 0.51 |
| 41:LL:69:GLU:HG2 | 41:LL:96:GLY:HA2 | 1.92 | 0.51 |
| 41:LL:114:ASP:OD1 | 41:LL:115:SER:N | 2.44 | 0.51 |
| 41:LM:341:PHE:HB3 | 41:LM:348:ASN:HD21 | 1.75 | 0.51 |
| 41:MB:31:ASP:OD1 | 41:MB:35:THR:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MD:195:LEU:HD21 | 40:MD:264:ARG:HH11 | 1.76 | 0.51 |
| 40:MG:63:PRO:HD3 | 40:MG:86:LEU:O | 2.11 | 0.51 |
| 41:MM:73:MET:HG3 | 41:MM:92:PHE:HB3 | 1.93 | 0.51 |
| 41:NB:100:ASN:HB3 | 41:NB:103:LYS:HB2 | 1.93 | 0.51 |
| 40:ND:104:ALA:HA | 40:ND:108:TYR:HD1 | 1.75 | 0.51 |
| 40:ND:366:ASP:O | 40:ND:367:LEU:C | 2.49 | 0.51 |
| 40:NF:206:ASN:OD1 | 42:NM:501:GTP:O2' | 2.25 | 0.51 |
| 41:NM:403:MET:HG2 | 41:NM:408:PHE:HE1 | 1.75 | 0.51 |
| 41:NO:239:CYS:HB3 | 41:NO:247:ASN:HB2 | 1.92 | 0.51 |
| 40:OA:73:THR:OG1 | 41:ON:46:ARG:NH1 | 2.44 | 0.51 |
| 40:OE:223:THR:OG1 | 40:OE:225:THR:OG1 | 2.29 | 0.51 |
| 40:OG:139:HIS:O | 40:OG:170:SER:HA | 2.10 | 0.51 |
| 40:PG:180:ALA:HB3 | 40:PG:183:GLU:HG3 | 1.92 | 0.51 |
| 41:PN:5:VAL:HG22 | 41:PN:62:ARG:HD2 | 1.93 | 0.51 |
| 40:QH:269:LEU:HD22 | 40:QH:303:VAL:HG21 | 1.93 | 0.51 |
| 41:QL:286:VAL:HG21 | 41:QL:325:GLU:HB3 | 1.93 | 0.51 |
| 41:QM:142:GLY:O | 41:QM:144:GLY:N | 2.43 | 0.51 |
| 41:QN:142:GLY:O | 41:QN:144:GLY:N | 2.44 | 0.51 |
| 41:QP:269:GLY:HA3 | 41:QP:367:PHE:N | 2.26 | 0.51 |
| 41:QP:426:GLY:O | 41:QP:427:ALA:C | 2.49 | 0.51 |
| 40:RA:436:MET:SD | 40:RA:436:MET:N | 2.81 | 0.51 |
| 40:RI:123:ARG:HH22 | 40:RI:124:LYS:HZ3 | 1.59 | 0.51 |
| 41:RM:293:MET:SD | 41:RM:367:PHE:HB2 | 2.51 | 0.51 |
| 41:SB:143:THR:OG1 | 43:SB:501:GDP:O2B | 2.29 | 0.51 |
| 40:SF:191:THR:HA | 40:SF:194:THR:HG22 | 1.93 | 0.51 |
| 40:SI:259:LEU:HD11 | 40:SI:377:LEU:HD13 | 1.93 | 0.51 |
| 40:SI:286:LEU:HB2 | 40:SI:372:ARG:HH21 | 1.75 | 0.51 |
| 41:SM:177:ASP:N | 41:SM:181:GLU:OE2 | 2.34 | 0.51 |
| 41:SO:258:VAL:HG12 | 41:SO:266:PHE:HZ | 1.76 | 0.51 |
| 40:TA:139:HIS:HE1 | 40:TA:168:GLU:HG2 | 1.76 | 0.51 |
| 40:TF:405:HIS:HA | 40:TF:408:VAL:HG12 | 1.92 | 0.51 |
| 41:TN:87:PRO:HD3 | 41:UN:281:TYR:HD2 | 1.76 | 0.51 |
| 40:UE:288:VAL:HG11 | 40:UE:327:ASP:HB3 | 1.93 | 0.51 |
| 40:UF:56:THR:HG21 | 40:VG:282:TYR:O | 2.10 | 0.51 |
| 40:UF:254:GLU:O | 40:UF:255:PHE:C | 2.50 | 0.51 |
| 40:UF:347:CYS:HA | 41:UN:388:MET:HE2 | 1.92 | 0.51 |
| 40:UG:141:PHE:HB2 | 40:UG:173:PRO:HD3 | 1.93 | 0.51 |
| 40:UH:98:ASP:O | 40:UH:105:ARG:NH1 | 2.43 | 0.51 |
| 40:VF:6:SER:O | 40:VF:65:ALA:HA | 2.09 | 0.51 |
| 41:VP:252:LYS:HD3 | 41:VP:350:LYS:HZ1 | 1.76 | 0.51 |
| 41:WB:202:ILE:HG21 | 41:WB:229:VAL:HG22 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WB:274:THR:HG22 | 41:WB:282:ARG:HH11 | 1.75 | 0.51 |
| 40:WI:346:TRP:CD1 | 41:WQ:391:ARG:HG3 | 2.46 | 0.51 |
| 8:1X:334:ALA:HA | 8:1X:337:MET:SD | 2.50 | 0.50 |
| 10:2F:159:TYR:HB3 | 41:VB:1:MET:HG3 | 1.92 | 0.50 |
| 13:2W:54:VAL:HG11 | 13:2W:86:TYR:HB2 | 1.92 | 0.50 |
| 17:3P:139:GLN:HG3 | 17:3Q:392:PHE:HD1 | 1.75 | 0.50 |
| 18:3T:189:LEU:HD21 | 18:3T:285:ILE:HD12 | 1.92 | 0.50 |
| 18:3U:313:ASP:HA | 18:3U:316:HIS:CE1 | 2.46 | 0.50 |
| 18:3V:231:TYR:HE1 | 18:3V:237:ASP:HB2 | 1.76 | 0.50 |
| 19:3Y:107:GLN:HE21 | 40:LG:362:VAL:HG21 | 1.76 | 0.50 |
| 23:4M:242:LEU:HD11 | 23:4M:265:THR:HB | 1.91 | 0.50 |
| 23:4N:260:THR:HB | 40:EF:219:ILE:HD13 | 1.93 | 0.50 |
| 24:4O:205:LEU:HD13 | 40:DE:221:ARG:CZ | 2.41 | 0.50 |
| 29:5D:72:GLU:HG3 | 40:GI:362:VAL:O | 2.10 | 0.50 |
| 31:5J:796:TYR:HA | 41:IM:227:HIS:CE1 | 2.46 | 0.50 |
| 34:5R:310:ASN:HA | 34:5R:313:LEU:HD12 | 1.93 | 0.50 |
| 34:5R:438:ALA:O | 34:5R:441:SER:N | 2.44 | 0.50 |
| 35:5T:144:GLU:OE2 | 35:5T:148:GLN:NE2 | 2.36 | 0.50 |
| 38:6C:203:PHE:CE1 | 41:VQ:331:LEU:HD23 | 2.46 | 0.50 |
| 39:6H:64:ASP:HA | 39:6H:67:ILE:HG12 | 1.93 | 0.50 |
| 40:AG:132:LEU:HB3 | 40:AG:164:LYS:HE3 | 1.92 | 0.50 |
| 40:AG:276:ILE:HD12 | 40:AG:281:ALA:HA | 1.93 | 0.50 |
| 41:AO:272:PRO:HG2 | 41:AO:361:LEU:HD13 | 1.93 | 0.50 |
| 40:BE:105:ARG:HA | 40:BE:109:THR:CG2 | 2.41 | 0.50 |
| 40:BG:258:ASN:ND2 | 41:BO:179:VAL:HB | 2.26 | 0.50 |
| 40:BI:180:ALA:HB3 | 40:BI:183:GLU:HG3 | 1.94 | 0.50 |
| 40:CE:398:TYR:HE2 | 40:CE:417:PHE:HB3 | 1.76 | 0.50 |
| 41:CM:64:VAL:HG11 | 41:CM:120:VAL:HG23 | 1.92 | 0.50 |
| 41:CM:193:VAL:HA | 41:CM:264:HIS:NE2 | 2.26 | 0.50 |
| 41:CO:66:VAL:HA | 41:CO:91:VAL:O | 2.11 | 0.50 |
| 41:CO:237:THR:HB | 41:CO:240:LEU:HD11 | 1.93 | 0.50 |
| 40:DA:313:MET:HB2 | 40:DA:346:TRP:CH2 | 2.45 | 0.50 |
| 40:DG:432:GLU:N | 40:DG:432:GLU:OE2 | 2.45 | 0.50 |
| 40:DH:104:ALA:O | 40:DH:105:ARG:C | 2.47 | 0.50 |
| 40:DH:334:ALA:O | 40:DH:337:THR:N | 2.43 | 0.50 |
| 41:DN:124:ALA:O | 41:DN:125:GLU:C | 2.48 | 0.50 |
| 41:DN:251:ARG:O | 41:DN:255:VAL:HG23 | 2.11 | 0.50 |
| 41:EB:176:SER:OG | 41:EB:178:THR:O | 2.29 | 0.50 |
| 40:EG:137:ILE:O | 40:EG:168:GLU:HA | 2.11 | 0.50 |
| 40:EH:222:PRO:CD | 41:EO:324:LYS:HG3 | 2.35 | 0.50 |
| 41:EL:207:LEU:HB3 | 41:EL:225:LEU:HD22 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EL:215:LEU:HD11 | 41:EL:228:LEU:HD11 | 1.92 | 0.50 |
| 41:EM:179:VAL:C | 41:EM:181:GLU:H | 2.15 | 0.50 |
| 40:GA:366:ASP:OD2 | 40:GA:367:LEU:N | 2.44 | 0.50 |
| 40:GF:53:PHE:HE1 | 40:GF:63:PRO:HG3 | 1.76 | 0.50 |
| 40:HH:141:PHE:HB2 | 40:HH:173:PRO:HD3 | 1.92 | 0.50 |
| 40:HH:269:LEU:HD11 | 40:HH:383:ILE:HD11 | 1.92 | 0.50 |
| 40:HI:177:VAL:HG21 | 41:HP:327:ASP:HB3 | 1.93 | 0.50 |
| 41:HQ:210:ILE:HD11 | 41:HQ:298:ASN:HA | 1.93 | 0.50 |
| 40:IA:91:GLN:HG2 | 40:IA:121:ARG:HH21 | 1.76 | 0.50 |
| 40:II:97:GLU:OE2 | 41:IP:251:ARG:NH2 | 2.33 | 0.50 |
| 41:IP:142:GLY:O | 41:IP:144:GLY:N | 2.44 | 0.50 |
| 41:IQ:1:MET:SD | 41:IQ:48:ASN:ND2 | 2.68 | 0.50 |
| 41:JO:354:CYS:SG | 41:JO:355:ASP:N | 2.84 | 0.50 |
| 40:KA:98:ASP:O | 40:KA:105:ARG:NH1 | 2.45 | 0.50 |
| 41:KL:391:ARG:O | 41:KL:393:ALA:N | 2.44 | 0.50 |
| 41:KP:215:LEU:HG | 41:KP:273:LEU:HD21 | 1.93 | 0.50 |
| 40:LF:16:ILE:HG12 | 40:LF:228:ASN:OD1 | 2.11 | 0.50 |
| 40:LF:273:ALA:HB3 | 40:LF:274:PRO:HD3 | 1.93 | 0.50 |
| 40:LF:335:ILE:HG23 | 40:LF:341:ILE:HD13 | 1.93 | 0.50 |
| 40:LG:274:PRO:HD2 | 40:LG:291:ILE:HB | 1.93 | 0.50 |
| 41:LN:16:ILE:HD11 | 41:LN:229:VAL:HG11 | 1.92 | 0.50 |
| 40:MG:217:LEU:HD21 | 40:MG:367:LEU:HD23 | 1.92 | 0.50 |
| 40:MH:49:PHE:CE1 | 40:MH:55:GLU:HB2 | 2.46 | 0.50 |
| 40:MH:139:HIS:ND1 | 40:MH:150:THR:HG21 | 2.26 | 0.50 |
| 41:MM:119:VAL:HA | 41:MM:122:LYS:HG2 | 1.92 | 0.50 |
| 41:MN:354:CYS:SG | 41:MN:355:ASP:N | 2.84 | 0.50 |
| 40:NE:122:ILE:HG21 | 40:NE:157:LEU:HD21 | 1.92 | 0.50 |
| 41:NO:134:GLN:HA | 41:NO:165:ASN:O | 2.11 | 0.50 |
| 41:OB:187:LEU:HD11 | 41:OB:408:PHE:HE1 | 1.75 | 0.50 |
| 40:OD:407:TYR:HB3 | 40:OD:412:MET:HB3 | 1.92 | 0.50 |
| 40:OG:180:ALA:HB3 | 40:OG:183:GLU:HG2 | 1.91 | 0.50 |
| 40:OH:294:ALA:O | 40:OH:295:CYS:C | 2.49 | 0.50 |
| 41:OL:12:CYS:SG | 41:OL:13:GLY:N | 2.83 | 0.50 |
| 41:OL:238:THR:HG21 | 41:OL:318:ARG:HD2 | 1.94 | 0.50 |
| 41:ON:20:PHE:HA | 41:ON:23:VAL:HG12 | 1.93 | 0.50 |
| 41:PB:99:ASN:HA | 41:PB:142:GLY:HA3 | 1.92 | 0.50 |
| 40:PD:288:VAL:HA | 40:PD:291:ILE:HG12 | 1.93 | 0.50 |
| 40:PG:120:ASP:OD2 | 40:PG:124:LYS:NZ | 2.40 | 0.50 |
| 40:PH:70:LEU:HB2 | 40:PH:145:THR:HG22 | 1.92 | 0.50 |
| 40:PH:101:ASN:OD1 | 40:PH:186:ASN:ND2 | 2.44 | 0.50 |
| 40:PH:141:PHE:HB2 | 40:PH:173:PRO:HD3 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PL:39:ASP:N | 41:PL:39:ASP:OD1 | 2.43 | 0.50 |
| 41:PM:337:ASN:HB2 | 41:PM:340:TYR:HD2 | 1.76 | 0.50 |
| 41:PO:49:VAL:O | 41:PO:62:ARG:NH1 | 2.44 | 0.50 |
| 41:PO:236:VAL:HG23 | 41:PO:237:THR:HG23 | 1.92 | 0.50 |
| 41:QB:88:ASP:O | 41:QB:89:ASN:C | 2.49 | 0.50 |
| 41:QB:157:GLU:O | 41:QB:158:GLU:C | 2.49 | 0.50 |
| 40:QE:137:ILE:HD11 | 40:QE:166:LYS:HB2 | 1.92 | 0.50 |
| 40:QG:54:SER:HG | 40:QG:64:ARG:HE | 1.59 | 0.50 |
| 40:QH:254:GLU:OE1 | 41:QP:98:GLY:HA2 | 2.10 | 0.50 |
| 41:QN:387:ALA:HA | 41:QN:390:ARG:HE | 1.76 | 0.50 |
| 41:RB:202:ILE:HG23 | 41:RB:300:MET:HB3 | 1.92 | 0.50 |
| 40:RF:167:LEU:HA | 40:RF:200:CYS:O | 2.11 | 0.50 |
| 40:RF:288:VAL:HA | 40:RF:291:ILE:HG12 | 1.93 | 0.50 |
| 40:RG:5:ILE:HD12 | 40:RG:125:LEU:HD12 | 1.94 | 0.50 |
| 40:RH:284:GLU:HG2 | 40:RH:286:LEU:HG | 1.92 | 0.50 |
| 40:SG:90:GLU:OE2 | 40:SG:121:ARG:NE | 2.43 | 0.50 |
| 41:SM:125:GLU:OE2 | 41:TM:291:GLN:NE2 | 2.42 | 0.50 |
| 41:SO:28:HIS:O | 41:SO:43:GLN:HB3 | 2.11 | 0.50 |
| 40:TA:6:SER:O | 40:TA:65:ALA:HA | 2.11 | 0.50 |
| 40:TA:210:TYR:CD1 | 41:TN:324:LYS:HD3 | 2.46 | 0.50 |
| 40:TE:138:PHE:HZ | 40:TE:235:VAL:HG11 | 1.76 | 0.50 |
| 40:TG:352:LYS:HZ3 | 41:TO:178:THR:N | 2.09 | 0.50 |
| 41:TM:3:GLU:HA | 41:TM:49:VAL:HG23 | 1.93 | 0.50 |
| 41:TN:178:THR:HG22 | 41:TN:180:VAL:H | 1.76 | 0.50 |
| 41:TO:27:GLU:O | 41:TO:43:GLN:NE2 | 2.44 | 0.50 |
| 41:TO:171:PRO:HG2 | 41:TO:381:ILE:HG12 | 1.93 | 0.50 |
| 41:TP:148:GLY:O | 41:TP:152:ILE:HG12 | 2.11 | 0.50 |
| 41:TP:372:THR:HB | 41:TP:375:GLN:HE22 | 1.76 | 0.50 |
| 41:UB:139:LEU:HD12 | 41:UB:170:VAL:HG12 | 1.92 | 0.50 |
| 40:UG:217:LEU:HA | 40:UG:277:SER:HB2 | 1.93 | 0.50 |
| 40:VG:177:VAL:HG13 | 40:VG:178:SER:H | 1.76 | 0.50 |
| 41:VP:296:ALA:HB1 | 41:VP:305:PRO:HD2 | 1.92 | 0.50 |
| 41:WB:331:LEU:HD13 | 40:WG:177:VAL:HG22 | 1.93 | 0.50 |
| 40:WH:139:HIS:ND1 | 40:WH:140:SER:O | 2.36 | 0.50 |
| 41:WM:6:HIS:HA | 41:WM:134:GLN:HG3 | 1.92 | 0.50 |
| 41:WM:108:GLU:O | 41:WM:111:GLU:HG3 | 2.11 | 0.50 |
| 7:1T:219:PHE:HB3 | 7:1T:231:LYS:HG3 | 1.94 | 0.50 |
| 7:1T:360:HIS:O | 7:1T:361:THR:C | 2.50 | 0.50 |
| 7:1T:544:LEU:HB2 | 8:1Y:164:GLU:HB3 | 1.92 | 0.50 |
| 12:2N:90:LYS:HA | 41:WB:108:GLU:HB3 | 1.93 | 0.50 |
| 12:2O:85:LEU:HB2 | 12:2O:126:PHE:CZ | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2V:15:TYR:CE2 | 13:2V:17:ILE:HB | 2.46 | 0.50 |
| 13:2V:171:LEU:O | 13:2V:172:TYR:C | 2.48 | 0.50 |
| 14:3C:103:LEU:O | 14:3C:110:ARG:NH1 | 2.45 | 0.50 |
| 21:4D:426:LEU:HD22 | 21:4D:428:SER:HB3 | 1.94 | 0.50 |
| 22:4I:10:SER:HB2 | 41:MO:217:LEU:CD1 | 2.42 | 0.50 |
| 22:4I:526:ASP:O | 22:4I:529:THR:OG1 | 2.25 | 0.50 |
| 22:4J:627:LEU:O | 22:4J:699:TRP:HZ3 | 1.94 | 0.50 |
| 22:4K:558:LYS:O | 22:4K:560:ARG:N | 2.43 | 0.50 |
| 24:4O:233:SER:O | 24:4O:234:ARG:C | 2.50 | 0.50 |
| 31:5J:857:VAL:HG11 | 33:5O:97:LEU:HD11 | 1.93 | 0.50 |
| 38:6D:287:SER:O | 38:6D:289:MET:N | 2.44 | 0.50 |
| 39:6H:61:ASN:HA | 41:OP:56:GLY:HA2 | 1.94 | 0.50 |
| 40:BF:170:SER:OG | 40:BF:203:MET:SD | 2.69 | 0.50 |
| 40:BH:102:ASN:HB3 | 40:BH:105:ARG:HB2 | 1.94 | 0.50 |
| 41:BO:209:ASP:C | 41:BO:211:CYS:H | 2.14 | 0.50 |
| 40:CG:260:VAL:HG13 | 41:CO:397:TRP:CH2 | 2.46 | 0.50 |
| 40:CH:137:ILE:HD12 | 40:CH:168:GLU:HG3 | 1.92 | 0.50 |
| 40:CI:167:LEU:HD22 | 40:CI:200:CYS:HB2 | 1.94 | 0.50 |
| 41:DB:188:SER:O | 41:DB:189:VAL:C | 2.50 | 0.50 |
| 41:DB:237:THR:HA | 41:DB:240:LEU:HD21 | 1.91 | 0.50 |
| 40:DE:176:GLN:HE22 | 41:DL:347:ASN:HD22 | 1.59 | 0.50 |
| 40:DE:419:GLU:O | 40:DE:422:GLU:HG3 | 2.11 | 0.50 |
| 41:DL:191:GLN:O | 41:DL:195:ASN:HB2 | 2.11 | 0.50 |
| 41:DN:67:ASP:HA | 41:DN:143:THR:HG21 | 1.93 | 0.50 |
| 41:DN:215:LEU:O | 41:DN:217:LEU:N | 2.44 | 0.50 |
| 40:EA:56:THR:HB | 40:EA:60:LYS:HB3 | 1.93 | 0.50 |
| 41:EB:142:GLY:O | 41:EB:144:GLY:N | 2.44 | 0.50 |
| 40:EE:288:VAL:HB | 40:EE:327:ASP:HB3 | 1.93 | 0.50 |
| 40:EH:277:SER:O | 40:EH:278:ALA:C | 2.49 | 0.50 |
| 40:EI:229:ARG:NH2 | 40:EI:366:ASP:HB2 | 2.26 | 0.50 |
| 41:EP:61:PRO:HG2 | 41:EP:84:ILE:HG23 | 1.93 | 0.50 |
| 41:EP:245:GLN:O | 41:EP:246:LEU:C | 2.49 | 0.50 |
| 40:FF:179:THR:HG21 | 41:FM:246:LEU:HD13 | 1.91 | 0.50 |
| 41:FO:289:LEU:HD11 | 41:FO:363:MET:HG2 | 1.92 | 0.50 |
| 41:FO:392:LYS:HD2 | 41:FO:395:LEU:HD13 | 1.93 | 0.50 |
| 41:FP:16:ILE:HD13 | 41:FP:226:ASN:ND2 | 2.24 | 0.50 |
| 40:GA:254:GLU:HA | 40:GA:257:THR:HG22 | 1.92 | 0.50 |
| 41:GB:248:ALA:HA | 41:GB:252:LYS:HD3 | 1.93 | 0.50 |
| 40:GG:102:ASN:ND2 | 40:GG:105:ARG:HD3 | 2.24 | 0.50 |
| 40:GI:85:GLN:O | 40:GI:87:PHE:N | 2.44 | 0.50 |
| 40:GI:217:LEU:O | 40:GI:219:ILE:N | 2.37 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GN:397:TRP:HA | 41:GN:397:TRP:HE3 | 1.75 | 0.50 |
| 41:GO:6:HIS:O | 41:GO:63:ALA:HA | 2.11 | 0.50 |
| 40:HA:273:ALA:HB3 | 40:HA:374:VAL:HG22 | 1.93 | 0.50 |
| 40:HF:20:CYS:HA | 40:HF:232:SER:HB2 | 1.92 | 0.50 |
| 40:HG:35:GLN:OE1 | 40:HG:35:GLN:N | 2.43 | 0.50 |
| 40:HI:318:LEU:O | 40:HI:374:VAL:HA | 2.11 | 0.50 |
| 41:HM:141:GLY:HA2 | 41:HM:178:THR:HG21 | 1.92 | 0.50 |
| 41:HP:286:VAL:HG21 | 41:HP:325:GLU:HB3 | 1.92 | 0.50 |
| 40:IG:274:PRO:HG3 | 40:IG:286:LEU:HD22 | 1.93 | 0.50 |
| 40:IH:26:LEU:HD21 | 40:IH:363:VAL:HG23 | 1.94 | 0.50 |
| 41:IM:222:TYR:O | 41:IM:226:ASN:ND2 | 2.44 | 0.50 |
| 41:IO:142:GLY:O | 41:IO:144:GLY:N | 2.44 | 0.50 |
| 41:IO:202:ILE:HG23 | 41:IO:300:MET:HB3 | 1.93 | 0.50 |
| 40:JD:238:ILE:HA | 40:JD:318:LEU:HD22 | 1.94 | 0.50 |
| 40:JH:228:ASN:ND2 | 42:JO:501:GTP:HN1 | 2.04 | 0.50 |
| 40:KE:98:ASP:OD1 | 40:KE:98:ASP:N | 2.45 | 0.50 |
| 40:KG:205:ASP:HB3 | 40:KG:303:VAL:HA | 1.92 | 0.50 |
| 41:KM:128:ASP:N | 41:KM:128:ASP:OD1 | 2.44 | 0.50 |
| 41:KO:274:THR:HB | 41:KO:282:ARG:HH11 | 1.76 | 0.50 |
| 41:LB:173:PRO:HD2 | 41:LB:205:GLU:HG3 | 1.93 | 0.50 |
| 40:LF:119:LEU:HD11 | 40:LF:156:ARG:HB3 | 1.92 | 0.50 |
| 40:LG:332:ILE:HG23 | 40:LG:351:PHE:CD2 | 2.44 | 0.50 |
| 40:MA:255:PHE:CE1 | 40:MA:318:LEU:HD21 | 2.47 | 0.50 |
| 40:MG:98:ASP:CG | 40:MG:100:ALA:H | 2.15 | 0.50 |
| 41:MN:8:GLN:HE21 | 41:MN:65:LEU:HG | 1.76 | 0.50 |
| 41:MO:262:ARG:O | 41:MO:263:LEU:C | 2.49 | 0.50 |
| 40:NA:247:ALA:HB3 | 40:NA:355:ILE:HB | 1.92 | 0.50 |
| 41:NB:330:MET:HB3 | 41:NB:349:VAL:HG21 | 1.93 | 0.50 |
| 40:NH:8:HIS:CD2 | 40:NH:138:PHE:HB2 | 2.46 | 0.50 |
| 41:NM:41:ASP:OD1 | 41:NM:41:ASP:N | 2.45 | 0.50 |
| 40:OA:241:SER:OG | 40:OA:249:ASN:OD1 | 2.28 | 0.50 |
| 41:OB:143:THR:O | 41:OB:147:MET:N | 2.40 | 0.50 |
| 40:OE:181:VAL:HG23 | 40:OE:182:VAL:HG13 | 1.93 | 0.50 |
| 40:OF:332:ILE:HG23 | 40:OF:351:PHE:HD1 | 1.76 | 0.50 |
| 40:OH:315:CYS:HG | 40:OH:351:PHE:HD2 | 1.57 | 0.50 |
| 41:OL:248:ALA:HA | 41:OL:252:LYS:HD2 | 1.93 | 0.50 |
| 41:ON:319:GLY:HA2 | 41:ON:357:PRO:HG3 | 1.94 | 0.50 |
| 41:PB:172:SER:OG | 41:PB:175:VAL:O | 2.28 | 0.50 |
| 41:PB:324:LYS:HG3 | 41:PB:325:GLU:N | 2.26 | 0.50 |
| 41:PP:398:TYR:HB3 | 41:PP:403:MET:HG3 | 1.93 | 0.50 |
| 40:QA:11:GLN:HG3 | 40:QA:74:VAL:HG21 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QB:181:GLU:O | 41:QB:182:PRO:C | 2.49 | 0.50 |
| 40:QE:311:LYS:NZ | 40:QE:437:ASP:OD1 | 2.44 | 0.50 |
| 41:QP:139:LEU:O | 41:QP:141:GLY:N | 2.44 | 0.50 |
| 41:QP:183:TYR:HD2 | 41:QP:183:TYR:H | 1.59 | 0.50 |
| 40:RA:436:MET:O | 41:RB:391:ARG:NH2 | 2.44 | 0.50 |
| 40:RF:224:TYR:HA | 40:RF:227:LEU:HG | 1.93 | 0.50 |
| 40:RI:180:ALA:HB3 | 40:RI:183:GLU:HG3 | 1.92 | 0.50 |
| 41:SB:139:LEU:HD12 | 41:SB:170:VAL:HG12 | 1.93 | 0.50 |
| 40:SE:55:GLU:OE2 | 40:SE:61:HIS:NE2 | 2.44 | 0.50 |
| 40:SH:138:PHE:HE2 | 40:SH:235:VAL:HG21 | 1.76 | 0.50 |
| 40:SH:139:HIS:NE2 | 40:SH:168:GLU:OE1 | 2.43 | 0.50 |
| 41:SO:318:ARG:HD2 | 41:SO:358:PRO:HD3 | 1.92 | 0.50 |
| 41:SP:379:LYS:O | 41:SP:382:SER:N | 2.44 | 0.50 |
| 41:TB:46:ARG:HH12 | 40:TG:72:PRO:HB2 | 1.75 | 0.50 |
| 40:TG:2:ARG:HH21 | 41:TO:69:GLU:HB2 | 1.75 | 0.50 |
| 40:TH:73:THR:HA | 40:TH:76:ASP:HB2 | 1.92 | 0.50 |
| 40:TH:90:GLU:HB3 | 40:TH:121:ARG:NH2 | 2.26 | 0.50 |
| 40:TH:239:THR:O | 40:TH:243:ARG:NH1 | 2.45 | 0.50 |
| 41:TM:165:ASN:ND2 | 41:TM:250:LEU:HD13 | 2.26 | 0.50 |
| 40:UG:311:LYS:NZ | 40:UG:342:GLN:OE1 | 2.43 | 0.50 |
| 40:UH:298:PRO:HG2 | 40:UH:308:ARG:HD3 | 1.94 | 0.50 |
| 40:UI:400:LYS:O | 40:UI:401:ARG:C | 2.50 | 0.50 |
| 41:VB:222:TYR:O | 41:VB:226:ASN:ND2 | 2.43 | 0.50 |
| 40:VH:109:THR:OG1 | 40:VH:410:GLU:O | 2.29 | 0.50 |
| 40:VJ:62:VAL:HG11 | 40:WI:283:HIS:HB3 | 1.93 | 0.50 |
| 40:WH:240:ALA:HA | 40:WH:243:ARG:HG3 | 1.93 | 0.50 |
| 41:WO:273:LEU:O | 41:WO:292:GLN:NE2 | 2.36 | 0.50 |
| 41:WQ:19:LYS:HG3 | 41:WQ:226:ASN:HB2 | 1.94 | 0.50 |
| 7:1T:512:PRO:HG2 | 7:1T:557:GLY:HA2 | 1.93 | 0.50 |
| 8:1W:480:VAL:HG21 | 40:VG:282:TYR:HE2 | 1.77 | 0.50 |
| 8:1X:140:VAL:CG1 | 8:1X:141:THR:N | 2.74 | 0.50 |
| 11:2I:24:PRO:HB2 | 11:2I:25:PRO:HD3 | 1.92 | 0.50 |
| 12:2M:168:THR:HA | 12:2M:171:VAL:HG22 | 1.93 | 0.50 |
| 13:2T:116:PRO:HG2 | 40:AA:264:ARG:HG2 | 1.93 | 0.50 |
| 21:4D:154:LEU:HD13 | 21:4D:176:ILE:HG21 | 1.93 | 0.50 |
| 21:4E:247:ALA:O | 21:4E:261:THR:HA | 2.11 | 0.50 |
| 21:4E:495:VAL:O | 21:4E:496:ILE:C | 2.50 | 0.50 |
| 22:4I:562:LEU:HD22 | 22:4I:589:LEU:HD21 | 1.93 | 0.50 |
| 22:4K:454:ILE:HG22 | 22:4K:465:VAL:HG22 | 1.93 | 0.50 |
| 23:4M:109:CYS:SG | 40:BG:218:ASP:CG | 2.90 | 0.50 |
| 23:4N:260:THR:CB | 40:EF:219:ILE:HD13 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4Q:199:GLY:H | 40:DH:221:ARG:HB3 | 1.76 | 0.50 |
| 23:4R:195:ARG:HD3 | 40:DI:221:ARG:HH12 | 1.76 | 0.50 |
| 26:4V:343:ARG:HH21 | 26:4V:356:HIS:HA | 1.76 | 0.50 |
| 31:5J:746:THR:N | 31:5J:749:SER:HG | 2.10 | 0.50 |
| 37:6A:113:ARG:HB2 | 40:TH:47:ASP:HB2 | 1.93 | 0.50 |
| 39:6K:99:LEU:HG | 39:6K:103:LYS:HE2 | 1.93 | 0.50 |
| 41:AB:124:ALA:HB1 | 41:AB:130:LEU:HD11 | 1.94 | 0.50 |
| 40:AF:259:LEU:O | 40:AF:379:ASN:ND2 | 2.43 | 0.50 |
| 41:AL:236:VAL:HG22 | 41:AL:368:ILE:HD11 | 1.92 | 0.50 |
| 40:BF:194:THR:O | 40:BF:198:SER:HB2 | 2.11 | 0.50 |
| 40:BG:217:LEU:HD21 | 40:BG:367:LEU:HD23 | 1.93 | 0.50 |
| 40:BI:265:ILE:HG23 | 40:BI:431:TYR:CE1 | 2.46 | 0.50 |
| 40:BI:406:TRP:HZ3 | 41:BP:258:VAL:HB | 1.75 | 0.50 |
| 41:BM:316:VAL:HA | 41:BM:352:ALA:HB3 | 1.93 | 0.50 |
| 41:BN:210:ILE:HD12 | 41:BN:298:ASN:HA | 1.93 | 0.50 |
| 41:BP:152:ILE:HG22 | 41:BP:195:ASN:HB3 | 1.94 | 0.50 |
| 41:CN:238:THR:HA | 41:CN:241:ARG:HH21 | 1.75 | 0.50 |
| 41:CN:268:PRO:HA | 41:CN:368:ILE:HD13 | 1.92 | 0.50 |
| 41:CP:21:TRP:HA | 41:CP:24:ILE:HG12 | 1.92 | 0.50 |
| 41:CP:238:THR:OG1 | 41:CP:239:CYS:N | 2.41 | 0.50 |
| 41:DB:420:ASN:HB2 | 41:DB:421:PRO:HD3 | 1.93 | 0.50 |
| 40:DE:101:ASN:HB3 | 40:DE:182:VAL:HG21 | 1.94 | 0.50 |
| 40:DF:70:LEU:HD12 | 40:DF:145:THR:HB | 1.93 | 0.50 |
| 40:DG:7:VAL:HG23 | 40:DG:66:VAL:HG23 | 1.93 | 0.50 |
| 40:DH:106:GLY:HA2 | 40:DH:110:ILE:O | 2.11 | 0.50 |
| 40:DI:177:VAL:HG13 | 41:DP:327:ASP:HB3 | 1.94 | 0.50 |
| 41:DP:98:GLY:O | 41:DP:99:ASN:C | 2.49 | 0.50 |
| 40:EF:400:LYS:NZ | 41:EM:344:TRP:HB2 | 2.27 | 0.50 |
| 40:EI:4:CYS:SG | 40:EI:51:THR:O | 2.69 | 0.50 |
| 40:FA:5:ILE:HD11 | 40:FA:126:ALA:HB2 | 1.93 | 0.50 |
| 40:FA:106:GLY:C | 40:FA:108:TYR:H | 2.14 | 0.50 |
| 40:FA:223:THR:OG1 | 40:FA:224:TYR:N | 2.41 | 0.50 |
| 40:FE:120:ASP:OD1 | 40:FE:124:LYS:NZ | 2.37 | 0.50 |
| 40:FE:247:ALA:HB3 | 40:FE:355:ILE:HB | 1.92 | 0.50 |
| 40:FG:223:THR:HG23 | 40:FG:225:THR:H | 1.76 | 0.50 |
| 41:FP:43:GLN:N | 41:FP:43:GLN:OE1 | 2.44 | 0.50 |
| 40:HG:17:GLY:HA2 | 40:HG:20:CYS:HB2 | 1.93 | 0.50 |
| 40:IF:56:THR:HG21 | 41:JL:281:TYR:HA | 1.92 | 0.50 |
| 41:IO:215:LEU:HD21 | 41:IO:273:LEU:HD22 | 1.93 | 0.50 |
| 40:JD:294:ALA:O | 40:JD:300:ASN:ND2 | 2.39 | 0.50 |
| 40:JG:3:GLU:OE1 | 40:JG:3:GLU:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JM:25:SER:HG | 41:JM:51:TYR:HH | 1.58 | 0.50 |
| 40:KH:24:TYR:O | 40:KH:28:HIS:HB2 | 2.11 | 0.50 |
| 41:KL:49:VAL:HG21 | 41:KL:240:LEU:O | 2.11 | 0.50 |
| 41:KM:68:LEU:HD23 | 41:KM:112:LEU:HD13 | 1.93 | 0.50 |
| 40:LE:177:VAL:HG11 | 41:LL:327:ASP:HB3 | 1.93 | 0.50 |
| 40:LH:324:VAL:HG12 | 40:LH:326:LYS:H | 1.75 | 0.50 |
| 41:LN:236:VAL:HG23 | 41:LN:237:THR:HG23 | 1.92 | 0.50 |
| 41:MB:67:ASP:OD2 | 41:MB:68:LEU:N | 2.43 | 0.50 |
| 40:ME:323:VAL:HG22 | 40:ME:372:ARG:HG2 | 1.92 | 0.50 |
| 41:MM:198:GLU:HG2 | 41:MM:266:PHE:HE2 | 1.76 | 0.50 |
| 41:MO:311:LEU:HD23 | 41:MO:342:VAL:HG11 | 1.91 | 0.50 |
| 41:MP:377:LEU:HD12 | 41:MP:380:ARG:HH21 | 1.75 | 0.50 |
| 40:NA:88:HIS:NE2 | 40:OA:284:GLU:OE2 | 2.45 | 0.50 |
| 40:NF:273:ALA:HB3 | 40:NF:374:VAL:H | 1.76 | 0.50 |
| 41:OB:86:ARG:HG2 | 41:OB:88:ASP:H | 1.77 | 0.50 |
| 40:OG:20:CYS:HA | 40:OG:232:SER:HB2 | 1.92 | 0.50 |
| 40:OG:88:HIS:HD2 | 40:PG:283:HIS:HB3 | 1.77 | 0.50 |
| 40:OH:209:ILE:HG23 | 40:OH:227:LEU:HD22 | 1.93 | 0.50 |
| 41:OM:244:GLY:O | 41:OM:247:ASN:ND2 | 2.43 | 0.50 |
| 41:OO:42:LEU:HD11 | 41:OO:243:PRO:HG3 | 1.93 | 0.50 |
| 41:QB:1:MET:O | 41:QB:2:ARG:C | 2.48 | 0.50 |
| 41:QB:290:THR:C | 41:QB:292:GLN:H | 2.14 | 0.50 |
| 41:QP:400:GLY:O | 41:QP:401:GLU:C | 2.50 | 0.50 |
| 41:QP:405:GLU:O | 41:QP:408:PHE:HB2 | 2.11 | 0.50 |
| 40:RE:222:PRO:HD2 | 41:RL:324:LYS:HZ1 | 1.76 | 0.50 |
| 40:SE:56:THR:HA | 40:TE:285:GLN:OE1 | 2.10 | 0.50 |
| 40:SF:221:ARG:HH22 | 41:SM:325:GLU:H | 1.60 | 0.50 |
| 40:SH:177:VAL:CG1 | 41:SO:327:ASP:HB3 | 2.42 | 0.50 |
| 41:SM:237:THR:HG23 | 41:SM:240:LEU:HD21 | 1.94 | 0.50 |
| 41:TP:383:GLU:HA | 41:TP:386:THR:HG22 | 1.92 | 0.50 |
| 41:TP:392:LYS:HG3 | 41:TP:395:LEU:HD23 | 1.93 | 0.50 |
| 40:UF:37:PRO:O | 40:UF:39:ASP:N | 2.45 | 0.50 |
| 40:UF:276:ILE:CG1 | 40:UF:280:LYS:HB2 | 2.42 | 0.50 |
| 41:UO:234:SER:OG | 41:UO:241:ARG:NH2 | 2.45 | 0.50 |
| 41:UP:309:ARG:HD3 | 41:UP:342:VAL:HA | 1.93 | 0.50 |
| 41:VB:27:GLU:O | 41:VB:43:GLN:NE2 | 2.43 | 0.50 |
| 40:VF:20:CYS:HA | 40:VF:232:SER:HB2 | 1.94 | 0.50 |
| 40:VI:326:LYS:HA | 40:VI:329:ASN:HB2 | 1.93 | 0.50 |
| 41:VN:211:CYS:HA | 41:VN:215:LEU:HB2 | 1.93 | 0.50 |
| 41:VP:189:VAL:HA | 41:VP:192:LEU:HB2 | 1.92 | 0.50 |
| 40:WI:244:PHE:HB2 | 40:WI:356:ASN:HD21 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WQ:103:LYS:O | 41:WQ:107:THR:OG1 | 2.29 | 0.50 |
| 7:1U:167:SER:OG | 7:1U:217:ASP:OD1 | 2.29 | 0.50 |
| 8:1X:174:LEU:CD1 | 41:UB:33:THR:HG22 | 2.42 | 0.50 |
| 12:2N:38:VAL:HG23 | 12:2N:52:VAL:HG13 | 1.93 | 0.50 |
| 12:2O:212:ASP:HB3 | 13:2W:37:ILE:HD11 | 1.93 | 0.50 |
| 15:3F:132:VAL:HG13 | 15:3F:264:PHE:HE1 | 1.75 | 0.50 |
| 16:3K:123:ARG:NH1 | 16:3K:131:ASP:OD2 | 2.40 | 0.50 |
| 17:3R:320:LYS:HG2 | 17:3R:324:ASP:OD2 | 2.11 | 0.50 |
| 19:3Y:264:ALA:HA | 19:3Y:274:VAL:HG12 | 1.93 | 0.50 |
| 22:4I:615:ASP:O | 22:4I:617:CYS:N | 2.42 | 0.50 |
| 22:4J:627:LEU:O | 22:4J:699:TRP:CZ3 | 2.65 | 0.50 |
| 34:5Q:292:LEU:HD12 | 40:GE:282:TYR:CZ | 2.47 | 0.50 |
| 36:5W:94:VAL:HA | 36:5W:97:ALA:HB3 | 1.93 | 0.50 |
| 38:6C:144:ASN:HB2 | 41:VP:336:LYS:HZ1 | 1.77 | 0.50 |
| 38:6C:198:TYR:CD2 | 38:6C:199:PRO:HD2 | 2.46 | 0.50 |
| 40:AG:97:GLU:HG2 | 40:AG:105:ARG:HH22 | 1.77 | 0.50 |
| 41:AL:211:CYS:HA | 41:AL:215:LEU:HD12 | 1.93 | 0.50 |
| 41:AP:139:LEU:HD22 | 41:AP:170:VAL:HG22 | 1.94 | 0.50 |
| 41:CB:95:SER:OG | 41:CB:96:GLY:N | 2.44 | 0.50 |
| 40:CH:317:LEU:HD11 | 40:CH:351:PHE:HB3 | 1.92 | 0.50 |
| 41:CL:172:SER:O | 41:CL:173:PRO:C | 2.49 | 0.50 |
| 40:DA:219:ILE:O | 40:DA:220:GLU:C | 2.50 | 0.50 |
| 40:DA:225:THR:HA | 40:DA:228:ASN:ND2 | 2.27 | 0.50 |
| 41:DB:293:MET:C | 41:DB:295:ASP:H | 2.15 | 0.50 |
| 40:DE:261:PRO:HB3 | 40:DE:346:TRP:CH2 | 2.44 | 0.50 |
| 40:DF:180:ALA:HB3 | 40:DF:183:GLU:HG3 | 1.94 | 0.50 |
| 40:DG:271:THR:HB | 40:DG:376:MET:HB3 | 1.92 | 0.50 |
| 40:DI:216:ASN:O | 40:DI:218:ASP:N | 2.44 | 0.50 |
| 41:DN:188:SER:O | 41:DN:189:VAL:C | 2.50 | 0.50 |
| 41:EB:313:VAL:O | 41:EB:349:VAL:HA | 2.12 | 0.50 |
| 40:EI:210:TYR:HD1 | 41:EP:324:LYS:HG2 | 1.77 | 0.50 |
| 41:EM:13:GLY:O | 41:EM:16:ILE:HG12 | 2.11 | 0.50 |
| 41:EO:313:VAL:HB | 41:EO:349:VAL:HG22 | 1.92 | 0.50 |
| 41:EP:27:GLU:O | 41:EP:28:HIS:C | 2.49 | 0.50 |
| 40:FA:176:GLN:O | 40:FA:177:VAL:C | 2.50 | 0.50 |
| 40:FA:217:LEU:HB3 | 40:FA:219:ILE:CG1 | 2.42 | 0.50 |
| 41:GB:331:LEU:HD12 | 40:GG:177:VAL:HB | 1.92 | 0.50 |
| 41:GO:292:GLN:O | 41:GO:298:ASN:ND2 | 2.44 | 0.50 |
| 40:HA:244:PHE:HD2 | 40:HA:356:ASN:HD21 | 1.60 | 0.50 |
| 42:HB:502:GTP:O2' | 40:HG:206:ASN:OD1 | 2.28 | 0.50 |
| 41:HN:142:GLY:O | 41:HN:144:GLY:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HO:2:ARG:HB3 | 41:HO:131:GLN:NE2 | 2.26 | 0.50 |
| 41:HO:112:LEU:HB3 | 41:HO:147:MET:HE2 | 1.92 | 0.50 |
| 40:IH:182:VAL:O | 40:IH:186:ASN:ND2 | 2.44 | 0.50 |
| 41:IM:107:THR:O | 41:IM:110:ALA:N | 2.34 | 0.50 |
| 41:IO:43:GLN:HA | 41:IO:242:PHE:HE1 | 1.76 | 0.50 |
| 41:IP:178:THR:HB | 41:IP:181:GLU:HG3 | 1.92 | 0.50 |
| 41:JB:99:ASN:HD21 | 41:JB:178:THR:HB | 1.77 | 0.50 |
| 40:JD:5:ILE:HG12 | 40:JD:132:LEU:HD11 | 1.94 | 0.50 |
| 40:JE:4:CYS:HB3 | 40:JE:133:GLN:HB3 | 1.92 | 0.50 |
| 41:JM:204:ASN:HA | 41:JM:207:LEU:HD12 | 1.92 | 0.50 |
| 41:JM:389:PHE:O | 41:JM:392:LYS:N | 2.43 | 0.50 |
| 41:JN:330:MET:HA | 41:JN:333:VAL:HG22 | 1.93 | 0.50 |
| 40:KG:271:THR:OG1 | 40:KG:300:ASN:O | 2.24 | 0.50 |
| 41:KL:180:VAL:O | 41:KL:181:GLU:C | 2.50 | 0.50 |
| 41:KL:362:LYS:HG2 | 41:KL:363:MET:HG3 | 1.93 | 0.50 |
| 40:LA:20:CYS:HA | 40:LA:232:SER:HB2 | 1.92 | 0.50 |
| 40:LD:255:PHE:HZ | 40:LD:318:LEU:HD21 | 1.77 | 0.50 |
| 40:LG:239:THR:O | 40:LG:243:ARG:HG3 | 2.11 | 0.50 |
| 41:LN:180:VAL:HG23 | 41:LN:184:ASN:HD21 | 1.77 | 0.50 |
| 40:MF:139:HIS:NE2 | 40:MF:168:GLU:HB3 | 2.26 | 0.50 |
| 40:MH:16:ILE:HD13 | 40:MH:231:ILE:HG21 | 1.92 | 0.50 |
| 41:MN:67:ASP:OD1 | 41:MN:72:THR:OG1 | 2.29 | 0.50 |
| 41:MO:207:LEU:HA | 41:MO:210:ILE:HD12 | 1.92 | 0.50 |
| 40:ND:88:HIS:HD2 | 40:ND:89:PRO:HD2 | 1.76 | 0.50 |
| 40:ND:102:ASN:HB3 | 40:ND:105:ARG:CB | 2.41 | 0.50 |
| 40:NH:438:SER:HB3 | 41:NP:390:ARG:HH12 | 1.76 | 0.50 |
| 41:NN:25:SER:OG | 41:NN:30:ILE:O | 2.28 | 0.50 |
| 41:NN:232:THR:HG21 | 41:NN:268:PRO:HB2 | 1.94 | 0.50 |
| 41:NO:89:ASN:HA | 41:NO:119:VAL:HG21 | 1.92 | 0.50 |
| 40:OE:31:GLN:HG2 | 40:OE:33:ASP:H | 1.76 | 0.50 |
| 40:OH:174:ALA:HB1 | 40:OH:207:GLU:HG3 | 1.94 | 0.50 |
| 41:OL:396:HIS:HA | 41:OL:399:THR:HG22 | 1.93 | 0.50 |
| 41:ON:39:ASP:OD2 | 41:ON:359:ARG:NH2 | 2.44 | 0.50 |
| 40:PA:205:ASP:HB2 | 40:PA:303:VAL:HA | 1.92 | 0.50 |
| 41:PB:21:TRP:HA | 41:PB:24:ILE:HG22 | 1.94 | 0.50 |
| 40:PE:316:CYS:HA | 40:PE:352:LYS:HB3 | 1.93 | 0.50 |
| 41:PO:27:GLU:OE1 | 41:PO:241:ARG:NH2 | 2.44 | 0.50 |
| 40:QA:88:HIS:CD2 | 40:QA:89:PRO:HD2 | 2.47 | 0.50 |
| 41:QB:170:VAL:HB | 41:QB:171:PRO:CD | 2.41 | 0.50 |
| 41:QB:399:THR:O | 41:QB:400:GLY:C | 2.49 | 0.50 |
| 41:QP:65:LEU:O | 41:QP:91:VAL:HG13 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QP:192:LEU:O | 41:QP:195:ASN:N | 2.44 | 0.50 |
| 40:RE:191:THR:O | 40:RE:195:LEU:HB2 | 2.12 | 0.50 |
| 40:RI:213:CYS:HA | 40:RI:217:LEU:HD12 | 1.92 | 0.50 |
| 41:RN:161:ASP:N | 41:RN:161:ASP:OD2 | 2.44 | 0.50 |
| 40:SE:65:ALA:O | 40:SE:91:GLN:NE2 | 2.39 | 0.50 |
| 40:SF:91:GLN:HE22 | 40:SF:125:LEU:HD11 | 1.77 | 0.50 |
| 41:SN:142:GLY:O | 41:SN:144:GLY:N | 2.45 | 0.50 |
| 41:SO:147:MET:O | 41:SO:148:GLY:C | 2.49 | 0.50 |
| 40:TA:134:GLY:HA3 | 40:TA:165:SER:O | 2.12 | 0.50 |
| 40:TA:371:GLN:OE1 | 40:TA:371:GLN:N | 2.41 | 0.50 |
| 41:TB:262:ARG:NH2 | 41:TB:414:ASN:OD1 | 2.45 | 0.50 |
| 40:TE:231:ILE:HA | 40:TE:234:ILE:HG22 | 1.93 | 0.50 |
| 41:TN:364:SER:OG | 41:TN:365:ALA:N | 2.43 | 0.50 |
| 41:TO:309:ARG:H | 41:TO:372:THR:HG1 | 1.58 | 0.50 |
| 40:UA:7:VAL:O | 40:UA:137:ILE:HA | 2.12 | 0.50 |
| 41:UB:62:ARG:NH1 | 41:UB:123:GLU:OE1 | 2.44 | 0.50 |
| 40:UE:215:ARG:NH2 | 40:UE:299:ALA:O | 2.45 | 0.50 |
| 40:UF:432:GLU:C | 40:UF:434:VAL:H | 2.14 | 0.50 |
| 40:UI:54:SER:OG | 40:UI:55:GLU:N | 2.45 | 0.50 |
| 40:VJ:195:LEU:O | 40:VJ:266:HIS:NE2 | 2.39 | 0.50 |
| 40:WE:342:GLN:NE2 | 40:WE:343:PHE:O | 2.44 | 0.50 |
| 40:WH:5:ILE:HD13 | 40:WH:64:ARG:HB3 | 1.93 | 0.50 |
| 41:WO:210:ILE:O | 41:WO:214:THR:OG1 | 2.27 | 0.50 |
| 7:1S:524:ARG:HD3 | 7:1S:546:GLY:H | 1.77 | 0.50 |
| 8:1W:305:GLN:HA | 8:1W:308:LYS:HE2 | 1.93 | 0.50 |
| 8:1X:294:GLU:OE2 | 8:1X:297:ARG:NH2 | 2.45 | 0.50 |
| 14:3A:108:GLY:O | 40:LF:159:VAL:HG13 | 2.12 | 0.50 |
| 16:3K:261:THR:OG1 | 16:3K:394:ARG:NH2 | 2.42 | 0.50 |
| 18:3T:325:THR:HG23 | 18:3U:71:ARG:HH22 | 1.77 | 0.50 |
| 19:3Y:186:GLU:OE2 | 41:KN:55:THR:OG1 | 2.29 | 0.50 |
| 21:4E:462:ILE:O | 21:4E:463:GLY:C | 2.50 | 0.50 |
| 21:4E:472:VAL:HG11 | 21:4E:498:VAL:HB | 1.94 | 0.50 |
| 23:4M:109:CYS:SG | 40:BG:218:ASP:OD1 | 2.70 | 0.50 |
| 23:4M:238:HIS:O | 23:4M:240:LEU:HG | 2.12 | 0.50 |
| 23:4M:240:LEU:HD13 | 23:4M:266:HIS:HA | 1.93 | 0.50 |
| 23:4R:113:TRP:O | 23:4R:114:ALA:C | 2.49 | 0.50 |
| 26:4W:362:GLU:O | 26:4W:364:GLY:N | 2.44 | 0.50 |
| 27:4Z:56:LEU:HD11 | 27:4Z:71:MET:HE2 | 1.94 | 0.50 |
| 30:5G:33:ASN:HD22 | 41:GN:227:HIS:CE1 | 2.29 | 0.50 |
| 31:5I:292:ILE:HG22 | 31:5I:313:VAL:HG23 | 1.92 | 0.50 |
| 41:AB:132:GLY:HA3 | 41:AB:163:ILE:O | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AB:382:SER:OG | 41:AB:412:GLU:OE2 | 2.21 | 0.50 |
| 40:AE:168:GLU:HB2 | 40:AE:201:ALA:HA | 1.94 | 0.50 |
| 40:AG:178:SER:OG | 40:AG:183:GLU:OE1 | 2.29 | 0.50 |
| 40:BI:273:ALA:O | 40:BI:275:VAL:N | 2.45 | 0.50 |
| 41:BM:36:TYR:HB2 | 41:BM:59:TYR:HE1 | 1.75 | 0.50 |
| 41:BM:98:GLY:O | 41:BM:100:ASN:HB2 | 2.11 | 0.50 |
| 41:BM:189:VAL:O | 41:BM:190:HIS:C | 2.50 | 0.50 |
| 41:BM:317:PHE:HB3 | 41:BM:321:MET:SD | 2.51 | 0.50 |
| 41:BP:286:VAL:HB | 41:BP:287:PRO:HD3 | 1.93 | 0.50 |
| 41:BP:420:ASN:HB2 | 41:BP:421:PRO:HD3 | 1.93 | 0.50 |
| 40:CA:305:CYS:O | 40:CA:306:ASP:C | 2.49 | 0.50 |
| 41:CB:211:CYS:HA | 41:CB:215:LEU:HB2 | 1.94 | 0.50 |
| 40:CE:217:LEU:HA | 40:CE:277:SER:HB3 | 1.93 | 0.50 |
| 40:CH:105:ARG:HA | 40:CH:109:THR:CG2 | 2.41 | 0.50 |
| 41:CL:13:GLY:HA3 | 41:CL:136:THR:O | 2.12 | 0.50 |
| 41:CM:192:LEU:HA | 41:CM:196:THR:HG23 | 1.93 | 0.50 |
| 41:CP:139:LEU:HA | 41:CP:145:SER:HB2 | 1.92 | 0.50 |
| 40:DA:253:THR:O | 40:DA:254:GLU:C | 2.50 | 0.50 |
| 40:DA:402:ALA:O | 40:DA:404:VAL:N | 2.43 | 0.50 |
| 41:DB:185:ALA:HB1 | 41:DB:381:ILE:HD11 | 1.94 | 0.50 |
| 40:DE:348:PRO:HB2 | 41:DM:384:GLN:OE1 | 2.12 | 0.50 |
| 40:DI:118:VAL:HG21 | 40:DI:149:PHE:HZ | 1.76 | 0.50 |
| 40:DI:210:TYR:O | 40:DI:211:ASP:C | 2.50 | 0.50 |
| 41:DP:36:TYR:CZ | 41:DP:44:LEU:HB2 | 2.46 | 0.50 |
| 41:EB:156:ARG:HD3 | 41:EB:164:MET:HG3 | 1.94 | 0.50 |
| 40:EE:174:ALA:HB3 | 40:EE:177:VAL:HG12 | 1.91 | 0.50 |
| 40:EH:13:GLY:O | 40:EH:16:ILE:HG12 | 2.11 | 0.50 |
| 41:EP:178:THR:CG2 | 41:EP:180:VAL:HG22 | 2.41 | 0.50 |
| 40:FA:240:ALA:HA | 40:FA:243:ARG:HG2 | 1.94 | 0.50 |
| 41:FB:131:GLN:HE22 | 41:FB:249:ASP:HB3 | 1.76 | 0.50 |
| 40:FE:271:THR:HG22 | 40:FE:376:MET:HB3 | 1.93 | 0.50 |
| 40:FG:326:LYS:HZ2 | 41:FO:212:PHE:HB2 | 1.76 | 0.50 |
| 40:FI:176:GLN:HG2 | 40:FI:177:VAL:HG13 | 1.93 | 0.50 |
| 40:GA:244:PHE:HD2 | 40:GA:356:ASN:HD21 | 1.58 | 0.50 |
| 41:GB:236:VAL:HG13 | 41:GB:237:THR:HG23 | 1.94 | 0.50 |
| 41:GB:274:THR:OG1 | 41:GB:279:GLN:OE1 | 2.27 | 0.50 |
| 40:GF:217:LEU:HA | 40:GF:277:SER:HB3 | 1.92 | 0.50 |
| 40:GH:224:TYR:O | 40:GH:225:THR:C | 2.50 | 0.50 |
| 40:GH:362:VAL:HG11 | 40:GH:369:LYS:HG3 | 1.93 | 0.50 |
| 40:GI:31:GLN:HE21 | 40:GI:37:PRO:HG3 | 1.77 | 0.50 |
| 40:GI:223:THR:HB | 40:GI:225:THR:HG22 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GI:411:GLY:O | 40:GI:412:MET:C | 2.50 | 0.50 |
| 41:GN:31:ASP:HB2 | 41:GN:32:PRO:HD2 | 1.94 | 0.50 |
| 40:HA:90:GLU:N | 40:HA:90:GLU:OE2 | 2.44 | 0.50 |
| 40:HF:228:ASN:ND2 | 42:HM:501:GTP:HN1 | 2.08 | 0.50 |
| 40:HF:370:VAL:HG22 | 40:HF:372:ARG:H | 1.77 | 0.50 |
| 41:HM:234:SER:O | 41:HM:238:THR:OG1 | 2.29 | 0.50 |
| 40:IF:105:ARG:HG2 | 40:IF:410:GLU:HG2 | 1.94 | 0.50 |
| 40:II:325:PRO:HA | 40:II:328:VAL:HG12 | 1.94 | 0.50 |
| 41:IM:285:THR:HB | 41:IM:287:PRO:HD2 | 1.93 | 0.50 |
| 41:IO:268:PRO:HG2 | 41:IO:300:MET:HB2 | 1.92 | 0.50 |
| 41:IP:237:THR:HG22 | 41:IP:250:LEU:HD21 | 1.94 | 0.50 |
| 41:JL:58:LYS:HD3 | 41:KL:281:TYR:CD1 | 2.47 | 0.50 |
| 41:JM:389:PHE:O | 41:JM:390:ARG:C | 2.50 | 0.50 |
| 40:KG:121:ARG:HE | 40:KG:124:LYS:HD2 | 1.77 | 0.50 |
| 40:KH:56:THR:OG1 | 40:KH:57:GLY:N | 2.45 | 0.50 |
| 41:KL:149:THR:HA | 41:KL:152:ILE:HD12 | 1.91 | 0.50 |
| 41:KL:260:PHE:HB2 | 41:KL:263:LEU:HD13 | 1.93 | 0.50 |
| 41:KL:395:LEU:O | 41:KL:396:HIS:C | 2.49 | 0.50 |
| 41:KM:202:ILE:HD13 | 41:KM:229:VAL:HG22 | 1.93 | 0.50 |
| 40:LA:206:ASN:OD1 | 42:LA:501:GTP:O2' | 2.30 | 0.50 |
| 40:MA:70:LEU:HB3 | 40:MA:110:ILE:HD12 | 1.93 | 0.50 |
| 40:MA:100:ALA:O | 40:MA:101:ASN:C | 2.50 | 0.50 |
| 41:MB:202:ILE:HG23 | 41:MB:300:MET:HB3 | 1.93 | 0.50 |
| 40:ME:209:ILE:HG12 | 40:ME:302:MET:HE3 | 1.93 | 0.50 |
| 40:ME:264:ARG:NE | 40:ME:430:ASP:OD2 | 2.42 | 0.50 |
| 41:MO:303:CYS:O | 41:MO:304:ASP:C | 2.50 | 0.50 |
| 40:NA:71:GLU:HB3 | 40:NA:98:ASP:HB2 | 1.92 | 0.50 |
| 40:NA:102:ASN:HB3 | 40:NA:105:ARG:HB2 | 1.93 | 0.50 |
| 40:NA:328:VAL:O | 40:NA:332:ILE:HG12 | 2.12 | 0.50 |
| 40:OD:306:ASP:OD1 | 40:OD:308:ARG:HG2 | 2.12 | 0.50 |
| 40:OE:122:ILE:HG21 | 40:OE:157:LEU:HD11 | 1.93 | 0.50 |
| 40:OH:28:HIS:HE1 | 40:OH:243:ARG:HD2 | 1.77 | 0.50 |
| 40:PA:115:ILE:HA | 40:PA:118:VAL:HG12 | 1.92 | 0.50 |
| 40:PG:2:ARG:HH22 | 41:PO:71:GLY:HA2 | 1.77 | 0.50 |
| 40:PH:34:GLY:HA2 | 40:PH:86:LEU:HD13 | 1.93 | 0.50 |
| 41:QB:24:ILE:HG22 | 41:QB:234:SER:HB2 | 1.93 | 0.50 |
| 41:QB:322:SER:O | 41:QB:324:LYS:N | 2.45 | 0.50 |
| 40:QE:73:THR:OG1 | 41:QL:46:ARG:NH1 | 2.31 | 0.50 |
| 40:QG:51:THR:HG21 | 40:QG:243:ARG:HG2 | 1.92 | 0.50 |
| 40:QG:140:SER:HA | 40:QG:171:ILE:H | 1.76 | 0.50 |
| 40:QG:213:CYS:HA | 40:QG:217:LEU:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QN:309:ARG:NH1 | 41:QN:339:SER:O | 2.44 | 0.50 |
| 41:QP:374:ILE:HG22 | 41:QP:422:VAL:HG21 | 1.93 | 0.50 |
| 40:RI:101:ASN:HD22 | 40:RI:143:GLY:HA2 | 1.77 | 0.50 |
| 41:RN:189:VAL:HG13 | 41:RN:265:PHE:HE1 | 1.75 | 0.50 |
| 41:RN:317:PHE:HE1 | 41:RN:326:VAL:HG13 | 1.74 | 0.50 |
| 40:SE:248:LEU:HB2 | 40:SE:355:ILE:H | 1.76 | 0.50 |
| 40:SH:223:THR:HG23 | 40:SH:225:THR:HG22 | 1.94 | 0.50 |
| 41:SO:322:SER:O | 41:SO:323:MET:C | 2.49 | 0.50 |
| 41:TB:173:PRO:HB3 | 41:TB:380:ARG:HD2 | 1.93 | 0.50 |
| 41:TB:345:ILE:O | 41:TB:348:ASN:ND2 | 2.45 | 0.50 |
| 41:TM:135:LEU:O | 41:TM:166:THR:HA | 2.10 | 0.50 |
| 41:TO:61:PRO:HD2 | 41:TO:84:ILE:HG12 | 1.94 | 0.50 |
| 40:UA:105:ARG:HG2 | 40:UA:410:GLU:HG2 | 1.94 | 0.50 |
| 41:UB:325:GLU:HG3 | 40:UG:221:ARG:NH2 | 2.27 | 0.50 |
| 40:UF:213:CYS:HA | 40:UF:217:LEU:HB2 | 1.94 | 0.50 |
| 40:UI:278:ALA:O | 40:UI:281:ALA:N | 2.44 | 0.50 |
| 40:UI:344:VAL:HG23 | 40:UI:347:CYS:HB2 | 1.93 | 0.50 |
| 40:VJ:10:GLY:HA2 | 40:VJ:145:THR:HG23 | 1.94 | 0.50 |
| 7:1U:345:ALA:HB1 | 7:1U:596:SER:HB2 | 1.94 | 0.50 |
| 8:1Z:480:VAL:HG21 | 40:UG:282:TYR:HE2 | 1.76 | 0.50 |
| 15:3E:320:ARG:NH2 | 15:3E:331:ASP:OD2 | 2.45 | 0.50 |
| 16:3M:183:LEU:O | 16:3M:187:ARG:HG3 | 2.11 | 0.50 |
| 21:4E:301:LEU:HD22 | 21:4E:305:ALA:HB2 | 1.92 | 0.50 |
| 22:4J:670:ASN:O | 22:4J:671:ASP:C | 2.50 | 0.50 |
| 22:4K:556:GLU:O | 22:4K:559:SER:N | 2.37 | 0.50 |
| 23:4M:60:LEU:HA | 40:BG:80:THR:O | 2.12 | 0.50 |
| 23:4Q:218:SER:O | 23:4Q:219:GLN:C | 2.50 | 0.50 |
| 23:4R:248:GLY:HA3 | 41:DP:45:GLU:HG2 | 1.93 | 0.50 |
| 29:5E:108:VAL:HG11 | 40:GE:114:LEU:HD21 | 1.93 | 0.50 |
| 31:5I:432:PHE:CE1 | 40:IG:282:TYR:HE1 | 2.29 | 0.50 |
| 34:5Q:246:GLN:OE1 | 34:5Q:249:ARG:NH2 | 2.44 | 0.50 |
| 34:5Q:266:VAL:HA | 41:GM:276:ARG:HH22 | 1.77 | 0.50 |
| 38:6C:157:ILE:HG12 | 38:6C:158:THR:H | 1.77 | 0.50 |
| 38:6C:171:ASP:O | 38:6C:173:ALA:N | 2.43 | 0.50 |
| 39:6K:122:ASP:HB3 | 39:6K:125:ASN:HB2 | 1.92 | 0.50 |
| 41:AP:330:MET:HB3 | 41:AP:349:VAL:HG11 | 1.93 | 0.50 |
| 41:BM:55:THR:HG23 | 41:CM:283:ALA:HA | 1.94 | 0.50 |
| 41:BN:275:SER:N | 41:BN:278:SER:O | 2.45 | 0.50 |
| 41:CM:12:CYS:SG | 41:CM:13:GLY:N | 2.84 | 0.50 |
| 41:CP:293:MET:HG2 | 41:CP:367:PHE:HB2 | 1.93 | 0.50 |
| 40:DA:59:GLY:O | 40:DA:61:HIS:ND1 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DH:101:ASN:HB3 | 40:DH:182:VAL:CG2 | 2.41 | 0.50 |
| 40:DH:309:HIS:HE1 | 40:DH:385:GLU:HG2 | 1.76 | 0.50 |
| 40:DH:356:ASN:OD1 | 40:DH:356:ASN:N | 2.45 | 0.50 |
| 40:DI:123:ARG:O | 40:DI:124:LYS:C | 2.49 | 0.50 |
| 41:DM:50:TYR:HE2 | 41:DM:237:THR:HG21 | 1.77 | 0.50 |
| 41:DM:393:ALA:O | 41:DM:394:PHE:C | 2.49 | 0.50 |
| 41:DP:238:THR:OG1 | 41:DP:239:CYS:N | 2.45 | 0.50 |
| 41:DP:382:SER:O | 41:DP:383:GLU:C | 2.50 | 0.50 |
| 40:EF:318:LEU:O | 40:EF:374:VAL:HA | 2.10 | 0.50 |
| 40:EG:138:PHE:HZ | 40:EG:235:VAL:HG21 | 1.77 | 0.50 |
| 40:EH:191:THR:O | 40:EH:194:THR:N | 2.44 | 0.50 |
| 40:EI:217:LEU:O | 40:EI:218:ASP:C | 2.49 | 0.50 |
| 41:EL:26:ASP:OD1 | 41:EL:359:ARG:NH2 | 2.37 | 0.50 |
| 41:EN:52:ASN:OD1 | 41:EN:62:ARG:NH2 | 2.40 | 0.50 |
| 40:FF:286:LEU:HD21 | 40:FF:371:GLN:H | 1.76 | 0.50 |
| 40:FG:7:VAL:O | 40:FG:137:ILE:HA | 2.12 | 0.50 |
| 40:FI:76:ASP:OD2 | 41:FP:46:ARG:NH2 | 2.37 | 0.50 |
| 41:GB:117:LEU:HD11 | 41:GB:154:LYS:HB3 | 1.92 | 0.50 |
| 40:GE:188:ILE:HG22 | 40:GE:420:ALA:HB1 | 1.93 | 0.50 |
| 40:GE:262:TYR:HE1 | 41:GM:393:ALA:HA | 1.75 | 0.50 |
| 40:GI:107:HIS:HA | 40:GI:152:LEU:HD22 | 1.94 | 0.50 |
| 41:GM:103:LYS:HA | 41:GM:107:THR:HG22 | 1.94 | 0.50 |
| 40:HE:246:GLY:HA2 | 40:HE:357:TYR:HB2 | 1.94 | 0.50 |
| 40:HH:433:GLU:O | 41:HP:391:ARG:NH2 | 2.44 | 0.50 |
| 41:HP:139:LEU:HD22 | 41:HP:170:VAL:HG22 | 1.93 | 0.50 |
| 40:IA:326:LYS:HZ3 | 41:IB:225:LEU:HD21 | 1.75 | 0.50 |
| 41:IB:39:ASP:N | 41:IB:39:ASP:OD1 | 2.44 | 0.50 |
| 40:JE:196:GLU:OE2 | 40:JE:196:GLU:N | 2.44 | 0.50 |
| 40:JF:11:GLN:HA | 40:JF:74:VAL:HG11 | 1.92 | 0.50 |
| 40:JF:260:VAL:HB | 41:JN:397:TRP:HH2 | 1.76 | 0.50 |
| 40:KD:36:MET:SD | 40:KD:61:HIS:NE2 | 2.79 | 0.50 |
| 40:KG:102:ASN:HB3 | 40:KG:105:ARG:HB2 | 1.93 | 0.50 |
| 41:KL:61:PRO:HG2 | 41:KL:84:ILE:HG23 | 1.93 | 0.50 |
| 41:KL:144:GLY:O | 41:KL:148:GLY:HA3 | 2.11 | 0.50 |
| 41:KM:161:ASP:OD2 | 41:KM:162:ARG:NH1 | 2.45 | 0.50 |
| 41:LB:2:ARG:NH1 | 40:LG:72:PRO:HD2 | 2.26 | 0.50 |
| 40:LE:329:ASN:HB3 | 41:LM:175:VAL:HG11 | 1.93 | 0.50 |
| 40:MF:223:THR:OG1 | 40:MF:224:TYR:N | 2.43 | 0.50 |
| 41:MM:142:GLY:O | 41:MM:144:GLY:N | 2.45 | 0.50 |
| 41:MO:20:PHE:HA | 41:MO:230:SER:HB3 | 1.92 | 0.50 |
| 41:MO:317:PHE:HB3 | 41:MO:321:MET:SD | 2.52 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NA:319:TYR:HB3 | 40:NA:323:VAL:HG21 | 1.92 | 0.50 |
| 40:NA:387:TRP:CD1 | 40:NA:431:TYR:HE2 | 2.29 | 0.50 |
| 41:NB:164:MET:HB2 | 41:NB:196:THR:HA | 1.94 | 0.50 |
| 41:NB:305:PRO:HB3 | 41:NB:310:TYR:HE2 | 1.76 | 0.50 |
| 40:ND:413:GLU:O | 40:ND:416:GLU:N | 2.41 | 0.50 |
| 40:NG:329:ASN:OD1 | 40:NG:330:ALA:N | 2.45 | 0.50 |
| 40:NH:7:VAL:HG13 | 40:NH:66:VAL:HB | 1.93 | 0.50 |
| 40:OA:219:ILE:HG13 | 40:OA:222:PRO:HG3 | 1.94 | 0.50 |
| 41:OB:202:ILE:HD13 | 41:OB:229:VAL:HG13 | 1.94 | 0.50 |
| 40:OD:326:LYS:HA | 40:OD:328:VAL:HB | 1.94 | 0.50 |
| 40:OH:403:PHE:HE1 | 41:OO:345:ILE:HD13 | 1.77 | 0.50 |
| 40:PD:8:HIS:CE1 | 40:PD:21:TRP:HE1 | 2.29 | 0.50 |
| 40:PE:2:ARG:HB2 | 40:PE:242:LEU:HD11 | 1.94 | 0.50 |
| 40:PG:102:ASN:HB3 | 40:PG:105:ARG:HB3 | 1.94 | 0.50 |
| 41:QB:181:GLU:HB3 | 41:QB:182:PRO:HD3 | 1.93 | 0.50 |
| 40:QE:141:PHE:HB2 | 40:QE:173:PRO:HD3 | 1.93 | 0.50 |
| 41:QL:49:VAL:O | 41:QL:62:ARG:NH2 | 2.45 | 0.50 |
| 41:QL:107:THR:O | 41:QL:110:ALA:N | 2.43 | 0.50 |
| 41:QM:165:ASN:ND2 | 41:QM:198:GLU:OE1 | 2.45 | 0.50 |
| 40:RA:49:PHE:HE2 | 40:RA:55:GLU:HB2 | 1.76 | 0.50 |
| 41:RM:171:PRO:HG3 | 41:RM:181:GLU:HB3 | 1.93 | 0.50 |
| 41:SB:385:PHE:HZ | 41:SB:408:PHE:HB3 | 1.76 | 0.50 |
| 41:SB:396:HIS:O | 41:SB:397:TRP:C | 2.50 | 0.50 |
| 40:SI:225:THR:O | 40:SI:229:ARG:HB3 | 2.11 | 0.50 |
| 41:SL:239:CYS:HB3 | 41:SL:247:ASN:HB2 | 1.94 | 0.50 |
| 41:SL:282:ARG:HE | 41:SL:284:LEU:HD23 | 1.77 | 0.50 |
| 40:TE:287:SER:N | 40:TE:290:GLU:OE2 | 2.37 | 0.50 |
| 40:TF:116:ASP:N | 40:TF:116:ASP:OD1 | 2.44 | 0.50 |
| 41:TL:337:ASN:HB3 | 41:TL:340:TYR:HB2 | 1.92 | 0.50 |
| 40:UF:293:ASN:HD22 | 40:UF:335:ILE:HD11 | 1.76 | 0.50 |
| 40:UH:20:CYS:HA | 40:UH:232:SER:HB2 | 1.94 | 0.50 |
| 40:UI:81:GLY:O | 40:UI:82:THR:C | 2.50 | 0.50 |
| 41:UO:313:VAL:HB | 41:UO:349:VAL:HG22 | 1.93 | 0.50 |
| 40:VF:136:LEU:HD22 | 40:VF:169:PHE:HE2 | 1.75 | 0.50 |
| 40:VI:238:ILE:HG13 | 40:VI:255:PHE:HE1 | 1.77 | 0.50 |
| 40:WE:191:THR:HA | 40:WE:194:THR:HG22 | 1.93 | 0.50 |
| 40:WF:260:VAL:HB | 41:WN:397:TRP:HZ3 | 1.77 | 0.50 |
| 40:WF:276:ILE:HG23 | 40:WF:280:LYS:HB2 | 1.94 | 0.50 |
| 40:WI:247:ALA:HB3 | 40:WI:355:ILE:HD11 | 1.94 | 0.50 |
| 41:WM:132:GLY:HA2 | 41:WM:162:ARG:HB3 | 1.93 | 0.50 |
| 41:WN:129:CYS:O | 41:WN:130:LEU:C | 2.49 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1S:373:PRO:HG2 | 10:2F:137:LYS:HA | 1.94 | 0.50 |
| 7:1T:69:CYS:O | 7:1T:81:SER:HA | 2.12 | 0.50 |
| 11:2I:109:ASN:OD1 | 41:LB:425:ARG:NH2 | 2.45 | 0.50 |
| 11:2J:37:ASP:OD1 | 11:2J:40:GLN:NE2 | 2.45 | 0.50 |
| 15:3E:198:ILE:HG22 | 15:3F:311:LYS:HB3 | 1.92 | 0.50 |
| 17:3R:251:GLN:O | 17:3R:252:HIS:C | 2.48 | 0.50 |
| 22:4J:633:GLU:O | 22:4J:634:ASN:C | 2.50 | 0.50 |
| 22:4J:701:ALA:O | 22:4J:702:ASN:C | 2.49 | 0.50 |
| 24:4O:171:PRO:C | 24:4O:173:SER:H | 2.15 | 0.50 |
| 23:4R:38:GLY:O | 23:4R:39:GLN:C | 2.48 | 0.50 |
| 30:5G:32:GLY:HA3 | 34:5Q:215:ARG:HD3 | 1.92 | 0.50 |
| 31:5I:304:THR:OG1 | 40:IF:369:LYS:NZ | 2.42 | 0.50 |
| 33:5N:291:THR:HA | 33:5N:294:LYS:HE2 | 1.94 | 0.50 |
| 34:5R:429:LEU:O | 34:5R:430:ASN:C | 2.50 | 0.50 |
| 36:5W:130:LEU:HD12 | 36:5W:135:GLU:HB3 | 1.93 | 0.50 |
| 41:AO:187:LEU:HD11 | 41:AO:408:PHE:CE2 | 2.46 | 0.50 |
| 41:AO:213:ARG:O | 41:AO:216:LYS:HG2 | 2.12 | 0.50 |
| 40:BE:72:PRO:O | 40:BE:73:THR:C | 2.49 | 0.50 |
| 40:BI:315:CYS:HA | 40:BI:378:SER:HA | 1.93 | 0.50 |
| 41:BM:319:GLY:HA2 | 41:BM:357:PRO:HB3 | 1.93 | 0.50 |
| 41:BN:36:TYR:OH | 41:BN:40:SER:O | 2.22 | 0.50 |
| 41:BN:187:LEU:O | 41:BN:191:GLN:NE2 | 2.45 | 0.50 |
| 41:BP:189:VAL:HG11 | 41:BP:415:MET:CE | 2.42 | 0.50 |
| 41:BP:285:THR:O | 41:BP:286:VAL:C | 2.49 | 0.50 |
| 40:CE:21:TRP:CH2 | 40:CE:52:PHE:HB3 | 2.47 | 0.50 |
| 41:CL:129:CYS:O | 41:CL:130:LEU:C | 2.49 | 0.50 |
| 41:CN:202:ILE:HD13 | 41:CN:229:VAL:HG11 | 1.93 | 0.50 |
| 41:CN:306:ARG:O | 41:CN:308:GLY:N | 2.45 | 0.50 |
| 41:CP:299:MET:O | 41:CP:301:ALA:N | 2.44 | 0.50 |
| 40:DA:294:ALA:O | 40:DA:295:CYS:C | 2.50 | 0.50 |
| 41:DB:109:GLY:O | 41:DB:110:ALA:C | 2.49 | 0.50 |
| 41:DB:392:LYS:HB3 | 41:DB:395:LEU:HD11 | 1.93 | 0.50 |
| 40:DE:397:MET:O | 40:DE:400:LYS:N | 2.43 | 0.50 |
| 40:DG:329:ASN:ND2 | 41:DO:205:GLU:OE2 | 2.44 | 0.50 |
| 41:DL:6:HIS:HA | 41:DL:134:GLN:HG3 | 1.93 | 0.50 |
| 41:DN:204:ASN:ND2 | 43:DN:501:GDP:N3 | 2.59 | 0.50 |
| 40:EE:332:ILE:HA | 40:EE:335:ILE:HG12 | 1.94 | 0.50 |
| 40:EF:76:ASP:HA | 40:EF:79:ARG:HG2 | 1.94 | 0.50 |
| 41:EL:77:ARG:HA | 41:EL:82:GLY:HA3 | 1.94 | 0.50 |
| 41:EL:167:PHE:HE1 | 41:EL:233:MET:HG2 | 1.77 | 0.50 |
| 41:EL:314:ALA:HA | 41:EL:350:LYS:HG2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EM:14:ASN:HB3 | 41:EM:76:VAL:CG2 | 2.33 | 0.50 |
| 41:EP:151:LEU:O | 41:EP:155:ILE:HG23 | 2.11 | 0.50 |
| 41:EP:420:ASN:O | 41:EP:421:PRO:C | 2.49 | 0.50 |
| 40:FF:168:GLU:OE1 | 40:FF:170:SER:OG | 2.20 | 0.50 |
| 40:FG:53:PHE:HB3 | 40:FG:61:HIS:HB3 | 1.93 | 0.50 |
| 40:HA:224:TYR:CE2 | 41:HN:323:MET:HG2 | 2.47 | 0.50 |
| 41:HM:337:ASN:HB2 | 41:HM:340:TYR:HD2 | 1.77 | 0.50 |
| 41:HO:114:ASP:OD1 | 41:HO:114:ASP:N | 2.45 | 0.50 |
| 40:IA:70:LEU:HD12 | 40:IA:110:ILE:HG12 | 1.94 | 0.50 |
| 40:IF:136:LEU:HG | 40:IF:169:PHE:HE2 | 1.76 | 0.50 |
| 41:IO:202:ILE:HG21 | 41:IO:229:VAL:HG22 | 1.94 | 0.50 |
| 41:IP:7:LEU:O | 41:IP:135:LEU:HA | 2.11 | 0.50 |
| 40:JD:140:SER:HA | 40:JD:171:ILE:HB | 1.94 | 0.50 |
| 40:JD:141:PHE:HB2 | 40:JD:173:PRO:HD3 | 1.93 | 0.50 |
| 40:JE:2:ARG:HH11 | 40:JE:242:LEU:HA | 1.76 | 0.50 |
| 41:JO:137:HIS:HE1 | 41:JO:166:THR:HB | 1.76 | 0.50 |
| 40:KD:168:GLU:HB2 | 40:KD:201:ALA:HA | 1.94 | 0.50 |
| 40:KF:406:TRP:CE2 | 41:KM:255:VAL:HA | 2.46 | 0.50 |
| 41:KP:385:PHE:HZ | 41:KP:408:PHE:HB3 | 1.76 | 0.50 |
| 40:LE:221:ARG:HG2 | 41:LL:322:SER:HB3 | 1.92 | 0.50 |
| 40:LE:224:TYR:HB3 | 42:LL:501:GTP:N1 | 2.26 | 0.50 |
| 40:LF:222:PRO:HD2 | 41:LM:324:LYS:HD3 | 1.94 | 0.50 |
| 41:LN:156:ARG:NH1 | 41:LN:195:ASN:O | 2.45 | 0.50 |
| 41:LO:311:LEU:HD23 | 41:LO:342:VAL:HG11 | 1.94 | 0.50 |
| 41:LP:58:LYS:NZ | 41:MP:280:GLN:OE1 | 2.44 | 0.50 |
| 40:MA:288:VAL:HG21 | 40:MA:323:VAL:HG13 | 1.94 | 0.50 |
| 40:MF:109:THR:OG1 | 40:MF:410:GLU:OE1 | 2.29 | 0.50 |
| 41:ML:207:LEU:HB3 | 41:ML:225:LEU:HD22 | 1.93 | 0.50 |
| 41:MM:156:ARG:NE | 41:MM:195:ASN:O | 2.38 | 0.50 |
| 41:MM:263:LEU:HD21 | 41:MM:421:PRO:HB2 | 1.94 | 0.50 |
| 41:MN:101:TRP:HB2 | 41:MN:184:ASN:HD22 | 1.75 | 0.50 |
| 41:NN:31:ASP:OD1 | 41:NN:35:THR:N | 2.45 | 0.50 |
| 41:NP:27:GLU:OE1 | 41:NP:318:ARG:NH2 | 2.26 | 0.50 |
| 40:OH:133:GLN:HA | 40:OH:164:LYS:HD2 | 1.92 | 0.50 |
| 40:PD:136:LEU:HD13 | 40:PD:167:LEU:HB2 | 1.93 | 0.50 |
| 40:PD:239:THR:OG1 | 40:PD:243:ARG:NH2 | 2.43 | 0.50 |
| 40:PF:2:ARG:HH11 | 40:PF:242:LEU:HD13 | 1.76 | 0.50 |
| 40:PG:244:PHE:HD2 | 40:PG:356:ASN:HD21 | 1.60 | 0.50 |
| 40:PH:24:TYR:HA | 40:PH:27:GLU:HG3 | 1.93 | 0.50 |
| 40:QE:20:CYS:HA | 40:QE:232:SER:HB2 | 1.94 | 0.50 |
| 40:QH:332:ILE:HA | 40:QH:335:ILE:HD12 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QM:173:PRO:HB3 | 41:QM:380:ARG:HG2 | 1.93 | 0.50 |
| 41:QP:100:ASN:O | 41:QP:101:TRP:C | 2.50 | 0.50 |
| 41:QP:110:ALA:C | 41:QP:112:LEU:H | 2.15 | 0.50 |
| 41:QP:148:GLY:O | 41:QP:149:THR:C | 2.50 | 0.50 |
| 40:RF:174:ALA:HB3 | 40:RF:178:SER:H | 1.75 | 0.50 |
| 41:RN:372:THR:OG1 | 41:RN:422:VAL:O | 2.28 | 0.50 |
| 40:SI:151:SER:OG | 40:SI:190:THR:OG1 | 2.24 | 0.50 |
| 41:SO:286:VAL:HB | 41:SO:325:GLU:HG2 | 1.94 | 0.50 |
| 41:SP:215:LEU:HD21 | 41:SP:273:LEU:HD22 | 1.93 | 0.50 |
| 40:TE:180:ALA:HB3 | 40:TE:183:GLU:HG3 | 1.93 | 0.50 |
| 40:TG:239:THR:O | 40:TG:243:ARG:NH1 | 2.44 | 0.50 |
| 40:TH:212:ILE:HD11 | 40:TH:275:VAL:HG21 | 1.94 | 0.50 |
| 40:TI:140:SER:OG | 42:TI:501:GTP:O1A | 2.26 | 0.50 |
| 40:TI:251:ASP:N | 40:TI:251:ASP:OD1 | 2.42 | 0.50 |
| 40:UA:90:GLU:HG2 | 40:UA:121:ARG:HH12 | 1.77 | 0.50 |
| 40:UA:226:ASN:ND2 | 40:UA:366:ASP:OD2 | 2.44 | 0.50 |
| 40:UG:215:ARG:NH2 | 40:UG:299:ALA:O | 2.45 | 0.50 |
| 40:UH:209:ILE:HG21 | 40:UH:227:LEU:HA | 1.94 | 0.50 |
| 40:UH:426:ALA:HA | 40:UH:429:LYS:HE2 | 1.93 | 0.50 |
| 40:UI:88:HIS:HB2 | 40:VJ:283:HIS:CB | 2.42 | 0.50 |
| 40:VH:6:SER:O | 40:VH:65:ALA:HA | 2.10 | 0.50 |
| 40:VI:70:LEU:HD23 | 40:VI:114:LEU:HD12 | 1.93 | 0.50 |
| 40:VJ:167:LEU:HD22 | 40:VJ:200:CYS:HB3 | 1.93 | 0.50 |
| 40:WA:323:VAL:HG22 | 40:WA:372:ARG:HG2 | 1.93 | 0.50 |
| 40:WE:401:ARG:NH1 | 40:WE:414:GLU:OE2 | 2.45 | 0.50 |
| 40:WI:98:ASP:O | 40:WI:105:ARG:NH1 | 2.44 | 0.50 |
| 41:WM:139:LEU:HD22 | 41:WM:170:VAL:HG12 | 1.92 | 0.50 |
| 7:1T:264:LEU:HD23 | 7:1T:281:TYR:HE1 | 1.75 | 0.50 |
| 7:1T:321:ASP:O | 7:1T:322:PHE:C | 2.50 | 0.50 |
| 8:1W:451:GLN:O | 8:1W:455:ILE:HG12 | 2.12 | 0.50 |
| 8:1Z:528:LEU:HD21 | 8:1Z:532:TYR:HB2 | 1.94 | 0.50 |
| 11:2I:187:ARG:HA | 11:2I:187:ARG:CZ | 2.42 | 0.50 |
| 17:3O:371:GLU:HG3 | 17:3R:114:ARG:HB3 | 1.94 | 0.50 |
| 20:4B:248:ILE:HG22 | 20:4B:249:THR:HG23 | 1.94 | 0.50 |
| 23:4M:253:TYR:O | 40:EG:221:ARG:NH2 | 2.45 | 0.50 |
| 23:4N:216:MET:O | 23:4N:219:GLN:N | 2.45 | 0.50 |
| 23:4N:261:TYR:HB2 | 40:EF:218:ASP:OD2 | 2.12 | 0.50 |
| 23:4Q:174:MET:HB2 | 23:4Q:180:ARG:O | 2.12 | 0.50 |
| 23:4Q:244:PRO:HA | 23:4Q:261:TYR:HD2 | 1.75 | 0.50 |
| 34:5Q:215:ARG:NH2 | 41:GN:217:LEU:HD21 | 2.26 | 0.50 |
| 38:6C:58:GLN:HE22 | 40:UA:117:LEU:HD21 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:6F:48:ILE:HB | 39:6F:108:HIS:HA | 1.92 | 0.50 |
| 39:6I:32:GLU:OE2 | 39:6I:35:ARG:NH2 | 2.45 | 0.50 |
| 39:6J:31:LEU:HD23 | 39:6J:136:TYR:HE1 | 1.77 | 0.50 |
| 41:AB:309:ARG:NH1 | 41:AB:426:GLY:O | 2.43 | 0.50 |
| 40:AG:332:ILE:HG23 | 40:AG:351:PHE:HD2 | 1.75 | 0.50 |
| 41:AL:237:THR:O | 41:AL:241:ARG:NH1 | 2.45 | 0.50 |
| 41:AP:64:VAL:HG12 | 41:AP:89:ASN:HB3 | 1.94 | 0.50 |
| 40:BH:324:VAL:HG22 | 41:BP:221:THR:HG22 | 1.94 | 0.50 |
| 41:BN:271:ALA:HB1 | 41:BN:292:GLN:HB3 | 1.93 | 0.50 |
| 41:BO:190:HIS:HD2 | 41:BO:411:ALA:HA | 1.77 | 0.50 |
| 41:BO:334:GLN:HE22 | 41:BO:347:ASN:HA | 1.77 | 0.50 |
| 41:BP:138:SER:O | 41:BP:139:LEU:C | 2.49 | 0.50 |
| 40:CA:123:ARG:HA | 40:CA:161:TYR:OH | 2.12 | 0.50 |
| 41:CB:375:GLN:HE21 | 41:CB:422:VAL:HG13 | 1.76 | 0.50 |
| 40:CI:224:TYR:CE2 | 41:CP:246:LEU:HD11 | 2.47 | 0.50 |
| 41:CO:97:ALA:O | 41:CO:98:GLY:C | 2.49 | 0.50 |
| 41:CO:284:LEU:HG | 41:CO:289:LEU:HD11 | 1.93 | 0.50 |
| 40:DA:232:SER:O | 40:DA:235:VAL:HG12 | 2.11 | 0.50 |
| 40:DA:413:GLU:O | 40:DA:414:GLU:C | 2.49 | 0.50 |
| 41:DB:312:THR:HA | 41:DB:348:ASN:HB2 | 1.92 | 0.50 |
| 40:DE:21:TRP:CZ3 | 40:DE:63:PRO:HB3 | 2.47 | 0.50 |
| 40:DH:385:GLU:HG3 | 40:DH:386:ALA:N | 2.27 | 0.50 |
| 40:DI:305:CYS:O | 40:DI:305:CYS:SG | 2.68 | 0.50 |
| 41:DL:2:ARG:HA | 41:DL:129:CYS:O | 2.11 | 0.50 |
| 41:DL:17:GLY:O | 41:DL:18:ALA:C | 2.50 | 0.50 |
| 41:DL:17:GLY:HA2 | 41:DL:20:PHE:HB3 | 1.94 | 0.50 |
| 41:DL:419:GLY:O | 41:DL:423:VAL:HG13 | 2.11 | 0.50 |
| 41:DN:21:TRP:CZ3 | 41:DN:50:TYR:HB3 | 2.47 | 0.50 |
| 40:EG:212:ILE:HD11 | 40:EG:300:ASN:HA | 1.92 | 0.50 |
| 40:EI:109:THR:HG1 | 40:EI:110:ILE:N | 2.09 | 0.50 |
| 40:EI:374:VAL:HG22 | 40:EI:375:CYS:H | 1.77 | 0.50 |
| 41:EM:226:ASN:HB2 | 43:EM:501:GDP:HN1 | 1.76 | 0.50 |
| 41:EP:131:GLN:HG2 | 41:EP:250:LEU:HD12 | 1.93 | 0.50 |
| 40:FF:271:THR:HA | 40:FF:302:MET:HG2 | 1.93 | 0.50 |
| 40:GA:265:ILE:HG21 | 40:GA:313:MET:HE1 | 1.93 | 0.50 |
| 40:GE:21:TRP:HZ2 | 40:GE:65:ALA:HB2 | 1.77 | 0.50 |
| 40:GF:122:ILE:HD12 | 40:GF:135:PHE:HE2 | 1.75 | 0.50 |
| 40:GG:237:SER:OG | 40:GG:320:ARG:NE | 2.39 | 0.50 |
| 41:GM:215:LEU:HD21 | 41:GM:273:LEU:HD22 | 1.94 | 0.50 |
| 40:HE:72:PRO:O | 40:HE:73:THR:C | 2.50 | 0.50 |
| 40:HI:251:ASP:H | 40:HI:254:GLU:HB2 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HN:135:LEU:HD11 | 41:HN:137:HIS:HB3 | 1.93 | 0.50 |
| 40:IA:314:ALA:N | 40:IA:379:ASN:OD1 | 2.45 | 0.50 |
| 41:IM:312:THR:OG1 | 41:IM:370:ASN:ND2 | 2.32 | 0.50 |
| 40:JF:136:LEU:HD11 | 40:JF:239:THR:HG21 | 1.94 | 0.50 |
| 40:JG:250:VAL:HG11 | 40:JG:318:LEU:HD22 | 1.94 | 0.50 |
| 40:JH:167:LEU:HD13 | 40:JH:202:PHE:HE2 | 1.77 | 0.50 |
| 41:JO:116:VAL:HG11 | 41:JO:151:LEU:HD11 | 1.94 | 0.50 |
| 40:KE:195:LEU:HD21 | 40:KE:427:LEU:HD21 | 1.94 | 0.50 |
| 40:KF:70:LEU:HD23 | 40:KF:114:LEU:HD12 | 1.93 | 0.50 |
| 40:KF:297:GLU:HA | 40:KF:298:PRO:HG2 | 1.93 | 0.50 |
| 41:KN:180:VAL:O | 41:KN:184:ASN:ND2 | 2.45 | 0.50 |
| 41:KO:39:ASP:OD1 | 41:KO:43:GLN:NE2 | 2.44 | 0.50 |
| 41:KP:210:ILE:HG12 | 41:KP:298:ASN:HA | 1.93 | 0.50 |
| 40:LE:70:LEU:HD23 | 40:LE:114:LEU:HD22 | 1.92 | 0.50 |
| 41:LO:6:HIS:O | 41:LO:63:ALA:HA | 2.12 | 0.50 |
| 41:LO:116:VAL:HG11 | 41:LO:151:LEU:HD21 | 1.94 | 0.50 |
| 40:MD:195:LEU:HG | 40:MD:264:ARG:HD2 | 1.94 | 0.50 |
| 41:MN:131:GLN:HE22 | 41:MN:249:ASP:HB2 | 1.76 | 0.50 |
| 40:ND:182:VAL:O | 40:ND:183:GLU:C | 2.50 | 0.50 |
| 40:NG:333:ALA:HB2 | 41:NO:174:LYS:NZ | 2.26 | 0.50 |
| 41:NL:334:GLN:HE22 | 41:NL:347:ASN:HA | 1.75 | 0.50 |
| 41:NM:271:ALA:O | 41:NM:292:GLN:NE2 | 2.45 | 0.50 |
| 41:NO:73:MET:HG3 | 41:NO:92:PHE:HB3 | 1.94 | 0.50 |
| 41:NO:142:GLY:O | 41:NO:144:GLY:N | 2.45 | 0.50 |
| 41:NP:178:THR:N | 41:NP:181:GLU:OE2 | 2.45 | 0.50 |
| 40:OA:362:VAL:HG21 | 40:OA:369:LYS:HA | 1.93 | 0.50 |
| 41:ON:211:CYS:HA | 41:ON:215:LEU:HB2 | 1.94 | 0.50 |
| 40:PA:102:ASN:HB3 | 40:PA:105:ARG:HD3 | 1.94 | 0.50 |
| 41:PB:140:GLY:HA3 | 41:PB:181:GLU:HG2 | 1.92 | 0.50 |
| 40:PE:6:SER:O | 40:PE:65:ALA:HA | 2.12 | 0.50 |
| 40:PF:34:GLY:O | 40:PF:61:HIS:N | 2.43 | 0.50 |
| 40:PF:438:SER:OG | 41:PN:390:ARG:NH2 | 2.45 | 0.50 |
| 41:PN:293:MET:HE2 | 41:PN:367:PHE:HB2 | 1.93 | 0.50 |
| 41:PO:140:GLY:HA3 | 41:PO:181:GLU:HG3 | 1.94 | 0.50 |
| 40:QA:188:ILE:HD12 | 40:QA:424:MET:HG3 | 1.93 | 0.50 |
| 41:QB:81:PHE:O | 41:QB:84:ILE:HG12 | 2.12 | 0.50 |
| 40:QE:272:TYR:O | 40:QE:300:ASN:ND2 | 2.38 | 0.50 |
| 40:QF:270:ALA:HA | 40:QF:376:MET:O | 2.11 | 0.50 |
| 40:RF:175:PRO:O | 40:RF:393:LYS:NZ | 2.37 | 0.50 |
| 40:RF:248:LEU:H | 40:RF:355:ILE:HB | 1.77 | 0.50 |
| 40:RG:132:LEU:HD23 | 40:RG:164:LYS:HZ2 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RM:73:MET:HG3 | 41:RM:92:PHE:HB3 | 1.94 | 0.50 |
| 41:RN:31:ASP:OD2 | 41:RN:35:THR:OG1 | 2.30 | 0.50 |
| 40:SE:137:ILE:HG22 | 40:SE:139:HIS:HD2 | 1.77 | 0.50 |
| 40:SG:151:SER:OG | 40:SG:190:THR:OG1 | 2.24 | 0.50 |
| 41:SO:385:PHE:CZ | 41:SO:408:PHE:HB3 | 2.42 | 0.50 |
| 41:TL:40:SER:OG | 41:TL:41:ASP:N | 2.45 | 0.50 |
| 40:UH:356:ASN:HD21 | 40:UH:358:GLN:HB3 | 1.77 | 0.50 |
| 40:UI:277:SER:O | 40:UI:278:ALA:C | 2.49 | 0.50 |
| 41:UO:350:LYS:HE3 | 41:UO:351:THR:H | 1.77 | 0.50 |
| 41:UP:272:PRO:HD3 | 41:UP:364:SER:HA | 1.92 | 0.50 |
| 40:VA:71:GLU:HB3 | 40:VA:98:ASP:HA | 1.94 | 0.50 |
| 41:WB:134:GLN:HA | 41:WB:165:ASN:O | 2.12 | 0.50 |
| 40:WH:64:ARG:NH1 | 40:WH:128:GLN:O | 2.44 | 0.50 |
| 41:WN:358:PRO:HG3 | 41:WN:364:SER:HB3 | 1.93 | 0.50 |
| 41:WP:285:THR:HG22 | 41:WP:287:PRO:HD2 | 1.93 | 0.50 |
| 7:1U:221:TYR:CE1 | 7:1U:231:LYS:HB2 | 2.47 | 0.50 |
| 9:2B:163:VAL:HG23 | 40:TH:369:LYS:HG3 | 1.94 | 0.50 |
| 9:2B:357:GLU:HB3 | 9:2B:361:ARG:NH1 | 2.27 | 0.50 |
| 11:2J:248:LYS:HA | 11:2J:248:LYS:HZ3 | 1.76 | 0.50 |
| 13:2U:54:VAL:HG22 | 13:2U:88:THR:HG22 | 1.93 | 0.50 |
| 13:2V:176:GLU:O | 13:2V:177:LEU:C | 2.50 | 0.50 |
| 13:2X:61:CYS:HB2 | 13:2X:154:VAL:HG13 | 1.94 | 0.50 |
| 13:2X:62:PRO:HG2 | 13:2X:153:ARG:CZ | 2.41 | 0.50 |
| 18:3U:415:ASP:OD2 | 18:3V:63:ARG:NE | 2.45 | 0.50 |
| 21:4E:429:PRO:HB3 | 22:4K:644:TYR:CB | 2.42 | 0.50 |
| 21:4F:194:LEU:HD22 | 21:4F:199:ILE:HD12 | 1.93 | 0.50 |
| 22:4K:556:GLU:O | 22:4K:558:LYS:N | 2.44 | 0.50 |
| 31:5J:807:LYS:HD2 | 33:5O:94:ALA:HB1 | 1.94 | 0.50 |
| 34:5R:414:GLU:HA | 34:5R:417:MET:HE3 | 1.94 | 0.50 |
| 41:AB:236:VAL:HG22 | 41:AB:368:ILE:HD11 | 1.93 | 0.50 |
| 40:AH:205:ASP:OD1 | 40:AH:206:ASN:N | 2.44 | 0.50 |
| 40:BA:212:ILE:HD11 | 40:BA:275:VAL:HG21 | 1.94 | 0.50 |
| 41:BB:73:MET:HG3 | 41:BB:92:PHE:HB3 | 1.94 | 0.50 |
| 41:BB:142:GLY:O | 41:BB:144:GLY:N | 2.45 | 0.50 |
| 40:BG:191:THR:O | 40:BG:195:LEU:HB2 | 2.12 | 0.50 |
| 40:BH:397:MET:HG3 | 41:BO:345:ILE:HA | 1.94 | 0.50 |
| 41:BO:28:HIS:O | 41:BO:43:GLN:HB3 | 2.11 | 0.50 |
| 40:CA:173:PRO:HG2 | 40:CA:390:LEU:HD11 | 1.94 | 0.50 |
| 40:CA:328:VAL:HG21 | 40:CA:355:ILE:HD11 | 1.94 | 0.50 |
| 40:CE:204:VAL:HG11 | 40:CE:231:ILE:HG12 | 1.94 | 0.50 |
| 41:CM:107:THR:HG21 | 41:CM:401:GLU:HB3 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CO:13:GLY:HA3 | 41:CO:136:THR:O | 2.12 | 0.50 |
| 41:CO:224:ASP:C | 41:CO:226:ASN:H | 2.14 | 0.50 |
| 41:CO:372:THR:HA | 41:CO:375:GLN:HE22 | 1.77 | 0.50 |
| 40:DA:103:TYR:CE1 | 40:DA:190:THR:HG22 | 2.47 | 0.50 |
| 40:DA:402:ALA:HB2 | 41:DN:344:TRP:CZ3 | 2.46 | 0.50 |
| 40:DA:402:ALA:HB2 | 41:DN:344:TRP:HZ3 | 1.76 | 0.50 |
| 41:DB:23:VAL:O | 41:DB:27:GLU:HG2 | 2.12 | 0.50 |
| 40:DH:338:LYS:C | 40:DH:340:SER:H | 2.15 | 0.50 |
| 40:DI:56:THR:OG1 | 40:DI:57:GLY:N | 2.44 | 0.50 |
| 40:DI:242:LEU:HD21 | 40:DI:252:LEU:HD13 | 1.93 | 0.50 |
| 41:DM:11:GLN:N | 43:DM:501:GDP:O2B | 2.38 | 0.50 |
| 41:DN:357:PRO:CB | 41:DN:362:LYS:HA | 2.42 | 0.50 |
| 41:DO:309:ARG:H | 41:DO:372:THR:HG22 | 1.77 | 0.50 |
| 41:DP:137:HIS:O | 41:DP:169:VAL:HG23 | 2.12 | 0.50 |
| 41:DP:334:GLN:HE22 | 41:DP:347:ASN:HA | 1.77 | 0.50 |
| 40:EH:27:GLU:CD | 40:EH:28:HIS:H | 2.14 | 0.50 |
| 40:EH:243:ARG:HG3 | 40:EH:244:PHE:H | 1.76 | 0.50 |
| 40:EI:219:ILE:O | 40:EI:222:PRO:HD3 | 2.12 | 0.50 |
| 40:FH:298:PRO:HG3 | 40:FH:308:ARG:HE | 1.77 | 0.50 |
| 40:FI:56:THR:OG1 | 40:FI:57:GLY:N | 2.45 | 0.50 |
| 40:FI:90:GLU:HB3 | 40:FI:121:ARG:HH22 | 1.76 | 0.50 |
| 41:FO:139:LEU:HG | 41:FO:168:SER:HB3 | 1.94 | 0.50 |
| 40:GE:132:LEU:HD22 | 40:GE:135:PHE:HE2 | 1.77 | 0.50 |
| 40:GE:347:CYS:O | 40:GE:347:CYS:SG | 2.68 | 0.50 |
| 40:GE:370:VAL:HG22 | 40:GE:372:ARG:H | 1.77 | 0.50 |
| 40:GH:376:MET:SD | 40:GH:378:SER:HB3 | 2.51 | 0.50 |
| 40:GH:405:HIS:CE1 | 41:GO:258:VAL:HG12 | 2.47 | 0.50 |
| 41:GN:36:TYR:CE1 | 41:GN:38:GLY:HA3 | 2.46 | 0.50 |
| 40:HE:28:HIS:O | 40:HE:29:GLY:C | 2.51 | 0.50 |
| 40:HE:236:SER:HA | 40:HE:243:ARG:HH22 | 1.77 | 0.50 |
| 40:HI:206:ASN:OD1 | 42:HP:501:GTP:O2' | 2.22 | 0.50 |
| 40:IH:85:GLN:O | 41:JB:281:TYR:OH | 2.30 | 0.50 |
| 40:IH:348:PRO:HG2 | 41:IP:384:GLN:HG2 | 1.93 | 0.50 |
| 41:IM:31:ASP:OD1 | 41:IM:35:THR:N | 2.44 | 0.50 |
| 40:JD:318:LEU:O | 40:JD:374:VAL:HA | 2.11 | 0.50 |
| 40:JF:180:ALA:HB3 | 40:JF:183:GLU:HG3 | 1.93 | 0.50 |
| 40:JG:195:LEU:HD21 | 40:JG:427:LEU:HD13 | 1.93 | 0.50 |
| 40:JG:219:ILE:HD12 | 40:JG:222:PRO:HB3 | 1.93 | 0.50 |
| 41:JO:421:PRO:HA | 41:JO:424:THR:HG22 | 1.93 | 0.50 |
| 41:KO:142:GLY:O | 41:KO:144:GLY:N | 2.45 | 0.50 |
| 40:LE:258:ASN:ND2 | 40:LE:352:LYS:HD3 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LF:183:GLU:HB3 | 40:LF:184:PRO:HD3 | 1.93 | 0.50 |
| 40:LH:20:CYS:HA | 40:LH:232:SER:HB2 | 1.94 | 0.50 |
| 41:LP:234:SER:O | 41:LP:238:THR:OG1 | 2.29 | 0.50 |
| 40:ME:139:HIS:NE2 | 40:ME:168:GLU:OE2 | 2.31 | 0.50 |
| 40:ME:192:HIS:ND1 | 40:ME:423:ASP:OD1 | 2.44 | 0.50 |
| 41:MN:2:ARG:HH21 | 41:MN:240:LEU:HA | 1.77 | 0.50 |
| 41:NN:313:VAL:HB | 41:NN:349:VAL:HG12 | 1.94 | 0.50 |
| 41:NO:7:LEU:HD22 | 41:NO:151:LEU:HD21 | 1.94 | 0.50 |
| 40:OD:7:VAL:HG13 | 40:OD:66:VAL:HB | 1.94 | 0.50 |
| 40:OH:21:TRP:HZ2 | 40:OH:65:ALA:HB2 | 1.77 | 0.50 |
| 41:OM:130:LEU:O | 41:OM:162:ARG:NE | 2.45 | 0.50 |
| 41:OO:174:LYS:HB3 | 41:OO:205:GLU:HG3 | 1.93 | 0.50 |
| 41:OO:325:GLU:HA | 41:OO:328:GLU:HB3 | 1.94 | 0.50 |
| 41:OP:85:PHE:HB2 | 41:OP:90:PHE:HE2 | 1.77 | 0.50 |
| 41:PN:226:ASN:ND2 | 43:PN:502:GDP:O6 | 2.42 | 0.50 |
| 41:PP:54:ALA:HA | 41:QP:283:ALA:CB | 2.41 | 0.50 |
| 41:PP:226:ASN:ND2 | 43:PP:501:GDP:O6 | 2.42 | 0.50 |
| 41:QP:67:ASP:HA | 41:QP:143:THR:HG21 | 1.93 | 0.50 |
| 41:RB:372:THR:OG1 | 41:RB:422:VAL:O | 2.30 | 0.50 |
| 40:RE:68:VAL:HA | 40:RE:93:ILE:HB | 1.93 | 0.50 |
| 40:RG:352:LYS:HD2 | 41:RO:178:THR:HG23 | 1.94 | 0.50 |
| 40:RG:366:ASP:OD2 | 40:RG:367:LEU:N | 2.45 | 0.50 |
| 41:SN:4:ILE:HB | 41:SN:50:TYR:HE1 | 1.76 | 0.50 |
| 41:SO:132:GLY:HA2 | 41:SO:162:ARG:HG3 | 1.94 | 0.50 |
| 41:SO:171:PRO:HB3 | 41:SO:181:GLU:HG3 | 1.94 | 0.50 |
| 40:TI:102:ASN:HB3 | 40:TI:105:ARG:HB2 | 1.94 | 0.50 |
| 41:TN:207:LEU:HA | 41:TN:210:ILE:HG22 | 1.94 | 0.50 |
| 41:TN:407:GLU:HA | 41:TN:410:GLU:HG2 | 1.94 | 0.50 |
| 40:UA:320:ARG:HE | 40:UA:360:PRO:HG3 | 1.77 | 0.50 |
| 40:UH:71:GLU:HB2 | 40:UH:98:ASP:HA | 1.94 | 0.50 |
| 41:UM:253:LEU:O | 41:UM:257:MET:CB | 2.48 | 0.50 |
| 40:VJ:139:HIS:O | 40:VJ:170:SER:HA | 2.11 | 0.50 |
| 41:WB:156:ARG:NH1 | 41:WB:162:ARG:O | 2.41 | 0.50 |
| 40:WF:342:GLN:NE2 | 40:WF:343:PHE:O | 2.45 | 0.50 |
| 2:1D:10:ARG:NH2 | 40:GH:401:ARG:HA | 2.26 | 0.49 |
| 8:1W:263:MET:HG2 | 40:VJ:282:TYR:OH | 2.11 | 0.49 |
| 8:1W:459:GLN:HA | 8:1W:462:GLU:HG3 | 1.94 | 0.49 |
| 13:2X:85:LYS:HB3 | 13:2X:159:ASN:HB3 | 1.93 | 0.49 |
| 15:3E:295:ASN:HD22 | 15:3H:38:VAL:HA | 1.75 | 0.49 |
| 16:3J:283:GLU:OE1 | 16:3J:374:GLN:NE2 | 2.45 | 0.49 |
| 17:3P:269:ASP:O | 17:3P:270:LYS:C | 2.51 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:3P:296:VAL:O | 17:3P:297:PRO:C | 2.50 | 0.49 |
| 17:3R:108:LEU:HA | 17:3R:111:ASN:HB2 | 1.94 | 0.49 |
| 21:4E:451:ILE:HD12 | 21:4E:503:PHE:CD2 | 2.47 | 0.49 |
| 22:4H:340:ILE:HD11 | 22:4H:356:CYS:HB3 | 1.94 | 0.49 |
| 22:4I:98:ARG:NH2 | 41:BO:279:GLN:HE21 | 2.10 | 0.49 |
| 22:4J:218:THR:O | 40:CF:371:GLN:NE2 | 2.42 | 0.49 |
| 22:4K:561:GLU:HG3 | 22:4K:562:LEU:N | 2.25 | 0.49 |
| 23:4N:236:TYR:CA | 23:4N:267:ASP:HB3 | 2.34 | 0.49 |
| 26:4V:51:LYS:HB2 | 31:5I:505:ARG:NH2 | 2.26 | 0.49 |
| 33:5N:322:GLU:OE2 | 34:5Q:131:LYS:NZ | 2.45 | 0.49 |
| 33:5N:392:MET:HG2 | 33:5N:396:LYS:HZ2 | 1.75 | 0.49 |
| 34:5Q:179:GLU:HG2 | 40:GA:369:LYS:HD3 | 1.93 | 0.49 |
| 36:5Y:123:ARG:HH12 | 40:KH:400:LYS:HA | 1.77 | 0.49 |
| 41:AB:324:LYS:NZ | 41:AB:328:GLU:OE2 | 2.32 | 0.49 |
| 40:AH:141:PHE:HB2 | 40:AH:173:PRO:HD3 | 1.94 | 0.49 |
| 41:AM:8:GLN:HB2 | 41:AM:65:LEU:HA | 1.94 | 0.49 |
| 41:AN:35:THR:HA | 41:AN:58:LYS:HB2 | 1.94 | 0.49 |
| 40:BA:12:ALA:HB1 | 40:BA:171:ILE:HD12 | 1.94 | 0.49 |
| 41:BB:107:THR:C | 41:BB:109:GLY:H | 2.15 | 0.49 |
| 40:BH:109:THR:OG1 | 40:BH:110:ILE:N | 2.45 | 0.49 |
| 41:BL:198:GLU:HA | 41:BL:264:HIS:HB2 | 1.94 | 0.49 |
| 40:CE:49:PHE:HE1 | 40:CE:55:GLU:HB2 | 1.76 | 0.49 |
| 40:CH:180:ALA:HA | 41:CO:256:ASN:ND2 | 2.20 | 0.49 |
| 41:CO:21:TRP:CE3 | 41:CO:24:ILE:HD11 | 2.47 | 0.49 |
| 41:CP:182:PRO:HB3 | 41:CP:384:GLN:HB2 | 1.93 | 0.49 |
| 40:DF:36:MET:O | 40:DF:38:SER:N | 2.44 | 0.49 |
| 41:DM:7:LEU:HD13 | 41:DM:135:LEU:HD12 | 1.94 | 0.49 |
| 41:DM:193:VAL:HA | 41:DM:264:HIS:CE1 | 2.47 | 0.49 |
| 41:DO:6:HIS:O | 41:DO:63:ALA:HA | 2.11 | 0.49 |
| 41:DP:54:ALA:HB1 | 41:EP:282:ARG:O | 2.12 | 0.49 |
| 40:EA:2:ARG:NH2 | 41:EB:69:GLU:OE2 | 2.44 | 0.49 |
| 40:EA:287:SER:H | 40:EA:290:GLU:HG3 | 1.76 | 0.49 |
| 41:EB:322:SER:HA | 40:EG:223:THR:HG22 | 1.93 | 0.49 |
| 40:EF:70:LEU:HD23 | 40:EF:114:LEU:HD12 | 1.93 | 0.49 |
| 40:EG:6:SER:O | 40:EG:65:ALA:HA | 2.12 | 0.49 |
| 40:EG:320:ARG:HH21 | 40:EG:360:PRO:HA | 1.77 | 0.49 |
| 40:EI:144:GLY:O | 40:EI:145:THR:C | 2.50 | 0.49 |
| 40:EI:320:ARG:HG2 | 40:EI:360:PRO:HD3 | 1.93 | 0.49 |
| 41:EL:202:ILE:HG12 | 41:EL:300:MET:HG3 | 1.94 | 0.49 |
| 41:EP:100:ASN:O | 41:EP:101:TRP:C | 2.50 | 0.49 |
| 40:FA:23:LEU:HA | 40:FA:26:LEU:HD23 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FE:211:ASP:HA | 40:FE:214:ARG:HG2 | 1.93 | 0.49 |
| 40:FF:182:VAL:O | 40:FF:186:ASN:ND2 | 2.45 | 0.49 |
| 41:FO:318:ARG:HB2 | 41:FO:364:SER:HB3 | 1.94 | 0.49 |
| 41:FP:215:LEU:HD11 | 41:FP:273:LEU:HD22 | 1.94 | 0.49 |
| 40:GA:438:SER:HB2 | 41:GB:391:ARG:HD3 | 1.94 | 0.49 |
| 40:GE:140:SER:O | 40:GE:141:PHE:C | 2.50 | 0.49 |
| 40:GH:72:PRO:HA | 40:GH:94:THR:HG22 | 1.93 | 0.49 |
| 41:GO:137:HIS:O | 41:GO:168:SER:HA | 2.12 | 0.49 |
| 41:GO:200:TYR:CD1 | 41:GO:266:PHE:HB2 | 2.47 | 0.49 |
| 41:HB:172:SER:OG | 41:HB:175:VAL:O | 2.31 | 0.49 |
| 40:HI:16:ILE:HD12 | 40:HI:231:ILE:HG21 | 1.94 | 0.49 |
| 41:HN:161:ASP:O | 41:HN:162:ARG:C | 2.49 | 0.49 |
| 41:HO:68:LEU:HB2 | 41:HO:143:THR:HG22 | 1.94 | 0.49 |
| 40:IF:224:TYR:HA | 40:IF:227:LEU:HB2 | 1.93 | 0.49 |
| 40:IG:73:THR:HA | 40:IG:76:ASP:HB2 | 1.94 | 0.49 |
| 40:IG:140:SER:OG | 42:IG:501:GTP:O2A | 2.29 | 0.49 |
| 40:IG:262:TYR:OH | 41:IO:391:ARG:O | 2.21 | 0.49 |
| 40:IH:51:THR:HG23 | 40:IH:52:PHE:HD1 | 1.77 | 0.49 |
| 41:IP:253:LEU:O | 41:IP:257:MET:HB2 | 2.12 | 0.49 |
| 41:IP:273:LEU:O | 41:IP:292:GLN:NE2 | 2.27 | 0.49 |
| 40:JG:234:ILE:HD11 | 40:JG:272:TYR:HB2 | 1.93 | 0.49 |
| 41:JL:100:ASN:HB3 | 41:JL:103:LYS:HB2 | 1.94 | 0.49 |
| 41:JL:180:VAL:O | 41:JL:184:ASN:ND2 | 2.43 | 0.49 |
| 41:JM:16:ILE:HG12 | 41:JM:226:ASN:HD21 | 1.76 | 0.49 |
| 41:JM:19:LYS:HG2 | 41:JM:227:HIS:HA | 1.92 | 0.49 |
| 41:JN:83:GLN:OE1 | 41:KN:281:TYR:OH | 2.27 | 0.49 |
| 40:KG:271:THR:HG22 | 40:KG:376:MET:HB3 | 1.94 | 0.49 |
| 41:KM:170:VAL:HG11 | 41:KM:377:LEU:HD21 | 1.94 | 0.49 |
| 41:KP:170:VAL:HG11 | 41:KP:377:LEU:HD21 | 1.93 | 0.49 |
| 41:KP:215:LEU:HB3 | 41:KP:217:LEU:HD23 | 1.94 | 0.49 |
| 40:LA:154:MET:HG3 | 40:LA:194:THR:HG22 | 1.94 | 0.49 |
| 40:LA:298:PRO:HB3 | 40:LA:307:PRO:HD2 | 1.94 | 0.49 |
| 41:LB:180:VAL:HG23 | 41:LB:184:ASN:HD21 | 1.77 | 0.49 |
| 40:LD:73:THR:HA | 40:LD:76:ASP:HB2 | 1.94 | 0.49 |
| 40:LD:167:LEU:HD23 | 40:LD:202:PHE:HE1 | 1.76 | 0.49 |
| 40:LG:398:TYR:CE1 | 40:LG:417:PHE:HB3 | 2.47 | 0.49 |
| 40:NE:238:ILE:HA | 40:NE:318:LEU:HD22 | 1.93 | 0.49 |
| 40:NF:211:ASP:OD2 | 40:NF:215:ARG:NH2 | 2.44 | 0.49 |
| 40:NH:20:CYS:HA | 40:NH:232:SER:HB2 | 1.93 | 0.49 |
| 41:NP:28:HIS:NE2 | 41:NP:241:ARG:HD2 | 2.27 | 0.49 |
| 40:OD:167:LEU:HD13 | 40:OD:202:PHE:HE2 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OE:60:LYS:HD2 | 40:OE:61:HIS:H | 1.76 | 0.49 |
| 40:OH:54:SER:OG | 40:OH:55:GLU:N | 2.44 | 0.49 |
| 41:OL:207:LEU:HD13 | 41:OL:225:LEU:HD12 | 1.93 | 0.49 |
| 41:PB:51:TYR:HB3 | 41:PB:59:TYR:HB3 | 1.94 | 0.49 |
| 41:PO:204:ASN:HA | 41:PO:207:LEU:HD12 | 1.93 | 0.49 |
| 41:PP:274:THR:HA | 41:PP:282:ARG:HH22 | 1.77 | 0.49 |
| 40:QA:51:THR:OG1 | 40:QA:52:PHE:N | 2.45 | 0.49 |
| 41:QB:253:LEU:O | 41:QB:257:MET:N | 2.44 | 0.49 |
| 41:QP:148:GLY:O | 41:QP:152:ILE:HG13 | 2.12 | 0.49 |
| 41:RB:141:GLY:O | 41:RB:184:ASN:ND2 | 2.44 | 0.49 |
| 40:RF:172:TYR:HB2 | 40:RF:203:MET:HB3 | 1.94 | 0.49 |
| 40:RG:154:MET:HG3 | 40:RG:194:THR:HG22 | 1.94 | 0.49 |
| 41:RP:300:MET:SD | 41:RP:300:MET:N | 2.84 | 0.49 |
| 41:SB:156:ARG:HG2 | 41:SB:195:ASN:HD22 | 1.77 | 0.49 |
| 40:SE:244:PHE:CG | 40:SE:358:GLN:HG3 | 2.47 | 0.49 |
| 40:SH:419:GLU:HA | 40:SH:422:GLU:HB2 | 1.94 | 0.49 |
| 41:SN:315:ALA:HB3 | 41:SN:351:THR:HG22 | 1.93 | 0.49 |
| 40:TF:101:ASN:HA | 40:TF:144:GLY:H | 1.77 | 0.49 |
| 41:TL:290:THR:HG21 | 41:TL:329:GLN:HB3 | 1.93 | 0.49 |
| 40:UE:262:TYR:HB2 | 40:UE:265:ILE:HG22 | 1.93 | 0.49 |
| 40:UI:287:SER:HA | 40:UI:372:ARG:HH11 | 1.77 | 0.49 |
| 41:UO:229:VAL:O | 41:UO:232:THR:OG1 | 2.22 | 0.49 |
| 41:UP:142:GLY:O | 41:UP:143:THR:C | 2.50 | 0.49 |
| 41:VB:60:VAL:HG21 | 41:VB:86:ARG:HG2 | 1.93 | 0.49 |
| 40:VF:3:GLU:HA | 40:VF:51:THR:HA | 1.93 | 0.49 |
| 40:VH:54:SER:HB3 | 40:VH:64:ARG:HD3 | 1.94 | 0.49 |
| 40:VJ:79:ARG:HH22 | 40:VJ:94:THR:HG23 | 1.76 | 0.49 |
| 40:VJ:109:THR:OG1 | 40:VJ:410:GLU:O | 2.28 | 0.49 |
| 41:VO:180:VAL:HG23 | 41:VO:184:ASN:HD21 | 1.76 | 0.49 |
| 41:VO:229:VAL:HA | 41:VO:232:THR:HG22 | 1.93 | 0.49 |
| 40:WE:16:ILE:HA | 40:WE:228:ASN:HB3 | 1.94 | 0.49 |
| 40:WE:30:ILE:HG13 | 40:WE:53:PHE:CD2 | 2.48 | 0.49 |
| 41:WM:193:VAL:HG23 | 41:WM:265:PHE:HE1 | 1.75 | 0.49 |
| 8:1W:256:ARG:HA | 8:1W:259:ILE:HG22 | 1.93 | 0.49 |
| 9:2B:43:LEU:C | 9:2B:45:GLN:H | 2.14 | 0.49 |
| 9:2B:47:THR:HB | 11:2K:246:LYS:HE3 | 1.94 | 0.49 |
| 9:2B:187:GLN:HE21 | 41:TO:360:GLY:HA2 | 1.78 | 0.49 |
| 9:2B:347:ILE:HG22 | 41:TM:360:GLY:HA2 | 1.94 | 0.49 |
| 10:2E:86:THR:HG21 | 40:AE:176:GLN:HG2 | 1.93 | 0.49 |
| 10:2G:97:GLN:O | 10:2G:101:GLN:CB | 2.58 | 0.49 |
| 12:2O:188:PRO:O | 12:2O:191:ARG:NH2 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2U:37:ILE:HG12 | 13:2U:38:THR:N | 2.26 | 0.49 |
| 17:3O:94:TYR:O | 17:3P:211:VAL:HG23 | 2.13 | 0.49 |
| 22:4I:652:VAL:HA | 22:4I:688:ILE:O | 2.11 | 0.49 |
| 23:4N:91:ILE:HG21 | 40:AF:84:ARG:HB2 | 1.94 | 0.49 |
| 23:4P:236:TYR:CA | 23:4P:267:ASP:HB3 | 2.34 | 0.49 |
| 23:4R:18:TYR:CD2 | 23:4R:45:LEU:HD21 | 2.47 | 0.49 |
| 26:4W:370:TYR:HD1 | 26:4W:374:ILE:HG13 | 1.77 | 0.49 |
| 28:5B:208:GLY:O | 41:KP:83:GLN:NE2 | 2.45 | 0.49 |
| 32:5L:98:VAL:HB | 32:5L:101:LEU:HB3 | 1.94 | 0.49 |
| 34:5R:333:GLU:HA | 34:5R:336:ILE:HD12 | 1.94 | 0.49 |
| 37:6A:85:THR:HB | 41:TO:320:ARG:HH21 | 1.76 | 0.49 |
| 39:6I:66:ARG:HH22 | 41:ON:38:GLY:H | 1.60 | 0.49 |
| 39:6I:79:SER:OG | 39:6I:80:LYS:NZ | 2.45 | 0.49 |
| 41:AB:142:GLY:O | 41:AB:144:GLY:N | 2.45 | 0.49 |
| 40:AE:89:PRO:HG2 | 40:BE:280:LYS:HG3 | 1.94 | 0.49 |
| 40:AE:271:THR:HA | 40:AE:302:MET:HG3 | 1.93 | 0.49 |
| 40:AF:71:GLU:HB3 | 40:AF:98:ASP:HA | 1.93 | 0.49 |
| 40:AH:20:CYS:HA | 40:AH:232:SER:HB2 | 1.94 | 0.49 |
| 41:AN:172:SER:OG | 41:AN:175:VAL:O | 2.29 | 0.49 |
| 40:BA:390:LEU:HD23 | 40:BA:393:LYS:HD2 | 1.94 | 0.49 |
| 40:BE:75:ILE:HB | 40:BE:94:THR:HG23 | 1.93 | 0.49 |
| 40:BE:315:CYS:HA | 40:BE:378:SER:HA | 1.94 | 0.49 |
| 40:BE:354:GLY:C | 40:BE:355:ILE:HG13 | 2.32 | 0.49 |
| 41:BL:95:SER:OG | 41:BL:96:GLY:N | 2.46 | 0.49 |
| 40:CA:109:THR:O | 40:CA:110:ILE:C | 2.51 | 0.49 |
| 40:CF:204:VAL:HG11 | 40:CF:231:ILE:HG12 | 1.94 | 0.49 |
| 40:CG:200:CYS:HA | 40:CG:266:HIS:HB2 | 1.93 | 0.49 |
| 40:CH:136:LEU:HD13 | 40:CH:167:LEU:HB2 | 1.95 | 0.49 |
| 41:CN:23:VAL:HA | 41:CN:26:ASP:OD1 | 2.11 | 0.49 |
| 41:CO:326:VAL:O | 41:CO:330:MET:HG2 | 2.12 | 0.49 |
| 40:DA:177:VAL:HG11 | 40:DA:207:GLU:HB2 | 1.93 | 0.49 |
| 40:DA:375:CYS:SG | 40:DA:375:CYS:O | 2.70 | 0.49 |
| 41:DB:24:ILE:HA | 41:DB:27:GLU:CG | 2.42 | 0.49 |
| 41:DB:142:GLY:O | 41:DB:145:SER:N | 2.43 | 0.49 |
| 41:DB:163:ILE:HG12 | 41:DB:251:ARG:HD3 | 1.93 | 0.49 |
| 41:DL:105:HIS:HA | 41:DL:150:LEU:HG | 1.94 | 0.49 |
| 41:DL:414:ASN:O | 41:DL:418:LEU:N | 2.45 | 0.49 |
| 41:EB:132:GLY:HA3 | 41:EB:163:ILE:O | 2.12 | 0.49 |
| 41:EB:155:ILE:HA | 41:EB:158:GLU:HB2 | 1.94 | 0.49 |
| 40:EF:151:SER:OG | 40:EF:190:THR:OG1 | 2.26 | 0.49 |
| 40:EG:168:GLU:N | 40:EG:168:GLU:OE1 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EG:258:ASN:HD21 | 41:EO:178:THR:HG23 | 1.77 | 0.49 |
| 41:EN:132:GLY:HA2 | 41:EN:162:ARG:HB3 | 1.94 | 0.49 |
| 41:EO:139:LEU:HG | 41:EO:168:SER:HB2 | 1.94 | 0.49 |
| 40:FG:298:PRO:HB3 | 40:FG:307:PRO:HD2 | 1.93 | 0.49 |
| 41:FN:310:TYR:HD1 | 41:FN:371:SER:HB3 | 1.76 | 0.49 |
| 41:FO:306:ARG:HA | 41:FO:340:TYR:HE2 | 1.76 | 0.49 |
| 41:GB:41:ASP:N | 41:GB:41:ASP:OD1 | 2.45 | 0.49 |
| 40:GE:317:LEU:HB3 | 40:GE:319:TYR:CE1 | 2.47 | 0.49 |
| 40:GF:121:ARG:NE | 40:GF:124:LYS:HE2 | 2.27 | 0.49 |
| 40:GI:101:ASN:HA | 40:GI:143:GLY:HA2 | 1.93 | 0.49 |
| 41:GO:142:GLY:O | 41:GO:144:GLY:N | 2.45 | 0.49 |
| 41:HB:139:LEU:HG | 41:HB:168:SER:HB2 | 1.94 | 0.49 |
| 40:HE:325:PRO:HB3 | 41:HM:222:TYR:CD2 | 2.47 | 0.49 |
| 41:HP:222:TYR:O | 41:HP:226:ASN:ND2 | 2.45 | 0.49 |
| 41:HP:290:THR:HG21 | 41:HP:329:GLN:HB3 | 1.94 | 0.49 |
| 40:IE:179:THR:N | 40:IE:183:GLU:OE2 | 2.41 | 0.49 |
| 40:IE:255:PHE:HZ | 40:IE:318:LEU:HD21 | 1.77 | 0.49 |
| 40:IG:313:MET:HE2 | 40:IG:381:THR:HG22 | 1.93 | 0.49 |
| 40:IG:395:ASP:OD2 | 40:IG:421:ARG:NH2 | 2.41 | 0.49 |
| 40:IH:79:ARG:HH12 | 40:IH:94:THR:HG21 | 1.76 | 0.49 |
| 41:IM:113:VAL:HG21 | 41:IM:150:LEU:HD23 | 1.94 | 0.49 |
| 41:IN:7:LEU:O | 41:IN:135:LEU:HA | 2.12 | 0.49 |
| 40:JF:406:TRP:HE1 | 41:JM:258:VAL:HG23 | 1.77 | 0.49 |
| 40:JH:79:ARG:HH21 | 40:JH:92:LEU:HB2 | 1.76 | 0.49 |
| 41:JM:372:THR:HA | 41:JM:422:VAL:HG22 | 1.94 | 0.49 |
| 41:JN:257:MET:HG3 | 41:JN:266:PHE:CE1 | 2.47 | 0.49 |
| 40:KA:24:TYR:HA | 40:KA:27:GLU:HG2 | 1.93 | 0.49 |
| 40:KE:20:CYS:HA | 40:KE:232:SER:HB2 | 1.94 | 0.49 |
| 41:KN:282:ARG:HG3 | 41:KN:284:LEU:HB2 | 1.92 | 0.49 |
| 40:LH:318:LEU:O | 40:LH:374:VAL:HA | 2.12 | 0.49 |
| 41:LL:86:ARG:HH12 | 41:LL:88:ASP:HB3 | 1.77 | 0.49 |
| 41:LP:6:HIS:O | 41:LP:63:ALA:HA | 2.11 | 0.49 |
| 40:MA:252:LEU:HD23 | 40:MA:255:PHE:HE2 | 1.76 | 0.49 |
| 40:MG:333:ALA:O | 40:MG:337:THR:HG23 | 2.13 | 0.49 |
| 41:MN:198:GLU:HG2 | 41:MN:266:PHE:HE2 | 1.74 | 0.49 |
| 40:NA:93:ILE:HD11 | 40:NA:121:ARG:HG3 | 1.94 | 0.49 |
| 40:ND:70:LEU:O | 40:ND:96:LYS:N | 2.45 | 0.49 |
| 40:ND:286:LEU:HD13 | 40:ND:290:GLU:HG3 | 1.94 | 0.49 |
| 40:NF:255:PHE:HZ | 40:NF:318:LEU:HD21 | 1.77 | 0.49 |
| 41:NP:2:ARG:NH1 | 41:NP:251:ARG:HH12 | 2.10 | 0.49 |
| 40:OD:173:PRO:HB3 | 40:OD:183:GLU:HG3 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OF:438:SER:HA | 41:ON:391:ARG:HH12 | 1.76 | 0.49 |
| 40:OH:49:PHE:HE2 | 40:OH:55:GLU:HB2 | 1.77 | 0.49 |
| 40:PA:260:VAL:HG13 | 41:PB:397:TRP:HE1 | 1.77 | 0.49 |
| 41:PL:313:VAL:HB | 41:PL:349:VAL:HG12 | 1.93 | 0.49 |
| 41:PO:49:VAL:HG11 | 41:PO:241:ARG:HG2 | 1.93 | 0.49 |
| 41:QB:190:HIS:HA | 41:QB:414:ASN:ND2 | 2.27 | 0.49 |
| 41:QM:183:TYR:HE2 | 41:QM:394:PHE:HB2 | 1.78 | 0.49 |
| 41:QN:163:ILE:HD13 | 41:QN:250:LEU:HB3 | 1.94 | 0.49 |
| 41:QP:311:LEU:HD22 | 41:QP:372:THR:HB | 1.92 | 0.49 |
| 41:QP:386:THR:O | 41:QP:388:MET:N | 2.44 | 0.49 |
| 40:RF:27:GLU:HA | 40:RF:361:THR:HG21 | 1.93 | 0.49 |
| 40:RG:88:HIS:NE2 | 40:SG:284:GLU:OE2 | 2.45 | 0.49 |
| 40:SF:215:ARG:NH2 | 40:SF:300:ASN:OD1 | 2.45 | 0.49 |
| 40:SF:224:TYR:HD2 | 41:SM:245:GLN:HG3 | 1.77 | 0.49 |
| 40:SG:56:THR:HG23 | 40:SG:60:LYS:HB3 | 1.94 | 0.49 |
| 40:SH:73:THR:HG23 | 41:SO:243:PRO:HB3 | 1.93 | 0.49 |
| 41:SN:246:LEU:HD22 | 41:SN:352:ALA:HA | 1.94 | 0.49 |
| 41:SN:290:THR:HG21 | 41:SN:329:GLN:HB3 | 1.94 | 0.49 |
| 41:SO:139:LEU:CB | 41:SO:171:PRO:HD3 | 2.41 | 0.49 |
| 41:SO:151:LEU:O | 41:SO:155:ILE:HG23 | 2.12 | 0.49 |
| 41:TN:131:GLN:HE22 | 41:TN:240:LEU:HD22 | 1.77 | 0.49 |
| 41:TO:237:THR:HB | 41:TO:240:LEU:HD11 | 1.94 | 0.49 |
| 41:TO:269:GLY:HA2 | 41:TO:300:MET:HG2 | 1.94 | 0.49 |
| 41:UB:74:ASP:N | 41:UB:74:ASP:OD2 | 2.43 | 0.49 |
| 41:UB:272:PRO:HG2 | 41:UB:364:SER:HA | 1.94 | 0.49 |
| 40:UG:371:GLN:HB2 | 40:UG:372:ARG:HD2 | 1.92 | 0.49 |
| 40:UH:247:ALA:HB3 | 40:UH:355:ILE:HB | 1.94 | 0.49 |
| 40:VA:188:ILE:HA | 40:VA:191:THR:HG22 | 1.94 | 0.49 |
| 40:VA:391:ASP:HB3 | 40:VA:421:ARG:HH12 | 1.76 | 0.49 |
| 41:VB:354:CYS:SG | 41:VB:355:ASP:N | 2.81 | 0.49 |
| 40:VG:318:LEU:O | 40:VG:374:VAL:HA | 2.11 | 0.49 |
| 40:VI:356:ASN:OD1 | 40:VI:357:TYR:N | 2.45 | 0.49 |
| 41:WM:342:VAL:HB | 41:WM:344:TRP:CD1 | 2.47 | 0.49 |
| 41:WN:6:HIS:CD2 | 41:WN:134:GLN:HE21 | 2.29 | 0.49 |
| 41:WO:47:ILE:HG12 | 41:WO:51:TYR:HB2 | 1.94 | 0.49 |
| 7:1T:46:THR:CG2 | 7:1T:59:PHE:HB3 | 2.41 | 0.49 |
| 7:1T:554:THR:HB | 7:1T:599:ASN:HD21 | 1.76 | 0.49 |
| 13:2W:24:ILE:O | 13:2W:63:ALA:HB2 | 2.12 | 0.49 |
| 14:3A:65:MET:O | 14:3A:107:ASN:ND2 | 2.40 | 0.49 |
| 15:3H:381:ASN:O | 15:3H:385:ILE:HG12 | 2.12 | 0.49 |
| 17:3R:165:ASP:O | 17:3R:166:ALA:C | 2.51 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:3U:169:ARG:HB2 | 18:3V:52:LEU:HD23 | 1.94 | 0.49 |
| 20:4A:80:LEU:O | 20:4A:83:GLU:HB2 | 2.13 | 0.49 |
| 21:4E:330:ILE:HB | 21:4E:333:LYS:HE2 | 1.94 | 0.49 |
| 22:4I:78:VAL:HG23 | 40:AG:41:THR:HG23 | 1.94 | 0.49 |
| 22:4J:90:PRO:HA | 41:BN:279:GLN:HA | 1.94 | 0.49 |
| 22:4J:585:ILE:O | 22:4J:589:LEU:HB2 | 2.12 | 0.49 |
| 22:4J:679:SER:O | 22:4J:680:LYS:C | 2.51 | 0.49 |
| 22:4K:556:GLU:O | 22:4K:557:SER:C | 2.50 | 0.49 |
| 23:4N:184:MET:O | 23:4N:185:SER:C | 2.49 | 0.49 |
| 23:4N:241:GLY:C | 23:4N:242:LEU:HG | 2.32 | 0.49 |
| 24:4O:236:TYR:HB3 | 24:4O:237:PRO:HD3 | 1.92 | 0.49 |
| 31:5I:346:PRO:HG2 | 40:IA:220:GLU:HB3 | 1.94 | 0.49 |
| 38:6C:48:PRO:HA | 41:VO:336:LYS:NZ | 2.27 | 0.49 |
| 40:AG:224:TYR:HD1 | 40:AG:227:LEU:HD12 | 1.77 | 0.49 |
| 40:BA:226:ASN:ND2 | 40:BA:366:ASP:OD2 | 2.45 | 0.49 |
| 40:BF:96:LYS:HD2 | 41:BM:129:CYS:SG | 2.53 | 0.49 |
| 40:BI:279:GLU:HG2 | 40:BI:280:LYS:N | 2.27 | 0.49 |
| 41:BO:61:PRO:HG2 | 41:BO:84:ILE:HG23 | 1.93 | 0.49 |
| 41:CB:7:LEU:O | 41:CB:135:LEU:HA | 2.11 | 0.49 |
| 41:CN:292:GLN:O | 41:CN:293:MET:C | 2.51 | 0.49 |
| 41:CP:172:SER:HB3 | 41:CP:203:ASP:OD1 | 2.12 | 0.49 |
| 40:DA:376:MET:O | 40:DA:376:MET:HG3 | 2.12 | 0.49 |
| 40:DA:398:TYR:O | 40:DA:399:ALA:C | 2.51 | 0.49 |
| 41:DB:242:PHE:HB3 | 41:DB:356:ILE:HD13 | 1.94 | 0.49 |
| 40:DE:59:GLY:O | 40:DE:61:HIS:N | 2.45 | 0.49 |
| 40:DE:99:ALA:HB3 | 40:DE:144:GLY:HA3 | 1.93 | 0.49 |
| 40:DE:141:PHE:O | 40:DE:142:GLY:C | 2.50 | 0.49 |
| 40:DH:402:ALA:C | 40:DH:404:VAL:H | 2.15 | 0.49 |
| 40:DI:270:ALA:CB | 40:DI:377:LEU:HA | 2.41 | 0.49 |
| 41:DM:121:ARG:O | 41:DM:122:LYS:C | 2.51 | 0.49 |
| 41:DN:6:HIS:CG | 41:DN:8:GLN:HE22 | 2.30 | 0.49 |
| 41:DN:134:GLN:HG3 | 41:DN:165:ASN:HB2 | 1.94 | 0.49 |
| 41:DP:240:LEU:H | 41:DP:240:LEU:HD23 | 1.77 | 0.49 |
| 40:EE:53:PHE:HB3 | 40:EE:61:HIS:HB3 | 1.93 | 0.49 |
| 40:EH:36:MET:O | 40:EH:37:PRO:C | 2.50 | 0.49 |
| 40:EI:274:PRO:HB3 | 40:EI:370:VAL:HG21 | 1.92 | 0.49 |
| 40:EI:399:ALA:C | 40:EI:401:ARG:H | 2.15 | 0.49 |
| 41:EM:88:ASP:O | 41:EM:89:ASN:C | 2.50 | 0.49 |
| 41:EM:268:PRO:C | 41:EM:300:MET:HB2 | 2.32 | 0.49 |
| 41:EO:380:ARG:HA | 41:EO:383:GLU:HG3 | 1.94 | 0.49 |
| 40:FF:298:PRO:HG3 | 40:FF:308:ARG:HE | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GB:61:PRO:HD3 | 41:GB:84:ILE:HG12 | 1.94 | 0.49 |
| 40:GI:99:ALA:O | 40:GI:100:ALA:C | 2.50 | 0.49 |
| 41:GO:6:HIS:HD2 | 41:GO:134:GLN:HB3 | 1.78 | 0.49 |
| 41:GO:189:VAL:HA | 41:GO:192:LEU:HB2 | 1.94 | 0.49 |
| 40:HA:26:LEU:HG | 40:HA:363:VAL:HG12 | 1.94 | 0.49 |
| 40:HE:85:GLN:O | 40:HE:87:PHE:N | 2.45 | 0.49 |
| 40:HG:60:LYS:HZ2 | 40:IG:282:TYR:HD2 | 1.59 | 0.49 |
| 40:IF:138:PHE:HE1 | 40:IF:235:VAL:HG11 | 1.78 | 0.49 |
| 41:IN:7:LEU:HD23 | 41:IN:64:VAL:HB | 1.93 | 0.49 |
| 41:IO:6:HIS:O | 41:IO:63:ALA:HA | 2.12 | 0.49 |
| 41:JL:226:ASN:ND2 | 43:JL:501:GDP:O6 | 2.46 | 0.49 |
| 41:KB:289:LEU:HD11 | 41:KB:363:MET:HG2 | 1.94 | 0.49 |
| 40:KD:188:ILE:HA | 40:KD:191:THR:HG22 | 1.94 | 0.49 |
| 40:KG:50:ASN:O | 40:KG:64:ARG:NH2 | 2.46 | 0.49 |
| 41:KN:178:THR:HB | 41:KN:181:GLU:HG3 | 1.93 | 0.49 |
| 40:LA:140:SER:OG | 42:LA:501:GTP:O2A | 2.24 | 0.49 |
| 41:LB:236:VAL:HG22 | 41:LB:368:ILE:HD11 | 1.94 | 0.49 |
| 40:LF:273:ALA:CB | 40:LF:374:VAL:HG13 | 2.42 | 0.49 |
| 40:LG:287:SER:O | 40:LG:291:ILE:HG23 | 2.13 | 0.49 |
| 41:LM:198:GLU:HG2 | 41:LM:266:PHE:HE2 | 1.77 | 0.49 |
| 41:LN:232:THR:HG21 | 41:LN:268:PRO:HB2 | 1.94 | 0.49 |
| 41:LP:7:LEU:O | 41:LP:135:LEU:HA | 2.12 | 0.49 |
| 40:MA:177:VAL:HG12 | 40:MA:178:SER:N | 2.28 | 0.49 |
| 41:MB:186:THR:HG23 | 41:MB:415:MET:HE3 | 1.94 | 0.49 |
| 40:MG:150:THR:O | 40:MG:154:MET:HG2 | 2.12 | 0.49 |
| 41:ML:204:ASN:OD1 | 43:ML:502:GDP:O2' | 2.31 | 0.49 |
| 41:MP:275:SER:O | 41:MP:279:GLN:HB2 | 2.12 | 0.49 |
| 41:NB:392:LYS:NZ | 41:NB:405:GLU:OE1 | 2.32 | 0.49 |
| 41:NN:165:ASN:HD21 | 41:NN:250:LEU:HD13 | 1.77 | 0.49 |
| 41:NO:3:GLU:HB2 | 41:NO:130:LEU:HD13 | 1.94 | 0.49 |
| 40:OG:140:SER:HA | 40:OG:171:ILE:H | 1.78 | 0.49 |
| 40:OG:209:ILE:HB | 40:OG:227:LEU:HD22 | 1.95 | 0.49 |
| 41:PB:8:GLN:OE1 | 41:PB:136:THR:OG1 | 2.30 | 0.49 |
| 40:PG:326:LYS:HA | 40:PG:329:ASN:HB2 | 1.94 | 0.49 |
| 41:PM:137:HIS:HE1 | 41:PM:166:THR:HB | 1.77 | 0.49 |
| 40:QA:112:LYS:HA | 40:QA:115:ILE:HG22 | 1.94 | 0.49 |
| 41:QB:70:PRO:HG3 | 41:QB:94:GLN:HE21 | 1.76 | 0.49 |
| 41:QB:397:TRP:O | 41:QB:398:TYR:C | 2.49 | 0.49 |
| 41:QN:182:PRO:O | 41:QN:186:THR:OG1 | 2.26 | 0.49 |
| 41:QP:239:CYS:HA | 41:QP:354:CYS:HB3 | 1.93 | 0.49 |
| 40:RA:73:THR:HB | 41:RN:243:PRO:HB3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RG:288:VAL:HA | 40:RG:291:ILE:HG12 | 1.93 | 0.49 |
| 40:RG:288:VAL:HB | 40:RG:372:ARG:HH22 | 1.77 | 0.49 |
| 41:RM:117:LEU:HA | 41:RM:120:VAL:HG22 | 1.94 | 0.49 |
| 41:RP:189:VAL:HG21 | 41:RP:378:PHE:HE1 | 1.77 | 0.49 |
| 40:SA:210:TYR:CE1 | 41:SN:324:LYS:HG3 | 2.47 | 0.49 |
| 41:SB:393:ALA:O | 41:SB:394:PHE:C | 2.50 | 0.49 |
| 40:SF:56:THR:HB | 40:TF:285:GLN:HA | 1.94 | 0.49 |
| 41:SL:55:THR:N | 41:TL:282:ARG:O | 2.40 | 0.49 |
| 41:SN:237:THR:HG23 | 41:SN:240:LEU:HD21 | 1.94 | 0.49 |
| 41:SN:271:ALA:HA | 41:SN:273:LEU:HG | 1.93 | 0.49 |
| 41:TB:2:ARG:HD2 | 41:TB:240:LEU:HB2 | 1.94 | 0.49 |
| 40:TI:177:VAL:HG12 | 41:TP:331:LEU:HB2 | 1.94 | 0.49 |
| 41:TO:248:ALA:HA | 41:TO:252:LYS:HG2 | 1.93 | 0.49 |
| 40:UA:7:VAL:HB | 40:UA:137:ILE:HG22 | 1.94 | 0.49 |
| 40:UE:133:GLN:O | 40:UE:165:SER:OG | 2.30 | 0.49 |
| 40:UH:217:LEU:HD22 | 40:UH:366:ASP:HB3 | 1.94 | 0.49 |
| 41:UP:143:THR:O | 41:UP:144:GLY:C | 2.51 | 0.49 |
| 40:VA:250:VAL:HG21 | 40:VA:318:LEU:HD22 | 1.95 | 0.49 |
| 41:VP:203:ASP:OD1 | 41:VP:204:ASN:N | 2.45 | 0.49 |
| 41:VQ:139:LEU:HD12 | 41:VQ:170:VAL:HG12 | 1.94 | 0.49 |
| 41:VQ:342:VAL:HG23 | 41:VQ:345:ILE:HG22 | 1.94 | 0.49 |
| 40:WA:104:ALA:HB2 | 40:WA:412:MET:HG2 | 1.94 | 0.49 |
| 40:WF:51:THR:HG21 | 40:WF:243:ARG:HG2 | 1.94 | 0.49 |
| 40:WF:274:PRO:HG3 | 40:WF:286:LEU:HD22 | 1.94 | 0.49 |
| 41:WM:371:SER:C | 41:WM:373:ALA:H | 2.16 | 0.49 |
| 41:WP:318:ARG:HB3 | 41:WP:357:PRO:HA | 1.93 | 0.49 |
| 12:2N:59:ALA:HB1 | 41:AN:423:VAL:HG13 | 1.94 | 0.49 |
| 12:2O:113:PHE:HA | 12:2O:131:ILE:HD11 | 1.95 | 0.49 |
| 14:3C:46:ARG:HH21 | 40:MG:264:ARG:NH1 | 2.10 | 0.49 |
| 17:3P:149:ARG:O | 17:3P:153:ILE:HG12 | 2.12 | 0.49 |
| 18:3U:188:GLU:HB2 | 18:3U:192:ARG:HH12 | 1.78 | 0.49 |
| 21:4D:502:ARG:HG2 | 22:4I:647:ARG:HH22 | 1.78 | 0.49 |
| 27:4Y:59:SER:OG | 27:4Y:61:ASP:O | 2.26 | 0.49 |
| 27:4Y:143:TYR:CD1 | 27:4Y:211:ILE:HG12 | 2.47 | 0.49 |
| 36:5X:131:VAL:HA | 40:KE:405:HIS:HB2 | 1.95 | 0.49 |
| 36:5X:186:TYR:HA | 36:5X:189:LEU:HD13 | 1.94 | 0.49 |
| 37:6A:79:ARG:NH2 | 37:6A:95:ASP:OD1 | 2.45 | 0.49 |
| 37:6A:124:LYS:HB3 | 41:UP:212:PHE:HZ | 1.78 | 0.49 |
| 40:AF:329:ASN:HB3 | 41:AN:175:VAL:HG11 | 1.94 | 0.49 |
| 40:BF:253:THR:HG21 | 41:BN:103:LYS:HZ2 | 1.77 | 0.49 |
| 40:BF:255:PHE:HZ | 40:BF:318:LEU:HD21 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BH:177:VAL:CG2 | 41:BO:327:ASP:HB3 | 2.42 | 0.49 |
| 40:BI:99:ALA:O | 40:BI:100:ALA:C | 2.50 | 0.49 |
| 41:BM:244:GLY:HA3 | 41:BM:354:CYS:HA | 1.93 | 0.49 |
| 40:CA:317:LEU:HD13 | 40:CA:332:ILE:HD11 | 1.95 | 0.49 |
| 41:CB:61:PRO:HD3 | 41:CB:84:ILE:HG12 | 1.94 | 0.49 |
| 40:CH:288:VAL:HG21 | 40:CH:327:ASP:OD1 | 2.13 | 0.49 |
| 41:CP:6:HIS:HA | 41:CP:134:GLN:O | 2.11 | 0.49 |
| 41:DB:45:GLU:C | 41:DB:47:ILE:H | 2.16 | 0.49 |
| 41:DB:173:PRO:O | 41:DB:174:LYS:C | 2.50 | 0.49 |
| 40:DE:262:TYR:HE2 | 40:DE:434:VAL:HG13 | 1.77 | 0.49 |
| 40:DF:68:VAL:HG21 | 40:DF:149:PHE:CE2 | 2.47 | 0.49 |
| 40:DF:264:ARG:O | 40:DF:266:HIS:N | 2.46 | 0.49 |
| 40:DH:400:LYS:O | 40:DH:401:ARG:C | 2.51 | 0.49 |
| 40:DI:262:TYR:CD2 | 40:DI:434:VAL:HG23 | 2.47 | 0.49 |
| 41:DN:204:ASN:HD22 | 41:DN:222:TYR:HE1 | 1.60 | 0.49 |
| 41:DP:145:SER:OG | 41:DP:146:GLY:N | 2.45 | 0.49 |
| 41:DP:317:PHE:HB3 | 41:DP:321:MET:SD | 2.52 | 0.49 |
| 40:EE:102:ASN:HB3 | 40:EE:105:ARG:HG3 | 1.94 | 0.49 |
| 40:EH:74:VAL:HG13 | 40:EH:75:ILE:HG12 | 1.95 | 0.49 |
| 40:EI:222:PRO:HD2 | 41:EP:324:LYS:HG3 | 1.95 | 0.49 |
| 40:EI:252:LEU:HA | 40:EI:255:PHE:HD2 | 1.75 | 0.49 |
| 41:EN:27:GLU:OE2 | 41:EN:318:ARG:NH2 | 2.40 | 0.49 |
| 41:EP:355:ASP:O | 41:EP:356:ILE:C | 2.50 | 0.49 |
| 40:FA:195:LEU:HA | 40:FA:266:HIS:NE2 | 2.26 | 0.49 |
| 40:FG:26:LEU:HD21 | 40:FG:363:VAL:HG23 | 1.95 | 0.49 |
| 40:FI:14:VAL:HG23 | 40:FI:67:PHE:HD2 | 1.77 | 0.49 |
| 41:FN:105:HIS:HA | 41:FN:150:LEU:HD22 | 1.94 | 0.49 |
| 40:GA:177:VAL:CG2 | 41:GN:331:LEU:HB2 | 2.43 | 0.49 |
| 40:GE:107:HIS:HA | 40:GE:152:LEU:HD22 | 1.94 | 0.49 |
| 40:GH:394:PHE:HZ | 40:GH:417:PHE:HB3 | 1.77 | 0.49 |
| 40:GH:439:VAL:O | 40:GH:440:GLU:C | 2.50 | 0.49 |
| 40:GI:263:PRO:O | 40:GI:264:ARG:HB2 | 2.11 | 0.49 |
| 41:GO:178:THR:N | 41:GO:181:GLU:OE2 | 2.36 | 0.49 |
| 40:II:28:HIS:CE1 | 40:II:243:ARG:HD2 | 2.48 | 0.49 |
| 41:IP:200:TYR:HE1 | 41:IP:368:ILE:HD12 | 1.78 | 0.49 |
| 40:JF:177:VAL:HA | 41:JM:331:LEU:HD13 | 1.94 | 0.49 |
| 41:JM:144:GLY:O | 41:JM:148:GLY:N | 2.42 | 0.49 |
| 41:KB:68:LEU:HB2 | 41:KB:143:THR:HG22 | 1.94 | 0.49 |
| 40:KE:320:ARG:HH21 | 40:KE:360:PRO:HA | 1.78 | 0.49 |
| 41:KL:141:GLY:HA3 | 43:KL:501:GDP:O1A | 2.12 | 0.49 |
| 41:KM:131:GLN:HE22 | 41:KM:249:ASP:HB2 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:LB:132:GLY:HA3 | 41:LB:163:ILE:O | 2.12 | 0.49 |
| 40:LF:228:ASN:OD1 | 42:LM:501:GTP:N2 | 2.40 | 0.49 |
| 40:LG:172:TYR:CE2 | 40:LG:386:ALA:HB1 | 2.48 | 0.49 |
| 41:LM:62:ARG:NH2 | 41:LM:127:CYS:SG | 2.85 | 0.49 |
| 40:MA:422:GLU:O | 40:MA:425:ALA:HB3 | 2.13 | 0.49 |
| 40:MD:223:THR:HG23 | 40:MD:225:THR:H | 1.76 | 0.49 |
| 40:MH:338:LYS:HB2 | 40:MH:341:ILE:HD11 | 1.94 | 0.49 |
| 41:MM:77:ARG:HH21 | 41:MM:90:PHE:HE2 | 1.59 | 0.49 |
| 41:NB:125:GLU:OE2 | 41:OB:291:GLN:NE2 | 2.44 | 0.49 |
| 40:NF:5:ILE:O | 40:NF:135:PHE:HA | 2.12 | 0.49 |
| 40:NF:101:ASN:OD1 | 41:NM:252:LYS:NZ | 2.31 | 0.49 |
| 40:NG:311:LYS:HZ2 | 40:NG:342:GLN:HG2 | 1.78 | 0.49 |
| 40:NH:119:LEU:HD11 | 40:NH:156:ARG:HG3 | 1.92 | 0.49 |
| 41:NN:257:MET:HA | 41:NN:312:THR:HG21 | 1.93 | 0.49 |
| 40:PA:215:ARG:NH2 | 40:PA:299:ALA:O | 2.45 | 0.49 |
| 41:PB:8:GLN:OE1 | 41:PB:8:GLN:HA | 2.06 | 0.49 |
| 41:PB:232:THR:HG21 | 41:PB:268:PRO:HB2 | 1.95 | 0.49 |
| 40:PF:206:ASN:HD22 | 40:PF:227:LEU:HD13 | 1.77 | 0.49 |
| 40:PG:324:VAL:HB | 40:PG:327:ASP:HB2 | 1.93 | 0.49 |
| 41:PL:74:ASP:OD1 | 41:PL:77:ARG:NH2 | 2.35 | 0.49 |
| 40:QA:190:THR:HA | 40:QA:193:THR:HG22 | 1.94 | 0.49 |
| 41:QB:244:GLY:HA3 | 41:QB:354:CYS:HA | 1.95 | 0.49 |
| 40:QF:238:ILE:HA | 40:QF:318:LEU:HD22 | 1.94 | 0.49 |
| 40:QG:326:LYS:HZ3 | 41:QO:220:PRO:HG2 | 1.76 | 0.49 |
| 41:QM:156:ARG:HH21 | 41:QM:196:THR:HA | 1.77 | 0.49 |
| 41:QM:267:MET:N | 41:QM:369:GLY:O | 2.40 | 0.49 |
| 41:QO:86:ARG:HG2 | 41:QO:89:ASN:H | 1.77 | 0.49 |
| 41:QP:271:ALA:HB2 | 41:QP:367:PHE:HE1 | 1.77 | 0.49 |
| 41:QP:312:THR:HA | 41:QP:348:ASN:HB2 | 1.95 | 0.49 |
| 40:RA:381:THR:O | 40:RA:431:TYR:OH | 2.30 | 0.49 |
| 41:RL:16:ILE:HA | 41:RL:226:ASN:HD21 | 1.76 | 0.49 |
| 41:RN:31:ASP:OD2 | 41:RN:37:HIS:NE2 | 2.45 | 0.49 |
| 41:RP:100:ASN:HB3 | 41:RP:103:LYS:HB2 | 1.94 | 0.49 |
| 40:SF:75:ILE:HG23 | 40:SF:92:LEU:HD12 | 1.94 | 0.49 |
| 40:SF:265:ILE:HG22 | 40:SF:379:ASN:HD21 | 1.78 | 0.49 |
| 40:SI:209:ILE:HD12 | 40:SI:230:LEU:HD23 | 1.95 | 0.49 |
| 41:SM:24:ILE:HA | 41:SM:27:GLU:HB2 | 1.93 | 0.49 |
| 41:SO:225:LEU:O | 41:SO:226:ASN:C | 2.49 | 0.49 |
| 40:TE:217:LEU:HA | 40:TE:277:SER:HB2 | 1.95 | 0.49 |
| 40:TG:139:HIS:O | 40:TG:170:SER:HA | 2.12 | 0.49 |
| 41:TL:180:VAL:O | 41:TL:184:ASN:ND2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UF:337:THR:O | 40:UF:338:LYS:C | 2.50 | 0.49 |
| 40:UF:352:LYS:HE3 | 41:UN:179:VAL:CG2 | 2.43 | 0.49 |
| 40:UI:288:VAL:O | 40:UI:291:ILE:HG12 | 2.12 | 0.49 |
| 40:UI:406:TRP:CZ3 | 41:UP:255:VAL:HA | 2.48 | 0.49 |
| 41:UO:259:PRO:HB2 | 41:UO:260:PHE:HD2 | 1.78 | 0.49 |
| 40:VH:79:ARG:HG2 | 40:VH:92:LEU:HD13 | 1.95 | 0.49 |
| 40:VH:169:PHE:HZ | 40:VH:238:ILE:HD11 | 1.76 | 0.49 |
| 40:VI:228:ASN:HA | 40:VI:231:ILE:HG22 | 1.94 | 0.49 |
| 41:VP:345:ILE:O | 41:VP:348:ASN:ND2 | 2.44 | 0.49 |
| 40:WF:93:ILE:HD11 | 40:WF:121:ARG:HG3 | 1.93 | 0.49 |
| 7:1T:384:ARG:O | 7:1T:385:ASP:C | 2.50 | 0.49 |
| 7:1U:317:VAL:HG12 | 7:1U:324:GLU:HG3 | 1.95 | 0.49 |
| 8:1W:310:GLN:O | 8:1W:314:LYS:HG2 | 2.12 | 0.49 |
| 8:1X:256:ARG:CZ | 40:UF:282:TYR:HA | 2.42 | 0.49 |
| 8:1Z:477:ARG:HH22 | 40:TG:60:LYS:HE3 | 1.78 | 0.49 |
| 9:2B:389:GLU:HG3 | 9:2B:392:ARG:HE | 1.75 | 0.49 |
| 11:2I:68:LYS:NZ | 41:LN:195:ASN:OD1 | 2.32 | 0.49 |
| 11:2K:43:LYS:HA | 41:MO:335:ASN:O | 2.11 | 0.49 |
| 12:2R:81:PHE:HB3 | 12:2R:83:ILE:HG12 | 1.93 | 0.49 |
| 13:2V:135:ASN:OD1 | 13:2V:135:ASN:N | 2.45 | 0.49 |
| 14:3B:79:VAL:HG21 | 14:3B:96:ILE:HD11 | 1.94 | 0.49 |
| 15:3E:48:ILE:HA | 15:3E:51:THR:HG22 | 1.94 | 0.49 |
| 17:3O:360:LYS:HA | 17:3O:363:ILE:HB | 1.94 | 0.49 |
| 17:3Q:409:ILE:O | 17:3Q:411:LEU:N | 2.46 | 0.49 |
| 18:3T:138:LEU:HD23 | 18:3T:286:LEU:HD21 | 1.95 | 0.49 |
| 20:4A:41:ASP:O | 20:4A:42:VAL:C | 2.51 | 0.49 |
| 20:4A:149:ARG:HH22 | 20:4A:150:SER:CA | 2.25 | 0.49 |
| 21:4F:446:THR:O | 21:4F:447:ASP:C | 2.50 | 0.49 |
| 22:4I:91:ASP:OD2 | 41:BO:279:GLN:NE2 | 2.45 | 0.49 |
| 22:4J:283:LYS:HE2 | 22:4J:332:PHE:HD2 | 1.76 | 0.49 |
| 23:4N:55:PRO:O | 23:4N:56:ALA:C | 2.51 | 0.49 |
| 24:4O:214:ASP:O | 24:4O:215:GLN:C | 2.51 | 0.49 |
| 24:4O:254:LYS:HE2 | 24:4O:255:PHE:HB3 | 1.93 | 0.49 |
| 24:4O:257:PHE:HB3 | 41:EL:322:SER:HB2 | 1.94 | 0.49 |
| 23:4P:185:SER:HA | 23:4P:202:PHE:HD2 | 1.76 | 0.49 |
| 23:4P:241:GLY:C | 23:4P:242:LEU:HG | 2.32 | 0.49 |
| 23:4P:258:GLY:O | 40:EA:226:ASN:ND2 | 2.46 | 0.49 |
| 23:4Q:253:TYR:O | 23:4Q:254:LYS:C | 2.49 | 0.49 |
| 39:6F:98:LEU:HD22 | 39:6F:153:TRP:HD1 | 1.77 | 0.49 |
| 40:AA:179:THR:HG23 | 41:AN:351:THR:HB | 1.94 | 0.49 |
| 41:AB:311:LEU:HD21 | 41:AB:425:ARG:HB3 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AE:104:ALA:O | 40:AE:108:TYR:HB2 | 2.13 | 0.49 |
| 40:AF:6:SER:O | 40:AF:65:ALA:HA | 2.13 | 0.49 |
| 41:AM:193:VAL:HG13 | 41:AM:262:ARG:HG2 | 1.93 | 0.49 |
| 41:BB:180:VAL:O | 41:BB:181:GLU:C | 2.51 | 0.49 |
| 40:BE:69:ASP:OD1 | 40:BE:74:VAL:HG11 | 2.13 | 0.49 |
| 40:BE:261:PRO:HD2 | 40:BE:265:ILE:O | 2.12 | 0.49 |
| 40:BF:118:VAL:HG21 | 40:BF:149:PHE:HZ | 1.77 | 0.49 |
| 40:BH:123:ARG:HA | 40:BH:161:TYR:OH | 2.11 | 0.49 |
| 40:BI:407:TYR:O | 40:BI:408:VAL:C | 2.51 | 0.49 |
| 41:BM:378:PHE:HA | 41:BM:415:MET:HE2 | 1.93 | 0.49 |
| 41:BN:290:THR:HG21 | 41:BN:329:GLN:HB3 | 1.94 | 0.49 |
| 40:CA:329:ASN:OD1 | 40:CA:330:ALA:N | 2.44 | 0.49 |
| 40:CA:339:ARG:O | 40:CA:340:SER:C | 2.50 | 0.49 |
| 40:CI:202:PHE:CE1 | 40:CI:377:LEU:HD23 | 2.46 | 0.49 |
| 41:CN:226:ASN:O | 41:CN:230:SER:N | 2.34 | 0.49 |
| 41:DB:128:ASP:O | 41:DB:129:CYS:HB2 | 2.12 | 0.49 |
| 41:DB:181:GLU:O | 41:DB:182:PRO:C | 2.50 | 0.49 |
| 40:DH:255:PHE:O | 40:DH:259:LEU:HB2 | 2.12 | 0.49 |
| 41:DM:55:THR:O | 41:DM:56:GLY:C | 2.51 | 0.49 |
| 41:DN:93:GLY:O | 41:DN:95:SER:N | 2.45 | 0.49 |
| 41:DN:149:THR:HA | 41:DN:152:ILE:HD12 | 1.94 | 0.49 |
| 41:DO:375:GLN:HE21 | 41:DO:379:LYS:HE3 | 1.77 | 0.49 |
| 41:EB:331:LEU:HD13 | 40:EG:177:VAL:HG23 | 1.93 | 0.49 |
| 40:EH:104:ALA:O | 40:EH:106:GLY:N | 2.45 | 0.49 |
| 40:EI:185:TYR:O | 40:EI:186:ASN:C | 2.51 | 0.49 |
| 41:EM:112:LEU:O | 41:EM:114:ASP:N | 2.45 | 0.49 |
| 41:EN:16:ILE:HA | 41:EN:226:ASN:HD21 | 1.77 | 0.49 |
| 41:EN:60:VAL:HG11 | 41:EN:86:ARG:HG2 | 1.95 | 0.49 |
| 41:EN:236:VAL:HG22 | 41:EN:368:ILE:HD11 | 1.94 | 0.49 |
| 40:FH:76:ASP:OD1 | 40:FH:79:ARG:NH2 | 2.46 | 0.49 |
| 40:FH:221:ARG:HG3 | 41:FO:322:SER:HB3 | 1.95 | 0.49 |
| 41:FO:103:LYS:O | 41:FO:107:THR:OG1 | 2.31 | 0.49 |
| 41:FP:226:ASN:H | 43:FP:501:GDP:HN21 | 1.61 | 0.49 |
| 40:GE:76:ASP:HA | 40:GE:79:ARG:HG2 | 1.95 | 0.49 |
| 40:GG:278:ALA:HA | 40:GG:368:ALA:HB2 | 1.94 | 0.49 |
| 40:GH:274:PRO:CB | 40:GH:370:VAL:HG11 | 2.42 | 0.49 |
| 40:HA:16:ILE:HD11 | 40:HA:138:PHE:HB3 | 1.95 | 0.49 |
| 40:HF:195:LEU:HD21 | 40:HF:264:ARG:HH21 | 1.77 | 0.49 |
| 41:HM:293:MET:HG2 | 41:HM:367:PHE:HB2 | 1.95 | 0.49 |
| 41:HQ:149:THR:HA | 41:HQ:152:ILE:HG22 | 1.94 | 0.49 |
| 40:IA:5:ILE:HD12 | 40:IA:125:LEU:HD22 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IB:285:THR:HB | 41:IB:287:PRO:HD2 | 1.94 | 0.49 |
| 41:IM:267:MET:HE3 | 41:IM:301:ALA:HB3 | 1.95 | 0.49 |
| 41:IP:316:VAL:HB | 41:IP:366:THR:HG22 | 1.93 | 0.49 |
| 40:JA:5:ILE:O | 40:JA:135:PHE:HA | 2.11 | 0.49 |
| 40:JG:182:VAL:O | 40:JG:186:ASN:ND2 | 2.45 | 0.49 |
| 40:KF:177:VAL:HG21 | 41:KM:327:ASP:HB3 | 1.93 | 0.49 |
| 41:KO:404:ASP:N | 41:KO:404:ASP:OD2 | 2.44 | 0.49 |
| 40:LA:325:PRO:HA | 40:LA:328:VAL:HG12 | 1.94 | 0.49 |
| 41:LB:25:SER:HB2 | 41:LB:81:PHE:HE2 | 1.78 | 0.49 |
| 40:LH:167:LEU:HD22 | 40:LH:200:CYS:HB3 | 1.95 | 0.49 |
| 41:LL:334:GLN:HG2 | 41:LL:341:PHE:CE2 | 2.48 | 0.49 |
| 40:MA:28:HIS:O | 40:MA:29:GLY:C | 2.50 | 0.49 |
| 40:MG:25:CYS:HB3 | 40:MG:30:ILE:O | 2.11 | 0.49 |
| 40:MG:348:PRO:HD2 | 41:MO:388:MET:HE3 | 1.94 | 0.49 |
| 40:MH:28:HIS:CE1 | 40:MH:243:ARG:HD2 | 2.48 | 0.49 |
| 40:NA:190:THR:O | 40:NA:194:THR:OG1 | 2.26 | 0.49 |
| 40:ND:191:THR:O | 40:ND:192:HIS:C | 2.50 | 0.49 |
| 40:NE:73:THR:OG1 | 41:NL:46:ARG:NH1 | 2.46 | 0.49 |
| 40:NG:238:ILE:HG13 | 40:NG:239:THR:HG23 | 1.94 | 0.49 |
| 41:NP:211:CYS:HA | 41:NP:215:LEU:HD12 | 1.93 | 0.49 |
| 40:OA:332:ILE:HD12 | 40:OA:351:PHE:HD2 | 1.76 | 0.49 |
| 40:OE:26:LEU:HD21 | 40:OE:363:VAL:HG22 | 1.94 | 0.49 |
| 40:OG:429:LYS:O | 40:OG:433:GLU:HG3 | 2.13 | 0.49 |
| 40:OH:248:LEU:O | 40:OH:354:GLY:HA2 | 2.12 | 0.49 |
| 41:OL:317:PHE:O | 41:OL:353:VAL:HA | 2.13 | 0.49 |
| 41:PB:211:CYS:HA | 41:PB:215:LEU:HB2 | 1.95 | 0.49 |
| 40:PG:288:VAL:HG11 | 40:PG:327:ASP:HB3 | 1.94 | 0.49 |
| 41:PL:190:HIS:CD2 | 41:PL:411:ALA:HA | 2.47 | 0.49 |
| 41:PL:317:PHE:HB2 | 41:PL:353:VAL:HG12 | 1.95 | 0.49 |
| 41:PO:8:GLN:OE1 | 41:PO:136:THR:OG1 | 2.27 | 0.49 |
| 41:PP:238:THR:HG21 | 41:PP:318:ARG:HG2 | 1.94 | 0.49 |
| 40:QA:21:TRP:CZ3 | 40:QA:52:PHE:HB3 | 2.47 | 0.49 |
| 40:QE:209:ILE:HB | 40:QE:227:LEU:HD22 | 1.94 | 0.49 |
| 40:QH:112:LYS:HA | 40:QH:115:ILE:HG22 | 1.95 | 0.49 |
| 41:QL:263:LEU:O | 41:QL:370:ASN:ND2 | 2.44 | 0.49 |
| 41:QL:278:SER:HA | 41:QL:281:TYR:HD2 | 1.77 | 0.49 |
| 41:QP:290:THR:C | 41:QP:292:GLN:H | 2.15 | 0.49 |
| 41:QP:342:VAL:HB | 41:QP:345:ILE:HG12 | 1.95 | 0.49 |
| 40:RF:319:TYR:HB3 | 40:RF:323:VAL:HG11 | 1.95 | 0.49 |
| 40:RH:263:PRO:HG3 | 41:RP:396:HIS:CG | 2.48 | 0.49 |
| 40:RI:47:ASP:OD1 | 40:RI:50:ASN:ND2 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RM:257:MET:O | 41:RM:370:ASN:ND2 | 2.45 | 0.49 |
| 41:RN:178:THR:HB | 41:RN:181:GLU:HG3 | 1.94 | 0.49 |
| 40:SE:3:GLU:N | 40:SE:3:GLU:OE2 | 2.46 | 0.49 |
| 40:SH:206:ASN:ND2 | 42:SH:501:GTP:O2' | 2.45 | 0.49 |
| 41:SL:139:LEU:HD12 | 41:SL:170:VAL:HB | 1.95 | 0.49 |
| 41:SM:73:MET:HA | 41:SM:76:VAL:HG12 | 1.93 | 0.49 |
| 41:SO:103:LYS:HA | 41:SO:107:THR:CB | 2.43 | 0.49 |
| 41:SO:343:GLU:C | 41:SO:345:ILE:H | 2.15 | 0.49 |
| 41:TB:139:LEU:HG | 41:TB:168:SER:HB3 | 1.94 | 0.49 |
| 40:TG:16:ILE:HG13 | 40:TG:228:ASN:HD22 | 1.78 | 0.49 |
| 41:TP:77:ARG:NH1 | 41:TP:82:GLY:O | 2.45 | 0.49 |
| 40:UH:325:PRO:HG2 | 41:UP:221:THR:HA | 1.94 | 0.49 |
| 40:UI:12:ALA:O | 40:UI:16:ILE:HG23 | 2.13 | 0.49 |
| 40:UI:294:ALA:O | 40:UI:295:CYS:C | 2.50 | 0.49 |
| 41:UO:311:LEU:H | 41:UO:371:SER:HA | 1.78 | 0.49 |
| 40:VA:177:VAL:HB | 41:VO:331:LEU:HD22 | 1.95 | 0.49 |
| 41:VN:282:ARG:NH2 | 41:VN:292:GLN:OE1 | 2.45 | 0.49 |
| 40:WA:76:ASP:O | 40:WA:80:THR:CB | 2.60 | 0.49 |
| 40:WF:140:SER:OG | 42:WF:501:GTP:O2A | 2.27 | 0.49 |
| 41:WM:310:TYR:CE1 | 41:WM:371:SER:HB3 | 2.47 | 0.49 |
| 7:1T:511:HIS:O | 7:1T:514:GLU:N | 2.46 | 0.49 |
| 7:1T:586:HIS:CE1 | 7:1T:590:ILE:HD11 | 2.47 | 0.49 |
| 7:1U:519:THR:HG1 | 7:1U:529:TRP:HE1 | 1.59 | 0.49 |
| 11:2I:197:LEU:O | 11:2I:198:GLN:C | 2.49 | 0.49 |
| 12:2R:45:LYS:HA | 12:2R:48:MET:HG2 | 1.94 | 0.49 |
| 14:3B:105:ALA:O | 14:3B:110:ARG:NH1 | 2.45 | 0.49 |
| 15:3F:128:VAL:HG23 | 15:3F:130:ASP:HB2 | 1.95 | 0.49 |
| 18:3W:188:GLU:HB2 | 18:3W:192:ARG:HH12 | 1.77 | 0.49 |
| 21:4F:473:VAL:HG11 | 21:4F:482:PRO:HG2 | 1.94 | 0.49 |
| 22:4I:104:ILE:HG12 | 22:4I:115:VAL:HG22 | 1.95 | 0.49 |
| 23:4N:94:TYR:OH | 41:AM:45:GLU:HG2 | 2.11 | 0.49 |
| 23:4R:108:ASN:O | 23:4R:109:CYS:C | 2.51 | 0.49 |
| 28:5B:190:THR:HG21 | 41:KP:70:PRO:HB2 | 1.95 | 0.49 |
| 30:5G:77:PRO:HD3 | 40:GA:361:THR:HA | 1.94 | 0.49 |
| 31:5J:803:ILE:HG21 | 33:5O:90:GLU:OE1 | 2.11 | 0.49 |
| 36:5X:258:ARG:NH1 | 40:LF:440:GLU:HA | 2.28 | 0.49 |
| 39:6I:127:LEU:HD21 | 39:6I:140:VAL:HG11 | 1.94 | 0.49 |
| 40:BE:76:ASP:HA | 40:BE:79:ARG:HH21 | 1.77 | 0.49 |
| 40:BF:177:VAL:HG23 | 40:BF:178:SER:H | 1.76 | 0.49 |
| 41:BN:207:LEU:HA | 41:BN:210:ILE:HG22 | 1.95 | 0.49 |
| 41:BO:299:MET:HG2 | 41:BO:305:PRO:HG3 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CH:76:ASP:HA | 40:CH:79:ARG:HB2 | 1.93 | 0.49 |
| 40:CH:109:THR:C | 40:CH:111:GLY:H | 2.14 | 0.49 |
| 41:CL:202:ILE:HG21 | 41:CL:229:VAL:HG22 | 1.94 | 0.49 |
| 41:CN:208:TYR:O | 41:CN:209:ASP:C | 2.51 | 0.49 |
| 41:CO:358:PRO:HD3 | 41:CO:364:SER:HB3 | 1.93 | 0.49 |
| 41:CP:105:HIS:HA | 41:CP:150:LEU:HD22 | 1.93 | 0.49 |
| 40:DA:403:PHE:CE1 | 41:DN:259:PRO:HA | 2.48 | 0.49 |
| 41:DB:163:ILE:HG21 | 41:DB:250:LEU:HB3 | 1.95 | 0.49 |
| 41:DB:245:GLN:O | 41:DB:247:ASN:N | 2.45 | 0.49 |
| 41:DB:347:ASN:O | 40:DG:181:VAL:HG12 | 2.12 | 0.49 |
| 40:DH:71:GLU:HG2 | 40:DH:98:ASP:HB2 | 1.93 | 0.49 |
| 40:DH:326:LYS:HG3 | 41:DP:220:PRO:HD2 | 1.93 | 0.49 |
| 40:DI:111:GLY:O | 40:DI:114:LEU:N | 2.45 | 0.49 |
| 41:DL:144:GLY:O | 41:DL:145:SER:C | 2.50 | 0.49 |
| 41:DL:256:ASN:ND2 | 41:DL:350:LYS:HD3 | 2.27 | 0.49 |
| 41:DN:141:GLY:HA3 | 43:DN:501:GDP:O1A | 2.11 | 0.49 |
| 41:DO:305:PRO:HB3 | 41:DO:310:TYR:HE1 | 1.77 | 0.49 |
| 41:DP:420:ASN:O | 41:DP:423:VAL:HG22 | 2.11 | 0.49 |
| 40:EH:9:VAL:HB | 40:EH:68:VAL:HG13 | 1.94 | 0.49 |
| 40:EH:27:GLU:HG3 | 40:EH:361:THR:OG1 | 2.12 | 0.49 |
| 40:EI:69:ASP:CG | 40:EI:74:VAL:HG11 | 2.32 | 0.49 |
| 40:EI:273:ALA:O | 40:EI:275:VAL:N | 2.38 | 0.49 |
| 40:EI:320:ARG:HG3 | 40:EI:356:ASN:HD21 | 1.78 | 0.49 |
| 41:EP:56:GLY:O | 41:EP:57:GLY:C | 2.50 | 0.49 |
| 41:EP:305:PRO:HA | 41:EP:373:ALA:CB | 2.41 | 0.49 |
| 40:FA:317:LEU:HD13 | 40:FA:332:ILE:HD11 | 1.95 | 0.49 |
| 41:FB:5:VAL:HG13 | 41:FB:62:ARG:HG2 | 1.95 | 0.49 |
| 41:FB:139:LEU:HD12 | 41:FB:170:VAL:HG22 | 1.94 | 0.49 |
| 41:FP:131:GLN:HE22 | 41:FP:249:ASP:HB2 | 1.76 | 0.49 |
| 40:GI:17:GLY:O | 40:GI:18:ASN:C | 2.51 | 0.49 |
| 41:GN:298:ASN:O | 41:GN:300:MET:N | 2.46 | 0.49 |
| 40:HI:138:PHE:HZ | 40:HI:235:VAL:HG21 | 1.78 | 0.49 |
| 41:HM:321:MET:HG2 | 41:HM:363:MET:HG2 | 1.94 | 0.49 |
| 41:HN:420:ASN:O | 41:HN:423:VAL:N | 2.45 | 0.49 |
| 40:IA:224:TYR:O | 40:IA:228:ASN:ND2 | 2.45 | 0.49 |
| 41:IO:299:MET:N | 41:IO:299:MET:SD | 2.86 | 0.49 |
| 41:IP:2:ARG:HB2 | 41:IP:131:GLN:HG3 | 1.95 | 0.49 |
| 41:IP:87:PRO:HG2 | 40:JG:280:LYS:HG3 | 1.94 | 0.49 |
| 41:IQ:73:MET:HG3 | 41:IQ:92:PHE:HB3 | 1.93 | 0.49 |
| 41:JB:324:LYS:HE3 | 40:JG:210:TYR:HA | 1.93 | 0.49 |
| 41:JL:222:TYR:O | 41:JL:226:ASN:CB | 2.38 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JM:49:VAL:HG11 | 41:JM:241:ARG:HG3 | 1.94 | 0.49 |
| 40:KA:103:TYR:HD2 | 40:KA:412:MET:HE1 | 1.78 | 0.49 |
| 40:KA:195:LEU:HD22 | 40:KA:427:LEU:HD11 | 1.94 | 0.49 |
| 41:KB:337:ASN:HB3 | 41:KB:340:TYR:HD2 | 1.77 | 0.49 |
| 40:LG:160:ASP:O | 40:LG:162:GLY:N | 2.46 | 0.49 |
| 41:LN:16:ILE:HG13 | 41:LN:226:ASN:HB3 | 1.95 | 0.49 |
| 41:LN:139:LEU:HG | 41:LN:168:SER:HB2 | 1.94 | 0.49 |
| 41:LO:52:ASN:OD1 | 41:LO:62:ARG:NH2 | 2.46 | 0.49 |
| 40:MA:430:ASP:O | 40:MA:434:VAL:HG13 | 2.13 | 0.49 |
| 40:MF:72:PRO:O | 40:MF:73:THR:C | 2.50 | 0.49 |
| 40:MH:5:ILE:HD12 | 40:MH:132:LEU:HD13 | 1.94 | 0.49 |
| 41:MN:316:VAL:HA | 41:MN:352:ALA:O | 2.13 | 0.49 |
| 41:MO:163:ILE:HG22 | 41:MO:164:MET:H | 1.77 | 0.49 |
| 41:NB:152:ILE:HG23 | 41:NB:164:MET:HG3 | 1.94 | 0.49 |
| 40:ND:172:TYR:CZ | 40:ND:386:ALA:HB1 | 2.47 | 0.49 |
| 40:ND:205:ASP:HB3 | 40:ND:303:VAL:HA | 1.93 | 0.49 |
| 41:OB:178:THR:HB | 41:OB:181:GLU:HG2 | 1.93 | 0.49 |
| 41:PB:222:TYR:O | 41:PB:226:ASN:ND2 | 2.46 | 0.49 |
| 40:PG:112:LYS:HA | 40:PG:115:ILE:HG22 | 1.94 | 0.49 |
| 41:PP:15:GLN:NE2 | 43:PP:501:GDP:O6 | 2.45 | 0.49 |
| 41:QB:209:ASP:HA | 41:QB:213:ARG:CZ | 2.42 | 0.49 |
| 41:QL:289:LEU:O | 41:QL:293:MET:HG2 | 2.13 | 0.49 |
| 41:QP:12:CYS:HB2 | 43:QP:501:GDP:N9 | 2.28 | 0.49 |
| 41:QP:236:VAL:HG12 | 41:QP:237:THR:HG22 | 1.94 | 0.49 |
| 40:RI:137:ILE:HB | 40:RI:168:GLU:HG2 | 1.95 | 0.49 |
| 40:SE:88:HIS:HB3 | 40:SE:91:GLN:HG2 | 1.93 | 0.49 |
| 40:SG:66:VAL:HG12 | 40:SG:68:VAL:HG23 | 1.94 | 0.49 |
| 41:SO:131:GLN:HE22 | 41:SO:249:ASP:HB2 | 1.77 | 0.49 |
| 41:SO:252:LYS:O | 41:SO:253:LEU:C | 2.51 | 0.49 |
| 41:SO:318:ARG:HB3 | 41:SO:358:PRO:HD3 | 1.94 | 0.49 |
| 40:TA:71:GLU:OE2 | 41:TN:247:ASN:ND2 | 2.43 | 0.49 |
| 40:TA:97:GLU:OE2 | 40:TA:105:ARG:NH1 | 2.45 | 0.49 |
| 40:TF:371:GLN:OE1 | 40:TF:371:GLN:N | 2.45 | 0.49 |
| 41:TP:41:ASP:OD1 | 41:TP:41:ASP:N | 2.46 | 0.49 |
| 41:UB:33:THR:O | 41:UB:58:LYS:NZ | 2.41 | 0.49 |
| 40:UE:73:THR:HA | 40:UE:76:ASP:HB2 | 1.95 | 0.49 |
| 40:UI:297:GLU:HG2 | 40:UI:299:ALA:H | 1.77 | 0.49 |
| 41:UN:30:ILE:HD11 | 41:UN:47:ILE:HD11 | 1.94 | 0.49 |
| 40:WE:76:ASP:HA | 40:WE:79:ARG:HG2 | 1.95 | 0.49 |
| 40:WE:288:VAL:HB | 40:WE:327:ASP:HB3 | 1.94 | 0.49 |
| 40:WE:325:PRO:O | 40:WE:328:VAL:HB | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:WF:318:LEU:O | 40:WF:374:VAL:HA | 2.11 | 0.49 |
| 40:WH:319:TYR:HB3 | 40:WH:323:VAL:HG11 | 1.94 | 0.49 |
| 13:2T:49:ILE:HG12 | 13:2T:157:HIS:O | 2.13 | 0.49 |
| 13:2U:131:GLN:HE22 | 13:2U:133:GLN:HG3 | 1.76 | 0.49 |
| 13:2V:137:SER:HA | 13:2V:148:TYR:HB2 | 1.95 | 0.49 |
| 14:3B:9:GLN:NE2 | 41:ML:304:ASP:HA | 2.27 | 0.49 |
| 14:3B:46:ARG:HG2 | 14:3B:48:HIS:CD2 | 2.47 | 0.49 |
| 19:3Y:300:LYS:NZ | 40:LE:366:ASP:OD1 | 2.44 | 0.49 |
| 22:4H:329:ASP:OD1 | 22:4H:329:ASP:N | 2.45 | 0.49 |
| 22:4I:232:PHE:HE2 | 22:4I:338:LEU:HB3 | 1.77 | 0.49 |
| 22:4I:476:THR:HA | 41:FO:216:LYS:HE3 | 1.94 | 0.49 |
| 22:4J:282:ARG:HH22 | 41:CN:80:PRO:HD3 | 1.77 | 0.49 |
| 23:4M:107:LYS:HE3 | 23:4M:115:GLU:HG2 | 1.94 | 0.49 |
| 23:4N:254:LYS:HD3 | 41:DM:53:GLU:HB2 | 1.95 | 0.49 |
| 23:4Q:19:ILE:CD1 | 40:BH:79:ARG:HB3 | 2.43 | 0.49 |
| 25:4T:349:LEU:HB3 | 34:5Q:83:ILE:HG12 | 1.94 | 0.49 |
| 26:4W:257:LYS:HB3 | 26:4W:346:PHE:HE1 | 1.77 | 0.49 |
| 40:AE:70:LEU:HD12 | 40:AE:99:ALA:HB2 | 1.94 | 0.49 |
| 40:AG:326:LYS:HE2 | 41:AO:218:THR:O | 2.13 | 0.49 |
| 41:AO:50:TYR:O | 41:AO:62:ARG:HB2 | 2.12 | 0.49 |
| 41:AP:52:ASN:OD1 | 41:AP:62:ARG:NH2 | 2.45 | 0.49 |
| 40:CA:115:ILE:HG21 | 40:CA:156:ARG:HH21 | 1.78 | 0.49 |
| 41:CB:262:ARG:O | 41:CB:264:HIS:ND1 | 2.46 | 0.49 |
| 40:CH:104:ALA:HA | 40:CH:108:TYR:HD2 | 1.78 | 0.49 |
| 41:CL:101:TRP:HZ2 | 41:CL:191:GLN:HE22 | 1.61 | 0.49 |
| 41:CN:218:THR:C | 41:CN:220:PRO:HD3 | 2.33 | 0.49 |
| 41:CN:311:LEU:HA | 41:CN:342:VAL:HG22 | 1.93 | 0.49 |
| 41:CP:311:LEU:HA | 41:CP:342:VAL:CG2 | 2.42 | 0.49 |
| 40:DA:183:GLU:O | 40:DA:184:PRO:C | 2.50 | 0.49 |
| 40:DE:187:SER:HB2 | 40:DE:390:LEU:HD11 | 1.95 | 0.49 |
| 40:DE:287:SER:O | 40:DE:288:VAL:C | 2.50 | 0.49 |
| 40:DF:183:GLU:O | 40:DF:184:PRO:C | 2.51 | 0.49 |
| 40:DG:73:THR:HA | 40:DG:76:ASP:HB3 | 1.95 | 0.49 |
| 40:DI:106:GLY:HA2 | 40:DI:110:ILE:O | 2.12 | 0.49 |
| 41:DL:211:CYS:O | 41:DL:213:ARG:N | 2.39 | 0.49 |
| 41:DL:335:ASN:O | 41:DL:336:LYS:C | 2.50 | 0.49 |
| 41:DN:137:HIS:CE1 | 41:DN:168:SER:HB3 | 2.47 | 0.49 |
| 41:DP:11:GLN:HB3 | 43:DP:501:GDP:O2B | 2.11 | 0.49 |
| 41:DP:31:ASP:C | 41:DP:33:THR:H | 2.14 | 0.49 |
| 41:DP:82:GLY:C | 41:DP:84:ILE:H | 2.16 | 0.49 |
| 40:EA:288:VAL:HA | 40:EA:291:ILE:HG12 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EH:402:ALA:HB2 | 41:EO:344:TRP:HZ3 | 1.77 | 0.49 |
| 41:EM:323:MET:SD | 41:EM:353:VAL:HG21 | 2.53 | 0.49 |
| 41:EN:202:ILE:HD13 | 41:EN:229:VAL:HG21 | 1.94 | 0.49 |
| 41:EP:107:THR:OG1 | 41:EP:108:GLU:N | 2.41 | 0.49 |
| 41:FB:236:VAL:HG13 | 41:FB:237:THR:HG23 | 1.94 | 0.49 |
| 40:FF:182:VAL:HG23 | 40:FF:186:ASN:HD21 | 1.78 | 0.49 |
| 40:FG:224:TYR:HB3 | 40:FG:228:ASN:HD21 | 1.77 | 0.49 |
| 40:FI:20:CYS:HA | 40:FI:232:SER:HB2 | 1.95 | 0.49 |
| 40:GA:88:HIS:CE1 | 40:GA:90:GLU:HB2 | 2.47 | 0.49 |
| 40:GI:303:VAL:O | 40:GI:305:CYS:N | 2.46 | 0.49 |
| 41:GP:309:ARG:NH1 | 41:GP:339:SER:O | 2.40 | 0.49 |
| 40:HA:100:ALA:O | 41:HN:255:VAL:HG11 | 2.13 | 0.49 |
| 40:HA:316:CYS:SG | 40:HA:377:LEU:HB2 | 2.53 | 0.49 |
| 40:HG:160:ASP:OD1 | 40:HG:161:TYR:N | 2.46 | 0.49 |
| 40:HI:28:HIS:O | 40:HI:40:LYS:NZ | 2.37 | 0.49 |
| 40:IE:258:ASN:N | 40:IE:258:ASN:HD22 | 2.11 | 0.49 |
| 40:IG:205:ASP:HB2 | 40:IG:303:VAL:HA | 1.95 | 0.49 |
| 41:JB:67:ASP:OD1 | 41:JB:68:LEU:N | 2.46 | 0.49 |
| 40:JF:438:SER:HB3 | 41:JN:391:ARG:HH11 | 1.77 | 0.49 |
| 40:JG:244:PHE:HD2 | 40:JG:356:ASN:HD21 | 1.58 | 0.49 |
| 41:JM:124:ALA:O | 41:JM:125:GLU:C | 2.51 | 0.49 |
| 40:KD:73:THR:HA | 40:KD:76:ASP:HB3 | 1.93 | 0.49 |
| 40:KF:366:ASP:OD2 | 40:KF:366:ASP:N | 2.38 | 0.49 |
| 40:KG:208:ALA:HB2 | 40:KG:304:LYS:HD2 | 1.94 | 0.49 |
| 41:KL:230:SER:HA | 41:KL:233:MET:HE3 | 1.95 | 0.49 |
| 40:MD:73:THR:HA | 40:MD:76:ASP:HB2 | 1.94 | 0.49 |
| 40:MG:58:ALA:O | 40:MG:59:GLY:C | 2.51 | 0.49 |
| 41:MO:54:ALA:O | 41:MO:55:THR:C | 2.51 | 0.49 |
| 41:NP:107:THR:O | 41:NP:110:ALA:N | 2.40 | 0.49 |
| 41:OB:3:GLU:N | 41:OB:131:GLN:HE22 | 2.11 | 0.49 |
| 40:OH:26:LEU:HD22 | 40:OH:363:VAL:HG13 | 1.93 | 0.49 |
| 40:OH:71:GLU:O | 40:OH:71:GLU:HG2 | 2.11 | 0.49 |
| 41:OM:87:PRO:HA | 41:OM:90:PHE:HD1 | 1.78 | 0.49 |
| 41:ON:198:GLU:HG2 | 41:ON:266:PHE:HE2 | 1.77 | 0.49 |
| 41:OP:410:GLU:HA | 41:OP:413:SER:HB3 | 1.94 | 0.49 |
| 40:PF:342:GLN:NE2 | 40:PF:343:PHE:O | 2.46 | 0.49 |
| 40:PH:16:ILE:HA | 40:PH:228:ASN:HB3 | 1.95 | 0.49 |
| 40:PH:154:MET:HB2 | 40:PH:166:LYS:HE2 | 1.94 | 0.49 |
| 41:PL:204:ASN:OD1 | 43:PL:501:GDP:O2' | 2.30 | 0.49 |
| 41:PM:238:THR:HG21 | 41:PM:318:ARG:HD2 | 1.94 | 0.49 |
| 40:QA:140:SER:HA | 40:QA:171:ILE:HB | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QB:87:PRO:O | 41:QB:90:PHE:HB2 | 2.12 | 0.49 |
| 40:QF:224:TYR:HD1 | 40:QF:227:LEU:HD12 | 1.78 | 0.49 |
| 41:QM:100:ASN:HB3 | 41:QM:103:LYS:HG2 | 1.94 | 0.49 |
| 41:QN:10:GLY:O | 41:QN:14:ASN:HB2 | 2.12 | 0.49 |
| 41:RB:247:ASN:H | 40:RG:11:GLN:HE22 | 1.60 | 0.49 |
| 40:RG:404:VAL:HG23 | 40:RG:417:PHE:HE2 | 1.77 | 0.49 |
| 41:SB:183:TYR:HE1 | 41:SB:388:MET:HB3 | 1.76 | 0.49 |
| 40:SG:139:HIS:CD2 | 40:SG:150:THR:HG21 | 2.48 | 0.49 |
| 40:SH:70:LEU:HD23 | 40:SH:114:LEU:HD12 | 1.95 | 0.49 |
| 40:SH:224:TYR:CD1 | 41:SO:323:MET:HG3 | 2.47 | 0.49 |
| 41:SN:216:LYS:HE2 | 41:SN:275:SER:HB3 | 1.95 | 0.49 |
| 41:SO:208:TYR:O | 41:SO:209:ASP:C | 2.51 | 0.49 |
| 41:SO:275:SER:HG | 41:SO:276:ARG:HH11 | 1.58 | 0.49 |
| 41:TB:290:THR:HG21 | 41:TB:329:GLN:HB3 | 1.94 | 0.49 |
| 40:TE:7:VAL:HG23 | 40:TE:66:VAL:HG23 | 1.95 | 0.49 |
| 40:TE:234:ILE:O | 40:TE:238:ILE:HD12 | 2.13 | 0.49 |
| 40:TG:277:SER:O | 40:TG:279:GLU:N | 2.46 | 0.49 |
| 41:TL:173:PRO:HB3 | 41:TL:380:ARG:HD2 | 1.94 | 0.49 |
| 41:TP:385:PHE:O | 41:TP:389:PHE:HB2 | 2.12 | 0.49 |
| 40:UE:3:GLU:N | 40:UE:3:GLU:OE1 | 2.45 | 0.49 |
| 40:UE:62:VAL:HG11 | 40:VF:283:HIS:HB3 | 1.94 | 0.49 |
| 41:UN:189:VAL:O | 41:UN:193:VAL:HG23 | 2.13 | 0.49 |
| 40:VG:121:ARG:NE | 40:VG:124:LYS:HD2 | 2.25 | 0.49 |
| 40:VH:20:CYS:HA | 40:VH:232:SER:HB2 | 1.93 | 0.49 |
| 40:VJ:318:LEU:O | 40:VJ:374:VAL:HA | 2.12 | 0.49 |
| 41:VP:287:PRO:HG3 | 41:VP:329:GLN:HE22 | 1.77 | 0.49 |
| 40:WH:177:VAL:HB | 41:WO:327:ASP:HB3 | 1.94 | 0.49 |
| 41:WN:2:ARG:HD2 | 41:WN:240:LEU:HD11 | 1.93 | 0.49 |
| 41:WN:173:PRO:HB3 | 41:WN:380:ARG:HD3 | 1.94 | 0.49 |
| 41:WP:421:PRO:HA | 41:WP:424:THR:HG22 | 1.95 | 0.49 |
| 7:1T:21:GLY:HA2 | 7:1T:330:CYS:SG | 2.52 | 0.49 |
| 7:1T:383:MET:O | 7:1T:385:ASP:N | 2.46 | 0.49 |
| 8:1W:475:GLU:OE1 | 8:1W:478:ARG:NH1 | 2.44 | 0.49 |
| 9:2C:428:ARG:HG2 | 40:SI:58:ALA:HB2 | 1.94 | 0.49 |
| 11:2K:217:PHE:O | 11:2K:219:ASP:N | 2.46 | 0.49 |
| 13:2T:34:ILE:HD11 | 13:2T:49:ILE:HD12 | 1.94 | 0.49 |
| 13:2U:34:ILE:HG12 | 13:2U:49:ILE:HG22 | 1.94 | 0.49 |
| 13:2W:104:ARG:HB2 | 13:2W:118:ILE:HD11 | 1.94 | 0.49 |
| 13:2X:2:PHE:O | 13:2X:7:GLN:NE2 | 2.46 | 0.49 |
| 14:3A:48:HIS:ND1 | 40:MF:433:GLU:HG3 | 2.28 | 0.49 |
| 14:3A:81:LEU:HA | 14:3A:84:ARG:HD3 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:3H:388:VAL:HG23 | 15:3H:389:LEU:HD12 | 1.94 | 0.49 |
| 17:3R:174:LEU:HD13 | 17:3R:322:ARG:HG2 | 1.95 | 0.49 |
| 21:4D:120:VAL:HG12 | 21:4D:135:GLU:HB2 | 1.94 | 0.49 |
| 22:4H:246:ARG:HH11 | 22:4H:379:LYS:HB3 | 1.78 | 0.49 |
| 24:4O:190:TYR:OH | 41:CL:53:GLU:HB2 | 2.13 | 0.49 |
| 23:4Q:20:PRO:HG3 | 40:CH:279:GLU:HG3 | 1.95 | 0.49 |
| 23:4R:19:ILE:CD1 | 40:BI:79:ARG:HB3 | 2.43 | 0.49 |
| 23:4R:261:TYR:HE1 | 23:4R:265:THR:HG21 | 1.77 | 0.49 |
| 31:5I:421:LEU:HD13 | 31:5I:425:LEU:HD23 | 1.94 | 0.49 |
| 33:5O:43:VAL:HG11 | 41:JL:94:GLN:HG2 | 1.94 | 0.49 |
| 34:5R:448:ARG:HE | 40:FG:58:ALA:HB3 | 1.77 | 0.49 |
| 38:6C:117:ILE:HD12 | 41:VB:331:LEU:HD11 | 1.95 | 0.49 |
| 41:AL:173:PRO:HD3 | 41:AL:380:ARG:NH1 | 2.28 | 0.49 |
| 41:BB:271:ALA:HB3 | 41:BB:272:PRO:HD3 | 1.94 | 0.49 |
| 41:BB:358:PRO:HB2 | 41:BB:361:LEU:HD12 | 1.95 | 0.49 |
| 40:CA:72:PRO:HD3 | 40:CA:96:LYS:O | 2.12 | 0.49 |
| 40:CF:116:ASP:OD1 | 40:CF:117:LEU:N | 2.46 | 0.49 |
| 40:CH:273:ALA:HB2 | 40:CH:374:VAL:HG13 | 1.94 | 0.49 |
| 40:CI:181:VAL:HG22 | 41:CP:256:ASN:ND2 | 2.28 | 0.49 |
| 41:CL:271:ALA:HB3 | 41:CL:272:PRO:CD | 2.42 | 0.49 |
| 41:CO:216:LYS:HB2 | 41:CO:275:SER:HB2 | 1.94 | 0.49 |
| 40:DA:149:PHE:CE2 | 40:DA:153:LEU:HD22 | 2.47 | 0.49 |
| 40:DE:240:ALA:O | 40:DE:243:ARG:N | 2.40 | 0.49 |
| 41:DL:3:GLU:C | 41:DL:4:ILE:HG12 | 2.31 | 0.49 |
| 41:DL:34:GLY:O | 41:DL:35:THR:C | 2.51 | 0.49 |
| 41:DL:101:TRP:HB3 | 41:DL:403:MET:HE2 | 1.95 | 0.49 |
| 41:DL:121:ARG:O | 41:DL:122:LYS:C | 2.51 | 0.49 |
| 41:DL:193:VAL:HG21 | 41:DL:418:LEU:HG | 1.95 | 0.49 |
| 41:DL:392:LYS:HB3 | 41:DL:395:LEU:HD22 | 1.95 | 0.49 |
| 41:DM:7:LEU:N | 41:DM:134:GLN:O | 2.38 | 0.49 |
| 41:DM:181:GLU:C | 41:DM:183:TYR:H | 2.15 | 0.49 |
| 41:DM:245:GLN:O | 41:DM:246:LEU:C | 2.50 | 0.49 |
| 41:DN:262:ARG:O | 41:DN:264:HIS:N | 2.46 | 0.49 |
| 40:EE:319:TYR:HB3 | 40:EE:323:VAL:HG21 | 1.95 | 0.49 |
| 40:EG:213:CYS:O | 40:EG:219:ILE:N | 2.40 | 0.49 |
| 40:EI:215:ARG:O | 40:EI:216:ASN:C | 2.51 | 0.49 |
| 40:EI:219:ILE:HG23 | 40:EI:222:PRO:HG3 | 1.95 | 0.49 |
| 41:EM:54:ALA:HB3 | 41:EM:58:LYS:CB | 2.41 | 0.49 |
| 41:EP:79:GLY:O | 41:EP:80:PRO:C | 2.51 | 0.49 |
| 40:FH:177:VAL:HG22 | 41:FO:331:LEU:HD22 | 1.94 | 0.49 |
| 40:FI:70:LEU:HD12 | 40:FI:145:THR:HG22 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FM:60:VAL:HG21 | 41:FM:86:ARG:HE | 1.77 | 0.49 |
| 41:FO:279:GLN:HA | 41:FO:282:ARG:HB2 | 1.94 | 0.49 |
| 41:GM:286:VAL:HG11 | 41:GM:326:VAL:HG22 | 1.95 | 0.49 |
| 41:GN:267:MET:HG2 | 41:GN:301:ALA:HB2 | 1.94 | 0.49 |
| 40:HA:104:ALA:O | 40:HA:108:TYR:HB2 | 2.12 | 0.49 |
| 40:HF:3:GLU:OE2 | 40:HF:130:THR:N | 2.46 | 0.49 |
| 41:HO:286:VAL:HA | 41:HO:289:LEU:HB2 | 1.94 | 0.49 |
| 41:HP:271:ALA:HB2 | 41:HP:298:ASN:HD22 | 1.77 | 0.49 |
| 41:IB:142:GLY:O | 41:IB:144:GLY:N | 2.46 | 0.49 |
| 40:IH:228:ASN:ND2 | 42:IH:501:GTP:HN1 | 2.09 | 0.49 |
| 41:IN:330:MET:HB3 | 41:IN:349:VAL:HG11 | 1.95 | 0.49 |
| 40:JE:206:ASN:OD1 | 42:JE:501:GTP:O2' | 2.29 | 0.49 |
| 40:JF:98:ASP:O | 40:JF:105:ARG:NH1 | 2.42 | 0.49 |
| 40:JF:151:SER:HB2 | 40:JF:193:THR:HG21 | 1.95 | 0.49 |
| 41:JN:159:TYR:HB3 | 41:JN:162:ARG:HG3 | 1.94 | 0.49 |
| 41:JO:8:GLN:HA | 41:JO:135:LEU:HD12 | 1.94 | 0.49 |
| 40:KA:174:ALA:HB3 | 40:KA:178:SER:H | 1.77 | 0.49 |
| 40:KE:88:HIS:HE1 | 40:KE:90:GLU:HG3 | 1.77 | 0.49 |
| 41:KL:322:SER:O | 41:KL:323:MET:C | 2.51 | 0.49 |
| 40:LF:171:ILE:HA | 40:LF:204:VAL:O | 2.13 | 0.49 |
| 40:LG:261:PRO:HG3 | 40:LG:313:MET:HE1 | 1.95 | 0.49 |
| 41:MB:117:LEU:HA | 41:MB:120:VAL:HG12 | 1.94 | 0.49 |
| 40:MF:104:ALA:HB1 | 40:MF:410:GLU:CD | 2.32 | 0.49 |
| 40:MG:147:SER:HB2 | 40:MG:190:THR:HB | 1.95 | 0.49 |
| 40:MG:288:VAL:HA | 40:MG:291:ILE:CD1 | 2.43 | 0.49 |
| 41:ML:167:PHE:HA | 41:ML:200:TYR:HB2 | 1.95 | 0.49 |
| 41:NB:269:GLY:HA3 | 41:NB:367:PHE:HB3 | 1.95 | 0.49 |
| 40:ND:328:VAL:HG21 | 40:ND:353:VAL:HG11 | 1.93 | 0.49 |
| 40:NH:71:GLU:HB3 | 40:NH:98:ASP:HA | 1.94 | 0.49 |
| 41:NM:318:ARG:HE | 41:NM:358:PRO:HD3 | 1.78 | 0.49 |
| 41:NO:272:PRO:HG3 | 41:NO:364:SER:HA | 1.95 | 0.49 |
| 40:OA:31:GLN:HG3 | 40:OA:33:ASP:HB3 | 1.95 | 0.49 |
| 40:OH:88:HIS:CE1 | 40:OH:121:ARG:HH12 | 2.31 | 0.49 |
| 41:OL:52:ASN:OD1 | 41:OL:62:ARG:NH2 | 2.45 | 0.49 |
| 40:PD:179:THR:OG1 | 40:PD:183:GLU:OE2 | 2.29 | 0.49 |
| 40:PF:401:ARG:HD2 | 40:PF:404:VAL:HG21 | 1.95 | 0.49 |
| 40:PG:256:GLN:HE21 | 41:PO:397:TRP:HZ2 | 1.61 | 0.49 |
| 41:PL:172:SER:OG | 41:PL:175:VAL:O | 2.30 | 0.49 |
| 41:PO:207:LEU:HB3 | 41:PO:225:LEU:HD22 | 1.95 | 0.49 |
| 40:QA:254:GLU:OE1 | 41:QB:99:ASN:HB2 | 2.12 | 0.49 |
| 41:QB:31:ASP:N | 41:QB:35:THR:O | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QE:251:ASP:H | 40:QE:254:GLU:HB2 | 1.77 | 0.49 |
| 40:QE:288:VAL:HA | 40:QE:291:ILE:HG22 | 1.95 | 0.49 |
| 40:QH:154:MET:HG3 | 40:QH:194:THR:HG22 | 1.95 | 0.49 |
| 40:QH:188:ILE:HD12 | 40:QH:424:MET:HG3 | 1.94 | 0.49 |
| 41:QL:8:GLN:HG2 | 41:QL:65:LEU:HA | 1.95 | 0.49 |
| 41:QM:36:TYR:OH | 41:QM:43:GLN:OE1 | 2.29 | 0.49 |
| 41:QO:7:LEU:HB3 | 41:QO:135:LEU:HD13 | 1.95 | 0.49 |
| 41:QP:110:ALA:C | 41:QP:112:LEU:N | 2.66 | 0.49 |
| 41:QP:417:ASP:O | 41:QP:418:LEU:C | 2.50 | 0.49 |
| 40:RG:260:VAL:HB | 41:RO:397:TRP:HE1 | 1.78 | 0.49 |
| 40:RH:137:ILE:HB | 40:RH:168:GLU:HG3 | 1.95 | 0.49 |
| 41:RO:203:ASP:N | 41:RO:300:MET:O | 2.36 | 0.49 |
| 41:RO:318:ARG:HD3 | 41:RO:358:PRO:HD3 | 1.93 | 0.49 |
| 41:RP:203:ASP:N | 41:RP:300:MET:O | 2.37 | 0.49 |
| 41:SB:325:GLU:HA | 41:SB:328:GLU:HG3 | 1.94 | 0.49 |
| 40:SG:85:GLN:NE2 | 40:TG:279:GLU:OE2 | 2.39 | 0.49 |
| 40:SH:242:LEU:H | 40:SH:242:LEU:HD23 | 1.78 | 0.49 |
| 41:TB:182:PRO:HA | 41:TB:381:ILE:HD11 | 1.94 | 0.49 |
| 41:TB:245:GLN:HG3 | 40:TG:15:GLN:HE22 | 1.78 | 0.49 |
| 40:TH:191:THR:O | 40:TH:195:LEU:HB2 | 2.13 | 0.49 |
| 41:TM:51:TYR:HB3 | 41:TM:59:TYR:HB3 | 1.94 | 0.49 |
| 40:UF:406:TRP:CG | 41:UM:255:VAL:HG23 | 2.47 | 0.49 |
| 40:UG:241:SER:OG | 40:UG:250:VAL:N | 2.44 | 0.49 |
| 40:UI:71:GLU:HG3 | 40:UI:98:ASP:HB2 | 1.95 | 0.49 |
| 41:UP:44:LEU:HD22 | 41:UP:47:ILE:HG21 | 1.93 | 0.49 |
| 41:UP:139:LEU:HD23 | 41:UP:188:SER:HB2 | 1.95 | 0.49 |
| 41:VB:330:MET:HB3 | 41:VB:349:VAL:HG11 | 1.95 | 0.49 |
| 40:VJ:239:THR:O | 40:VJ:243:ARG:NH1 | 2.46 | 0.49 |
| 41:VO:22:GLU:HG3 | 41:VO:81:PHE:HD1 | 1.77 | 0.49 |
| 41:VO:260:PHE:HE2 | 41:VO:425:ARG:HE | 1.59 | 0.49 |
| 40:WH:62:VAL:HG21 | 40:WH:88:HIS:HB2 | 1.93 | 0.49 |
| 41:WQ:396:HIS:HA | 41:WQ:399:THR:HG22 | 1.94 | 0.49 |
| 7:1T:290:GLN:HE22 | 7:1T:369:ARG:HH12 | 1.61 | 0.49 |
| 8:1W:346:MET:HA | 8:1W:349:GLU:HG3 | 1.94 | 0.49 |
| 9:2B:308:GLN:O | 9:2B:311:LYS:HG3 | 2.12 | 0.49 |
| 10:2F:47:LEU:HD11 | 40:MA:434:VAL:HG12 | 1.95 | 0.49 |
| 11:2K:221:ILE:N | 11:2K:222:PRO:HD2 | 2.28 | 0.49 |
| 16:3J:17:TRP:CD1 | 16:3K:127:ASP:HA | 2.48 | 0.49 |
| 20:4A:201:LYS:HE2 | 21:4F:42:ARG:HH21 | 1.77 | 0.49 |
| 21:4E:477:SER:HB2 | 21:4E:482:PRO:HB3 | 1.94 | 0.49 |
| 22:4K:659:LYS:HB2 | 22:4K:678:LEU:HD11 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4N:116:ALA:O | 23:4N:117:LEU:C | 2.50 | 0.49 |
| 26:4V:23:ARG:HG3 | 26:4V:40:VAL:HG21 | 1.94 | 0.49 |
| 26:4V:282:VAL:HG21 | 26:4V:304:TYR:HB3 | 1.95 | 0.49 |
| 34:5R:438:ALA:O | 34:5R:439:ARG:C | 2.50 | 0.49 |
| 36:5Y:116:ARG:NH2 | 41:KO:417:ASP:OD1 | 2.39 | 0.49 |
| 40:AE:187:SER:HA | 40:AE:190:THR:HG22 | 1.95 | 0.49 |
| 40:AF:402:ALA:HB2 | 41:AM:344:TRP:HZ3 | 1.78 | 0.49 |
| 40:AG:27:GLU:OE1 | 40:AG:243:ARG:NH1 | 2.37 | 0.49 |
| 41:AM:142:GLY:O | 41:AM:144:GLY:N | 2.46 | 0.49 |
| 40:BF:326:LYS:HD3 | 41:BN:208:TYR:HD1 | 1.78 | 0.49 |
| 40:BG:208:ALA:HA | 40:BG:304:LYS:NZ | 2.27 | 0.49 |
| 40:BG:307:PRO:HB3 | 40:BG:312:TYR:HE1 | 1.78 | 0.49 |
| 41:CN:64:VAL:HG11 | 41:CN:120:VAL:HG22 | 1.95 | 0.49 |
| 41:CN:87:PRO:HD3 | 41:DN:281:TYR:CD2 | 2.46 | 0.49 |
| 40:DA:9:VAL:HG12 | 40:DA:145:THR:HG22 | 1.94 | 0.49 |
| 40:DA:181:VAL:HG12 | 41:DN:347:ASN:O | 2.13 | 0.49 |
| 41:DB:19:LYS:HA | 41:DB:22:GLU:HB2 | 1.93 | 0.49 |
| 41:DB:105:HIS:CE1 | 41:DB:191:GLN:HG3 | 2.48 | 0.49 |
| 40:DE:181:VAL:HG22 | 41:DL:256:ASN:OD1 | 2.13 | 0.49 |
| 40:DH:56:THR:OG1 | 40:DH:60:LYS:HB2 | 2.13 | 0.49 |
| 41:DN:31:ASP:HB2 | 41:DN:33:THR:HG23 | 1.95 | 0.49 |
| 41:DN:248:ALA:HB1 | 41:DN:252:LYS:HG2 | 1.95 | 0.49 |
| 40:EF:90:GLU:C | 40:EF:121:ARG:HH12 | 2.16 | 0.49 |
| 40:EG:241:SER:OG | 40:EG:249:ASN:OD1 | 2.24 | 0.49 |
| 41:EP:1:MET:SD | 41:EP:128:ASP:HB2 | 2.52 | 0.49 |
| 41:EP:42:LEU:HA | 41:EP:45:GLU:HB3 | 1.94 | 0.49 |
| 41:EP:109:GLY:O | 41:EP:110:ALA:C | 2.51 | 0.49 |
| 41:EP:318:ARG:HE | 41:EP:318:ARG:HB3 | 1.45 | 0.49 |
| 41:EP:413:SER:O | 41:EP:417:ASP:N | 2.44 | 0.49 |
| 41:FB:49:VAL:HG11 | 41:FB:241:ARG:HG2 | 1.94 | 0.49 |
| 40:FF:191:THR:O | 40:FF:195:LEU:HB2 | 2.13 | 0.49 |
| 40:FI:228:ASN:ND2 | 42:FI:501:GTP:HN1 | 2.05 | 0.49 |
| 40:GE:287:SER:O | 40:GE:288:VAL:C | 2.51 | 0.49 |
| 40:GE:305:CYS:O | 40:GE:306:ASP:C | 2.51 | 0.49 |
| 40:GH:132:LEU:O | 40:GH:133:GLN:C | 2.49 | 0.49 |
| 40:GI:217:LEU:O | 40:GI:219:ILE:HG12 | 2.13 | 0.49 |
| 40:GI:259:LEU:HG | 40:GI:316:CYS:HB2 | 1.94 | 0.49 |
| 41:GN:54:ALA:O | 41:GN:56:GLY:N | 2.46 | 0.49 |
| 40:HA:254:GLU:O | 40:HA:258:ASN:ND2 | 2.45 | 0.49 |
| 40:HE:79:ARG:C | 40:HE:84:ARG:HB2 | 2.34 | 0.49 |
| 40:HE:346:TRP:NE1 | 40:HE:434:VAL:O | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HF:6:SER:O | 40:HF:65:ALA:HA | 2.13 | 0.49 |
| 40:HF:222:PRO:HG2 | 41:HM:324:LYS:HE2 | 1.95 | 0.49 |
| 40:IA:318:LEU:O | 40:IA:374:VAL:HA | 2.12 | 0.49 |
| 40:II:215:ARG:HH21 | 40:II:299:ALA:HB1 | 1.77 | 0.49 |
| 41:JB:235:GLY:HA3 | 41:JB:366:THR:HG21 | 1.93 | 0.49 |
| 40:JD:238:ILE:HG13 | 40:JD:239:THR:HG23 | 1.93 | 0.49 |
| 40:JH:88:HIS:HB3 | 40:JH:91:GLN:HB2 | 1.94 | 0.49 |
| 40:KG:238:ILE:HA | 40:KG:318:LEU:HD22 | 1.94 | 0.49 |
| 40:LF:104:ALA:C | 40:LF:106:GLY:H | 2.16 | 0.49 |
| 40:LF:298:PRO:HB3 | 40:LF:307:PRO:HD2 | 1.94 | 0.49 |
| 40:LG:255:PHE:O | 40:LG:259:LEU:HB2 | 2.13 | 0.49 |
| 41:LN:194:GLU:OE2 | 41:LN:262:ARG:NH1 | 2.45 | 0.49 |
| 41:LN:253:LEU:O | 41:LN:257:MET:CB | 2.58 | 0.49 |
| 40:MF:105:ARG:HB3 | 40:MF:110:ILE:HD13 | 1.95 | 0.49 |
| 40:MF:217:LEU:HA | 40:MF:277:SER:HB3 | 1.93 | 0.49 |
| 40:MF:326:LYS:HB2 | 41:MN:208:TYR:CE1 | 2.48 | 0.49 |
| 40:MG:266:HIS:O | 40:MG:268:PRO:HD3 | 2.13 | 0.49 |
| 40:MG:430:ASP:O | 40:MG:434:VAL:HG22 | 2.12 | 0.49 |
| 41:MN:380:ARG:NH2 | 41:MN:383:GLU:OE2 | 2.45 | 0.49 |
| 41:MO:33:THR:OG1 | 41:MO:34:GLY:N | 2.46 | 0.49 |
| 41:MO:211:CYS:HA | 41:MO:215:LEU:HD12 | 1.94 | 0.49 |
| 41:MO:294:PHE:CZ | 41:MO:313:VAL:HG11 | 2.48 | 0.49 |
| 41:NB:87:PRO:HD3 | 41:OB:281:TYR:HD2 | 1.77 | 0.49 |
| 40:NH:323:VAL:HG22 | 40:NH:372:ARG:HG2 | 1.95 | 0.49 |
| 41:NM:107:THR:O | 41:NM:110:ALA:N | 2.46 | 0.49 |
| 41:NP:272:PRO:HG3 | 41:NP:364:SER:HA | 1.95 | 0.49 |
| 40:OH:136:LEU:HD23 | 40:OH:169:PHE:HE2 | 1.78 | 0.49 |
| 40:OH:201:ALA:O | 40:OH:203:MET:HG3 | 2.13 | 0.49 |
| 40:OH:339:ARG:O | 40:OH:340:SER:C | 2.51 | 0.49 |
| 40:OH:438:SER:HB2 | 41:OP:391:ARG:HH21 | 1.78 | 0.49 |
| 41:ON:256:ASN:HD22 | 41:ON:350:LYS:HD3 | 1.78 | 0.49 |
| 41:OO:8:GLN:NE2 | 41:OO:21:TRP:HE1 | 2.11 | 0.49 |
| 41:PB:134:GLN:HA | 41:PB:165:ASN:O | 2.13 | 0.49 |
| 40:PE:296:PHE:HE1 | 40:PE:376:MET:HG3 | 1.78 | 0.49 |
| 40:PF:272:TYR:HD2 | 40:PF:275:VAL:HG22 | 1.77 | 0.49 |
| 41:PO:165:ASN:HA | 41:PO:198:GLU:O | 2.12 | 0.49 |
| 41:QB:54:ALA:HB1 | 41:RB:282:ARG:O | 2.13 | 0.49 |
| 40:QE:60:LYS:HZ2 | 40:RE:283:HIS:HA | 1.77 | 0.49 |
| 40:QF:88:HIS:HB3 | 40:QF:91:GLN:HB2 | 1.95 | 0.49 |
| 40:RE:296:PHE:CE2 | 40:RE:335:ILE:HG12 | 2.48 | 0.49 |
| 40:RG:90:GLU:O | 40:RG:121:ARG:NH1 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RN:142:GLY:O | 41:RN:144:GLY:N | 2.46 | 0.49 |
| 40:SA:102:ASN:ND2 | 40:SA:105:ARG:HG3 | 2.28 | 0.49 |
| 41:SB:296:ALA:O | 41:SB:306:ARG:NH2 | 2.46 | 0.49 |
| 40:SF:70:LEU:HD23 | 40:SF:114:LEU:HD12 | 1.94 | 0.49 |
| 40:SF:401:ARG:HD2 | 40:SF:404:VAL:HG11 | 1.95 | 0.49 |
| 41:SO:97:ALA:O | 41:SO:98:GLY:C | 2.51 | 0.49 |
| 40:TA:274:PRO:HG2 | 40:TA:370:VAL:HG21 | 1.95 | 0.49 |
| 40:TH:10:GLY:HA2 | 40:TH:145:THR:HG22 | 1.95 | 0.49 |
| 40:TI:269:LEU:HB2 | 40:TI:383:ILE:HD11 | 1.95 | 0.49 |
| 41:TL:6:HIS:HD2 | 41:TL:8:GLN:HE21 | 1.61 | 0.49 |
| 41:TN:271:ALA:HB2 | 41:TN:298:ASN:HD22 | 1.77 | 0.49 |
| 41:UB:101:TRP:HB2 | 41:UB:184:ASN:HD22 | 1.78 | 0.49 |
| 40:UF:56:THR:OG1 | 40:UF:57:GLY:N | 2.45 | 0.49 |
| 40:UF:71:GLU:HB3 | 40:UF:98:ASP:CA | 2.41 | 0.49 |
| 41:UN:139:LEU:HD21 | 41:UN:192:LEU:HD22 | 1.95 | 0.49 |
| 40:VA:141:PHE:HB2 | 40:VA:173:PRO:HD3 | 1.94 | 0.49 |
| 40:VG:431:TYR:HA | 40:VG:434:VAL:HG12 | 1.95 | 0.49 |
| 41:VO:375:GLN:HG2 | 41:VO:422:VAL:HG13 | 1.95 | 0.49 |
| 40:WF:260:VAL:HG12 | 41:WN:396:HIS:CE1 | 2.47 | 0.49 |
| 41:WO:2:ARG:HB2 | 41:WO:240:LEU:HD11 | 1.95 | 0.49 |
| 41:WQ:142:GLY:O | 41:WQ:144:GLY:N | 2.46 | 0.49 |
| 8:1W:393:GLN:NE2 | 41:VB:360:GLY:O | 2.46 | 0.49 |
| 10:2F:44:TRP:CG | 41:MB:391:ARG:HD2 | 2.48 | 0.49 |
| 10:2F:162:LYS:HA | 10:2F:162:LYS:HD3 | 1.72 | 0.49 |
| 12:2R:158:ASN:O | 12:2R:160:ARG:NH1 | 2.44 | 0.49 |
| 13:2W:115:LYS:HB3 | 13:2W:116:PRO:HD2 | 1.94 | 0.49 |
| 15:3E:319:THR:HG22 | 15:3H:184:ILE:HG23 | 1.95 | 0.49 |
| 15:3F:146:VAL:HG21 | 15:3F:253:LEU:HD11 | 1.95 | 0.49 |
| 16:3J:194:LEU:O | 16:3J:195:LYS:HG3 | 2.13 | 0.49 |
| 17:3O:263:ALA:HB3 | 17:3P:407:PRO:HG3 | 1.95 | 0.49 |
| 17:3P:192:LEU:HD11 | 17:3P:223:VAL:HA | 1.94 | 0.49 |
| 18:3T:253:THR:O | 18:3T:257:TRP:N | 2.40 | 0.49 |
| 18:3U:318:LEU:HD23 | 18:3V:64:TYR:HE1 | 1.77 | 0.49 |
| 21:4E:96:VAL:O | 40:AH:41:THR:OG1 | 2.23 | 0.49 |
| 22:4K:455:SER:OG | 22:4K:464:SER:OG | 2.27 | 0.49 |
| 22:4K:680:LYS:HA | 22:4K:680:LYS:HD2 | 1.52 | 0.49 |
| 23:4M:263:HIS:HA | 23:4M:266:HIS:CE1 | 2.47 | 0.49 |
| 23:4N:205:LEU:O | 23:4N:208:GLN:HG2 | 2.12 | 0.49 |
| 24:4O:186:GLY:O | 24:4O:187:PHE:C | 2.51 | 0.49 |
| 23:4Q:184:MET:O | 23:4Q:185:SER:C | 2.51 | 0.49 |
| 23:4R:110:ASN:O | 23:4R:111:GLN:C | 2.51 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:4Y:70:VAL:HG22 | 27:4Y:268:THR:HG22 | 1.94 | 0.49 |
| 33:5N:236:GLU:HA | 33:5N:239:LYS:HG2 | 1.95 | 0.49 |
| 33:5N:412:ILE:HG13 | 40:HF:282:TYR:HE2 | 1.78 | 0.49 |
| 39:6G:31:LEU:HD21 | 39:6G:45:ILE:HG13 | 1.95 | 0.49 |
| 40:AA:29:GLY:HA2 | 40:AA:42:ILE:HG23 | 1.95 | 0.49 |
| 40:AE:141:PHE:HB2 | 40:AE:173:PRO:HD3 | 1.95 | 0.49 |
| 40:AE:323:VAL:HG22 | 40:AE:372:ARG:HG2 | 1.95 | 0.49 |
| 40:AG:140:SER:OG | 42:AG:501:GTP:O2A | 2.30 | 0.49 |
| 40:AH:179:THR:HG21 | 41:AO:246:LEU:CD1 | 2.42 | 0.49 |
| 41:AM:106:TYR:OH | 41:AM:407:GLU:OE2 | 2.29 | 0.49 |
| 41:AM:213:ARG:HH12 | 41:AM:297:LYS:HD3 | 1.78 | 0.49 |
| 40:BF:98:ASP:OD1 | 40:BF:99:ALA:N | 2.46 | 0.49 |
| 41:BM:321:MET:CE | 41:BM:363:MET:HG2 | 2.43 | 0.49 |
| 41:CB:226:ASN:ND2 | 43:CB:501:GDP:O6 | 2.45 | 0.49 |
| 40:CG:405:HIS:HA | 40:CG:408:VAL:HG12 | 1.95 | 0.49 |
| 40:CH:55:GLU:HG2 | 40:CH:61:HIS:CD2 | 2.48 | 0.49 |
| 41:CL:311:LEU:HD23 | 41:CL:344:TRP:CZ2 | 2.47 | 0.49 |
| 41:CM:102:ALA:O | 41:CM:107:THR:HG22 | 2.13 | 0.49 |
| 41:CM:377:LEU:HA | 41:CM:380:ARG:HE | 1.77 | 0.49 |
| 41:CN:137:HIS:H | 41:CN:137:HIS:HD2 | 1.61 | 0.49 |
| 41:CN:293:MET:HG2 | 41:CN:367:PHE:HB2 | 1.94 | 0.49 |
| 41:CN:375:GLN:HG3 | 41:CN:376:GLU:H | 1.78 | 0.49 |
| 40:DA:191:THR:O | 40:DA:192:HIS:C | 2.50 | 0.49 |
| 40:DA:294:ALA:O | 40:DA:297:GLU:N | 2.46 | 0.49 |
| 40:DH:218:ASP:O | 40:DH:219:ILE:C | 2.50 | 0.49 |
| 40:DI:270:ALA:HB2 | 40:DI:377:LEU:HA | 1.94 | 0.49 |
| 41:DL:3:GLU:HB3 | 41:DL:130:LEU:HD12 | 1.94 | 0.49 |
| 41:DL:203:ASP:HB3 | 41:DL:301:ALA:HA | 1.94 | 0.49 |
| 41:DL:375:GLN:O | 41:DL:376:GLU:C | 2.52 | 0.49 |
| 41:DM:268:PRO:O | 41:DM:299:MET:HA | 2.13 | 0.49 |
| 41:DN:142:GLY:O | 41:DN:145:SER:N | 2.41 | 0.49 |
| 41:EB:271:ALA:HA | 41:EB:273:LEU:HD23 | 1.94 | 0.49 |
| 40:EF:269:LEU:HD22 | 40:EF:303:VAL:HG11 | 1.94 | 0.49 |
| 40:EH:101:ASN:N | 41:EO:252:LYS:HZ3 | 2.11 | 0.49 |
| 40:EH:219:ILE:O | 40:EH:222:PRO:HD3 | 2.12 | 0.49 |
| 40:EH:387:TRP:HB3 | 40:EH:424:MET:SD | 2.53 | 0.49 |
| 41:EM:142:GLY:O | 41:EM:143:THR:C | 2.51 | 0.49 |
| 40:FA:153:LEU:O | 40:FA:154:MET:C | 2.51 | 0.49 |
| 40:FE:269:LEU:HD22 | 40:FE:303:VAL:HG21 | 1.95 | 0.49 |
| 41:FM:326:VAL:O | 41:FM:330:MET:HG2 | 2.12 | 0.49 |
| 41:GB:309:ARG:NH1 | 41:GB:339:SER:O | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GF:352:LYS:HD2 | 41:GN:179:VAL:CG1 | 2.43 | 0.49 |
| 40:GG:150:THR:O | 40:GG:154:MET:HG2 | 2.13 | 0.49 |
| 40:GH:139:HIS:CD2 | 40:GH:170:SER:HB3 | 2.48 | 0.49 |
| 40:GH:223:THR:O | 40:GH:227:LEU:HG | 2.13 | 0.49 |
| 40:GI:5:ILE:HG13 | 40:GI:132:LEU:HD11 | 1.94 | 0.49 |
| 40:GI:132:LEU:O | 40:GI:133:GLN:C | 2.51 | 0.49 |
| 40:GI:273:ALA:HB3 | 40:GI:374:VAL:H | 1.78 | 0.49 |
| 40:HF:397:MET:HG3 | 41:HM:346:PRO:HD2 | 1.95 | 0.49 |
| 41:HN:3:GLU:C | 41:HN:4:ILE:HG12 | 2.31 | 0.49 |
| 41:HO:7:LEU:HD13 | 41:HO:64:VAL:HG23 | 1.95 | 0.49 |
| 41:HQ:139:LEU:HD12 | 41:HQ:170:VAL:HG12 | 1.93 | 0.49 |
| 41:IN:22:GLU:HG2 | 41:IN:81:PHE:HD1 | 1.78 | 0.49 |
| 40:JE:71:GLU:N | 40:JE:71:GLU:OE2 | 2.46 | 0.49 |
| 40:JG:70:LEU:HD23 | 40:JG:114:LEU:HD12 | 1.95 | 0.49 |
| 40:KG:75:ILE:HG23 | 40:KG:92:LEU:HB3 | 1.95 | 0.49 |
| 41:KN:198:GLU:HG2 | 41:KN:266:PHE:HE2 | 1.77 | 0.49 |
| 41:LB:128:ASP:OD2 | 41:LB:128:ASP:N | 2.45 | 0.49 |
| 40:LG:207:GLU:HG2 | 40:LG:304:LYS:HD3 | 1.95 | 0.49 |
| 40:LG:315:CYS:HB3 | 40:LG:376:MET:SD | 2.53 | 0.49 |
| 40:MG:225:THR:HA | 40:MG:228:ASN:ND2 | 2.28 | 0.49 |
| 41:MO:112:LEU:HB3 | 41:MO:147:MET:HE1 | 1.94 | 0.49 |
| 41:MP:290:THR:HG21 | 41:MP:329:GLN:HB3 | 1.94 | 0.49 |
| 40:NA:179:THR:HG21 | 41:NN:246:LEU:HD11 | 1.94 | 0.49 |
| 40:ND:207:GLU:O | 40:ND:210:TYR:HB2 | 2.13 | 0.49 |
| 40:ND:297:GLU:O | 40:ND:299:ALA:N | 2.44 | 0.49 |
| 40:OD:241:SER:OG | 40:OD:249:ASN:OD1 | 2.31 | 0.49 |
| 40:OH:326:LYS:HE3 | 41:OP:225:LEU:HD11 | 1.94 | 0.49 |
| 41:OP:316:VAL:HB | 41:OP:366:THR:HG22 | 1.95 | 0.49 |
| 40:PD:73:THR:HA | 40:PD:76:ASP:HB2 | 1.95 | 0.49 |
| 40:PE:194:THR:O | 40:PE:198:SER:CB | 2.61 | 0.49 |
| 40:PH:241:SER:OG | 40:PH:250:VAL:N | 2.41 | 0.49 |
| 40:PH:405:HIS:HA | 40:PH:408:VAL:HG22 | 1.94 | 0.49 |
| 41:PM:182:PRO:O | 41:PM:186:THR:OG1 | 2.25 | 0.49 |
| 41:PO:113:VAL:HG21 | 41:PO:150:LEU:HD23 | 1.94 | 0.49 |
| 40:QA:67:PHE:HB2 | 40:QA:92:LEU:HD23 | 1.95 | 0.49 |
| 41:QB:290:THR:HG21 | 41:QB:329:GLN:CB | 2.43 | 0.49 |
| 40:QE:177:VAL:HG21 | 41:QL:327:ASP:HB3 | 1.95 | 0.49 |
| 40:QE:319:TYR:CD2 | 40:QE:323:VAL:HG21 | 2.47 | 0.49 |
| 40:QG:349:THR:OG1 | 40:QG:352:LYS:NZ | 2.46 | 0.49 |
| 41:QL:19:LYS:HZ3 | 41:QL:227:HIS:HA | 1.77 | 0.49 |
| 41:QM:6:HIS:HA | 41:QM:134:GLN:HB3 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QM:7:LEU:O | 41:QM:135:LEU:HA | 2.13 | 0.49 |
| 41:QN:232:THR:HG22 | 41:QN:270:PHE:HB2 | 1.94 | 0.49 |
| 41:QO:156:ARG:HH21 | 41:QO:196:THR:HA | 1.77 | 0.49 |
| 41:QO:198:GLU:OE1 | 41:QO:200:TYR:OH | 2.27 | 0.49 |
| 41:RB:64:VAL:HG21 | 41:RB:120:VAL:HG12 | 1.93 | 0.49 |
| 40:RE:116:ASP:N | 40:RE:116:ASP:OD1 | 2.44 | 0.49 |
| 40:RE:248:LEU:HD23 | 40:RE:355:ILE:HD12 | 1.94 | 0.49 |
| 40:RH:274:PRO:HA | 40:RH:276:ILE:HD12 | 1.95 | 0.49 |
| 40:RI:188:ILE:HG23 | 40:RI:424:MET:HG3 | 1.94 | 0.49 |
| 40:SG:70:LEU:HD12 | 40:SG:145:THR:HG22 | 1.95 | 0.49 |
| 41:SM:330:MET:HE2 | 41:SM:349:VAL:HG21 | 1.95 | 0.49 |
| 41:SO:250:LEU:O | 41:SO:251:ARG:C | 2.51 | 0.49 |
| 40:TG:54:SER:O | 40:TG:61:HIS:HA | 2.13 | 0.49 |
| 40:TH:101:ASN:HA | 40:TH:144:GLY:H | 1.77 | 0.49 |
| 40:TI:118:VAL:HG21 | 40:TI:149:PHE:HZ | 1.77 | 0.49 |
| 40:UG:251:ASP:OD1 | 40:UG:252:LEU:N | 2.43 | 0.49 |
| 40:UH:217:LEU:HD21 | 40:UH:367:LEU:HD23 | 1.95 | 0.49 |
| 40:UI:88:HIS:O | 40:UI:89:PRO:C | 2.50 | 0.49 |
| 41:UM:375:GLN:HG3 | 41:UM:379:LYS:HD2 | 1.94 | 0.49 |
| 41:UN:234:SER:OG | 41:UN:241:ARG:NH2 | 2.46 | 0.49 |
| 41:UP:180:VAL:O | 41:UP:181:GLU:C | 2.50 | 0.49 |
| 41:VB:327:ASP:HB3 | 40:VH:177:VAL:HG13 | 1.94 | 0.49 |
| 41:VN:222:TYR:O | 41:VN:226:ASN:ND2 | 2.44 | 0.49 |
| 40:WE:102:ASN:HB3 | 40:WE:105:ARG:HB3 | 1.95 | 0.49 |
| 40:WG:240:ALA:HA | 40:WG:243:ARG:HG3 | 1.94 | 0.49 |
| 40:WH:195:LEU:HD21 | 40:WH:264:ARG:HE | 1.78 | 0.49 |
| 40:WH:298:PRO:HB3 | 40:WH:307:PRO:HD2 | 1.94 | 0.49 |
| 40:WI:239:THR:O | 40:WI:243:ARG:NH1 | 2.46 | 0.49 |
| 41:WO:318:ARG:HG2 | 41:WO:357:PRO:HA | 1.95 | 0.49 |
| 41:WP:238:THR:HG21 | 41:WP:318:ARG:HG2 | 1.95 | 0.49 |
| 41:WQ:159:TYR:HB3 | 41:WQ:162:ARG:HD3 | 1.94 | 0.49 |
| 7:1S:508:VAL:HG23 | 7:1S:519:THR:HG22 | 1.95 | 0.48 |
| 7:1T:79:ILE:O | 7:1T:96:TRP:HB2 | 2.13 | 0.48 |
| 9:2B:403:LEU:O | 9:2B:407:LYS:HD2 | 2.12 | 0.48 |
| 13:2V:173:SER:O | 13:2V:174:GLU:C | 2.51 | 0.48 |
| 13:2X:28:LYS:HZ3 | 13:2X:56:THR:HA | 1.78 | 0.48 |
| 17:3R:97:ASP:O | 17:3R:101:ARG:N | 2.35 | 0.48 |
| 20:4B:253:LEU:HD21 | 41:MP:215:LEU:HD22 | 1.95 | 0.48 |
| 21:4D:50:ASP:OD1 | 21:4D:50:ASP:N | 2.45 | 0.48 |
| 21:4F:361:ILE:HD12 | 21:4F:364:LEU:HD13 | 1.95 | 0.48 |
| 21:4F:428:SER:HB3 | 21:4F:433:ASP:HB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4H:266:MET:HG3 | 22:4H:270:SER:HB2 | 1.95 | 0.48 |
| 23:4M:240:LEU:HB2 | 23:4M:266:HIS:HA | 1.94 | 0.48 |
| 26:4V:125:MET:HA | 26:4V:158:ILE:O | 2.12 | 0.48 |
| 31:5I:602:LYS:HD3 | 31:5I:673:ASN:N | 2.27 | 0.48 |
| 31:5J:793:GLY:H | 41:IM:276:ARG:HH11 | 1.61 | 0.48 |
| 36:5W:38:ASP:OD1 | 36:5W:39:ILE:N | 2.42 | 0.48 |
| 37:6A:119:THR:HG22 | 37:6A:122:LYS:HE3 | 1.95 | 0.48 |
| 40:AH:236:SER:O | 40:AH:240:ALA:HB2 | 2.13 | 0.48 |
| 40:BF:101:ASN:ND2 | 41:BM:256:ASN:OD1 | 2.46 | 0.48 |
| 40:BI:109:THR:O | 40:BI:111:GLY:N | 2.46 | 0.48 |
| 41:BM:427:ALA:O | 41:BM:428:CYS:C | 2.51 | 0.48 |
| 41:BP:143:THR:O | 41:BP:144:GLY:C | 2.51 | 0.48 |
| 41:CB:170:VAL:HG21 | 41:CB:377:LEU:HD11 | 1.94 | 0.48 |
| 41:CB:202:ILE:HG23 | 41:CB:300:MET:HB3 | 1.94 | 0.48 |
| 40:CF:188:ILE:HG21 | 40:CF:394:PHE:CD2 | 2.48 | 0.48 |
| 40:CF:387:TRP:CD1 | 40:CF:431:TYR:HE2 | 2.31 | 0.48 |
| 40:CH:182:VAL:O | 40:CH:183:GLU:C | 2.50 | 0.48 |
| 40:CH:390:LEU:HD12 | 40:CH:393:LYS:HD3 | 1.95 | 0.48 |
| 41:CM:107:THR:O | 41:CM:110:ALA:N | 2.41 | 0.48 |
| 41:CN:393:ALA:O | 41:CN:394:PHE:C | 2.51 | 0.48 |
| 41:CP:19:LYS:HG3 | 41:CP:226:ASN:HB3 | 1.95 | 0.48 |
| 40:DA:103:TYR:N | 40:DA:186:ASN:OD1 | 2.46 | 0.48 |
| 40:DA:259:LEU:HD21 | 40:DA:377:LEU:O | 2.13 | 0.48 |
| 41:DB:101:TRP:N | 41:DB:184:ASN:OD1 | 2.46 | 0.48 |
| 40:DI:112:LYS:C | 40:DI:114:LEU:H | 2.16 | 0.48 |
| 40:DI:162:GLY:O | 40:DI:163:LYS:C | 2.51 | 0.48 |
| 41:DL:48:ASN:O | 41:DL:49:VAL:C | 2.51 | 0.48 |
| 41:DL:182:PRO:HB3 | 41:DL:385:PHE:HA | 1.95 | 0.48 |
| 41:DP:192:LEU:O | 41:DP:193:VAL:C | 2.51 | 0.48 |
| 41:EB:207:LEU:HB3 | 41:EB:225:LEU:HD22 | 1.95 | 0.48 |
| 40:EG:231:ILE:HA | 40:EG:234:ILE:HD12 | 1.94 | 0.48 |
| 40:EI:217:LEU:O | 40:EI:219:ILE:HG22 | 2.13 | 0.48 |
| 41:EN:107:THR:O | 41:EN:110:ALA:N | 2.46 | 0.48 |
| 41:EO:114:ASP:OD1 | 41:EO:115:SER:N | 2.45 | 0.48 |
| 40:FA:335:ILE:HG23 | 40:FA:341:ILE:HD13 | 1.93 | 0.48 |
| 40:FE:26:LEU:HD21 | 40:FE:363:VAL:HG23 | 1.94 | 0.48 |
| 41:FN:139:LEU:HG | 41:FN:168:SER:HB3 | 1.94 | 0.48 |
| 41:FN:239:CYS:HB3 | 41:FN:248:ALA:H | 1.78 | 0.48 |
| 40:GA:204:VAL:HG11 | 40:GA:231:ILE:HD11 | 1.94 | 0.48 |
| 40:GE:262:TYR:CE1 | 41:GM:393:ALA:HA | 2.48 | 0.48 |
| 40:GG:297:GLU:OE1 | 40:GG:300:ASN:ND2 | 2.45 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GI:224:TYR:CE2 | 42:GP:501:GTP:H2' | 2.47 | 0.48 |
| 41:GM:226:ASN:ND2 | 43:GM:501:GDP:O6 | 2.41 | 0.48 |
| 41:HB:156:ARG:NH2 | 41:HB:197:ASP:OD2 | 2.47 | 0.48 |
| 40:HE:12:ALA:HB3 | 40:HE:140:SER:HB2 | 1.94 | 0.48 |
| 40:HE:90:GLU:HG3 | 40:HE:121:ARG:HD2 | 1.95 | 0.48 |
| 40:HE:242:LEU:O | 40:HE:243:ARG:C | 2.51 | 0.48 |
| 40:HF:252:LEU:HA | 40:HF:255:PHE:HD2 | 1.78 | 0.48 |
| 41:HM:20:PHE:HA | 41:HM:230:SER:HB2 | 1.94 | 0.48 |
| 41:HN:23:VAL:O | 41:HN:27:GLU:HB3 | 2.13 | 0.48 |
| 40:IE:20:CYS:HA | 40:IE:232:SER:HB2 | 1.95 | 0.48 |
| 40:IE:108:TYR:O | 40:IE:112:LYS:NZ | 2.44 | 0.48 |
| 40:IE:235:VAL:HA | 40:IE:238:ILE:HG22 | 1.93 | 0.48 |
| 40:IF:109:THR:HG21 | 40:IF:410:GLU:HG3 | 1.95 | 0.48 |
| 41:IM:173:PRO:HA | 41:IM:380:ARG:CZ | 2.43 | 0.48 |
| 41:IQ:398:TYR:HB3 | 41:IQ:403:MET:HG3 | 1.95 | 0.48 |
| 41:JB:189:VAL:HA | 41:JB:192:LEU:HB2 | 1.95 | 0.48 |
| 40:JD:335:ILE:HG23 | 40:JD:341:ILE:HG21 | 1.95 | 0.48 |
| 40:JE:326:LYS:CE | 41:JM:208:TYR:HB2 | 2.43 | 0.48 |
| 40:JG:121:ARG:HH12 | 40:JG:124:LYS:HG3 | 1.78 | 0.48 |
| 41:JN:73:MET:O | 41:JN:77:ARG:HG3 | 2.13 | 0.48 |
| 41:KB:132:GLY:HA2 | 41:KB:162:ARG:HB3 | 1.95 | 0.48 |
| 40:KE:116:ASP:OD1 | 40:KE:117:LEU:N | 2.47 | 0.48 |
| 40:KF:238:ILE:HG13 | 40:KF:239:THR:HG23 | 1.95 | 0.48 |
| 40:KG:200:CYS:HA | 40:KG:266:HIS:HB2 | 1.94 | 0.48 |
| 40:LG:167:LEU:HB3 | 40:LG:202:PHE:CE1 | 2.48 | 0.48 |
| 40:LH:16:ILE:HA | 40:LH:228:ASN:HB3 | 1.95 | 0.48 |
| 41:LM:207:LEU:HB3 | 41:LM:225:LEU:HG | 1.95 | 0.48 |
| 40:MG:433:GLU:C | 40:MG:435:GLY:H | 2.15 | 0.48 |
| 40:MH:366:ASP:O | 40:MH:367:LEU:C | 2.50 | 0.48 |
| 41:ML:27:GLU:OE1 | 41:ML:318:ARG:NH2 | 2.33 | 0.48 |
| 41:MN:142:GLY:O | 41:MN:144:GLY:N | 2.46 | 0.48 |
| 41:MN:317:PHE:CD2 | 41:MN:365:ALA:HB2 | 2.48 | 0.48 |
| 41:NB:167:PHE:CE2 | 41:NB:233:MET:HG2 | 2.48 | 0.48 |
| 40:ND:148:GLY:O | 40:ND:151:SER:N | 2.46 | 0.48 |
| 40:NF:2:ARG:HB3 | 40:NF:133:GLN:HE21 | 1.78 | 0.48 |
| 41:OB:20:PHE:HA | 41:OB:230:SER:HB3 | 1.95 | 0.48 |
| 40:OD:81:GLY:O | 40:OD:82:THR:C | 2.50 | 0.48 |
| 40:OH:281:ALA:HA | 40:OH:284:GLU:HG2 | 1.95 | 0.48 |
| 40:OH:328:VAL:HG11 | 40:OH:353:VAL:HG11 | 1.94 | 0.48 |
| 41:OL:385:PHE:O | 41:OL:389:PHE:CB | 2.60 | 0.48 |
| 41:OO:178:THR:HB | 41:OO:181:GLU:HG2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PL:113:VAL:HG11 | 41:PL:150:LEU:HD22 | 1.94 | 0.48 |
| 40:QA:238:ILE:HD11 | 40:QA:377:LEU:HD21 | 1.95 | 0.48 |
| 40:QA:260:VAL:HB | 41:QB:397:TRP:CZ2 | 2.46 | 0.48 |
| 41:QB:31:ASP:C | 41:QB:33:THR:H | 2.17 | 0.48 |
| 41:QB:209:ASP:HA | 41:QB:213:ARG:NH1 | 2.27 | 0.48 |
| 40:RI:16:ILE:HD11 | 40:RI:138:PHE:HB3 | 1.94 | 0.48 |
| 40:RI:207:GLU:HA | 40:RI:210:TYR:CD2 | 2.48 | 0.48 |
| 41:RN:170:VAL:HG11 | 41:RN:377:LEU:HD21 | 1.94 | 0.48 |
| 40:SE:21:TRP:HZ2 | 40:SE:65:ALA:HB2 | 1.78 | 0.48 |
| 40:SI:224:TYR:HA | 40:SI:227:LEU:HB2 | 1.94 | 0.48 |
| 41:SL:142:GLY:O | 41:SL:144:GLY:N | 2.46 | 0.48 |
| 41:SO:146:GLY:O | 41:SO:147:MET:C | 2.52 | 0.48 |
| 41:SO:401:GLU:HG3 | 41:SO:402:GLY:N | 2.28 | 0.48 |
| 41:SO:425:ARG:O | 41:SO:426:GLY:C | 2.51 | 0.48 |
| 41:TN:274:THR:OG1 | 41:TN:279:GLN:OE1 | 2.31 | 0.48 |
| 40:UF:28:HIS:HB2 | 40:UF:30:ILE:HG12 | 1.94 | 0.48 |
| 40:UF:138:PHE:CD1 | 40:UF:169:PHE:HB2 | 2.48 | 0.48 |
| 40:UH:172:TYR:HB3 | 40:UH:205:ASP:HB3 | 1.94 | 0.48 |
| 40:UH:270:ALA:HA | 40:UH:377:LEU:HD23 | 1.95 | 0.48 |
| 41:UN:282:ARG:NH2 | 41:UN:292:GLN:OE1 | 2.46 | 0.48 |
| 40:VJ:71:GLU:HB3 | 40:VJ:98:ASP:HA | 1.93 | 0.48 |
| 41:VP:22:GLU:HG2 | 41:VP:81:PHE:HB2 | 1.95 | 0.48 |
| 40:WA:96:LYS:NZ | 41:WN:1:MET:H3 | 2.10 | 0.48 |
| 40:WI:406:TRP:CG | 41:WP:255:VAL:HG23 | 2.48 | 0.48 |
| 41:WM:1:MET:HE1 | 41:WM:46:ARG:HA | 1.95 | 0.48 |
| 41:WN:263:LEU:HD21 | 41:WN:421:PRO:HB2 | 1.94 | 0.48 |
| 5:1N:167:ARG:HD2 | 41:HQ:338:SER:HB2 | 1.94 | 0.48 |
| 8:1Z:379:ASP:N | 8:1Z:379:ASP:OD1 | 2.46 | 0.48 |
| 21:4E:411:LYS:HA | 21:4E:411:LYS:HD3 | 1.53 | 0.48 |
| 21:4E:477:SER:O | 21:4E:479:MET:N | 2.45 | 0.48 |
| 22:4J:533:MET:HG3 | 22:4J:597:GLN:HE22 | 1.78 | 0.48 |
| 23:4M:186:GLY:O | 23:4M:187:PHE:C | 2.52 | 0.48 |
| 31:5I:684:GLU:O | 31:5I:687:ILE:HG13 | 2.12 | 0.48 |
| 31:5J:802:THR:HG23 | 31:5J:804:PHE:H | 1.78 | 0.48 |
| 34:5R:358:LYS:HE2 | 34:5R:358:LYS:HB2 | 1.58 | 0.48 |
| 35:5T:94:LEU:HD21 | 41:JL:40:SER:HB2 | 1.96 | 0.48 |
| 36:5W:67:GLY:HA2 | 40:OF:222:PRO:HA | 1.95 | 0.48 |
| 36:5W:226:LYS:HD2 | 36:5W:227:PRO:HD2 | 1.94 | 0.48 |
| 36:5X:119:ILE:O | 36:5X:123:ARG:NE | 2.45 | 0.48 |
| 39:6I:18:ARG:HA | 39:6I:21:GLN:HG2 | 1.94 | 0.48 |
| 40:AG:3:GLU:HA | 40:AG:51:THR:HA | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AG:319:TYR:HB3 | 40:AG:323:VAL:HG21 | 1.94 | 0.48 |
| 41:AM:132:GLY:HA3 | 41:AM:163:ILE:O | 2.13 | 0.48 |
| 41:AM:180:VAL:O | 41:AM:184:ASN:ND2 | 2.46 | 0.48 |
| 40:BE:74:VAL:HG13 | 40:BE:75:ILE:H | 1.79 | 0.48 |
| 40:BF:236:SER:O | 40:BF:240:ALA:HB2 | 2.13 | 0.48 |
| 40:BG:67:PHE:HB3 | 40:BG:75:ILE:HD12 | 1.94 | 0.48 |
| 40:BH:204:VAL:HG12 | 40:BH:209:ILE:HD11 | 1.95 | 0.48 |
| 40:BH:325:PRO:O | 40:BH:326:LYS:C | 2.51 | 0.48 |
| 41:BM:245:GLN:O | 41:BM:247:ASN:N | 2.46 | 0.48 |
| 40:CG:153:LEU:O | 40:CG:157:LEU:HB2 | 2.13 | 0.48 |
| 40:CG:333:ALA:HB2 | 41:CO:174:LYS:HE3 | 1.95 | 0.48 |
| 41:CM:44:LEU:HA | 41:CM:47:ILE:HD13 | 1.94 | 0.48 |
| 41:CO:253:LEU:O | 41:CO:257:MET:HB2 | 2.13 | 0.48 |
| 41:CP:311:LEU:HA | 41:CP:342:VAL:HG22 | 1.94 | 0.48 |
| 41:DB:88:ASP:O | 41:DB:90:PHE:N | 2.46 | 0.48 |
| 41:DB:139:LEU:O | 41:DB:141:GLY:N | 2.46 | 0.48 |
| 40:DE:314:ALA:HB2 | 41:DM:394:PHE:HZ | 1.77 | 0.48 |
| 40:DF:187:SER:HB2 | 40:DF:390:LEU:HD11 | 1.95 | 0.48 |
| 40:DF:326:LYS:NZ | 41:DN:212:PHE:H | 2.11 | 0.48 |
| 40:DH:113:GLU:H | 40:DH:113:GLU:HG3 | 1.42 | 0.48 |
| 40:DH:273:ALA:HB2 | 40:DH:374:VAL:HG22 | 1.95 | 0.48 |
| 40:DI:69:ASP:HB2 | 40:DI:75:ILE:HG13 | 1.95 | 0.48 |
| 40:DI:185:TYR:O | 40:DI:186:ASN:C | 2.52 | 0.48 |
| 41:DL:71:GLY:O | 41:DL:72:THR:C | 2.52 | 0.48 |
| 41:DM:141:GLY:HA3 | 43:DM:501:GDP:O1A | 2.12 | 0.48 |
| 41:DN:260:PHE:C | 41:DN:262:ARG:H | 2.17 | 0.48 |
| 41:DN:392:LYS:HB2 | 41:DN:392:LYS:HE2 | 1.51 | 0.48 |
| 41:DP:1:MET:SD | 41:DP:48:ASN:ND2 | 2.85 | 0.48 |
| 40:EA:318:LEU:HB2 | 40:EA:375:CYS:O | 2.14 | 0.48 |
| 40:EF:390:LEU:HD23 | 40:EF:393:LYS:HE2 | 1.95 | 0.48 |
| 40:EH:27:GLU:C | 40:EH:29:GLY:H | 2.16 | 0.48 |
| 40:EH:71:GLU:HB3 | 40:EH:98:ASP:CG | 2.33 | 0.48 |
| 40:EH:363:VAL:O | 40:EH:365:GLY:N | 2.46 | 0.48 |
| 40:EI:70:LEU:HD12 | 40:EI:145:THR:HG23 | 1.94 | 0.48 |
| 41:EN:103:LYS:O | 41:EN:107:THR:OG1 | 2.30 | 0.48 |
| 41:EP:417:ASP:O | 41:EP:420:ASN:N | 2.30 | 0.48 |
| 40:FA:30:ILE:HG13 | 40:FA:53:PHE:CZ | 2.48 | 0.48 |
| 40:FA:228:ASN:CG | 42:FN:501:GTP:HN21 | 2.17 | 0.48 |
| 40:FA:326:LYS:HD3 | 40:FA:326:LYS:HA | 1.64 | 0.48 |
| 41:FB:148:GLY:O | 41:FB:152:ILE:HG12 | 2.14 | 0.48 |
| 40:FE:76:ASP:HA | 40:FE:79:ARG:HG2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FO:7:LEU:O | 41:FO:135:LEU:HA | 2.13 | 0.48 |
| 41:FO:113:VAL:HG22 | 41:FO:117:LEU:HD23 | 1.94 | 0.48 |
| 40:GG:265:ILE:HG22 | 40:GG:379:ASN:HD21 | 1.78 | 0.48 |
| 40:GH:363:VAL:O | 40:GH:365:GLY:N | 2.46 | 0.48 |
| 40:GI:104:ALA:HA | 40:GI:108:TYR:CD2 | 2.45 | 0.48 |
| 41:GM:19:LYS:HG3 | 41:GM:226:ASN:HB2 | 1.95 | 0.48 |
| 41:HB:396:HIS:HA | 41:HB:399:THR:HG22 | 1.95 | 0.48 |
| 40:HF:260:VAL:HB | 41:HN:397:TRP:HH2 | 1.77 | 0.48 |
| 40:HF:262:TYR:HE2 | 41:HN:393:ALA:HA | 1.78 | 0.48 |
| 41:HN:376:GLU:O | 41:HN:377:LEU:C | 2.51 | 0.48 |
| 40:IE:170:SER:OG | 40:IE:203:MET:SD | 2.70 | 0.48 |
| 40:IF:6:SER:O | 40:IF:65:ALA:HA | 2.13 | 0.48 |
| 40:IF:20:CYS:HA | 40:IF:232:SER:HB2 | 1.94 | 0.48 |
| 40:II:38:SER:OG | 40:II:39:ASP:N | 2.45 | 0.48 |
| 41:IO:104:GLY:HA3 | 41:IO:146:GLY:HA3 | 1.94 | 0.48 |
| 40:JA:323:VAL:HG22 | 40:JA:372:ARG:HG2 | 1.95 | 0.48 |
| 41:JB:276:ARG:HA | 41:JB:279:GLN:HB2 | 1.94 | 0.48 |
| 40:JG:88:HIS:HB3 | 40:JG:91:GLN:HB2 | 1.94 | 0.48 |
| 40:JH:223:THR:OG1 | 40:JH:224:TYR:N | 2.47 | 0.48 |
| 41:JL:39:ASP:OD1 | 41:JL:39:ASP:N | 2.45 | 0.48 |
| 41:JL:91:VAL:HG11 | 41:JL:116:VAL:HG22 | 1.95 | 0.48 |
| 40:KA:288:VAL:HA | 40:KA:291:ILE:HG12 | 1.94 | 0.48 |
| 41:KB:25:SER:OG | 41:KB:30:ILE:O | 2.29 | 0.48 |
| 41:KB:172:SER:OG | 41:KB:203:ASP:OD1 | 2.24 | 0.48 |
| 41:KL:142:GLY:O | 41:KL:144:GLY:N | 2.46 | 0.48 |
| 41:KL:271:ALA:O | 41:KL:273:LEU:N | 2.43 | 0.48 |
| 40:LG:208:ALA:HB2 | 40:LG:304:LYS:HG2 | 1.95 | 0.48 |
| 41:LL:139:LEU:HD23 | 41:LL:170:VAL:HG13 | 1.95 | 0.48 |
| 41:LP:107:THR:O | 41:LP:110:ALA:N | 2.39 | 0.48 |
| 41:MB:245:GLN:HA | 40:MG:11:GLN:HE22 | 1.77 | 0.48 |
| 41:MB:257:MET:SD | 41:MB:314:ALA:HB2 | 2.53 | 0.48 |
| 41:MB:341:PHE:HB3 | 41:MB:348:ASN:HD21 | 1.78 | 0.48 |
| 40:ME:262:TYR:OH | 41:MM:391:ARG:O | 2.28 | 0.48 |
| 40:MF:406:TRP:HE1 | 41:MM:258:VAL:HG23 | 1.78 | 0.48 |
| 41:MN:243:PRO:HD2 | 41:MN:356:ILE:HD13 | 1.94 | 0.48 |
| 41:MO:39:ASP:O | 41:MO:40:SER:C | 2.50 | 0.48 |
| 41:MO:178:THR:O | 41:MO:181:GLU:HB3 | 2.13 | 0.48 |
| 40:NA:222:PRO:HB2 | 40:NA:227:LEU:HG | 1.95 | 0.48 |
| 41:NB:202:ILE:HG12 | 41:NB:268:PRO:HG3 | 1.95 | 0.48 |
| 41:NB:258:VAL:HG13 | 40:NG:406:TRP:HE1 | 1.78 | 0.48 |
| 40:ND:88:HIS:CD2 | 40:ND:89:PRO:HD2 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NE:70:LEU:HD12 | 40:NE:99:ALA:HB2 | 1.95 | 0.48 |
| 40:NF:70:LEU:HD12 | 40:NF:145:THR:HG22 | 1.95 | 0.48 |
| 41:NL:154:LYS:O | 41:NL:158:GLU:HG2 | 2.13 | 0.48 |
| 41:NM:229:VAL:HG12 | 41:NM:233:MET:HE2 | 1.94 | 0.48 |
| 40:OA:138:PHE:HZ | 40:OA:235:VAL:HG21 | 1.77 | 0.48 |
| 40:OE:109:THR:OG1 | 40:OE:410:GLU:O | 2.30 | 0.48 |
| 40:OE:191:THR:O | 40:OE:195:LEU:HB2 | 2.13 | 0.48 |
| 40:OG:5:ILE:HG12 | 40:OG:132:LEU:HD11 | 1.94 | 0.48 |
| 40:OG:104:ALA:O | 40:OG:108:TYR:HB2 | 2.13 | 0.48 |
| 40:OG:307:PRO:HB3 | 40:OG:312:TYR:HE1 | 1.77 | 0.48 |
| 41:OL:169:VAL:HG11 | 43:OL:502:GDP:H1' | 1.95 | 0.48 |
| 40:PD:255:PHE:HE1 | 40:PD:318:LEU:HD11 | 1.77 | 0.48 |
| 40:PE:31:GLN:HB2 | 40:PE:37:PRO:HD3 | 1.95 | 0.48 |
| 40:PE:194:THR:O | 40:PE:198:SER:HB3 | 2.14 | 0.48 |
| 40:QA:30:ILE:HG13 | 40:QA:53:PHE:CD2 | 2.48 | 0.48 |
| 41:QB:145:SER:O | 41:QB:148:GLY:N | 2.47 | 0.48 |
| 40:QE:31:GLN:HG3 | 40:QE:34:GLY:H | 1.78 | 0.48 |
| 40:QF:112:LYS:HA | 40:QF:115:ILE:HG22 | 1.94 | 0.48 |
| 41:QM:117:LEU:HA | 41:QM:120:VAL:HG12 | 1.95 | 0.48 |
| 41:RB:383:GLU:HA | 41:RB:386:THR:HG22 | 1.95 | 0.48 |
| 40:RG:311:LYS:N | 40:RG:381:THR:OG1 | 2.42 | 0.48 |
| 40:RH:88:HIS:NE2 | 40:SH:284:GLU:OE2 | 2.45 | 0.48 |
| 40:RH:184:PRO:O | 40:RH:188:ILE:HG12 | 2.13 | 0.48 |
| 41:RL:6:HIS:O | 41:RL:63:ALA:HA | 2.13 | 0.48 |
| 41:RN:221:THR:HG23 | 41:RN:224:ASP:H | 1.78 | 0.48 |
| 41:RO:118:ASP:O | 41:RO:122:LYS:HG2 | 2.13 | 0.48 |
| 41:RP:132:GLY:HA2 | 41:RP:162:ARG:HB3 | 1.94 | 0.48 |
| 40:SF:288:VAL:HG21 | 40:SF:328:VAL:HG23 | 1.94 | 0.48 |
| 40:SG:109:THR:O | 40:SG:112:LYS:NZ | 2.46 | 0.48 |
| 40:SI:11:GLN:HE22 | 41:SP:246:LEU:N | 2.07 | 0.48 |
| 41:SL:61:PRO:HG2 | 41:SL:85:PHE:HA | 1.94 | 0.48 |
| 41:SO:234:SER:OG | 41:SO:235:GLY:N | 2.46 | 0.48 |
| 41:SP:86:ARG:HD3 | 41:SP:88:ASP:H | 1.78 | 0.48 |
| 40:TA:210:TYR:OH | 41:TN:327:ASP:OD2 | 2.30 | 0.48 |
| 40:TG:3:GLU:OE1 | 40:TG:3:GLU:N | 2.42 | 0.48 |
| 40:TG:55:GLU:HG2 | 40:TG:61:HIS:CE1 | 2.48 | 0.48 |
| 41:TN:53:GLU:HG3 | 41:TN:59:TYR:HE1 | 1.79 | 0.48 |
| 41:TN:318:ARG:HB2 | 41:TN:358:PRO:HD3 | 1.95 | 0.48 |
| 41:TO:269:GLY:O | 41:TO:367:PHE:N | 2.44 | 0.48 |
| 40:UF:111:GLY:C | 40:UF:113:GLU:H | 2.17 | 0.48 |
| 40:UF:288:VAL:HG11 | 40:UF:327:ASP:HB3 | 1.93 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UI:88:HIS:O | 40:UI:91:GLN:N | 2.45 | 0.48 |
| 40:VF:112:LYS:HA | 40:VF:115:ILE:HG22 | 1.95 | 0.48 |
| 40:VH:12:ALA:HB1 | 40:VH:171:ILE:HD12 | 1.95 | 0.48 |
| 41:VN:178:THR:N | 41:VN:181:GLU:OE2 | 2.36 | 0.48 |
| 41:VN:314:ALA:HB3 | 41:VN:368:ILE:HB | 1.94 | 0.48 |
| 41:WN:21:TRP:CZ2 | 41:WN:63:ALA:HB2 | 2.48 | 0.48 |
| 41:WO:171:PRO:O | 41:WO:380:ARG:NH2 | 2.45 | 0.48 |
| 7:1S:587:SER:OG | 7:1S:608:ASP:OD1 | 2.29 | 0.48 |
| 7:1T:16:LEU:HD21 | 7:1T:612:LEU:HD23 | 1.94 | 0.48 |
| 7:1T:394:ASP:O | 7:1T:395:ASP:C | 2.51 | 0.48 |
| 8:1W:522:GLU:O | 8:1W:525:ALA:C | 2.52 | 0.48 |
| 13:2X:173:SER:O | 13:2X:175:ASP:N | 2.47 | 0.48 |
| 13:2X:177:LEU:HG | 13:2X:178:PRO:HD2 | 1.95 | 0.48 |
| 16:3J:315:HIS:HB3 | 16:3L:202:LYS:HB2 | 1.95 | 0.48 |
| 16:3K:326:ASN:OD1 | 16:3K:327:VAL:N | 2.46 | 0.48 |
| 18:3W:308:CYS:SG | 18:3W:427:ARG:NH1 | 2.86 | 0.48 |
| 18:3W:347:GLU:OE1 | 18:3W:351:LYS:NZ | 2.37 | 0.48 |
| 21:4E:154:LEU:HD13 | 21:4E:176:ILE:HG12 | 1.95 | 0.48 |
| 21:4F:458:ASN:H | 41:FM:218:THR:HG1 | 1.62 | 0.48 |
| 22:4I:37:SER:HB3 | 22:4I:40:LYS:HD2 | 1.94 | 0.48 |
| 22:4J:257:ASP:OD2 | 22:4J:281:ARG:NH1 | 2.46 | 0.48 |
| 22:4K:700:ARG:HE | 22:4K:701:ALA:H | 1.61 | 0.48 |
| 23:4N:58:ARG:H | 41:BM:41:ASP:CG | 2.17 | 0.48 |
| 23:4P:260:THR:O | 23:4P:264:LEU:HB2 | 2.13 | 0.48 |
| 23:4R:216:MET:O | 23:4R:217:LYS:C | 2.51 | 0.48 |
| 31:5I:602:LYS:HZ1 | 41:IQ:33:THR:HG21 | 1.78 | 0.48 |
| 40:AA:89:PRO:HD2 | 40:BA:280:LYS:HG2 | 1.95 | 0.48 |
| 41:BB:226:ASN:CG | 43:BB:501:GDP:HN1 | 2.16 | 0.48 |
| 40:BE:189:LEU:HD11 | 40:BE:417:PHE:CE1 | 2.48 | 0.48 |
| 41:BL:100:ASN:HB3 | 41:BL:103:LYS:HB2 | 1.96 | 0.48 |
| 41:BM:235:GLY:O | 41:BM:238:THR:HG22 | 2.13 | 0.48 |
| 41:BM:325:GLU:O | 41:BM:329:GLN:HB2 | 2.14 | 0.48 |
| 41:BN:149:THR:HG21 | 41:BN:188:SER:HA | 1.96 | 0.48 |
| 41:BP:291:GLN:C | 41:BP:293:MET:H | 2.16 | 0.48 |
| 40:CA:108:TYR:HD1 | 40:CA:412:MET:HE2 | 1.78 | 0.48 |
| 41:CB:58:LYS:HG3 | 41:DB:280:GLN:HG3 | 1.96 | 0.48 |
| 40:CE:88:HIS:HD2 | 40:DE:283:HIS:O | 1.96 | 0.48 |
| 40:CG:20:CYS:HA | 40:CG:232:SER:HB2 | 1.95 | 0.48 |
| 40:CH:255:PHE:O | 40:CH:259:LEU:HB2 | 2.13 | 0.48 |
| 41:CL:171:PRO:HB3 | 41:CL:181:GLU:HG2 | 1.94 | 0.48 |
| 41:CP:10:GLY:HA2 | 41:CP:143:THR:HB | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CP:185:ALA:O | 41:CP:186:THR:C | 2.51 | 0.48 |
| 40:DA:1:GLN:O | 40:DA:3:GLU:N | 2.46 | 0.48 |
| 40:DA:99:ALA:HB3 | 40:DA:144:GLY:HA3 | 1.95 | 0.48 |
| 41:DB:350:LYS:HA | 41:DB:350:LYS:HD2 | 1.60 | 0.48 |
| 40:DE:11:GLN:HB2 | 42:DE:501:GTP:O1B | 2.13 | 0.48 |
| 40:DE:258:ASN:O | 40:DE:314:ALA:HB1 | 2.13 | 0.48 |
| 40:DG:346:TRP:HB3 | 41:DO:391:ARG:HH11 | 1.77 | 0.48 |
| 40:DH:230:LEU:HD21 | 40:DH:275:VAL:HG12 | 1.95 | 0.48 |
| 40:DH:271:THR:OG1 | 40:DH:301:GLN:HA | 2.13 | 0.48 |
| 40:DH:350:GLY:HA2 | 41:DP:179:VAL:HB | 1.95 | 0.48 |
| 40:DI:70:LEU:HD23 | 40:DI:70:LEU:HA | 1.73 | 0.48 |
| 40:DI:403:PHE:CZ | 41:DP:345:ILE:HD13 | 2.49 | 0.48 |
| 41:DL:222:TYR:O | 41:DL:225:LEU:HB2 | 2.13 | 0.48 |
| 41:DM:156:ARG:HH21 | 41:DM:164:MET:HB3 | 1.78 | 0.48 |
| 41:DM:286:VAL:HB | 41:DM:287:PRO:HD3 | 1.95 | 0.48 |
| 41:DN:167:PHE:HD2 | 41:DN:202:ILE:HD11 | 1.78 | 0.48 |
| 41:DN:172:SER:HB2 | 41:DN:205:GLU:HB2 | 1.95 | 0.48 |
| 41:DN:271:ALA:HB3 | 41:DN:272:PRO:CD | 2.43 | 0.48 |
| 40:EF:6:SER:O | 40:EF:65:ALA:HA | 2.13 | 0.48 |
| 40:EF:188:ILE:HD12 | 40:EF:424:MET:HG3 | 1.95 | 0.48 |
| 40:EI:182:VAL:O | 40:EI:183:GLU:C | 2.52 | 0.48 |
| 40:EI:394:PHE:CD2 | 40:EI:421:ARG:HD2 | 2.48 | 0.48 |
| 41:EM:200:TYR:CZ | 41:EM:368:ILE:HG21 | 2.48 | 0.48 |
| 41:EM:400:GLY:O | 41:EM:401:GLU:C | 2.51 | 0.48 |
| 40:FA:99:ALA:HB3 | 40:FA:145:THR:HG23 | 1.96 | 0.48 |
| 40:FI:278:ALA:H | 40:FI:368:ALA:HB2 | 1.78 | 0.48 |
| 40:FI:406:TRP:CG | 41:FP:255:VAL:HG23 | 2.48 | 0.48 |
| 40:GE:104:ALA:HB2 | 40:GE:412:MET:HB3 | 1.94 | 0.48 |
| 40:GE:352:LYS:HB2 | 41:GM:179:VAL:HG23 | 1.94 | 0.48 |
| 40:GG:273:ALA:CB | 40:GG:274:PRO:HD2 | 2.43 | 0.48 |
| 40:GH:115:ILE:O | 40:GH:118:VAL:HG12 | 2.13 | 0.48 |
| 41:GM:213:ARG:HG2 | 41:GM:297:LYS:HE3 | 1.94 | 0.48 |
| 41:GO:11:GLN:HA | 41:GO:72:THR:HG21 | 1.96 | 0.48 |
| 40:HF:51:THR:HG21 | 40:HF:243:ARG:HG2 | 1.95 | 0.48 |
| 40:HI:328:VAL:O | 40:HI:332:ILE:HG12 | 2.13 | 0.48 |
| 41:HN:170:VAL:HG11 | 41:HN:377:LEU:HD21 | 1.95 | 0.48 |
| 41:HN:416:ASN:C | 41:HN:418:LEU:H | 2.17 | 0.48 |
| 41:HO:135:LEU:HD22 | 41:HO:152:ILE:HD11 | 1.95 | 0.48 |
| 41:HP:282:ARG:NH1 | 41:HP:292:GLN:OE1 | 2.41 | 0.48 |
| 40:IE:90:GLU:OE1 | 40:IE:121:ARG:NH1 | 2.47 | 0.48 |
| 41:IM:21:TRP:CH2 | 41:IM:61:PRO:HB3 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JA:64:ARG:NH1 | 40:JA:129:CYS:SG | 2.86 | 0.48 |
| 40:JE:352:LYS:HD2 | 41:JM:179:VAL:N | 2.28 | 0.48 |
| 40:JH:90:GLU:HG3 | 40:KH:280:LYS:HD2 | 1.95 | 0.48 |
| 41:JN:286:VAL:HG11 | 41:JN:326:VAL:HA | 1.94 | 0.48 |
| 41:KB:414:ASN:HA | 41:KB:417:ASP:HB2 | 1.95 | 0.48 |
| 40:KD:438:SER:HB2 | 41:KL:391:ARG:HH11 | 1.79 | 0.48 |
| 40:KE:231:ILE:O | 40:KE:235:VAL:HG23 | 2.13 | 0.48 |
| 40:KF:166:LYS:HE3 | 40:KF:166:LYS:HB2 | 1.70 | 0.48 |
| 41:KP:142:GLY:O | 41:KP:144:GLY:N | 2.45 | 0.48 |
| 40:LF:77:GLU:HA | 40:LF:80:THR:HG22 | 1.95 | 0.48 |
| 40:LF:166:LYS:HE3 | 40:LF:166:LYS:HB2 | 1.40 | 0.48 |
| 41:LM:173:PRO:HD3 | 41:LM:380:ARG:NH1 | 2.29 | 0.48 |
| 41:LM:174:LYS:HG3 | 41:LM:175:VAL:HG13 | 1.96 | 0.48 |
| 40:MA:224:TYR:O | 42:MN:501:GTP:N2 | 2.45 | 0.48 |
| 41:MB:100:ASN:HB3 | 41:MB:103:LYS:HB3 | 1.94 | 0.48 |
| 40:MD:70:LEU:HD22 | 40:MD:110:ILE:HG22 | 1.95 | 0.48 |
| 40:MF:162:GLY:O | 40:MF:164:LYS:N | 2.46 | 0.48 |
| 40:MF:200:CYS:SG | 40:MF:268:PRO:HG2 | 2.54 | 0.48 |
| 40:MF:228:ASN:CB | 42:MM:501:GTP:N2 | 2.75 | 0.48 |
| 40:MG:416:GLU:O | 40:MG:417:PHE:C | 2.51 | 0.48 |
| 40:MH:261:PRO:HD2 | 40:MH:265:ILE:O | 2.13 | 0.48 |
| 41:ML:137:HIS:NE2 | 41:ML:168:SER:OG | 2.38 | 0.48 |
| 41:ML:180:VAL:HG23 | 41:ML:184:ASN:HD21 | 1.77 | 0.48 |
| 41:NB:191:GLN:O | 41:NB:195:ASN:ND2 | 2.42 | 0.48 |
| 40:ND:31:GLN:O | 40:ND:32:PRO:C | 2.51 | 0.48 |
| 40:ND:246:GLY:O | 40:ND:247:ALA:C | 2.51 | 0.48 |
| 40:NE:247:ALA:HB3 | 40:NE:355:ILE:HB | 1.95 | 0.48 |
| 40:NG:271:THR:HG22 | 40:NG:376:MET:HB3 | 1.94 | 0.48 |
| 41:NL:86:ARG:HA | 41:OL:281:TYR:HD2 | 1.78 | 0.48 |
| 41:NN:330:MET:HB3 | 41:NN:349:VAL:HG21 | 1.95 | 0.48 |
| 41:NO:322:SER:OG | 41:NO:325:GLU:OE2 | 2.31 | 0.48 |
| 41:NP:198:GLU:HG2 | 41:NP:266:PHE:HE2 | 1.78 | 0.48 |
| 41:OL:256:ASN:ND2 | 41:OL:350:LYS:HD3 | 2.28 | 0.48 |
| 41:ON:137:HIS:CE1 | 41:ON:139:LEU:HD23 | 2.48 | 0.48 |
| 41:OO:207:LEU:HD21 | 41:OO:300:MET:HB3 | 1.95 | 0.48 |
| 41:OP:113:VAL:HA | 41:OP:116:VAL:HG22 | 1.95 | 0.48 |
| 41:PB:289:LEU:HD11 | 41:PB:363:MET:HG3 | 1.94 | 0.48 |
| 41:PB:348:ASN:HA | 41:PB:350:LYS:HZ1 | 1.79 | 0.48 |
| 40:PF:202:PHE:CD1 | 40:PF:268:PRO:HG2 | 2.48 | 0.48 |
| 40:PF:265:ILE:HD11 | 40:PF:430:ASP:HB3 | 1.95 | 0.48 |
| 40:PG:24:TYR:HA | 40:PG:27:GLU:HG2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PP:132:GLY:CA | 41:PP:163:ILE:O | 2.61 | 0.48 |
| 41:PP:249:ASP:OD1 | 41:PP:250:LEU:N | 2.43 | 0.48 |
| 41:QB:20:PHE:HA | 41:QB:230:SER:OG | 2.14 | 0.48 |
| 41:QB:188:SER:O | 41:QB:189:VAL:C | 2.51 | 0.48 |
| 40:QG:345:ASP:OD1 | 40:QG:345:ASP:N | 2.47 | 0.48 |
| 41:QM:107:THR:O | 41:QM:110:ALA:N | 2.30 | 0.48 |
| 41:QM:309:ARG:NH1 | 41:QM:339:SER:O | 2.46 | 0.48 |
| 41:QO:170:VAL:HG11 | 41:QO:377:LEU:HD21 | 1.95 | 0.48 |
| 40:RI:123:ARG:HH12 | 40:RI:124:LYS:HZ2 | 1.61 | 0.48 |
| 41:RP:46:ARG:HH12 | 41:RP:243:PRO:HD3 | 1.78 | 0.48 |
| 40:SF:16:ILE:HD11 | 40:SF:171:ILE:HD11 | 1.95 | 0.48 |
| 40:SG:352:LYS:HZ2 | 41:SO:179:VAL:HA | 1.77 | 0.48 |
| 41:SO:394:PHE:HD1 | 41:SO:397:TRP:CH2 | 2.32 | 0.48 |
| 41:SO:398:TYR:HB3 | 41:SO:403:MET:HE3 | 1.94 | 0.48 |
| 41:SP:184:ASN:OD1 | 41:SP:398:TYR:OH | 2.30 | 0.48 |
| 40:TA:238:ILE:HA | 40:TA:318:LEU:HD22 | 1.95 | 0.48 |
| 40:TE:371:GLN:OE1 | 40:TE:371:GLN:N | 2.38 | 0.48 |
| 40:TF:317:LEU:HD13 | 40:TF:376:MET:HB3 | 1.94 | 0.48 |
| 40:TF:332:ILE:HG21 | 41:TN:175:VAL:HG21 | 1.95 | 0.48 |
| 41:TL:142:GLY:O | 41:TL:144:GLY:N | 2.47 | 0.48 |
| 41:TL:176:SER:OG | 41:TL:178:THR:O | 2.31 | 0.48 |
| 40:UI:107:HIS:HB2 | 40:UI:148:GLY:HA2 | 1.95 | 0.48 |
| 40:UI:273:ALA:HB1 | 40:UI:291:ILE:HB | 1.94 | 0.48 |
| 41:UO:44:LEU:HA | 41:UO:47:ILE:HB | 1.94 | 0.48 |
| 40:VF:53:PHE:HB3 | 40:VF:61:HIS:HB3 | 1.94 | 0.48 |
| 41:VN:10:GLY:HA2 | 41:VN:143:THR:HG23 | 1.96 | 0.48 |
| 41:VO:193:VAL:HG11 | 41:VO:262:ARG:HH21 | 1.77 | 0.48 |
| 41:VO:273:LEU:O | 41:VO:292:GLN:NE2 | 2.44 | 0.48 |
| 41:VP:182:PRO:HG3 | 41:VP:384:GLN:HB3 | 1.94 | 0.48 |
| 41:VP:237:THR:O | 41:VP:241:ARG:NE | 2.32 | 0.48 |
| 40:WG:76:ASP:HA | 40:WG:79:ARG:HG2 | 1.94 | 0.48 |
| 40:WG:205:ASP:HB2 | 40:WG:303:VAL:HA | 1.93 | 0.48 |
| 41:WN:101:TRP:O | 41:WN:102:ALA:C | 2.51 | 0.48 |
| 41:WN:271:ALA:HB3 | 41:WN:272:PRO:HD3 | 1.95 | 0.48 |
| 5:1N:157:SER:HB2 | 41:HQ:306:ARG:HG2 | 1.96 | 0.48 |
| 10:2E:96:HIS:O | 10:2E:99:THR:OG1 | 2.22 | 0.48 |
| 10:2G:68:PRO:HD2 | 10:2G:72:LEU:HG | 1.94 | 0.48 |
| 11:2J:114:ILE:HA | 40:LF:414:GLU:HG2 | 1.96 | 0.48 |
| 13:2U:88:THR:OG1 | 13:2U:104:ARG:NH1 | 2.45 | 0.48 |
| 13:2W:65:PRO:HB2 | 13:2W:66:LYS:HE3 | 1.95 | 0.48 |
| 13:2W:176:GLU:O | 13:2W:177:LEU:C | 2.51 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:3F:49:GLU:OE2 | 15:3F:53:ARG:NH1 | 2.40 | 0.48 |
| 16:3J:319:GLU:HB2 | 16:3L:202:LYS:HG2 | 1.94 | 0.48 |
| 16:3K:387:ASP:O | 16:3K:391:MET:HG2 | 2.14 | 0.48 |
| 16:3L:89:ILE:HD12 | 16:3L:169:ARG:HD2 | 1.93 | 0.48 |
| 17:3R:164:LEU:CD2 | 17:3R:254:LEU:HB3 | 2.43 | 0.48 |
| 17:3R:166:ALA:HB1 | 17:3R:315:ARG:CZ | 2.42 | 0.48 |
| 18:3T:121:VAL:HG23 | 18:3T:208:LYS:HG2 | 1.95 | 0.48 |
| 20:4B:237:GLN:HA | 20:4B:240:ASN:HB2 | 1.94 | 0.48 |
| 21:4D:305:ALA:HA | 21:4D:308:PHE:HB3 | 1.96 | 0.48 |
| 23:4N:260:THR:O | 23:4N:264:LEU:HB2 | 2.13 | 0.48 |
| 23:4R:171:PRO:C | 23:4R:173:SER:H | 2.16 | 0.48 |
| 23:4R:259:ARG:HB3 | 23:4R:263:HIS:ND1 | 2.28 | 0.48 |
| 26:4V:9:PHE:HZ | 26:4V:87:LEU:HD11 | 1.77 | 0.48 |
| 26:4W:185:ARG:NH2 | 26:4W:197:GLY:O | 2.44 | 0.48 |
| 41:AB:273:LEU:HB2 | 41:AB:292:GLN:HE22 | 1.77 | 0.48 |
| 40:AE:176:GLN:HG3 | 41:AL:331:LEU:HD11 | 1.95 | 0.48 |
| 41:AP:385:PHE:HZ | 41:AP:408:PHE:HB3 | 1.77 | 0.48 |
| 41:BB:303:CYS:O | 41:BB:304:ASP:C | 2.51 | 0.48 |
| 40:BE:17:GLY:HA2 | 40:BE:20:CYS:HB2 | 1.94 | 0.48 |
| 40:BE:287:SER:O | 40:BE:288:VAL:C | 2.50 | 0.48 |
| 41:BL:285:THR:N | 41:BL:288:GLU:OE2 | 2.46 | 0.48 |
| 41:BO:143:THR:O | 41:BO:144:GLY:C | 2.51 | 0.48 |
| 41:BP:246:LEU:HA | 41:BP:246:LEU:HD13 | 1.72 | 0.48 |
| 40:CE:274:PRO:HG3 | 40:CE:286:LEU:HD11 | 1.96 | 0.48 |
| 41:CL:139:LEU:HG | 41:CL:168:SER:HB2 | 1.95 | 0.48 |
| 41:CN:374:ILE:H | 41:CN:374:ILE:HG12 | 1.46 | 0.48 |
| 40:DA:310:GLY:HA3 | 40:DA:382:ALA:HB2 | 1.95 | 0.48 |
| 40:DE:269:LEU:HD23 | 40:DE:380:THR:HB | 1.96 | 0.48 |
| 40:DG:326:LYS:HG2 | 41:DO:208:TYR:CE1 | 2.47 | 0.48 |
| 40:DI:210:TYR:HB2 | 41:DP:324:LYS:HZ2 | 1.75 | 0.48 |
| 41:DM:142:GLY:O | 41:DM:143:THR:C | 2.51 | 0.48 |
| 41:DN:108:GLU:O | 41:DN:111:GLU:N | 2.46 | 0.48 |
| 41:DN:144:GLY:O | 41:DN:148:GLY:HA3 | 2.13 | 0.48 |
| 40:EA:101:ASN:HD21 | 41:EN:252:LYS:NZ | 2.11 | 0.48 |
| 40:EA:239:THR:O | 40:EA:243:ARG:NE | 2.42 | 0.48 |
| 40:EE:166:LYS:H | 40:EE:199:ASP:HB3 | 1.77 | 0.48 |
| 40:EF:107:HIS:HD2 | 40:EF:152:LEU:HB2 | 1.76 | 0.48 |
| 40:EG:271:THR:HA | 40:EG:302:MET:HE1 | 1.94 | 0.48 |
| 40:EI:205:ASP:O | 40:EI:206:ASN:C | 2.52 | 0.48 |
| 41:EM:224:ASP:N | 41:EM:224:ASP:OD1 | 2.46 | 0.48 |
| 41:EP:329:GLN:C | 41:EP:331:LEU:H | 2.17 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FE:2:ARG:NE | 40:FE:242:LEU:O | 2.42 | 0.48 |
| 40:FG:286:LEU:O | 40:FG:372:ARG:NH2 | 2.46 | 0.48 |
| 40:FH:233:GLN:HE21 | 40:FH:367:LEU:HD22 | 1.79 | 0.48 |
| 40:FI:318:LEU:O | 40:FI:374:VAL:HA | 2.13 | 0.48 |
| 41:FN:4:ILE:HA | 41:FN:132:GLY:O | 2.12 | 0.48 |
| 41:GB:268:PRO:HG2 | 41:GB:300:MET:HB3 | 1.95 | 0.48 |
| 40:GF:274:PRO:HG3 | 40:GF:286:LEU:HD12 | 1.94 | 0.48 |
| 40:GF:326:LYS:HB3 | 41:GN:208:TYR:CZ | 2.48 | 0.48 |
| 40:GG:174:ALA:HB3 | 40:GG:178:SER:H | 1.77 | 0.48 |
| 41:GN:285:THR:O | 41:GN:286:VAL:C | 2.51 | 0.48 |
| 41:GO:68:LEU:HD12 | 41:GO:97:ALA:HB2 | 1.94 | 0.48 |
| 41:GP:239:CYS:HB3 | 41:GP:247:ASN:HB2 | 1.94 | 0.48 |
| 40:HE:14:VAL:HG11 | 40:HE:74:VAL:HG23 | 1.94 | 0.48 |
| 40:HE:305:CYS:O | 40:HE:306:ASP:C | 2.52 | 0.48 |
| 40:HH:376:MET:SD | 40:HH:378:SER:HB3 | 2.53 | 0.48 |
| 40:HI:167:LEU:HD11 | 40:HI:252:LEU:HD22 | 1.95 | 0.48 |
| 41:IB:323:MET:HG3 | 40:IG:224:TYR:CE2 | 2.49 | 0.48 |
| 40:IF:134:GLY:HA3 | 40:IF:252:LEU:HD22 | 1.95 | 0.48 |
| 40:IF:352:LYS:NZ | 41:IN:178:THR:OG1 | 2.43 | 0.48 |
| 40:IH:319:TYR:HB3 | 40:IH:323:VAL:HG21 | 1.95 | 0.48 |
| 41:IO:15:GLN:NE2 | 43:IO:501:GDP:O6 | 2.42 | 0.48 |
| 41:IQ:107:THR:O | 41:IQ:110:ALA:N | 2.35 | 0.48 |
| 40:JD:157:LEU:HD11 | 40:JD:166:LYS:HZ2 | 1.78 | 0.48 |
| 40:JE:73:THR:HA | 41:JL:46:ARG:HH22 | 1.78 | 0.48 |
| 41:JL:40:SER:OG | 41:JL:41:ASP:N | 2.46 | 0.48 |
| 40:KG:73:THR:HA | 40:KG:76:ASP:HB2 | 1.94 | 0.48 |
| 41:KL:336:LYS:HE2 | 41:KL:336:LYS:HB2 | 1.45 | 0.48 |
| 41:LM:142:GLY:O | 41:LM:144:GLY:N | 2.46 | 0.48 |
| 41:LN:234:SER:O | 41:LN:318:ARG:NH2 | 2.46 | 0.48 |
| 40:MA:2:ARG:H | 40:MA:2:ARG:HG2 | 1.36 | 0.48 |
| 40:MD:255:PHE:HZ | 40:MD:318:LEU:HD21 | 1.76 | 0.48 |
| 40:MG:397:MET:C | 40:MG:399:ALA:H | 2.16 | 0.48 |
| 40:NF:177:VAL:HG12 | 41:NM:331:LEU:HD22 | 1.96 | 0.48 |
| 41:NN:11:GLN:HA | 41:NN:72:THR:HG21 | 1.96 | 0.48 |
| 41:NP:196:THR:OG1 | 41:NP:197:ASP:N | 2.46 | 0.48 |
| 41:OB:252:LYS:O | 41:OB:256:ASN:ND2 | 2.46 | 0.48 |
| 41:OB:316:VAL:HA | 41:OB:352:ALA:O | 2.13 | 0.48 |
| 40:OD:332:ILE:HG23 | 40:OD:351:PHE:CD2 | 2.48 | 0.48 |
| 40:PD:119:LEU:HD21 | 40:PD:156:ARG:HB3 | 1.95 | 0.48 |
| 40:PF:319:TYR:HB3 | 40:PF:323:VAL:HG21 | 1.94 | 0.48 |
| 40:PH:60:LYS:HZ2 | 40:PH:62:VAL:HG22 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PN:238:THR:HG21 | 41:PN:318:ARG:HD2 | 1.95 | 0.48 |
| 41:QB:221:THR:O | 41:QB:222:TYR:C | 2.51 | 0.48 |
| 41:QB:426:GLY:O | 41:QB:427:ALA:C | 2.51 | 0.48 |
| 40:QE:79:ARG:O | 40:QE:84:ARG:NH1 | 2.46 | 0.48 |
| 40:QE:139:HIS:HB2 | 40:QE:150:THR:HG21 | 1.94 | 0.48 |
| 40:QF:180:ALA:HB3 | 40:QF:183:GLU:HG3 | 1.95 | 0.48 |
| 40:QG:79:ARG:O | 40:QG:84:ARG:NH1 | 2.46 | 0.48 |
| 41:QO:135:LEU:O | 41:QO:166:THR:HA | 2.13 | 0.48 |
| 41:QP:54:ALA:HB3 | 41:QP:58:LYS:HD2 | 1.96 | 0.48 |
| 41:QP:54:ALA:HB1 | 41:RP:282:ARG:O | 2.13 | 0.48 |
| 41:QP:221:THR:O | 41:QP:223:GLY:N | 2.46 | 0.48 |
| 41:RB:378:PHE:HA | 41:RB:381:ILE:HG12 | 1.95 | 0.48 |
| 40:RH:70:LEU:HD23 | 40:RH:114:LEU:HD12 | 1.95 | 0.48 |
| 41:RP:267:MET:N | 41:RP:369:GLY:O | 2.46 | 0.48 |
| 40:SG:130:THR:OG1 | 40:SG:131:GLY:N | 2.46 | 0.48 |
| 40:SI:180:ALA:HA | 41:SP:350:LYS:HD2 | 1.95 | 0.48 |
| 41:SO:406:MET:SD | 41:SO:406:MET:N | 2.87 | 0.48 |
| 41:SP:238:THR:HG21 | 41:SP:318:ARG:HD2 | 1.94 | 0.48 |
| 41:TM:282:ARG:HD3 | 41:TM:283:ALA:H | 1.77 | 0.48 |
| 41:TN:19:LYS:NZ | 41:TN:227:HIS:HB2 | 2.27 | 0.48 |
| 41:TO:179:VAL:HG23 | 41:TO:180:VAL:HG13 | 1.95 | 0.48 |
| 41:TP:105:HIS:CD2 | 41:TP:150:LEU:HB2 | 2.49 | 0.48 |
| 40:UA:76:ASP:HA | 40:UA:79:ARG:HG2 | 1.96 | 0.48 |
| 40:UF:156:ARG:C | 40:UF:158:SER:H | 2.17 | 0.48 |
| 40:UF:207:GLU:HA | 40:UF:210:TYR:HD1 | 1.77 | 0.48 |
| 40:UH:235:VAL:HA | 40:UH:238:ILE:HG22 | 1.93 | 0.48 |
| 41:UP:211:CYS:SG | 41:UP:220:PRO:HB3 | 2.53 | 0.48 |
| 40:VH:362:VAL:HB | 40:VH:369:LYS:HB3 | 1.95 | 0.48 |
| 40:VI:70:LEU:HD12 | 40:VI:99:ALA:HB2 | 1.95 | 0.48 |
| 40:VI:286:LEU:O | 40:VI:372:ARG:NH1 | 2.46 | 0.48 |
| 41:VO:304:ASP:HB2 | 41:VO:306:ARG:HH21 | 1.78 | 0.48 |
| 41:WB:202:ILE:HD13 | 41:WB:229:VAL:HG13 | 1.95 | 0.48 |
| 41:WB:331:LEU:HD11 | 40:WG:176:GLN:HG3 | 1.93 | 0.48 |
| 40:WE:255:PHE:O | 40:WE:259:LEU:HB2 | 2.14 | 0.48 |
| 40:WF:256:GLN:HB3 | 41:WN:397:TRP:CH2 | 2.49 | 0.48 |
| 40:WG:172:TYR:CD1 | 40:WG:173:PRO:HD2 | 2.49 | 0.48 |
| 40:WI:70:LEU:HD23 | 40:WI:114:LEU:HD12 | 1.94 | 0.48 |
| 40:WI:206:ASN:HD22 | 40:WI:209:ILE:HD12 | 1.79 | 0.48 |
| 7:1T:293:ILE:HG23 | 7:1T:307:VAL:HG13 | 1.94 | 0.48 |
| 7:1U:140:TRP:HA | 7:1U:147:ALA:HA | 1.96 | 0.48 |
| 11:2I:245:GLU:O | 11:2I:246:LYS:C | 2.51 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:2J:54:LEU:HD23 | 41:LL:113:VAL:HG13 | 1.95 | 0.48 |
| 11:2K:157:TYR:OH | 11:2K:161:ARG:NH2 | 2.36 | 0.48 |
| 12:2N:75:PHE:HD2 | 12:2N:111:LEU:HD11 | 1.78 | 0.48 |
| 13:2T:118:ILE:HG12 | 13:2T:120:THR:HG23 | 1.95 | 0.48 |
| 15:3F:48:ILE:HG13 | 15:3G:351:LEU:HD21 | 1.94 | 0.48 |
| 15:3F:184:ILE:HG23 | 15:3G:319:THR:HG22 | 1.96 | 0.48 |
| 16:3J:275:VAL:HG11 | 16:3J:380:LYS:HE2 | 1.95 | 0.48 |
| 17:3R:225:ILE:HD12 | 17:3R:339:GLN:HG2 | 1.94 | 0.48 |
| 21:4F:170:ARG:HD2 | 21:4F:204:PRO:HB3 | 1.94 | 0.48 |
| 21:4F:487:PRO:HA | 21:4F:490:PHE:HD1 | 1.78 | 0.48 |
| 22:4H:243:PHE:H | 41:DL:280:GLN:HE22 | 1.60 | 0.48 |
| 22:4I:249:LEU:HD12 | 22:4I:351:VAL:HG21 | 1.95 | 0.48 |
| 22:4J:436:PHE:HB2 | 22:4J:454:ILE:HB | 1.95 | 0.48 |
| 22:4J:632:PHE:HB2 | 22:4J:668:PRO:HG2 | 1.96 | 0.48 |
| 23:4R:254:LYS:NZ | 41:EP:283:ALA:HB1 | 2.29 | 0.48 |
| 26:4V:12:GLU:OE1 | 26:4V:23:ARG:NE | 2.46 | 0.48 |
| 39:6G:62:ALA:HB1 | 41:OB:35:THR:HG23 | 1.94 | 0.48 |
| 39:6H:115:LEU:HD23 | 39:6H:142:LEU:HA | 1.95 | 0.48 |
| 40:AG:20:CYS:HA | 40:AG:232:SER:HB2 | 1.95 | 0.48 |
| 41:AL:289:LEU:O | 41:AL:293:MET:HB2 | 2.13 | 0.48 |
| 41:AL:307:HIS:ND1 | 41:AL:376:GLU:OE2 | 2.46 | 0.48 |
| 41:AM:128:ASP:OD1 | 41:AM:129:CYS:N | 2.46 | 0.48 |
| 41:AN:290:THR:HG21 | 41:AN:329:GLN:HB3 | 1.96 | 0.48 |
| 41:AO:358:PRO:CG | 41:AO:364:SER:HB3 | 2.37 | 0.48 |
| 40:BA:7:VAL:HB | 40:BA:137:ILE:HG22 | 1.96 | 0.48 |
| 40:BA:257:THR:HA | 41:BB:397:TRP:CZ2 | 2.48 | 0.48 |
| 40:BG:18:ASN:HD21 | 40:BG:78:VAL:HG22 | 1.79 | 0.48 |
| 41:BL:238:THR:HG21 | 41:BL:318:ARG:HD2 | 1.96 | 0.48 |
| 40:CF:73:THR:OG1 | 40:CF:74:VAL:N | 2.45 | 0.48 |
| 41:CM:86:ARG:HB2 | 41:CM:89:ASN:HB3 | 1.95 | 0.48 |
| 41:CN:107:THR:O | 41:CN:108:GLU:C | 2.52 | 0.48 |
| 41:CN:252:LYS:HE3 | 41:CN:252:LYS:HB2 | 1.46 | 0.48 |
| 41:CN:289:LEU:HD11 | 41:CN:363:MET:O | 2.12 | 0.48 |
| 40:DA:36:MET:O | 40:DA:37:PRO:C | 2.51 | 0.48 |
| 40:DA:178:SER:C | 40:DA:180:ALA:H | 2.17 | 0.48 |
| 40:DA:280:LYS:O | 40:DA:281:ALA:C | 2.51 | 0.48 |
| 41:DB:101:TRP:O | 41:DB:104:GLY:N | 2.44 | 0.48 |
| 40:DG:3:GLU:HG2 | 40:DG:64:ARG:HE | 1.79 | 0.48 |
| 40:DH:213:CYS:HB3 | 40:DH:219:ILE:CD1 | 2.41 | 0.48 |
| 40:DI:144:GLY:O | 40:DI:145:THR:C | 2.51 | 0.48 |
| 40:DI:224:TYR:HB3 | 42:DI:501:GTP:N1 | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DI:398:TYR:O | 40:DI:401:ARG:N | 2.36 | 0.48 |
| 41:DO:16:ILE:HG12 | 41:DO:226:ASN:HB3 | 1.94 | 0.48 |
| 41:DO:161:ASP:O | 41:DO:251:ARG:NH2 | 2.47 | 0.48 |
| 41:DP:82:GLY:O | 41:DP:84:ILE:N | 2.42 | 0.48 |
| 40:EE:168:GLU:OE1 | 40:EE:198:SER:OG | 2.29 | 0.48 |
| 40:EI:9:VAL:HG13 | 40:EI:68:VAL:HG13 | 1.96 | 0.48 |
| 41:EL:139:LEU:HD12 | 41:EL:170:VAL:HG12 | 1.94 | 0.48 |
| 41:EO:210:ILE:O | 41:EO:214:THR:OG1 | 2.22 | 0.48 |
| 40:FE:30:ILE:HD13 | 40:FE:36:MET:HG2 | 1.95 | 0.48 |
| 40:FG:20:CYS:HA | 40:FG:232:SER:HB2 | 1.95 | 0.48 |
| 40:FG:27:GLU:OE1 | 40:FG:236:SER:OG | 2.27 | 0.48 |
| 40:GF:71:GLU:HB3 | 40:GF:98:ASP:HA | 1.94 | 0.48 |
| 40:GG:130:THR:HG22 | 41:GO:94:GLN:HG2 | 1.95 | 0.48 |
| 40:GI:218:ASP:O | 40:GI:219:ILE:C | 2.50 | 0.48 |
| 41:GO:134:GLN:HA | 41:GO:165:ASN:O | 2.13 | 0.48 |
| 41:GO:180:VAL:O | 41:GO:184:ASN:ND2 | 2.46 | 0.48 |
| 41:GP:172:SER:OG | 41:GP:175:VAL:O | 2.27 | 0.48 |
| 40:HE:385:GLU:H | 40:HE:385:GLU:HG3 | 1.47 | 0.48 |
| 41:HM:207:LEU:HA | 41:HM:210:ILE:HG22 | 1.96 | 0.48 |
| 41:HM:257:MET:HA | 41:HM:312:THR:HG21 | 1.95 | 0.48 |
| 41:HQ:20:PHE:CD1 | 41:HQ:233:MET:HB3 | 2.48 | 0.48 |
| 40:II:4:CYS:HB2 | 40:II:52:PHE:HE2 | 1.79 | 0.48 |
| 40:II:198:SER:HG | 40:II:266:HIS:HE2 | 1.60 | 0.48 |
| 41:IQ:52:ASN:OD1 | 41:IQ:62:ARG:NH1 | 2.47 | 0.48 |
| 40:JA:101:ASN:HB3 | 40:JA:182:VAL:HG21 | 1.96 | 0.48 |
| 40:JD:128:GLN:HE21 | 40:JD:128:GLN:HA | 1.78 | 0.48 |
| 40:KA:141:PHE:HB2 | 40:KA:173:PRO:HD3 | 1.96 | 0.48 |
| 41:KB:142:GLY:O | 41:KB:144:GLY:N | 2.47 | 0.48 |
| 41:KB:170:VAL:HG11 | 41:KB:377:LEU:HD21 | 1.96 | 0.48 |
| 40:KF:288:VAL:HG11 | 40:KF:328:VAL:HG12 | 1.96 | 0.48 |
| 40:KG:211:ASP:OD2 | 40:KG:215:ARG:NH2 | 2.46 | 0.48 |
| 40:KG:405:HIS:HA | 40:KG:408:VAL:HG12 | 1.93 | 0.48 |
| 41:KL:400:GLY:C | 41:KL:402:GLY:H | 2.17 | 0.48 |
| 41:KM:211:CYS:HA | 41:KM:215:LEU:HB2 | 1.95 | 0.48 |
| 40:MG:264:ARG:O | 40:MG:266:HIS:N | 2.46 | 0.48 |
| 40:MH:20:CYS:HA | 40:MH:232:SER:HB2 | 1.96 | 0.48 |
| 40:MH:299:ALA:C | 40:MH:301:GLN:H | 2.17 | 0.48 |
| 41:MM:152:ILE:HG12 | 41:MM:164:MET:HE1 | 1.94 | 0.48 |
| 41:MO:44:LEU:HD12 | 41:MO:47:ILE:HD13 | 1.95 | 0.48 |
| 41:MP:309:ARG:H | 41:MP:372:THR:HG1 | 1.58 | 0.48 |
| 41:NM:165:ASN:HB3 | 41:NM:167:PHE:HE1 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:NP:137:HIS:NE2 | 41:NP:166:THR:OG1 | 2.45 | 0.48 |
| 40:OH:146:GLY:O | 40:OH:147:SER:C | 2.52 | 0.48 |
| 41:OL:7:LEU:HD23 | 41:OL:64:VAL:HB | 1.96 | 0.48 |
| 41:OL:128:ASP:OD2 | 41:OL:129:CYS:N | 2.46 | 0.48 |
| 40:PF:356:ASN:OD1 | 40:PF:357:TYR:N | 2.46 | 0.48 |
| 40:PH:317:LEU:HD11 | 40:PH:332:ILE:HD11 | 1.95 | 0.48 |
| 41:PL:11:GLN:HA | 41:PL:72:THR:HG21 | 1.96 | 0.48 |
| 41:PO:299:MET:SD | 41:PO:299:MET:N | 2.81 | 0.48 |
| 41:PP:8:GLN:NE2 | 41:PP:64:VAL:O | 2.46 | 0.48 |
| 41:QB:35:THR:OG1 | 41:QB:36:TYR:N | 2.45 | 0.48 |
| 41:QB:65:LEU:O | 41:QB:91:VAL:HG13 | 2.14 | 0.48 |
| 41:QB:190:HIS:HA | 41:QB:414:ASN:HD22 | 1.78 | 0.48 |
| 40:QE:5:ILE:HG12 | 40:QE:132:LEU:HD11 | 1.95 | 0.48 |
| 40:QE:15:GLN:HE22 | 40:QE:228:ASN:HD21 | 1.61 | 0.48 |
| 41:QM:113:VAL:HG23 | 41:QM:151:LEU:HD22 | 1.95 | 0.48 |
| 41:QP:58:LYS:HB3 | 41:QP:58:LYS:HE3 | 1.48 | 0.48 |
| 41:RB:21:TRP:CZ3 | 41:RB:61:PRO:HB3 | 2.49 | 0.48 |
| 41:RM:101:TRP:CD1 | 41:RM:146:GLY:HA2 | 2.49 | 0.48 |
| 41:RN:138:SER:HA | 41:RN:169:VAL:HB | 1.96 | 0.48 |
| 40:SF:171:ILE:HD13 | 40:SF:204:VAL:HG23 | 1.95 | 0.48 |
| 40:SG:204:VAL:HG13 | 40:SG:302:MET:HB3 | 1.95 | 0.48 |
| 41:SO:19:LYS:HG3 | 41:SO:227:HIS:HA | 1.95 | 0.48 |
| 41:SO:42:LEU:HD12 | 41:SO:42:LEU:HA | 1.73 | 0.48 |
| 41:SO:290:THR:HG21 | 41:SO:329:GLN:HB3 | 1.93 | 0.48 |
| 40:TI:6:SER:O | 40:TI:65:ALA:HA | 2.13 | 0.48 |
| 40:TI:294:ALA:O | 40:TI:300:ASN:ND2 | 2.44 | 0.48 |
| 41:TN:407:GLU:OE2 | 41:TN:407:GLU:N | 2.45 | 0.48 |
| 41:TO:214:THR:O | 41:TO:275:SER:OG | 2.23 | 0.48 |
| 40:UE:28:HIS:HE1 | 40:UE:243:ARG:HD3 | 1.79 | 0.48 |
| 40:UG:224:TYR:HA | 40:UG:227:LEU:HD12 | 1.95 | 0.48 |
| 40:UI:304:LYS:HA | 40:UI:304:LYS:HD2 | 1.53 | 0.48 |
| 41:UN:142:GLY:O | 41:UN:144:GLY:N | 2.46 | 0.48 |
| 41:UP:70:PRO:HB3 | 41:UP:92:PHE:HD2 | 1.77 | 0.48 |
| 40:VJ:88:HIS:CD2 | 40:VJ:90:GLU:HB2 | 2.48 | 0.48 |
| 40:VJ:214:ARG:HH21 | 41:VQ:324:LYS:HE3 | 1.77 | 0.48 |
| 40:WG:48:SER:O | 40:WG:51:THR:HG22 | 2.14 | 0.48 |
| 41:WM:70:PRO:HB3 | 41:WM:92:PHE:CE2 | 2.49 | 0.48 |
| 41:WO:113:VAL:HA | 41:WO:116:VAL:HG12 | 1.95 | 0.48 |
| 8:1W:313:ILE:HA | 8:1W:316:ILE:HG22 | 1.95 | 0.48 |
| 9:2B:169:ALA:HB1 | 37:6A:99:LEU:HD22 | 1.96 | 0.48 |
| 13:2U:160:CYS:SG | 13:2U:162:ILE:HG12 | 2.54 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2V:156:ILE:H | 13:2V:156:ILE:HG12 | 1.50 | 0.48 |
| 15:3H:268:LEU:HG | 15:3H:272:LYS:HE3 | 1.94 | 0.48 |
| 17:3R:181:LEU:HG | 17:3R:237:LEU:HD23 | 1.95 | 0.48 |
| 18:3T:431:MET:HB3 | 40:LA:42:ILE:HD11 | 1.96 | 0.48 |
| 20:4B:277:MET:HB3 | 20:4B:282:ARG:CZ | 2.43 | 0.48 |
| 21:4E:420:LEU:HG | 21:4E:444:LEU:HD21 | 1.96 | 0.48 |
| 21:4F:97:LEU:HB2 | 21:4F:124:TYR:HB3 | 1.96 | 0.48 |
| 22:4H:251:LEU:HA | 22:4H:262:ILE:HG22 | 1.95 | 0.48 |
| 22:4J:627:LEU:HG | 22:4J:632:PHE:HB3 | 1.96 | 0.48 |
| 22:4K:615:ASP:O | 22:4K:616:THR:C | 2.50 | 0.48 |
| 23:4N:19:ILE:HD11 | 40:BF:79:ARG:HB3 | 1.95 | 0.48 |
| 23:4P:236:TYR:HA | 23:4P:267:ASP:CB | 2.36 | 0.48 |
| 23:4R:246:TYR:HD1 | 40:DI:79:ARG:HD2 | 1.77 | 0.48 |
| 25:4T:382:LEU:O | 25:4T:384:HIS:N | 2.46 | 0.48 |
| 26:4V:128:LEU:HB3 | 26:4V:133:ALA:HB2 | 1.96 | 0.48 |
| 26:4V:210:SER:HG | 26:4V:213:CYS:HG | 1.48 | 0.48 |
| 32:5L:37:MET:SD | 41:KO:218:THR:HG23 | 2.52 | 0.48 |
| 33:5O:119:ILE:HD13 | 33:5O:122:ARG:HH21 | 1.79 | 0.48 |
| 34:5Q:167:GLU:CB | 34:5R:491:LEU:HD22 | 2.42 | 0.48 |
| 34:5R:451:LEU:HD22 | 34:5R:451:LEU:HA | 1.69 | 0.48 |
| 35:5T:102:TYR:O | 35:5T:104:ARG:N | 2.39 | 0.48 |
| 39:6K:128:SER:O | 39:6K:132:ALA:N | 2.41 | 0.48 |
| 40:AA:60:LYS:NZ | 40:AA:85:GLN:O | 2.37 | 0.48 |
| 41:AL:268:PRO:HG2 | 41:AL:300:MET:HB2 | 1.94 | 0.48 |
| 41:AO:2:ARG:HH11 | 41:AO:2:ARG:H | 1.62 | 0.48 |
| 41:AO:91:VAL:HG11 | 41:AO:116:VAL:HG22 | 1.95 | 0.48 |
| 40:BF:53:PHE:HB3 | 40:BF:61:HIS:HB3 | 1.94 | 0.48 |
| 40:BH:285:GLN:O | 40:BH:286:LEU:C | 2.51 | 0.48 |
| 40:BI:306:ASP:O | 40:BI:309:HIS:N | 2.46 | 0.48 |
| 40:CA:65:ALA:H | 40:CA:91:GLN:HE21 | 1.61 | 0.48 |
| 40:CA:153:LEU:HG | 40:CA:157:LEU:HG | 1.95 | 0.48 |
| 40:CA:329:ASN:ND2 | 41:CB:174:LYS:HE2 | 2.29 | 0.48 |
| 40:CG:398:TYR:O | 40:CG:401:ARG:NH1 | 2.46 | 0.48 |
| 40:CI:104:ALA:HB2 | 40:CI:412:MET:HB2 | 1.95 | 0.48 |
| 41:CN:107:THR:HG21 | 41:CN:401:GLU:HB3 | 1.96 | 0.48 |
| 40:DA:102:ASN:O | 40:DA:103:TYR:C | 2.51 | 0.48 |
| 40:DA:328:VAL:HG11 | 40:DA:353:VAL:HG11 | 1.96 | 0.48 |
| 41:DB:99:ASN:ND2 | 41:DB:178:THR:HG21 | 2.28 | 0.48 |
| 40:DE:73:THR:O | 40:DE:76:ASP:N | 2.46 | 0.48 |
| 40:DE:209:ILE:H | 40:DE:209:ILE:HG12 | 1.50 | 0.48 |
| 40:DF:324:VAL:O | 40:DF:325:PRO:C | 2.50 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DG:15:GLN:HG3 | 40:DG:228:ASN:ND2 | 2.28 | 0.48 |
| 40:DG:322:ASP:N | 40:DG:371:GLN:O | 2.42 | 0.48 |
| 41:DL:102:ALA:HA | 41:DL:106:TYR:HD2 | 1.79 | 0.48 |
| 41:DM:259:PRO:HG2 | 41:DM:260:PHE:H | 1.78 | 0.48 |
| 40:EA:118:VAL:O | 40:EA:122:ILE:HG12 | 2.14 | 0.48 |
| 40:EE:71:GLU:HG3 | 40:EE:98:ASP:HA | 1.96 | 0.48 |
| 40:EE:76:ASP:OD2 | 41:EL:46:ARG:NH2 | 2.44 | 0.48 |
| 40:EG:97:GLU:HG2 | 40:EG:105:ARG:HH22 | 1.78 | 0.48 |
| 40:EH:141:PHE:HE2 | 40:EH:194:THR:HG21 | 1.78 | 0.48 |
| 40:EI:341:ILE:H | 40:EI:341:ILE:HG12 | 1.43 | 0.48 |
| 41:EM:96:GLY:O | 41:EM:98:GLY:N | 2.47 | 0.48 |
| 41:EN:142:GLY:O | 41:EN:144:GLY:N | 2.46 | 0.48 |
| 40:FA:315:CYS:HB3 | 40:FA:351:PHE:HD1 | 1.78 | 0.48 |
| 40:FF:336:LYS:HE3 | 40:FF:351:PHE:HE1 | 1.79 | 0.48 |
| 40:FI:14:VAL:HG23 | 40:FI:67:PHE:CD2 | 2.49 | 0.48 |
| 40:FI:212:ILE:HD11 | 40:FI:275:VAL:HG21 | 1.96 | 0.48 |
| 40:FI:431:TYR:HA | 40:FI:434:VAL:HG12 | 1.95 | 0.48 |
| 41:FO:99:ASN:HA | 41:FO:142:GLY:H | 1.78 | 0.48 |
| 41:FP:228:LEU:HD11 | 41:FP:273:LEU:HD11 | 1.94 | 0.48 |
| 40:GA:70:LEU:HD22 | 40:GA:110:ILE:HG22 | 1.95 | 0.48 |
| 40:GE:112:LYS:O | 40:GE:115:ILE:HG22 | 2.13 | 0.48 |
| 40:GG:152:LEU:O | 40:GG:156:ARG:HG2 | 2.13 | 0.48 |
| 40:GH:260:VAL:CG2 | 41:GP:397:TRP:HZ2 | 2.26 | 0.48 |
| 41:GN:171:PRO:HB3 | 41:GN:181:GLU:HG2 | 1.94 | 0.48 |
| 41:GP:142:GLY:O | 41:GP:144:GLY:N | 2.47 | 0.48 |
| 40:IH:223:THR:OG1 | 40:IH:224:TYR:N | 2.45 | 0.48 |
| 40:II:70:LEU:HD12 | 40:II:110:ILE:HD12 | 1.94 | 0.48 |
| 41:IQ:186:THR:HG22 | 41:IQ:411:ALA:HB1 | 1.95 | 0.48 |
| 41:IQ:256:ASN:ND2 | 41:IQ:256:ASN:O | 2.47 | 0.48 |
| 40:JA:405:HIS:HA | 40:JA:408:VAL:HG12 | 1.96 | 0.48 |
| 41:JB:139:LEU:HD12 | 41:JB:170:VAL:HG12 | 1.94 | 0.48 |
| 41:JB:198:GLU:HG3 | 41:JB:266:PHE:HE2 | 1.79 | 0.48 |
| 41:JM:303:CYS:O | 41:JM:304:ASP:C | 2.52 | 0.48 |
| 41:JN:142:GLY:O | 41:JN:144:GLY:N | 2.46 | 0.48 |
| 41:JO:198:GLU:HG2 | 41:JO:266:PHE:HE2 | 1.77 | 0.48 |
| 40:KA:116:ASP:OD1 | 40:KA:117:LEU:N | 2.47 | 0.48 |
| 40:KE:51:THR:HG23 | 40:KE:52:PHE:HD1 | 1.77 | 0.48 |
| 40:KE:139:HIS:NE2 | 40:KE:168:GLU:OE2 | 2.34 | 0.48 |
| 40:KH:18:ASN:HD21 | 40:KH:78:VAL:HG22 | 1.79 | 0.48 |
| 41:KM:117:LEU:HB3 | 41:KM:121:ARG:NH1 | 2.28 | 0.48 |
| 40:LE:294:ALA:O | 40:LE:300:ASN:ND2 | 2.38 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LG:200:CYS:SG | 40:LG:200:CYS:O | 2.72 | 0.48 |
| 40:LH:326:LYS:HD3 | 41:LP:220:PRO:HD2 | 1.96 | 0.48 |
| 41:LN:8:GLN:HG3 | 41:LN:14:ASN:HD22 | 1.78 | 0.48 |
| 41:LO:285:THR:HG23 | 41:LO:288:GLU:H | 1.79 | 0.48 |
| 42:MB:502:GTP:H2' | 40:MG:224:TYR:CZ | 2.47 | 0.48 |
| 40:MF:326:LYS:O | 40:MF:329:ASN:N | 2.47 | 0.48 |
| 41:ML:67:ASP:HA | 41:ML:143:THR:HG21 | 1.96 | 0.48 |
| 40:NA:88:HIS:CE1 | 40:NA:90:GLU:HB2 | 2.48 | 0.48 |
| 40:NF:240:ALA:HB1 | 40:NF:356:ASN:HD22 | 1.79 | 0.48 |
| 40:NG:20:CYS:HA | 40:NG:232:SER:HB2 | 1.96 | 0.48 |
| 40:NG:73:THR:H | 40:NG:76:ASP:HB2 | 1.77 | 0.48 |
| 40:OD:30:ILE:HG13 | 40:OD:53:PHE:CE2 | 2.49 | 0.48 |
| 40:OD:211:ASP:HA | 40:OD:214:ARG:HG2 | 1.94 | 0.48 |
| 40:OF:224:TYR:HA | 40:OF:227:LEU:HB2 | 1.95 | 0.48 |
| 40:OF:332:ILE:HG23 | 40:OF:351:PHE:CD1 | 2.49 | 0.48 |
| 41:ON:29:GLY:O | 41:ON:37:HIS:N | 2.41 | 0.48 |
| 41:PN:31:ASP:OD1 | 41:PN:31:ASP:N | 2.42 | 0.48 |
| 41:PN:122:LYS:HD3 | 41:QN:291:GLN:HE22 | 1.79 | 0.48 |
| 41:PN:132:GLY:HA3 | 41:PN:163:ILE:O | 2.13 | 0.48 |
| 41:PO:287:PRO:O | 41:PO:291:GLN:HG2 | 2.13 | 0.48 |
| 40:QE:108:TYR:O | 40:QE:112:LYS:NZ | 2.44 | 0.48 |
| 40:QE:273:ALA:HB1 | 40:QE:294:ALA:HB3 | 1.95 | 0.48 |
| 40:QH:70:LEU:HD23 | 40:QH:114:LEU:HD12 | 1.94 | 0.48 |
| 41:QO:300:MET:SD | 41:QO:300:MET:N | 2.70 | 0.48 |
| 41:QP:282:ARG:HA | 41:QP:282:ARG:HD2 | 1.55 | 0.48 |
| 41:RO:209:ASP:HB3 | 41:RO:213:ARG:HH22 | 1.78 | 0.48 |
| 40:SA:273:ALA:HB3 | 40:SA:374:VAL:H | 1.78 | 0.48 |
| 41:SB:314:ALA:HB3 | 41:SB:368:ILE:HB | 1.95 | 0.48 |
| 40:SE:67:PHE:HB2 | 40:SE:92:LEU:HD13 | 1.96 | 0.48 |
| 40:SH:20:CYS:HA | 40:SH:232:SER:HB2 | 1.96 | 0.48 |
| 40:SH:329:ASN:HD21 | 41:SP:175:VAL:HG21 | 1.77 | 0.48 |
| 41:SO:364:SER:OG | 41:SO:365:ALA:N | 2.47 | 0.48 |
| 41:TB:425:ARG:HH22 | 40:TG:400:LYS:HG3 | 1.79 | 0.48 |
| 42:TI:501:GTP:O1G | 41:TP:252:LYS:NZ | 2.37 | 0.48 |
| 41:UB:237:THR:O | 41:UB:241:ARG:NH1 | 2.47 | 0.48 |
| 40:UE:88:HIS:CE1 | 40:UE:90:GLU:HB2 | 2.49 | 0.48 |
| 40:UE:135:PHE:HD1 | 40:UE:166:LYS:HG2 | 1.77 | 0.48 |
| 40:UG:252:LEU:HD12 | 40:UG:255:PHE:HD2 | 1.79 | 0.48 |
| 40:UG:324:VAL:HG23 | 40:UG:327:ASP:HB2 | 1.96 | 0.48 |
| 41:UP:301:ALA:O | 41:UP:302:ALA:C | 2.51 | 0.48 |
| 41:UP:386:THR:O | 41:UP:390:ARG:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VJ:54:SER:HB2 | 40:VJ:64:ARG:HE | 1.79 | 0.48 |
| 40:WA:405:HIS:CD2 | 41:WN:261:PRO:HD3 | 2.48 | 0.48 |
| 41:WN:29:GLY:O | 41:WN:30:ILE:C | 2.51 | 0.48 |
| 7:1S:606:SER:HB3 | 7:1S:610:ALA:HB3 | 1.96 | 0.48 |
| 10:2E:89:ASN:HA | 40:AE:214:ARG:HH12 | 1.78 | 0.48 |
| 11:2I:188:LEU:HD22 | 11:2I:188:LEU:HA | 1.73 | 0.48 |
| 11:2J:248:LYS:O | 11:2J:250:ILE:HG12 | 2.13 | 0.48 |
| 12:2M:130:GLY:O | 12:2M:134:MET:HG2 | 2.14 | 0.48 |
| 13:2V:99:VAL:HG23 | 13:2V:101:ARG:HD2 | 1.95 | 0.48 |
| 15:3H:119:ARG:O | 15:3H:122:ARG:NE | 2.42 | 0.48 |
| 16:3L:110:LEU:HB2 | 16:3L:144:ILE:HG21 | 1.95 | 0.48 |
| 17:3O:202:ARG:NH1 | 17:3O:469:ASP:OD1 | 2.47 | 0.48 |
| 17:3P:192:LEU:HD12 | 17:3P:192:LEU:HA | 1.73 | 0.48 |
| 17:3R:182:GLU:HG2 | 17:3R:237:LEU:HD21 | 1.95 | 0.48 |
| 22:4H:98:ARG:HH21 | 22:4H:100:ARG:HD3 | 1.78 | 0.48 |
| 22:4I:261:GLU:HB2 | 22:4I:281:ARG:HD2 | 1.96 | 0.48 |
| 22:4I:562:LEU:HA | 22:4I:565:VAL:HG22 | 1.96 | 0.48 |
| 23:4M:20:PRO:HG2 | 40:BG:89:PRO:HB2 | 1.96 | 0.48 |
| 30:5G:46:HIS:HA | 30:5G:57:ILE:HG12 | 1.94 | 0.48 |
| 34:5Q:188:GLU:HB3 | 34:5Q:192:ARG:NH1 | 2.28 | 0.48 |
| 39:6J:32:GLU:OE2 | 39:6J:35:ARG:NH2 | 2.47 | 0.48 |
| 41:AB:49:VAL:O | 41:AB:62:ARG:NH1 | 2.46 | 0.48 |
| 40:AE:280:LYS:HG2 | 40:ME:89:PRO:HG2 | 1.95 | 0.48 |
| 41:AM:226:ASN:ND2 | 43:AM:501:GDP:O6 | 2.37 | 0.48 |
| 41:AM:385:PHE:HZ | 41:AM:408:PHE:HB3 | 1.77 | 0.48 |
| 41:AO:260:PHE:O | 41:AO:261:PRO:C | 2.52 | 0.48 |
| 40:BH:206:ASN:HD22 | 40:BH:206:ASN:HA | 1.49 | 0.48 |
| 41:BP:224:ASP:C | 41:BP:226:ASN:H | 2.17 | 0.48 |
| 40:CG:128:GLN:NE2 | 40:DG:290:GLU:OE2 | 2.45 | 0.48 |
| 40:CH:211:ASP:C | 40:CH:213:CYS:H | 2.17 | 0.48 |
| 40:CI:269:LEU:HD22 | 40:CI:383:ILE:HD11 | 1.95 | 0.48 |
| 41:CN:86:ARG:NH2 | 41:DN:282:ARG:HB2 | 2.26 | 0.48 |
| 41:CN:103:LYS:HA | 41:CN:107:THR:CG2 | 2.44 | 0.48 |
| 41:CN:132:GLY:HA3 | 41:CN:163:ILE:HG22 | 1.96 | 0.48 |
| 41:CN:288:GLU:HG3 | 41:CN:289:LEU:N | 2.29 | 0.48 |
| 41:CN:425:ARG:O | 41:CN:426:GLY:C | 2.52 | 0.48 |
| 41:CO:107:THR:O | 41:CO:108:GLU:C | 2.50 | 0.48 |
| 41:CO:385:PHE:O | 41:CO:386:THR:C | 2.52 | 0.48 |
| 41:CP:322:SER:O | 41:CP:323:MET:C | 2.52 | 0.48 |
| 40:DA:259:LEU:HA | 40:DA:314:ALA:HB1 | 1.96 | 0.48 |
| 40:DI:118:VAL:HG21 | 40:DI:149:PHE:CZ | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DL:99:ASN:C | 41:DL:184:ASN:HD21 | 2.17 | 0.48 |
| 41:DM:47:ILE:O | 41:DM:49:VAL:N | 2.46 | 0.48 |
| 41:DN:171:PRO:HG2 | 41:DN:185:ALA:HB2 | 1.96 | 0.48 |
| 41:DP:346:PRO:O | 41:DP:347:ASN:C | 2.52 | 0.48 |
| 40:EF:212:ILE:HD13 | 40:EF:300:ASN:HA | 1.96 | 0.48 |
| 40:EI:3:GLU:CG | 40:EI:129:CYS:HB3 | 2.40 | 0.48 |
| 40:EI:122:ILE:HD13 | 40:EI:122:ILE:HA | 1.78 | 0.48 |
| 40:EI:154:MET:HA | 40:EI:154:MET:HE3 | 1.96 | 0.48 |
| 40:EI:387:TRP:O | 40:EI:391:ASP:N | 2.42 | 0.48 |
| 41:EP:285:THR:O | 41:EP:286:VAL:C | 2.51 | 0.48 |
| 40:FA:315:CYS:SG | 40:FA:316:CYS:N | 2.87 | 0.48 |
| 40:FH:398:TYR:OH | 40:FH:414:GLU:OE2 | 2.28 | 0.48 |
| 41:FM:39:ASP:N | 41:FM:39:ASP:OD1 | 2.47 | 0.48 |
| 41:FO:335:ASN:O | 41:FO:338:SER:OG | 2.31 | 0.48 |
| 40:GG:205:ASP:HB3 | 40:GG:303:VAL:HA | 1.96 | 0.48 |
| 40:GH:386:ALA:HA | 40:GH:389:ARG:HD3 | 1.95 | 0.48 |
| 40:GI:25:CYS:O | 40:GI:26:LEU:C | 2.52 | 0.48 |
| 41:GM:170:VAL:HG21 | 41:GM:377:LEU:HD21 | 1.96 | 0.48 |
| 40:IF:104:ALA:HB2 | 40:IF:412:MET:HG2 | 1.96 | 0.48 |
| 41:IN:322:SER:OG | 41:IN:323:MET:N | 2.47 | 0.48 |
| 41:IQ:170:VAL:HG11 | 41:IQ:377:LEU:HD21 | 1.95 | 0.48 |
| 41:IQ:173:PRO:HG2 | 41:IQ:380:ARG:HG2 | 1.96 | 0.48 |
| 40:JA:141:PHE:HB2 | 40:JA:173:PRO:HD3 | 1.96 | 0.48 |
| 40:JD:135:PHE:HB2 | 40:JD:166:LYS:HD2 | 1.95 | 0.48 |
| 40:JE:138:PHE:HZ | 40:JE:235:VAL:HG21 | 1.78 | 0.48 |
| 40:JH:16:ILE:HA | 40:JH:228:ASN:HB3 | 1.96 | 0.48 |
| 41:JL:309:ARG:NH1 | 41:JL:339:SER:O | 2.46 | 0.48 |
| 41:JM:107:THR:OG1 | 41:JM:108:GLU:N | 2.47 | 0.48 |
| 41:KL:139:LEU:HA | 41:KL:139:LEU:HD12 | 1.72 | 0.48 |
| 40:MF:11:GLN:HE22 | 41:MM:246:LEU:H | 1.60 | 0.48 |
| 40:MG:250:VAL:HG23 | 40:MG:254:GLU:HB2 | 1.95 | 0.48 |
| 40:MG:348:PRO:HD2 | 41:MO:388:MET:CE | 2.43 | 0.48 |
| 40:NA:181:VAL:HG22 | 41:NN:256:ASN:HD22 | 1.79 | 0.48 |
| 41:NB:73:MET:HG3 | 41:NB:92:PHE:HB3 | 1.95 | 0.48 |
| 40:ND:170:SER:OG | 40:ND:171:ILE:N | 2.47 | 0.48 |
| 40:NF:115:ILE:HA | 40:NF:118:VAL:HG12 | 1.96 | 0.48 |
| 40:NG:180:ALA:HB3 | 40:NG:183:GLU:HG3 | 1.96 | 0.48 |
| 41:NN:95:SER:OG | 41:NN:96:GLY:N | 2.46 | 0.48 |
| 41:NP:10:GLY:O | 41:NP:14:ASN:ND2 | 2.46 | 0.48 |
| 41:NP:142:GLY:O | 41:NP:144:GLY:N | 2.47 | 0.48 |
| 40:OD:239:THR:O | 40:OD:243:ARG:NH1 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OH:326:LYS:NZ | 41:OP:208:TYR:HB2 | 2.29 | 0.48 |
| 41:ON:132:GLY:CA | 41:ON:163:ILE:O | 2.55 | 0.48 |
| 40:PF:68:VAL:HG12 | 40:PF:93:ILE:HB | 1.95 | 0.48 |
| 40:PF:394:PHE:HD2 | 40:PF:421:ARG:HD3 | 1.79 | 0.48 |
| 40:PH:4:CYS:HB3 | 40:PH:52:PHE:HE1 | 1.77 | 0.48 |
| 41:PL:87:PRO:HG2 | 41:QL:278:SER:HB3 | 1.95 | 0.48 |
| 40:QA:177:VAL:HA | 41:QN:331:LEU:HD12 | 1.96 | 0.48 |
| 40:QF:100:ALA:HB2 | 41:QM:251:ARG:HG3 | 1.95 | 0.48 |
| 40:QF:260:VAL:HB | 41:QN:397:TRP:HH2 | 1.78 | 0.48 |
| 41:QO:26:ASP:OD1 | 41:QO:359:ARG:NH1 | 2.46 | 0.48 |
| 41:QP:414:ASN:O | 41:QP:417:ASP:HB2 | 2.13 | 0.48 |
| 40:RA:121:ARG:HA | 40:RA:124:LYS:HB2 | 1.96 | 0.48 |
| 40:RE:324:VAL:HG13 | 40:RE:327:ASP:H | 1.79 | 0.48 |
| 40:RG:174:ALA:HB2 | 40:RG:206:ASN:H | 1.79 | 0.48 |
| 40:RG:311:LYS:NZ | 40:RG:435:GLY:O | 2.45 | 0.48 |
| 41:RN:31:ASP:OD1 | 41:RN:35:THR:N | 2.47 | 0.48 |
| 41:RN:323:MET:HA | 41:RN:326:VAL:HB | 1.96 | 0.48 |
| 40:SF:102:ASN:HB3 | 40:SF:105:ARG:HB2 | 1.96 | 0.48 |
| 40:SH:2:ARG:HD3 | 40:SH:242:LEU:HB2 | 1.96 | 0.48 |
| 40:SH:395:ASP:OD1 | 40:SH:421:ARG:NE | 2.46 | 0.48 |
| 41:TB:139:LEU:HD12 | 41:TB:170:VAL:HG12 | 1.95 | 0.48 |
| 41:UP:286:VAL:HG13 | 41:UP:287:PRO:HD3 | 1.95 | 0.48 |
| 41:WB:180:VAL:O | 41:WB:184:ASN:ND2 | 2.47 | 0.48 |
| 40:WF:55:GLU:OE1 | 40:WF:61:HIS:NE2 | 2.47 | 0.48 |
| 40:WF:103:TYR:HB3 | 40:WF:407:TYR:HE1 | 1.78 | 0.48 |
| 40:WF:191:THR:HA | 40:WF:194:THR:HG22 | 1.95 | 0.48 |
| 40:WG:298:PRO:HB3 | 40:WG:307:PRO:HD2 | 1.96 | 0.48 |
| 41:WN:70:PRO:HD3 | 41:WN:94:GLN:HA | 1.94 | 0.48 |
| 41:WQ:19:LYS:HE2 | 41:WQ:223:GLY:HA2 | 1.95 | 0.48 |
| 7:1S:427:SER:H | 7:1S:473:ASN:ND2 | 2.11 | 0.48 |
| 9:2C:492:LEU:HD12 | 40:SH:58:ALA:HB2 | 1.95 | 0.48 |
| 12:2R:78:ARG:HH12 | 13:2V:149:ILE:HG22 | 1.79 | 0.48 |
| 13:2U:42:ILE:HD13 | 13:2U:183:LEU:HD11 | 1.95 | 0.48 |
| 13:2X:53:ASN:O | 13:2X:55:SER:N | 2.47 | 0.48 |
| 17:3P:296:VAL:HG22 | 17:3P:297:PRO:HD2 | 1.94 | 0.48 |
| 17:3R:164:LEU:HD21 | 17:3R:254:LEU:HB3 | 1.96 | 0.48 |
| 20:4A:78:GLN:NE2 | 41:MN:276:ARG:O | 2.47 | 0.48 |
| 21:4F:425:ALA:HB3 | 21:4F:504:VAL:HG13 | 1.95 | 0.48 |
| 23:4N:236:TYR:HA | 23:4N:267:ASP:CB | 2.36 | 0.48 |
| 23:4N:242:LEU:HD11 | 23:4N:265:THR:HB | 1.96 | 0.48 |
| 23:4P:193:ARG:NH2 | 41:CN:56:GLY:H | 2.11 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4P:242:LEU:HD11 | 23:4P:265:THR:HB | 1.96 | 0.48 |
| 23:4P:260:THR:HB | 40:EA:219:ILE:HD13 | 1.96 | 0.48 |
| 26:4V:270:SER:OG | 26:4V:312:GLU:OE2 | 2.32 | 0.48 |
| 32:5L:34:LEU:O | 32:5L:38:THR:HG22 | 2.14 | 0.48 |
| 36:5W:74:SER:OG | 36:5W:75:SER:N | 2.47 | 0.48 |
| 36:5W:110:CYS:SG | 36:5W:112:HIS:ND1 | 2.83 | 0.48 |
| 36:5W:116:ARG:HA | 36:5W:146:ARG:HA | 1.95 | 0.48 |
| 38:6C:48:PRO:HB3 | 41:VO:333:VAL:HG23 | 1.96 | 0.48 |
| 40:AF:211:ASP:OD1 | 40:AF:215:ARG:NH1 | 2.47 | 0.48 |
| 40:AG:280:LYS:HG2 | 40:MG:88:HIS:CE1 | 2.49 | 0.48 |
| 40:AH:284:GLU:OE2 | 40:AH:284:GLU:N | 2.46 | 0.48 |
| 41:BB:53:GLU:HG3 | 41:BB:54:ALA:N | 2.27 | 0.48 |
| 40:BH:152:LEU:O | 40:BH:156:ARG:HG2 | 2.13 | 0.48 |
| 40:BH:156:ARG:O | 40:BH:160:ASP:HB3 | 2.14 | 0.48 |
| 41:BM:256:ASN:O | 41:BM:312:THR:HG21 | 2.14 | 0.48 |
| 40:CA:3:GLU:HG3 | 40:CA:129:CYS:HB3 | 1.95 | 0.48 |
| 40:CA:75:ILE:HA | 40:CA:78:VAL:HG23 | 1.96 | 0.48 |
| 40:CH:212:ILE:HA | 40:CH:215:ARG:HD2 | 1.96 | 0.48 |
| 40:CI:108:TYR:O | 40:CI:112:LYS:NZ | 2.40 | 0.48 |
| 41:CN:97:ALA:O | 41:CN:99:ASN:N | 2.47 | 0.48 |
| 41:CP:22:GLU:HA | 41:CP:81:PHE:HD2 | 1.79 | 0.48 |
| 41:CP:134:GLN:HA | 41:CP:165:ASN:O | 2.14 | 0.48 |
| 40:DA:265:ILE:HG23 | 40:DA:431:TYR:CZ | 2.48 | 0.48 |
| 40:DE:90:GLU:HB3 | 40:DE:121:ARG:HD3 | 1.95 | 0.48 |
| 40:DF:252:LEU:HD23 | 40:DF:255:PHE:CE2 | 2.48 | 0.48 |
| 40:DI:327:ASP:O | 40:DI:328:VAL:C | 2.52 | 0.48 |
| 41:DL:7:LEU:CB | 41:DL:135:LEU:HD13 | 2.41 | 0.48 |
| 41:DL:254:ALA:O | 41:DL:257:MET:N | 2.44 | 0.48 |
| 41:DM:147:MET:HG3 | 41:DM:151:LEU:HD23 | 1.95 | 0.48 |
| 41:DN:66:VAL:HG12 | 41:DN:91:VAL:HB | 1.96 | 0.48 |
| 41:DO:178:THR:HB | 41:DO:181:GLU:HB2 | 1.95 | 0.48 |
| 41:DP:375:GLN:HG3 | 41:DP:379:LYS:HD2 | 1.96 | 0.48 |
| 41:EB:113:VAL:HG23 | 41:EB:151:LEU:HD12 | 1.96 | 0.48 |
| 41:EB:180:VAL:O | 41:EB:184:ASN:ND2 | 2.46 | 0.48 |
| 40:EG:376:MET:SD | 40:EG:378:SER:HB3 | 2.53 | 0.48 |
| 40:EH:139:HIS:CE1 | 40:EH:170:SER:HB3 | 2.49 | 0.48 |
| 41:EM:382:SER:O | 41:EM:386:THR:HG23 | 2.13 | 0.48 |
| 41:EP:286:VAL:HG12 | 41:EP:329:GLN:HG3 | 1.95 | 0.48 |
| 40:FA:352:LYS:HD2 | 41:FB:179:VAL:N | 2.29 | 0.48 |
| 41:FO:142:GLY:O | 41:FO:144:GLY:N | 2.47 | 0.48 |
| 40:GA:254:GLU:HG2 | 41:GB:98:GLY:HA2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GH:22:GLU:O | 40:GH:26:LEU:HG | 2.14 | 0.48 |
| 40:GI:207:GLU:HG2 | 40:GI:304:LYS:HG2 | 1.96 | 0.48 |
| 40:GI:326:LYS:HE3 | 40:GI:326:LYS:HB3 | 1.44 | 0.48 |
| 41:GM:107:THR:O | 41:GM:110:ALA:N | 2.34 | 0.48 |
| 41:GP:189:VAL:O | 41:GP:193:VAL:HG23 | 2.14 | 0.48 |
| 40:HE:88:HIS:HB3 | 40:HE:91:GLN:H | 1.79 | 0.48 |
| 40:HE:303:VAL:O | 40:HE:305:CYS:N | 2.47 | 0.48 |
| 40:HE:363:VAL:O | 40:HE:364:PRO:C | 2.52 | 0.48 |
| 40:HH:67:PHE:HB3 | 40:HH:75:ILE:HD12 | 1.96 | 0.48 |
| 41:HM:180:VAL:HG12 | 41:HM:183:TYR:HB2 | 1.95 | 0.48 |
| 40:IF:88:HIS:HB3 | 40:IF:91:GLN:HB2 | 1.94 | 0.48 |
| 40:IH:235:VAL:HA | 40:IH:238:ILE:HG22 | 1.96 | 0.48 |
| 40:II:70:LEU:HD13 | 40:II:114:LEU:HD12 | 1.96 | 0.48 |
| 40:JG:348:PRO:HB2 | 41:JO:384:GLN:HE22 | 1.78 | 0.48 |
| 41:JM:11:GLN:N | 43:JM:501:GDP:O2B | 2.46 | 0.48 |
| 41:JM:61:PRO:HG2 | 41:JM:84:ILE:HG23 | 1.95 | 0.48 |
| 41:JM:389:PHE:HE1 | 41:JM:395:LEU:HD13 | 1.79 | 0.48 |
| 41:JN:178:THR:HB | 41:JN:181:GLU:HG3 | 1.95 | 0.48 |
| 40:KA:271:THR:HG22 | 40:KA:376:MET:HB3 | 1.96 | 0.48 |
| 40:KF:156:ARG:HA | 40:KF:159:VAL:HG22 | 1.94 | 0.48 |
| 41:KO:208:TYR:O | 41:KO:212:PHE:CB | 2.60 | 0.48 |
| 40:LE:217:LEU:HD21 | 40:LE:367:LEU:HD23 | 1.96 | 0.48 |
| 40:LF:104:ALA:CB | 40:LF:410:GLU:HG2 | 2.43 | 0.48 |
| 40:LF:105:ARG:HA | 40:LF:109:THR:OG1 | 2.14 | 0.48 |
| 40:LG:51:THR:HG21 | 40:LG:243:ARG:CG | 2.43 | 0.48 |
| 41:LM:21:TRP:HA | 41:LM:24:ILE:HG22 | 1.95 | 0.48 |
| 40:MD:53:PHE:HB3 | 40:MD:61:HIS:HB3 | 1.94 | 0.48 |
| 40:MH:303:VAL:HG12 | 40:MH:305:CYS:HB3 | 1.95 | 0.48 |
| 41:ML:107:THR:HG22 | 41:ML:108:GLU:H | 1.79 | 0.48 |
| 40:ND:52:PHE:HE1 | 40:ND:239:THR:HG21 | 1.77 | 0.48 |
| 40:ND:261:PRO:HD2 | 40:ND:265:ILE:O | 2.13 | 0.48 |
| 40:NE:90:GLU:HG3 | 40:NE:121:ARG:HH22 | 1.79 | 0.48 |
| 40:NG:298:PRO:HB3 | 40:NG:307:PRO:HD2 | 1.96 | 0.48 |
| 41:NM:54:ALA:HB3 | 41:NM:58:LYS:O | 2.13 | 0.48 |
| 40:OA:154:MET:HE2 | 40:OA:194:THR:HG22 | 1.96 | 0.48 |
| 41:OB:260:PHE:HE1 | 40:OG:402:ALA:HA | 1.78 | 0.48 |
| 40:OD:255:PHE:O | 40:OD:259:LEU:HB2 | 2.14 | 0.48 |
| 40:OH:10:GLY:H | 40:OH:69:ASP:HB2 | 1.79 | 0.48 |
| 40:OH:406:TRP:HE1 | 41:OO:258:VAL:CG2 | 2.27 | 0.48 |
| 41:OM:171:PRO:HB3 | 41:OM:181:GLU:HG2 | 1.95 | 0.48 |
| 41:OP:137:HIS:O | 41:OP:168:SER:HA | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OP:333:VAL:HA | 41:OP:336:LYS:HG2 | 1.95 | 0.48 |
| 40:QE:179:THR:OG1 | 40:QE:183:GLU:OE2 | 2.31 | 0.48 |
| 40:QE:188:ILE:HD12 | 40:QE:424:MET:HG3 | 1.95 | 0.48 |
| 40:QF:209:ILE:HB | 40:QF:227:LEU:HD22 | 1.95 | 0.48 |
| 41:QM:313:VAL:O | 41:QM:349:VAL:HA | 2.13 | 0.48 |
| 41:QO:271:ALA:O | 41:QO:292:GLN:NE2 | 2.47 | 0.48 |
| 41:QP:142:GLY:O | 41:QP:143:THR:C | 2.51 | 0.48 |
| 41:QP:314:ALA:HA | 41:QP:349:VAL:HA | 1.95 | 0.48 |
| 41:RB:222:TYR:O | 41:RB:226:ASN:ND2 | 2.47 | 0.48 |
| 40:RF:2:ARG:HH22 | 40:RF:48:SER:HA | 1.79 | 0.48 |
| 40:RG:145:THR:OG1 | 40:RG:146:GLY:N | 2.46 | 0.48 |
| 41:RL:209:ASP:O | 41:RL:213:ARG:NH1 | 2.47 | 0.48 |
| 41:RL:308:GLY:HA3 | 41:RL:373:ALA:HB2 | 1.96 | 0.48 |
| 40:SA:6:SER:O | 40:SA:65:ALA:HA | 2.13 | 0.48 |
| 41:SB:105:HIS:HA | 41:SB:150:LEU:HD13 | 1.96 | 0.48 |
| 40:SE:6:SER:O | 40:SE:65:ALA:HA | 2.14 | 0.48 |
| 41:SN:309:ARG:NH1 | 41:SN:339:SER:O | 2.46 | 0.48 |
| 41:SO:271:ALA:HB2 | 41:SO:365:ALA:HB3 | 1.96 | 0.48 |
| 41:SP:103:LYS:HG2 | 41:SP:107:THR:HG21 | 1.95 | 0.48 |
| 40:TH:177:VAL:HB | 41:TO:331:LEU:HD12 | 1.96 | 0.48 |
| 41:TN:139:LEU:HG | 41:TN:168:SER:HB3 | 1.95 | 0.48 |
| 40:UA:271:THR:HG22 | 40:UA:301:GLN:HA | 1.94 | 0.48 |
| 41:UB:183:TYR:OH | 41:UB:393:ALA:O | 2.22 | 0.48 |
| 40:UF:287:SER:O | 40:UF:288:VAL:C | 2.52 | 0.48 |
| 40:UF:402:ALA:O | 40:UF:403:PHE:C | 2.52 | 0.48 |
| 40:UG:196:GLU:N | 40:UG:196:GLU:OE2 | 2.42 | 0.48 |
| 40:UG:386:ALA:HA | 40:UG:389:ARG:HE | 1.79 | 0.48 |
| 40:UH:91:GLN:HE21 | 40:UH:125:LEU:HD21 | 1.79 | 0.48 |
| 40:UH:133:GLN:N | 40:UH:133:GLN:OE1 | 2.47 | 0.48 |
| 40:UH:315:CYS:HA | 40:UH:377:LEU:O | 2.14 | 0.48 |
| 40:UI:10:GLY:O | 40:UI:11:GLN:C | 2.51 | 0.48 |
| 41:UO:21:TRP:HZ2 | 41:UO:63:ALA:HB2 | 1.79 | 0.48 |
| 40:VA:332:ILE:HG23 | 40:VA:351:PHE:HD2 | 1.79 | 0.48 |
| 40:VF:39:ASP:HB2 | 40:VF:42:ILE:HD12 | 1.96 | 0.48 |
| 40:VG:96:LYS:HD3 | 41:VN:129:CYS:HB2 | 1.95 | 0.48 |
| 40:VJ:212:ILE:HD11 | 40:VJ:300:ASN:HA | 1.94 | 0.48 |
| 41:VO:107:THR:HG22 | 41:VO:108:GLU:H | 1.79 | 0.48 |
| 41:VQ:383:GLU:HA | 41:VQ:386:THR:HG22 | 1.95 | 0.48 |
| 40:WH:20:CYS:HA | 40:WH:232:SER:HB2 | 1.95 | 0.48 |
| 40:WH:185:TYR:HE1 | 40:WH:403:PHE:HB2 | 1.79 | 0.48 |
| 40:WH:241:SER:OG | 40:WH:249:ASN:OD1 | 2.32 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WN:371:SER:C | 41:WN:373:ALA:H | 2.17 | 0.48 |
| 41:WP:375:GLN:HE21 | 41:WP:423:VAL:HB | 1.79 | 0.48 |
| 7:1T:140:TRP:HA | 7:1T:147:ALA:HA | 1.95 | 0.48 |
| 10:2G:94:LEU:HG | 40:MH:116:ASP:HB3 | 1.95 | 0.48 |
| 11:2K:186:LYS:HA | 11:2K:186:LYS:HD3 | 1.51 | 0.48 |
| 13:2U:24:ILE:O | 13:2U:63:ALA:HB2 | 2.14 | 0.48 |
| 13:2X:97:LYS:O | 13:2X:98:ASN:C | 2.52 | 0.48 |
| 14:3A:48:HIS:HA | 40:MF:433:GLU:CD | 2.34 | 0.48 |
| 16:3J:325:PRO:HG3 | 16:3L:181:GLU:OE2 | 2.13 | 0.48 |
| 16:3L:243:ILE:O | 16:3L:247:ILE:HD12 | 2.12 | 0.48 |
| 17:3Q:419:ARG:HA | 17:3Q:419:ARG:HD3 | 1.55 | 0.48 |
| 21:4E:248:ILE:HG22 | 21:4E:261:THR:HG22 | 1.95 | 0.48 |
| 21:4F:34:ARG:O | 21:4F:36:GLY:N | 2.44 | 0.48 |
| 22:4H:161:TYR:CE1 | 41:AL:80:PRO:HB3 | 2.49 | 0.48 |
| 22:4J:75:ASP:O | 22:4J:77:GLN:N | 2.47 | 0.48 |
| 22:4J:649:LYS:O | 22:4J:651:LYS:N | 2.47 | 0.48 |
| 22:4K:486:VAL:O | 22:4K:503:LYS:NZ | 2.41 | 0.48 |
| 24:4O:205:LEU:O | 24:4O:206:SER:C | 2.51 | 0.48 |
| 23:4Q:259:ARG:CZ | 40:EH:366:ASP:H | 2.27 | 0.48 |
| 26:4V:210:SER:OG | 26:4V:213:CYS:SG | 2.62 | 0.48 |
| 26:4W:91:LYS:HD2 | 26:4W:164:LEU:HD13 | 1.95 | 0.48 |
| 39:6L:147:LEU:HD13 | 39:6L:150:MET:HG2 | 1.95 | 0.48 |
| 40:AH:283:HIS:HB3 | 40:MH:88:HIS:HB2 | 1.94 | 0.48 |
| 41:BL:142:GLY:O | 41:BL:144:GLY:N | 2.46 | 0.48 |
| 40:CE:2:ARG:HB3 | 40:CE:242:LEU:HD22 | 1.96 | 0.48 |
| 41:CL:376:GLU:HA | 41:CL:379:LYS:HB2 | 1.96 | 0.48 |
| 41:CM:107:THR:OG1 | 41:CM:108:GLU:N | 2.47 | 0.48 |
| 41:CM:287:PRO:HA | 41:CM:329:GLN:HG2 | 1.95 | 0.48 |
| 41:CN:7:LEU:HB2 | 41:CN:135:LEU:HB2 | 1.95 | 0.48 |
| 41:CN:11:GLN:N | 43:CN:501:GDP:O2B | 2.45 | 0.48 |
| 41:CO:3:GLU:OE2 | 41:CO:48:ASN:HB2 | 2.14 | 0.48 |
| 41:CO:69:GLU:HB2 | 41:CO:96:GLY:HA2 | 1.95 | 0.48 |
| 41:CO:393:ALA:O | 41:CO:394:PHE:C | 2.51 | 0.48 |
| 41:CP:8:GLN:HG2 | 41:CP:14:ASN:HA | 1.96 | 0.48 |
| 41:CP:226:ASN:CG | 43:CP:501:GDP:HN1 | 2.17 | 0.48 |
| 40:DA:106:GLY:HA2 | 40:DA:110:ILE:O | 2.14 | 0.48 |
| 40:DA:311:LYS:H | 40:DA:381:THR:HG22 | 1.79 | 0.48 |
| 41:DB:103:LYS:HA | 41:DB:108:GLU:HB2 | 1.96 | 0.48 |
| 41:DB:153:SER:O | 41:DB:157:GLU:HG2 | 2.13 | 0.48 |
| 41:DB:305:PRO:O | 41:DB:306:ARG:C | 2.52 | 0.48 |
| 40:DF:333:ALA:HB2 | 41:DN:175:VAL:CG1 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DH:96:LYS:HB3 | 40:DH:96:LYS:HE3 | 1.39 | 0.48 |
| 40:DI:143:GLY:O | 40:DI:144:GLY:C | 2.51 | 0.48 |
| 40:DI:210:TYR:CG | 41:DP:324:LYS:HD3 | 2.49 | 0.48 |
| 41:DL:3:GLU:CB | 41:DL:130:LEU:HA | 2.44 | 0.48 |
| 41:DL:152:ILE:O | 41:DL:155:ILE:HG12 | 2.14 | 0.48 |
| 41:DL:331:LEU:HD22 | 41:DL:331:LEU:HA | 1.71 | 0.48 |
| 41:DM:42:LEU:HD12 | 41:DM:43:GLN:HG2 | 1.95 | 0.48 |
| 41:DM:82:GLY:O | 41:DM:84:ILE:N | 2.45 | 0.48 |
| 41:DM:87:PRO:HA | 41:DM:90:PHE:CZ | 2.48 | 0.48 |
| 41:DM:112:LEU:HG | 41:DM:147:MET:HE1 | 1.96 | 0.48 |
| 41:DN:98:GLY:O | 41:DN:99:ASN:C | 2.52 | 0.48 |
| 41:DN:123:GLU:O | 41:DN:126:SER:N | 2.43 | 0.48 |
| 41:DN:257:MET:HA | 41:DN:312:THR:CB | 2.44 | 0.48 |
| 41:DP:358:PRO:HG2 | 41:DP:361:LEU:HB2 | 1.96 | 0.48 |
| 40:EE:217:LEU:HD11 | 40:EE:230:LEU:HD21 | 1.96 | 0.48 |
| 40:EE:288:VAL:HA | 40:EE:291:ILE:HG12 | 1.96 | 0.48 |
| 40:EH:258:ASN:HD21 | 41:EP:179:VAL:H | 1.62 | 0.48 |
| 40:EH:402:ALA:HB2 | 41:EO:344:TRP:CZ3 | 2.49 | 0.48 |
| 41:EM:311:LEU:HD12 | 41:EM:342:VAL:HG11 | 1.95 | 0.48 |
| 40:FA:278:ALA:H | 40:FA:368:ALA:HB2 | 1.79 | 0.48 |
| 40:FH:395:ASP:OD1 | 40:FH:421:ARG:NH1 | 2.47 | 0.48 |
| 41:FM:171:PRO:HG3 | 41:FM:185:ALA:HB2 | 1.95 | 0.48 |
| 40:GE:37:PRO:O | 40:GE:38:SER:C | 2.50 | 0.48 |
| 40:GE:141:PHE:HB3 | 40:GE:173:PRO:HD3 | 1.95 | 0.48 |
| 40:GF:105:ARG:NH1 | 40:GF:410:GLU:OE2 | 2.47 | 0.48 |
| 40:GH:228:ASN:CG | 42:GH:501:GTP:HN21 | 2.15 | 0.48 |
| 40:HA:269:LEU:HD21 | 40:HA:301:GLN:HB2 | 1.94 | 0.48 |
| 41:HB:331:LEU:HD22 | 40:HG:177:VAL:HG22 | 1.95 | 0.48 |
| 41:HM:142:GLY:O | 41:HM:144:GLY:N | 2.47 | 0.48 |
| 41:HN:371:SER:C | 41:HN:373:ALA:H | 2.16 | 0.48 |
| 41:HO:309:ARG:HD3 | 41:HO:342:VAL:HA | 1.95 | 0.48 |
| 40:IA:105:ARG:CZ | 41:IN:251:ARG:HH22 | 2.27 | 0.48 |
| 41:IB:113:VAL:HG21 | 41:IB:150:LEU:HD23 | 1.94 | 0.48 |
| 40:IF:115:ILE:HA | 40:IF:118:VAL:HG12 | 1.96 | 0.48 |
| 41:IN:326:VAL:O | 41:IN:330:MET:HG2 | 2.14 | 0.48 |
| 40:JD:150:THR:O | 40:JD:154:MET:HG2 | 2.14 | 0.48 |
| 41:KB:7:LEU:O | 41:KB:135:LEU:HA | 2.14 | 0.48 |
| 41:KB:200:TYR:HE2 | 41:KB:236:VAL:HG21 | 1.78 | 0.48 |
| 40:LH:174:ALA:HB3 | 40:LH:178:SER:H | 1.79 | 0.48 |
| 40:LH:270:ALA:HA | 40:LH:376:MET:O | 2.14 | 0.48 |
| 41:LM:245:GLN:HG3 | 41:LM:323:MET:HE2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:ME:177:VAL:HA | 41:ML:331:LEU:HD12 | 1.95 | 0.48 |
| 40:ME:277:SER:O | 40:ME:279:GLU:N | 2.47 | 0.48 |
| 41:MO:27:GLU:HA | 41:MO:359:ARG:HD2 | 1.95 | 0.48 |
| 41:MO:243:PRO:HD2 | 41:MO:356:ILE:HD13 | 1.96 | 0.48 |
| 40:NA:73:THR:HG23 | 41:NN:46:ARG:HH12 | 1.79 | 0.48 |
| 40:ND:273:ALA:HB3 | 40:ND:374:VAL:H | 1.79 | 0.48 |
| 40:ND:348:PRO:HB2 | 41:NL:384:GLN:OE1 | 2.14 | 0.48 |
| 40:NE:2:ARG:NH2 | 41:NM:71:GLY:HA3 | 2.29 | 0.48 |
| 41:NP:304:ASP:OD1 | 41:NP:307:HIS:ND1 | 2.47 | 0.48 |
| 40:OE:138:PHE:HZ | 40:OE:235:VAL:HG21 | 1.78 | 0.48 |
| 40:OF:76:ASP:HA | 40:OF:79:ARG:HG2 | 1.94 | 0.48 |
| 40:OH:12:ALA:HA | 42:OO:501:GTP:C5 | 2.49 | 0.48 |
| 41:ON:142:GLY:O | 41:ON:144:GLY:N | 2.47 | 0.48 |
| 41:PB:323:MET:HA | 41:PB:326:VAL:HB | 1.96 | 0.48 |
| 41:QB:262:ARG:O | 41:QB:263:LEU:C | 2.52 | 0.48 |
| 40:QE:3:GLU:HA | 40:QE:51:THR:HA | 1.94 | 0.48 |
| 40:QF:319:TYR:HB3 | 40:QF:323:VAL:HG11 | 1.95 | 0.48 |
| 40:QG:116:ASP:OD1 | 40:QG:116:ASP:N | 2.47 | 0.48 |
| 41:QM:116:VAL:HA | 41:QM:119:VAL:HG22 | 1.96 | 0.48 |
| 41:QO:117:LEU:HD11 | 41:QO:154:LYS:HG2 | 1.96 | 0.48 |
| 41:QO:260:PHE:HD2 | 41:QO:263:LEU:HD12 | 1.79 | 0.48 |
| 40:RA:260:VAL:HB | 41:RB:397:TRP:HH2 | 1.79 | 0.48 |
| 40:RF:88:HIS:HD2 | 40:SF:283:HIS:HB3 | 1.79 | 0.48 |
| 40:RH:101:ASN:O | 40:RH:186:ASN:ND2 | 2.30 | 0.48 |
| 40:SA:228:ASN:HB3 | 40:SA:231:ILE:HD12 | 1.96 | 0.48 |
| 40:SF:178:SER:OG | 40:SF:179:THR:N | 2.46 | 0.48 |
| 40:SH:234:ILE:HG13 | 40:SH:272:TYR:HB2 | 1.95 | 0.48 |
| 40:SI:20:CYS:HA | 40:SI:232:SER:HB2 | 1.96 | 0.48 |
| 41:SO:36:TYR:OH | 41:SO:43:GLN:HB2 | 2.13 | 0.48 |
| 41:SO:64:VAL:O | 41:SO:66:VAL:HG23 | 2.14 | 0.48 |
| 40:TF:7:VAL:O | 40:TF:137:ILE:HA | 2.13 | 0.48 |
| 40:TH:274:PRO:HB3 | 40:TH:370:VAL:HG21 | 1.96 | 0.48 |
| 40:TH:349:THR:HB | 41:TP:176:SER:HB3 | 1.95 | 0.48 |
| 41:TN:282:ARG:HD3 | 41:TN:283:ALA:H | 1.79 | 0.48 |
| 40:UF:337:THR:OG1 | 40:UF:338:LYS:N | 2.47 | 0.48 |
| 41:UN:125:GLU:OE1 | 41:UN:159:TYR:OH | 2.26 | 0.48 |
| 41:UO:130:LEU:HG | 41:UO:162:ARG:HD2 | 1.96 | 0.48 |
| 40:VG:349:THR:HG1 | 41:VO:176:SER:HG | 1.54 | 0.48 |
| 41:VQ:287:PRO:HG3 | 41:VQ:329:GLN:HE22 | 1.78 | 0.48 |
| 40:WF:117:LEU:O | 40:WF:121:ARG:HG2 | 2.13 | 0.48 |
| 40:WI:180:ALA:HB3 | 40:WI:183:GLU:HG2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WM:299:MET:O | 41:WM:301:ALA:N | 2.46 | 0.48 |
| 10:2F:86:THR:HB | 40:AA:176:GLN:HG3 | 1.95 | 0.48 |
| 12:2M:76:TYR:OH | 40:WG:127:ASP:OD2 | 2.31 | 0.48 |
| 13:2W:77:VAL:HG22 | 13:2W:133:GLN:HG3 | 1.95 | 0.48 |
| 17:3P:359:ASN:O | 17:3P:363:ILE:HG12 | 2.14 | 0.48 |
| 21:4D:34:ARG:HD2 | 21:4D:39:VAL:HG13 | 1.95 | 0.48 |
| 21:4D:472:VAL:O | 21:4D:484:TYR:HA | 2.14 | 0.48 |
| 22:4J:48:LEU:H | 22:4J:51:GLN:HE21 | 1.62 | 0.48 |
| 23:4N:218:SER:O | 23:4N:219:GLN:C | 2.52 | 0.48 |
| 23:4Q:240:LEU:HB2 | 23:4Q:262:GLY:HA2 | 1.95 | 0.48 |
| 26:4W:97:LEU:HD12 | 26:4W:158:ILE:HD12 | 1.95 | 0.48 |
| 33:5O:134:ASN:HA | 33:5O:137:ARG:HG3 | 1.96 | 0.48 |
| 35:5T:162:MET:HE2 | 41:KL:320:ARG:HG3 | 1.96 | 0.48 |
| 40:BA:274:PRO:HD3 | 40:BA:291:ILE:HD12 | 1.96 | 0.48 |
| 40:BH:161:TYR:O | 40:BH:162:GLY:C | 2.52 | 0.48 |
| 41:BN:170:VAL:HG11 | 41:BN:377:LEU:HD21 | 1.96 | 0.48 |
| 41:BN:292:GLN:HG2 | 41:BN:298:ASN:HD21 | 1.79 | 0.48 |
| 41:BP:33:THR:OG1 | 41:BP:34:GLY:N | 2.47 | 0.48 |
| 40:CE:405:HIS:HA | 40:CE:408:VAL:HG12 | 1.94 | 0.48 |
| 40:CH:435:GLY:O | 40:CH:436:MET:C | 2.52 | 0.48 |
| 40:CI:317:LEU:HD23 | 40:CI:376:MET:HB2 | 1.95 | 0.48 |
| 41:CL:7:LEU:CB | 41:CL:135:LEU:HD13 | 2.42 | 0.48 |
| 41:CM:33:THR:OG1 | 41:CM:34:GLY:N | 2.45 | 0.48 |
| 41:CM:162:ARG:HA | 41:CM:162:ARG:HD3 | 1.53 | 0.48 |
| 41:CO:333:VAL:HG13 | 41:CO:337:ASN:HD21 | 1.78 | 0.48 |
| 40:DA:213:CYS:O | 40:DA:214:ARG:C | 2.52 | 0.48 |
| 40:DE:104:ALA:C | 40:DE:106:GLY:N | 2.67 | 0.48 |
| 40:DE:106:GLY:CA | 40:DE:148:GLY:CA | 2.78 | 0.48 |
| 40:DE:363:VAL:O | 40:DE:365:GLY:N | 2.47 | 0.48 |
| 40:DF:305:CYS:O | 40:DF:306:ASP:C | 2.52 | 0.48 |
| 40:DI:208:ALA:HB2 | 40:DI:304:LYS:H | 1.78 | 0.48 |
| 41:DL:11:GLN:O | 41:DL:12:CYS:C | 2.52 | 0.48 |
| 41:DO:375:GLN:NE2 | 41:DO:379:LYS:HB3 | 2.29 | 0.48 |
| 41:DP:73:MET:HG3 | 41:DP:90:PHE:HD1 | 1.77 | 0.48 |
| 40:EA:217:LEU:HG | 40:EA:275:VAL:HG12 | 1.96 | 0.48 |
| 40:EG:2:ARG:HH22 | 40:EG:249:ASN:ND2 | 2.12 | 0.48 |
| 40:EH:287:SER:O | 40:EH:291:ILE:HG23 | 2.13 | 0.48 |
| 40:EI:224:TYR:H | 41:EP:323:MET:HG2 | 1.79 | 0.48 |
| 40:EI:317:LEU:HD13 | 40:EI:376:MET:HB2 | 1.95 | 0.48 |
| 41:EL:152:ILE:HG22 | 41:EL:156:ARG:HH11 | 1.78 | 0.48 |
| 41:EN:203:ASP:N | 41:EN:300:MET:O | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EO:207:LEU:HB3 | 41:EO:225:LEU:HD22 | 1.95 | 0.48 |
| 40:FA:219:ILE:HB | 40:FA:222:PRO:CG | 2.44 | 0.48 |
| 41:FB:247:ASN:OD1 | 40:FG:11:GLN:NE2 | 2.47 | 0.48 |
| 40:FH:141:PHE:HB2 | 40:FH:173:PRO:HD3 | 1.95 | 0.48 |
| 41:FN:7:LEU:O | 41:FN:135:LEU:HA | 2.14 | 0.48 |
| 40:GA:326:LYS:HE3 | 41:GB:208:TYR:HB2 | 1.96 | 0.48 |
| 40:GE:363:VAL:O | 40:GE:365:GLY:N | 2.47 | 0.48 |
| 40:GG:259:LEU:O | 40:GG:379:ASN:ND2 | 2.38 | 0.48 |
| 41:GO:132:GLY:HA2 | 41:GO:163:ILE:O | 2.14 | 0.48 |
| 40:HH:167:LEU:HD23 | 40:HH:202:PHE:HE2 | 1.78 | 0.48 |
| 41:HN:256:ASN:HB2 | 41:HN:350:LYS:HE3 | 1.96 | 0.48 |
| 41:HO:248:ALA:HA | 41:HO:252:LYS:HD3 | 1.95 | 0.48 |
| 40:IA:132:LEU:HD21 | 40:IA:135:PHE:HE2 | 1.79 | 0.48 |
| 41:IB:271:ALA:HB3 | 41:IB:293:MET:HG2 | 1.96 | 0.48 |
| 40:IF:199:ASP:HB3 | 40:IF:256:GLN:HG3 | 1.95 | 0.48 |
| 40:IG:167:LEU:HG | 40:IG:200:CYS:HB3 | 1.95 | 0.48 |
| 40:IG:172:TYR:N | 40:IG:204:VAL:O | 2.41 | 0.48 |
| 41:IN:230:SER:HA | 41:IN:233:MET:HB2 | 1.95 | 0.48 |
| 40:JA:56:THR:HA | 40:KA:285:GLN:HG2 | 1.96 | 0.48 |
| 40:JE:190:THR:HA | 40:JE:193:THR:HG22 | 1.95 | 0.48 |
| 41:JM:271:ALA:HB3 | 41:JM:272:PRO:HD3 | 1.96 | 0.48 |
| 41:JO:6:HIS:O | 41:JO:63:ALA:HA | 2.13 | 0.48 |
| 40:KA:270:ALA:HA | 40:KA:376:MET:O | 2.14 | 0.48 |
| 42:KB:502:GTP:HN1 | 40:KG:228:ASN:ND2 | 2.08 | 0.48 |
| 40:KF:73:THR:HA | 40:KF:76:ASP:HB2 | 1.94 | 0.48 |
| 41:KL:7:LEU:O | 41:KL:135:LEU:HA | 2.14 | 0.48 |
| 41:KL:16:ILE:HG13 | 41:KL:229:VAL:CG1 | 2.43 | 0.48 |
| 41:KN:170:VAL:HG11 | 41:KN:377:LEU:HD11 | 1.96 | 0.48 |
| 41:KN:215:LEU:HD11 | 41:KN:228:LEU:HD11 | 1.96 | 0.48 |
| 40:LD:150:THR:O | 40:LD:154:MET:HG2 | 2.14 | 0.48 |
| 40:LE:136:LEU:HD23 | 40:LE:167:LEU:HB2 | 1.96 | 0.48 |
| 40:LE:318:LEU:O | 40:LE:374:VAL:HA | 2.14 | 0.48 |
| 40:LG:261:PRO:HG3 | 40:LG:313:MET:CE | 2.44 | 0.48 |
| 40:LH:294:ALA:O | 40:LH:300:ASN:ND2 | 2.44 | 0.48 |
| 41:LM:307:HIS:ND1 | 41:LM:376:GLU:OE2 | 2.44 | 0.48 |
| 41:LN:54:ALA:HA | 41:MN:283:ALA:HB2 | 1.95 | 0.48 |
| 41:LP:61:PRO:HD3 | 41:LP:84:ILE:HG12 | 1.95 | 0.48 |
| 41:LP:237:THR:HG22 | 41:LP:250:LEU:HD21 | 1.96 | 0.48 |
| 41:MB:255:VAL:HG23 | 40:MG:406:TRP:CG | 2.49 | 0.48 |
| 41:MB:311:LEU:HD23 | 41:MB:342:VAL:HG11 | 1.96 | 0.48 |
| 40:ME:2:ARG:NE | 40:ME:242:LEU:O | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:ML:142:GLY:O | 41:ML:144:GLY:N | 2.46 | 0.48 |
| 41:NB:252:LYS:O | 41:NB:256:ASN:ND2 | 2.43 | 0.48 |
| 40:ND:348:PRO:HD2 | 41:NL:388:MET:HG3 | 1.96 | 0.48 |
| 41:NN:100:ASN:HB3 | 41:NN:103:LYS:HB3 | 1.96 | 0.48 |
| 40:OA:393:LYS:HG3 | 41:ON:346:PRO:HG2 | 1.94 | 0.48 |
| 42:OB:502:GTP:HN1 | 40:OG:228:ASN:ND2 | 2.07 | 0.48 |
| 40:OG:76:ASP:HA | 40:OG:79:ARG:HG2 | 1.95 | 0.48 |
| 40:OH:398:TYR:O | 40:OH:399:ALA:C | 2.52 | 0.48 |
| 40:PD:225:THR:O | 40:PD:229:ARG:HG3 | 2.13 | 0.48 |
| 40:PF:72:PRO:HG2 | 41:PM:2:ARG:NH1 | 2.28 | 0.48 |
| 41:PL:19:LYS:NZ | 41:PL:223:GLY:O | 2.47 | 0.48 |
| 41:PL:202:ILE:HG21 | 41:PL:229:VAL:HG22 | 1.96 | 0.48 |
| 41:PP:22:GLU:HG3 | 41:PP:81:PHE:CD1 | 2.49 | 0.48 |
| 41:QB:66:VAL:HB | 41:QB:91:VAL:CG2 | 2.44 | 0.48 |
| 41:QB:81:PHE:O | 41:QB:82:GLY:C | 2.52 | 0.48 |
| 41:QB:124:ALA:HB1 | 41:QB:130:LEU:HD22 | 1.95 | 0.48 |
| 41:QB:183:TYR:CE2 | 41:QB:388:MET:HB3 | 2.49 | 0.48 |
| 41:QL:348:ASN:C | 41:QL:348:ASN:HD22 | 2.18 | 0.48 |
| 41:QN:193:VAL:HG22 | 41:QN:418:LEU:HD22 | 1.96 | 0.48 |
| 41:QO:217:LEU:HB3 | 41:QO:220:PRO:HD3 | 1.96 | 0.48 |
| 40:RH:405:HIS:CD2 | 41:RO:261:PRO:HG3 | 2.49 | 0.48 |
| 40:RI:76:ASP:HA | 40:RI:79:ARG:HG2 | 1.95 | 0.48 |
| 41:SB:322:SER:HB2 | 40:SG:223:THR:HG22 | 1.95 | 0.48 |
| 40:SE:141:PHE:HB2 | 40:SE:173:PRO:HD3 | 1.95 | 0.48 |
| 40:SG:187:SER:O | 40:SG:191:THR:OG1 | 2.24 | 0.48 |
| 40:SH:127:ASP:OD1 | 40:TH:293:ASN:ND2 | 2.47 | 0.48 |
| 41:SO:226:ASN:CB | 43:SO:501:GDP:HN1 | 2.27 | 0.48 |
| 40:TE:257:THR:HA | 41:TM:397:TRP:CH2 | 2.49 | 0.48 |
| 40:TG:404:VAL:HG23 | 40:TG:417:PHE:HE2 | 1.79 | 0.48 |
| 41:TL:4:ILE:HA | 41:TL:132:GLY:O | 2.13 | 0.48 |
| 41:TP:341:PHE:HB3 | 41:TP:348:ASN:HD21 | 1.79 | 0.48 |
| 41:TP:424:THR:OG1 | 41:TP:425:ARG:NH1 | 2.46 | 0.48 |
| 41:UB:107:THR:O | 41:UB:110:ALA:N | 2.47 | 0.48 |
| 40:UE:319:TYR:HB3 | 40:UE:323:VAL:HG11 | 1.96 | 0.48 |
| 40:UF:221:ARG:HB2 | 41:UM:322:SER:HB3 | 1.95 | 0.48 |
| 40:UG:274:PRO:HB3 | 40:UG:370:VAL:HG11 | 1.96 | 0.48 |
| 41:UO:316:VAL:HG12 | 41:UO:352:ALA:HB3 | 1.94 | 0.48 |
| 41:UP:142:GLY:O | 41:UP:144:GLY:N | 2.47 | 0.48 |
| 41:VB:43:GLN:HA | 41:VB:242:PHE:HE2 | 1.79 | 0.48 |
| 40:VF:70:LEU:HD13 | 40:VF:114:LEU:HD12 | 1.94 | 0.48 |
| 40:VJ:11:GLN:HG3 | 40:VJ:74:VAL:HG11 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:WA:171:ILE:HG21 | 42:WA:501:GTP:H1' | 1.95 | 0.48 |
| 40:WA:349:THR:OG1 | 41:WB:176:SER:OG | 2.20 | 0.48 |
| 40:WI:316:CYS:SG | 40:WI:377:LEU:HB2 | 2.54 | 0.48 |
| 41:WM:297:LYS:C | 41:WM:299:MET:H | 2.17 | 0.48 |
| 41:WN:362:LYS:HA | 41:WN:362:LYS:HD3 | 1.65 | 0.48 |
| 7:1T:264:LEU:HB3 | 7:1T:276:CYS:SG | 2.54 | 0.47 |
| 7:1T:523:ASP:O | 7:1T:524:ARG:C | 2.52 | 0.47 |
| 11:2I:87:PRO:HD3 | 40:LA:264:ARG:HD2 | 1.96 | 0.47 |
| 13:2T:85:LYS:HB2 | 13:2T:85:LYS:HE2 | 1.53 | 0.47 |
| 13:2U:92:GLN:HB3 | 13:2U:152:LEU:HG | 1.95 | 0.47 |
| 13:2W:144:TYR:O | 13:2W:146:THR:N | 2.47 | 0.47 |
| 13:2X:96:ASP:HA | 13:2X:149:ILE:HD11 | 1.96 | 0.47 |
| 13:2X:137:SER:O | 13:2X:140:THR:HG22 | 2.13 | 0.47 |
| 14:3B:94:LYS:HA | 14:3B:97:GLN:HG3 | 1.95 | 0.47 |
| 16:3L:99:ALA:HB2 | 16:3L:247:ILE:HD11 | 1.96 | 0.47 |
| 17:3R:229:CYS:O | 17:3R:232:ARG:HG2 | 2.14 | 0.47 |
| 20:4A:21:ASN:HA | 20:4A:24:LYS:HD2 | 1.96 | 0.47 |
| 22:4I:137:SER:HA | 22:4I:146:PHE:HA | 1.96 | 0.47 |
| 22:4J:91:ASP:C | 41:BN:280:GLN:H | 2.18 | 0.47 |
| 23:4M:245:LYS:HE3 | 40:DG:79:ARG:HH22 | 1.79 | 0.47 |
| 24:4O:259:ARG:HD3 | 40:EE:365:GLY:HA2 | 1.96 | 0.47 |
| 23:4R:30:ARG:HH21 | 41:BP:53:GLU:HG3 | 1.79 | 0.47 |
| 35:5T:160:GLU:HG2 | 35:5T:161:SER:H | 1.79 | 0.47 |
| 37:6A:57:ASP:OD1 | 37:6A:58:ASN:ND2 | 2.47 | 0.47 |
| 39:6G:105:LEU:HD13 | 39:6G:146:VAL:HG22 | 1.96 | 0.47 |
| 40:AA:7:VAL:HG11 | 40:AA:153:LEU:HD21 | 1.96 | 0.47 |
| 40:AA:259:LEU:HD13 | 40:AA:316:CYS:HB2 | 1.96 | 0.47 |
| 40:AE:11:GLN:N | 42:AE:501:GTP:O1B | 2.43 | 0.47 |
| 41:AL:67:ASP:OD1 | 41:AL:68:LEU:N | 2.47 | 0.47 |
| 41:AL:142:GLY:O | 41:AL:144:GLY:N | 2.47 | 0.47 |
| 40:BA:98:ASP:OD1 | 40:BA:99:ALA:N | 2.47 | 0.47 |
| 40:BA:102:ASN:HB3 | 40:BA:105:ARG:H | 1.79 | 0.47 |
| 41:BB:337:ASN:N | 41:BB:337:ASN:OD1 | 2.47 | 0.47 |
| 41:BL:89:ASN:ND2 | 41:BL:123:GLU:OE2 | 2.44 | 0.47 |
| 41:BL:143:THR:OG1 | 43:BL:502:GDP:O1B | 2.31 | 0.47 |
| 40:CA:160:ASP:O | 40:CA:161:TYR:C | 2.52 | 0.47 |
| 41:CB:67:ASP:HA | 41:CB:143:THR:HG21 | 1.96 | 0.47 |
| 41:CB:268:PRO:HG2 | 41:CB:300:MET:HB2 | 1.96 | 0.47 |
| 40:CF:360:PRO:HG3 | 40:CF:373:ALA:HB2 | 1.96 | 0.47 |
| 41:CO:238:THR:HA | 41:CO:241:ARG:HH21 | 1.79 | 0.47 |
| 41:CO:272:PRO:HB2 | 41:CO:361:LEU:CD1 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CP:124:ALA:O | 41:CP:125:GLU:C | 2.52 | 0.47 |
| 41:CP:355:ASP:O | 41:CP:356:ILE:C | 2.52 | 0.47 |
| 40:DA:183:GLU:HB3 | 40:DA:184:PRO:HD3 | 1.96 | 0.47 |
| 41:DB:102:ALA:HB1 | 41:DB:401:GLU:HB3 | 1.96 | 0.47 |
| 40:DF:2:ARG:HB3 | 40:DF:133:GLN:NE2 | 2.29 | 0.47 |
| 40:DF:89:PRO:HG2 | 40:EF:280:LYS:HG2 | 1.95 | 0.47 |
| 40:DF:238:ILE:HD11 | 40:DF:377:LEU:HD21 | 1.96 | 0.47 |
| 40:DF:384:ALA:O | 40:DF:385:GLU:C | 2.53 | 0.47 |
| 40:DH:211:ASP:OD1 | 40:DH:212:ILE:N | 2.47 | 0.47 |
| 41:DL:72:THR:O | 41:DL:73:MET:C | 2.52 | 0.47 |
| 41:DL:374:ILE:HG23 | 41:DL:378:PHE:CE2 | 2.49 | 0.47 |
| 41:DM:259:PRO:HD3 | 41:DM:311:LEU:HD21 | 1.95 | 0.47 |
| 41:DN:21:TRP:CZ2 | 41:DN:63:ALA:HB2 | 2.49 | 0.47 |
| 41:DN:211:CYS:O | 41:DN:213:ARG:N | 2.47 | 0.47 |
| 41:DP:290:THR:HG21 | 41:DP:329:GLN:HB3 | 1.95 | 0.47 |
| 40:EA:16:ILE:HA | 40:EA:228:ASN:HB3 | 1.95 | 0.47 |
| 40:EE:169:PHE:CE1 | 40:EE:235:VAL:HG22 | 2.49 | 0.47 |
| 40:EF:274:PRO:HG3 | 40:EF:286:LEU:HD23 | 1.96 | 0.47 |
| 40:EG:314:ALA:HA | 40:EG:350:GLY:O | 2.14 | 0.47 |
| 40:EI:105:ARG:HE | 40:EI:105:ARG:HB3 | 1.45 | 0.47 |
| 40:EI:121:ARG:O | 40:EI:122:ILE:C | 2.52 | 0.47 |
| 41:EL:237:THR:HG23 | 41:EL:240:LEU:HD21 | 1.95 | 0.47 |
| 41:EM:171:PRO:HB3 | 41:EM:181:GLU:CG | 2.43 | 0.47 |
| 41:EM:345:ILE:O | 41:EM:348:ASN:ND2 | 2.46 | 0.47 |
| 40:FA:93:ILE:HG12 | 40:FA:117:LEU:HD22 | 1.96 | 0.47 |
| 40:FA:333:ALA:C | 40:FA:335:ILE:H | 2.18 | 0.47 |
| 41:FO:192:LEU:HD13 | 41:FO:199:THR:HG21 | 1.95 | 0.47 |
| 41:FP:203:ASP:HB2 | 41:FP:302:ALA:H | 1.79 | 0.47 |
| 40:GA:116:ASP:N | 40:GA:116:ASP:OD1 | 2.47 | 0.47 |
| 41:GB:324:LYS:HA | 40:GG:210:TYR:HE1 | 1.79 | 0.47 |
| 40:GF:347:CYS:HA | 41:GN:388:MET:HE1 | 1.96 | 0.47 |
| 40:GG:136:LEU:HD11 | 40:GG:239:THR:HG21 | 1.96 | 0.47 |
| 40:GI:383:ILE:HD11 | 40:GI:387:TRP:CE2 | 2.49 | 0.47 |
| 41:GN:54:ALA:O | 41:GN:55:THR:C | 2.52 | 0.47 |
| 41:GN:391:ARG:O | 41:GN:392:LYS:C | 2.52 | 0.47 |
| 40:HE:19:ALA:O | 40:HE:20:CYS:C | 2.53 | 0.47 |
| 40:HG:88:HIS:CE1 | 40:HG:90:GLU:HB2 | 2.49 | 0.47 |
| 40:HG:209:ILE:HA | 40:HG:212:ILE:HG22 | 1.95 | 0.47 |
| 40:HG:326:LYS:NZ | 41:HO:208:TYR:HB2 | 2.29 | 0.47 |
| 40:HI:2:ARG:HA | 40:HI:133:GLN:HE21 | 1.79 | 0.47 |
| 40:IE:141:PHE:HB2 | 40:IE:173:PRO:HD3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IG:184:PRO:HG3 | 40:IG:393:LYS:HD2 | 1.96 | 0.47 |
| 40:JA:438:SER:HB2 | 41:JB:390:ARG:HH12 | 1.78 | 0.47 |
| 40:JD:11:GLN:HG2 | 40:JD:74:VAL:HG11 | 1.96 | 0.47 |
| 40:JE:30:ILE:HD13 | 40:JE:36:MET:HB3 | 1.96 | 0.47 |
| 40:JE:107:HIS:HD2 | 40:JE:152:LEU:HB2 | 1.79 | 0.47 |
| 41:JM:44:LEU:HG | 41:JM:44:LEU:O | 2.13 | 0.47 |
| 40:KA:11:GLN:HG3 | 40:KA:74:VAL:HG11 | 1.95 | 0.47 |
| 41:KL:122:LYS:HD2 | 41:LL:291:GLN:HE21 | 1.79 | 0.47 |
| 41:KM:95:SER:OG | 41:KM:96:GLY:N | 2.46 | 0.47 |
| 41:KM:404:ASP:N | 41:KM:404:ASP:OD1 | 2.46 | 0.47 |
| 41:KN:117:LEU:HA | 41:KN:120:VAL:HG12 | 1.96 | 0.47 |
| 41:KP:401:GLU:N | 41:KP:401:GLU:OE2 | 2.47 | 0.47 |
| 41:LB:271:ALA:HB1 | 41:LB:292:GLN:HB3 | 1.95 | 0.47 |
| 41:LL:107:THR:O | 41:LL:110:ALA:N | 2.46 | 0.47 |
| 41:LM:249:ASP:OD2 | 41:LM:249:ASP:N | 2.45 | 0.47 |
| 40:MA:160:ASP:O | 40:MA:162:GLY:N | 2.46 | 0.47 |
| 40:ME:406:TRP:CG | 41:ML:255:VAL:HG23 | 2.49 | 0.47 |
| 40:MF:177:VAL:CG1 | 41:MM:327:ASP:HB3 | 2.44 | 0.47 |
| 40:MG:413:GLU:O | 40:MG:414:GLU:C | 2.52 | 0.47 |
| 40:ND:188:ILE:HD13 | 40:ND:424:MET:HG3 | 1.95 | 0.47 |
| 40:NE:213:CYS:HA | 40:NE:217:LEU:HB2 | 1.95 | 0.47 |
| 40:NE:333:ALA:HB2 | 41:NM:174:LYS:HE2 | 1.96 | 0.47 |
| 41:NN:223:GLY:O | 41:NN:227:HIS:HB2 | 2.13 | 0.47 |
| 41:NN:332:ASN:HB3 | 41:NN:336:LYS:NZ | 2.28 | 0.47 |
| 41:OB:19:LYS:HG3 | 41:OB:226:ASN:HB2 | 1.96 | 0.47 |
| 40:OF:172:TYR:N | 40:OF:204:VAL:O | 2.44 | 0.47 |
| 40:OH:261:PRO:O | 40:OH:262:TYR:C | 2.52 | 0.47 |
| 41:OM:19:LYS:HD2 | 41:OM:227:HIS:HD2 | 1.79 | 0.47 |
| 41:OO:236:VAL:HG12 | 41:OO:368:ILE:HD11 | 1.96 | 0.47 |
| 41:OP:183:TYR:OH | 41:OP:393:ALA:O | 2.25 | 0.47 |
| 41:PB:322:SER:HB3 | 41:PB:325:GLU:OE1 | 2.14 | 0.47 |
| 40:PE:167:LEU:HD22 | 40:PE:200:CYS:HB3 | 1.96 | 0.47 |
| 40:PH:5:ILE:HD12 | 40:PH:125:LEU:HD23 | 1.95 | 0.47 |
| 40:QA:415:GLY:O | 40:QA:419:GLU:HG3 | 2.14 | 0.47 |
| 41:QB:420:ASN:O | 41:QB:423:VAL:N | 2.39 | 0.47 |
| 40:QH:237:SER:OG | 40:QH:375:CYS:SG | 2.53 | 0.47 |
| 41:QO:309:ARG:NH1 | 41:QO:339:SER:O | 2.47 | 0.47 |
| 41:QP:42:LEU:HG | 41:QP:43:GLN:N | 2.28 | 0.47 |
| 40:RI:11:GLN:HG2 | 40:RI:74:VAL:HG11 | 1.96 | 0.47 |
| 41:RL:135:LEU:O | 41:RL:166:THR:HA | 2.14 | 0.47 |
| 40:SA:145:THR:OG1 | 42:SN:501:GTP:O2B | 2.31 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SA:413:GLU:OE1 | 40:SA:415:GLY:N | 2.45 | 0.47 |
| 41:SM:170:VAL:HG21 | 41:SM:377:LEU:HD21 | 1.96 | 0.47 |
| 41:SN:375:GLN:HE21 | 41:SN:423:VAL:HB | 1.79 | 0.47 |
| 41:SP:12:CYS:HA | 43:SP:502:GDP:C8 | 2.49 | 0.47 |
| 40:UI:236:SER:O | 40:UI:240:ALA:HB2 | 2.13 | 0.47 |
| 41:UP:41:ASP:O | 41:UP:42:LEU:C | 2.51 | 0.47 |
| 41:UP:137:HIS:CD2 | 41:UP:168:SER:HB3 | 2.49 | 0.47 |
| 41:UP:221:THR:C | 41:UP:223:GLY:H | 2.17 | 0.47 |
| 40:VA:150:THR:O | 40:VA:154:MET:HG2 | 2.14 | 0.47 |
| 41:VO:343:GLU:N | 41:VO:343:GLU:OE2 | 2.47 | 0.47 |
| 41:VQ:42:LEU:HD23 | 41:VQ:356:ILE:HD11 | 1.96 | 0.47 |
| 40:WA:76:ASP:OD1 | 40:WA:79:ARG:NH2 | 2.45 | 0.47 |
| 41:WM:13:GLY:HA2 | 41:WM:136:THR:CB | 2.33 | 0.47 |
| 41:WM:181:GLU:HB2 | 41:WM:182:PRO:HD3 | 1.95 | 0.47 |
| 41:WN:101:TRP:NE1 | 41:WN:145:SER:O | 2.46 | 0.47 |
| 41:WN:165:ASN:HB3 | 41:WN:200:TYR:HE1 | 1.79 | 0.47 |
| 41:WQ:262:ARG:NH2 | 41:WQ:417:ASP:O | 2.47 | 0.47 |
| 7:1T:210:SER:HB2 | 7:1T:256:ILE:HG22 | 1.96 | 0.47 |
| 8:1W:522:GLU:O | 8:1W:525:ALA:O | 2.33 | 0.47 |
| 13:2V:135:ASN:HB2 | 13:2V:138:ASP:HB3 | 1.96 | 0.47 |
| 16:3K:179:LYS:NZ | 16:3K:222:SER:OG | 2.33 | 0.47 |
| 19:3Y:19:GLY:O | 19:3Y:23:LYS:HG2 | 2.13 | 0.47 |
| 21:4D:334:PRO:HA | 21:4D:343:PHE:HA | 1.96 | 0.47 |
| 22:4H:113:ILE:HB | 22:4H:136:ILE:HD12 | 1.95 | 0.47 |
| 23:4M:240:LEU:HG | 23:4M:240:LEU:H | 1.49 | 0.47 |
| 24:4O:253:TYR:O | 24:4O:254:LYS:C | 2.52 | 0.47 |
| 23:4P:260:THR:CB | 40:EA:219:ILE:HD13 | 2.44 | 0.47 |
| 27:4Z:225:ASN:HB2 | 41:KO:32:PRO:HG3 | 1.96 | 0.47 |
| 34:5Q:122:THR:O | 34:5Q:125:GLU:N | 2.47 | 0.47 |
| 36:5X:26:ILE:HD11 | 36:5X:81:PHE:HA | 1.96 | 0.47 |
| 37:6A:56:HIS:CE1 | 41:UO:243:PRO:HG2 | 2.50 | 0.47 |
| 39:6I:66:ARG:NH2 | 41:ON:38:GLY:H | 2.11 | 0.47 |
| 39:6K:111:ASP:N | 39:6K:111:ASP:OD2 | 2.47 | 0.47 |
| 40:AE:217:LEU:HA | 40:AE:277:SER:HB3 | 1.95 | 0.47 |
| 40:AF:237:SER:HA | 40:AF:320:ARG:HD2 | 1.96 | 0.47 |
| 41:BB:173:PRO:HA | 41:BB:380:ARG:HD2 | 1.95 | 0.47 |
| 41:BB:286:VAL:HB | 41:BB:287:PRO:HD3 | 1.95 | 0.47 |
| 40:BI:268:PRO:HB2 | 40:BI:377:LEU:HD12 | 1.95 | 0.47 |
| 41:BM:61:PRO:HG2 | 41:BM:84:ILE:HG23 | 1.96 | 0.47 |
| 40:CE:104:ALA:HB2 | 40:CE:412:MET:HG2 | 1.96 | 0.47 |
| 40:CE:176:GLN:HE21 | 41:CL:331:LEU:HD11 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CN:80:PRO:HG2 | 41:CN:81:PHE:H | 1.79 | 0.47 |
| 41:CN:98:GLY:O | 41:CN:99:ASN:C | 2.52 | 0.47 |
| 41:CN:320:ARG:HH11 | 41:CN:355:ASP:HB3 | 1.77 | 0.47 |
| 41:CP:322:SER:O | 41:CP:324:LYS:N | 2.47 | 0.47 |
| 40:DA:403:PHE:O | 40:DA:406:TRP:HB2 | 2.14 | 0.47 |
| 40:DE:100:ALA:O | 40:DE:101:ASN:C | 2.52 | 0.47 |
| 40:DE:126:ALA:HB1 | 40:DE:132:LEU:HD22 | 1.96 | 0.47 |
| 40:DE:429:LYS:O | 40:DE:430:ASP:C | 2.52 | 0.47 |
| 40:DE:430:ASP:O | 40:DE:431:TYR:C | 2.53 | 0.47 |
| 40:DF:175:PRO:HG3 | 40:DF:304:LYS:HB3 | 1.95 | 0.47 |
| 40:DF:224:TYR:OH | 42:DF:501:GTP:H2' | 2.14 | 0.47 |
| 40:DF:326:LYS:HZ1 | 41:DN:211:CYS:HB2 | 1.78 | 0.47 |
| 40:DI:63:PRO:HG2 | 40:DI:87:PHE:CD2 | 2.49 | 0.47 |
| 40:DI:225:THR:HA | 40:DI:228:ASN:ND2 | 2.28 | 0.47 |
| 40:DI:332:ILE:HD13 | 40:DI:332:ILE:HA | 1.74 | 0.47 |
| 41:DL:420:ASN:HA | 41:DL:423:VAL:HG22 | 1.96 | 0.47 |
| 41:DN:257:MET:SD | 41:DN:314:ALA:N | 2.85 | 0.47 |
| 41:DO:111:GLU:OE1 | 41:DO:111:GLU:N | 2.47 | 0.47 |
| 40:EE:438:SER:HB2 | 41:EM:391:ARG:HD2 | 1.95 | 0.47 |
| 40:EH:433:GLU:O | 40:EH:436:MET:HG2 | 2.15 | 0.47 |
| 41:EN:68:LEU:HD23 | 41:EN:143:THR:HG23 | 1.96 | 0.47 |
| 41:EP:28:HIS:HA | 41:EP:242:PHE:HZ | 1.79 | 0.47 |
| 40:FA:262:TYR:HD1 | 40:FA:262:TYR:N | 2.11 | 0.47 |
| 41:FM:334:GLN:NE2 | 41:FM:348:ASN:OD1 | 2.47 | 0.47 |
| 42:GB:502:GTP:O2' | 40:GG:206:ASN:OD1 | 2.24 | 0.47 |
| 40:GE:274:PRO:CG | 40:GE:373:ALA:HA | 2.44 | 0.47 |
| 41:GM:119:VAL:HG23 | 41:GM:122:LYS:HE3 | 1.94 | 0.47 |
| 41:GP:200:TYR:HE2 | 41:GP:368:ILE:HD12 | 1.78 | 0.47 |
| 40:HE:31:GLN:HG2 | 40:HE:37:PRO:HD3 | 1.95 | 0.47 |
| 40:HE:366:ASP:O | 40:HE:367:LEU:C | 2.52 | 0.47 |
| 40:HG:264:ARG:NH2 | 40:HG:423:ASP:OD1 | 2.48 | 0.47 |
| 40:HH:102:ASN:HB3 | 40:HH:105:ARG:HB2 | 1.95 | 0.47 |
| 40:HI:223:THR:HB | 41:HP:322:SER:HB2 | 1.96 | 0.47 |
| 41:HN:61:PRO:HD2 | 41:HN:84:ILE:O | 2.14 | 0.47 |
| 41:HN:267:MET:HB3 | 41:HN:301:ALA:CB | 2.44 | 0.47 |
| 41:HN:284:LEU:HA | 41:HN:288:GLU:HG2 | 1.96 | 0.47 |
| 41:HO:132:GLY:HA3 | 41:HO:163:ILE:O | 2.14 | 0.47 |
| 41:HO:213:ARG:O | 41:HO:216:LYS:NZ | 2.45 | 0.47 |
| 41:IB:296:ALA:HB1 | 41:IB:305:PRO:HD2 | 1.96 | 0.47 |
| 40:IE:316:CYS:SG | 40:IE:377:LEU:HB2 | 2.54 | 0.47 |
| 41:IP:86:ARG:HH12 | 41:IP:122:LYS:HD3 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JB:252:LYS:HD3 | 40:JG:100:ALA:HA | 1.97 | 0.47 |
| 40:JD:14:VAL:HG23 | 40:JD:67:PHE:HD2 | 1.78 | 0.47 |
| 40:JD:405:HIS:HA | 40:JD:408:VAL:HG12 | 1.96 | 0.47 |
| 40:JE:172:TYR:OH | 40:JE:386:ALA:O | 2.33 | 0.47 |
| 41:JN:20:PHE:HA | 41:JN:23:VAL:HG12 | 1.96 | 0.47 |
| 41:JO:309:ARG:NH1 | 41:JO:339:SER:O | 2.47 | 0.47 |
| 41:KM:238:THR:HG1 | 41:KM:354:CYS:HG | 1.56 | 0.47 |
| 41:KN:165:ASN:ND2 | 41:KN:198:GLU:OE1 | 2.47 | 0.47 |
| 41:LM:91:VAL:HG11 | 41:LM:116:VAL:HG22 | 1.96 | 0.47 |
| 41:LO:257:MET:SD | 41:LO:314:ALA:HB2 | 2.54 | 0.47 |
| 40:MD:235:VAL:HA | 40:MD:238:ILE:HG22 | 1.96 | 0.47 |
| 40:MH:25:CYS:HB3 | 40:MH:30:ILE:O | 2.14 | 0.47 |
| 41:MN:236:VAL:HG22 | 41:MN:368:ILE:HD11 | 1.96 | 0.47 |
| 40:NA:81:GLY:O | 40:NA:84:ARG:NH1 | 2.43 | 0.47 |
| 40:ND:298:PRO:HG2 | 40:ND:308:ARG:NH2 | 2.29 | 0.47 |
| 40:NH:79:ARG:HG2 | 40:NH:92:LEU:HD13 | 1.96 | 0.47 |
| 41:NP:86:ARG:HG2 | 41:OP:281:TYR:HB3 | 1.96 | 0.47 |
| 40:OE:181:VAL:HG12 | 41:OL:348:ASN:HA | 1.96 | 0.47 |
| 40:OG:260:VAL:HG23 | 40:OG:265:ILE:O | 2.14 | 0.47 |
| 41:OM:289:LEU:HD11 | 41:OM:363:MET:HG2 | 1.96 | 0.47 |
| 41:OM:372:THR:OG1 | 41:OM:422:VAL:O | 2.32 | 0.47 |
| 41:OO:248:ALA:HA | 41:OO:252:LYS:HD3 | 1.96 | 0.47 |
| 40:PA:211:ASP:HB3 | 40:PA:215:ARG:NH1 | 2.29 | 0.47 |
| 40:PA:240:ALA:HA | 40:PA:243:ARG:HE | 1.79 | 0.47 |
| 41:PB:7:LEU:HD11 | 41:PB:133:PHE:HB3 | 1.96 | 0.47 |
| 40:PF:394:PHE:HE2 | 40:PF:421:ARG:HB2 | 1.79 | 0.47 |
| 41:PL:398:TYR:HB3 | 41:PL:403:MET:HB3 | 1.96 | 0.47 |
| 41:QB:186:THR:OG1 | 41:QB:187:LEU:N | 2.47 | 0.47 |
| 40:QE:70:LEU:HD23 | 40:QE:114:LEU:HD12 | 1.96 | 0.47 |
| 40:QF:21:TRP:CH2 | 40:QF:52:PHE:HB3 | 2.49 | 0.47 |
| 40:QF:70:LEU:HD22 | 40:QF:110:ILE:HG22 | 1.95 | 0.47 |
| 40:QG:2:ARG:HH12 | 40:QG:131:GLY:HA3 | 1.78 | 0.47 |
| 41:QL:73:MET:HB3 | 41:QL:90:PHE:CZ | 2.48 | 0.47 |
| 41:QL:114:ASP:OD1 | 41:QL:115:SER:N | 2.47 | 0.47 |
| 41:QP:3:GLU:O | 41:QP:131:GLN:N | 2.39 | 0.47 |
| 41:QP:88:ASP:OD1 | 41:QP:88:ASP:N | 2.44 | 0.47 |
| 41:QP:138:SER:HB3 | 41:QP:169:VAL:HG21 | 1.95 | 0.47 |
| 41:QP:272:PRO:CG | 41:QP:364:SER:HB2 | 2.25 | 0.47 |
| 41:RM:271:ALA:HB1 | 41:RM:292:GLN:HG3 | 1.96 | 0.47 |
| 40:SA:72:PRO:HB2 | 41:SN:46:ARG:HH21 | 1.78 | 0.47 |
| 40:SA:167:LEU:HD13 | 40:SA:200:CYS:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SB:171:PRO:HB3 | 41:SB:181:GLU:HG2 | 1.96 | 0.47 |
| 40:SG:194:THR:OG1 | 40:SG:198:SER:OG | 2.32 | 0.47 |
| 40:SG:249:ASN:O | 40:SG:249:ASN:ND2 | 2.43 | 0.47 |
| 41:SO:185:ALA:O | 41:SO:188:SER:N | 2.43 | 0.47 |
| 41:SO:298:ASN:O | 41:SO:300:MET:N | 2.47 | 0.47 |
| 40:TF:259:LEU:HD21 | 40:TF:316:CYS:HB2 | 1.95 | 0.47 |
| 40:UF:53:PHE:CE1 | 40:UF:63:PRO:HG3 | 2.49 | 0.47 |
| 40:UG:145:THR:OG1 | 40:UG:146:GLY:N | 2.46 | 0.47 |
| 40:UG:235:VAL:HA | 40:UG:238:ILE:HG22 | 1.95 | 0.47 |
| 40:UG:332:ILE:HG21 | 41:UO:175:VAL:HG12 | 1.96 | 0.47 |
| 40:UH:171:ILE:HG21 | 42:UO:501:GTP:H1' | 1.97 | 0.47 |
| 40:UI:11:GLN:N | 42:UI:501:GTP:O2B | 2.46 | 0.47 |
| 41:UM:257:MET:HG3 | 41:UM:266:PHE:CE1 | 2.48 | 0.47 |
| 41:UO:100:ASN:OD1 | 41:UO:102:ALA:N | 2.46 | 0.47 |
| 40:VA:195:LEU:HD12 | 40:VA:266:HIS:HE1 | 1.79 | 0.47 |
| 40:VA:352:LYS:HE2 | 41:VB:178:THR:HG22 | 1.97 | 0.47 |
| 41:VO:20:PHE:HB2 | 41:VO:233:MET:HE3 | 1.96 | 0.47 |
| 41:VP:156:ARG:NH2 | 41:VP:197:ASP:OD2 | 2.47 | 0.47 |
| 40:WF:53:PHE:HE1 | 40:WF:86:LEU:HD11 | 1.79 | 0.47 |
| 40:WF:319:TYR:CE2 | 40:WF:328:VAL:HG22 | 2.49 | 0.47 |
| 40:WG:326:LYS:HE2 | 41:WO:208:TYR:HB2 | 1.96 | 0.47 |
| 40:WG:394:PHE:HD1 | 40:WG:421:ARG:HD3 | 1.79 | 0.47 |
| 40:WH:137:ILE:HG22 | 40:WH:139:HIS:HD2 | 1.80 | 0.47 |
| 41:WQ:272:PRO:HG3 | 41:WQ:364:SER:HA | 1.95 | 0.47 |
| 7:1T:321:ASP:O | 7:1T:323:LYS:N | 2.47 | 0.47 |
| 7:1T:368:LEU:HD12 | 10:2E:130:ARG:HB3 | 1.97 | 0.47 |
| 11:2J:185:MET:HA | 11:2J:254:ASN:OD1 | 2.13 | 0.47 |
| 13:2U:172:TYR:HB3 | 13:2U:176:GLU:HB2 | 1.96 | 0.47 |
| 14:3C:26:LYS:HD3 | 40:MG:342:GLN:HE22 | 1.78 | 0.47 |
| 17:3P:192:LEU:CD1 | 17:3P:223:VAL:HA | 2.45 | 0.47 |
| 18:3T:147:LEU:HD22 | 18:3T:438:PRO:HD3 | 1.96 | 0.47 |
| 18:3W:329:ILE:HG12 | 18:3W:405:LEU:HB3 | 1.96 | 0.47 |
| 20:4A:168:LEU:HB3 | 20:4A:172:GLN:NE2 | 2.30 | 0.47 |
| 21:4D:474:LYS:HG2 | 21:4D:485:TYR:OH | 2.14 | 0.47 |
| 21:4D:476:ASP:O | 21:4D:477:SER:HB2 | 2.13 | 0.47 |
| 21:4D:477:SER:O | 21:4D:479:MET:N | 2.46 | 0.47 |
| 21:4E:116:ARG:NH2 | 41:BP:276:ARG:O | 2.48 | 0.47 |
| 22:4H:262:ILE:HG12 | 22:4H:279:LEU:HB2 | 1.95 | 0.47 |
| 23:4N:171:PRO:C | 23:4N:173:SER:H | 2.18 | 0.47 |
| 23:4R:89:SER:O | 23:4R:90:MET:HG2 | 2.15 | 0.47 |
| 26:4W:247:PRO:HG3 | 26:4W:308:CYS:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:4Z:41:GLN:O | 27:4Z:43:ASN:N | 2.44 | 0.47 |
| 36:5X:118:TYR:HE2 | 41:KL:421:PRO:HD3 | 1.79 | 0.47 |
| 41:AB:256:ASN:OD1 | 40:AG:101:ASN:ND2 | 2.32 | 0.47 |
| 40:AE:240:ALA:HB1 | 40:AE:356:ASN:HD22 | 1.78 | 0.47 |
| 40:AG:188:ILE:HG22 | 40:AG:420:ALA:HB1 | 1.96 | 0.47 |
| 40:AG:352:LYS:HZ2 | 41:AO:179:VAL:HA | 1.79 | 0.47 |
| 40:BF:102:ASN:H | 40:BF:144:GLY:HA3 | 1.79 | 0.47 |
| 40:BI:222:PRO:HB2 | 40:BI:226:ASN:HB2 | 1.96 | 0.47 |
| 40:BI:393:LYS:HG3 | 41:BP:346:PRO:HB2 | 1.95 | 0.47 |
| 41:BO:210:ILE:H | 41:BO:210:ILE:HG13 | 1.52 | 0.47 |
| 41:CB:248:ALA:HA | 41:CB:252:LYS:HD2 | 1.96 | 0.47 |
| 40:CE:273:ALA:HB1 | 40:CE:291:ILE:HB | 1.97 | 0.47 |
| 40:CF:269:LEU:O | 40:CF:377:LEU:HA | 2.15 | 0.47 |
| 40:CI:206:ASN:ND2 | 42:CI:501:GTP:O2' | 2.47 | 0.47 |
| 41:CL:135:LEU:HG | 41:CL:137:HIS:HB3 | 1.94 | 0.47 |
| 41:CM:416:ASN:C | 41:CM:418:LEU:H | 2.17 | 0.47 |
| 41:CM:420:ASN:HB2 | 41:CM:421:PRO:HD3 | 1.94 | 0.47 |
| 41:CN:375:GLN:HG3 | 41:CN:376:GLU:N | 2.29 | 0.47 |
| 41:CO:70:PRO:HB3 | 41:CO:92:PHE:CE2 | 2.49 | 0.47 |
| 41:CP:272:PRO:HG3 | 41:CP:364:SER:HA | 1.96 | 0.47 |
| 40:DA:169:PHE:HE2 | 40:DA:238:ILE:HG21 | 1.80 | 0.47 |
| 41:DB:105:HIS:NE2 | 41:DB:191:GLN:HG3 | 2.28 | 0.47 |
| 40:DE:122:ILE:HA | 40:DE:125:LEU:HD12 | 1.97 | 0.47 |
| 40:DE:173:PRO:HG3 | 40:DE:187:SER:HB3 | 1.96 | 0.47 |
| 40:DE:320:ARG:HB3 | 40:DE:356:ASN:ND2 | 2.29 | 0.47 |
| 40:DE:403:PHE:CZ | 41:DL:312:THR:HG21 | 2.49 | 0.47 |
| 40:DF:73:THR:O | 40:DF:76:ASP:N | 2.47 | 0.47 |
| 40:DF:194:THR:O | 40:DF:198:SER:HB3 | 2.13 | 0.47 |
| 41:DM:119:VAL:O | 41:DM:120:VAL:C | 2.51 | 0.47 |
| 41:DM:174:LYS:HE2 | 41:DM:174:LYS:HB3 | 1.47 | 0.47 |
| 41:DP:293:MET:CG | 41:DP:367:PHE:HB2 | 2.41 | 0.47 |
| 41:DP:391:ARG:HD3 | 41:DP:391:ARG:HA | 1.50 | 0.47 |
| 41:DP:417:ASP:O | 41:DP:418:LEU:C | 2.52 | 0.47 |
| 40:EA:20:CYS:HA | 40:EA:232:SER:HB2 | 1.96 | 0.47 |
| 40:EH:189:LEU:HD13 | 40:EH:189:LEU:HA | 1.75 | 0.47 |
| 41:EP:112:LEU:O | 41:EP:113:VAL:C | 2.52 | 0.47 |
| 40:FE:175:PRO:HD2 | 40:FE:207:GLU:HG3 | 1.96 | 0.47 |
| 40:FH:104:ALA:O | 40:FH:108:TYR:HB2 | 2.13 | 0.47 |
| 40:FH:254:GLU:HA | 40:FH:257:THR:HG22 | 1.95 | 0.47 |
| 41:FM:232:THR:HG21 | 41:FM:268:PRO:HB2 | 1.97 | 0.47 |
| 40:GE:226:ASN:HA | 40:GE:229:ARG:HD2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GF:271:THR:OG1 | 40:GF:376:MET:HB3 | 2.14 | 0.47 |
| 40:GH:289:ALA:O | 40:GH:290:GLU:C | 2.52 | 0.47 |
| 40:GH:398:TYR:CE1 | 40:GH:417:PHE:HB2 | 2.49 | 0.47 |
| 40:GI:254:GLU:HG3 | 40:GI:255:PHE:N | 2.29 | 0.47 |
| 41:GM:248:ALA:HA | 41:GM:252:LYS:HD2 | 1.95 | 0.47 |
| 41:GN:47:ILE:C | 41:GN:49:VAL:H | 2.18 | 0.47 |
| 41:GO:278:SER:O | 41:GO:279:GLN:C | 2.52 | 0.47 |
| 41:GP:41:ASP:N | 41:GP:41:ASP:OD1 | 2.45 | 0.47 |
| 40:HE:8:HIS:HE1 | 40:HE:21:TRP:HE1 | 1.62 | 0.47 |
| 40:HE:21:TRP:O | 40:HE:22:GLU:C | 2.52 | 0.47 |
| 40:HE:338:LYS:HE2 | 40:HE:338:LYS:HB2 | 1.44 | 0.47 |
| 40:HF:136:LEU:HD11 | 40:HF:239:THR:HG21 | 1.96 | 0.47 |
| 40:II:67:PHE:HE1 | 40:II:78:VAL:HG11 | 1.78 | 0.47 |
| 41:IM:49:VAL:HG21 | 41:IM:241:ARG:HG3 | 1.95 | 0.47 |
| 41:IO:232:THR:HG21 | 41:IO:268:PRO:HB2 | 1.96 | 0.47 |
| 42:JB:502:GTP:O2A | 40:JG:140:SER:OG | 2.29 | 0.47 |
| 40:JE:79:ARG:HH22 | 40:JE:94:THR:HG21 | 1.78 | 0.47 |
| 41:JL:396:HIS:HA | 41:JL:399:THR:HG22 | 1.96 | 0.47 |
| 41:KN:236:VAL:HG22 | 41:KN:368:ILE:HD11 | 1.96 | 0.47 |
| 40:LG:277:SER:O | 40:LG:279:GLU:N | 2.47 | 0.47 |
| 40:LG:400:LYS:O | 40:LG:401:ARG:C | 2.52 | 0.47 |
| 40:LH:213:CYS:HA | 40:LH:217:LEU:HD13 | 1.96 | 0.47 |
| 41:LN:237:THR:HG22 | 41:LN:250:LEU:HD21 | 1.96 | 0.47 |
| 40:MF:183:GLU:HB3 | 40:MF:184:PRO:HD3 | 1.96 | 0.47 |
| 40:MG:269:LEU:HD23 | 40:MG:303:VAL:CG1 | 2.45 | 0.47 |
| 41:MM:149:THR:HA | 41:MM:152:ILE:HD12 | 1.96 | 0.47 |
| 41:NB:142:GLY:O | 41:NB:144:GLY:N | 2.47 | 0.47 |
| 40:NF:209:ILE:HA | 40:NF:212:ILE:HG22 | 1.95 | 0.47 |
| 41:NL:185:ALA:O | 41:NL:189:VAL:HG12 | 2.14 | 0.47 |
| 40:OF:284:GLU:HG2 | 40:OF:286:LEU:HD12 | 1.96 | 0.47 |
| 40:OH:88:HIS:O | 40:OH:91:GLN:N | 2.46 | 0.47 |
| 40:PA:233:GLN:HB3 | 40:PA:272:TYR:CZ | 2.49 | 0.47 |
| 40:PG:7:VAL:HG12 | 40:PG:66:VAL:HB | 1.97 | 0.47 |
| 40:PH:228:ASN:ND2 | 42:PO:501:GTP:HN1 | 2.06 | 0.47 |
| 41:PL:165:ASN:HA | 41:PL:198:GLU:O | 2.13 | 0.47 |
| 41:PM:137:HIS:CE1 | 41:PM:168:SER:HB3 | 2.49 | 0.47 |
| 40:QE:181:VAL:HG22 | 41:QL:256:ASN:ND2 | 2.29 | 0.47 |
| 40:QF:405:HIS:HA | 40:QF:408:VAL:HG12 | 1.97 | 0.47 |
| 40:QH:319:TYR:HB3 | 40:QH:323:VAL:HG11 | 1.96 | 0.47 |
| 41:RM:53:GLU:HG3 | 41:RM:59:TYR:HE1 | 1.78 | 0.47 |
| 41:RM:362:LYS:HG3 | 41:RM:363:MET:HG2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RM:392:LYS:NZ | 41:RM:405:GLU:OE2 | 2.35 | 0.47 |
| 40:SE:332:ILE:HD12 | 40:SE:351:PHE:HB3 | 1.96 | 0.47 |
| 40:SF:65:ALA:O | 40:SF:91:GLN:NE2 | 2.44 | 0.47 |
| 40:SG:140:SER:HA | 40:SG:171:ILE:HB | 1.97 | 0.47 |
| 40:SI:111:GLY:O | 40:SI:115:ILE:HG12 | 2.15 | 0.47 |
| 41:SL:217:LEU:HB2 | 41:SL:220:PRO:HG3 | 1.96 | 0.47 |
| 41:SL:288:GLU:HA | 41:SL:291:GLN:HG3 | 1.96 | 0.47 |
| 41:SM:7:LEU:O | 41:SM:135:LEU:HA | 2.14 | 0.47 |
| 41:SN:323:MET:HB2 | 41:SN:326:VAL:HB | 1.95 | 0.47 |
| 41:SO:393:ALA:O | 41:SO:394:PHE:C | 2.53 | 0.47 |
| 41:TB:142:GLY:O | 41:TB:144:GLY:N | 2.47 | 0.47 |
| 40:TF:311:LYS:N | 40:TF:381:THR:OG1 | 2.35 | 0.47 |
| 40:TI:269:LEU:HD21 | 40:TI:301:GLN:HB3 | 1.95 | 0.47 |
| 41:TO:238:THR:HG21 | 41:TO:318:ARG:HE | 1.79 | 0.47 |
| 41:UM:21:TRP:HA | 41:UM:24:ILE:HG22 | 1.95 | 0.47 |
| 41:UN:193:VAL:O | 41:UN:264:HIS:NE2 | 2.45 | 0.47 |
| 41:UN:210:ILE:HG13 | 41:UN:298:ASN:HA | 1.96 | 0.47 |
| 41:UP:110:ALA:O | 41:UP:111:GLU:C | 2.52 | 0.47 |
| 41:UP:167:PHE:HZ | 41:UP:236:VAL:HG11 | 1.78 | 0.47 |
| 42:VB:502:GTP:O2A | 40:VH:140:SER:OG | 2.31 | 0.47 |
| 40:VF:76:ASP:HA | 40:VF:79:ARG:HG2 | 1.95 | 0.47 |
| 40:VG:211:ASP:O | 40:VG:215:ARG:HB2 | 2.14 | 0.47 |
| 41:VN:200:TYR:HE1 | 41:VN:266:PHE:HD2 | 1.62 | 0.47 |
| 41:VO:68:LEU:HD13 | 41:VO:112:LEU:HD13 | 1.96 | 0.47 |
| 41:VO:237:THR:O | 41:VO:241:ARG:NE | 2.39 | 0.47 |
| 41:VP:211:CYS:HA | 41:VP:215:LEU:HB2 | 1.96 | 0.47 |
| 40:WE:370:VAL:HG22 | 40:WE:372:ARG:H | 1.79 | 0.47 |
| 40:WG:49:PHE:O | 40:WG:53:PHE:N | 2.40 | 0.47 |
| 40:WG:134:GLY:HA2 | 40:WG:164:LYS:HG3 | 1.96 | 0.47 |
| 40:WH:142:GLY:O | 40:WH:186:ASN:ND2 | 2.47 | 0.47 |
| 40:WI:223:THR:OG1 | 41:WP:245:GLN:NE2 | 2.40 | 0.47 |
| 41:WN:141:GLY:HA3 | 43:WN:501:GDP:O1A | 2.14 | 0.47 |
| 41:WO:379:LYS:HA | 41:WO:382:SER:HB3 | 1.97 | 0.47 |
| 7:1T:278:SER:O | 7:1T:280:SER:N | 2.47 | 0.47 |
| 7:1T:353:LYS:HA | 7:1T:376:THR:HG23 | 1.96 | 0.47 |
| 8:1X:93:LYS:HB2 | 8:1X:93:LYS:HE2 | 1.50 | 0.47 |
| 8:1X:192:MET:HA | 8:1X:195:ILE:HG22 | 1.95 | 0.47 |
| 11:2I:119:LYS:NZ | 40:LG:410:GLU:N | 2.63 | 0.47 |
| 12:2N:76:TYR:OH | 40:WA:127:ASP:OD1 | 2.30 | 0.47 |
| 13:2W:119:CYS:O | 13:2W:120:THR:C | 2.53 | 0.47 |
| 16:3J:366:LEU:HD21 | 16:3L:35:SER:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:3O:393:LEU:HB3 | 17:3R:283:TYR:CE2 | 2.49 | 0.47 |
| 17:3R:164:LEU:HD11 | 17:3R:255:GLU:HA | 1.96 | 0.47 |
| 18:3V:77:GLN:O | 18:3V:81:SER:HB3 | 2.15 | 0.47 |
| 19:3Y:167:TRP:HZ2 | 25:4T:399:GLU:HB3 | 1.75 | 0.47 |
| 19:3Y:216:ALA:CB | 40:KF:58:ALA:HB2 | 2.45 | 0.47 |
| 21:4D:35:ASN:ND2 | 40:MF:326:LYS:HG2 | 2.29 | 0.47 |
| 21:4D:35:ASN:HD22 | 40:MF:326:LYS:HG2 | 1.79 | 0.47 |
| 21:4D:474:LYS:HB3 | 21:4D:475:PRO:HD2 | 1.95 | 0.47 |
| 22:4I:154:ILE:HB | 22:4I:186:ASN:HB2 | 1.97 | 0.47 |
| 22:4I:195:PRO:HA | 22:4I:198:LYS:HB2 | 1.97 | 0.47 |
| 23:4R:101:ALA:O | 23:4R:104:ILE:HG12 | 2.14 | 0.47 |
| 23:4R:113:TRP:O | 23:4R:117:LEU:HG | 2.14 | 0.47 |
| 26:4V:282:VAL:HG12 | 26:4V:300:VAL:HG13 | 1.97 | 0.47 |
| 27:4Z:101:ALA:O | 27:4Z:103:LEU:N | 2.47 | 0.47 |
| 37:6A:43:ARG:NH2 | 41:TO:41:ASP:OD2 | 2.47 | 0.47 |
| 38:6D:276:PRO:HB3 | 41:VN:291:GLN:HE22 | 1.79 | 0.47 |
| 41:AL:163:ILE:HG21 | 41:AL:250:LEU:HB3 | 1.95 | 0.47 |
| 41:AN:314:ALA:HB3 | 41:AN:368:ILE:HB | 1.95 | 0.47 |
| 41:AO:238:THR:O | 41:AO:242:PHE:N | 2.47 | 0.47 |
| 41:AP:41:ASP:N | 41:AP:41:ASP:OD1 | 2.47 | 0.47 |
| 41:BB:109:GLY:O | 41:BB:113:VAL:HG23 | 2.13 | 0.47 |
| 40:BE:136:LEU:HD23 | 40:BE:167:LEU:HD13 | 1.97 | 0.47 |
| 40:BI:261:PRO:HD2 | 40:BI:265:ILE:HB | 1.96 | 0.47 |
| 41:BN:142:GLY:O | 41:BN:144:GLY:N | 2.47 | 0.47 |
| 40:CE:271:THR:OG1 | 40:CE:300:ASN:O | 2.28 | 0.47 |
| 40:CG:101:ASN:HD21 | 40:CG:180:ALA:HB1 | 1.79 | 0.47 |
| 40:CG:238:ILE:HG12 | 40:CG:377:LEU:HD11 | 1.96 | 0.47 |
| 40:CH:20:CYS:CA | 40:CH:232:SER:HB2 | 2.42 | 0.47 |
| 41:CL:7:LEU:HA | 41:CL:64:VAL:HG13 | 1.97 | 0.47 |
| 41:CM:178:THR:HB | 41:CM:181:GLU:HG2 | 1.96 | 0.47 |
| 41:CN:20:PHE:O | 41:CN:20:PHE:CG | 2.67 | 0.47 |
| 41:CP:260:PHE:CE2 | 41:CP:425:ARG:HD3 | 2.49 | 0.47 |
| 41:CP:330:MET:HG3 | 41:CP:349:VAL:HG21 | 1.97 | 0.47 |
| 40:DF:73:THR:O | 40:DF:74:VAL:C | 2.52 | 0.47 |
| 40:DI:281:ALA:O | 40:DI:282:TYR:C | 2.52 | 0.47 |
| 41:DL:137:HIS:CE1 | 41:DL:168:SER:HB2 | 2.48 | 0.47 |
| 41:DM:156:ARG:HA | 41:DM:156:ARG:HD3 | 1.41 | 0.47 |
| 41:DM:323:MET:HE2 | 41:DM:323:MET:HB2 | 1.53 | 0.47 |
| 41:DN:20:PHE:HA | 41:DN:230:SER:HB2 | 1.96 | 0.47 |
| 41:DN:372:THR:HA | 41:DN:422:VAL:HG22 | 1.96 | 0.47 |
| 41:DO:210:ILE:O | 41:DO:214:THR:OG1 | 2.22 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EE:20:CYS:HA | 40:EE:232:SER:HB2 | 1.96 | 0.47 |
| 40:EE:136:LEU:HD23 | 40:EE:167:LEU:HB2 | 1.96 | 0.47 |
| 40:EI:291:ILE:HD11 | 40:EI:319:TYR:CD1 | 2.49 | 0.47 |
| 40:EI:319:TYR:HB3 | 40:EI:323:VAL:HG11 | 1.95 | 0.47 |
| 41:EM:20:PHE:HA | 41:EM:230:SER:HB3 | 1.97 | 0.47 |
| 41:EM:91:VAL:HG11 | 41:EM:116:VAL:HG22 | 1.96 | 0.47 |
| 40:FA:168:GLU:O | 40:FA:170:SER:N | 2.41 | 0.47 |
| 41:FB:178:THR:N | 41:FB:181:GLU:OE2 | 2.37 | 0.47 |
| 40:FE:295:CYS:O | 40:FE:301:GLN:NE2 | 2.48 | 0.47 |
| 40:FE:312:TYR:HD1 | 40:FE:380:THR:HB | 1.79 | 0.47 |
| 40:FE:326:LYS:HB3 | 41:FM:208:TYR:HE1 | 1.78 | 0.47 |
| 41:FN:395:LEU:HA | 41:FN:398:TYR:HD2 | 1.78 | 0.47 |
| 41:FO:309:ARG:H | 41:FO:372:THR:HG1 | 1.60 | 0.47 |
| 41:FP:139:LEU:HG | 41:FP:168:SER:HB3 | 1.95 | 0.47 |
| 41:FP:316:VAL:HG23 | 41:FP:366:THR:HB | 1.95 | 0.47 |
| 40:GH:303:VAL:O | 40:GH:305:CYS:N | 2.48 | 0.47 |
| 40:GI:274:PRO:HB3 | 40:GI:370:VAL:HG11 | 1.96 | 0.47 |
| 41:GN:193:VAL:HG22 | 41:GN:265:PHE:HE1 | 1.80 | 0.47 |
| 40:HE:401:ARG:HD3 | 40:HE:401:ARG:HA | 1.59 | 0.47 |
| 40:HG:20:CYS:HA | 40:HG:232:SER:HB2 | 1.97 | 0.47 |
| 40:HI:54:SER:O | 40:HI:61:HIS:HA | 2.14 | 0.47 |
| 40:HI:241:SER:OG | 40:HI:249:ASN:OD1 | 2.31 | 0.47 |
| 41:HO:86:ARG:HH11 | 41:HO:89:ASN:HD21 | 1.60 | 0.47 |
| 40:II:73:THR:HA | 40:II:76:ASP:HB3 | 1.96 | 0.47 |
| 41:IN:142:GLY:O | 41:IN:144:GLY:N | 2.47 | 0.47 |
| 41:IO:149:THR:HG21 | 41:IO:188:SER:HA | 1.96 | 0.47 |
| 41:IO:236:VAL:HG23 | 41:IO:237:THR:HG23 | 1.96 | 0.47 |
| 41:IO:274:THR:HG22 | 41:IO:282:ARG:HE | 1.79 | 0.47 |
| 40:JF:268:PRO:HA | 40:JF:379:ASN:HA | 1.96 | 0.47 |
| 41:JL:60:VAL:HG11 | 41:JL:86:ARG:HG3 | 1.95 | 0.47 |
| 41:KL:102:ALA:O | 41:KL:104:GLY:N | 2.48 | 0.47 |
| 41:KO:107:THR:O | 41:KO:110:ALA:N | 2.43 | 0.47 |
| 41:KP:248:ALA:HA | 41:KP:252:LYS:HD3 | 1.96 | 0.47 |
| 41:LB:376:GLU:O | 41:LB:380:ARG:HG3 | 2.14 | 0.47 |
| 40:LD:426:ALA:O | 40:LD:430:ASP:HB2 | 2.13 | 0.47 |
| 40:LG:91:GLN:HG2 | 40:LG:121:ARG:HD2 | 1.95 | 0.47 |
| 41:LM:246:LEU:HD21 | 42:LM:501:GTP:H3' | 1.94 | 0.47 |
| 41:LN:117:LEU:O | 41:LN:121:ARG:HB2 | 2.15 | 0.47 |
| 40:MD:288:VAL:HB | 40:MD:327:ASP:HB3 | 1.96 | 0.47 |
| 40:MF:23:LEU:HD12 | 40:MF:363:VAL:HG13 | 1.95 | 0.47 |
| 40:MF:252:LEU:HA | 40:MF:255:PHE:HD2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MG:144:GLY:O | 40:MG:148:GLY:N | 2.47 | 0.47 |
| 41:ML:31:ASP:OD2 | 41:ML:35:THR:OG1 | 2.30 | 0.47 |
| 41:ML:137:HIS:ND1 | 41:ML:144:GLY:O | 2.47 | 0.47 |
| 41:MO:323:MET:SD | 41:MO:353:VAL:HG21 | 2.54 | 0.47 |
| 40:NA:254:GLU:HB3 | 40:NA:352:LYS:NZ | 2.30 | 0.47 |
| 40:ND:282:TYR:C | 40:ND:284:GLU:H | 2.16 | 0.47 |
| 40:NH:172:TYR:N | 40:NH:204:VAL:O | 2.40 | 0.47 |
| 41:NO:50:TYR:HE2 | 41:NO:241:ARG:HH21 | 1.62 | 0.47 |
| 41:NO:285:THR:HG23 | 41:NO:287:PRO:HD2 | 1.96 | 0.47 |
| 40:OA:205:ASP:OD1 | 40:OA:206:ASN:N | 2.42 | 0.47 |
| 40:OD:217:LEU:HA | 40:OD:277:SER:HB2 | 1.95 | 0.47 |
| 40:OE:2:ARG:HB3 | 40:OE:133:GLN:NE2 | 2.28 | 0.47 |
| 40:OE:167:LEU:HD12 | 40:OE:202:PHE:HE2 | 1.80 | 0.47 |
| 41:OL:237:THR:HG22 | 41:OL:250:LEU:HD21 | 1.95 | 0.47 |
| 41:OO:398:TYR:HB3 | 41:OO:403:MET:HB2 | 1.96 | 0.47 |
| 41:OP:165:ASN:HD21 | 41:OP:250:LEU:HD13 | 1.78 | 0.47 |
| 40:PD:24:TYR:HA | 40:PD:27:GLU:HG2 | 1.96 | 0.47 |
| 40:PG:294:ALA:O | 40:PG:300:ASN:ND2 | 2.39 | 0.47 |
| 40:PH:401:ARG:NH2 | 40:PH:414:GLU:OE1 | 2.40 | 0.47 |
| 41:PP:309:ARG:NH1 | 41:PP:339:SER:O | 2.48 | 0.47 |
| 40:QA:228:ASN:HD21 | 42:QN:501:GTP:HN1 | 1.61 | 0.47 |
| 41:QB:66:VAL:HG21 | 41:QB:147:MET:HE2 | 1.95 | 0.47 |
| 41:QB:257:MET:HA | 41:QB:312:THR:OG1 | 2.15 | 0.47 |
| 40:QE:109:THR:OG1 | 40:QE:410:GLU:O | 2.32 | 0.47 |
| 40:QH:136:LEU:HB3 | 40:QH:138:PHE:HE1 | 1.78 | 0.47 |
| 41:QL:172:SER:OG | 41:QL:175:VAL:O | 2.31 | 0.47 |
| 41:QM:314:ALA:HB3 | 41:QM:368:ILE:HB | 1.97 | 0.47 |
| 40:RA:311:LYS:N | 40:RA:381:THR:OG1 | 2.41 | 0.47 |
| 40:RE:64:ARG:NH2 | 40:RE:129:CYS:SG | 2.77 | 0.47 |
| 40:RI:115:ILE:HA | 40:RI:118:VAL:HG22 | 1.95 | 0.47 |
| 41:RN:139:LEU:HD12 | 41:RN:170:VAL:HG22 | 1.96 | 0.47 |
| 41:RO:311:LEU:N | 41:RO:370:ASN:O | 2.47 | 0.47 |
| 40:SA:56:THR:OG1 | 40:TA:284:GLU:O | 2.29 | 0.47 |
| 40:SA:265:ILE:HB | 40:SA:431:TYR:CE1 | 2.48 | 0.47 |
| 40:SE:371:GLN:OE1 | 40:SE:371:GLN:N | 2.41 | 0.47 |
| 40:SG:138:PHE:HE2 | 40:SG:235:VAL:HG21 | 1.79 | 0.47 |
| 40:SG:311:LYS:N | 40:SG:381:THR:OG1 | 2.41 | 0.47 |
| 41:SM:200:TYR:CD1 | 41:SM:266:PHE:HB2 | 2.50 | 0.47 |
| 41:SO:317:PHE:HB3 | 41:SO:321:MET:SD | 2.54 | 0.47 |
| 40:TE:285:GLN:HB2 | 40:TE:290:GLU:OE2 | 2.15 | 0.47 |
| 40:TG:51:THR:O | 40:TG:64:ARG:NH1 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UE:217:LEU:HA | 40:UE:277:SER:HB2 | 1.95 | 0.47 |
| 40:UE:310:GLY:HA3 | 40:UE:382:ALA:HB2 | 1.96 | 0.47 |
| 40:UG:315:CYS:HA | 40:UG:377:LEU:O | 2.14 | 0.47 |
| 41:UN:149:THR:HG21 | 41:UN:188:SER:HA | 1.97 | 0.47 |
| 41:UN:309:ARG:NH1 | 41:UN:338:SER:O | 2.47 | 0.47 |
| 40:VF:21:TRP:HZ3 | 40:VF:52:PHE:HB3 | 1.79 | 0.47 |
| 40:VG:255:PHE:HZ | 40:VG:318:LEU:HD11 | 1.78 | 0.47 |
| 40:VI:295:CYS:O | 40:VI:301:GLN:NE2 | 2.47 | 0.47 |
| 41:VO:6:HIS:O | 41:VO:63:ALA:HA | 2.15 | 0.47 |
| 40:WF:205:ASP:HB2 | 40:WF:303:VAL:HA | 1.97 | 0.47 |
| 7:1T:256:ILE:HD12 | 7:1T:266:VAL:HG12 | 1.96 | 0.47 |
| 15:3F:46:ASP:OD2 | 16:3M:43:ARG:NH2 | 2.47 | 0.47 |
| 16:3J:52:GLN:OE1 | 16:3K:344:GLN:NE2 | 2.46 | 0.47 |
| 17:3R:233:MET:HA | 17:3R:328:LEU:HD11 | 1.97 | 0.47 |
| 18:3V:246:LYS:HA | 18:3V:249:GLU:HG2 | 1.97 | 0.47 |
| 20:4B:241:LEU:HA | 20:4B:244:ILE:HD12 | 1.95 | 0.47 |
| 21:4D:409:VAL:HG21 | 40:DA:57:GLY:HA3 | 1.96 | 0.47 |
| 21:4F:426:LEU:O | 21:4F:427:GLU:C | 2.52 | 0.47 |
| 22:4J:642:CYS:CB | 22:4J:690:TYR:HB3 | 2.45 | 0.47 |
| 22:4K:678:LEU:O | 22:4K:683:ASP:HB2 | 2.15 | 0.47 |
| 23:4M:254:LYS:HE2 | 23:4M:254:LYS:HB3 | 1.54 | 0.47 |
| 23:4N:260:THR:CB | 40:EF:219:ILE:CD1 | 2.93 | 0.47 |
| 24:4O:242:LEU:O | 24:4O:246:TYR:HB2 | 2.15 | 0.47 |
| 23:4R:184:MET:O | 23:4R:185:SER:C | 2.52 | 0.47 |
| 36:5W:146:ARG:HG3 | 36:5W:147:ILE:H | 1.78 | 0.47 |
| 38:6C:37:ASN:OD1 | 41:VO:213:ARG:NH2 | 2.48 | 0.47 |
| 38:6C:105:LYS:HD2 | 38:6C:105:LYS:O | 2.14 | 0.47 |
| 40:AA:269:LEU:O | 40:AA:377:LEU:HA | 2.15 | 0.47 |
| 40:AE:3:GLU:HA | 40:AE:51:THR:HA | 1.96 | 0.47 |
| 40:AE:302:MET:HE3 | 40:AE:302:MET:HB3 | 1.82 | 0.47 |
| 41:AN:341:PHE:HB3 | 41:AN:348:ASN:HD21 | 1.79 | 0.47 |
| 40:BA:398:TYR:O | 40:BA:401:ARG:NH1 | 2.48 | 0.47 |
| 40:BG:301:GLN:HE21 | 40:BG:307:PRO:HG3 | 1.80 | 0.47 |
| 40:BI:10:GLY:O | 40:BI:11:GLN:C | 2.53 | 0.47 |
| 41:BN:73:MET:HG3 | 41:BN:92:PHE:HB3 | 1.96 | 0.47 |
| 41:BP:97:ALA:O | 41:BP:98:GLY:C | 2.52 | 0.47 |
| 40:CA:244:PHE:HB2 | 40:CA:356:ASN:HD21 | 1.80 | 0.47 |
| 41:CN:372:THR:O | 41:CN:375:GLN:HG2 | 2.15 | 0.47 |
| 41:CO:373:ALA:C | 41:CO:375:GLN:H | 2.15 | 0.47 |
| 41:DB:204:ASN:CG | 43:DB:501:GDP:HN22 | 2.18 | 0.47 |
| 40:DF:333:ALA:HB2 | 41:DN:175:VAL:HG11 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DH:75:ILE:HG21 | 40:DH:94:THR:HB | 1.96 | 0.47 |
| 40:DH:239:THR:O | 40:DH:239:THR:OG1 | 2.30 | 0.47 |
| 40:DI:102:ASN:O | 40:DI:105:ARG:N | 2.48 | 0.47 |
| 41:DL:213:ARG:HB3 | 41:DL:297:LYS:HE3 | 1.95 | 0.47 |
| 41:DM:3:GLU:H | 41:DM:131:GLN:H | 1.63 | 0.47 |
| 41:DM:52:ASN:O | 41:DM:59:TYR:HA | 2.15 | 0.47 |
| 41:DN:156:ARG:HD3 | 41:DN:156:ARG:HA | 1.64 | 0.47 |
| 41:DN:338:SER:O | 41:DN:339:SER:C | 2.52 | 0.47 |
| 40:EA:228:ASN:HD21 | 42:EA:501:GTP:HN1 | 1.63 | 0.47 |
| 40:EE:231:ILE:O | 40:EE:235:VAL:HG23 | 2.14 | 0.47 |
| 40:EE:245:ASP:N | 40:EE:245:ASP:OD1 | 2.46 | 0.47 |
| 40:EH:305:CYS:O | 40:EH:306:ASP:C | 2.53 | 0.47 |
| 40:EI:28:HIS:CE1 | 40:EI:243:ARG:HD2 | 2.49 | 0.47 |
| 40:EI:346:TRP:HZ2 | 40:EI:434:VAL:HG13 | 1.80 | 0.47 |
| 41:EL:271:ALA:HB1 | 41:EL:292:GLN:HG3 | 1.97 | 0.47 |
| 41:EP:424:THR:OG1 | 41:EP:425:ARG:N | 2.48 | 0.47 |
| 41:FB:4:ILE:HD11 | 41:FB:240:LEU:HD11 | 1.95 | 0.47 |
| 40:FE:326:LYS:HB3 | 41:FM:208:TYR:CE1 | 2.49 | 0.47 |
| 40:FF:352:LYS:HD2 | 41:FN:179:VAL:HG13 | 1.96 | 0.47 |
| 41:FM:6:HIS:O | 41:FM:63:ALA:HA | 2.13 | 0.47 |
| 41:FO:8:GLN:HE21 | 41:FO:65:LEU:HG | 1.79 | 0.47 |
| 41:FP:210:ILE:HG12 | 41:FP:298:ASN:HA | 1.95 | 0.47 |
| 40:GE:397:MET:H | 40:GE:397:MET:HG2 | 1.53 | 0.47 |
| 40:GH:319:TYR:O | 40:GH:355:ILE:HA | 2.14 | 0.47 |
| 40:GI:175:PRO:HB3 | 40:GI:389:ARG:CZ | 2.44 | 0.47 |
| 41:GN:56:GLY:O | 41:GN:57:GLY:C | 2.52 | 0.47 |
| 41:GP:257:MET:HG2 | 41:GP:266:PHE:CZ | 2.49 | 0.47 |
| 40:HF:2:ARG:HA | 40:HF:133:GLN:HE22 | 1.80 | 0.47 |
| 40:HH:138:PHE:HE2 | 40:HH:235:VAL:HG11 | 1.79 | 0.47 |
| 40:HI:371:GLN:OE1 | 40:HI:371:GLN:N | 2.44 | 0.47 |
| 41:HN:142:GLY:O | 41:HN:143:THR:C | 2.53 | 0.47 |
| 41:IB:171:PRO:HB3 | 41:IB:181:GLU:HG2 | 1.97 | 0.47 |
| 40:IH:11:GLN:NE2 | 40:IH:15:GLN:OE1 | 2.47 | 0.47 |
| 40:II:67:PHE:HB3 | 40:II:75:ILE:HD12 | 1.96 | 0.47 |
| 41:IN:287:PRO:HA | 41:IN:329:GLN:HE22 | 1.79 | 0.47 |
| 41:IP:11:GLN:HA | 41:IP:72:THR:HG21 | 1.94 | 0.47 |
| 41:IQ:7:LEU:HD13 | 41:IQ:64:VAL:HB | 1.96 | 0.47 |
| 40:JF:70:LEU:HD23 | 40:JF:114:LEU:HD12 | 1.97 | 0.47 |
| 40:JH:119:LEU:HD11 | 40:JH:156:ARG:HB3 | 1.97 | 0.47 |
| 41:JM:178:THR:O | 41:JM:181:GLU:HB2 | 2.14 | 0.47 |
| 41:JO:135:LEU:O | 41:JO:166:THR:HA | 2.13 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KE:71:GLU:HG2 | 40:KE:98:ASP:HB3 | 1.96 | 0.47 |
| 40:KE:234:ILE:O | 40:KE:238:ILE:HG12 | 2.15 | 0.47 |
| 40:KE:401:ARG:HD2 | 40:KE:404:VAL:HG21 | 1.95 | 0.47 |
| 41:KN:207:LEU:HD13 | 41:KN:225:LEU:HB3 | 1.95 | 0.47 |
| 41:LB:77:ARG:NH1 | 41:LB:82:GLY:O | 2.48 | 0.47 |
| 41:LB:134:GLN:HE21 | 41:LB:167:PHE:HE1 | 1.63 | 0.47 |
| 40:LD:254:GLU:HG2 | 40:LD:352:LYS:HE2 | 1.97 | 0.47 |
| 40:LF:12:ALA:O | 40:LF:16:ILE:HG13 | 2.13 | 0.47 |
| 40:LF:262:TYR:CZ | 41:LN:393:ALA:HB2 | 2.49 | 0.47 |
| 40:LG:160:ASP:HB2 | 40:LG:161:TYR:H | 1.57 | 0.47 |
| 41:LO:289:LEU:HD11 | 41:LO:363:MET:HB3 | 1.95 | 0.47 |
| 40:MA:71:GLU:HG2 | 40:MA:72:PRO:CD | 2.42 | 0.47 |
| 40:MA:252:LEU:HA | 40:MA:255:PHE:CD2 | 2.50 | 0.47 |
| 40:MG:199:ASP:O | 40:MG:266:HIS:HB2 | 2.13 | 0.47 |
| 40:MG:363:VAL:O | 40:MG:364:PRO:C | 2.52 | 0.47 |
| 40:MH:70:LEU:HD23 | 40:MH:114:LEU:HD12 | 1.97 | 0.47 |
| 41:MM:7:LEU:HD23 | 41:MM:64:VAL:HB | 1.94 | 0.47 |
| 41:MO:152:ILE:HG12 | 41:MO:164:MET:HE1 | 1.97 | 0.47 |
| 41:MO:286:VAL:HG11 | 41:MO:326:VAL:HG22 | 1.96 | 0.47 |
| 41:MP:51:TYR:HB3 | 41:MP:59:TYR:HB3 | 1.96 | 0.47 |
| 40:NA:194:THR:HG22 | 40:NA:198:SER:HB2 | 1.95 | 0.47 |
| 40:NA:224:TYR:HB3 | 42:NN:501:GTP:N1 | 2.30 | 0.47 |
| 40:ND:224:TYR:HA | 40:ND:227:LEU:HD12 | 1.97 | 0.47 |
| 40:NH:51:THR:HG22 | 40:NH:52:PHE:H | 1.78 | 0.47 |
| 40:NH:222:PRO:HG2 | 41:NO:324:LYS:HB2 | 1.97 | 0.47 |
| 40:NH:235:VAL:HA | 40:NH:238:ILE:HG22 | 1.95 | 0.47 |
| 41:NL:152:ILE:HG23 | 41:NL:164:MET:HG3 | 1.95 | 0.47 |
| 40:OA:298:PRO:HB3 | 40:OA:307:PRO:HD2 | 1.95 | 0.47 |
| 40:OD:362:VAL:HG13 | 40:OD:367:LEU:HB3 | 1.96 | 0.47 |
| 41:OL:186:THR:HG23 | 41:OL:415:MET:HG3 | 1.97 | 0.47 |
| 41:OO:378:PHE:HA | 41:OO:381:ILE:HG22 | 1.97 | 0.47 |
| 40:PD:70:LEU:HD23 | 40:PD:114:LEU:HD12 | 1.96 | 0.47 |
| 40:PH:235:VAL:O | 40:PH:239:THR:HG22 | 2.15 | 0.47 |
| 41:PN:177:ASP:N | 41:PN:181:GLU:OE2 | 2.48 | 0.47 |
| 41:PO:334:GLN:NE2 | 41:PO:348:ASN:OD1 | 2.48 | 0.47 |
| 40:QE:247:ALA:O | 41:QM:11:GLN:NE2 | 2.47 | 0.47 |
| 40:QG:101:ASN:HA | 40:QG:144:GLY:N | 2.29 | 0.47 |
| 40:QG:238:ILE:HA | 40:QG:318:LEU:HD22 | 1.96 | 0.47 |
| 41:QN:36:TYR:O | 41:QN:37:HIS:ND1 | 2.46 | 0.47 |
| 41:RB:139:LEU:HD21 | 41:RB:192:LEU:HD11 | 1.96 | 0.47 |
| 40:RG:258:ASN:HB3 | 40:RG:352:LYS:HD3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RH:26:LEU:HD23 | 40:RH:363:VAL:HG22 | 1.97 | 0.47 |
| 40:RI:88:HIS:CD2 | 40:SI:283:HIS:HB2 | 2.49 | 0.47 |
| 41:RL:285:THR:HB | 41:RL:287:PRO:HD2 | 1.96 | 0.47 |
| 40:SH:398:TYR:O | 40:SH:401:ARG:NH2 | 2.47 | 0.47 |
| 41:SL:131:GLN:NE2 | 41:SL:249:ASP:OD2 | 2.46 | 0.47 |
| 41:SO:342:VAL:HB | 41:SO:344:TRP:CD1 | 2.49 | 0.47 |
| 41:TL:165:ASN:HD22 | 41:TL:198:GLU:HB2 | 1.79 | 0.47 |
| 40:UA:98:ASP:HB3 | 41:UN:249:ASP:OD1 | 2.15 | 0.47 |
| 40:UI:223:THR:HG21 | 41:UP:320:ARG:NH1 | 2.29 | 0.47 |
| 40:UI:228:ASN:CG | 42:UI:501:GTP:HN21 | 2.16 | 0.47 |
| 40:UI:407:TYR:O | 40:UI:412:MET:HB2 | 2.14 | 0.47 |
| 41:UO:293:MET:HG2 | 41:UO:367:PHE:HB2 | 1.95 | 0.47 |
| 40:VA:20:CYS:HA | 40:VA:232:SER:HB2 | 1.97 | 0.47 |
| 40:VA:73:THR:HA | 40:VA:76:ASP:HB2 | 1.96 | 0.47 |
| 41:VB:100:ASN:HB3 | 41:VB:103:LYS:HB2 | 1.95 | 0.47 |
| 40:VF:142:GLY:O | 40:VF:186:ASN:ND2 | 2.34 | 0.47 |
| 40:VH:258:ASN:HD21 | 41:VP:99:ASN:HD22 | 1.61 | 0.47 |
| 40:VJ:204:VAL:HG11 | 40:VJ:231:ILE:HG12 | 1.96 | 0.47 |
| 40:VJ:236:SER:O | 40:VJ:320:ARG:NH2 | 2.45 | 0.47 |
| 40:VJ:332:ILE:HG23 | 40:VJ:351:PHE:HD2 | 1.79 | 0.47 |
| 41:VQ:87:PRO:HD3 | 41:WP:281:TYR:HD1 | 1.79 | 0.47 |
| 41:VQ:240:LEU:HD11 | 41:VQ:250:LEU:HG | 1.95 | 0.47 |
| 41:VQ:292:GLN:HG2 | 41:VQ:298:ASN:ND2 | 2.29 | 0.47 |
| 40:WA:101:ASN:HB2 | 41:WN:255:VAL:CG1 | 2.44 | 0.47 |
| 40:WH:12:ALA:HB1 | 40:WH:171:ILE:HD12 | 1.96 | 0.47 |
| 41:WP:173:PRO:HD3 | 41:WP:380:ARG:NH1 | 2.29 | 0.47 |
| 9:2B:115:GLU:OE2 | 9:2B:119:GLN:NE2 | 2.47 | 0.47 |
| 11:2I:161:ARG:NH1 | 40:MG:398:TYR:O | 2.42 | 0.47 |
| 11:2I:186:LYS:HA | 11:2I:251:TYR:HB3 | 1.96 | 0.47 |
| 11:2K:243:VAL:HG22 | 11:2K:246:LYS:HE2 | 1.97 | 0.47 |
| 12:2P:109:LEU:HD13 | 12:2P:134:MET:HE2 | 1.96 | 0.47 |
| 13:2W:119:CYS:O | 13:2W:119:CYS:SG | 2.72 | 0.47 |
| 13:2X:49:ILE:HD13 | 13:2X:59:ILE:HG12 | 1.95 | 0.47 |
| 13:2X:172:TYR:HD2 | 13:2X:176:GLU:HB2 | 1.79 | 0.47 |
| 15:3E:67:LEU:HB3 | 15:3E:71:ARG:NH1 | 2.28 | 0.47 |
| 16:3J:31:GLN:HE21 | 16:3K:366:LEU:HD22 | 1.79 | 0.47 |
| 16:3J:276:TYR:HE2 | 16:3J:381:ALA:HB2 | 1.78 | 0.47 |
| 16:3K:168:ALA:HB2 | 16:3K:228:ARG:HH12 | 1.80 | 0.47 |
| 17:3O:99:TRP:CD1 | 17:3P:208:ILE:HG13 | 2.49 | 0.47 |
| 19:3Y:140:VAL:HG11 | 41:LB:22:GLU:HG3 | 1.96 | 0.47 |
| 22:4I:625:GLU:O | 22:4I:629:LYS:HG3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:4V:368:VAL:O | 26:4V:372:PHE:HB2 | 2.15 | 0.47 |
| 31:5J:826:ILE:O | 31:5J:830:ILE:HG12 | 2.14 | 0.47 |
| 38:6C:9:ASP:OD1 | 38:6C:17:SER:N | 2.48 | 0.47 |
| 40:AF:20:CYS:HA | 40:AF:232:SER:HB2 | 1.97 | 0.47 |
| 40:AG:279:GLU:O | 40:MG:89:PRO:HG3 | 2.14 | 0.47 |
| 40:BA:7:VAL:HG13 | 40:BA:66:VAL:HG13 | 1.96 | 0.47 |
| 41:BB:61:PRO:HD2 | 41:BB:84:ILE:O | 2.15 | 0.47 |
| 40:BE:440:GLU:HB2 | 41:BM:390:ARG:HD3 | 1.97 | 0.47 |
| 40:BF:405:HIS:HE1 | 41:BM:259:PRO:O | 1.98 | 0.47 |
| 40:BG:102:ASN:HD22 | 40:BG:105:ARG:HD3 | 1.79 | 0.47 |
| 40:CG:27:GLU:HG2 | 40:CG:243:ARG:HH12 | 1.80 | 0.47 |
| 40:CI:140:SER:OG | 42:CI:501:GTP:O1A | 2.22 | 0.47 |
| 41:CL:156:ARG:O | 41:CL:157:GLU:C | 2.53 | 0.47 |
| 41:CN:376:GLU:HA | 41:CN:379:LYS:HB2 | 1.95 | 0.47 |
| 41:CP:284:LEU:HD23 | 41:CP:284:LEU:HA | 1.73 | 0.47 |
| 40:DE:9:VAL:HG21 | 40:DE:153:LEU:HD22 | 1.95 | 0.47 |
| 40:DF:75:ILE:O | 40:DF:78:VAL:HG12 | 2.15 | 0.47 |
| 40:DF:402:ALA:O | 40:DF:403:PHE:C | 2.52 | 0.47 |
| 40:DH:88:HIS:O | 40:DH:89:PRO:C | 2.53 | 0.47 |
| 40:DH:334:ALA:O | 40:DH:335:ILE:C | 2.52 | 0.47 |
| 41:DL:397:TRP:O | 41:DL:401:GLU:HG2 | 2.14 | 0.47 |
| 41:DL:414:ASN:O | 41:DL:415:MET:C | 2.52 | 0.47 |
| 40:EA:238:ILE:HG23 | 40:EA:255:PHE:CE2 | 2.48 | 0.47 |
| 40:EF:241:SER:OG | 40:EF:356:ASN:ND2 | 2.48 | 0.47 |
| 40:EF:370:VAL:HG22 | 40:EF:372:ARG:H | 1.79 | 0.47 |
| 40:EH:307:PRO:HA | 40:EH:382:ALA:CB | 2.44 | 0.47 |
| 40:EH:308:ARG:C | 40:EH:310:GLY:H | 2.16 | 0.47 |
| 40:EH:387:TRP:HB3 | 40:EH:424:MET:CE | 2.45 | 0.47 |
| 40:EI:137:ILE:HG12 | 40:EI:168:GLU:HG3 | 1.97 | 0.47 |
| 40:EI:177:VAL:O | 40:EI:178:SER:HB3 | 2.13 | 0.47 |
| 40:EI:308:ARG:O | 40:EI:310:GLY:N | 2.46 | 0.47 |
| 41:EM:358:PRO:HB2 | 41:EM:361:LEU:HD12 | 1.96 | 0.47 |
| 41:EP:130:LEU:HB3 | 41:EP:162:ARG:HG2 | 1.97 | 0.47 |
| 40:FA:132:LEU:HD22 | 40:FA:132:LEU:HA | 1.72 | 0.47 |
| 40:FH:235:VAL:HA | 40:FH:238:ILE:HG22 | 1.97 | 0.47 |
| 41:FM:60:VAL:HG21 | 41:FM:86:ARG:NE | 2.30 | 0.47 |
| 40:GE:207:GLU:HB3 | 40:GE:304:LYS:HZ2 | 1.80 | 0.47 |
| 40:GE:217:LEU:O | 40:GE:219:ILE:N | 2.45 | 0.47 |
| 40:GE:278:ALA:O | 40:GE:279:GLU:C | 2.53 | 0.47 |
| 40:GE:305:CYS:O | 40:GE:305:CYS:SG | 2.72 | 0.47 |
| 40:GG:142:GLY:HA2 | 40:GG:183:GLU:HG2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GM:20:PHE:HA | 41:GM:230:SER:HB2 | 1.96 | 0.47 |
| 41:GN:70:PRO:HD2 | 41:GN:94:GLN:HA | 1.95 | 0.47 |
| 41:GN:383:GLU:O | 41:GN:386:THR:HB | 2.14 | 0.47 |
| 41:GP:275:SER:OG | 41:GP:276:ARG:N | 2.47 | 0.47 |
| 41:GP:313:VAL:HB | 41:GP:349:VAL:HA | 1.95 | 0.47 |
| 41:HB:170:VAL:HG11 | 41:HB:377:LEU:HD21 | 1.96 | 0.47 |
| 40:HE:241:SER:CB | 40:HE:250:VAL:H | 2.28 | 0.47 |
| 40:HE:278:ALA:O | 40:HE:281:ALA:N | 2.48 | 0.47 |
| 40:HF:180:ALA:HB3 | 40:HF:183:GLU:HG3 | 1.97 | 0.47 |
| 40:HF:221:ARG:NE | 41:HM:322:SER:OG | 2.47 | 0.47 |
| 40:HI:271:THR:HG22 | 40:HI:376:MET:HB3 | 1.96 | 0.47 |
| 41:HO:392:LYS:NZ | 41:HO:405:GLU:OE2 | 2.47 | 0.47 |
| 40:IA:139:HIS:NE2 | 40:IA:168:GLU:OE2 | 2.47 | 0.47 |
| 40:IF:121:ARG:HH12 | 40:IF:125:LEU:HG | 1.79 | 0.47 |
| 40:IF:326:LYS:HA | 40:IF:326:LYS:HD3 | 1.54 | 0.47 |
| 40:II:109:THR:HG23 | 40:II:110:ILE:H | 1.78 | 0.47 |
| 40:II:165:SER:OG | 40:II:256:GLN:OE1 | 2.29 | 0.47 |
| 40:JE:200:CYS:HA | 40:JE:266:HIS:HB2 | 1.97 | 0.47 |
| 40:JF:249:ASN:HB2 | 41:JN:11:GLN:HE22 | 1.79 | 0.47 |
| 40:KE:45:GLY:N | 40:KE:48:SER:HG | 2.12 | 0.47 |
| 40:KE:139:HIS:O | 40:KE:170:SER:HA | 2.15 | 0.47 |
| 40:KF:205:ASP:HB2 | 40:KF:303:VAL:HA | 1.96 | 0.47 |
| 40:KF:318:LEU:O | 40:KF:374:VAL:HA | 2.13 | 0.47 |
| 41:KL:212:PHE:CE1 | 41:KL:220:PRO:HG2 | 2.49 | 0.47 |
| 41:KN:204:ASN:OD1 | 43:KN:502:GDP:O2' | 2.23 | 0.47 |
| 40:LF:320:ARG:HG3 | 40:LF:373:ALA:HB3 | 1.94 | 0.47 |
| 40:LG:285:GLN:H | 40:LG:285:GLN:HG2 | 1.45 | 0.47 |
| 40:LH:401:ARG:NH2 | 40:LH:414:GLU:OE1 | 2.48 | 0.47 |
| 40:MF:88:HIS:HD2 | 40:MF:91:GLN:HE21 | 1.61 | 0.47 |
| 40:MF:105:ARG:HA | 40:MF:109:THR:OG1 | 2.14 | 0.47 |
| 41:MO:116:VAL:HB | 41:MO:151:LEU:HD21 | 1.97 | 0.47 |
| 41:MP:194:GLU:N | 41:MP:194:GLU:OE2 | 2.48 | 0.47 |
| 40:NE:207:GLU:HB3 | 40:NE:304:LYS:NZ | 2.29 | 0.47 |
| 40:NG:140:SER:OG | 42:NG:501:GTP:O2A | 2.32 | 0.47 |
| 40:NH:245:ASP:HA | 40:NH:249:ASN:HD21 | 1.80 | 0.47 |
| 40:NH:400:LYS:NZ | 41:NO:425:ARG:HH21 | 2.12 | 0.47 |
| 41:NN:73:MET:HG3 | 41:NN:92:PHE:HB3 | 1.95 | 0.47 |
| 41:NN:290:THR:HG21 | 41:NN:329:GLN:HB3 | 1.96 | 0.47 |
| 41:NO:161:ASP:O | 41:NO:251:ARG:NH2 | 2.48 | 0.47 |
| 41:NO:204:ASN:OD1 | 43:NO:502:GDP:O2' | 2.30 | 0.47 |
| 40:OE:254:GLU:HA | 40:OE:257:THR:HG22 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OM:237:THR:O | 41:OM:241:ARG:NH1 | 2.47 | 0.47 |
| 41:OO:28:HIS:HE1 | 41:OO:47:ILE:HA | 1.78 | 0.47 |
| 40:PE:206:ASN:HA | 40:PE:209:ILE:HG22 | 1.96 | 0.47 |
| 40:QA:385:GLU:O | 40:QA:389:ARG:NE | 2.47 | 0.47 |
| 41:QN:222:TYR:HD1 | 41:QN:225:LEU:HD12 | 1.78 | 0.47 |
| 41:QO:313:VAL:HG12 | 41:QO:369:GLY:HA2 | 1.95 | 0.47 |
| 40:RA:117:LEU:HD23 | 40:RA:121:ARG:NH2 | 2.24 | 0.47 |
| 40:RE:209:ILE:HA | 40:RE:212:ILE:HG12 | 1.96 | 0.47 |
| 40:RE:329:ASN:HB2 | 41:RM:175:VAL:HG11 | 1.97 | 0.47 |
| 41:RN:2:ARG:HG3 | 41:RN:240:LEU:HD12 | 1.97 | 0.47 |
| 41:RN:28:HIS:CE1 | 41:RN:241:ARG:HH21 | 2.33 | 0.47 |
| 41:RO:293:MET:SD | 41:RO:367:PHE:HB2 | 2.55 | 0.47 |
| 41:RP:8:GLN:HE21 | 41:RP:14:ASN:HD22 | 1.60 | 0.47 |
| 40:SA:250:VAL:HB | 40:SA:255:PHE:CE2 | 2.50 | 0.47 |
| 40:SE:188:ILE:HG21 | 40:SE:394:PHE:CE2 | 2.49 | 0.47 |
| 40:SE:262:TYR:OH | 41:SM:391:ARG:O | 2.33 | 0.47 |
| 40:SF:209:ILE:HA | 40:SF:212:ILE:HG22 | 1.97 | 0.47 |
| 41:SO:342:VAL:HB | 41:SO:344:TRP:NE1 | 2.29 | 0.47 |
| 40:TA:107:HIS:HD2 | 40:TA:152:LEU:HB2 | 1.80 | 0.47 |
| 41:TO:178:THR:HB | 41:TO:181:GLU:HG3 | 1.97 | 0.47 |
| 41:TO:372:THR:HG22 | 41:TO:422:VAL:HG22 | 1.97 | 0.47 |
| 40:UA:143:GLY:N | 42:UA:501:GTP:O2A | 2.45 | 0.47 |
| 40:UF:239:THR:O | 40:UF:243:ARG:NH1 | 2.48 | 0.47 |
| 40:UF:273:ALA:HB3 | 40:UF:274:PRO:HD3 | 1.97 | 0.47 |
| 40:UI:63:PRO:HD2 | 40:UI:86:LEU:O | 2.15 | 0.47 |
| 40:UI:177:VAL:CG1 | 41:UP:327:ASP:HB3 | 2.45 | 0.47 |
| 40:UI:228:ASN:OD1 | 42:UI:501:GTP:N2 | 2.37 | 0.47 |
| 40:UI:376:MET:O | 40:UI:377:LEU:C | 2.51 | 0.47 |
| 41:UN:376:GLU:O | 41:UN:380:ARG:HG2 | 2.14 | 0.47 |
| 41:UP:54:ALA:O | 41:UP:55:THR:C | 2.52 | 0.47 |
| 40:VA:100:ALA:HA | 41:VO:252:LYS:HG2 | 1.96 | 0.47 |
| 40:VA:128:GLN:HG2 | 40:WA:285:GLN:HG3 | 1.95 | 0.47 |
| 41:VB:187:LEU:HD11 | 41:VB:408:PHE:HE1 | 1.80 | 0.47 |
| 41:VQ:170:VAL:HG21 | 41:VQ:377:LEU:HD11 | 1.97 | 0.47 |
| 41:WB:6:HIS:O | 41:WB:63:ALA:HA | 2.14 | 0.47 |
| 40:WE:70:LEU:HD23 | 40:WE:114:LEU:HD12 | 1.97 | 0.47 |
| 41:WN:244:GLY:CA | 41:WN:355:ASP:HB3 | 2.43 | 0.47 |
| 41:WP:134:GLN:HA | 41:WP:165:ASN:O | 2.15 | 0.47 |
| 7:1S:20:ILE:HB | 7:1S:611:ILE:HB | 1.96 | 0.47 |
| 7:1U:440:GLU:HA | 7:1U:458:LYS:HB3 | 1.97 | 0.47 |
| 8:1X:204:ILE:HD11 | 40:UA:369:LYS:HD3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:1Z:455:ILE:HD13 | 41:UO:276:ARG:HD2 | 1.97 | 0.47 |
| 10:2E:151:HIS:CG | 10:2E:157:ARG:HB2 | 2.50 | 0.47 |
| 10:2F:61:CYS:SG | 10:2F:62:PHE:N | 2.87 | 0.47 |
| 11:2J:185:MET:HG2 | 11:2J:186:LYS:H | 1.77 | 0.47 |
| 11:2K:63:LEU:O | 41:LO:190:HIS:NE2 | 2.41 | 0.47 |
| 11:2K:221:ILE:CG2 | 11:2K:222:PRO:N | 2.77 | 0.47 |
| 12:2O:48:MET:HB2 | 12:2O:51:SER:HB2 | 1.97 | 0.47 |
| 12:2O:216:GLN:NE2 | 41:WN:118:ASP:OD2 | 2.47 | 0.47 |
| 13:2T:82:ASN:ND2 | 13:2T:126:ASP:O | 2.45 | 0.47 |
| 13:2U:90:GLU:HB2 | 13:2U:104:ARG:NH1 | 2.30 | 0.47 |
| 13:2V:79:ILE:HD12 | 13:2V:164:ARG:HB3 | 1.97 | 0.47 |
| 13:2W:139:PHE:HA | 13:2W:142:ARG:CG | 2.44 | 0.47 |
| 13:2W:157:HIS:HB3 | 13:2W:158:ALA:H | 1.53 | 0.47 |
| 13:2X:115:LYS:HG2 | 13:2X:118:ILE:O | 2.13 | 0.47 |
| 13:2X:172:TYR:O | 13:2X:173:SER:C | 2.53 | 0.47 |
| 14:3A:70:MET:HE1 | 40:LF:159:VAL:HG21 | 1.97 | 0.47 |
| 14:3C:24:LEU:CD1 | 40:LG:162:GLY:H | 2.28 | 0.47 |
| 16:3M:37:GLN:O | 16:3M:41:GLU:HG2 | 2.15 | 0.47 |
| 17:3O:361:MET:HE3 | 17:3O:361:MET:HB3 | 1.74 | 0.47 |
| 18:3U:346:LYS:HZ3 | 18:3V:92:ALA:HB2 | 1.78 | 0.47 |
| 21:4D:188:LYS:HB3 | 40:AA:39:ASP:HB2 | 1.96 | 0.47 |
| 21:4D:521:ALA:O | 21:4D:522:GLN:C | 2.53 | 0.47 |
| 21:4E:264:ILE:HG12 | 21:4E:275:ILE:HG23 | 1.97 | 0.47 |
| 21:4E:435:GLY:O | 21:4E:436:ARG:C | 2.53 | 0.47 |
| 21:4E:487:PRO:HA | 21:4E:490:PHE:HD2 | 1.79 | 0.47 |
| 21:4F:425:ALA:HB2 | 21:4F:506:LEU:HD21 | 1.96 | 0.47 |
| 21:4F:439:VAL:HG22 | 21:4F:454:PRO:HD3 | 1.96 | 0.47 |
| 22:4H:349:ARG:NH2 | 41:CL:32:PRO:O | 2.46 | 0.47 |
| 22:4I:52:LYS:HD2 | 22:4I:52:LYS:HA | 1.75 | 0.47 |
| 22:4J:533:MET:HG3 | 22:4J:597:GLN:NE2 | 2.30 | 0.47 |
| 22:4J:633:GLU:HB2 | 22:4J:699:TRP:CZ2 | 2.49 | 0.47 |
| 23:4M:100:GLN:HB3 | 23:4M:103:PHE:CZ | 2.50 | 0.47 |
| 23:4N:210:LEU:HD12 | 23:4N:210:LEU:HA | 1.81 | 0.47 |
| 24:4O:193:ARG:HD3 | 41:CL:57:GLY:H | 1.79 | 0.47 |
| 24:4O:199:GLY:N | 40:DE:221:ARG:HG3 | 2.26 | 0.47 |
| 23:4P:194:ALA:HA | 23:4P:197:LEU:HD22 | 1.96 | 0.47 |
| 23:4Q:171:PRO:C | 23:4Q:173:SER:H | 2.17 | 0.47 |
| 23:4Q:193:ARG:NH1 | 41:CO:56:GLY:H | 2.13 | 0.47 |
| 23:4Q:259:ARG:HH21 | 40:EH:366:ASP:CG | 2.17 | 0.47 |
| 23:4R:113:TRP:O | 23:4R:116:ALA:N | 2.48 | 0.47 |
| 26:4V:123:LEU:HD23 | 26:4V:309:VAL:HG21 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:5X:101:TRP:HB2 | 41:OL:361:LEU:HD23 | 1.95 | 0.47 |
| 36:5Z:255:ASP:HA | 36:5Z:258:ARG:HG2 | 1.97 | 0.47 |
| 39:6F:23:GLN:OE1 | 39:6F:66:ARG:NH1 | 2.47 | 0.47 |
| 39:6J:129:CYS:HG | 40:PF:283:HIS:HE2 | 1.63 | 0.47 |
| 39:6L:127:LEU:O | 40:OD:84:ARG:NH2 | 2.47 | 0.47 |
| 40:AA:7:VAL:HB | 40:AA:137:ILE:HG22 | 1.97 | 0.47 |
| 41:AB:237:THR:HG22 | 41:AB:250:LEU:HD21 | 1.96 | 0.47 |
| 40:AF:70:LEU:HD22 | 40:AF:110:ILE:HG22 | 1.96 | 0.47 |
| 40:AH:188:ILE:HG22 | 40:AH:420:ALA:HB1 | 1.96 | 0.47 |
| 40:AH:294:ALA:HA | 40:AH:297:GLU:HG3 | 1.97 | 0.47 |
| 41:AL:269:GLY:HA3 | 41:AL:367:PHE:HB3 | 1.95 | 0.47 |
| 41:AN:6:HIS:HD2 | 41:AN:134:GLN:HE21 | 1.63 | 0.47 |
| 41:AN:86:ARG:HH11 | 41:BN:282:ARG:HG2 | 1.79 | 0.47 |
| 41:AN:232:THR:HG21 | 41:AN:268:PRO:HB2 | 1.97 | 0.47 |
| 41:AO:98:GLY:O | 41:AO:99:ASN:C | 2.53 | 0.47 |
| 41:AO:313:VAL:HA | 41:AO:369:GLY:HA2 | 1.97 | 0.47 |
| 41:AP:222:TYR:HA | 41:AP:225:LEU:HD12 | 1.97 | 0.47 |
| 40:BA:12:ALA:O | 40:BA:16:ILE:HG12 | 2.14 | 0.47 |
| 41:BB:392:LYS:HB3 | 41:BB:392:LYS:HE3 | 1.42 | 0.47 |
| 40:BE:311:LYS:HE3 | 40:BE:311:LYS:HB3 | 1.40 | 0.47 |
| 40:BH:121:ARG:HD2 | 40:BH:124:LYS:HD3 | 1.96 | 0.47 |
| 40:BH:301:GLN:HG3 | 40:BH:307:PRO:HG2 | 1.95 | 0.47 |
| 41:BL:107:THR:O | 41:BL:110:ALA:N | 2.40 | 0.47 |
| 41:BL:404:ASP:OD1 | 41:BL:404:ASP:N | 2.48 | 0.47 |
| 41:BM:107:THR:O | 41:BM:109:GLY:N | 2.47 | 0.47 |
| 41:BM:311:LEU:HD23 | 41:BM:342:VAL:HG11 | 1.96 | 0.47 |
| 41:BN:421:PRO:HA | 41:BN:424:THR:HG22 | 1.97 | 0.47 |
| 41:BO:102:ALA:HB2 | 41:BO:403:MET:HG3 | 1.97 | 0.47 |
| 41:BO:238:THR:HG21 | 41:BO:318:ARG:HG2 | 1.97 | 0.47 |
| 41:BO:297:LYS:HE3 | 41:BO:297:LYS:HB2 | 1.44 | 0.47 |
| 41:BP:201:CYS:O | 41:BP:268:PRO:HD3 | 2.15 | 0.47 |
| 40:CA:363:VAL:O | 40:CA:365:GLY:N | 2.48 | 0.47 |
| 41:CB:107:THR:OG1 | 41:CB:108:GLU:N | 2.47 | 0.47 |
| 40:CE:62:VAL:CG2 | 40:DE:283:HIS:HB3 | 2.44 | 0.47 |
| 40:CE:76:ASP:HA | 40:CE:79:ARG:HG2 | 1.96 | 0.47 |
| 40:CE:177:VAL:HG23 | 41:CL:331:LEU:CB | 2.45 | 0.47 |
| 40:CH:119:LEU:HD11 | 40:CH:156:ARG:HB3 | 1.97 | 0.47 |
| 40:CH:209:ILE:H | 40:CH:209:ILE:HG12 | 1.43 | 0.47 |
| 40:CH:315:CYS:HB3 | 40:CH:378:SER:HB3 | 1.97 | 0.47 |
| 41:CM:65:LEU:HD21 | 41:CM:76:VAL:HG11 | 1.95 | 0.47 |
| 41:CN:122:LYS:HB3 | 41:CN:122:LYS:HE2 | 1.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CO:57:GLY:O | 41:CO:58:LYS:C | 2.52 | 0.47 |
| 41:CO:107:THR:OG1 | 41:CO:108:GLU:N | 2.47 | 0.47 |
| 41:CO:182:PRO:HB2 | 41:CO:388:MET:SD | 2.54 | 0.47 |
| 41:CP:6:HIS:HB2 | 41:CP:134:GLN:CD | 2.35 | 0.47 |
| 41:CP:110:ALA:O | 41:CP:113:VAL:HG22 | 2.14 | 0.47 |
| 41:CP:227:HIS:HA | 41:CP:230:SER:HB3 | 1.97 | 0.47 |
| 41:CP:272:PRO:HB3 | 41:CP:284:LEU:HD21 | 1.97 | 0.47 |
| 40:DA:20:CYS:HA | 40:DA:232:SER:HB2 | 1.97 | 0.47 |
| 40:DA:326:LYS:HG3 | 41:DB:212:PHE:HE1 | 1.79 | 0.47 |
| 41:DB:333:VAL:HA | 41:DB:336:LYS:HE2 | 1.97 | 0.47 |
| 40:DE:99:ALA:O | 40:DE:100:ALA:C | 2.53 | 0.47 |
| 40:DE:181:VAL:HG12 | 41:DL:349:VAL:H | 1.80 | 0.47 |
| 40:DE:272:TYR:O | 40:DE:300:ASN:ND2 | 2.48 | 0.47 |
| 40:DF:31:GLN:O | 40:DF:33:ASP:N | 2.48 | 0.47 |
| 40:DF:132:LEU:O | 40:DF:134:GLY:N | 2.47 | 0.47 |
| 40:DF:181:VAL:HG12 | 41:DM:349:VAL:H | 1.79 | 0.47 |
| 40:DF:263:PRO:O | 40:DF:264:ARG:C | 2.53 | 0.47 |
| 40:DG:20:CYS:HA | 40:DG:232:SER:HB2 | 1.95 | 0.47 |
| 40:DG:69:ASP:HA | 40:DG:145:THR:HG21 | 1.97 | 0.47 |
| 40:DI:402:ALA:O | 40:DI:403:PHE:C | 2.51 | 0.47 |
| 41:DL:12:CYS:HB3 | 41:DL:138:SER:HB2 | 1.96 | 0.47 |
| 41:DL:170:VAL:HG21 | 41:DL:377:LEU:HD21 | 1.97 | 0.47 |
| 41:DL:372:THR:HB | 41:DL:426:GLY:HA3 | 1.97 | 0.47 |
| 41:DL:380:ARG:HE | 41:DL:380:ARG:HB3 | 1.58 | 0.47 |
| 41:DM:157:GLU:O | 41:DM:158:GLU:C | 2.52 | 0.47 |
| 41:DM:174:LYS:HE2 | 41:DM:175:VAL:H | 1.79 | 0.47 |
| 41:DM:252:LYS:O | 41:DM:255:VAL:HG22 | 2.15 | 0.47 |
| 41:DN:3:GLU:CD | 41:DN:62:ARG:HH12 | 2.18 | 0.47 |
| 41:DN:190:HIS:HD2 | 41:DN:411:ALA:HA | 1.78 | 0.47 |
| 41:DP:278:SER:C | 41:DP:280:GLN:H | 2.18 | 0.47 |
| 41:DP:382:SER:OG | 41:DP:383:GLU:N | 2.46 | 0.47 |
| 41:DP:386:THR:C | 41:DP:388:MET:H | 2.18 | 0.47 |
| 40:EE:2:ARG:HH11 | 40:EE:242:LEU:HA | 1.80 | 0.47 |
| 40:EH:28:HIS:NE2 | 40:EH:243:ARG:HB2 | 2.30 | 0.47 |
| 40:EH:156:ARG:HA | 40:EH:156:ARG:HD3 | 1.71 | 0.47 |
| 40:EH:437:ASP:O | 40:EH:438:SER:C | 2.52 | 0.47 |
| 40:EI:191:THR:HB | 40:EI:387:TRP:CZ3 | 2.43 | 0.47 |
| 40:EI:385:GLU:O | 40:EI:389:ARG:N | 2.41 | 0.47 |
| 40:EI:395:ASP:O | 40:EI:396:LEU:C | 2.53 | 0.47 |
| 41:EM:222:TYR:O | 41:EM:226:ASN:N | 2.45 | 0.47 |
| 41:EO:7:LEU:HG | 41:EO:135:LEU:HD13 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EP:163:ILE:CD1 | 41:EP:251:ARG:HG2 | 2.43 | 0.47 |
| 41:EP:391:ARG:O | 41:EP:392:LYS:C | 2.53 | 0.47 |
| 40:FA:222:PRO:CD | 41:FN:324:LYS:NZ | 2.78 | 0.47 |
| 40:FE:235:VAL:HA | 40:FE:238:ILE:HG22 | 1.97 | 0.47 |
| 40:FE:347:CYS:HA | 41:FM:388:MET:HE2 | 1.97 | 0.47 |
| 40:FI:51:THR:HG21 | 40:FI:243:ARG:HB2 | 1.97 | 0.47 |
| 41:FO:174:LYS:HG2 | 41:FO:205:GLU:OE2 | 2.15 | 0.47 |
| 41:FP:12:CYS:O | 41:FP:16:ILE:HG12 | 2.15 | 0.47 |
| 41:GB:189:VAL:O | 41:GB:193:VAL:HG23 | 2.14 | 0.47 |
| 40:GE:127:ASP:O | 40:GE:129:CYS:N | 2.47 | 0.47 |
| 40:GE:380:THR:OG1 | 40:GE:381:THR:N | 2.47 | 0.47 |
| 40:GE:383:ILE:H | 40:GE:383:ILE:HG12 | 1.33 | 0.47 |
| 40:GE:430:ASP:O | 40:GE:434:VAL:HG13 | 2.15 | 0.47 |
| 40:GF:241:SER:HG | 40:GF:250:VAL:H | 1.57 | 0.47 |
| 40:GG:286:LEU:HD13 | 40:GG:286:LEU:HA | 1.76 | 0.47 |
| 40:GI:32:PRO:O | 40:GI:33:ASP:C | 2.52 | 0.47 |
| 40:GI:182:VAL:HG22 | 41:GP:256:ASN:HB3 | 1.95 | 0.47 |
| 41:GM:404:ASP:HB3 | 41:GM:407:GLU:HG2 | 1.97 | 0.47 |
| 41:GM:412:GLU:OE2 | 41:GM:416:ASN:ND2 | 2.48 | 0.47 |
| 41:GN:19:LYS:HA | 41:GN:19:LYS:HD3 | 1.71 | 0.47 |
| 40:HE:101:ASN:HA | 40:HE:143:GLY:C | 2.35 | 0.47 |
| 40:HE:195:LEU:HD13 | 40:HE:427:LEU:HD11 | 1.97 | 0.47 |
| 40:HF:205:ASP:OD1 | 40:HF:206:ASN:N | 2.47 | 0.47 |
| 40:HG:20:CYS:O | 40:HG:23:LEU:N | 2.47 | 0.47 |
| 40:HH:204:VAL:HG11 | 40:HH:231:ILE:HD11 | 1.97 | 0.47 |
| 40:HH:217:LEU:HA | 40:HH:277:SER:HB3 | 1.96 | 0.47 |
| 40:HI:205:ASP:HB3 | 40:HI:303:VAL:HA | 1.95 | 0.47 |
| 41:HN:260:PHE:HE2 | 41:HN:344:TRP:CZ3 | 2.32 | 0.47 |
| 41:HO:189:VAL:HA | 41:HO:192:LEU:HB2 | 1.96 | 0.47 |
| 41:HQ:162:ARG:HD3 | 41:HQ:162:ARG:HA | 1.71 | 0.47 |
| 41:IB:68:LEU:HD21 | 41:IB:109:GLY:HA2 | 1.96 | 0.47 |
| 41:IB:171:PRO:HG3 | 41:IB:181:GLU:HB3 | 1.95 | 0.47 |
| 40:IF:16:ILE:HA | 40:IF:228:ASN:HB3 | 1.97 | 0.47 |
| 40:IF:107:HIS:HD2 | 40:IF:152:LEU:HB2 | 1.79 | 0.47 |
| 40:IG:20:CYS:HA | 40:IG:232:SER:HB2 | 1.97 | 0.47 |
| 40:IH:9:VAL:HG12 | 40:IH:68:VAL:HG13 | 1.96 | 0.47 |
| 40:JA:70:LEU:HB2 | 40:JA:145:THR:HG22 | 1.97 | 0.47 |
| 41:JL:139:LEU:HD12 | 41:JL:170:VAL:HG12 | 1.97 | 0.47 |
| 41:JL:237:THR:O | 41:JL:241:ARG:NH1 | 2.47 | 0.47 |
| 41:JM:246:LEU:HB3 | 41:JM:353:VAL:HG13 | 1.97 | 0.47 |
| 41:JM:323:MET:H | 41:JM:323:MET:HG2 | 1.53 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JN:135:LEU:HB3 | 41:JN:166:THR:HG22 | 1.97 | 0.47 |
| 41:KB:138:SER:HA | 41:KB:169:VAL:HB | 1.97 | 0.47 |
| 41:KB:255:VAL:HA | 40:KG:406:TRP:CE2 | 2.50 | 0.47 |
| 40:KE:278:ALA:H | 40:KE:368:ALA:HB2 | 1.79 | 0.47 |
| 40:KF:326:LYS:HE2 | 41:KN:225:LEU:HD11 | 1.96 | 0.47 |
| 40:KH:139:HIS:O | 40:KH:170:SER:HA | 2.14 | 0.47 |
| 41:KL:2:ARG:HB3 | 41:KL:131:GLN:HB2 | 1.96 | 0.47 |
| 41:KL:16:ILE:HD13 | 41:KL:136:THR:HB | 1.96 | 0.47 |
| 41:KL:226:ASN:CG | 43:KL:501:GDP:HN1 | 2.17 | 0.47 |
| 40:LA:179:THR:OG1 | 41:LN:351:THR:OG1 | 2.30 | 0.47 |
| 40:LA:320:ARG:HD3 | 40:LA:360:PRO:HG3 | 1.95 | 0.47 |
| 41:LB:17:GLY:HA2 | 41:LB:20:PHE:HB3 | 1.97 | 0.47 |
| 40:LD:397:MET:HB3 | 40:LD:402:ALA:HB3 | 1.97 | 0.47 |
| 40:LF:339:ARG:O | 40:LF:340:SER:C | 2.53 | 0.47 |
| 40:LG:326:LYS:HE2 | 40:LG:326:LYS:HB3 | 1.59 | 0.47 |
| 40:LH:109:THR:OG1 | 40:LH:410:GLU:OE2 | 2.26 | 0.47 |
| 41:LN:53:GLU:HA | 41:LN:59:TYR:HD1 | 1.79 | 0.47 |
| 41:LO:36:TYR:O | 41:LO:37:HIS:ND1 | 2.47 | 0.47 |
| 41:LP:54:ALA:HA | 41:MP:283:ALA:HB2 | 1.97 | 0.47 |
| 40:MA:96:LYS:HB2 | 40:MA:96:LYS:HE3 | 1.53 | 0.47 |
| 40:MF:231:ILE:O | 40:MF:235:VAL:HG23 | 2.15 | 0.47 |
| 40:MG:288:VAL:O | 40:MG:291:ILE:HG12 | 2.15 | 0.47 |
| 41:ML:113:VAL:HA | 41:ML:116:VAL:HG12 | 1.95 | 0.47 |
| 41:MN:5:VAL:HG23 | 41:MN:130:LEU:HD11 | 1.96 | 0.47 |
| 41:MP:142:GLY:O | 41:MP:144:GLY:N | 2.47 | 0.47 |
| 41:MP:337:ASN:HB3 | 41:MP:340:TYR:HD2 | 1.79 | 0.47 |
| 40:NA:49:PHE:O | 40:NA:53:PHE:HB2 | 2.14 | 0.47 |
| 40:ND:108:TYR:HB3 | 40:ND:411:GLY:HA3 | 1.96 | 0.47 |
| 40:ND:287:SER:O | 40:ND:372:ARG:HD2 | 2.14 | 0.47 |
| 40:NG:88:HIS:HB3 | 40:NG:91:GLN:HE22 | 1.80 | 0.47 |
| 40:NH:33:ASP:OD1 | 40:NH:34:GLY:N | 2.48 | 0.47 |
| 40:NH:429:LYS:O | 40:NH:433:GLU:HG3 | 2.15 | 0.47 |
| 41:NL:67:ASP:OD2 | 41:NL:72:THR:OG1 | 2.33 | 0.47 |
| 41:NO:25:SER:OG | 41:NO:30:ILE:O | 2.32 | 0.47 |
| 41:NO:215:LEU:HB3 | 41:NO:217:LEU:HD23 | 1.95 | 0.47 |
| 40:OD:384:ALA:HA | 40:OD:387:TRP:HD1 | 1.80 | 0.47 |
| 40:OE:76:ASP:HA | 40:OE:79:ARG:HG2 | 1.96 | 0.47 |
| 40:OE:405:HIS:HA | 40:OE:408:VAL:HG22 | 1.97 | 0.47 |
| 40:OF:406:TRP:CD2 | 41:OM:255:VAL:HG22 | 2.50 | 0.47 |
| 40:OH:16:ILE:HG12 | 40:OH:228:ASN:HB3 | 1.97 | 0.47 |
| 40:OH:292:THR:O | 40:OH:295:CYS:SG | 2.70 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OH:295:CYS:HB2 | 40:OH:376:MET:HB2 | 1.96 | 0.47 |
| 41:OL:8:GLN:NE2 | 41:OL:65:LEU:HD22 | 2.28 | 0.47 |
| 41:OL:309:ARG:H | 41:OL:372:THR:HG1 | 1.57 | 0.47 |
| 41:OL:313:VAL:O | 41:OL:349:VAL:HA | 2.15 | 0.47 |
| 41:ON:133:PHE:HZ | 41:ON:159:TYR:HD2 | 1.61 | 0.47 |
| 40:PE:70:LEU:HD12 | 40:PE:145:THR:HG22 | 1.97 | 0.47 |
| 40:PF:256:GLN:HA | 40:PF:259:LEU:HB2 | 1.97 | 0.47 |
| 40:PH:311:LYS:HE3 | 40:PH:344:VAL:HG12 | 1.97 | 0.47 |
| 41:PL:1:MET:HG3 | 41:PL:48:ASN:HD22 | 1.80 | 0.47 |
| 41:QB:12:CYS:HB2 | 43:QB:501:GDP:C8 | 2.50 | 0.47 |
| 41:QB:124:ALA:HA | 41:QB:130:LEU:HD13 | 1.96 | 0.47 |
| 41:QB:138:SER:O | 41:QB:139:LEU:C | 2.51 | 0.47 |
| 41:QB:153:SER:OG | 41:QB:154:LYS:N | 2.48 | 0.47 |
| 41:QB:254:ALA:HB1 | 40:QG:406:TRP:CZ2 | 2.50 | 0.47 |
| 41:QB:332:ASN:O | 41:QB:336:LYS:N | 2.46 | 0.47 |
| 40:QG:228:ASN:ND2 | 42:QG:501:GTP:HN1 | 2.06 | 0.47 |
| 40:QG:233:GLN:NE2 | 40:QG:237:SER:OG | 2.47 | 0.47 |
| 40:QH:89:PRO:HA | 40:QH:92:LEU:HD23 | 1.97 | 0.47 |
| 40:QH:185:TYR:OH | 40:QH:397:MET:O | 2.33 | 0.47 |
| 41:QN:293:MET:HG3 | 41:QN:367:PHE:HB2 | 1.97 | 0.47 |
| 41:QP:82:GLY:C | 41:QP:84:ILE:H | 2.18 | 0.47 |
| 41:QP:117:LEU:HD22 | 41:QP:154:LYS:HD3 | 1.96 | 0.47 |
| 41:QP:298:ASN:O | 41:QP:300:MET:N | 2.48 | 0.47 |
| 41:QP:314:ALA:N | 41:QP:368:ILE:O | 2.47 | 0.47 |
| 41:RB:7:LEU:HD23 | 41:RB:64:VAL:HB | 1.97 | 0.47 |
| 40:RE:15:GLN:HG3 | 40:RE:228:ASN:HD21 | 1.80 | 0.47 |
| 40:RE:20:CYS:O | 40:RE:24:TYR:HD2 | 1.98 | 0.47 |
| 40:RE:85:GLN:O | 40:SE:283:HIS:HE1 | 1.98 | 0.47 |
| 40:RE:161:TYR:HH | 40:SE:338:LYS:HZ1 | 1.56 | 0.47 |
| 40:RF:176:GLN:OE1 | 40:RF:176:GLN:N | 2.48 | 0.47 |
| 40:RH:2:ARG:HG3 | 40:RH:51:THR:HG22 | 1.95 | 0.47 |
| 41:RM:268:PRO:HG2 | 41:RM:300:MET:HB2 | 1.95 | 0.47 |
| 41:RO:4:ILE:HD11 | 41:RO:50:TYR:HE1 | 1.79 | 0.47 |
| 41:RO:156:ARG:HE | 41:RO:164:MET:HG2 | 1.80 | 0.47 |
| 41:RP:200:TYR:HB3 | 41:RP:268:PRO:HG3 | 1.97 | 0.47 |
| 41:RP:260:PHE:HE2 | 41:RP:425:ARG:HH11 | 1.62 | 0.47 |
| 40:SA:310:GLY:HA3 | 40:SA:382:ALA:HB2 | 1.97 | 0.47 |
| 41:SB:133:PHE:CG | 41:SB:155:ILE:HD11 | 2.50 | 0.47 |
| 41:SB:178:THR:O | 41:SB:180:VAL:N | 2.47 | 0.47 |
| 40:SF:257:THR:HA | 41:SN:397:TRP:CZ3 | 2.50 | 0.47 |
| 40:SG:229:ARG:HH12 | 40:SG:365:GLY:HA3 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SL:86:ARG:NH1 | 41:SL:89:ASN:OD1 | 2.47 | 0.47 |
| 41:SL:87:PRO:HA | 41:SL:90:PHE:HD2 | 1.79 | 0.47 |
| 41:SL:276:ARG:HA | 41:SL:279:GLN:HG2 | 1.97 | 0.47 |
| 41:SO:124:ALA:O | 41:SO:125:GLU:C | 2.52 | 0.47 |
| 41:SO:298:ASN:O | 41:SO:299:MET:C | 2.53 | 0.47 |
| 41:SP:108:GLU:HA | 41:SP:111:GLU:HB2 | 1.97 | 0.47 |
| 41:TB:23:VAL:HG13 | 41:TB:359:ARG:HH12 | 1.80 | 0.47 |
| 41:TB:96:GLY:O | 41:TB:103:LYS:NZ | 2.45 | 0.47 |
| 40:TE:220:GLU:O | 40:TE:221:ARG:NE | 2.46 | 0.47 |
| 40:TF:73:THR:HG22 | 41:TM:46:ARG:HE | 1.80 | 0.47 |
| 40:TG:5:ILE:HD13 | 40:TG:125:LEU:HB3 | 1.97 | 0.47 |
| 41:TM:304:ASP:OD1 | 41:TM:307:HIS:ND1 | 2.39 | 0.47 |
| 41:TO:27:GLU:OE2 | 41:TO:241:ARG:NH1 | 2.43 | 0.47 |
| 41:TO:221:THR:HG23 | 41:TO:223:GLY:H | 1.79 | 0.47 |
| 41:TO:325:GLU:HA | 41:TO:328:GLU:HG2 | 1.95 | 0.47 |
| 41:TP:269:GLY:O | 41:TP:367:PHE:N | 2.43 | 0.47 |
| 40:UA:338:LYS:HZ2 | 40:UA:340:SER:H | 1.63 | 0.47 |
| 41:UB:313:VAL:O | 41:UB:349:VAL:HA | 2.15 | 0.47 |
| 40:UE:20:CYS:HA | 40:UE:232:SER:HB2 | 1.96 | 0.47 |
| 40:UE:88:HIS:HE1 | 40:UE:90:GLU:HB2 | 1.80 | 0.47 |
| 40:UF:201:ALA:O | 40:UF:203:MET:N | 2.47 | 0.47 |
| 40:UF:276:ILE:HG13 | 40:UF:280:LYS:HB2 | 1.95 | 0.47 |
| 40:UF:294:ALA:O | 40:UF:297:GLU:HB2 | 2.15 | 0.47 |
| 40:UF:323:VAL:HG23 | 40:UF:355:ILE:HG23 | 1.96 | 0.47 |
| 40:UF:400:LYS:O | 40:UF:401:ARG:C | 2.52 | 0.47 |
| 40:UH:222:PRO:HD2 | 41:UO:324:LYS:HG3 | 1.97 | 0.47 |
| 40:UI:123:ARG:HA | 40:UI:123:ARG:HD2 | 1.44 | 0.47 |
| 41:UM:40:SER:OG | 41:UM:41:ASP:N | 2.47 | 0.47 |
| 41:UM:172:SER:OG | 41:UM:175:VAL:O | 2.31 | 0.47 |
| 41:UO:66:VAL:HG22 | 41:UO:91:VAL:HB | 1.96 | 0.47 |
| 41:UP:315:ALA:O | 41:UP:317:PHE:N | 2.47 | 0.47 |
| 40:VA:6:SER:O | 40:VA:65:ALA:HA | 2.14 | 0.47 |
| 41:VP:176:SER:OG | 41:VP:178:THR:O | 2.31 | 0.47 |
| 41:VQ:288:GLU:HA | 41:VQ:291:GLN:HG3 | 1.97 | 0.47 |
| 40:WA:100:ALA:O | 41:WN:255:VAL:HG11 | 2.14 | 0.47 |
| 40:WE:265:ILE:HG23 | 40:WE:431:TYR:CZ | 2.50 | 0.47 |
| 40:WG:187:SER:HA | 40:WG:190:THR:HG22 | 1.97 | 0.47 |
| 40:WG:284:GLU:N | 40:WG:284:GLU:OE1 | 2.48 | 0.47 |
| 40:WH:181:VAL:HG12 | 41:WO:347:ASN:O | 2.15 | 0.47 |
| 40:WH:238:ILE:HA | 40:WH:318:LEU:HD22 | 1.96 | 0.47 |
| 40:WH:326:LYS:HD2 | 41:WP:212:PHE:CZ | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WM:12:CYS:O | 41:WM:13:GLY:C | 2.53 | 0.47 |
| 41:WN:107:THR:HB | 41:WN:108:GLU:H | 1.56 | 0.47 |
| 41:WN:214:THR:HG22 | 41:WN:215:LEU:HG | 1.97 | 0.47 |
| 41:WO:202:ILE:HG23 | 41:WO:300:MET:HB3 | 1.97 | 0.47 |
| 41:WO:398:TYR:HB3 | 41:WO:403:MET:HG3 | 1.97 | 0.47 |
| 41:WP:142:GLY:O | 41:WP:144:GLY:N | 2.47 | 0.47 |
| 41:WP:326:VAL:O | 41:WP:330:MET:HG2 | 2.14 | 0.47 |
| 41:WQ:105:HIS:HE1 | 41:WQ:191:GLN:HE22 | 1.62 | 0.47 |
| 41:WQ:155:ILE:HA | 41:WQ:158:GLU:HG2 | 1.97 | 0.47 |
| 4:1H:161:ARG:HH12 | 41:GO:121:ARG:CZ | 2.27 | 0.47 |
| 7:1S:586:HIS:NE2 | 7:1S:604:SER:OG | 2.46 | 0.47 |
| 7:1T:435:GLY:HA3 | 7:1T:464:VAL:HG21 | 1.96 | 0.47 |
| 9:2C:457:ARG:NE | 41:SP:55:THR:OG1 | 2.48 | 0.47 |
| 10:2E:46:ARG:NH2 | 40:ME:433:GLU:OE2 | 2.48 | 0.47 |
| 11:2J:88:VAL:HG11 | 41:LM:392:LYS:HD2 | 1.96 | 0.47 |
| 12:2Q:215:GLN:HE22 | 13:2V:37:ILE:HG23 | 1.80 | 0.47 |
| 13:2W:83:LEU:HD11 | 13:2W:161:ARG:HG2 | 1.95 | 0.47 |
| 15:3E:48:ILE:HD11 | 15:3F:350:ARG:HH12 | 1.80 | 0.47 |
| 17:3Q:383:LYS:HE2 | 17:3Q:383:LYS:HB2 | 1.71 | 0.47 |
| 21:4D:407:LYS:HE3 | 21:4D:407:LYS:HB2 | 1.50 | 0.47 |
| 21:4F:472:VAL:O | 21:4F:484:TYR:HA | 2.15 | 0.47 |
| 22:4J:155:ASN:CA | 22:4J:167:ILE:O | 2.63 | 0.47 |
| 26:4V:29:TYR:O | 26:4V:33:GLY:HA2 | 2.14 | 0.47 |
| 27:4Z:41:GLN:HA | 27:4Z:44:ARG:HG3 | 1.96 | 0.47 |
| 31:5J:822:GLU:O | 31:5J:826:ILE:HG12 | 2.14 | 0.47 |
| 37:6A:126:TRP:HE1 | 41:TP:94:GLN:CD | 2.17 | 0.47 |
| 39:6I:48:ILE:HB | 39:6I:108:HIS:HA | 1.96 | 0.47 |
| 39:6I:99:LEU:HG | 39:6I:103:LYS:HE2 | 1.97 | 0.47 |
| 40:AH:138:PHE:HE2 | 40:AH:235:VAL:HG21 | 1.80 | 0.47 |
| 40:BE:287:SER:H | 40:BE:290:GLU:HG3 | 1.79 | 0.47 |
| 40:BF:150:THR:O | 40:BF:154:MET:HB2 | 2.14 | 0.47 |
| 41:BO:64:VAL:O | 41:BO:66:VAL:HG13 | 2.15 | 0.47 |
| 41:BO:294:PHE:HE2 | 41:BO:313:VAL:HG11 | 1.80 | 0.47 |
| 41:BP:13:GLY:HA3 | 41:BP:136:THR:O | 2.15 | 0.47 |
| 40:CA:60:LYS:O | 40:CA:62:VAL:N | 2.47 | 0.47 |
| 40:CA:210:TYR:O | 40:CA:214:ARG:HG3 | 2.14 | 0.47 |
| 40:CH:150:THR:O | 40:CH:151:SER:C | 2.53 | 0.47 |
| 41:CN:154:LYS:HA | 41:CN:154:LYS:HD2 | 1.68 | 0.47 |
| 41:CN:253:LEU:O | 41:CN:257:MET:HB2 | 2.15 | 0.47 |
| 41:CN:330:MET:HG3 | 41:CN:351:THR:CG2 | 2.44 | 0.47 |
| 41:CO:165:ASN:HA | 41:CO:198:GLU:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CO:251:ARG:O | 41:CO:255:VAL:HG23 | 2.15 | 0.47 |
| 41:CP:82:GLY:O | 41:CP:84:ILE:N | 2.45 | 0.47 |
| 40:DA:273:ALA:HB2 | 40:DA:374:VAL:HG13 | 1.97 | 0.47 |
| 41:DB:263:LEU:HD13 | 41:DB:263:LEU:HA | 1.72 | 0.47 |
| 40:DI:102:ASN:O | 40:DI:103:TYR:C | 2.52 | 0.47 |
| 41:DL:25:SER:O | 41:DL:30:ILE:N | 2.48 | 0.47 |
| 41:DL:88:ASP:O | 41:DL:89:ASN:C | 2.53 | 0.47 |
| 41:DM:20:PHE:HA | 41:DM:230:SER:OG | 2.14 | 0.47 |
| 41:DM:207:LEU:O | 41:DM:208:TYR:C | 2.53 | 0.47 |
| 41:DN:41:ASP:O | 41:DN:44:LEU:N | 2.48 | 0.47 |
| 41:DN:190:HIS:HA | 41:DN:414:ASN:ND2 | 2.30 | 0.47 |
| 41:DN:357:PRO:HB2 | 41:DN:362:LYS:HA | 1.97 | 0.47 |
| 41:DN:397:TRP:O | 41:DN:398:TYR:C | 2.52 | 0.47 |
| 41:DO:226:ASN:ND2 | 43:DO:501:GDP:O6 | 2.48 | 0.47 |
| 41:DP:69:GLU:H | 41:DP:69:GLU:HG3 | 1.43 | 0.47 |
| 40:EF:21:TRP:HZ3 | 40:EF:53:PHE:CE1 | 2.33 | 0.47 |
| 40:EG:70:LEU:HD23 | 40:EG:114:LEU:HD22 | 1.97 | 0.47 |
| 40:EH:238:ILE:H | 40:EH:238:ILE:HG12 | 1.47 | 0.47 |
| 40:EI:262:TYR:O | 40:EI:263:PRO:C | 2.53 | 0.47 |
| 41:EL:192:LEU:HA | 41:EL:195:ASN:HB2 | 1.96 | 0.47 |
| 41:EP:346:PRO:O | 41:EP:347:ASN:C | 2.52 | 0.47 |
| 40:FA:33:ASP:HA | 40:FA:85:GLN:HB2 | 1.96 | 0.47 |
| 40:FA:262:TYR:N | 40:FA:262:TYR:CD1 | 2.82 | 0.47 |
| 40:FH:172:TYR:HB2 | 40:FH:203:MET:HE3 | 1.97 | 0.47 |
| 41:FN:109:GLY:O | 41:FN:113:VAL:HG23 | 2.15 | 0.47 |
| 40:GE:223:THR:O | 40:GE:224:TYR:C | 2.53 | 0.47 |
| 41:GN:130:LEU:O | 41:GN:131:GLN:C | 2.52 | 0.47 |
| 41:HB:259:PRO:HG3 | 41:HB:311:LEU:HD23 | 1.96 | 0.47 |
| 40:HE:8:HIS:CE1 | 40:HE:21:TRP:HE1 | 2.33 | 0.47 |
| 40:HE:73:THR:O | 40:HE:74:VAL:C | 2.53 | 0.47 |
| 40:HH:181:VAL:HG23 | 41:HO:348:ASN:HA | 1.97 | 0.47 |
| 41:HN:102:ALA:HB1 | 41:HN:401:GLU:HB2 | 1.96 | 0.47 |
| 40:IE:98:ASP:O | 40:IE:105:ARG:NH2 | 2.42 | 0.47 |
| 40:IE:101:ASN:HA | 40:IE:144:GLY:H | 1.80 | 0.47 |
| 40:IF:326:LYS:HD2 | 41:IN:208:TYR:CD1 | 2.43 | 0.47 |
| 40:IF:326:LYS:NZ | 41:IN:225:LEU:HD21 | 2.29 | 0.47 |
| 40:IG:109:THR:HG23 | 40:IG:110:ILE:H | 1.80 | 0.47 |
| 41:IM:22:GLU:HG3 | 41:IM:81:PHE:CD2 | 2.46 | 0.47 |
| 41:IP:113:VAL:HG22 | 41:IP:117:LEU:HD23 | 1.97 | 0.47 |
| 40:JA:128:GLN:NE2 | 40:KA:290:GLU:HG3 | 2.29 | 0.47 |
| 40:JH:205:ASP:OD1 | 40:JH:206:ASN:N | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JL:134:GLN:HA | 41:JL:165:ASN:O | 2.15 | 0.47 |
| 41:JM:286:VAL:HG22 | 41:JM:363:MET:HE1 | 1.95 | 0.47 |
| 41:JM:397:TRP:O | 41:JM:398:TYR:C | 2.54 | 0.47 |
| 41:JN:179:VAL:HG23 | 41:JN:180:VAL:HG13 | 1.97 | 0.47 |
| 40:KD:136:LEU:HD11 | 40:KD:239:THR:HG21 | 1.97 | 0.47 |
| 40:KE:11:GLN:HE22 | 41:KL:247:ASN:H | 1.63 | 0.47 |
| 41:KL:6:HIS:HB3 | 41:KL:21:TRP:HZ2 | 1.80 | 0.47 |
| 41:KN:317:PHE:HB2 | 41:KN:353:VAL:HG22 | 1.97 | 0.47 |
| 40:LD:207:GLU:HA | 40:LD:210:TYR:HB2 | 1.97 | 0.47 |
| 41:LM:238:THR:HG21 | 41:LM:318:ARG:HD3 | 1.97 | 0.47 |
| 41:LN:417:ASP:OD1 | 41:LN:420:ASN:ND2 | 2.48 | 0.47 |
| 41:LO:30:ILE:HD11 | 41:LO:47:ILE:HD11 | 1.96 | 0.47 |
| 41:LO:100:ASN:HB3 | 41:LO:103:LYS:H | 1.79 | 0.47 |
| 41:LP:213:ARG:HH21 | 41:LP:297:LYS:HD2 | 1.80 | 0.47 |
| 41:MB:142:GLY:O | 41:MB:144:GLY:N | 2.48 | 0.47 |
| 40:ME:3:GLU:N | 40:ME:3:GLU:OE1 | 2.48 | 0.47 |
| 40:ME:217:LEU:HA | 40:ME:277:SER:HB3 | 1.96 | 0.47 |
| 40:MF:239:THR:HB | 40:MF:242:LEU:HD11 | 1.96 | 0.47 |
| 40:MF:256:GLN:C | 40:MF:258:ASN:H | 2.18 | 0.47 |
| 40:MG:429:LYS:HB3 | 40:MG:429:LYS:HE3 | 1.56 | 0.47 |
| 41:MN:282:ARG:HD3 | 41:MN:283:ALA:H | 1.80 | 0.47 |
| 40:NA:73:THR:HA | 40:NA:76:ASP:HB2 | 1.97 | 0.47 |
| 40:NA:142:GLY:HA2 | 40:NA:183:GLU:HG2 | 1.96 | 0.47 |
| 40:ND:2:ARG:H | 40:ND:2:ARG:HG2 | 1.46 | 0.47 |
| 40:NF:2:ARG:HB3 | 40:NF:133:GLN:NE2 | 2.30 | 0.47 |
| 41:NO:35:THR:HB | 41:NO:58:LYS:HG2 | 1.95 | 0.47 |
| 41:OM:19:LYS:HD2 | 41:OM:227:HIS:CD2 | 2.50 | 0.47 |
| 40:PA:254:GLU:HB2 | 41:PB:98:GLY:HA2 | 1.97 | 0.47 |
| 41:PB:271:ALA:HA | 41:PB:273:LEU:HG | 1.97 | 0.47 |
| 41:PB:305:PRO:HB3 | 41:PB:310:TYR:HE1 | 1.80 | 0.47 |
| 41:PM:8:GLN:HG2 | 41:PM:17:GLY:HA3 | 1.95 | 0.47 |
| 41:PM:20:PHE:HA | 41:PM:230:SER:HB3 | 1.97 | 0.47 |
| 41:PM:101:TRP:CZ3 | 41:PM:187:LEU:HB3 | 2.47 | 0.47 |
| 41:PN:120:VAL:HG11 | 41:PN:155:ILE:HG12 | 1.97 | 0.47 |
| 41:PN:342:VAL:HG23 | 41:PN:345:ILE:HG22 | 1.96 | 0.47 |
| 41:PO:171:PRO:O | 41:PO:380:ARG:NH2 | 2.48 | 0.47 |
| 41:QB:81:PHE:HB3 | 41:QB:84:ILE:HD13 | 1.97 | 0.47 |
| 41:QB:156:ARG:HD2 | 41:QB:156:ARG:HA | 1.55 | 0.47 |
| 40:QE:406:TRP:HE1 | 41:QL:258:VAL:HB | 1.79 | 0.47 |
| 41:QL:107:THR:O | 41:QL:109:GLY:N | 2.47 | 0.47 |
| 41:QN:86:ARG:HG2 | 41:QN:89:ASN:H | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QN:237:THR:HG22 | 41:QN:250:LEU:HD21 | 1.96 | 0.47 |
| 40:RF:311:LYS:NZ | 40:RF:435:GLY:O | 2.47 | 0.47 |
| 40:RH:213:CYS:HA | 40:RH:217:LEU:HD13 | 1.97 | 0.47 |
| 40:RI:69:ASP:HB3 | 40:RI:75:ILE:HD11 | 1.97 | 0.47 |
| 40:RI:207:GLU:OE1 | 40:RI:304:LYS:NZ | 2.43 | 0.47 |
| 41:RO:6:HIS:O | 41:RO:63:ALA:HA | 2.14 | 0.47 |
| 40:SI:217:LEU:HB3 | 40:SI:219:ILE:HD12 | 1.97 | 0.47 |
| 41:SN:6:HIS:O | 41:SN:63:ALA:HA | 2.15 | 0.47 |
| 41:SO:9:ALA:HB2 | 41:SO:66:VAL:HB | 1.97 | 0.47 |
| 41:SO:310:TYR:O | 41:SO:311:LEU:C | 2.53 | 0.47 |
| 41:SP:73:MET:HA | 41:SP:76:VAL:HG12 | 1.96 | 0.47 |
| 40:TI:301:GLN:HE21 | 40:TI:307:PRO:HD3 | 1.78 | 0.47 |
| 41:TL:325:GLU:HA | 41:TL:328:GLU:HG2 | 1.97 | 0.47 |
| 41:TM:313:VAL:HG13 | 41:TM:367:PHE:CE2 | 2.50 | 0.47 |
| 40:UA:315:CYS:HA | 40:UA:377:LEU:O | 2.15 | 0.47 |
| 40:UF:138:PHE:CZ | 40:UF:235:VAL:HG21 | 2.50 | 0.47 |
| 40:UF:145:THR:OG1 | 42:UM:501:GTP:O2B | 2.29 | 0.47 |
| 40:UF:207:GLU:O | 40:UF:210:TYR:HB2 | 2.14 | 0.47 |
| 41:UP:275:SER:OG | 41:UP:276:ARG:N | 2.45 | 0.47 |
| 40:VF:102:ASN:HB3 | 40:VF:105:ARG:HB2 | 1.97 | 0.47 |
| 40:VJ:237:SER:HA | 40:VJ:320:ARG:NH2 | 2.30 | 0.47 |
| 40:WA:5:ILE:HD13 | 40:WA:64:ARG:HB3 | 1.97 | 0.47 |
| 40:WE:174:ALA:HB3 | 40:WE:178:SER:H | 1.79 | 0.47 |
| 40:WI:213:CYS:HA | 40:WI:217:LEU:HB3 | 1.97 | 0.47 |
| 41:WQ:67:ASP:OD2 | 41:WQ:68:LEU:N | 2.48 | 0.47 |
| 41:WQ:170:VAL:HG11 | 41:WQ:377:LEU:HD21 | 1.97 | 0.47 |
| 7:1T:48:LEU:HG | 7:1T:59:PHE:CD1 | 2.50 | 0.47 |
| 7:1T:111:LYS:HE2 | 7:1T:111:LYS:HB2 | 1.55 | 0.47 |
| 7:1T:142:ILE:H | 7:1T:142:ILE:HG12 | 1.64 | 0.47 |
| 7:1T:220:PHE:HD1 | 7:1T:234:PRO:HD3 | 1.80 | 0.47 |
| 10:2G:164:ASP:HB2 | 40:VJ:117:LEU:HD23 | 1.96 | 0.47 |
| 15:3F:264:PHE:HE2 | 15:3F:394:ARG:HG3 | 1.80 | 0.47 |
| 17:3O:402:GLU:HA | 17:3O:405:ARG:HE | 1.79 | 0.47 |
| 17:3P:178:LYS:HE3 | 17:3P:178:LYS:HB3 | 1.36 | 0.47 |
| 17:3P:391:ALA:O | 17:3P:395:VAL:HG12 | 2.15 | 0.47 |
| 17:3R:156:TRP:HA | 17:3R:156:TRP:HE3 | 1.76 | 0.47 |
| 17:3R:308:ILE:O | 17:3R:312:GLN:HG3 | 2.15 | 0.47 |
| 18:3T:131:LEU:HD13 | 18:3T:279:ARG:HG2 | 1.97 | 0.47 |
| 20:4B:324:LEU:HD13 | 22:4I:13:ARG:HG3 | 1.97 | 0.47 |
| 21:4D:492:ILE:HG12 | 21:4D:531:ILE:HD13 | 1.95 | 0.47 |
| 21:4F:331:VAL:HG21 | 21:4F:347:CYS:HB3 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4I:80:SER:HB3 | 40:AG:41:THR:HG21 | 1.97 | 0.47 |
| 22:4I:440:LEU:HB2 | 22:4I:452:PHE:HE2 | 1.80 | 0.47 |
| 22:4J:324:LYS:HD2 | 22:4J:328:LEU:HD11 | 1.97 | 0.47 |
| 23:4Q:175:ASP:O | 23:4Q:176:ASP:C | 2.52 | 0.47 |
| 23:4Q:201:SER:O | 23:4Q:202:PHE:C | 2.52 | 0.47 |
| 25:4T:398:THR:O | 25:4T:399:GLU:C | 2.53 | 0.47 |
| 27:4Z:73:VAL:HA | 27:4Z:91:SER:HA | 1.96 | 0.47 |
| 30:5G:85:GLN:NE2 | 41:GB:70:PRO:O | 2.48 | 0.47 |
| 37:6A:122:LYS:HZ2 | 40:TH:1:GLN:HG2 | 1.80 | 0.47 |
| 40:AH:283:HIS:CD2 | 40:MH:62:VAL:HG23 | 2.50 | 0.47 |
| 41:AP:134:GLN:HA | 41:AP:165:ASN:O | 2.14 | 0.47 |
| 40:BA:76:ASP:OD2 | 41:BN:46:ARG:NH2 | 2.47 | 0.47 |
| 40:BA:180:ALA:HB3 | 40:BA:183:GLU:HG3 | 1.97 | 0.47 |
| 40:BE:386:ALA:HA | 40:BE:389:ARG:HD3 | 1.96 | 0.47 |
| 40:BH:79:ARG:HG2 | 40:BH:92:LEU:HD13 | 1.97 | 0.47 |
| 40:BH:362:VAL:HG21 | 40:BH:369:LYS:HG2 | 1.96 | 0.47 |
| 41:BM:393:ALA:O | 41:BM:394:PHE:C | 2.52 | 0.47 |
| 41:BP:330:MET:HB3 | 41:BP:349:VAL:HG11 | 1.96 | 0.47 |
| 40:CA:96:LYS:HA | 40:CA:96:LYS:HD2 | 1.57 | 0.47 |
| 41:CB:165:ASN:ND2 | 41:CB:198:GLU:OE1 | 2.48 | 0.47 |
| 40:CF:10:GLY:HA2 | 40:CF:145:THR:HG23 | 1.97 | 0.47 |
| 40:CH:3:GLU:H | 40:CH:3:GLU:HG2 | 1.51 | 0.47 |
| 41:CL:49:VAL:HG21 | 41:CL:241:ARG:HG2 | 1.97 | 0.47 |
| 41:CL:233:MET:O | 41:CL:236:VAL:HG12 | 2.15 | 0.47 |
| 41:CP:193:VAL:HG13 | 41:CP:265:PHE:HE1 | 1.80 | 0.47 |
| 41:CP:271:ALA:HB3 | 41:CP:272:PRO:CD | 2.45 | 0.47 |
| 41:DB:338:SER:O | 41:DB:339:SER:C | 2.53 | 0.47 |
| 41:DB:394:PHE:HA | 41:DB:396:HIS:CE1 | 2.49 | 0.47 |
| 40:DH:74:VAL:O | 40:DH:77:GLU:N | 2.45 | 0.47 |
| 40:DH:104:ALA:O | 40:DH:107:HIS:N | 2.48 | 0.47 |
| 40:DI:23:LEU:HD12 | 40:DI:26:LEU:HD11 | 1.96 | 0.47 |
| 40:DI:144:GLY:O | 40:DI:147:SER:N | 2.29 | 0.47 |
| 41:DL:62:ARG:HG2 | 41:DL:123:GLU:CG | 2.45 | 0.47 |
| 41:DM:142:GLY:O | 41:DM:144:GLY:N | 2.48 | 0.47 |
| 41:DM:163:ILE:H | 41:DM:163:ILE:HG13 | 1.52 | 0.47 |
| 41:DO:263:LEU:HD21 | 41:DO:421:PRO:HB2 | 1.97 | 0.47 |
| 41:DP:375:GLN:OE1 | 41:DP:419:GLY:HA2 | 2.15 | 0.47 |
| 40:EA:100:ALA:O | 41:EN:255:VAL:HG11 | 2.15 | 0.47 |
| 40:EA:391:ASP:OD1 | 40:EA:421:ARG:NH2 | 2.48 | 0.47 |
| 40:EF:213:CYS:HA | 40:EF:217:LEU:HB2 | 1.97 | 0.47 |
| 40:EH:69:ASP:OD2 | 40:EH:74:VAL:HG11 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EH:278:ALA:HA | 40:EH:368:ALA:HB2 | 1.97 | 0.47 |
| 40:EH:326:LYS:HE3 | 40:EH:326:LYS:HB3 | 1.74 | 0.47 |
| 40:EH:400:LYS:H | 40:EH:400:LYS:HG2 | 1.35 | 0.47 |
| 40:EI:2:ARG:O | 40:EI:51:THR:HA | 2.15 | 0.47 |
| 40:EI:35:GLN:C | 40:EI:37:PRO:HD3 | 2.35 | 0.47 |
| 40:EI:274:PRO:CG | 40:EI:373:ALA:HA | 2.28 | 0.47 |
| 40:FA:313:MET:HG3 | 40:FA:381:THR:HG22 | 1.95 | 0.47 |
| 40:FG:239:THR:HB | 40:FG:242:LEU:HD11 | 1.97 | 0.47 |
| 40:FI:319:TYR:HB3 | 40:FI:323:VAL:HG21 | 1.97 | 0.47 |
| 41:FO:203:ASP:HB2 | 41:FO:301:ALA:HA | 1.97 | 0.47 |
| 40:GA:90:GLU:OE2 | 40:HA:280:LYS:NZ | 2.44 | 0.47 |
| 40:GH:262:TYR:HB3 | 40:GH:263:PRO:HD2 | 1.96 | 0.47 |
| 41:GM:73:MET:HA | 41:GM:76:VAL:HG12 | 1.96 | 0.47 |
| 41:HB:8:GLN:HE21 | 41:HB:65:LEU:HD13 | 1.80 | 0.47 |
| 40:HE:261:PRO:HA | 41:HM:394:PHE:CD2 | 2.49 | 0.47 |
| 40:HF:326:LYS:HZ2 | 41:HN:208:TYR:HB2 | 1.80 | 0.47 |
| 40:HG:3:GLU:OE2 | 40:HG:3:GLU:N | 2.47 | 0.47 |
| 41:HO:149:THR:HG21 | 41:HO:188:SER:HA | 1.96 | 0.47 |
| 41:HP:316:VAL:HG12 | 41:HP:352:ALA:HB3 | 1.97 | 0.47 |
| 40:IA:248:LEU:HD22 | 40:IA:353:VAL:HG23 | 1.97 | 0.47 |
| 41:IB:22:GLU:HG2 | 41:IB:81:PHE:HB2 | 1.97 | 0.47 |
| 40:IF:221:ARG:HA | 40:IF:221:ARG:HD3 | 1.65 | 0.47 |
| 40:IG:208:ALA:HB2 | 40:IG:304:LYS:HG2 | 1.97 | 0.47 |
| 40:IH:253:THR:HG21 | 41:IP:103:LYS:HE2 | 1.96 | 0.47 |
| 40:II:88:HIS:HB3 | 40:II:91:GLN:HE22 | 1.80 | 0.47 |
| 41:IM:237:THR:O | 41:IM:241:ARG:NH1 | 2.48 | 0.47 |
| 41:IO:113:VAL:HG22 | 41:IO:117:LEU:HD23 | 1.97 | 0.47 |
| 41:IP:229:VAL:HG12 | 41:IP:233:MET:HE2 | 1.95 | 0.47 |
| 41:JB:3:GLU:HA | 41:JB:49:VAL:HA | 1.96 | 0.47 |
| 41:JB:342:VAL:HG23 | 41:JB:345:ILE:HG22 | 1.97 | 0.47 |
| 40:JF:321:GLY:HA2 | 40:JF:359:PRO:HD3 | 1.97 | 0.47 |
| 40:JG:139:HIS:CG | 40:JG:150:THR:HG21 | 2.50 | 0.47 |
| 41:JM:5:VAL:HG23 | 41:JM:130:LEU:HD11 | 1.97 | 0.47 |
| 41:JM:358:PRO:O | 41:JM:359:ARG:C | 2.53 | 0.47 |
| 41:JN:316:VAL:HG23 | 41:JN:366:THR:HB | 1.96 | 0.47 |
| 40:KA:20:CYS:HA | 40:KA:232:SER:HB2 | 1.96 | 0.47 |
| 41:KB:271:ALA:HB1 | 41:KB:292:GLN:HG2 | 1.96 | 0.47 |
| 40:KD:318:LEU:O | 40:KD:374:VAL:HA | 2.14 | 0.47 |
| 40:KH:228:ASN:ND2 | 42:KO:501:GTP:HN1 | 2.12 | 0.47 |
| 41:KL:173:PRO:HA | 41:KL:380:ARG:HD3 | 1.97 | 0.47 |
| 41:KN:101:TRP:HD1 | 41:KN:145:SER:HB2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KO:27:GLU:OE2 | 41:KO:318:ARG:NH2 | 2.34 | 0.47 |
| 41:KO:348:ASN:C | 41:KO:348:ASN:HD22 | 2.18 | 0.47 |
| 40:LA:88:HIS:HD2 | 40:MA:283:HIS:HB2 | 1.79 | 0.47 |
| 40:LF:16:ILE:HD11 | 40:LF:171:ILE:HD11 | 1.96 | 0.47 |
| 40:LF:264:ARG:H | 40:LF:264:ARG:HG3 | 1.34 | 0.47 |
| 40:LG:49:PHE:HD1 | 40:LG:53:PHE:HB2 | 1.79 | 0.47 |
| 40:LG:301:GLN:C | 40:LG:303:VAL:H | 2.19 | 0.47 |
| 40:LG:438:SER:HB3 | 41:LO:390:ARG:HH22 | 1.80 | 0.47 |
| 40:MA:141:PHE:CE1 | 40:MA:194:THR:HG21 | 2.50 | 0.47 |
| 41:MB:10:GLY:O | 41:MB:14:ASN:ND2 | 2.47 | 0.47 |
| 40:MD:311:LYS:H | 40:MD:381:THR:HB | 1.80 | 0.47 |
| 40:ME:70:LEU:HD23 | 40:ME:114:LEU:HD12 | 1.97 | 0.47 |
| 40:ME:319:TYR:HB3 | 40:ME:323:VAL:HG21 | 1.97 | 0.47 |
| 40:ME:329:ASN:HB3 | 41:MM:175:VAL:HG11 | 1.97 | 0.47 |
| 40:MF:71:GLU:HB3 | 40:MF:98:ASP:HB3 | 1.96 | 0.47 |
| 40:MF:273:ALA:HB3 | 40:MF:274:PRO:CD | 2.45 | 0.47 |
| 40:MG:198:SER:OG | 40:MG:199:ASP:N | 2.48 | 0.47 |
| 41:MP:202:ILE:HD13 | 41:MP:229:VAL:HG22 | 1.97 | 0.47 |
| 41:NB:19:LYS:HE2 | 41:NB:223:GLY:HA2 | 1.97 | 0.47 |
| 41:NB:248:ALA:HA | 41:NB:252:LYS:HG2 | 1.96 | 0.47 |
| 40:NE:191:THR:O | 40:NE:195:LEU:HB2 | 2.15 | 0.47 |
| 41:NL:362:LYS:HA | 41:NL:362:LYS:HD3 | 1.80 | 0.47 |
| 41:NN:200:TYR:HE2 | 41:NN:368:ILE:HD12 | 1.78 | 0.47 |
| 41:NP:318:ARG:HH21 | 41:NP:358:PRO:HB3 | 1.79 | 0.47 |
| 40:OA:73:THR:HA | 40:OA:76:ASP:HB3 | 1.97 | 0.47 |
| 41:OB:14:ASN:HD21 | 41:OB:67:ASP:HB2 | 1.79 | 0.47 |
| 41:OB:204:ASN:HA | 41:OB:207:LEU:HD12 | 1.97 | 0.47 |
| 40:OG:210:TYR:CE1 | 40:OG:227:LEU:HD11 | 2.50 | 0.47 |
| 40:OG:323:VAL:HG22 | 40:OG:372:ARG:HG2 | 1.95 | 0.47 |
| 40:OH:68:VAL:HG21 | 40:OH:118:VAL:HG21 | 1.97 | 0.47 |
| 40:OH:74:VAL:O | 40:OH:77:GLU:N | 2.47 | 0.47 |
| 40:OH:199:ASP:O | 40:OH:266:HIS:HB2 | 2.14 | 0.47 |
| 40:OH:313:MET:HB3 | 40:OH:314:ALA:H | 1.49 | 0.47 |
| 41:OO:4:ILE:HB | 41:OO:50:TYR:HE1 | 1.80 | 0.47 |
| 41:OO:309:ARG:NH1 | 41:OO:426:GLY:O | 2.48 | 0.47 |
| 41:OO:325:GLU:O | 41:OO:329:GLN:OE1 | 2.32 | 0.47 |
| 41:OP:171:PRO:HG2 | 41:OP:381:ILE:HD11 | 1.97 | 0.47 |
| 40:PD:322:ASP:OD1 | 40:PD:372:ARG:NH1 | 2.48 | 0.47 |
| 40:PF:211:ASP:OD2 | 40:PF:215:ARG:HD3 | 2.14 | 0.47 |
| 40:PH:137:ILE:HG22 | 40:PH:139:HIS:HD2 | 1.80 | 0.47 |
| 40:PH:239:THR:O | 40:PH:243:ARG:NH1 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PM:3:GLU:HB3 | 41:PM:62:ARG:HH12 | 1.79 | 0.47 |
| 41:PN:306:ARG:HG3 | 41:PN:340:TYR:HE1 | 1.79 | 0.47 |
| 40:QE:221:ARG:HH22 | 41:QL:325:GLU:HB2 | 1.80 | 0.47 |
| 40:QE:318:LEU:O | 40:QE:374:VAL:HA | 2.15 | 0.47 |
| 41:QM:313:VAL:HG13 | 41:QM:349:VAL:HG22 | 1.97 | 0.47 |
| 41:QP:36:TYR:O | 41:QP:37:HIS:C | 2.53 | 0.47 |
| 40:RA:139:HIS:O | 40:RA:170:SER:HA | 2.14 | 0.47 |
| 40:RA:306:ASP:OD2 | 40:RA:308:ARG:NH2 | 2.48 | 0.47 |
| 40:RF:234:ILE:HD11 | 40:RF:272:TYR:HB2 | 1.97 | 0.47 |
| 40:RF:269:LEU:HD21 | 40:RF:301:GLN:HB3 | 1.97 | 0.47 |
| 40:RH:116:ASP:N | 40:RH:116:ASP:OD1 | 2.47 | 0.47 |
| 41:RN:263:LEU:HD21 | 41:RN:422:VAL:HB | 1.96 | 0.47 |
| 40:SE:326:LYS:HE3 | 41:SM:208:TYR:HB2 | 1.97 | 0.47 |
| 40:SF:90:GLU:O | 40:SF:121:ARG:NH1 | 2.48 | 0.47 |
| 41:SM:113:VAL:HA | 41:SM:116:VAL:HG12 | 1.97 | 0.47 |
| 41:SM:139:LEU:HG | 41:SM:168:SER:HB3 | 1.96 | 0.47 |
| 41:SO:152:ILE:HA | 41:SO:155:ILE:HG12 | 1.97 | 0.47 |
| 41:SO:418:LEU:O | 41:SO:419:GLY:C | 2.53 | 0.47 |
| 40:TH:97:GLU:HG2 | 41:TO:251:ARG:HH22 | 1.80 | 0.47 |
| 41:TM:114:ASP:OD1 | 41:TM:115:SER:N | 2.47 | 0.47 |
| 41:TN:187:LEU:HD21 | 41:TN:403:MET:HE2 | 1.97 | 0.47 |
| 40:UF:84:ARG:HG3 | 40:UF:85:GLN:H | 1.80 | 0.47 |
| 40:UI:116:ASP:HA | 40:UI:119:LEU:HD23 | 1.97 | 0.47 |
| 40:UI:228:ASN:O | 40:UI:229:ARG:C | 2.52 | 0.47 |
| 41:UN:314:ALA:HA | 41:UN:350:LYS:HB3 | 1.96 | 0.47 |
| 40:VA:206:ASN:OD1 | 42:VA:501:GTP:O2' | 2.32 | 0.47 |
| 40:VF:138:PHE:HE2 | 40:VF:235:VAL:HG21 | 1.80 | 0.47 |
| 40:VG:238:ILE:HG23 | 40:VG:255:PHE:CE2 | 2.50 | 0.47 |
| 40:VJ:271:THR:OG1 | 40:VJ:300:ASN:O | 2.26 | 0.47 |
| 41:VQ:142:GLY:O | 41:VQ:144:GLY:N | 2.48 | 0.47 |
| 40:WA:172:TYR:OH | 40:WA:386:ALA:O | 2.33 | 0.47 |
| 40:WA:253:THR:O | 40:WA:257:THR:OG1 | 2.26 | 0.47 |
| 40:WI:384:ALA:HB2 | 40:WI:431:TYR:HD1 | 1.79 | 0.47 |
| 41:WM:186:THR:HG21 | 41:WM:385:PHE:HB2 | 1.96 | 0.47 |
| 41:WM:404:ASP:HB2 | 41:WM:406:MET:HG2 | 1.96 | 0.47 |
| 41:WP:215:LEU:HB3 | 41:WP:217:LEU:HG | 1.97 | 0.47 |
| 2:1C:14:PRO:HB2 | 41:GM:262:ARG:HH12 | 1.79 | 0.47 |
| 7:1S:59:PHE:CE1 | 7:1S:585:GLY:HA2 | 2.50 | 0.47 |
| 7:1S:480:SER:OG | 7:1S:484:THR:OG1 | 2.33 | 0.47 |
| 7:1U:292:GLY:H | 7:1U:310:GLU:HG2 | 1.78 | 0.47 |
| 8:1X:284:MET:HA | 8:1X:287:TYR:CE1 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:1Z:400:TRP:HH2 | 41:UP:276:ARG:CB | 2.28 | 0.47 |
| 12:2R:59:ALA:HB1 | 41:AP:423:VAL:HG13 | 1.97 | 0.47 |
| 13:2T:49:ILE:HG23 | 13:2T:160:CYS:SG | 2.55 | 0.47 |
| 13:2T:72:LYS:HE3 | 13:2T:72:LYS:HB3 | 1.45 | 0.47 |
| 14:3B:80:THR:O | 14:3B:84:ARG:NH1 | 2.47 | 0.47 |
| 17:3R:183:ARG:HH11 | 17:3R:186:MET:HB2 | 1.79 | 0.47 |
| 21:4D:140:ASN:HB3 | 21:4D:216:ARG:HE | 1.80 | 0.47 |
| 21:4E:41:ARG:O | 41:LO:77:ARG:NH1 | 2.46 | 0.47 |
| 21:4E:409:VAL:HA | 21:4E:412:MET:HE2 | 1.97 | 0.47 |
| 21:4E:423:LEU:HB3 | 21:4E:507:ASP:HB3 | 1.97 | 0.47 |
| 21:4F:276:LEU:HD11 | 40:CE:45:GLY:HA3 | 1.97 | 0.47 |
| 22:4H:303:VAL:HB | 41:CL:216:LYS:HB3 | 1.96 | 0.47 |
| 23:4N:170:SER:N | 23:4N:171:PRO:HD2 | 2.30 | 0.47 |
| 23:4R:36:THR:O | 23:4R:37:TYR:C | 2.53 | 0.47 |
| 26:4W:333:ILE:HD13 | 31:5I:392:GLN:OE1 | 2.15 | 0.47 |
| 31:5I:744:TYR:HA | 41:IQ:356:ILE:HG12 | 1.97 | 0.47 |
| 34:5Q:216:GLU:HG3 | 41:GN:276:ARG:HD3 | 1.97 | 0.47 |
| 39:6H:17:TYR:O | 39:6H:21:GLN:OE1 | 2.33 | 0.47 |
| 39:6H:43:ARG:NH1 | 39:6H:46:SER:OG | 2.48 | 0.47 |
| 40:AA:262:TYR:OH | 41:AB:391:ARG:O | 2.29 | 0.47 |
| 41:AM:172:SER:OG | 41:AM:175:VAL:O | 2.26 | 0.47 |
| 41:AP:117:LEU:O | 41:AP:121:ARG:HB2 | 2.15 | 0.47 |
| 40:BF:120:ASP:OD1 | 40:BF:124:LYS:NZ | 2.48 | 0.47 |
| 40:BG:20:CYS:HA | 40:BG:232:SER:HB2 | 1.97 | 0.47 |
| 40:BG:205:ASP:HB2 | 40:BG:303:VAL:HG13 | 1.97 | 0.47 |
| 40:BI:70:LEU:HD22 | 40:BI:145:THR:HG23 | 1.97 | 0.47 |
| 40:BI:231:ILE:O | 40:BI:235:VAL:HG23 | 2.15 | 0.47 |
| 41:BM:112:LEU:O | 41:BM:116:VAL:HG23 | 2.14 | 0.47 |
| 40:CA:65:ALA:H | 40:CA:91:GLN:NE2 | 2.13 | 0.47 |
| 41:CB:197:ASP:OD2 | 41:CB:197:ASP:N | 2.45 | 0.47 |
| 40:CF:326:LYS:HE3 | 41:CN:208:TYR:HB2 | 1.96 | 0.47 |
| 40:CI:56:THR:OG1 | 40:CI:59:GLY:O | 2.33 | 0.47 |
| 41:CL:271:ALA:CB | 41:CL:365:ALA:HB3 | 2.44 | 0.47 |
| 41:CL:362:LYS:HD3 | 41:CL:362:LYS:HA | 1.57 | 0.47 |
| 41:CM:393:ALA:O | 41:CM:394:PHE:C | 2.53 | 0.47 |
| 41:CN:208:TYR:O | 41:CN:211:CYS:N | 2.48 | 0.47 |
| 41:CN:359:ARG:CZ | 41:CN:359:ARG:HB2 | 2.45 | 0.47 |
| 41:CO:56:GLY:C | 41:CO:58:LYS:H | 2.18 | 0.47 |
| 41:CP:74:ASP:HA | 41:CP:77:ARG:NH1 | 2.29 | 0.47 |
| 41:CP:250:LEU:HD23 | 41:CP:250:LEU:HA | 1.76 | 0.47 |
| 41:DB:288:GLU:O | 41:DB:291:GLN:HG3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DE:7:VAL:N | 40:DE:136:LEU:O | 2.38 | 0.47 |
| 40:DE:288:VAL:HG23 | 40:DE:372:ARG:HD3 | 1.96 | 0.47 |
| 40:DE:413:GLU:HG2 | 40:DE:416:GLU:H | 1.79 | 0.47 |
| 40:DF:225:THR:HA | 40:DF:228:ASN:HB2 | 1.96 | 0.47 |
| 40:DF:273:ALA:H | 40:DF:274:PRO:HD2 | 1.80 | 0.47 |
| 40:DF:297:GLU:O | 40:DF:299:ALA:N | 2.47 | 0.47 |
| 41:DL:36:TYR:CE1 | 41:DL:38:GLY:HA3 | 2.50 | 0.47 |
| 41:DP:42:LEU:HD13 | 41:DP:356:ILE:CG1 | 2.43 | 0.47 |
| 40:EA:145:THR:OG1 | 42:EA:501:GTP:O2B | 2.33 | 0.47 |
| 40:EA:210:TYR:HB3 | 41:EN:324:LYS:NZ | 2.30 | 0.47 |
| 41:EB:234:SER:O | 41:EB:238:THR:HB | 2.15 | 0.47 |
| 40:EH:339:ARG:HA | 40:EH:339:ARG:HD3 | 1.41 | 0.47 |
| 41:EM:334:GLN:OE1 | 41:EM:348:ASN:N | 2.48 | 0.47 |
| 41:EM:395:LEU:O | 41:EM:396:HIS:C | 2.53 | 0.47 |
| 41:EP:226:ASN:HB2 | 43:EP:501:GDP:HN1 | 1.80 | 0.47 |
| 41:EP:341:PHE:HD1 | 41:EP:348:ASN:HD21 | 1.63 | 0.47 |
| 40:FA:208:ALA:O | 40:FA:211:ASP:N | 2.48 | 0.47 |
| 41:FM:148:GLY:O | 41:FM:152:ILE:HG12 | 2.15 | 0.47 |
| 41:FM:207:LEU:HD13 | 41:FM:210:ILE:HD11 | 1.96 | 0.47 |
| 41:FN:200:TYR:HE2 | 41:FN:236:VAL:HG21 | 1.79 | 0.47 |
| 41:FN:392:LYS:HD2 | 41:FN:395:LEU:HD23 | 1.97 | 0.47 |
| 40:GA:141:PHE:HD1 | 40:GA:172:TYR:HA | 1.79 | 0.47 |
| 40:GG:376:MET:SD | 40:GG:378:SER:HB3 | 2.55 | 0.47 |
| 40:GH:12:ALA:O | 40:GH:16:ILE:HG23 | 2.15 | 0.47 |
| 40:GI:224:TYR:HB2 | 41:GP:245:GLN:OE1 | 2.14 | 0.47 |
| 41:GN:108:GLU:O | 41:GN:111:GLU:HG2 | 2.15 | 0.47 |
| 41:GO:252:LYS:O | 41:GO:256:ASN:HB2 | 2.15 | 0.47 |
| 40:HH:274:PRO:HG3 | 40:HH:286:LEU:HD12 | 1.97 | 0.47 |
| 40:HI:12:ALA:O | 40:HI:16:ILE:HG12 | 2.14 | 0.47 |
| 41:HN:69:GLU:O | 41:HN:71:GLY:N | 2.48 | 0.47 |
| 41:HN:160:PRO:O | 41:HN:161:ASP:C | 2.53 | 0.47 |
| 41:HP:204:ASN:HB3 | 41:HP:208:TYR:CZ | 2.49 | 0.47 |
| 40:IE:304:LYS:HA | 40:IE:304:LYS:HD3 | 1.79 | 0.47 |
| 40:II:213:CYS:HA | 40:II:217:LEU:HB2 | 1.96 | 0.47 |
| 41:IN:6:HIS:O | 41:IN:63:ALA:HA | 2.15 | 0.47 |
| 40:JE:209:ILE:HD12 | 40:JE:230:LEU:HD23 | 1.97 | 0.47 |
| 40:JG:150:THR:O | 40:JG:154:MET:HG2 | 2.15 | 0.47 |
| 41:JN:20:PHE:HA | 41:JN:230:SER:HB2 | 1.96 | 0.47 |
| 41:KB:139:LEU:HG | 41:KB:168:SER:HB2 | 1.97 | 0.47 |
| 41:KL:413:SER:OG | 41:KL:414:ASN:N | 2.48 | 0.47 |
| 40:LA:93:ILE:HD11 | 40:LA:121:ARG:HG3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LF:326:LYS:CE | 41:LN:208:TYR:HB2 | 2.45 | 0.47 |
| 40:LG:352:LYS:HD3 | 40:LG:352:LYS:HA | 1.21 | 0.47 |
| 40:LH:288:VAL:HA | 40:LH:291:ILE:HG12 | 1.97 | 0.47 |
| 41:MB:258:VAL:HB | 40:MG:406:TRP:HZ2 | 1.79 | 0.47 |
| 40:MD:231:ILE:O | 40:MD:235:VAL:HG23 | 2.15 | 0.47 |
| 40:MF:159:VAL:O | 40:MF:160:ASP:C | 2.53 | 0.47 |
| 40:ND:151:SER:O | 40:ND:152:LEU:C | 2.53 | 0.47 |
| 40:ND:235:VAL:O | 40:ND:239:THR:HG22 | 2.14 | 0.47 |
| 40:NG:206:ASN:OD1 | 42:NG:501:GTP:O2' | 2.30 | 0.47 |
| 40:OA:191:THR:HA | 40:OA:194:THR:HG1 | 1.80 | 0.47 |
| 40:OD:405:HIS:HA | 40:OD:408:VAL:HG22 | 1.97 | 0.47 |
| 40:OE:139:HIS:CE1 | 40:OE:150:THR:HG21 | 2.50 | 0.47 |
| 40:OE:288:VAL:HG22 | 40:OE:372:ARG:HD3 | 1.97 | 0.47 |
| 40:OE:296:PHE:HD2 | 40:OE:341:ILE:HG12 | 1.80 | 0.47 |
| 40:OH:261:PRO:HB2 | 40:OH:346:TRP:CZ3 | 2.51 | 0.47 |
| 40:PF:238:ILE:HG12 | 40:PF:377:LEU:HD21 | 1.97 | 0.47 |
| 41:QB:218:THR:OG1 | 41:QB:219:THR:N | 2.48 | 0.47 |
| 41:QL:136:THR:HG22 | 41:QL:167:PHE:HB2 | 1.97 | 0.47 |
| 40:RE:269:LEU:HD13 | 40:RE:303:VAL:HB | 1.96 | 0.47 |
| 40:RH:20:CYS:HA | 40:RH:232:SER:HB2 | 1.97 | 0.47 |
| 41:RL:268:PRO:HG2 | 41:RL:300:MET:HB2 | 1.96 | 0.47 |
| 41:RM:31:ASP:OD1 | 41:RM:34:GLY:N | 2.45 | 0.47 |
| 41:RM:271:ALA:O | 41:RM:292:GLN:NE2 | 2.47 | 0.47 |
| 41:RN:16:ILE:HG12 | 43:RN:502:GDP:N2 | 2.29 | 0.47 |
| 41:RO:156:ARG:HH21 | 41:RO:164:MET:H | 1.63 | 0.47 |
| 40:SE:91:GLN:OE1 | 40:SE:121:ARG:NH1 | 2.47 | 0.47 |
| 40:SE:222:PRO:O | 41:SL:322:SER:OG | 2.29 | 0.47 |
| 40:SI:90:GLU:HB3 | 40:SI:121:ARG:NH2 | 2.29 | 0.47 |
| 41:SL:272:PRO:HG3 | 41:SL:364:SER:HA | 1.95 | 0.47 |
| 41:SO:97:ALA:O | 41:SO:100:ASN:N | 2.46 | 0.47 |
| 40:TA:209:ILE:HA | 40:TA:212:ILE:HG22 | 1.96 | 0.47 |
| 41:UB:77:ARG:HH12 | 41:UB:83:GLN:HA | 1.80 | 0.47 |
| 40:UF:191:THR:HG21 | 40:UF:424:MET:SD | 2.55 | 0.47 |
| 40:UF:328:VAL:HG11 | 40:UF:353:VAL:HG13 | 1.97 | 0.47 |
| 41:UP:85:PHE:O | 41:UP:86:ARG:C | 2.52 | 0.47 |
| 40:VA:225:THR:HG22 | 40:VA:229:ARG:HE | 1.79 | 0.47 |
| 40:VG:205:ASP:OD2 | 40:VG:207:GLU:N | 2.47 | 0.47 |
| 40:VH:70:LEU:HD12 | 40:VH:99:ALA:HB2 | 1.97 | 0.47 |
| 41:VP:139:LEU:HD12 | 41:VP:170:VAL:HG12 | 1.97 | 0.47 |
| 40:WA:188:ILE:HD11 | 40:WA:424:MET:HG3 | 1.96 | 0.47 |
| 40:WH:182:VAL:HG22 | 40:WH:185:TYR:HB2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WN:58:LYS:HA | 41:WN:58:LYS:HD2 | 1.54 | 0.47 |
| 7:1U:162:THR:N | 7:1U:177:ALA:O | 2.41 | 0.46 |
| 8:1Y:202:HIS:HA | 8:1Y:205:ARG:HD3 | 1.98 | 0.46 |
| 9:2B:45:GLN:O | 9:2B:46:VAL:C | 2.53 | 0.46 |
| 11:2I:209:LYS:HD3 | 11:2I:209:LYS:HA | 1.35 | 0.46 |
| 15:3F:194:ASN:HD22 | 17:3R:168:ILE:HD13 | 1.71 | 0.46 |
| 16:3K:214:THR:HG22 | 16:3K:216:GLN:H | 1.80 | 0.46 |
| 17:3R:218:GLU:O | 17:3R:222:GLU:N | 2.47 | 0.46 |
| 17:3R:254:LEU:HD23 | 17:3R:307:ASN:HB3 | 1.97 | 0.46 |
| 17:3R:327:ASN:O | 17:3R:328:LEU:C | 2.54 | 0.46 |
| 21:4F:495:VAL:HA | 21:4F:503:PHE:O | 2.15 | 0.46 |
| 22:4K:651:LYS:HA | 22:4K:651:LYS:HD3 | 1.48 | 0.46 |
| 23:4M:21:GLY:O | 40:BG:79:ARG:NE | 2.48 | 0.46 |
| 23:4Q:209:ALA:C | 23:4Q:211:GLN:H | 2.18 | 0.46 |
| 23:4R:184:MET:HB3 | 40:CI:79:ARG:HD3 | 1.96 | 0.46 |
| 23:4R:198:PHE:HB3 | 40:DI:221:ARG:HD2 | 1.96 | 0.46 |
| 23:4R:204:VAL:O | 23:4R:207:ASN:HB3 | 2.15 | 0.46 |
| 23:4R:259:ARG:HH21 | 40:EI:365:GLY:CA | 2.28 | 0.46 |
| 26:4V:201:ILE:HG23 | 26:4V:202:ARG:HG3 | 1.97 | 0.46 |
| 28:5B:56:GLU:OE2 | 41:JB:276:ARG:N | 2.48 | 0.46 |
| 33:5N:248:PHE:HD1 | 40:HH:369:LYS:HE2 | 1.80 | 0.46 |
| 34:5Q:180:ARG:HH22 | 40:GA:370:VAL:HG12 | 1.80 | 0.46 |
| 35:5T:162:MET:CE | 41:KL:320:ARG:HA | 2.46 | 0.46 |
| 38:6C:98:PHE:CZ | 41:VB:294:PHE:HB3 | 2.50 | 0.46 |
| 39:6F:98:LEU:HD22 | 39:6F:153:TRP:CD1 | 2.50 | 0.46 |
| 39:6I:78:LEU:HD13 | 39:6I:146:VAL:HG11 | 1.98 | 0.46 |
| 39:6L:99:LEU:HG | 39:6L:103:LYS:HE2 | 1.96 | 0.46 |
| 41:AB:193:VAL:HG22 | 41:AB:418:LEU:HD22 | 1.96 | 0.46 |
| 40:AG:134:GLY:HA3 | 40:AG:165:SER:O | 2.15 | 0.46 |
| 41:BB:107:THR:OG1 | 41:BB:108:GLU:N | 2.48 | 0.46 |
| 40:BE:231:ILE:O | 40:BE:235:VAL:HG23 | 2.15 | 0.46 |
| 40:BF:220:GLU:HG2 | 40:BF:221:ARG:HG3 | 1.97 | 0.46 |
| 40:BF:431:TYR:HA | 40:BF:434:VAL:HG12 | 1.96 | 0.46 |
| 40:BG:84:ARG:HG3 | 40:BG:85:GLN:HG3 | 1.97 | 0.46 |
| 40:BG:211:ASP:OD1 | 40:BG:214:ARG:NH2 | 2.48 | 0.46 |
| 40:BH:163:LYS:HE2 | 40:BH:163:LYS:HB2 | 1.40 | 0.46 |
| 40:BI:207:GLU:HB3 | 40:BI:304:LYS:HG2 | 1.95 | 0.46 |
| 41:BL:103:LYS:HA | 41:BL:107:THR:HB | 1.97 | 0.46 |
| 41:BM:58:LYS:O | 41:BM:59:TYR:C | 2.52 | 0.46 |
| 41:BM:303:CYS:SG | 41:BM:374:ILE:HA | 2.55 | 0.46 |
| 41:BN:310:TYR:HD1 | 41:BN:371:SER:HB2 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BP:100:ASN:ND2 | 41:BP:397:TRP:HB3 | 2.31 | 0.46 |
| 40:CA:406:TRP:NE1 | 41:CN:258:VAL:HG13 | 2.25 | 0.46 |
| 41:CB:132:GLY:CA | 41:CB:163:ILE:O | 2.61 | 0.46 |
| 41:CB:358:PRO:HG2 | 41:CB:361:LEU:HB2 | 1.97 | 0.46 |
| 40:CF:329:ASN:HB3 | 41:CN:175:VAL:HG21 | 1.97 | 0.46 |
| 40:CH:195:LEU:HD11 | 40:CH:427:LEU:HD22 | 1.96 | 0.46 |
| 40:CI:276:ILE:HB | 40:CI:281:ALA:HB2 | 1.96 | 0.46 |
| 41:CL:222:TYR:HA | 41:CL:225:LEU:HD12 | 1.97 | 0.46 |
| 41:CM:61:PRO:HG2 | 41:CM:85:PHE:HA | 1.96 | 0.46 |
| 41:CN:193:VAL:HG22 | 41:CN:265:PHE:HZ | 1.80 | 0.46 |
| 41:CN:385:PHE:O | 41:CN:386:THR:C | 2.54 | 0.46 |
| 41:CO:294:PHE:CD1 | 41:CO:333:VAL:HG11 | 2.50 | 0.46 |
| 41:CO:315:ALA:O | 41:CO:317:PHE:N | 2.49 | 0.46 |
| 41:CP:98:GLY:O | 41:CP:99:ASN:C | 2.53 | 0.46 |
| 41:CP:358:PRO:HG2 | 41:CP:361:LEU:HB2 | 1.97 | 0.46 |
| 40:DA:50:ASN:O | 40:DA:51:THR:C | 2.53 | 0.46 |
| 40:DA:211:ASP:O | 40:DA:212:ILE:C | 2.54 | 0.46 |
| 40:DA:315:CYS:SG | 40:DA:350:GLY:O | 2.73 | 0.46 |
| 41:DB:186:THR:HG21 | 41:DB:385:PHE:HB2 | 1.96 | 0.46 |
| 40:DE:88:HIS:O | 40:DE:89:PRO:C | 2.53 | 0.46 |
| 40:DF:269:LEU:HD23 | 40:DF:303:VAL:HG11 | 1.97 | 0.46 |
| 40:DH:132:LEU:HB3 | 40:DH:164:LYS:NZ | 2.30 | 0.46 |
| 40:DI:34:GLY:HA3 | 40:DI:60:LYS:HD3 | 1.96 | 0.46 |
| 41:DL:293:MET:O | 41:DL:295:ASP:N | 2.48 | 0.46 |
| 41:DM:239:CYS:HA | 41:DM:354:CYS:HB2 | 1.97 | 0.46 |
| 41:DN:382:SER:O | 41:DN:383:GLU:C | 2.52 | 0.46 |
| 41:DP:88:ASP:O | 41:DP:89:ASN:C | 2.53 | 0.46 |
| 40:EA:224:TYR:HA | 40:EA:227:LEU:HB2 | 1.97 | 0.46 |
| 41:EB:322:SER:O | 41:EB:326:VAL:HG23 | 2.15 | 0.46 |
| 40:EI:7:VAL:O | 40:EI:8:HIS:C | 2.54 | 0.46 |
| 41:EP:226:ASN:CB | 43:EP:501:GDP:HN1 | 2.27 | 0.46 |
| 40:FA:9:VAL:HG23 | 40:FA:139:HIS:HB3 | 1.97 | 0.46 |
| 40:FA:230:LEU:HD11 | 40:FA:275:VAL:HG12 | 1.97 | 0.46 |
| 40:FA:258:ASN:HD21 | 41:FB:178:THR:HG23 | 1.80 | 0.46 |
| 40:FA:363:VAL:O | 40:FA:364:PRO:C | 2.54 | 0.46 |
| 40:FF:11:GLN:NE2 | 41:FM:247:ASN:OD1 | 2.48 | 0.46 |
| 40:FH:60:LYS:HZ1 | 40:GH:283:HIS:CE1 | 2.34 | 0.46 |
| 41:FO:101:TRP:CE3 | 41:FO:187:LEU:HD13 | 2.50 | 0.46 |
| 41:FP:318:ARG:HB2 | 41:FP:364:SER:HB3 | 1.97 | 0.46 |
| 40:GA:332:ILE:HA | 40:GA:335:ILE:HG22 | 1.96 | 0.46 |
| 41:GB:170:VAL:HG11 | 41:GB:377:LEU:HD21 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GF:121:ARG:HE | 40:GF:124:LYS:HE2 | 1.80 | 0.46 |
| 40:GH:49:PHE:CE2 | 40:GH:55:GLU:HB2 | 2.50 | 0.46 |
| 40:GH:316:CYS:O | 40:GH:317:LEU:C | 2.54 | 0.46 |
| 40:GI:119:LEU:HA | 40:GI:122:ILE:HD12 | 1.96 | 0.46 |
| 40:GI:250:VAL:HG12 | 40:GI:254:GLU:CD | 2.36 | 0.46 |
| 40:GI:306:ASP:OD2 | 40:GI:308:ARG:HB2 | 2.14 | 0.46 |
| 41:GO:163:ILE:HD11 | 41:GO:251:ARG:HG3 | 1.97 | 0.46 |
| 40:HF:48:SER:O | 40:HF:51:THR:HG22 | 2.15 | 0.46 |
| 40:HI:332:ILE:HD12 | 40:HI:351:PHE:HD2 | 1.80 | 0.46 |
| 41:HM:163:ILE:HD11 | 41:HM:251:ARG:HG2 | 1.98 | 0.46 |
| 41:HN:61:PRO:HG2 | 41:HN:84:ILE:HG23 | 1.98 | 0.46 |
| 41:HO:202:ILE:HG23 | 41:HO:300:MET:HB3 | 1.96 | 0.46 |
| 40:IH:123:ARG:HH21 | 40:IH:161:TYR:HE2 | 1.63 | 0.46 |
| 40:II:105:ARG:HA | 40:II:109:THR:HG22 | 1.97 | 0.46 |
| 40:II:247:ALA:HB3 | 40:II:355:ILE:HB | 1.97 | 0.46 |
| 40:II:278:ALA:HA | 40:II:368:ALA:HB2 | 1.97 | 0.46 |
| 41:IM:314:ALA:HB3 | 41:IM:368:ILE:HB | 1.97 | 0.46 |
| 41:IN:42:LEU:HD22 | 41:IN:356:ILE:HD11 | 1.98 | 0.46 |
| 41:IN:101:TRP:HB2 | 41:IN:184:ASN:HD22 | 1.80 | 0.46 |
| 41:IN:186:THR:HA | 41:IN:415:MET:HE1 | 1.97 | 0.46 |
| 41:IN:238:THR:HG21 | 41:IN:318:ARG:HD3 | 1.96 | 0.46 |
| 40:JD:12:ALA:O | 40:JD:16:ILE:HG12 | 2.14 | 0.46 |
| 41:JM:164:MET:HE2 | 41:JM:164:MET:HB2 | 1.82 | 0.46 |
| 40:KA:177:VAL:HA | 41:KN:331:LEU:HD13 | 1.96 | 0.46 |
| 40:KA:177:VAL:HG23 | 41:KN:331:LEU:HB2 | 1.97 | 0.46 |
| 41:KB:229:VAL:O | 41:KB:233:MET:HG3 | 2.15 | 0.46 |
| 40:KE:51:THR:HG21 | 40:KE:243:ARG:HG2 | 1.97 | 0.46 |
| 40:KE:413:GLU:HG2 | 40:KE:415:GLY:H | 1.79 | 0.46 |
| 41:KL:8:GLN:HG3 | 41:KL:65:LEU:HA | 1.97 | 0.46 |
| 41:KM:230:SER:HA | 41:KM:233:MET:HB3 | 1.97 | 0.46 |
| 41:KN:346:PRO:O | 41:KN:347:ASN:ND2 | 2.45 | 0.46 |
| 41:KP:202:ILE:HG21 | 41:KP:229:VAL:HG22 | 1.97 | 0.46 |
| 40:LA:81:GLY:O | 40:LA:84:ARG:NH1 | 2.44 | 0.46 |
| 40:LA:96:LYS:HD3 | 41:LN:129:CYS:HB2 | 1.97 | 0.46 |
| 40:LE:210:TYR:HE1 | 40:LE:227:LEU:HD21 | 1.80 | 0.46 |
| 40:LE:291:ILE:HD13 | 40:LE:372:ARG:HB3 | 1.97 | 0.46 |
| 40:LG:298:PRO:HB3 | 40:LG:307:PRO:HD2 | 1.97 | 0.46 |
| 40:LG:311:LYS:HG2 | 40:LG:342:GLN:HG2 | 1.96 | 0.46 |
| 40:LG:337:THR:OG1 | 40:LG:338:LYS:N | 2.48 | 0.46 |
| 41:LM:173:PRO:HD3 | 41:LM:380:ARG:CZ | 2.45 | 0.46 |
| 41:LN:202:ILE:HD13 | 41:LN:229:VAL:HG22 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MA:286:LEU:O | 40:MA:372:ARG:HD2 | 2.16 | 0.46 |
| 40:MF:348:PRO:HB3 | 41:MN:384:GLN:HG2 | 1.97 | 0.46 |
| 40:MH:58:ALA:O | 40:MH:59:GLY:C | 2.53 | 0.46 |
| 40:MH:337:THR:OG1 | 40:MH:338:LYS:N | 2.48 | 0.46 |
| 41:MO:245:GLN:O | 41:MO:246:LEU:C | 2.53 | 0.46 |
| 41:MP:12:CYS:HB3 | 41:MP:138:SER:HB2 | 1.97 | 0.46 |
| 40:NE:112:LYS:HA | 40:NE:115:ILE:HG22 | 1.97 | 0.46 |
| 40:NF:440:GLU:HB2 | 41:NN:390:ARG:HH21 | 1.80 | 0.46 |
| 40:NG:238:ILE:HA | 40:NG:318:LEU:HD22 | 1.97 | 0.46 |
| 40:NG:265:ILE:HG21 | 40:NG:313:MET:HE1 | 1.97 | 0.46 |
| 40:NH:51:THR:O | 40:NH:64:ARG:NH1 | 2.48 | 0.46 |
| 41:NM:334:GLN:HE22 | 41:NM:348:ASN:N | 2.14 | 0.46 |
| 41:NO:244:GLY:HA3 | 41:NO:354:CYS:HA | 1.97 | 0.46 |
| 40:OD:182:VAL:HG22 | 40:OD:185:TYR:HB2 | 1.97 | 0.46 |
| 40:OG:438:SER:HA | 41:OO:391:ARG:HH22 | 1.80 | 0.46 |
| 40:OH:10:GLY:O | 40:OH:14:VAL:HG23 | 2.14 | 0.46 |
| 40:OH:187:SER:O | 40:OH:188:ILE:C | 2.54 | 0.46 |
| 40:OH:224:TYR:CD1 | 40:OH:227:LEU:HD12 | 2.50 | 0.46 |
| 41:PL:3:GLU:OE2 | 41:PL:127:CYS:HB3 | 2.15 | 0.46 |
| 41:QB:317:PHE:HB3 | 41:QB:321:MET:SD | 2.55 | 0.46 |
| 40:QF:391:ASP:HB3 | 40:QF:421:ARG:HH12 | 1.79 | 0.46 |
| 40:QG:79:ARG:HH22 | 40:QG:94:THR:HG21 | 1.80 | 0.46 |
| 41:QO:86:ARG:HD2 | 41:QO:89:ASN:HB2 | 1.95 | 0.46 |
| 41:QP:222:TYR:O | 41:QP:225:LEU:N | 2.49 | 0.46 |
| 41:RB:137:HIS:HE1 | 41:RB:139:LEU:CD2 | 2.28 | 0.46 |
| 40:RF:31:GLN:HG2 | 40:RF:37:PRO:HG2 | 1.97 | 0.46 |
| 40:RF:310:GLY:HA3 | 40:RF:382:ALA:HB2 | 1.96 | 0.46 |
| 41:RO:113:VAL:HG22 | 41:RO:117:LEU:HD23 | 1.97 | 0.46 |
| 41:RP:269:GLY:HA2 | 41:RP:300:MET:HE1 | 1.96 | 0.46 |
| 41:SB:322:SER:OG | 40:SG:222:PRO:O | 2.25 | 0.46 |
| 40:SG:386:ALA:HA | 40:SG:389:ARG:NH2 | 2.30 | 0.46 |
| 40:SH:221:ARG:NH1 | 41:SO:325:GLU:HB2 | 2.29 | 0.46 |
| 40:SH:274:PRO:HB2 | 40:SH:370:VAL:HG11 | 1.97 | 0.46 |
| 40:SI:271:THR:HG22 | 40:SI:376:MET:HB3 | 1.97 | 0.46 |
| 40:TA:105:ARG:HD3 | 40:TA:109:THR:HB | 1.97 | 0.46 |
| 40:TF:22:GLU:OE2 | 40:TF:229:ARG:NH1 | 2.48 | 0.46 |
| 40:TG:234:ILE:HD11 | 40:TG:272:TYR:HB2 | 1.98 | 0.46 |
| 40:TG:293:ASN:HB3 | 40:TG:335:ILE:HD11 | 1.95 | 0.46 |
| 41:TM:142:GLY:O | 41:TM:144:GLY:N | 2.48 | 0.46 |
| 41:TM:335:ASN:O | 41:TM:338:SER:OG | 2.33 | 0.46 |
| 41:TN:417:ASP:O | 41:TN:421:PRO:HD3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TO:285:THR:HB | 41:TO:287:PRO:HD2 | 1.97 | 0.46 |
| 41:TP:421:PRO:O | 41:TP:425:ARG:HG2 | 2.15 | 0.46 |
| 40:UA:136:LEU:HD11 | 40:UA:239:THR:HG21 | 1.97 | 0.46 |
| 40:UE:136:LEU:HB3 | 40:UE:138:PHE:HE1 | 1.80 | 0.46 |
| 40:UI:56:THR:OG1 | 40:UI:57:GLY:N | 2.47 | 0.46 |
| 40:UI:100:ALA:O | 40:UI:101:ASN:C | 2.54 | 0.46 |
| 40:VA:352:LYS:HD2 | 41:VB:178:THR:HA | 1.96 | 0.46 |
| 41:VB:276:ARG:NH1 | 41:VB:279:GLN:OE1 | 2.48 | 0.46 |
| 41:VO:189:VAL:O | 41:VO:193:VAL:HG23 | 2.15 | 0.46 |
| 40:WG:241:SER:HA | 40:WG:356:ASN:HD22 | 1.79 | 0.46 |
| 40:WG:326:LYS:HG2 | 41:WO:208:TYR:CD1 | 2.49 | 0.46 |
| 7:1T:203:GLN:O | 41:WM:78:SER:HB2 | 2.15 | 0.46 |
| 7:1U:468:ARG:HA | 7:1U:468:ARG:HD2 | 1.85 | 0.46 |
| 8:1W:258:HIS:CG | 40:VJ:369:LYS:HE2 | 2.50 | 0.46 |
| 9:2B:389:GLU:HA | 9:2B:392:ARG:HG2 | 1.97 | 0.46 |
| 11:2I:186:LYS:CG | 11:2I:251:TYR:HB3 | 2.44 | 0.46 |
| 11:2I:234:MET:HB3 | 41:WO:276:ARG:HH12 | 1.79 | 0.46 |
| 11:2J:188:LEU:HG | 11:2J:251:TYR:HA | 1.97 | 0.46 |
| 11:2J:247:HIS:O | 11:2J:248:LYS:C | 2.53 | 0.46 |
| 13:2T:177:LEU:HD23 | 13:2T:182:LYS:HA | 1.97 | 0.46 |
| 14:3A:111:PRO:HG2 | 14:3A:113:ILE:HD11 | 1.98 | 0.46 |
| 14:3C:14:PHE:HB3 | 41:MO:174:LYS:HE2 | 1.97 | 0.46 |
| 15:3F:380:GLU:O | 17:3O:467:TYR:OH | 2.33 | 0.46 |
| 16:3J:17:TRP:HB2 | 16:3K:129:VAL:HG11 | 1.97 | 0.46 |
| 16:3K:131:ASP:N | 16:3K:134:GLU:OE1 | 2.48 | 0.46 |
| 17:3P:235:LEU:HD13 | 17:3P:235:LEU:HA | 1.82 | 0.46 |
| 19:3Y:103:GLN:HG3 | 40:LG:282:TYR:HE1 | 1.79 | 0.46 |
| 19:3Y:150:ASP:OD1 | 25:4T:408:ARG:NH2 | 2.47 | 0.46 |
| 19:3Y:318:ARG:HH22 | 41:LL:282:ARG:HB3 | 1.81 | 0.46 |
| 20:4B:286:ARG:HA | 20:4B:286:ARG:HD2 | 1.50 | 0.46 |
| 21:4D:97:LEU:HB2 | 21:4D:124:TYR:HB3 | 1.97 | 0.46 |
| 21:4E:233:LYS:HZ1 | 40:BH:58:ALA:HB1 | 1.80 | 0.46 |
| 21:4E:456:VAL:HB | 21:4E:459:SER:HB3 | 1.97 | 0.46 |
| 22:4J:92:LYS:H | 41:BN:279:GLN:N | 1.98 | 0.46 |
| 22:4J:693:PHE:HA | 22:4J:696:ALA:HB3 | 1.97 | 0.46 |
| 23:4R:37:TYR:CE2 | 23:4R:41:THR:HG21 | 2.50 | 0.46 |
| 26:4W:8:VAL:HG13 | 26:4W:79:GLY:HA3 | 1.97 | 0.46 |
| 27:4Y:176:SER:OG | 27:4Y:177:TRP:N | 2.47 | 0.46 |
| 30:5G:85:GLN:NE2 | 41:GB:74:ASP:OD2 | 2.48 | 0.46 |
| 31:5I:646:LYS:HG2 | 31:5I:650:GLN:HE21 | 1.81 | 0.46 |
| 31:5I:683:TYR:O | 31:5I:684:GLU:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 31:5J:795:ALA:HA | 31:5J:798:LEU:HB2 | 1.96 | 0.46 |
| 38:6C:89:GLU:HB2 | 41:VB:307:HIS:CE1 | 2.46 | 0.46 |
| 39:6L:117:ALA:HB1 | 39:6L:121:HIS:HB3 | 1.97 | 0.46 |
| 40:AA:235:VAL:O | 40:AA:239:THR:HG22 | 2.15 | 0.46 |
| 40:AF:398:TYR:O | 40:AF:401:ARG:NH1 | 2.46 | 0.46 |
| 41:AM:203:ASP:OD1 | 41:AM:204:ASN:N | 2.49 | 0.46 |
| 41:AO:266:PHE:HB3 | 41:AO:368:ILE:HG22 | 1.96 | 0.46 |
| 41:BB:393:ALA:O | 41:BB:395:LEU:N | 2.48 | 0.46 |
| 40:BF:88:HIS:HB3 | 40:BF:91:GLN:HG3 | 1.97 | 0.46 |
| 41:BL:107:THR:HG22 | 41:BL:108:GLU:H | 1.81 | 0.46 |
| 41:BO:138:SER:O | 41:BO:140:GLY:N | 2.48 | 0.46 |
| 41:BP:220:PRO:HB2 | 41:BP:225:LEU:HD21 | 1.96 | 0.46 |
| 41:BP:237:THR:HB | 41:BP:240:LEU:HD11 | 1.97 | 0.46 |
| 41:CB:398:TYR:HB3 | 41:CB:403:MET:HG3 | 1.96 | 0.46 |
| 40:CE:236:SER:HB2 | 40:CE:243:ARG:HH22 | 1.81 | 0.46 |
| 40:CH:109:THR:O | 40:CH:111:GLY:N | 2.47 | 0.46 |
| 41:CN:11:GLN:H | 43:CN:501:GDP:PB | 2.38 | 0.46 |
| 41:CN:60:VAL:HG11 | 41:DN:281:TYR:CB | 2.42 | 0.46 |
| 41:CN:135:LEU:HD11 | 41:CN:137:HIS:HB3 | 1.98 | 0.46 |
| 41:CO:273:LEU:H | 41:CO:292:GLN:NE2 | 2.13 | 0.46 |
| 41:CO:320:ARG:H | 41:CO:320:ARG:HG2 | 1.48 | 0.46 |
| 40:DA:164:LYS:HA | 40:DA:164:LYS:HD3 | 1.40 | 0.46 |
| 41:DB:123:GLU:O | 41:DB:124:ALA:C | 2.53 | 0.46 |
| 40:DE:47:ASP:C | 40:DE:49:PHE:H | 2.18 | 0.46 |
| 40:DE:181:VAL:HB | 41:DL:348:ASN:HA | 1.97 | 0.46 |
| 40:DF:248:LEU:H | 40:DF:355:ILE:HB | 1.80 | 0.46 |
| 40:DG:315:CYS:HB2 | 40:DG:350:GLY:O | 2.16 | 0.46 |
| 41:DM:232:THR:O | 41:DM:233:MET:C | 2.53 | 0.46 |
| 41:DM:412:GLU:HG2 | 41:DM:416:ASN:HD21 | 1.80 | 0.46 |
| 41:DN:62:ARG:HD2 | 41:DN:123:GLU:HB3 | 1.97 | 0.46 |
| 41:DN:173:PRO:O | 41:DN:174:LYS:C | 2.53 | 0.46 |
| 40:EA:11:GLN:OE1 | 41:EN:246:LEU:N | 2.48 | 0.46 |
| 40:EA:167:LEU:HD13 | 40:EA:200:CYS:HB3 | 1.96 | 0.46 |
| 41:EB:117:LEU:HD11 | 41:EB:154:LYS:HE3 | 1.97 | 0.46 |
| 40:EE:68:VAL:HG12 | 40:EE:93:ILE:HB | 1.98 | 0.46 |
| 40:EE:73:THR:HG22 | 41:EL:46:ARG:CZ | 2.45 | 0.46 |
| 40:EE:274:PRO:HA | 40:EE:276:ILE:HD12 | 1.97 | 0.46 |
| 40:EF:39:ASP:OD2 | 40:EF:39:ASP:N | 2.46 | 0.46 |
| 40:EH:413:GLU:H | 40:EH:413:GLU:HG3 | 1.51 | 0.46 |
| 40:EI:70:LEU:HD22 | 40:EI:110:ILE:HB | 1.96 | 0.46 |
| 40:EI:308:ARG:HE | 40:EI:308:ARG:HB2 | 1.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EM:413:SER:OG | 41:EM:414:ASN:N | 2.48 | 0.46 |
| 41:EN:26:ASP:HB3 | 41:EN:359:ARG:HH22 | 1.80 | 0.46 |
| 41:EO:103:LYS:O | 41:EO:107:THR:OG1 | 2.33 | 0.46 |
| 41:EO:238:THR:OG1 | 41:EO:318:ARG:NH2 | 2.48 | 0.46 |
| 40:FA:352:LYS:HA | 40:FA:352:LYS:HD3 | 1.61 | 0.46 |
| 41:FB:7:LEU:HD23 | 41:FB:64:VAL:HB | 1.97 | 0.46 |
| 41:FB:171:PRO:HB3 | 41:FB:181:GLU:HG2 | 1.97 | 0.46 |
| 41:FN:248:ALA:HA | 41:FN:252:LYS:HG2 | 1.97 | 0.46 |
| 40:GE:57:GLY:O | 40:GE:58:ALA:HB3 | 2.15 | 0.46 |
| 40:GE:430:ASP:O | 40:GE:431:TYR:C | 2.53 | 0.46 |
| 40:GF:7:VAL:HG13 | 40:GF:66:VAL:HG13 | 1.97 | 0.46 |
| 40:GG:22:GLU:OE2 | 40:GG:363:VAL:HG21 | 2.15 | 0.46 |
| 40:GI:255:PHE:O | 40:GI:259:LEU:HB2 | 2.15 | 0.46 |
| 41:GN:245:GLN:O | 41:GN:247:ASN:N | 2.49 | 0.46 |
| 41:GN:414:ASN:O | 41:GN:418:LEU:N | 2.48 | 0.46 |
| 40:HE:49:PHE:O | 40:HE:51:THR:N | 2.48 | 0.46 |
| 40:HH:139:HIS:ND1 | 40:HH:146:GLY:O | 2.48 | 0.46 |
| 41:HN:21:TRP:CZ2 | 41:HN:63:ALA:HB2 | 2.50 | 0.46 |
| 40:II:171:ILE:HD13 | 40:II:204:VAL:HG23 | 1.97 | 0.46 |
| 41:IP:132:GLY:HA2 | 41:IP:162:ARG:HB3 | 1.97 | 0.46 |
| 41:IP:406:MET:O | 41:IP:409:THR:OG1 | 2.27 | 0.46 |
| 40:JA:386:ALA:HA | 40:JA:389:ARG:HH21 | 1.80 | 0.46 |
| 41:JB:189:VAL:O | 41:JB:193:VAL:HG23 | 2.15 | 0.46 |
| 40:JE:14:VAL:HG21 | 40:JE:75:ILE:HD11 | 1.98 | 0.46 |
| 40:JE:312:TYR:CE2 | 40:JE:341:ILE:HG13 | 2.49 | 0.46 |
| 40:JF:26:LEU:HG | 40:JF:363:VAL:HG12 | 1.97 | 0.46 |
| 41:JM:297:LYS:HB3 | 41:JM:297:LYS:HE2 | 1.43 | 0.46 |
| 40:KD:51:THR:HG23 | 40:KD:52:PHE:HD1 | 1.80 | 0.46 |
| 40:KE:169:PHE:CE2 | 40:KE:235:VAL:HG22 | 2.50 | 0.46 |
| 41:KO:193:VAL:HG11 | 41:KO:418:LEU:HD21 | 1.96 | 0.46 |
| 41:KO:313:VAL:HB | 41:KO:349:VAL:HG12 | 1.97 | 0.46 |
| 40:LA:6:SER:O | 40:LA:65:ALA:HA | 2.14 | 0.46 |
| 40:LD:223:THR:HG23 | 40:LD:225:THR:HG22 | 1.95 | 0.46 |
| 40:LE:319:TYR:HB3 | 40:LE:323:VAL:HG21 | 1.97 | 0.46 |
| 41:LL:142:GLY:O | 41:LL:144:GLY:N | 2.48 | 0.46 |
| 41:LL:334:GLN:HE22 | 41:LL:347:ASN:HA | 1.80 | 0.46 |
| 41:LM:226:ASN:ND2 | 43:LM:502:GDP:O6 | 2.40 | 0.46 |
| 41:LM:236:VAL:HG22 | 41:LM:368:ILE:HD11 | 1.98 | 0.46 |
| 41:LP:58:LYS:NZ | 41:MP:280:GLN:O | 2.37 | 0.46 |
| 40:MF:132:LEU:HB3 | 40:MF:164:LYS:HE2 | 1.96 | 0.46 |
| 40:MF:254:GLU:HG2 | 41:MN:98:GLY:HA2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MF:419:GLU:O | 40:MF:422:GLU:HB2 | 2.15 | 0.46 |
| 40:MF:431:TYR:O | 40:MF:434:VAL:HG22 | 2.16 | 0.46 |
| 40:MH:30:ILE:HG12 | 40:MH:61:HIS:CB | 2.45 | 0.46 |
| 40:MH:251:ASP:H | 40:MH:254:GLU:HG3 | 1.80 | 0.46 |
| 41:ML:401:GLU:N | 41:ML:401:GLU:OE2 | 2.47 | 0.46 |
| 41:MP:284:LEU:HD11 | 41:MP:362:LYS:HD3 | 1.96 | 0.46 |
| 40:NE:328:VAL:O | 40:NE:332:ILE:HG13 | 2.15 | 0.46 |
| 40:NG:440:GLU:O | 41:NO:390:ARG:NH1 | 2.48 | 0.46 |
| 40:NH:143:GLY:N | 42:NO:501:GTP:O2A | 2.40 | 0.46 |
| 41:NL:26:ASP:HB3 | 41:NL:359:ARG:NH2 | 2.31 | 0.46 |
| 41:NL:387:ALA:HA | 41:NL:390:ARG:NH2 | 2.30 | 0.46 |
| 40:OG:311:LYS:HE3 | 40:OG:344:VAL:HA | 1.98 | 0.46 |
| 41:ON:179:VAL:HG13 | 41:ON:180:VAL:HG13 | 1.96 | 0.46 |
| 40:PH:295:CYS:SG | 40:PH:376:MET:HG3 | 2.55 | 0.46 |
| 41:PP:253:LEU:O | 41:PP:257:MET:HB2 | 2.15 | 0.46 |
| 40:QA:124:LYS:NZ | 40:RA:290:GLU:OE1 | 2.46 | 0.46 |
| 41:QL:52:ASN:OD1 | 41:QL:62:ARG:HD3 | 2.15 | 0.46 |
| 41:QM:137:HIS:O | 41:QM:168:SER:HA | 2.15 | 0.46 |
| 41:QM:172:SER:OG | 41:QM:175:VAL:O | 2.25 | 0.46 |
| 41:QP:226:ASN:HB2 | 43:QP:501:GDP:N1 | 2.30 | 0.46 |
| 40:RA:238:ILE:HD11 | 40:RA:377:LEU:HD21 | 1.98 | 0.46 |
| 41:RB:258:VAL:HB | 40:RG:406:TRP:HH2 | 1.80 | 0.46 |
| 40:RE:63:PRO:HG2 | 40:RE:87:PHE:HA | 1.97 | 0.46 |
| 40:RG:317:LEU:HD13 | 40:RG:376:MET:HG3 | 1.98 | 0.46 |
| 41:RM:66:VAL:HG12 | 41:RM:91:VAL:HB | 1.97 | 0.46 |
| 40:SA:141:PHE:HB2 | 40:SA:173:PRO:HD3 | 1.97 | 0.46 |
| 41:SB:139:LEU:HG | 41:SB:168:SER:HB3 | 1.96 | 0.46 |
| 41:SB:170:VAL:HG21 | 41:SB:377:LEU:HD11 | 1.97 | 0.46 |
| 40:SF:177:VAL:HB | 41:SM:331:LEU:HD12 | 1.96 | 0.46 |
| 40:SG:319:TYR:CE2 | 40:SG:328:VAL:HB | 2.50 | 0.46 |
| 41:SM:74:ASP:OD1 | 41:SM:77:ARG:NH2 | 2.48 | 0.46 |
| 41:SO:180:VAL:O | 41:SO:181:GLU:C | 2.53 | 0.46 |
| 41:SO:316:VAL:HA | 41:SO:352:ALA:HB3 | 1.96 | 0.46 |
| 40:TA:262:TYR:HB2 | 40:TA:265:ILE:HG22 | 1.96 | 0.46 |
| 40:TA:264:ARG:NH2 | 40:TA:430:ASP:OD2 | 2.31 | 0.46 |
| 40:TG:11:GLN:O | 40:TG:15:GLN:HG2 | 2.15 | 0.46 |
| 41:TP:166:THR:O | 41:TP:199:THR:HA | 2.15 | 0.46 |
| 40:UA:90:GLU:HG2 | 40:UA:121:ARG:NH1 | 2.29 | 0.46 |
| 40:UF:47:ASP:O | 40:UF:48:SER:C | 2.53 | 0.46 |
| 40:UH:222:PRO:HG2 | 41:UO:324:LYS:HE2 | 1.98 | 0.46 |
| 41:UM:156:ARG:NH1 | 41:UM:195:ASN:O | 2.43 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UO:396:HIS:HA | 41:UO:399:THR:HG22 | 1.97 | 0.46 |
| 40:VA:105:ARG:HD2 | 41:VO:251:ARG:HH21 | 1.81 | 0.46 |
| 41:VB:194:GLU:O | 41:VB:195:ASN:ND2 | 2.40 | 0.46 |
| 40:VF:238:ILE:HG12 | 40:VF:377:LEU:HD21 | 1.98 | 0.46 |
| 40:VF:319:TYR:HE2 | 40:VF:328:VAL:HG13 | 1.79 | 0.46 |
| 40:VG:298:PRO:HB3 | 40:VG:307:PRO:HD2 | 1.96 | 0.46 |
| 41:VQ:101:TRP:HB2 | 41:VQ:184:ASN:HD22 | 1.79 | 0.46 |
| 41:WO:66:VAL:HG22 | 41:WO:91:VAL:HB | 1.96 | 0.46 |
| 7:1T:139:VAL:O | 7:1T:148:ILE:HG13 | 2.15 | 0.46 |
| 12:2P:160:ARG:NH2 | 41:AL:420:ASN:OD1 | 2.38 | 0.46 |
| 12:2R:40:GLU:OE1 | 12:2R:54:ARG:NH1 | 2.49 | 0.46 |
| 13:2X:95:ASP:HB3 | 13:2X:146:THR:HB | 1.97 | 0.46 |
| 15:3E:81:LEU:HD11 | 15:3E:168:LYS:HG3 | 1.98 | 0.46 |
| 15:3H:21:LYS:HA | 15:3H:24:TYR:HD2 | 1.80 | 0.46 |
| 16:3K:71:VAL:HG13 | 16:3K:179:LYS:HG3 | 1.97 | 0.46 |
| 17:3P:182:GLU:HG3 | 17:3P:237:LEU:HD11 | 1.98 | 0.46 |
| 18:3V:222:TYR:O | 18:3V:225:ASP:HB3 | 2.15 | 0.46 |
| 19:3Y:112:ARG:HD3 | 40:LG:366:ASP:HB3 | 1.98 | 0.46 |
| 22:4I:680:LYS:HD2 | 22:4I:680:LYS:HA | 1.48 | 0.46 |
| 23:4R:86:LEU:HA | 23:4R:117:LEU:HD13 | 1.96 | 0.46 |
| 28:5B:226:PRO:HD2 | 41:KP:227:HIS:ND1 | 2.31 | 0.46 |
| 31:5J:800:TYR:HE2 | 41:IM:23:VAL:HG13 | 1.80 | 0.46 |
| 37:6A:16:GLN:O | 37:6A:20:LEU:HG | 2.15 | 0.46 |
| 37:6A:125:MET:O | 37:6A:127:SER:N | 2.48 | 0.46 |
| 39:6H:35:ARG:HH12 | 39:6H:135:HIS:HB3 | 1.80 | 0.46 |
| 40:AH:284:GLU:HB2 | 40:AH:286:LEU:HD22 | 1.97 | 0.46 |
| 40:BI:88:HIS:O | 40:BI:89:PRO:C | 2.54 | 0.46 |
| 40:CA:29:GLY:HA3 | 40:CA:42:ILE:HG21 | 1.96 | 0.46 |
| 40:CA:258:ASN:HD21 | 41:CB:180:VAL:H | 1.62 | 0.46 |
| 41:CB:145:SER:O | 41:CB:149:THR:OG1 | 2.31 | 0.46 |
| 40:CH:109:THR:OG1 | 40:CH:110:ILE:N | 2.44 | 0.46 |
| 41:CL:58:LYS:O | 41:CL:60:VAL:N | 2.48 | 0.46 |
| 41:CM:100:ASN:HB3 | 41:CM:103:LYS:HG3 | 1.98 | 0.46 |
| 41:CO:4:ILE:HD11 | 41:CO:240:LEU:HD13 | 1.98 | 0.46 |
| 41:CO:258:VAL:HG13 | 41:CO:266:PHE:CZ | 2.50 | 0.46 |
| 41:CP:293:MET:O | 41:CP:295:ASP:N | 2.40 | 0.46 |
| 41:DB:11:GLN:HA | 41:DB:72:THR:HG21 | 1.98 | 0.46 |
| 41:DB:56:GLY:O | 41:DB:58:LYS:HG2 | 2.15 | 0.46 |
| 41:DB:282:ARG:HH22 | 41:DB:288:GLU:HB3 | 1.81 | 0.46 |
| 40:DH:88:HIS:HB3 | 40:DH:91:GLN:HG3 | 1.98 | 0.46 |
| 40:DH:223:THR:OG1 | 40:DH:224:TYR:N | 2.44 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DI:387:TRP:HB3 | 40:DI:424:MET:SD | 2.55 | 0.46 |
| 41:DL:41:ASP:O | 41:DL:42:LEU:C | 2.53 | 0.46 |
| 41:DL:218:THR:OG1 | 41:DL:219:THR:N | 2.48 | 0.46 |
| 41:DM:137:HIS:CD2 | 41:DM:168:SER:HB3 | 2.50 | 0.46 |
| 41:DN:131:GLN:HG3 | 41:DN:163:ILE:HD12 | 1.97 | 0.46 |
| 41:DO:199:THR:OG1 | 41:DO:264:HIS:O | 2.33 | 0.46 |
| 41:DP:154:LYS:HB2 | 41:DP:154:LYS:HE2 | 1.47 | 0.46 |
| 41:DP:407:GLU:O | 41:DP:408:PHE:C | 2.53 | 0.46 |
| 40:EA:217:LEU:HA | 40:EA:277:SER:HB2 | 1.97 | 0.46 |
| 40:EF:238:ILE:HD12 | 40:EF:318:LEU:HD22 | 1.97 | 0.46 |
| 40:EH:337:THR:OG1 | 40:EH:338:LYS:N | 2.48 | 0.46 |
| 40:EI:27:GLU:O | 40:EI:28:HIS:C | 2.53 | 0.46 |
| 40:EI:90:GLU:O | 40:EI:92:LEU:N | 2.48 | 0.46 |
| 41:EN:122:LYS:HD3 | 41:FN:291:GLN:NE2 | 2.30 | 0.46 |
| 41:EP:21:TRP:CE3 | 41:EP:61:PRO:HB3 | 2.50 | 0.46 |
| 41:EP:108:GLU:O | 41:EP:109:GLY:C | 2.53 | 0.46 |
| 40:FF:271:THR:OG1 | 40:FF:300:ASN:O | 2.25 | 0.46 |
| 41:FN:103:LYS:HG2 | 41:FN:107:THR:HG21 | 1.96 | 0.46 |
| 40:GE:13:GLY:O | 40:GE:17:GLY:N | 2.47 | 0.46 |
| 40:GE:108:TYR:HB3 | 40:GE:411:GLY:HA3 | 1.98 | 0.46 |
| 40:GF:107:HIS:HD2 | 40:GF:152:LEU:HB2 | 1.81 | 0.46 |
| 40:GG:70:LEU:HB2 | 40:GG:145:THR:HG22 | 1.96 | 0.46 |
| 40:HA:11:GLN:HA | 40:HA:14:VAL:HG12 | 1.98 | 0.46 |
| 40:HA:112:LYS:HA | 40:HA:115:ILE:HG22 | 1.98 | 0.46 |
| 41:HM:226:ASN:ND2 | 43:HM:502:GDP:O6 | 2.41 | 0.46 |
| 41:HP:173:PRO:HB3 | 41:HP:380:ARG:HD3 | 1.96 | 0.46 |
| 41:IB:109:GLY:O | 41:IB:113:VAL:HG23 | 2.15 | 0.46 |
| 40:IF:349:THR:HG22 | 41:IN:179:VAL:HA | 1.97 | 0.46 |
| 40:IH:175:PRO:HG3 | 40:IH:304:LYS:HB3 | 1.97 | 0.46 |
| 40:IH:269:LEU:HD21 | 40:IH:383:ILE:HD12 | 1.97 | 0.46 |
| 41:IM:87:PRO:HA | 41:IM:90:PHE:HD2 | 1.80 | 0.46 |
| 41:IN:149:THR:HG21 | 41:IN:188:SER:HA | 1.98 | 0.46 |
| 41:IP:150:LEU:O | 41:IP:154:LYS:HG2 | 2.15 | 0.46 |
| 40:JD:9:VAL:HG11 | 40:JD:150:THR:HB | 1.98 | 0.46 |
| 40:JD:196:GLU:N | 40:JD:196:GLU:OE2 | 2.48 | 0.46 |
| 40:JG:217:LEU:HA | 40:JG:277:SER:HB2 | 1.98 | 0.46 |
| 40:JH:145:THR:OG1 | 42:JO:501:GTP:O2B | 2.32 | 0.46 |
| 41:JL:73:MET:HG3 | 41:JL:92:PHE:CD1 | 2.50 | 0.46 |
| 41:JO:64:VAL:HG21 | 41:JO:120:VAL:HG22 | 1.98 | 0.46 |
| 41:JO:222:TYR:HD1 | 41:JO:225:LEU:HD12 | 1.80 | 0.46 |
| 41:KB:288:GLU:N | 41:KB:288:GLU:OE2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KD:260:VAL:HG23 | 41:KL:397:TRP:HZ2 | 1.79 | 0.46 |
| 40:KE:296:PHE:CD2 | 40:KE:335:ILE:HG12 | 2.50 | 0.46 |
| 40:KF:239:THR:HG22 | 40:KF:252:LEU:HD11 | 1.97 | 0.46 |
| 41:KL:117:LEU:HD13 | 41:KL:117:LEU:HA | 1.68 | 0.46 |
| 41:KM:204:ASN:HD22 | 41:KM:207:LEU:HD12 | 1.79 | 0.46 |
| 41:KO:313:VAL:HG21 | 41:KO:341:PHE:HE2 | 1.80 | 0.46 |
| 41:LB:316:VAL:HB | 41:LB:366:THR:HG22 | 1.96 | 0.46 |
| 40:LF:112:LYS:HB3 | 40:LF:112:LYS:HE3 | 1.58 | 0.46 |
| 40:LF:320:ARG:HD3 | 40:LF:360:PRO:HG3 | 1.98 | 0.46 |
| 40:LF:402:ALA:O | 40:LF:403:PHE:C | 2.54 | 0.46 |
| 40:LG:239:THR:HG23 | 40:LG:243:ARG:HD3 | 1.98 | 0.46 |
| 40:LH:101:ASN:OD1 | 41:LO:350:LYS:NZ | 2.48 | 0.46 |
| 40:LH:141:PHE:HB2 | 40:LH:173:PRO:HD3 | 1.97 | 0.46 |
| 41:LM:7:LEU:HD22 | 41:LM:151:LEU:HD21 | 1.97 | 0.46 |
| 41:LN:204:ASN:OD1 | 43:LN:501:GDP:O2' | 2.29 | 0.46 |
| 41:LP:222:TYR:O | 41:LP:226:ASN:ND2 | 2.48 | 0.46 |
| 40:MA:315:CYS:HA | 40:MA:378:SER:HA | 1.97 | 0.46 |
| 40:MD:324:VAL:HG11 | 41:ML:219:THR:HB | 1.97 | 0.46 |
| 40:MF:104:ALA:HB1 | 40:MF:410:GLU:OE2 | 2.15 | 0.46 |
| 40:MH:209:ILE:HB | 40:MH:227:LEU:HG | 1.96 | 0.46 |
| 40:MH:259:LEU:O | 40:MH:260:VAL:C | 2.54 | 0.46 |
| 41:MN:272:PRO:CG | 41:MN:364:SER:HA | 2.45 | 0.46 |
| 40:ND:377:LEU:H | 40:ND:377:LEU:HG | 1.54 | 0.46 |
| 40:ND:429:LYS:HE3 | 40:ND:429:LYS:HB3 | 1.62 | 0.46 |
| 41:NN:135:LEU:O | 41:NN:166:THR:HA | 2.15 | 0.46 |
| 41:NP:41:ASP:N | 41:NP:41:ASP:OD1 | 2.48 | 0.46 |
| 40:OA:187:SER:O | 40:OA:191:THR:HG22 | 2.16 | 0.46 |
| 41:OB:202:ILE:HG12 | 41:OB:268:PRO:HG3 | 1.97 | 0.46 |
| 41:OL:143:THR:OG1 | 41:OL:144:GLY:N | 2.48 | 0.46 |
| 41:OL:334:GLN:HE22 | 41:OL:347:ASN:HA | 1.80 | 0.46 |
| 41:OM:287:PRO:O | 41:OM:291:GLN:HG2 | 2.15 | 0.46 |
| 41:OO:230:SER:HA | 41:OO:233:MET:HB3 | 1.97 | 0.46 |
| 40:PD:3:GLU:N | 40:PD:3:GLU:OE2 | 2.48 | 0.46 |
| 40:PD:256:GLN:HG3 | 41:PL:397:TRP:CZ2 | 2.51 | 0.46 |
| 40:PD:258:ASN:HB2 | 40:PD:352:LYS:HE3 | 1.97 | 0.46 |
| 40:PE:73:THR:OG1 | 41:PL:46:ARG:NH1 | 2.48 | 0.46 |
| 40:PE:209:ILE:HD11 | 40:PE:230:LEU:HD13 | 1.97 | 0.46 |
| 40:PF:101:ASN:HB3 | 40:PF:182:VAL:HG21 | 1.97 | 0.46 |
| 41:PL:14:ASN:HD21 | 41:PL:67:ASP:HB2 | 1.81 | 0.46 |
| 41:PL:137:HIS:O | 41:PL:168:SER:HA | 2.15 | 0.46 |
| 41:PM:271:ALA:O | 41:PM:292:GLN:NE2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QA:238:ILE:HG12 | 40:QA:377:LEU:HD11 | 1.98 | 0.46 |
| 41:QB:156:ARG:HD3 | 41:QB:164:MET:HG2 | 1.97 | 0.46 |
| 41:QB:286:VAL:HA | 41:QB:289:LEU:HD12 | 1.98 | 0.46 |
| 41:QN:184:ASN:O | 41:QN:188:SER:OG | 2.29 | 0.46 |
| 41:QP:399:THR:O | 41:QP:400:GLY:C | 2.53 | 0.46 |
| 40:RE:16:ILE:HD11 | 40:RE:231:ILE:HG21 | 1.97 | 0.46 |
| 40:RF:28:HIS:CE1 | 40:RF:48:SER:HB2 | 2.50 | 0.46 |
| 41:RN:107:THR:O | 41:RN:110:ALA:N | 2.48 | 0.46 |
| 41:RP:8:GLN:NE2 | 41:RP:14:ASN:HD22 | 2.13 | 0.46 |
| 41:RP:148:GLY:O | 41:RP:152:ILE:HD12 | 2.15 | 0.46 |
| 40:SG:192:HIS:ND1 | 40:SG:423:ASP:OD2 | 2.40 | 0.46 |
| 40:SG:436:MET:SD | 40:SG:436:MET:N | 2.87 | 0.46 |
| 41:SM:406:MET:O | 41:SM:409:THR:OG1 | 2.26 | 0.46 |
| 41:SO:221:THR:HG23 | 41:SO:224:ASP:HB2 | 1.97 | 0.46 |
| 41:TN:143:THR:O | 41:TN:147:MET:N | 2.48 | 0.46 |
| 41:TN:317:PHE:HB2 | 41:TN:353:VAL:HG12 | 1.97 | 0.46 |
| 41:TO:237:THR:O | 41:TO:241:ARG:NE | 2.39 | 0.46 |
| 41:UB:256:ASN:HB3 | 40:UG:181:VAL:HG22 | 1.97 | 0.46 |
| 40:UE:235:VAL:HA | 40:UE:238:ILE:HG12 | 1.96 | 0.46 |
| 40:UF:177:VAL:HG23 | 41:UM:327:ASP:HB2 | 1.96 | 0.46 |
| 40:UG:76:ASP:HA | 40:UG:79:ARG:HB2 | 1.97 | 0.46 |
| 40:UG:277:SER:O | 40:UG:279:GLU:N | 2.49 | 0.46 |
| 40:UI:193:THR:OG1 | 40:UI:194:THR:N | 2.48 | 0.46 |
| 40:UI:196:GLU:H | 40:UI:196:GLU:HG3 | 1.47 | 0.46 |
| 41:UN:403:MET:HE1 | 41:UN:407:GLU:HG3 | 1.97 | 0.46 |
| 41:UP:7:LEU:O | 41:UP:8:GLN:C | 2.54 | 0.46 |
| 41:UP:173:PRO:HD2 | 41:UP:205:GLU:HB2 | 1.97 | 0.46 |
| 40:VI:14:VAL:HG22 | 40:VI:67:PHE:HD1 | 1.80 | 0.46 |
| 40:VJ:169:PHE:HE2 | 40:VJ:235:VAL:HG13 | 1.80 | 0.46 |
| 41:VO:4:ILE:HA | 41:VO:132:GLY:O | 2.15 | 0.46 |
| 41:WB:324:LYS:HA | 41:WB:324:LYS:HD3 | 1.76 | 0.46 |
| 40:WG:274:PRO:HG3 | 40:WG:286:LEU:HD22 | 1.97 | 0.46 |
| 40:WI:221:ARG:HB3 | 41:WP:322:SER:HB2 | 1.97 | 0.46 |
| 41:WN:296:ALA:CB | 41:WN:305:PRO:HD2 | 2.36 | 0.46 |
| 41:WO:139:LEU:HD12 | 41:WO:170:VAL:HG12 | 1.97 | 0.46 |
| 7:1T:51:ALA:HB1 | 7:1T:54:THR:HG23 | 1.97 | 0.46 |
| 8:1X:183:MET:O | 8:1X:186:GLU:HB2 | 2.15 | 0.46 |
| 8:1X:318:ASP:HA | 8:1X:321:GLN:HG3 | 1.96 | 0.46 |
| 8:1Z:512:ILE:O | 8:1Z:516:LYS:HG2 | 2.15 | 0.46 |
| 12:2O:99:GLU:HG3 | 12:2O:102:LYS:HB2 | 1.98 | 0.46 |
| 13:2X:97:LYS:H | 13:2X:97:LYS:HG2 | 1.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:3F:4:LEU:HB3 | 15:3F:5:LEU:H | 1.52 | 0.46 |
| 15:3G:130:ASP:N | 15:3G:130:ASP:OD1 | 2.47 | 0.46 |
| 17:3O:406:ARG:HB2 | 17:3O:411:LEU:HG | 1.97 | 0.46 |
| 17:3O:415:MET:SD | 17:3O:415:MET:N | 2.84 | 0.46 |
| 17:3R:183:ARG:HH11 | 17:3R:186:MET:HE2 | 1.80 | 0.46 |
| 18:3U:267:GLY:HA2 | 18:3U:270:ARG:HG2 | 1.96 | 0.46 |
| 20:4A:201:LYS:HE2 | 21:4F:42:ARG:NH2 | 2.30 | 0.46 |
| 21:4E:34:ARG:O | 21:4E:36:GLY:N | 2.48 | 0.46 |
| 21:4F:243:LEU:O | 21:4F:265:HIS:HA | 2.15 | 0.46 |
| 22:4K:509:VAL:N | 22:4K:597:GLN:HB2 | 2.31 | 0.46 |
| 22:4K:677:LEU:O | 22:4K:678:LEU:C | 2.53 | 0.46 |
| 23:4M:253:TYR:O | 23:4M:254:LYS:C | 2.53 | 0.46 |
| 23:4M:260:THR:O | 23:4M:262:GLY:N | 2.43 | 0.46 |
| 23:4Q:170:SER:C | 23:4Q:172:TYR:H | 2.19 | 0.46 |
| 26:4V:9:PHE:CZ | 26:4V:87:LEU:HD11 | 2.50 | 0.46 |
| 26:4V:98:ILE:HB | 26:4V:159:ILE:HG23 | 1.98 | 0.46 |
| 27:4Z:104:SER:OG | 27:4Z:105:ASP:N | 2.47 | 0.46 |
| 28:5B:118:GLU:HG2 | 28:5B:119:THR:HG23 | 1.97 | 0.46 |
| 33:5N:440:VAL:O | 33:5N:444:ILE:HG12 | 2.14 | 0.46 |
| 33:5O:134:ASN:HD21 | 40:GE:58:ALA:HB1 | 1.80 | 0.46 |
| 36:5Y:66:LEU:HB3 | 40:OG:221:ARG:HD3 | 1.98 | 0.46 |
| 38:6D:256:ASP:OD1 | 38:6D:256:ASP:N | 2.42 | 0.46 |
| 40:AA:271:THR:HB | 40:AA:376:MET:HB3 | 1.97 | 0.46 |
| 40:AG:102:ASN:HB3 | 40:AG:105:ARG:HB2 | 1.96 | 0.46 |
| 41:BB:248:ALA:HA | 41:BB:252:LYS:HD3 | 1.97 | 0.46 |
| 40:BE:44:GLY:O | 40:BE:45:GLY:C | 2.54 | 0.46 |
| 40:BE:363:VAL:O | 40:BE:365:GLY:N | 2.49 | 0.46 |
| 40:BG:316:CYS:SG | 40:BG:377:LEU:HB2 | 2.56 | 0.46 |
| 41:BL:245:GLN:N | 41:BL:245:GLN:OE1 | 2.43 | 0.46 |
| 41:BM:3:GLU:HG3 | 41:BM:127:CYS:HB3 | 1.97 | 0.46 |
| 41:BO:8:GLN:O | 41:BO:66:VAL:HG22 | 2.15 | 0.46 |
| 41:BP:178:THR:HB | 41:BP:181:GLU:HG3 | 1.96 | 0.46 |
| 41:BP:393:ALA:O | 41:BP:394:PHE:C | 2.53 | 0.46 |
| 40:CA:278:ALA:O | 40:CA:281:ALA:N | 2.47 | 0.46 |
| 40:CE:219:ILE:HG22 | 40:CE:221:ARG:H | 1.80 | 0.46 |
| 40:CH:89:PRO:HD3 | 40:DH:283:HIS:CD2 | 2.51 | 0.46 |
| 41:CN:31:ASP:C | 41:CN:33:THR:H | 2.18 | 0.46 |
| 41:CN:204:ASN:HD22 | 41:CN:204:ASN:HA | 1.48 | 0.46 |
| 41:CN:231:ALA:C | 41:CN:233:MET:H | 2.17 | 0.46 |
| 40:DA:99:ALA:O | 40:DA:100:ALA:HB3 | 2.15 | 0.46 |
| 41:DB:344:TRP:CZ3 | 40:DG:402:ALA:HB2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DB:382:SER:O | 41:DB:383:GLU:C | 2.54 | 0.46 |
| 40:DE:101:ASN:OD1 | 40:DE:143:GLY:HA2 | 2.16 | 0.46 |
| 40:DF:62:VAL:HG11 | 40:EF:283:HIS:HB3 | 1.97 | 0.46 |
| 40:DF:224:TYR:O | 40:DF:228:ASN:N | 2.48 | 0.46 |
| 40:DG:217:LEU:HD21 | 40:DG:275:VAL:HG12 | 1.96 | 0.46 |
| 40:DG:230:LEU:HD11 | 40:DG:275:VAL:HG13 | 1.97 | 0.46 |
| 40:DH:173:PRO:HG3 | 40:DH:183:GLU:HG2 | 1.98 | 0.46 |
| 40:DI:112:LYS:HA | 40:DI:112:LYS:HD3 | 1.51 | 0.46 |
| 41:DL:31:ASP:O | 41:DL:84:ILE:HD11 | 2.16 | 0.46 |
| 41:DL:344:TRP:CD1 | 41:DL:344:TRP:N | 2.83 | 0.46 |
| 41:DL:425:ARG:H | 41:DL:425:ARG:HG2 | 1.45 | 0.46 |
| 41:DM:100:ASN:O | 41:DM:101:TRP:C | 2.54 | 0.46 |
| 41:DP:298:ASN:O | 41:DP:299:MET:C | 2.54 | 0.46 |
| 41:DP:399:THR:O | 41:DP:401:GLU:N | 2.47 | 0.46 |
| 40:EE:181:VAL:HG23 | 40:EE:182:VAL:HG13 | 1.97 | 0.46 |
| 40:EH:277:SER:O | 40:EH:280:LYS:N | 2.42 | 0.46 |
| 40:EI:139:HIS:CG | 40:EI:170:SER:HB3 | 2.50 | 0.46 |
| 40:EI:226:ASN:HA | 40:EI:229:ARG:NH2 | 2.30 | 0.46 |
| 41:EM:87:PRO:HG3 | 41:FM:278:SER:HB3 | 1.98 | 0.46 |
| 41:EM:239:CYS:HB3 | 41:EM:248:ALA:O | 2.14 | 0.46 |
| 41:EN:323:MET:HA | 41:EN:326:VAL:HB | 1.98 | 0.46 |
| 41:EP:5:VAL:HG23 | 41:EP:130:LEU:HD11 | 1.95 | 0.46 |
| 40:FA:255:PHE:CE1 | 40:FA:318:LEU:HD11 | 2.51 | 0.46 |
| 41:FB:207:LEU:HB3 | 41:FB:225:LEU:HD22 | 1.96 | 0.46 |
| 40:FF:398:TYR:OH | 40:FF:414:GLU:OE1 | 2.32 | 0.46 |
| 41:FO:133:PHE:HB2 | 41:FO:164:MET:SD | 2.55 | 0.46 |
| 41:FO:313:VAL:O | 41:FO:349:VAL:HA | 2.15 | 0.46 |
| 40:GF:285:GLN:HB3 | 40:GF:287:SER:HB3 | 1.96 | 0.46 |
| 40:GH:166:LYS:HB2 | 40:GH:166:LYS:HE2 | 1.38 | 0.46 |
| 40:GH:275:VAL:HA | 40:GH:367:LEU:HD11 | 1.98 | 0.46 |
| 40:GH:276:ILE:HD11 | 40:GH:280:LYS:HD2 | 1.98 | 0.46 |
| 40:GH:402:ALA:O | 40:GH:404:VAL:N | 2.49 | 0.46 |
| 40:GI:73:THR:OG1 | 40:GI:74:VAL:N | 2.48 | 0.46 |
| 41:GN:7:LEU:H | 41:GN:7:LEU:HG | 1.46 | 0.46 |
| 41:GN:152:ILE:HD12 | 41:GN:152:ILE:HA | 1.72 | 0.46 |
| 41:GO:207:LEU:HD13 | 41:GO:225:LEU:HD12 | 1.97 | 0.46 |
| 41:HN:107:THR:O | 41:HN:109:GLY:N | 2.49 | 0.46 |
| 40:IG:424:MET:SD | 40:IG:427:LEU:HD13 | 2.56 | 0.46 |
| 40:II:97:GLU:HG2 | 40:II:105:ARG:HH22 | 1.81 | 0.46 |
| 41:IM:149:THR:HG21 | 41:IM:188:SER:HA | 1.96 | 0.46 |
| 41:IQ:222:TYR:O | 41:IQ:226:ASN:ND2 | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JB:20:PHE:HA | 41:JB:230:SER:HB2 | 1.98 | 0.46 |
| 40:JF:247:ALA:HB3 | 40:JF:355:ILE:HB | 1.97 | 0.46 |
| 40:JG:318:LEU:O | 40:JG:374:VAL:HA | 2.15 | 0.46 |
| 40:JH:183:GLU:HG2 | 40:JH:184:PRO:HD3 | 1.97 | 0.46 |
| 41:JM:36:TYR:CE2 | 41:JM:44:LEU:HB2 | 2.50 | 0.46 |
| 41:KB:256:ASN:HD22 | 41:KB:350:LYS:HD3 | 1.80 | 0.46 |
| 40:KD:234:ILE:O | 40:KD:238:ILE:HG12 | 2.15 | 0.46 |
| 40:KF:238:ILE:HA | 40:KF:318:LEU:HD22 | 1.97 | 0.46 |
| 40:KG:116:ASP:OD1 | 40:KG:117:LEU:N | 2.47 | 0.46 |
| 41:KL:355:ASP:O | 41:KL:356:ILE:C | 2.54 | 0.46 |
| 41:KP:395:LEU:HA | 41:KP:398:TYR:HD2 | 1.81 | 0.46 |
| 41:LB:241:ARG:HH22 | 41:LB:318:ARG:HH22 | 1.64 | 0.46 |
| 40:LE:214:ARG:HH21 | 41:LL:324:LYS:HE2 | 1.80 | 0.46 |
| 40:LF:29:GLY:O | 40:LF:30:ILE:C | 2.53 | 0.46 |
| 40:LG:66:VAL:HG21 | 40:LG:122:ILE:HG13 | 1.98 | 0.46 |
| 41:LO:8:GLN:HE21 | 41:LO:65:LEU:HG | 1.79 | 0.46 |
| 40:MA:363:VAL:O | 40:MA:364:PRO:C | 2.53 | 0.46 |
| 40:MF:123:ARG:HA | 40:MF:161:TYR:OH | 2.14 | 0.46 |
| 40:MH:88:HIS:O | 40:MH:89:PRO:C | 2.53 | 0.46 |
| 40:MH:411:GLY:O | 40:MH:412:MET:C | 2.52 | 0.46 |
| 41:MO:274:THR:HB | 41:MO:279:GLN:HG3 | 1.98 | 0.46 |
| 40:NA:112:LYS:HA | 40:NA:115:ILE:HG22 | 1.96 | 0.46 |
| 40:NA:189:LEU:HD11 | 40:NA:417:PHE:HD2 | 1.81 | 0.46 |
| 40:ND:124:LYS:HE2 | 40:ND:124:LYS:HB2 | 1.58 | 0.46 |
| 40:NH:105:ARG:HG2 | 40:NH:410:GLU:HG3 | 1.97 | 0.46 |
| 41:NN:103:LYS:O | 41:NN:107:THR:OG1 | 2.33 | 0.46 |
| 41:NO:212:PHE:HD2 | 41:NO:213:ARG:HG2 | 1.80 | 0.46 |
| 40:OD:261:PRO:HD2 | 40:OD:379:ASN:HD22 | 1.81 | 0.46 |
| 40:OH:143:GLY:O | 40:OH:144:GLY:C | 2.54 | 0.46 |
| 41:OL:11:GLN:HA | 41:OL:72:THR:HG21 | 1.97 | 0.46 |
| 41:OM:170:VAL:HG11 | 41:OM:377:LEU:HD21 | 1.98 | 0.46 |
| 41:OO:3:GLU:OE2 | 41:OO:129:CYS:N | 2.49 | 0.46 |
| 40:PF:195:LEU:HD12 | 40:PF:427:LEU:HD12 | 1.98 | 0.46 |
| 40:PF:212:ILE:HG23 | 40:PF:216:ASN:HD21 | 1.81 | 0.46 |
| 40:PH:3:GLU:OE2 | 40:PH:131:GLY:N | 2.48 | 0.46 |
| 41:PM:39:ASP:OD1 | 41:PM:39:ASP:N | 2.49 | 0.46 |
| 41:PN:103:LYS:HA | 41:PN:107:THR:HG22 | 1.97 | 0.46 |
| 40:QA:212:ILE:HD11 | 40:QA:300:ASN:HA | 1.96 | 0.46 |
| 41:QB:328:GLU:HA | 41:QB:331:LEU:HD23 | 1.97 | 0.46 |
| 40:QE:238:ILE:HA | 40:QE:318:LEU:HD22 | 1.96 | 0.46 |
| 40:QF:386:ALA:HA | 40:QF:389:ARG:HH21 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QG:238:ILE:HG23 | 40:QG:239:THR:HG23 | 1.97 | 0.46 |
| 40:QG:240:ALA:HA | 40:QG:243:ARG:HE | 1.79 | 0.46 |
| 40:QH:35:GLN:NE2 | 40:QH:58:ALA:O | 2.41 | 0.46 |
| 41:QM:167:PHE:CE1 | 41:QM:233:MET:HG2 | 2.50 | 0.46 |
| 41:QN:152:ILE:O | 41:QN:156:ARG:HG3 | 2.16 | 0.46 |
| 41:QP:420:ASN:O | 41:QP:423:VAL:N | 2.42 | 0.46 |
| 40:RF:51:THR:HG21 | 40:RF:243:ARG:HG2 | 1.98 | 0.46 |
| 40:RH:180:ALA:HB3 | 40:RH:183:GLU:HG3 | 1.96 | 0.46 |
| 41:RL:5:VAL:HB | 41:RL:133:PHE:HD1 | 1.80 | 0.46 |
| 41:SB:222:TYR:HD1 | 41:SB:225:LEU:HD12 | 1.80 | 0.46 |
| 41:SB:305:PRO:HB3 | 41:SB:310:TYR:HE1 | 1.80 | 0.46 |
| 40:SI:276:ILE:HD12 | 40:SI:280:LYS:HG3 | 1.97 | 0.46 |
| 40:TG:345:ASP:N | 40:TG:345:ASP:OD1 | 2.49 | 0.46 |
| 40:TI:141:PHE:HB2 | 40:TI:173:PRO:HD3 | 1.96 | 0.46 |
| 40:UA:73:THR:HA | 40:UA:76:ASP:HB2 | 1.97 | 0.46 |
| 40:UE:284:GLU:HG3 | 40:UE:286:LEU:H | 1.80 | 0.46 |
| 40:UI:191:THR:O | 40:UI:192:HIS:C | 2.53 | 0.46 |
| 41:UO:183:TYR:CE1 | 41:UO:388:MET:HG3 | 2.50 | 0.46 |
| 40:VA:406:TRP:CD1 | 41:VO:255:VAL:HG23 | 2.51 | 0.46 |
| 40:VG:6:SER:O | 40:VG:65:ALA:HA | 2.15 | 0.46 |
| 41:VP:139:LEU:HG | 41:VP:168:SER:HB2 | 1.96 | 0.46 |
| 41:VQ:248:ALA:HA | 41:VQ:252:LYS:HE2 | 1.97 | 0.46 |
| 40:WA:103:TYR:CD2 | 40:WA:189:LEU:HD23 | 2.50 | 0.46 |
| 41:WB:142:GLY:O | 41:WB:144:GLY:N | 2.49 | 0.46 |
| 40:WE:306:ASP:OD1 | 40:WE:309:HIS:ND1 | 2.39 | 0.46 |
| 40:WF:109:THR:OG1 | 40:WF:410:GLU:O | 2.34 | 0.46 |
| 41:WM:172:SER:HB3 | 41:WM:205:GLU:HB2 | 1.96 | 0.46 |
| 41:WM:337:ASN:O | 41:WM:338:SER:C | 2.53 | 0.46 |
| 41:WN:193:VAL:HG23 | 41:WN:265:PHE:CE1 | 2.48 | 0.46 |
| 41:WO:202:ILE:HD12 | 41:WO:229:VAL:HG13 | 1.98 | 0.46 |
| 8:1Y:107:PHE:HA | 8:1Y:110:ILE:HG12 | 1.97 | 0.46 |
| 13:2V:101:ARG:HE | 13:2V:101:ARG:HB3 | 1.43 | 0.46 |
| 17:3P:157:LYS:HB3 | 17:3P:157:LYS:HE2 | 1.83 | 0.46 |
| 17:3P:217:THR:OG1 | 17:3P:218:GLU:N | 2.47 | 0.46 |
| 17:3R:178:LYS:O | 17:3R:182:GLU:HG3 | 2.15 | 0.46 |
| 17:3R:298:GLU:O | 17:3R:299:SER:C | 2.54 | 0.46 |
| 18:3T:368:LEU:HD22 | 18:3U:249:GLU:HB2 | 1.97 | 0.46 |
| 21:4E:255:MET:H | 21:4E:255:MET:HE3 | 1.81 | 0.46 |
| 21:4F:531:ILE:O | 21:4F:532:GLN:C | 2.54 | 0.46 |
| 23:4R:245:LYS:HE2 | 23:4R:245:LYS:HB3 | 1.32 | 0.46 |
| 25:4T:344:MET:HE3 | 26:4W:374:ILE:HB | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:4W:4:SER:OG | 26:4W:5:GLU:N | 2.48 | 0.46 |
| 26:4W:363:ASP:OD1 | 34:5Q:97:ARG:NH2 | 2.47 | 0.46 |
| 31:5I:360:ASP:OD2 | 40:HA:84:ARG:NH2 | 2.42 | 0.46 |
| 31:5I:388:ILE:HD11 | 41:IB:359:ARG:NH2 | 2.30 | 0.46 |
| 33:5O:109:LYS:NZ | 41:HM:80:PRO:HA | 2.31 | 0.46 |
| 34:5R:431:ARG:HE | 34:5R:435:GLU:HG2 | 1.81 | 0.46 |
| 36:5X:247:LEU:HD12 | 40:LF:430:ASP:OD1 | 2.16 | 0.46 |
| 41:AL:385:PHE:HZ | 41:AL:408:PHE:HB3 | 1.79 | 0.46 |
| 41:AN:33:THR:O | 41:AN:58:LYS:NZ | 2.42 | 0.46 |
| 41:AP:142:GLY:O | 41:AP:144:GLY:N | 2.48 | 0.46 |
| 40:BA:274:PRO:HB3 | 40:BA:370:VAL:HG11 | 1.98 | 0.46 |
| 40:BE:31:GLN:O | 40:BE:32:PRO:C | 2.53 | 0.46 |
| 40:BE:141:PHE:HB3 | 40:BE:173:PRO:HD3 | 1.98 | 0.46 |
| 40:BE:186:ASN:N | 40:BE:186:ASN:OD1 | 2.49 | 0.46 |
| 40:BE:248:LEU:HA | 40:BE:248:LEU:HD13 | 1.72 | 0.46 |
| 40:BE:390:LEU:HD23 | 40:BE:390:LEU:HA | 1.76 | 0.46 |
| 40:BF:20:CYS:HA | 40:BF:232:SER:HB2 | 1.97 | 0.46 |
| 40:BF:101:ASN:HB2 | 41:BM:252:LYS:HZ1 | 1.81 | 0.46 |
| 40:BH:184:PRO:HA | 40:BH:390:LEU:HD13 | 1.96 | 0.46 |
| 41:BO:393:ALA:O | 41:BO:394:PHE:C | 2.54 | 0.46 |
| 41:BP:425:ARG:H | 41:BP:425:ARG:HG2 | 1.57 | 0.46 |
| 41:CB:64:VAL:HG12 | 41:CB:89:ASN:HB2 | 1.98 | 0.46 |
| 40:CG:49:PHE:HE2 | 40:CG:55:GLU:HB2 | 1.81 | 0.46 |
| 40:CH:335:ILE:HG23 | 40:CH:341:ILE:HD13 | 1.96 | 0.46 |
| 40:DA:114:LEU:HD23 | 40:DA:114:LEU:HA | 1.71 | 0.46 |
| 40:DA:248:LEU:HA | 41:DB:11:GLN:HE22 | 1.79 | 0.46 |
| 40:DA:307:PRO:O | 40:DA:310:GLY:N | 2.49 | 0.46 |
| 40:DE:1:GLN:HB2 | 40:DE:2:ARG:H | 1.61 | 0.46 |
| 40:DE:164:LYS:HD3 | 40:DE:164:LYS:HA | 1.54 | 0.46 |
| 40:DF:1:GLN:HG2 | 40:DF:2:ARG:HG3 | 1.97 | 0.46 |
| 40:DF:55:GLU:HG2 | 40:DF:61:HIS:HD2 | 1.80 | 0.46 |
| 40:DF:66:VAL:O | 40:DF:67:PHE:C | 2.53 | 0.46 |
| 40:DF:86:LEU:O | 40:DF:87:PHE:C | 2.53 | 0.46 |
| 40:DH:195:LEU:HA | 40:DH:195:LEU:HD13 | 1.69 | 0.46 |
| 40:DH:254:GLU:OE1 | 41:DP:99:ASN:ND2 | 2.49 | 0.46 |
| 40:DH:351:PHE:N | 41:DP:179:VAL:HG12 | 2.30 | 0.46 |
| 40:DI:140:SER:O | 40:DI:142:GLY:N | 2.49 | 0.46 |
| 40:DI:313:MET:HG3 | 40:DI:380:THR:HA | 1.98 | 0.46 |
| 41:DL:54:ALA:HA | 41:EL:283:ALA:CB | 2.45 | 0.46 |
| 41:DL:279:GLN:O | 41:DL:281:TYR:N | 2.49 | 0.46 |
| 41:DL:312:THR:HA | 41:DL:348:ASN:HB2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DN:170:VAL:HG12 | 41:DN:171:PRO:HD2 | 1.98 | 0.46 |
| 41:DN:228:LEU:HD12 | 41:DN:228:LEU:HA | 1.80 | 0.46 |
| 41:DN:266:PHE:HA | 41:DN:370:ASN:HA | 1.97 | 0.46 |
| 41:DO:8:GLN:HG3 | 41:DO:136:THR:HB | 1.97 | 0.46 |
| 40:EA:185:TYR:HE2 | 40:EA:403:PHE:HB2 | 1.80 | 0.46 |
| 40:EA:248:LEU:HD13 | 40:EA:355:ILE:HD13 | 1.96 | 0.46 |
| 40:EE:88:HIS:CE1 | 40:EE:90:GLU:HB2 | 2.51 | 0.46 |
| 40:EG:271:THR:HG22 | 40:EG:301:GLN:HA | 1.97 | 0.46 |
| 40:EH:291:ILE:HG13 | 40:EH:374:VAL:HG12 | 1.98 | 0.46 |
| 40:EI:102:ASN:HD22 | 40:EI:105:ARG:H | 1.63 | 0.46 |
| 40:EI:357:TYR:O | 40:EI:358:GLN:C | 2.54 | 0.46 |
| 41:EM:293:MET:HG2 | 41:EM:367:PHE:HB3 | 1.98 | 0.46 |
| 41:EN:114:ASP:N | 41:EN:114:ASP:OD1 | 2.49 | 0.46 |
| 40:FG:185:TYR:HE2 | 40:FG:397:MET:HB3 | 1.79 | 0.46 |
| 40:FH:319:TYR:HA | 40:FH:373:ALA:O | 2.15 | 0.46 |
| 41:FO:253:LEU:HD23 | 41:FO:350:LYS:HD3 | 1.97 | 0.46 |
| 41:FP:104:GLY:HA3 | 41:FP:146:GLY:HA3 | 1.98 | 0.46 |
| 40:GA:274:PRO:HB3 | 40:GA:370:VAL:HG11 | 1.97 | 0.46 |
| 41:GM:138:SER:OG | 43:GM:501:GDP:O1A | 2.33 | 0.46 |
| 41:GM:149:THR:HG21 | 41:GM:188:SER:HA | 1.97 | 0.46 |
| 41:GP:398:TYR:HD2 | 41:GP:408:PHE:HZ | 1.63 | 0.46 |
| 40:HA:234:ILE:HD11 | 40:HA:272:TYR:HB2 | 1.98 | 0.46 |
| 40:HE:129:CYS:O | 40:HE:129:CYS:SG | 2.74 | 0.46 |
| 40:HE:255:PHE:HE1 | 40:HE:318:LEU:HD11 | 1.80 | 0.46 |
| 40:HF:76:ASP:HA | 40:HF:79:ARG:HG2 | 1.97 | 0.46 |
| 40:HI:7:VAL:HG11 | 40:HI:153:LEU:HD21 | 1.96 | 0.46 |
| 41:HN:165:ASN:OD1 | 41:HN:250:LEU:HD21 | 2.14 | 0.46 |
| 41:IN:43:GLN:HA | 41:IN:242:PHE:HE1 | 1.80 | 0.46 |
| 40:JE:211:ASP:HB3 | 40:JE:215:ARG:HH12 | 1.81 | 0.46 |
| 40:JG:229:ARG:O | 40:JG:232:SER:OG | 2.24 | 0.46 |
| 41:JM:12:CYS:HB2 | 43:JM:501:GDP:C8 | 2.51 | 0.46 |
| 40:KA:224:TYR:HB3 | 42:KN:501:GTP:N1 | 2.31 | 0.46 |
| 40:KD:60:LYS:HE2 | 40:KD:85:GLN:HG3 | 1.96 | 0.46 |
| 41:KO:132:GLY:HA3 | 41:KO:163:ILE:O | 2.16 | 0.46 |
| 41:KP:20:PHE:HA | 41:KP:230:SER:HB2 | 1.96 | 0.46 |
| 41:LB:242:PHE:HB3 | 41:LB:356:ILE:HD12 | 1.97 | 0.46 |
| 40:LF:10:GLY:O | 40:LF:11:GLN:C | 2.54 | 0.46 |
| 40:LF:136:LEU:HD21 | 40:LF:252:LEU:HD21 | 1.98 | 0.46 |
| 40:LF:174:ALA:CB | 40:LF:177:VAL:HG23 | 2.46 | 0.46 |
| 40:LG:177:VAL:HG22 | 40:LG:207:GLU:OE1 | 2.15 | 0.46 |
| 40:LG:288:VAL:HG21 | 40:LG:327:ASP:HB2 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LG:313:MET:HB3 | 40:LG:313:MET:HE3 | 1.80 | 0.46 |
| 40:LG:431:TYR:HA | 40:LG:434:VAL:HG22 | 1.96 | 0.46 |
| 40:LH:228:ASN:ND2 | 42:LO:501:GTP:HN1 | 2.11 | 0.46 |
| 40:MF:12:ALA:HB3 | 40:MF:140:SER:HB2 | 1.98 | 0.46 |
| 40:MH:69:ASP:HA | 40:MH:145:THR:HG21 | 1.97 | 0.46 |
| 40:MH:153:LEU:HD22 | 40:MH:157:LEU:HD13 | 1.98 | 0.46 |
| 41:ML:122:LYS:HE2 | 41:ML:122:LYS:HB2 | 1.68 | 0.46 |
| 41:MM:6:HIS:O | 41:MM:63:ALA:HA | 2.15 | 0.46 |
| 41:MM:7:LEU:O | 41:MM:135:LEU:HA | 2.15 | 0.46 |
| 41:MM:86:ARG:NH1 | 41:MM:123:GLU:OE2 | 2.49 | 0.46 |
| 40:ND:295:CYS:SG | 40:ND:376:MET:HB2 | 2.55 | 0.46 |
| 40:NH:185:TYR:HE1 | 40:NH:397:MET:HB3 | 1.80 | 0.46 |
| 41:NP:117:LEU:HD21 | 41:NP:154:LYS:HB3 | 1.98 | 0.46 |
| 41:OM:404:ASP:OD1 | 41:OM:405:GLU:N | 2.45 | 0.46 |
| 41:OO:263:LEU:HD21 | 41:OO:421:PRO:HB2 | 1.97 | 0.46 |
| 41:OO:317:PHE:HB2 | 41:OO:353:VAL:HG12 | 1.97 | 0.46 |
| 40:PA:25:CYS:HA | 40:PA:30:ILE:HB | 1.98 | 0.46 |
| 40:PA:206:ASN:HA | 40:PA:209:ILE:HG22 | 1.96 | 0.46 |
| 40:PD:31:GLN:HB2 | 40:PD:37:PRO:HD3 | 1.98 | 0.46 |
| 41:PO:136:THR:HA | 41:PO:167:PHE:O | 2.15 | 0.46 |
| 40:QA:150:THR:O | 40:QA:154:MET:HG2 | 2.16 | 0.46 |
| 41:QB:103:LYS:HB2 | 41:QB:104:GLY:H | 1.46 | 0.46 |
| 41:QB:182:PRO:O | 41:QB:186:THR:HG23 | 2.15 | 0.46 |
| 40:QF:212:ILE:O | 40:QF:216:ASN:HB2 | 2.16 | 0.46 |
| 41:QM:390:ARG:HH12 | 41:QM:391:ARG:HE | 1.63 | 0.46 |
| 41:QO:404:ASP:OD1 | 41:QO:405:GLU:N | 2.48 | 0.46 |
| 41:QP:314:ALA:HA | 41:QP:350:LYS:H | 1.80 | 0.46 |
| 40:RA:383:ILE:HG12 | 40:RA:387:TRP:CD1 | 2.50 | 0.46 |
| 40:RE:56:THR:HB | 40:SE:285:GLN:HA | 1.96 | 0.46 |
| 40:RF:239:THR:O | 40:RF:243:ARG:NE | 2.49 | 0.46 |
| 41:RL:134:GLN:HG3 | 41:RL:165:ASN:HB2 | 1.96 | 0.46 |
| 41:RO:2:ARG:HB2 | 41:RO:131:GLN:HG2 | 1.98 | 0.46 |
| 41:SB:142:GLY:O | 41:SB:144:GLY:N | 2.48 | 0.46 |
| 40:SF:406:TRP:HH2 | 41:SM:258:VAL:HB | 1.81 | 0.46 |
| 40:SG:50:ASN:O | 40:SG:64:ARG:NH2 | 2.49 | 0.46 |
| 40:SH:145:THR:OG1 | 40:SH:146:GLY:N | 2.49 | 0.46 |
| 41:SN:26:ASP:O | 41:SN:359:ARG:NH1 | 2.48 | 0.46 |
| 41:SO:225:LEU:O | 41:SO:227:HIS:N | 2.49 | 0.46 |
| 40:TA:2:ARG:HB3 | 40:TA:242:LEU:HD22 | 1.97 | 0.46 |
| 40:TA:391:ASP:OD1 | 40:TA:421:ARG:NH1 | 2.49 | 0.46 |
| 40:TF:356:ASN:OD1 | 40:TF:357:TYR:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:TI:222:PRO:HB3 | 40:TI:226:ASN:HB3 | 1.96 | 0.46 |
| 41:TP:156:ARG:NH1 | 41:TP:195:ASN:O | 2.48 | 0.46 |
| 41:UB:244:GLY:O | 41:UB:247:ASN:ND2 | 2.42 | 0.46 |
| 40:UF:10:GLY:O | 40:UF:11:GLN:C | 2.53 | 0.46 |
| 40:UG:247:ALA:HB3 | 40:UG:355:ILE:HD11 | 1.97 | 0.46 |
| 41:UM:117:LEU:HA | 41:UM:120:VAL:HG12 | 1.96 | 0.46 |
| 40:VA:247:ALA:O | 41:VB:11:GLN:NE2 | 2.47 | 0.46 |
| 40:VF:139:HIS:NE2 | 40:VF:168:GLU:OE2 | 2.31 | 0.46 |
| 41:VN:27:GLU:HA | 41:VN:359:ARG:NH1 | 2.31 | 0.46 |
| 41:VN:167:PHE:CE2 | 41:VN:233:MET:HG2 | 2.50 | 0.46 |
| 40:WA:76:ASP:O | 40:WA:80:THR:OG1 | 2.29 | 0.46 |
| 41:WB:324:LYS:HE3 | 40:WG:222:PRO:HG2 | 1.98 | 0.46 |
| 7:1T:513:GLU:O | 7:1T:514:GLU:C | 2.54 | 0.46 |
| 7:1U:47:ILE:O | 7:1U:60:LEU:HB2 | 2.15 | 0.46 |
| 8:1Y:101:ILE:HD12 | 11:2J:250:ILE:C | 2.36 | 0.46 |
| 11:2J:186:LYS:O | 11:2J:187:ARG:NE | 2.48 | 0.46 |
| 13:2T:141:ARG:HH21 | 13:2T:148:TYR:H | 1.64 | 0.46 |
| 13:2V:115:LYS:HE3 | 13:2V:117:PHE:H | 1.80 | 0.46 |
| 13:2W:178:PRO:O | 13:2W:179:ALA:C | 2.54 | 0.46 |
| 13:2X:182:LYS:HE3 | 13:2X:182:LYS:HB3 | 1.68 | 0.46 |
| 16:3K:168:ALA:CB | 16:3K:228:ARG:HH12 | 2.28 | 0.46 |
| 17:3P:408:ASN:HB3 | 17:3P:409:ILE:H | 1.44 | 0.46 |
| 17:3Q:470:GLN:O | 17:3Q:472:LYS:N | 2.48 | 0.46 |
| 17:3R:168:ILE:HG13 | 17:3R:251:GLN:HE22 | 1.80 | 0.46 |
| 18:3T:349:PRO:HA | 18:3T:352:VAL:HG12 | 1.98 | 0.46 |
| 20:4A:189:ARG:H | 20:4A:189:ARG:HG3 | 1.58 | 0.46 |
| 20:4B:258:GLN:O | 20:4B:259:VAL:C | 2.54 | 0.46 |
| 21:4E:90:VAL:HG22 | 40:AH:369:LYS:HB3 | 1.97 | 0.46 |
| 21:4F:320:VAL:HG21 | 21:4F:323:TRP:CE2 | 2.50 | 0.46 |
| 22:4I:619:VAL:HG11 | 22:4I:680:LYS:HG3 | 1.98 | 0.46 |
| 22:4J:304:LEU:HD11 | 41:BN:77:ARG:HG2 | 1.96 | 0.46 |
| 22:4J:680:LYS:HA | 22:4J:680:LYS:HD2 | 1.75 | 0.46 |
| 23:4M:172:TYR:C | 23:4M:174:MET:H | 2.18 | 0.46 |
| 23:4P:197:LEU:HD21 | 23:4P:208:GLN:HB2 | 1.97 | 0.46 |
| 26:4V:300:VAL:HG12 | 26:4V:304:TYR:HE1 | 1.81 | 0.46 |
| 27:4Z:33:ARG:NH1 | 32:5L:65:GLN:OE1 | 2.48 | 0.46 |
| 29:5D:63:TYR:OH | 40:GI:228:ASN:ND2 | 2.48 | 0.46 |
| 39:6G:104:SER:O | 39:6G:110:ASN:ND2 | 2.49 | 0.46 |
| 40:AA:231:ILE:O | 40:AA:235:VAL:HG23 | 2.15 | 0.46 |
| 40:AF:429:LYS:O | 40:AF:433:GLU:HG3 | 2.15 | 0.46 |
| 41:AN:107:THR:O | 41:AN:109:GLY:N | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AO:354:CYS:SG | 41:AO:355:ASP:N | 2.88 | 0.46 |
| 40:BA:181:VAL:HG23 | 40:BA:182:VAL:HG13 | 1.97 | 0.46 |
| 40:BF:205:ASP:OD1 | 40:BF:206:ASN:N | 2.48 | 0.46 |
| 40:BH:265:ILE:HG23 | 40:BH:431:TYR:CE1 | 2.51 | 0.46 |
| 41:BL:86:ARG:NH1 | 41:CL:281:TYR:O | 2.45 | 0.46 |
| 41:BN:292:GLN:HG2 | 41:BN:298:ASN:ND2 | 2.31 | 0.46 |
| 41:BN:322:SER:OG | 41:BN:323:MET:N | 2.48 | 0.46 |
| 40:CA:104:ALA:C | 40:CA:106:GLY:H | 2.19 | 0.46 |
| 40:CA:184:PRO:HA | 40:CA:390:LEU:HD21 | 1.97 | 0.46 |
| 40:CF:258:ASN:ND2 | 41:CN:99:ASN:OD1 | 2.48 | 0.46 |
| 40:CF:319:TYR:HB3 | 40:CF:323:VAL:HG11 | 1.96 | 0.46 |
| 40:CH:51:THR:OG1 | 40:CH:52:PHE:N | 2.49 | 0.46 |
| 40:CH:115:ILE:HD11 | 40:CH:152:LEU:HB3 | 1.97 | 0.46 |
| 40:CH:278:ALA:O | 40:CH:279:GLU:C | 2.54 | 0.46 |
| 41:CL:386:THR:O | 41:CL:389:PHE:N | 2.49 | 0.46 |
| 41:CM:325:GLU:O | 41:CM:329:GLN:HB2 | 2.16 | 0.46 |
| 41:CO:7:LEU:O | 41:CO:135:LEU:HD12 | 2.16 | 0.46 |
| 41:CO:97:ALA:O | 41:CO:99:ASN:N | 2.48 | 0.46 |
| 41:CO:208:TYR:CE1 | 41:CO:212:PHE:HB2 | 2.50 | 0.46 |
| 41:CP:156:ARG:HD2 | 41:CP:156:ARG:HA | 1.76 | 0.46 |
| 41:CP:251:ARG:O | 41:CP:255:VAL:HG23 | 2.15 | 0.46 |
| 41:CP:317:PHE:HB3 | 41:CP:321:MET:SD | 2.56 | 0.46 |
| 40:DA:73:THR:O | 40:DA:75:ILE:N | 2.49 | 0.46 |
| 40:DE:118:VAL:HG21 | 40:DE:149:PHE:CZ | 2.51 | 0.46 |
| 40:DE:144:GLY:O | 40:DE:145:THR:C | 2.54 | 0.46 |
| 40:DF:181:VAL:HG13 | 41:DM:256:ASN:OD1 | 2.15 | 0.46 |
| 40:DH:19:ALA:O | 40:DH:22:GLU:HB3 | 2.16 | 0.46 |
| 40:DH:313:MET:HG2 | 40:DH:379:ASN:HB3 | 1.97 | 0.46 |
| 40:DI:168:GLU:HB2 | 40:DI:201:ALA:HA | 1.96 | 0.46 |
| 41:DL:55:THR:O | 41:DL:56:GLY:C | 2.54 | 0.46 |
| 41:DL:306:ARG:C | 41:DL:308:GLY:H | 2.18 | 0.46 |
| 41:DM:41:ASP:C | 41:DM:43:GLN:H | 2.17 | 0.46 |
| 41:DM:138:SER:O | 41:DM:139:LEU:C | 2.54 | 0.46 |
| 41:DP:238:THR:O | 41:DP:239:CYS:C | 2.52 | 0.46 |
| 40:EA:21:TRP:CZ2 | 40:EA:65:ALA:HB2 | 2.50 | 0.46 |
| 40:EA:228:ASN:ND2 | 42:EA:501:GTP:HN1 | 2.13 | 0.46 |
| 41:EB:287:PRO:O | 41:EB:291:GLN:HG2 | 2.15 | 0.46 |
| 40:EH:82:THR:C | 40:EH:84:ARG:H | 2.19 | 0.46 |
| 40:EI:30:ILE:HG21 | 40:EI:61:HIS:HB2 | 1.97 | 0.46 |
| 41:EL:221:THR:HG23 | 41:EL:224:ASP:H | 1.80 | 0.46 |
| 41:EL:290:THR:HG21 | 41:EL:329:GLN:HB3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EM:193:VAL:HG22 | 41:EM:265:PHE:HZ | 1.81 | 0.46 |
| 41:EM:330:MET:O | 41:EM:334:GLN:HG3 | 2.16 | 0.46 |
| 41:EP:377:LEU:HD12 | 41:EP:377:LEU:HA | 1.68 | 0.46 |
| 40:FA:49:PHE:O | 40:FA:50:ASN:C | 2.54 | 0.46 |
| 40:FA:123:ARG:HH12 | 40:GA:297:GLU:HG2 | 1.81 | 0.46 |
| 42:FB:502:GTP:O2A | 40:FG:140:SER:OG | 2.32 | 0.46 |
| 40:FH:73:THR:HG22 | 41:FO:46:ARG:HE | 1.80 | 0.46 |
| 40:FI:320:ARG:HH21 | 40:FI:360:PRO:HA | 1.81 | 0.46 |
| 41:FM:330:MET:HA | 41:FM:333:VAL:HG22 | 1.97 | 0.46 |
| 41:FN:309:ARG:NH1 | 41:FN:339:SER:O | 2.48 | 0.46 |
| 41:FP:87:PRO:HA | 41:FP:90:PHE:HD2 | 1.81 | 0.46 |
| 41:FP:178:THR:HB | 41:FP:181:GLU:HG3 | 1.98 | 0.46 |
| 41:GB:287:PRO:O | 41:GB:291:GLN:HG2 | 2.15 | 0.46 |
| 40:GE:247:ALA:O | 40:GE:248:LEU:C | 2.53 | 0.46 |
| 40:GE:344:VAL:HG23 | 40:GE:347:CYS:HB3 | 1.96 | 0.46 |
| 40:GI:173:PRO:HG2 | 40:GI:390:LEU:HD21 | 1.96 | 0.46 |
| 40:GI:213:CYS:O | 40:GI:214:ARG:C | 2.53 | 0.46 |
| 41:GO:42:LEU:HD23 | 41:GO:356:ILE:HD11 | 1.97 | 0.46 |
| 41:GP:207:LEU:HA | 41:GP:210:ILE:HG12 | 1.97 | 0.46 |
| 40:HA:405:HIS:HA | 40:HA:408:VAL:HG12 | 1.98 | 0.46 |
| 40:HE:346:TRP:HZ2 | 40:HE:434:VAL:HG13 | 1.81 | 0.46 |
| 41:HP:256:ASN:CG | 41:HP:350:LYS:HZ2 | 2.18 | 0.46 |
| 41:IB:31:ASP:OD2 | 41:IB:35:THR:OG1 | 2.30 | 0.46 |
| 40:IG:49:PHE:HE2 | 40:IG:55:GLU:HB2 | 1.81 | 0.46 |
| 41:IM:207:LEU:HA | 41:IM:210:ILE:HG22 | 1.96 | 0.46 |
| 41:IM:323:MET:SD | 41:IM:353:VAL:HG21 | 2.55 | 0.46 |
| 40:JD:101:ASN:HA | 40:JD:144:GLY:H | 1.81 | 0.46 |
| 40:JE:332:ILE:HG23 | 40:JE:351:PHE:CD2 | 2.50 | 0.46 |
| 40:JF:6:SER:O | 40:JF:65:ALA:HA | 2.15 | 0.46 |
| 41:JM:109:GLY:O | 41:JM:110:ALA:C | 2.53 | 0.46 |
| 41:JM:305:PRO:HB2 | 41:JM:306:ARG:HH21 | 1.80 | 0.46 |
| 40:KD:192:HIS:NE2 | 40:KD:419:GLU:OE1 | 2.49 | 0.46 |
| 40:KE:3:GLU:OE1 | 40:KE:3:GLU:N | 2.47 | 0.46 |
| 41:KO:413:SER:O | 41:KO:417:ASP:HB2 | 2.16 | 0.46 |
| 40:LD:141:PHE:HB2 | 40:LD:173:PRO:HD3 | 1.97 | 0.46 |
| 40:LH:142:GLY:HA2 | 40:LH:183:GLU:HG2 | 1.97 | 0.46 |
| 41:LL:215:LEU:HB3 | 41:LL:217:LEU:HD13 | 1.98 | 0.46 |
| 41:LN:142:GLY:O | 41:LN:144:GLY:N | 2.48 | 0.46 |
| 41:LO:193:VAL:HG11 | 41:LO:262:ARG:HH21 | 1.80 | 0.46 |
| 40:MF:139:HIS:H | 40:MF:139:HIS:HD2 | 1.60 | 0.46 |
| 40:MF:416:GLU:O | 40:MF:417:PHE:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:ND:306:ASP:HB3 | 40:ND:309:HIS:HB2 | 1.97 | 0.46 |
| 41:NM:244:GLY:HA3 | 41:NM:354:CYS:HA | 1.97 | 0.46 |
| 41:NP:288:GLU:O | 41:NP:291:GLN:NE2 | 2.49 | 0.46 |
| 40:OF:287:SER:HA | 40:OF:372:ARG:HH12 | 1.81 | 0.46 |
| 40:OG:8:HIS:HB2 | 40:OG:67:PHE:HD1 | 1.79 | 0.46 |
| 41:OM:2:ARG:HD2 | 41:OM:240:LEU:HD12 | 1.98 | 0.46 |
| 41:ON:21:TRP:CE3 | 41:ON:24:ILE:HD11 | 2.51 | 0.46 |
| 41:ON:152:ILE:HG12 | 41:ON:164:MET:HE1 | 1.96 | 0.46 |
| 41:OO:141:GLY:O | 41:OO:184:ASN:ND2 | 2.49 | 0.46 |
| 41:OP:19:LYS:HG3 | 41:OP:226:ASN:HB2 | 1.96 | 0.46 |
| 40:PA:137:ILE:HB | 40:PA:168:GLU:HG3 | 1.98 | 0.46 |
| 41:PB:73:MET:HA | 41:PB:76:VAL:HG12 | 1.97 | 0.46 |
| 40:PG:259:LEU:O | 40:PG:379:ASN:ND2 | 2.49 | 0.46 |
| 41:PM:142:GLY:O | 41:PM:144:GLY:N | 2.48 | 0.46 |
| 41:PM:268:PRO:HG2 | 41:PM:300:MET:HB2 | 1.97 | 0.46 |
| 41:PN:142:GLY:O | 41:PN:144:GLY:N | 2.48 | 0.46 |
| 41:PN:172:SER:HB2 | 41:PN:205:GLU:HB2 | 1.98 | 0.46 |
| 41:PP:86:ARG:NE | 41:QP:281:TYR:O | 2.49 | 0.46 |
| 40:QE:229:ARG:HH21 | 40:QE:363:VAL:HG13 | 1.81 | 0.46 |
| 40:QE:352:LYS:NZ | 40:QE:353:VAL:O | 2.49 | 0.46 |
| 40:QH:296:PHE:HE1 | 40:QH:376:MET:HG3 | 1.80 | 0.46 |
| 41:QL:23:VAL:HG23 | 41:QL:359:ARG:HH22 | 1.81 | 0.46 |
| 41:QM:286:VAL:HB | 41:QM:325:GLU:HG2 | 1.98 | 0.46 |
| 41:QN:3:GLU:O | 41:QN:131:GLN:N | 2.42 | 0.46 |
| 40:RA:56:THR:OG1 | 40:RA:57:GLY:N | 2.48 | 0.46 |
| 40:RA:185:TYR:HA | 40:RA:394:PHE:CE2 | 2.51 | 0.46 |
| 40:RA:298:PRO:HA | 40:RA:301:GLN:HG2 | 1.97 | 0.46 |
| 40:RE:224:TYR:CZ | 41:RL:323:MET:HG3 | 2.51 | 0.46 |
| 40:RH:195:LEU:HD11 | 40:RH:427:LEU:HD13 | 1.98 | 0.46 |
| 41:RN:282:ARG:HH22 | 41:RN:291:GLN:HE22 | 1.63 | 0.46 |
| 41:RP:267:MET:SD | 41:RP:299:MET:HB2 | 2.55 | 0.46 |
| 41:SB:87:PRO:HD3 | 41:TB:281:TYR:HD2 | 1.80 | 0.46 |
| 40:SF:108:TYR:O | 40:SF:112:LYS:NZ | 2.49 | 0.46 |
| 40:SH:185:TYR:HE2 | 40:SH:403:PHE:HB2 | 1.80 | 0.46 |
| 41:SO:61:PRO:HG2 | 41:SO:85:PHE:CD1 | 2.50 | 0.46 |
| 41:SO:87:PRO:O | 41:SO:90:PHE:N | 2.48 | 0.46 |
| 41:SO:117:LEU:HD13 | 41:SO:117:LEU:HA | 1.71 | 0.46 |
| 41:SO:210:ILE:O | 41:SO:214:THR:N | 2.48 | 0.46 |
| 41:TB:16:ILE:HD13 | 41:TB:226:ASN:ND2 | 2.30 | 0.46 |
| 41:TP:130:LEU:O | 41:TP:162:ARG:NE | 2.47 | 0.46 |
| 40:UE:11:GLN:OE1 | 40:UE:11:GLN:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UF:21:TRP:O | 40:UF:25:CYS:HB2 | 2.15 | 0.46 |
| 40:UF:317:LEU:HB3 | 40:UF:319:TYR:CE1 | 2.51 | 0.46 |
| 40:UI:160:ASP:HB2 | 40:UI:161:TYR:H | 1.54 | 0.46 |
| 41:UM:294:PHE:HZ | 41:UM:313:VAL:HG11 | 1.80 | 0.46 |
| 41:UN:262:ARG:HH21 | 41:UN:418:LEU:HA | 1.80 | 0.46 |
| 41:UO:74:ASP:HA | 41:UO:77:ARG:HG2 | 1.98 | 0.46 |
| 41:UP:164:MET:HB2 | 41:UP:196:THR:HA | 1.97 | 0.46 |
| 40:VA:115:ILE:HA | 40:VA:118:VAL:HG12 | 1.97 | 0.46 |
| 40:VF:239:THR:O | 40:VF:243:ARG:NE | 2.35 | 0.46 |
| 40:VF:431:TYR:HA | 40:VF:434:VAL:HG12 | 1.98 | 0.46 |
| 40:VJ:235:VAL:HA | 40:VJ:238:ILE:HG22 | 1.97 | 0.46 |
| 41:WB:63:ALA:O | 41:WB:89:ASN:ND2 | 2.49 | 0.46 |
| 41:WB:324:LYS:O | 41:WB:328:GLU:HG3 | 2.15 | 0.46 |
| 40:WE:234:ILE:HD11 | 40:WE:272:TYR:HB2 | 1.97 | 0.46 |
| 40:WF:171:ILE:HD13 | 40:WF:204:VAL:HG23 | 1.98 | 0.46 |
| 40:WG:200:CYS:HA | 40:WG:266:HIS:HB2 | 1.97 | 0.46 |
| 41:WN:215:LEU:HD21 | 41:WN:273:LEU:HD22 | 1.97 | 0.46 |
| 41:WO:202:ILE:HG12 | 41:WO:268:PRO:HG3 | 1.98 | 0.46 |
| 5:1M:241:LEU:HD12 | 40:GH:159:VAL:HG11 | 1.97 | 0.46 |
| 7:1T:43:LEU:HB3 | 7:1T:48:LEU:HD13 | 1.98 | 0.46 |
| 8:1X:174:LEU:HD12 | 41:UB:33:THR:HG22 | 1.98 | 0.46 |
| 9:2B:46:VAL:HG12 | 9:2B:48:ILE:HG12 | 1.96 | 0.46 |
| 10:2F:54:THR:HG21 | 40:MA:198:SER:O | 2.16 | 0.46 |
| 10:2F:150:PRO:HD2 | 40:WG:221:ARG:NH1 | 2.31 | 0.46 |
| 10:2F:162:LYS:HZ2 | 40:WG:214:ARG:HG3 | 1.81 | 0.46 |
| 11:2I:186:LYS:HA | 11:2I:251:TYR:CB | 2.45 | 0.46 |
| 11:2I:188:LEU:HB2 | 11:2I:250:ILE:O | 2.16 | 0.46 |
| 11:2K:197:LEU:HD13 | 11:2K:197:LEU:HA | 1.72 | 0.46 |
| 11:2K:235:LYS:O | 11:2K:238:GLU:HG3 | 2.16 | 0.46 |
| 13:2U:38:THR:HA | 13:2U:44:SER:O | 2.16 | 0.46 |
| 15:3E:188:CYS:SG | 15:3F:319:THR:OG1 | 2.73 | 0.46 |
| 15:3F:189:PHE:C | 15:3F:191:LEU:H | 2.19 | 0.46 |
| 15:3F:205:VAL:O | 15:3F:206:ARG:NE | 2.49 | 0.46 |
| 15:3G:282:LEU:HD13 | 15:3G:376:ILE:HD12 | 1.97 | 0.46 |
| 18:3T:305:GLY:HA3 | 25:4T:421:LEU:HD11 | 1.97 | 0.46 |
| 20:4A:155:MET:N | 20:4A:155:MET:SD | 2.89 | 0.46 |
| 20:4B:278:THR:C | 20:4B:280:GLU:H | 2.19 | 0.46 |
| 21:4E:233:LYS:NZ | 40:BH:58:ALA:O | 2.49 | 0.46 |
| 22:4I:236:TRP:CE2 | 22:4I:349:ARG:HB3 | 2.51 | 0.46 |
| 22:4J:693:PHE:O | 22:4J:696:ALA:N | 2.48 | 0.46 |
| 22:4K:438:ALA:HB2 | 22:4K:454:ILE:HG23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4K:549:LEU:O | 22:4K:550:GLN:C | 2.54 | 0.46 |
| 23:4N:18:TYR:HE1 | 40:BF:80:THR:HG22 | 1.81 | 0.46 |
| 23:4R:108:ASN:ND2 | 23:4R:111:GLN:H | 2.13 | 0.46 |
| 27:4Z:153:GLY:H | 27:4Z:157:GLY:HA3 | 1.80 | 0.46 |
| 39:6G:115:LEU:HD11 | 39:6G:145:VAL:HG21 | 1.97 | 0.46 |
| 41:AO:162:ARG:H | 41:AO:162:ARG:HG2 | 1.45 | 0.46 |
| 40:BE:139:HIS:NE2 | 40:BE:170:SER:HB3 | 2.30 | 0.46 |
| 40:BF:181:VAL:HG12 | 41:BM:347:ASN:O | 2.15 | 0.46 |
| 40:BG:174:ALA:HB3 | 40:BG:178:SER:H | 1.81 | 0.46 |
| 40:BH:31:GLN:O | 40:BH:32:PRO:C | 2.54 | 0.46 |
| 40:BI:369:LYS:HD2 | 40:BI:369:LYS:HA | 1.53 | 0.46 |
| 41:BM:143:THR:HB | 41:BM:144:GLY:H | 1.63 | 0.46 |
| 41:BO:329:GLN:HA | 41:BO:332:ASN:HD21 | 1.81 | 0.46 |
| 41:BO:357:PRO:HB2 | 41:BO:358:PRO:HD2 | 1.97 | 0.46 |
| 40:CA:54:SER:OG | 40:CA:55:GLU:N | 2.48 | 0.46 |
| 40:CE:100:ALA:HB3 | 40:CE:105:ARG:HD3 | 1.98 | 0.46 |
| 40:CH:177:VAL:HG12 | 41:CO:327:ASP:HB3 | 1.98 | 0.46 |
| 40:CH:267:PHE:HB2 | 40:CH:431:TYR:OH | 2.16 | 0.46 |
| 40:CI:27:GLU:OE1 | 40:CI:243:ARG:NH1 | 2.48 | 0.46 |
| 41:CL:271:ALA:HB2 | 41:CL:365:ALA:HB3 | 1.98 | 0.46 |
| 41:CM:260:PHE:HB2 | 41:CM:263:LEU:HD11 | 1.97 | 0.46 |
| 41:CN:243:PRO:HD2 | 41:CN:356:ILE:HG13 | 1.97 | 0.46 |
| 41:CN:251:ARG:O | 41:CN:255:VAL:HG23 | 2.16 | 0.46 |
| 41:CN:286:VAL:HB | 41:CN:287:PRO:HD3 | 1.98 | 0.46 |
| 41:CO:88:ASP:C | 41:CO:90:PHE:H | 2.19 | 0.46 |
| 41:CO:111:GLU:H | 41:CO:111:GLU:HG2 | 1.47 | 0.46 |
| 40:DA:220:GLU:O | 40:DA:222:PRO:HD3 | 2.14 | 0.46 |
| 40:DA:331:ALA:O | 40:DA:332:ILE:C | 2.53 | 0.46 |
| 40:DA:419:GLU:H | 40:DA:419:GLU:HG3 | 1.59 | 0.46 |
| 40:DH:212:ILE:HA | 40:DH:215:ARG:HD2 | 1.98 | 0.46 |
| 40:DI:11:GLN:HE22 | 41:DP:246:LEU:HD22 | 1.81 | 0.46 |
| 41:DM:285:THR:O | 41:DM:286:VAL:C | 2.53 | 0.46 |
| 41:DN:252:LYS:O | 41:DN:256:ASN:ND2 | 2.49 | 0.46 |
| 41:DN:393:ALA:O | 41:DN:395:LEU:N | 2.45 | 0.46 |
| 41:DO:198:GLU:HG2 | 41:DO:266:PHE:HE2 | 1.79 | 0.46 |
| 41:DO:282:ARG:NH1 | 41:DO:288:GLU:OE1 | 2.46 | 0.46 |
| 41:DP:323:MET:O | 41:DP:324:LYS:C | 2.54 | 0.46 |
| 40:EG:2:ARG:O | 40:EG:51:THR:OG1 | 2.21 | 0.46 |
| 40:EG:98:ASP:O | 40:EG:105:ARG:NH1 | 2.38 | 0.46 |
| 40:EH:100:ALA:C | 40:EH:102:ASN:N | 2.69 | 0.46 |
| 40:EH:323:VAL:HG22 | 40:EH:372:ARG:HG3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EI:247:ALA:O | 40:EI:249:ASN:N | 2.49 | 0.46 |
| 41:EM:178:THR:HG22 | 41:EM:180:VAL:HG23 | 1.98 | 0.46 |
| 41:EM:262:ARG:HB2 | 41:EM:263:LEU:H | 1.51 | 0.46 |
| 41:EN:178:THR:HB | 41:EN:181:GLU:HB2 | 1.97 | 0.46 |
| 40:FA:48:SER:O | 40:FA:50:ASN:N | 2.48 | 0.46 |
| 41:FO:131:GLN:HE22 | 41:FO:249:ASP:HB3 | 1.81 | 0.46 |
| 41:FP:95:SER:OG | 41:FP:96:GLY:N | 2.49 | 0.46 |
| 41:FP:269:GLY:HA2 | 41:FP:300:MET:HG2 | 1.97 | 0.46 |
| 40:GE:269:LEU:HD22 | 40:GE:303:VAL:HG11 | 1.97 | 0.46 |
| 40:GF:319:TYR:HB3 | 40:GF:323:VAL:HG11 | 1.98 | 0.46 |
| 40:GG:79:ARG:NH2 | 40:GG:94:THR:OG1 | 2.49 | 0.46 |
| 40:GH:341:ILE:H | 40:GH:341:ILE:HG12 | 1.30 | 0.46 |
| 40:GH:406:TRP:CD1 | 41:GO:255:VAL:HA | 2.51 | 0.46 |
| 40:GI:332:ILE:HG12 | 40:GI:333:ALA:N | 2.29 | 0.46 |
| 40:HE:251:ASP:H | 40:HE:254:GLU:HG3 | 1.80 | 0.46 |
| 40:HF:141:PHE:HB2 | 40:HF:173:PRO:HD3 | 1.98 | 0.46 |
| 40:HI:213:CYS:HA | 40:HI:217:LEU:HD23 | 1.98 | 0.46 |
| 41:HN:104:GLY:O | 41:HN:147:MET:N | 2.49 | 0.46 |
| 41:IB:95:SER:OG | 41:IB:96:GLY:N | 2.48 | 0.46 |
| 41:IB:167:PHE:CE2 | 41:IB:200:TYR:HD2 | 2.34 | 0.46 |
| 40:IE:224:TYR:HA | 40:IE:227:LEU:HB2 | 1.97 | 0.46 |
| 40:IF:264:ARG:NE | 40:IF:430:ASP:OD2 | 2.45 | 0.46 |
| 40:IG:2:ARG:HH21 | 40:IG:242:LEU:HA | 1.81 | 0.46 |
| 40:II:177:VAL:HG12 | 41:IP:331:LEU:HB2 | 1.97 | 0.46 |
| 40:II:319:TYR:HB2 | 40:II:355:ILE:HD13 | 1.98 | 0.46 |
| 41:IM:87:PRO:HB2 | 40:JD:280:LYS:HG2 | 1.98 | 0.46 |
| 41:IN:41:ASP:N | 41:IN:41:ASP:OD1 | 2.49 | 0.46 |
| 41:IP:148:GLY:O | 41:IP:152:ILE:HG12 | 2.16 | 0.46 |
| 40:JA:310:GLY:HA3 | 40:JA:382:ALA:HB2 | 1.96 | 0.46 |
| 41:JB:272:PRO:HG3 | 41:JB:364:SER:HA | 1.96 | 0.46 |
| 40:JE:210:TYR:CE1 | 40:JE:227:LEU:HD21 | 2.50 | 0.46 |
| 40:JE:213:CYS:HA | 40:JE:217:LEU:HB3 | 1.98 | 0.46 |
| 41:JM:131:GLN:HE22 | 41:JM:250:LEU:HD12 | 1.80 | 0.46 |
| 40:KA:73:THR:HA | 40:KA:76:ASP:HB3 | 1.98 | 0.46 |
| 40:KA:274:PRO:HA | 40:KA:276:ILE:HD12 | 1.97 | 0.46 |
| 41:KB:316:VAL:HB | 41:KB:366:THR:HG22 | 1.96 | 0.46 |
| 40:KD:20:CYS:HA | 40:KD:232:SER:HB2 | 1.96 | 0.46 |
| 40:LF:23:LEU:HD12 | 40:LF:26:LEU:HD11 | 1.98 | 0.46 |
| 40:LF:223:THR:O | 40:LF:224:TYR:C | 2.54 | 0.46 |
| 40:LF:247:ALA:HB1 | 41:LN:222:TYR:CD2 | 2.51 | 0.46 |
| 40:LF:259:LEU:HD12 | 40:LF:259:LEU:HA | 1.76 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LH:177:VAL:HG21 | 41:LO:327:ASP:HB3 | 1.98 | 0.46 |
| 41:LL:266:PHE:HE2 | 41:LL:370:ASN:HD22 | 1.64 | 0.46 |
| 41:LO:282:ARG:HD2 | 41:LO:288:GLU:OE2 | 2.16 | 0.46 |
| 41:LP:189:VAL:O | 41:LP:193:VAL:HG23 | 2.16 | 0.46 |
| 41:MB:316:VAL:HB | 41:MB:366:THR:HG22 | 1.98 | 0.46 |
| 40:MH:57:GLY:O | 40:MH:58:ALA:HB3 | 2.16 | 0.46 |
| 41:MN:143:THR:O | 41:MN:147:MET:N | 2.48 | 0.46 |
| 41:NB:68:LEU:HD23 | 41:NB:143:THR:HG23 | 1.97 | 0.46 |
| 40:ND:382:ALA:O | 40:ND:383:ILE:C | 2.54 | 0.46 |
| 40:NE:2:ARG:HD3 | 40:NE:242:LEU:HB2 | 1.96 | 0.46 |
| 40:NG:140:SER:HA | 40:NG:171:ILE:H | 1.81 | 0.46 |
| 40:NH:113:GLU:HG2 | 40:NH:114:LEU:HD22 | 1.96 | 0.46 |
| 41:OB:10:GLY:O | 41:OB:14:ASN:HB2 | 2.16 | 0.46 |
| 41:OB:99:ASN:HA | 41:OB:142:GLY:HA3 | 1.98 | 0.46 |
| 41:OL:99:ASN:HA | 41:OL:142:GLY:HA3 | 1.98 | 0.46 |
| 41:OL:130:LEU:HD21 | 41:OL:133:PHE:HE1 | 1.80 | 0.46 |
| 41:OL:289:LEU:O | 41:OL:293:MET:HG3 | 2.16 | 0.46 |
| 41:ON:98:GLY:O | 41:ON:99:ASN:ND2 | 2.48 | 0.46 |
| 41:OO:63:ALA:O | 41:OO:89:ASN:ND2 | 2.48 | 0.46 |
| 41:OO:142:GLY:O | 41:OO:144:GLY:N | 2.49 | 0.46 |
| 41:PB:5:VAL:HB | 41:PB:133:PHE:HD1 | 1.81 | 0.46 |
| 40:PD:217:LEU:HA | 40:PD:277:SER:HB3 | 1.98 | 0.46 |
| 40:PH:170:SER:HB2 | 40:PH:203:MET:HE1 | 1.98 | 0.46 |
| 41:PN:139:LEU:HG | 41:PN:168:SER:HB2 | 1.97 | 0.46 |
| 41:PN:190:HIS:CE1 | 41:PN:414:ASN:HD22 | 2.34 | 0.46 |
| 41:PO:121:ARG:NE | 41:PO:158:GLU:OE1 | 2.46 | 0.46 |
| 41:QB:31:ASP:O | 41:QB:33:THR:N | 2.49 | 0.46 |
| 41:QB:130:LEU:O | 41:QB:131:GLN:C | 2.53 | 0.46 |
| 40:QE:21:TRP:HZ3 | 40:QE:52:PHE:CD2 | 2.34 | 0.46 |
| 41:QP:19:LYS:HB2 | 41:QP:226:ASN:OD1 | 2.15 | 0.46 |
| 41:QP:395:LEU:HD22 | 41:QP:408:PHE:CE2 | 2.50 | 0.46 |
| 41:RB:62:ARG:NH1 | 41:RB:127:CYS:SG | 2.79 | 0.46 |
| 41:RB:230:SER:HA | 41:RB:233:MET:HE3 | 1.97 | 0.46 |
| 41:RB:313:VAL:HG23 | 41:RB:349:VAL:HG22 | 1.97 | 0.46 |
| 40:RI:224:TYR:HE1 | 41:RP:323:MET:HG3 | 1.80 | 0.46 |
| 41:SB:31:ASP:OD2 | 41:SB:35:THR:OG1 | 2.34 | 0.46 |
| 41:SB:102:ALA:HB1 | 41:SB:401:GLU:HB2 | 1.98 | 0.46 |
| 41:SB:189:VAL:O | 41:SB:193:VAL:HG23 | 2.16 | 0.46 |
| 40:SE:137:ILE:HB | 40:SE:168:GLU:HG3 | 1.98 | 0.46 |
| 40:SF:26:LEU:HD21 | 40:SF:363:VAL:HG22 | 1.96 | 0.46 |
| 40:SG:6:SER:O | 40:SG:65:ALA:HA | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SI:101:ASN:HA | 40:SI:144:GLY:H | 1.80 | 0.46 |
| 40:SI:179:THR:OG1 | 41:SP:351:THR:OG1 | 2.28 | 0.46 |
| 41:SN:309:ARG:N | 41:SN:372:THR:OG1 | 2.48 | 0.46 |
| 41:SO:242:PHE:HB3 | 41:SO:356:ILE:HB | 1.96 | 0.46 |
| 41:SO:276:ARG:O | 41:SO:277:GLY:C | 2.54 | 0.46 |
| 40:TA:117:LEU:O | 40:TA:121:ARG:HG2 | 2.16 | 0.46 |
| 40:TF:380:THR:HG23 | 40:TF:382:ALA:H | 1.81 | 0.46 |
| 40:TG:322:ASP:H | 40:TG:371:GLN:HB3 | 1.80 | 0.46 |
| 41:TL:237:THR:HG23 | 41:TL:240:LEU:HD21 | 1.96 | 0.46 |
| 41:TM:375:GLN:O | 41:TM:379:LYS:HB2 | 2.16 | 0.46 |
| 40:UA:20:CYS:HA | 40:UA:232:SER:HB2 | 1.97 | 0.46 |
| 41:UB:229:VAL:O | 41:UB:233:MET:HG2 | 2.16 | 0.46 |
| 40:UE:132:LEU:O | 40:UE:164:LYS:NZ | 2.38 | 0.46 |
| 40:UF:104:ALA:HA | 40:UF:108:TYR:HD2 | 1.81 | 0.46 |
| 40:UH:101:ASN:HD22 | 41:UO:256:ASN:HD21 | 1.63 | 0.46 |
| 40:UI:277:SER:O | 40:UI:280:LYS:N | 2.36 | 0.46 |
| 41:UO:226:ASN:ND2 | 43:UO:502:GDP:O6 | 2.44 | 0.46 |
| 41:UO:385:PHE:CE2 | 41:UO:412:GLU:HB2 | 2.50 | 0.46 |
| 40:VA:97:GLU:HG3 | 40:VA:105:ARG:HH22 | 1.79 | 0.46 |
| 40:VF:139:HIS:CE1 | 40:VF:170:SER:HG | 2.34 | 0.46 |
| 40:VH:16:ILE:HA | 40:VH:228:ASN:HB3 | 1.98 | 0.46 |
| 40:VH:251:ASP:H | 40:VH:254:GLU:HB2 | 1.80 | 0.46 |
| 40:VJ:172:TYR:CD1 | 40:VJ:173:PRO:HD2 | 2.50 | 0.46 |
| 41:WB:246:LEU:HD22 | 41:WB:352:ALA:HA | 1.98 | 0.46 |
| 40:WF:403:PHE:HZ | 41:WM:312:THR:HG21 | 1.81 | 0.46 |
| 41:WN:174:LYS:HE3 | 41:WN:174:LYS:HB2 | 1.35 | 0.46 |
| 41:WN:286:VAL:O | 41:WN:290:THR:HG23 | 2.16 | 0.46 |
| 41:WQ:292:GLN:OE1 | 41:WQ:298:ASN:ND2 | 2.48 | 0.46 |
| 7:1S:14:LEU:HD13 | 7:1S:583:GLY:N | 2.30 | 0.46 |
| 7:1T:14:LEU:HD12 | 7:1T:581:HIS:HB3 | 1.98 | 0.46 |
| 7:1T:470:LYS:HB3 | 7:1T:472:ASN:OD1 | 2.15 | 0.46 |
| 8:1Y:99:SER:O | 8:1Y:101:ILE:HG23 | 2.15 | 0.46 |
| 9:2B:165:LYS:HE2 | 9:2C:489:MET:HE3 | 1.96 | 0.46 |
| 10:2E:151:HIS:CD2 | 10:2E:157:ARG:HB2 | 2.51 | 0.46 |
| 12:2Q:215:GLN:NE2 | 13:2V:37:ILE:HG23 | 2.31 | 0.46 |
| 13:2U:71:ILE:HG21 | 13:2U:167:PHE:CG | 2.51 | 0.46 |
| 15:3E:232:ARG:HH22 | 16:3J:259:VAL:HG21 | 1.81 | 0.46 |
| 17:3P:369:LEU:HD13 | 17:3P:369:LEU:HA | 1.76 | 0.46 |
| 17:3R:292:ALA:O | 17:3R:293:THR:C | 2.54 | 0.46 |
| 20:4B:250:SER:O | 20:4B:251:ASP:C | 2.52 | 0.46 |
| 22:4J:659:LYS:HB2 | 22:4J:659:LYS:HE2 | 1.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:4M:109:CYS:HG | 40:BG:218:ASP:CG | 2.19 | 0.46 |
| 23:4M:198:PHE:HD1 | 40:DG:221:ARG:HD2 | 1.81 | 0.46 |
| 24:4O:195:ARG:NH2 | 40:DE:221:ARG:HD2 | 2.31 | 0.46 |
| 23:4P:242:LEU:CD1 | 23:4P:250:VAL:HB | 2.46 | 0.46 |
| 23:4R:217:LYS:HA | 23:4R:217:LYS:HD2 | 1.41 | 0.46 |
| 27:4Y:149:LEU:HD12 | 27:4Y:162:LEU:HD22 | 1.97 | 0.46 |
| 28:5B:202:THR:HG23 | 28:5B:203:TRP:CD1 | 2.51 | 0.46 |
| 33:5N:453:LYS:HG2 | 33:5N:476:MET:HB3 | 1.98 | 0.46 |
| 38:6C:36:PHE:CZ | 41:VO:174:LYS:HD3 | 2.51 | 0.46 |
| 39:6F:116:ARG:HD3 | 39:6F:116:ARG:HA | 1.57 | 0.46 |
| 40:AF:100:ALA:O | 41:AM:255:VAL:HG11 | 2.16 | 0.46 |
| 40:AF:190:THR:O | 40:AF:194:THR:OG1 | 2.21 | 0.46 |
| 41:AO:174:LYS:HE3 | 41:AO:175:VAL:HG12 | 1.98 | 0.46 |
| 40:BE:177:VAL:CG2 | 41:BL:327:ASP:HB3 | 2.46 | 0.46 |
| 40:BF:100:ALA:HA | 41:BM:252:LYS:HG3 | 1.96 | 0.46 |
| 40:BH:332:ILE:HG23 | 40:BH:351:PHE:CD2 | 2.51 | 0.46 |
| 41:BO:16:ILE:HD11 | 41:BO:229:VAL:HG21 | 1.97 | 0.46 |
| 40:CA:59:GLY:O | 40:CA:61:HIS:N | 2.48 | 0.46 |
| 40:CA:188:ILE:HG23 | 40:CA:390:LEU:HD22 | 1.98 | 0.46 |
| 40:CH:320:ARG:HD3 | 40:CH:373:ALA:HB3 | 1.96 | 0.46 |
| 41:CL:105:HIS:O | 41:CL:107:THR:N | 2.44 | 0.46 |
| 41:CL:192:LEU:HD13 | 41:CL:192:LEU:HA | 1.73 | 0.46 |
| 41:CN:75:SER:O | 41:CN:78:SER:N | 2.48 | 0.46 |
| 41:CN:107:THR:OG1 | 41:CN:108:GLU:N | 2.49 | 0.46 |
| 40:DA:261:PRO:O | 41:DB:396:HIS:NE2 | 2.48 | 0.46 |
| 40:DA:324:VAL:O | 40:DA:326:LYS:N | 2.49 | 0.46 |
| 41:DB:204:ASN:OD1 | 43:DB:501:GDP:N2 | 2.49 | 0.46 |
| 40:DF:111:GLY:C | 40:DF:113:GLU:H | 2.19 | 0.46 |
| 40:DI:288:VAL:O | 40:DI:291:ILE:HG12 | 2.16 | 0.46 |
| 40:DI:406:TRP:CG | 41:DP:255:VAL:HG23 | 2.51 | 0.46 |
| 41:DL:117:LEU:HD23 | 41:DL:117:LEU:HA | 1.77 | 0.46 |
| 41:DL:209:ASP:O | 41:DL:210:ILE:C | 2.53 | 0.46 |
| 41:DL:385:PHE:HE2 | 41:DL:412:GLU:HB2 | 1.81 | 0.46 |
| 41:DM:145:SER:OG | 41:DM:146:GLY:N | 2.49 | 0.46 |
| 41:DM:180:VAL:O | 41:DM:184:ASN:ND2 | 2.49 | 0.46 |
| 41:DM:386:THR:OG1 | 41:DM:387:ALA:N | 2.49 | 0.46 |
| 41:DP:257:MET:HA | 41:DP:312:THR:HB | 1.96 | 0.46 |
| 40:EG:217:LEU:HA | 40:EG:277:SER:HB3 | 1.97 | 0.46 |
| 41:EL:142:GLY:O | 41:EL:144:GLY:N | 2.49 | 0.46 |
| 41:EM:331:LEU:HG | 41:EM:335:ASN:HD21 | 1.81 | 0.46 |
| 41:EN:237:THR:HG23 | 41:EN:240:LEU:HD21 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FG:205:ASP:HB3 | 40:FG:303:VAL:HA | 1.98 | 0.46 |
| 40:FG:252:LEU:HA | 40:FG:255:PHE:HD2 | 1.80 | 0.46 |
| 41:FM:73:MET:HG3 | 41:FM:92:PHE:HB3 | 1.98 | 0.46 |
| 40:GA:242:LEU:H | 40:GA:242:LEU:HD23 | 1.81 | 0.46 |
| 40:GE:23:LEU:HA | 40:GE:26:LEU:HD23 | 1.98 | 0.46 |
| 40:GE:280:LYS:HB3 | 40:GE:280:LYS:HE3 | 1.63 | 0.46 |
| 40:GH:102:ASN:O | 40:GH:105:ARG:N | 2.49 | 0.46 |
| 40:GI:420:ALA:HA | 40:GI:423:ASP:OD2 | 2.15 | 0.46 |
| 41:GO:167:PHE:CE2 | 41:GO:233:MET:HG3 | 2.51 | 0.46 |
| 40:HI:238:ILE:HD12 | 40:HI:318:LEU:HD11 | 1.98 | 0.46 |
| 41:HN:71:GLY:O | 41:HN:72:THR:C | 2.54 | 0.46 |
| 41:HQ:24:ILE:HG21 | 41:HQ:241:ARG:HH12 | 1.81 | 0.46 |
| 41:HQ:292:GLN:O | 41:HQ:298:ASN:ND2 | 2.48 | 0.46 |
| 40:IE:93:ILE:HD11 | 40:IE:121:ARG:HG3 | 1.97 | 0.46 |
| 40:IF:11:GLN:HE21 | 40:IF:74:VAL:HG21 | 1.81 | 0.46 |
| 41:IM:7:LEU:HD23 | 41:IM:64:VAL:HB | 1.97 | 0.46 |
| 41:IM:164:MET:HG2 | 41:IM:196:THR:HG22 | 1.98 | 0.46 |
| 40:JA:11:GLN:NE2 | 42:JA:501:GTP:O3G | 2.48 | 0.46 |
| 40:JE:14:VAL:HG22 | 40:JE:67:PHE:HD1 | 1.81 | 0.46 |
| 40:JG:16:ILE:HG21 | 40:JG:138:PHE:CD2 | 2.50 | 0.46 |
| 41:JM:185:ALA:CB | 41:JM:381:ILE:HD11 | 2.44 | 0.46 |
| 40:KG:265:ILE:HG23 | 40:KG:431:TYR:HE1 | 1.80 | 0.46 |
| 40:KH:262:TYR:HB2 | 40:KH:265:ILE:HG22 | 1.98 | 0.46 |
| 41:KL:285:THR:O | 41:KL:286:VAL:C | 2.54 | 0.46 |
| 41:KO:2:ARG:NH1 | 41:KO:249:ASP:OD2 | 2.49 | 0.46 |
| 41:KO:215:LEU:HD21 | 41:KO:273:LEU:HD22 | 1.98 | 0.46 |
| 40:LG:172:TYR:HE2 | 40:LG:386:ALA:HB1 | 1.81 | 0.46 |
| 41:LL:326:VAL:O | 41:LL:330:MET:HG2 | 2.16 | 0.46 |
| 41:LP:180:VAL:O | 41:LP:184:ASN:ND2 | 2.49 | 0.46 |
| 40:MF:320:ARG:HG3 | 40:MF:358:GLN:O | 2.15 | 0.46 |
| 40:MG:352:LYS:HE2 | 40:MG:352:LYS:HB2 | 1.54 | 0.46 |
| 41:MP:226:ASN:ND2 | 43:MP:501:GDP:O6 | 2.43 | 0.46 |
| 41:NB:139:LEU:HD23 | 41:NB:170:VAL:HG22 | 1.96 | 0.46 |
| 40:ND:426:ALA:HA | 40:ND:429:LYS:HD2 | 1.97 | 0.46 |
| 40:NF:235:VAL:HA | 40:NF:238:ILE:HG22 | 1.97 | 0.46 |
| 40:NG:98:ASP:O | 40:NG:105:ARG:NH1 | 2.47 | 0.46 |
| 41:NN:39:ASP:OD1 | 41:NN:39:ASP:N | 2.49 | 0.46 |
| 40:OA:122:ILE:HG21 | 40:OA:157:LEU:HD11 | 1.98 | 0.46 |
| 41:OB:260:PHE:HE2 | 41:OB:425:ARG:HE | 1.62 | 0.46 |
| 40:OD:326:LYS:HB2 | 40:OD:329:ASN:CB | 2.46 | 0.46 |
| 40:OG:205:ASP:O | 40:OG:209:ILE:HG12 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OH:17:GLY:O | 40:OH:18:ASN:C | 2.54 | 0.46 |
| 41:OO:169:VAL:HG12 | 41:OO:202:ILE:HB | 1.97 | 0.46 |
| 40:PD:192:HIS:CE1 | 40:PD:423:ASP:HB3 | 2.51 | 0.46 |
| 40:PD:311:LYS:HZ3 | 40:PD:342:GLN:HB3 | 1.81 | 0.46 |
| 40:PG:3:GLU:HG3 | 40:PG:129:CYS:HB2 | 1.98 | 0.46 |
| 41:PL:138:SER:HA | 41:PL:169:VAL:HG22 | 1.98 | 0.46 |
| 41:PP:229:VAL:O | 41:PP:232:THR:OG1 | 2.26 | 0.46 |
| 41:QB:141:GLY:HA3 | 43:QB:501:GDP:O1A | 2.15 | 0.46 |
| 41:QB:308:GLY:HA3 | 41:QB:373:ALA:HA | 1.98 | 0.46 |
| 41:QB:350:LYS:NZ | 40:QG:180:ALA:HB1 | 2.31 | 0.46 |
| 41:QB:417:ASP:O | 41:QB:420:ASN:N | 2.40 | 0.46 |
| 40:QG:205:ASP:HB3 | 40:QG:303:VAL:HA | 1.98 | 0.46 |
| 40:QG:318:LEU:O | 40:QG:374:VAL:HA | 2.16 | 0.46 |
| 40:QH:116:ASP:OD1 | 40:QH:117:LEU:N | 2.49 | 0.46 |
| 40:QH:260:VAL:HB | 41:QP:397:TRP:CZ2 | 2.51 | 0.46 |
| 41:QP:1:MET:O | 41:QP:129:CYS:HB3 | 2.16 | 0.46 |
| 41:QP:139:LEU:O | 41:QP:140:GLY:C | 2.54 | 0.46 |
| 41:QP:156:ARG:HD2 | 41:QP:195:ASN:HB2 | 1.98 | 0.46 |
| 41:QP:222:TYR:CZ | 43:QP:501:GDP:H2' | 2.51 | 0.46 |
| 41:QP:384:GLN:O | 41:QP:387:ALA:N | 2.49 | 0.46 |
| 41:RB:51:TYR:HA | 41:RB:60:VAL:O | 2.16 | 0.46 |
| 40:RF:413:GLU:N | 40:RF:413:GLU:OE2 | 2.49 | 0.46 |
| 41:RL:240:LEU:HD23 | 41:RL:240:LEU:H | 1.80 | 0.46 |
| 41:RN:206:ALA:O | 41:RN:210:ILE:HD12 | 2.16 | 0.46 |
| 41:RO:77:ARG:HH21 | 41:RO:90:PHE:HE2 | 1.64 | 0.46 |
| 41:RO:238:THR:HA | 41:RO:241:ARG:HB3 | 1.98 | 0.46 |
| 41:RP:257:MET:HB3 | 41:RP:266:PHE:CZ | 2.51 | 0.46 |
| 40:SA:67:PHE:HB2 | 40:SA:92:LEU:HD13 | 1.98 | 0.46 |
| 40:SA:217:LEU:HB3 | 40:SA:219:ILE:HG22 | 1.98 | 0.46 |
| 41:SB:189:VAL:HA | 41:SB:192:LEU:HB3 | 1.98 | 0.46 |
| 40:SH:38:SER:OG | 40:SH:39:ASP:N | 2.49 | 0.46 |
| 41:SO:359:ARG:HA | 41:SO:359:ARG:HD3 | 1.73 | 0.46 |
| 41:SP:229:VAL:O | 41:SP:233:MET:HG2 | 2.15 | 0.46 |
| 40:TI:212:ILE:HD11 | 40:TI:300:ASN:HA | 1.98 | 0.46 |
| 41:TL:240:LEU:HD13 | 41:TL:249:ASP:HB2 | 1.98 | 0.46 |
| 41:TM:330:MET:HB3 | 41:TM:349:VAL:HG11 | 1.98 | 0.46 |
| 41:TN:121:ARG:NH1 | 41:TN:158:GLU:OE2 | 2.49 | 0.46 |
| 41:TO:7:LEU:HD23 | 41:TO:133:PHE:HB3 | 1.98 | 0.46 |
| 41:TP:210:ILE:HD13 | 41:TP:228:LEU:HD21 | 1.97 | 0.46 |
| 40:UH:100:ALA:O | 41:UO:255:VAL:HG11 | 2.16 | 0.46 |
| 40:UI:223:THR:HG21 | 41:UP:320:ARG:HH12 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UP:182:PRO:O | 41:UP:183:TYR:C | 2.53 | 0.46 |
| 40:VF:297:GLU:HA | 40:VF:298:PRO:HD3 | 1.79 | 0.46 |
| 40:WE:3:GLU:HG3 | 40:WE:50:ASN:O | 2.16 | 0.46 |
| 40:WE:98:ASP:OD1 | 40:WE:99:ALA:N | 2.48 | 0.46 |
| 40:WG:238:ILE:HA | 40:WG:318:LEU:HD22 | 1.96 | 0.46 |
| 41:WM:391:ARG:HE | 41:WM:391:ARG:HB3 | 1.47 | 0.46 |
| 41:WQ:202:ILE:HG23 | 41:WQ:300:MET:HB3 | 1.97 | 0.46 |
| 7:1U:77:VAL:HG23 | 7:1U:78:TYR:HD1 | 1.81 | 0.46 |
| 7:1U:332:PHE:HZ | 7:1U:354:LYS:HB2 | 1.80 | 0.46 |
| 8:1W:329:ALA:HA | 8:1W:332:LYS:HG2 | 1.98 | 0.46 |
| 8:1X:109:ARG:O | 8:1X:112:TRP:HB3 | 2.16 | 0.46 |
| 9:2B:54:TRP:HB2 | 11:2K:252:ILE:HD11 | 1.96 | 0.46 |
| 10:2G:147:ILE:HD11 | 40:WI:221:ARG:HB3 | 1.97 | 0.46 |
| 11:2I:186:LYS:HE3 | 11:2I:187:ARG:HD2 | 1.97 | 0.46 |
| 11:2K:200:LEU:HD23 | 11:2K:237:LEU:HD23 | 1.98 | 0.46 |
| 12:2R:41:GLY:HA2 | 41:AP:340:TYR:HE2 | 1.79 | 0.46 |
| 13:2U:177:LEU:HB3 | 13:2U:182:LYS:HG2 | 1.97 | 0.46 |
| 13:2X:95:ASP:HB2 | 13:2X:99:VAL:HG23 | 1.98 | 0.46 |
| 15:3F:219:ASP:O | 15:3F:223:THR:OG1 | 2.27 | 0.46 |
| 16:3J:341:GLU:HB2 | 16:3L:60:ASN:HD21 | 1.81 | 0.46 |
| 17:3O:386:ILE:HG12 | 17:3O:434:LEU:HB3 | 1.98 | 0.46 |
| 17:3O:437:ARG:NH2 | 17:3R:123:ASP:HB3 | 2.31 | 0.46 |
| 17:3R:94:TYR:O | 17:3R:95:THR:C | 2.55 | 0.46 |
| 18:3T:259:LYS:HE2 | 18:3T:259:LYS:HB3 | 1.79 | 0.46 |
| 22:4H:26:TRP:CZ2 | 41:ML:77:ARG:HD2 | 2.51 | 0.46 |
| 22:4J:619:VAL:HG11 | 22:4J:680:LYS:HG2 | 1.97 | 0.46 |
| 22:4K:686:LYS:HA | 22:4K:686:LYS:HD2 | 1.38 | 0.46 |
| 22:4K:697:LEU:HD13 | 22:4K:697:LEU:HA | 1.71 | 0.46 |
| 24:4O:244:PRO:HD2 | 40:DE:89:PRO:HG3 | 1.97 | 0.46 |
| 25:4T:306:GLN:N | 25:4T:306:GLN:OE1 | 2.48 | 0.46 |
| 26:4V:22:ARG:NH1 | 40:JG:279:GLU:OE2 | 2.48 | 0.46 |
| 33:5N:464:PRO:HB2 | 33:5O:127:LYS:HE3 | 1.98 | 0.46 |
| 34:5Q:164:LEU:HD21 | 34:5R:490:ILE:CG2 | 2.45 | 0.46 |
| 36:5X:194:GLN:O | 36:5X:197:THR:OG1 | 2.33 | 0.46 |
| 39:6I:116:ARG:HA | 39:6I:116:ARG:HD3 | 1.79 | 0.46 |
| 39:6K:25:PHE:HE1 | 40:OE:80:THR:HB | 1.81 | 0.46 |
| 40:AA:73:THR:HA | 40:AA:76:ASP:HB2 | 1.98 | 0.46 |
| 41:AB:344:TRP:HZ3 | 40:AG:402:ALA:HB2 | 1.80 | 0.46 |
| 40:AH:274:PRO:HG3 | 40:AH:286:LEU:HD12 | 1.98 | 0.46 |
| 41:AO:135:LEU:HB3 | 41:AO:166:THR:HG22 | 1.98 | 0.46 |
| 40:BE:429:LYS:HA | 40:BE:429:LYS:HD3 | 1.43 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BF:51:THR:HB | 40:BF:243:ARG:HD3 | 1.98 | 0.46 |
| 40:BH:11:GLN:N | 42:BH:501:GTP:O1B | 2.47 | 0.46 |
| 40:BI:217:LEU:O | 40:BI:218:ASP:HB2 | 2.14 | 0.46 |
| 40:BI:429:LYS:HA | 40:BI:429:LYS:HD2 | 1.35 | 0.46 |
| 41:BM:204:ASN:HD22 | 41:BM:204:ASN:HA | 1.53 | 0.46 |
| 41:BO:336:LYS:HE2 | 41:BO:336:LYS:HB2 | 1.52 | 0.46 |
| 41:BP:355:ASP:O | 41:BP:356:ILE:C | 2.54 | 0.46 |
| 41:BP:358:PRO:HG3 | 41:BP:364:SER:HB3 | 1.97 | 0.46 |
| 40:CA:315:CYS:HA | 40:CA:378:SER:HA | 1.97 | 0.46 |
| 41:CB:174:LYS:HE3 | 41:CB:205:GLU:HG3 | 1.98 | 0.46 |
| 40:CE:52:PHE:O | 40:CE:64:ARG:HG2 | 2.15 | 0.46 |
| 40:CE:101:ASN:HA | 40:CE:144:GLY:H | 1.80 | 0.46 |
| 40:CG:182:VAL:O | 40:CG:186:ASN:ND2 | 2.49 | 0.46 |
| 40:CG:326:LYS:HA | 40:CG:329:ASN:HB2 | 1.98 | 0.46 |
| 40:CH:339:ARG:HH22 | 40:CH:342:GLN:HE21 | 1.64 | 0.46 |
| 41:CL:121:ARG:O | 41:CL:122:LYS:C | 2.55 | 0.46 |
| 41:CM:389:PHE:O | 41:CM:390:ARG:C | 2.54 | 0.46 |
| 41:CN:178:THR:HG22 | 41:CN:180:VAL:H | 1.80 | 0.46 |
| 41:CO:57:GLY:O | 41:CO:59:TYR:N | 2.49 | 0.46 |
| 40:DA:159:VAL:O | 40:DA:160:ASP:C | 2.53 | 0.46 |
| 41:DB:263:LEU:HD21 | 41:DB:422:VAL:HG23 | 1.98 | 0.46 |
| 40:DF:28:HIS:CE1 | 40:DF:49:PHE:HA | 2.51 | 0.46 |
| 40:DF:326:LYS:HE3 | 41:DN:220:PRO:CB | 2.44 | 0.46 |
| 40:DF:400:LYS:HG3 | 41:DM:344:TRP:HB2 | 1.98 | 0.46 |
| 40:DF:406:TRP:CE2 | 41:DM:255:VAL:HA | 2.50 | 0.46 |
| 40:DI:83:TYR:O | 40:DI:84:ARG:C | 2.53 | 0.46 |
| 41:DM:51:TYR:CE2 | 41:DM:61:PRO:HG3 | 2.50 | 0.46 |
| 41:DM:178:THR:O | 41:DM:181:GLU:HB2 | 2.16 | 0.46 |
| 41:DO:140:GLY:HA3 | 41:DO:181:GLU:HG3 | 1.98 | 0.46 |
| 41:DP:420:ASN:O | 41:DP:421:PRO:C | 2.54 | 0.46 |
| 40:EE:252:LEU:HA | 40:EE:255:PHE:HD2 | 1.80 | 0.46 |
| 40:EI:156:ARG:HE | 40:EI:156:ARG:HB2 | 1.39 | 0.46 |
| 40:EI:167:LEU:HD22 | 40:EI:200:CYS:HB2 | 1.98 | 0.46 |
| 40:EI:247:ALA:O | 40:EI:248:LEU:C | 2.53 | 0.46 |
| 41:EM:56:GLY:O | 41:EM:57:GLY:C | 2.54 | 0.46 |
| 41:EP:60:VAL:HG11 | 41:FP:281:TYR:HB3 | 1.98 | 0.46 |
| 41:EP:418:LEU:O | 41:EP:420:ASN:N | 2.48 | 0.46 |
| 41:FB:134:GLN:HA | 41:FB:165:ASN:O | 2.16 | 0.46 |
| 41:FM:49:VAL:HG11 | 41:FM:241:ARG:HG2 | 1.98 | 0.46 |
| 40:GA:396:LEU:HD23 | 41:GN:346:PRO:CG | 2.43 | 0.46 |
| 40:GE:172:TYR:HD2 | 40:GE:205:ASP:HB2 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GE:382:ALA:O | 40:GE:383:ILE:C | 2.54 | 0.46 |
| 40:GI:304:LYS:HA | 40:GI:304:LYS:HD2 | 1.52 | 0.46 |
| 40:HF:2:ARG:HH21 | 41:HN:70:PRO:C | 2.18 | 0.46 |
| 40:HF:223:THR:OG1 | 40:HF:224:TYR:N | 2.49 | 0.46 |
| 40:HF:406:TRP:CG | 41:HM:255:VAL:HG23 | 2.51 | 0.46 |
| 40:HH:318:LEU:O | 40:HH:374:VAL:HA | 2.16 | 0.46 |
| 41:HN:405:GLU:HA | 41:HN:408:PHE:HD2 | 1.80 | 0.46 |
| 40:IG:306:ASP:OD1 | 40:IG:308:ARG:HG2 | 2.15 | 0.46 |
| 41:IQ:39:ASP:OD1 | 41:IQ:39:ASP:N | 2.48 | 0.46 |
| 41:IQ:316:VAL:HG23 | 41:IQ:366:THR:HB | 1.97 | 0.46 |
| 40:JA:234:ILE:HD11 | 40:JA:272:TYR:HB2 | 1.98 | 0.46 |
| 41:JB:22:GLU:HG2 | 41:JB:81:PHE:HD2 | 1.81 | 0.46 |
| 40:JD:394:PHE:HE2 | 40:JD:421:ARG:HB2 | 1.80 | 0.46 |
| 40:JG:16:ILE:HD13 | 40:JG:228:ASN:HD22 | 1.81 | 0.46 |
| 40:JH:318:LEU:O | 40:JH:374:VAL:HA | 2.16 | 0.46 |
| 41:JM:193:VAL:HA | 41:JM:264:HIS:HE1 | 1.79 | 0.46 |
| 41:JN:139:LEU:HD12 | 41:JN:170:VAL:HG12 | 1.98 | 0.46 |
| 41:KM:142:GLY:O | 41:KM:144:GLY:N | 2.49 | 0.46 |
| 40:LF:167:LEU:HD22 | 40:LF:200:CYS:HB3 | 1.98 | 0.46 |
| 40:MD:169:PHE:HE1 | 40:MD:202:PHE:HD1 | 1.64 | 0.46 |
| 40:MD:393:LYS:HD2 | 40:MD:396:LEU:HD12 | 1.98 | 0.46 |
| 40:MG:273:ALA:CB | 40:MG:274:PRO:CD | 2.92 | 0.46 |
| 40:MG:276:ILE:HG22 | 40:MG:280:LYS:HB3 | 1.98 | 0.46 |
| 40:MH:58:ALA:O | 40:MH:60:LYS:N | 2.49 | 0.46 |
| 40:NA:3:GLU:HG2 | 40:NA:64:ARG:NH2 | 2.31 | 0.46 |
| 40:NA:221:ARG:NH2 | 41:NN:325:GLU:H | 2.13 | 0.46 |
| 41:NB:25:SER:OG | 41:NB:30:ILE:O | 2.33 | 0.46 |
| 40:ND:339:ARG:O | 40:ND:340:SER:C | 2.53 | 0.46 |
| 41:NM:205:GLU:HB3 | 41:NM:302:ALA:HB2 | 1.98 | 0.46 |
| 41:NO:6:HIS:O | 41:NO:63:ALA:HA | 2.16 | 0.46 |
| 41:NP:85:PHE:HB2 | 41:NP:90:PHE:HE1 | 1.81 | 0.46 |
| 40:OA:406:TRP:HE1 | 41:ON:258:VAL:HB | 1.81 | 0.46 |
| 40:OF:55:GLU:O | 40:PF:285:GLN:NE2 | 2.37 | 0.46 |
| 40:OH:86:LEU:O | 40:OH:87:PHE:C | 2.54 | 0.46 |
| 40:OH:136:LEU:HD23 | 40:OH:169:PHE:CE2 | 2.51 | 0.46 |
| 40:OH:328:VAL:HG11 | 40:OH:353:VAL:CG1 | 2.46 | 0.46 |
| 40:PA:76:ASP:OD1 | 40:PA:77:GLU:N | 2.49 | 0.46 |
| 40:PD:5:ILE:HD13 | 40:PD:64:ARG:HD3 | 1.98 | 0.46 |
| 40:PD:230:LEU:O | 40:PD:234:ILE:HD12 | 2.16 | 0.46 |
| 40:PE:328:VAL:O | 40:PE:332:ILE:HG12 | 2.16 | 0.46 |
| 40:PG:271:THR:OG1 | 40:PG:376:MET:HB3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PL:273:LEU:HD23 | 41:PL:273:LEU:HA | 1.85 | 0.46 |
| 41:PO:86:ARG:HB2 | 41:PO:89:ASN:HB2 | 1.97 | 0.46 |
| 41:PP:4:ILE:HD11 | 41:PP:240:LEU:HD13 | 1.98 | 0.46 |
| 40:QE:51:THR:HG21 | 40:QE:243:ARG:HG2 | 1.98 | 0.46 |
| 40:QE:90:GLU:HG3 | 40:RE:280:LYS:HZ1 | 1.80 | 0.46 |
| 40:QE:311:LYS:HE2 | 40:QE:344:VAL:HA | 1.98 | 0.46 |
| 40:QF:274:PRO:HG3 | 40:QF:291:ILE:HG21 | 1.97 | 0.46 |
| 40:QG:52:PHE:HE2 | 40:QG:243:ARG:HD3 | 1.81 | 0.46 |
| 41:QM:136:THR:HA | 41:QM:167:PHE:O | 2.15 | 0.46 |
| 41:QN:91:VAL:HG11 | 41:QN:116:VAL:HG22 | 1.97 | 0.46 |
| 41:QO:138:SER:HA | 41:QO:169:VAL:HB | 1.97 | 0.46 |
| 41:RB:130:LEU:HD21 | 41:RB:133:PHE:HE1 | 1.81 | 0.46 |
| 40:RE:112:LYS:HA | 40:RE:115:ILE:HG22 | 1.97 | 0.46 |
| 41:RL:64:VAL:HG21 | 41:RL:120:VAL:HG22 | 1.97 | 0.46 |
| 41:RN:149:THR:HB | 41:RN:191:GLN:HG2 | 1.97 | 0.46 |
| 40:SA:88:HIS:HB3 | 40:SA:91:GLN:HG2 | 1.97 | 0.46 |
| 41:SM:256:ASN:HD22 | 41:SM:350:LYS:HD2 | 1.80 | 0.46 |
| 41:SO:254:ALA:O | 41:SO:256:ASN:N | 2.49 | 0.46 |
| 41:SO:317:PHE:HB2 | 41:SO:352:ALA:O | 2.16 | 0.46 |
| 41:SP:173:PRO:HB3 | 41:SP:380:ARG:HD3 | 1.97 | 0.46 |
| 40:TF:224:TYR:HA | 40:TF:227:LEU:HB3 | 1.97 | 0.46 |
| 40:TI:75:ILE:HG21 | 40:TI:92:LEU:HB3 | 1.97 | 0.46 |
| 41:TN:55:THR:HG21 | 41:UN:284:LEU:HD12 | 1.96 | 0.46 |
| 41:TO:36:TYR:CZ | 41:TO:38:GLY:HA3 | 2.50 | 0.46 |
| 41:UB:318:ARG:HA | 41:UB:354:CYS:HB3 | 1.98 | 0.46 |
| 40:UF:136:LEU:HD23 | 40:UF:136:LEU:HA | 1.76 | 0.46 |
| 40:UF:195:LEU:O | 40:UF:266:HIS:NE2 | 2.48 | 0.46 |
| 40:UG:175:PRO:HB3 | 40:UG:389:ARG:HD2 | 1.96 | 0.46 |
| 40:UI:106:GLY:CA | 40:UI:148:GLY:HA3 | 2.46 | 0.46 |
| 40:UI:432:GLU:H | 40:UI:432:GLU:HG3 | 1.61 | 0.46 |
| 41:UM:327:ASP:OD1 | 41:UM:328:GLU:N | 2.49 | 0.46 |
| 41:UP:213:ARG:HE | 41:UP:213:ARG:HB2 | 1.62 | 0.46 |
| 41:UP:325:GLU:O | 41:UP:326:VAL:C | 2.53 | 0.46 |
| 42:VB:502:GTP:HN1 | 40:VH:228:ASN:ND2 | 2.09 | 0.46 |
| 40:VG:311:LYS:N | 40:VG:381:THR:OG1 | 2.44 | 0.46 |
| 40:WA:5:ILE:HD12 | 40:WA:125:LEU:HG | 1.98 | 0.46 |
| 40:WF:400:LYS:HZ1 | 41:WM:344:TRP:CB | 2.28 | 0.46 |
| 41:WM:190:HIS:HA | 41:WM:414:ASN:HD22 | 1.81 | 0.46 |
| 41:WM:379:LYS:HE2 | 41:WM:379:LYS:HB2 | 1.45 | 0.46 |
| 41:WN:186:THR:HG21 | 41:WN:385:PHE:CD1 | 2.51 | 0.46 |
| 7:1T:31:LYS:HD2 | 7:1T:71:THR:HA | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:2K:229:LYS:HD3 | 11:2K:229:LYS:HA | 1.65 | 0.46 |
| 13:2T:35:LYS:HZ3 | 13:2T:37:ILE:HG12 | 1.81 | 0.46 |
| 13:2T:63:ALA:O | 13:2T:64:ASP:C | 2.55 | 0.46 |
| 15:3F:178:LYS:HA | 15:3G:327:GLU:OE1 | 2.15 | 0.46 |
| 17:3R:159:GLU:HA | 17:3R:162:HIS:ND1 | 2.30 | 0.46 |
| 18:3U:207:HIS:CE1 | 18:3U:211:CYS:SG | 3.09 | 0.46 |
| 21:4D:316:SER:OG | 21:4D:317:ASP:N | 2.49 | 0.46 |
| 21:4D:465:LYS:HB3 | 21:4D:465:LYS:HE3 | 1.49 | 0.46 |
| 21:4F:513:LEU:H | 21:4F:513:LEU:HD23 | 1.79 | 0.46 |
| 22:4I:125:LEU:HD23 | 41:BO:277:GLY:CA | 2.46 | 0.46 |
| 23:4M:90:MET:H | 23:4M:90:MET:HG2 | 1.54 | 0.46 |
| 23:4N:242:LEU:CD1 | 23:4N:250:VAL:HB | 2.46 | 0.46 |
| 23:4P:198:PHE:HA | 40:DA:221:ARG:HG3 | 1.98 | 0.46 |
| 23:4Q:241:GLY:HA2 | 23:4Q:261:TYR:HB3 | 1.98 | 0.46 |
| 23:4R:117:LEU:HG | 23:4R:117:LEU:H | 1.46 | 0.46 |
| 26:4W:180:ASN:HB3 | 26:4W:183:LEU:HB2 | 1.97 | 0.46 |
| 26:4W:370:TYR:HA | 26:4W:374:ILE:HG13 | 1.98 | 0.46 |
| 39:6H:82:CYS:SG | 39:6H:103:LYS:HG2 | 2.56 | 0.46 |
| 40:AA:167:LEU:HD22 | 40:AA:200:CYS:HB3 | 1.96 | 0.46 |
| 40:AE:280:LYS:NZ | 40:ME:90:GLU:OE2 | 2.34 | 0.46 |
| 40:AF:195:LEU:HD13 | 40:AF:264:ARG:HH21 | 1.81 | 0.46 |
| 41:AN:91:VAL:HG11 | 41:AN:116:VAL:HG22 | 1.98 | 0.46 |
| 41:AN:313:VAL:HB | 41:AN:349:VAL:HG22 | 1.97 | 0.46 |
| 41:AO:102:ALA:HB1 | 41:AO:401:GLU:OE1 | 2.16 | 0.46 |
| 41:BB:35:THR:HA | 41:BB:57:GLY:O | 2.15 | 0.46 |
| 41:BB:215:LEU:O | 41:BB:216:LYS:C | 2.54 | 0.46 |
| 40:BE:171:ILE:HA | 40:BE:204:VAL:O | 2.16 | 0.46 |
| 40:BF:265:ILE:HG22 | 40:BF:379:ASN:HD21 | 1.81 | 0.46 |
| 40:BG:12:ALA:HB3 | 40:BG:140:SER:HB2 | 1.96 | 0.46 |
| 40:BH:273:ALA:HB2 | 40:BH:374:VAL:HG13 | 1.98 | 0.46 |
| 40:BH:298:PRO:HG2 | 40:BH:308:ARG:CZ | 2.46 | 0.46 |
| 40:BI:306:ASP:O | 40:BI:307:PRO:C | 2.54 | 0.46 |
| 41:BM:271:ALA:HB3 | 41:BM:272:PRO:HD3 | 1.97 | 0.46 |
| 41:BP:174:LYS:HD3 | 41:BP:175:VAL:H | 1.81 | 0.46 |
| 41:BP:322:SER:O | 41:BP:323:MET:C | 2.54 | 0.46 |
| 40:CA:107:HIS:HA | 40:CA:152:LEU:HG | 1.98 | 0.46 |
| 40:CA:201:ALA:O | 40:CA:203:MET:N | 2.49 | 0.46 |
| 40:CH:124:LYS:HB3 | 40:CH:124:LYS:HE3 | 1.42 | 0.46 |
| 40:CH:199:ASP:HB2 | 40:CH:200:CYS:H | 1.51 | 0.46 |
| 40:CI:212:ILE:O | 40:CI:216:ASN:HB2 | 2.15 | 0.46 |
| 41:CL:385:PHE:O | 41:CL:386:THR:C | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CO:6:HIS:CE1 | 41:CO:21:TRP:HE1 | 2.34 | 0.46 |
| 40:DA:137:ILE:HD11 | 40:DA:139:HIS:HD2 | 1.81 | 0.46 |
| 40:DA:172:TYR:CD1 | 40:DA:173:PRO:HD2 | 2.51 | 0.46 |
| 41:DB:26:ASP:O | 41:DB:27:GLU:C | 2.53 | 0.46 |
| 41:DB:107:THR:O | 41:DB:108:GLU:C | 2.54 | 0.46 |
| 41:DB:144:GLY:O | 41:DB:148:GLY:HA3 | 2.16 | 0.46 |
| 40:DF:123:ARG:HH12 | 40:DF:161:TYR:HD2 | 1.64 | 0.46 |
| 40:DF:139:HIS:ND1 | 40:DF:140:SER:O | 2.48 | 0.46 |
| 40:DI:283:HIS:CD2 | 40:DI:283:HIS:N | 2.84 | 0.46 |
| 41:DM:22:GLU:CD | 41:DM:81:PHE:HB2 | 2.35 | 0.46 |
| 41:DN:377:LEU:O | 41:DN:378:PHE:C | 2.54 | 0.46 |
| 41:DP:420:ASN:HB2 | 41:DP:421:PRO:CD | 2.44 | 0.46 |
| 40:EF:288:VAL:HA | 40:EF:291:ILE:HG22 | 1.96 | 0.46 |
| 40:EG:150:THR:O | 40:EG:154:MET:HG2 | 2.16 | 0.46 |
| 40:EH:173:PRO:HB3 | 40:EH:183:GLU:OE1 | 2.16 | 0.46 |
| 40:EH:229:ARG:HE | 40:EH:229:ARG:HB2 | 1.46 | 0.46 |
| 41:EM:68:LEU:HB2 | 41:EM:143:THR:HG22 | 1.97 | 0.46 |
| 41:EM:144:GLY:O | 41:EM:148:GLY:HA3 | 2.16 | 0.46 |
| 41:EM:325:GLU:O | 41:EM:328:GLU:HG3 | 2.16 | 0.46 |
| 41:EM:380:ARG:O | 41:EM:383:GLU:HG3 | 2.16 | 0.46 |
| 41:EM:420:ASN:O | 41:EM:423:VAL:N | 2.47 | 0.46 |
| 41:EN:262:ARG:NH2 | 41:EN:417:ASP:OD2 | 2.49 | 0.46 |
| 40:FI:54:SER:OG | 40:FI:55:GLU:N | 2.47 | 0.46 |
| 40:GH:141:PHE:HE1 | 40:GH:191:THR:HB | 1.80 | 0.46 |
| 40:GH:228:ASN:OD1 | 40:GH:228:ASN:N | 2.49 | 0.46 |
| 40:GI:221:ARG:HA | 40:GI:221:ARG:HD3 | 1.57 | 0.46 |
| 41:GM:5:VAL:HB | 41:GM:133:PHE:HD1 | 1.81 | 0.46 |
| 41:GM:156:ARG:NH1 | 41:GM:162:ARG:O | 2.49 | 0.46 |
| 41:GN:193:VAL:HG22 | 41:GN:265:PHE:CE1 | 2.51 | 0.46 |
| 41:GN:358:PRO:HG2 | 41:GN:361:LEU:HB2 | 1.98 | 0.46 |
| 41:GP:27:GLU:OE2 | 41:GP:241:ARG:NH2 | 2.49 | 0.46 |
| 41:GP:114:ASP:OD1 | 41:GP:115:SER:N | 2.49 | 0.46 |
| 41:GP:341:PHE:HB3 | 41:GP:348:ASN:HD21 | 1.81 | 0.46 |
| 41:HB:272:PRO:HG3 | 41:HB:364:SER:HA | 1.98 | 0.46 |
| 40:HE:281:ALA:HA | 40:HE:284:GLU:CG | 2.46 | 0.46 |
| 40:HH:79:ARG:HH22 | 40:HH:94:THR:HG21 | 1.81 | 0.46 |
| 40:IA:22:GLU:HG3 | 40:IA:363:VAL:HG21 | 1.98 | 0.46 |
| 40:II:288:VAL:HA | 40:II:291:ILE:HG12 | 1.96 | 0.46 |
| 41:IM:272:PRO:HG3 | 41:IM:364:SER:HB2 | 1.98 | 0.46 |
| 40:JD:288:VAL:HA | 40:JD:291:ILE:HG22 | 1.98 | 0.46 |
| 40:JE:209:ILE:HA | 40:JE:212:ILE:HG22 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JH:141:PHE:HB2 | 40:JH:173:PRO:HD3 | 1.98 | 0.46 |
| 41:JM:425:ARG:HE | 41:JM:425:ARG:HB3 | 1.53 | 0.46 |
| 41:JN:22:GLU:HG3 | 41:JN:81:PHE:CD2 | 2.50 | 0.46 |
| 41:JN:132:GLY:HA3 | 41:JN:163:ILE:O | 2.16 | 0.46 |
| 40:KG:112:LYS:HA | 40:KG:115:ILE:HG22 | 1.97 | 0.46 |
| 40:KH:112:LYS:HA | 40:KH:115:ILE:HG22 | 1.97 | 0.46 |
| 41:KM:45:GLU:HG2 | 41:KM:46:ARG:HG2 | 1.98 | 0.46 |
| 40:LD:20:CYS:HA | 40:LD:232:SER:HB2 | 1.98 | 0.46 |
| 40:LF:20:CYS:HA | 40:LF:232:SER:HB2 | 1.98 | 0.46 |
| 40:LF:164:LYS:HB2 | 40:LF:164:LYS:HE2 | 1.63 | 0.46 |
| 40:LF:326:LYS:HG3 | 41:LN:208:TYR:CD1 | 2.51 | 0.46 |
| 41:LM:117:LEU:O | 41:LM:121:ARG:HG2 | 2.16 | 0.46 |
| 40:MA:163:LYS:HE2 | 40:MA:163:LYS:HB2 | 1.60 | 0.46 |
| 40:MF:278:ALA:O | 40:MF:279:GLU:C | 2.54 | 0.46 |
| 40:NA:258:ASN:ND2 | 40:NA:352:LYS:HE3 | 2.30 | 0.46 |
| 40:ND:269:LEU:HD21 | 40:ND:380:THR:H | 1.81 | 0.46 |
| 40:NH:53:PHE:O | 40:NH:64:ARG:NH1 | 2.49 | 0.46 |
| 41:NP:156:ARG:NH1 | 41:NP:195:ASN:O | 2.49 | 0.46 |
| 40:OG:191:THR:HG23 | 40:OG:424:MET:HE1 | 1.98 | 0.46 |
| 40:OH:59:GLY:O | 40:OH:61:HIS:N | 2.47 | 0.46 |
| 41:OM:179:VAL:HG23 | 41:OM:180:VAL:HG13 | 1.97 | 0.46 |
| 40:PA:84:ARG:NH2 | 40:PA:85:GLN:OE1 | 2.49 | 0.46 |
| 40:PA:318:LEU:O | 40:PA:374:VAL:HA | 2.16 | 0.46 |
| 40:PD:174:ALA:HB3 | 40:PD:178:SER:H | 1.81 | 0.46 |
| 40:PD:187:SER:O | 40:PD:191:THR:OG1 | 2.28 | 0.46 |
| 40:PD:432:GLU:OE1 | 40:PD:432:GLU:N | 2.49 | 0.46 |
| 40:PE:224:TYR:CE1 | 41:PL:323:MET:HG2 | 2.51 | 0.46 |
| 40:PE:241:SER:OG | 40:PE:250:VAL:N | 2.39 | 0.46 |
| 40:PF:138:PHE:HE2 | 40:PF:235:VAL:HG11 | 1.80 | 0.46 |
| 40:PG:116:ASP:OD1 | 40:PG:117:LEU:N | 2.49 | 0.46 |
| 40:PG:251:ASP:OD1 | 40:PG:252:LEU:N | 2.44 | 0.46 |
| 40:PH:239:THR:HG23 | 40:PH:243:ARG:HH22 | 1.81 | 0.46 |
| 41:PL:142:GLY:O | 41:PL:144:GLY:N | 2.49 | 0.46 |
| 41:PN:27:GLU:OE1 | 41:PN:234:SER:OG | 2.34 | 0.46 |
| 41:PP:170:VAL:HG11 | 41:PP:377:LEU:HD21 | 1.98 | 0.46 |
| 41:QB:25:SER:HA | 41:QB:51:TYR:OH | 2.16 | 0.46 |
| 40:QE:230:LEU:O | 40:QE:234:ILE:HG12 | 2.16 | 0.46 |
| 40:QH:73:THR:HA | 40:QH:76:ASP:HB3 | 1.98 | 0.46 |
| 41:QP:224:ASP:O | 41:QP:225:LEU:C | 2.54 | 0.46 |
| 40:RA:182:VAL:HG22 | 41:RN:256:ASN:HD21 | 1.81 | 0.46 |
| 40:RE:254:GLU:HG2 | 41:RM:98:GLY:HA2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RF:352:LYS:HD2 | 41:RN:178:THR:HA | 1.97 | 0.46 |
| 41:RO:222:TYR:HA | 41:RO:225:LEU:HG | 1.97 | 0.46 |
| 41:RO:328:GLU:HA | 41:RO:331:LEU:HG | 1.97 | 0.46 |
| 40:SF:121:ARG:HE | 40:SF:124:LYS:HB3 | 1.80 | 0.46 |
| 40:SF:237:SER:HB3 | 40:SF:375:CYS:HB2 | 1.98 | 0.46 |
| 40:SG:316:CYS:HA | 40:SG:352:LYS:HB2 | 1.98 | 0.46 |
| 41:SM:215:LEU:HD21 | 41:SM:273:LEU:HD12 | 1.97 | 0.46 |
| 41:TB:237:THR:HG23 | 41:TB:240:LEU:HD21 | 1.98 | 0.46 |
| 40:TE:212:ILE:HD13 | 40:TE:300:ASN:HA | 1.98 | 0.46 |
| 40:TG:235:VAL:O | 40:TG:239:THR:HG22 | 2.15 | 0.46 |
| 41:TN:262:ARG:HB3 | 41:TN:418:LEU:HD11 | 1.98 | 0.46 |
| 41:TP:141:GLY:HA2 | 41:TP:178:THR:HG21 | 1.98 | 0.46 |
| 41:UB:285:THR:N | 41:UB:288:GLU:OE2 | 2.47 | 0.46 |
| 41:UB:318:ARG:HD3 | 41:UB:358:PRO:HD3 | 1.97 | 0.46 |
| 40:UE:260:VAL:HG11 | 40:UE:266:HIS:HA | 1.98 | 0.46 |
| 40:UF:160:ASP:O | 40:UF:161:TYR:C | 2.55 | 0.46 |
| 40:UF:243:ARG:HB3 | 40:UF:244:PHE:H | 1.60 | 0.46 |
| 40:UG:288:VAL:HG11 | 40:UG:327:ASP:HB3 | 1.97 | 0.46 |
| 40:UH:2:ARG:HH22 | 41:UP:71:GLY:HA2 | 1.79 | 0.46 |
| 40:UI:31:GLN:HE22 | 40:UI:37:PRO:HG3 | 1.81 | 0.46 |
| 40:UI:62:VAL:HG11 | 40:VJ:283:HIS:HB3 | 1.98 | 0.46 |
| 41:UO:5:VAL:O | 41:UO:133:PHE:HA | 2.16 | 0.46 |
| 41:UP:101:TRP:O | 41:UP:102:ALA:C | 2.54 | 0.46 |
| 41:UP:263:LEU:HD12 | 41:UP:263:LEU:HA | 1.72 | 0.46 |
| 41:UP:305:PRO:HB3 | 41:UP:310:TYR:CE2 | 2.50 | 0.46 |
| 41:UP:323:MET:O | 41:UP:324:LYS:C | 2.54 | 0.46 |
| 40:VF:181:VAL:HG13 | 40:VF:182:VAL:HG13 | 1.97 | 0.46 |
| 40:VJ:284:GLU:OE2 | 40:VJ:284:GLU:N | 2.49 | 0.46 |
| 40:WA:397:MET:SD | 41:WN:346:PRO:HD2 | 2.56 | 0.46 |
| 40:WA:407:TYR:HB3 | 40:WA:412:MET:HG3 | 1.97 | 0.46 |
| 40:WF:112:LYS:HA | 40:WF:115:ILE:HG22 | 1.98 | 0.46 |
| 40:WI:288:VAL:HG13 | 40:WI:319:TYR:HE2 | 1.80 | 0.46 |
| 7:1U:111:LYS:N | 7:1U:134:ASP:OD1 | 2.49 | 0.45 |
| 7:1U:246:LYS:HB3 | 7:1U:246:LYS:HE3 | 1.54 | 0.45 |
| 8:1X:100:LEU:HB3 | 11:2I:249:ILE:O | 2.16 | 0.45 |
| 8:1Y:101:ILE:HD13 | 11:2J:249:ILE:O | 2.16 | 0.45 |
| 9:2B:321:MET:HA | 9:2B:324:ARG:HD3 | 1.98 | 0.45 |
| 12:2O:180:GLU:HG3 | 12:2O:181:MET:HG3 | 1.98 | 0.45 |
| 13:2U:47:LEU:HD13 | 13:2U:47:LEU:HA | 1.82 | 0.45 |
| 13:2W:82:ASN:HB3 | 13:2W:127:ASP:O | 2.16 | 0.45 |
| 17:3P:104:LEU:HD22 | 17:3P:104:LEU:HA | 1.70 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:3P:238:ASP:HA | 17:3P:241:ILE:HD12 | 1.97 | 0.45 |
| 19:3Y:337:ARG:O | 19:3Y:341:ARG:HG2 | 2.16 | 0.45 |
| 21:4D:331:VAL:HG11 | 21:4D:347:CYS:HB3 | 1.98 | 0.45 |
| 21:4F:122:ILE:HG12 | 21:4F:133:VAL:HG22 | 1.98 | 0.45 |
| 22:4H:163:ARG:HH22 | 41:AL:83:GLN:HB2 | 1.81 | 0.45 |
| 22:4K:502:VAL:HG12 | 22:4K:503:LYS:HZ3 | 1.81 | 0.45 |
| 22:4K:628:LYS:HA | 22:4K:628:LYS:HD2 | 1.44 | 0.45 |
| 28:5B:55:ARG:NH1 | 40:IH:79:ARG:O | 2.44 | 0.45 |
| 36:5Y:48:LEU:O | 41:NB:35:THR:OG1 | 2.34 | 0.45 |
| 37:6A:66:ARG:O | 37:6A:70:LEU:CB | 2.65 | 0.45 |
| 39:6H:78:LEU:HD22 | 39:6H:150:MET:HE3 | 1.98 | 0.45 |
| 40:AA:139:HIS:NE2 | 40:AA:168:GLU:OE1 | 2.46 | 0.45 |
| 40:AE:231:ILE:O | 40:AE:235:VAL:HG23 | 2.16 | 0.45 |
| 41:AM:65:LEU:HD21 | 41:AM:76:VAL:HG11 | 1.98 | 0.45 |
| 41:AO:46:ARG:HG3 | 41:AO:49:VAL:CG2 | 2.46 | 0.45 |
| 40:BE:206:ASN:HD21 | 42:BL:501:GTP:HN22 | 1.64 | 0.45 |
| 40:BI:397:MET:HE2 | 40:BI:397:MET:HB2 | 1.82 | 0.45 |
| 41:BP:101:TRP:HD1 | 41:BP:145:SER:HB2 | 1.81 | 0.45 |
| 41:BP:362:LYS:HA | 41:BP:362:LYS:HD3 | 1.84 | 0.45 |
| 40:CA:76:ASP:HA | 40:CA:79:ARG:HD2 | 1.97 | 0.45 |
| 40:CA:367:LEU:HA | 40:CA:367:LEU:HD13 | 1.82 | 0.45 |
| 40:CE:255:PHE:HZ | 40:CE:318:LEU:HD21 | 1.81 | 0.45 |
| 40:CH:136:LEU:HD22 | 40:CH:167:LEU:HD13 | 1.99 | 0.45 |
| 40:CH:412:MET:HG2 | 40:CH:416:GLU:HG3 | 1.98 | 0.45 |
| 41:CM:139:LEU:HD22 | 41:CM:139:LEU:HA | 1.73 | 0.45 |
| 41:CM:359:ARG:H | 41:CM:359:ARG:HG3 | 1.68 | 0.45 |
| 41:CM:391:ARG:O | 41:CM:393:ALA:N | 2.49 | 0.45 |
| 40:DA:105:ARG:O | 40:DA:110:ILE:N | 2.49 | 0.45 |
| 41:DB:102:ALA:C | 41:DB:104:GLY:H | 2.19 | 0.45 |
| 40:DE:223:THR:H | 40:DE:226:ASN:HD22 | 1.64 | 0.45 |
| 40:DE:336:LYS:HE2 | 40:DE:336:LYS:HB2 | 1.39 | 0.45 |
| 40:DF:1:GLN:NE2 | 41:DN:70:PRO:O | 2.49 | 0.45 |
| 40:DF:315:CYS:HA | 40:DF:378:SER:HA | 1.97 | 0.45 |
| 40:DG:75:ILE:HG22 | 40:DG:79:ARG:HE | 1.81 | 0.45 |
| 40:DG:220:GLU:HB3 | 40:DG:221:ARG:HH21 | 1.82 | 0.45 |
| 40:DH:141:PHE:HB3 | 40:DH:173:PRO:HD3 | 1.98 | 0.45 |
| 40:DH:167:LEU:HD22 | 40:DH:200:CYS:HB2 | 1.99 | 0.45 |
| 40:DH:326:LYS:HE3 | 41:DP:208:TYR:HB2 | 1.98 | 0.45 |
| 40:DI:167:LEU:HD12 | 40:DI:200:CYS:HB3 | 1.98 | 0.45 |
| 40:DI:330:ALA:O | 40:DI:333:ALA:HB3 | 2.17 | 0.45 |
| 41:DL:107:THR:OG1 | 41:DL:108:GLU:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DM:15:GLN:O | 41:DM:18:ALA:N | 2.49 | 0.45 |
| 41:DM:306:ARG:HA | 41:DM:306:ARG:HD3 | 1.66 | 0.45 |
| 41:DN:1:MET:HE3 | 41:DN:1:MET:HB3 | 1.91 | 0.45 |
| 41:DN:68:LEU:O | 41:DN:69:GLU:HB2 | 2.15 | 0.45 |
| 41:DP:107:THR:O | 41:DP:108:GLU:C | 2.55 | 0.45 |
| 41:DP:215:LEU:HD21 | 41:DP:273:LEU:HD12 | 1.98 | 0.45 |
| 41:DP:313:VAL:HA | 41:DP:369:GLY:HA2 | 1.96 | 0.45 |
| 40:EG:248:LEU:HD23 | 40:EG:355:ILE:HD13 | 1.98 | 0.45 |
| 40:EH:75:ILE:CG2 | 40:EH:92:LEU:HB3 | 2.47 | 0.45 |
| 40:EH:100:ALA:O | 40:EH:102:ASN:N | 2.49 | 0.45 |
| 40:EH:100:ALA:HB3 | 40:EH:102:ASN:ND2 | 2.31 | 0.45 |
| 40:EH:193:THR:OG1 | 40:EH:194:THR:N | 2.48 | 0.45 |
| 40:EH:199:ASP:N | 40:EH:199:ASP:OD1 | 2.48 | 0.45 |
| 40:EH:323:VAL:HB | 40:EH:355:ILE:HG23 | 1.99 | 0.45 |
| 40:EI:229:ARG:O | 40:EI:230:LEU:C | 2.55 | 0.45 |
| 41:EM:19:LYS:HD3 | 41:EM:19:LYS:HA | 1.42 | 0.45 |
| 41:EM:249:ASP:O | 41:EM:253:LEU:HB2 | 2.16 | 0.45 |
| 41:EO:8:GLN:HE21 | 41:EO:14:ASN:HA | 1.81 | 0.45 |
| 41:EP:8:GLN:HE21 | 41:EP:14:ASN:HA | 1.81 | 0.45 |
| 41:EP:335:ASN:O | 41:EP:336:LYS:C | 2.53 | 0.45 |
| 40:FA:99:ALA:HA | 40:FA:105:ARG:HG2 | 1.97 | 0.45 |
| 40:FA:222:PRO:HB2 | 40:FA:226:ASN:HB2 | 1.97 | 0.45 |
| 41:FB:165:ASN:ND2 | 41:FB:198:GLU:OE1 | 2.49 | 0.45 |
| 42:FB:502:GTP:HN1 | 40:FG:228:ASN:HD21 | 1.62 | 0.45 |
| 40:FG:113:GLU:HG2 | 40:FG:114:LEU:HG | 1.98 | 0.45 |
| 41:FO:25:SER:OG | 41:FO:30:ILE:O | 2.34 | 0.45 |
| 41:FP:182:PRO:HA | 41:FP:381:ILE:HD11 | 1.97 | 0.45 |
| 40:GA:273:ALA:HB1 | 40:GA:274:PRO:HD2 | 1.99 | 0.45 |
| 40:GG:371:GLN:O | 40:GG:372:ARG:HG3 | 2.17 | 0.45 |
| 40:GH:16:ILE:HD11 | 40:GH:138:PHE:HB3 | 1.98 | 0.45 |
| 41:GO:152:ILE:HD13 | 41:GO:164:MET:CE | 2.46 | 0.45 |
| 40:HH:179:THR:HB | 41:HO:246:LEU:HD21 | 1.97 | 0.45 |
| 41:HN:156:ARG:HH11 | 41:HN:164:MET:HG3 | 1.81 | 0.45 |
| 41:HN:338:SER:O | 41:HN:339:SER:C | 2.54 | 0.45 |
| 41:HN:392:LYS:HB3 | 41:HN:392:LYS:HE2 | 1.72 | 0.45 |
| 41:HQ:13:GLY:HA2 | 41:HQ:16:ILE:HG22 | 1.98 | 0.45 |
| 41:IB:134:GLN:HA | 41:IB:165:ASN:O | 2.16 | 0.45 |
| 41:IN:252:LYS:O | 41:IN:256:ASN:ND2 | 2.49 | 0.45 |
| 41:IP:137:HIS:O | 41:IP:168:SER:HA | 2.16 | 0.45 |
| 40:JD:193:THR:HG23 | 40:JD:194:THR:HG23 | 1.97 | 0.45 |
| 40:JG:64:ARG:HG3 | 40:JG:125:LEU:HD12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JM:143:THR:OG1 | 43:JM:501:GDP:O1B | 2.34 | 0.45 |
| 41:JM:404:ASP:O | 41:JM:405:GLU:C | 2.54 | 0.45 |
| 40:KA:222:PRO:O | 41:KN:322:SER:OG | 2.32 | 0.45 |
| 40:KH:116:ASP:N | 40:KH:116:ASP:OD1 | 2.48 | 0.45 |
| 41:KM:138:SER:HA | 41:KM:169:VAL:HB | 1.97 | 0.45 |
| 40:LA:217:LEU:HD23 | 40:LA:277:SER:HB3 | 1.98 | 0.45 |
| 41:LB:322:SER:CB | 40:LG:221:ARG:HB3 | 2.46 | 0.45 |
| 40:LG:419:GLU:H | 40:LG:419:GLU:HG3 | 1.61 | 0.45 |
| 41:LO:178:THR:HB | 41:LO:181:GLU:HG3 | 1.98 | 0.45 |
| 40:MA:326:LYS:HA | 40:MA:329:ASN:HD22 | 1.81 | 0.45 |
| 41:MB:133:PHE:HB2 | 41:MB:164:MET:SD | 2.57 | 0.45 |
| 40:MD:326:LYS:HG2 | 41:ML:212:PHE:CE2 | 2.52 | 0.45 |
| 41:MN:272:PRO:HG2 | 41:MN:364:SER:HA | 1.98 | 0.45 |
| 41:NB:36:TYR:CD2 | 41:NB:44:LEU:HD23 | 2.51 | 0.45 |
| 41:NB:119:VAL:HA | 41:NB:122:LYS:HG2 | 1.98 | 0.45 |
| 41:NN:174:LYS:HB2 | 41:NN:205:GLU:HG3 | 1.97 | 0.45 |
| 41:OB:252:LYS:HD3 | 40:OG:100:ALA:HA | 1.98 | 0.45 |
| 40:OD:76:ASP:O | 40:OD:79:ARG:HB3 | 2.17 | 0.45 |
| 40:OH:236:SER:O | 40:OH:240:ALA:HB2 | 2.16 | 0.45 |
| 41:OL:236:VAL:HG12 | 41:OL:368:ILE:HD11 | 1.97 | 0.45 |
| 41:OM:133:PHE:HB2 | 41:OM:164:MET:HB3 | 1.98 | 0.45 |
| 41:ON:122:LYS:HD2 | 41:ON:122:LYS:HA | 1.72 | 0.45 |
| 40:PF:247:ALA:HB3 | 40:PF:355:ILE:HB | 1.98 | 0.45 |
| 41:PL:203:ASP:N | 41:PL:203:ASP:OD1 | 2.49 | 0.45 |
| 41:PN:116:VAL:HA | 41:PN:119:VAL:HG12 | 1.98 | 0.45 |
| 41:PO:313:VAL:O | 41:PO:349:VAL:HA | 2.16 | 0.45 |
| 41:PP:107:THR:O | 41:PP:110:ALA:N | 2.49 | 0.45 |
| 41:PP:142:GLY:O | 41:PP:144:GLY:N | 2.49 | 0.45 |
| 41:PP:171:PRO:HG3 | 41:PP:181:GLU:HB3 | 1.97 | 0.45 |
| 40:QA:87:PHE:HB3 | 40:QA:92:LEU:HD11 | 1.97 | 0.45 |
| 41:QO:27:GLU:OE1 | 41:QO:241:ARG:NH2 | 2.49 | 0.45 |
| 41:QO:36:TYR:O | 41:QO:37:HIS:ND1 | 2.49 | 0.45 |
| 40:RA:88:HIS:NE2 | 40:SA:280:LYS:HD3 | 2.31 | 0.45 |
| 40:RG:9:VAL:HG12 | 40:RG:146:GLY:HA2 | 1.97 | 0.45 |
| 40:RG:231:ILE:O | 40:RG:235:VAL:HG23 | 2.16 | 0.45 |
| 41:RL:224:ASP:O | 41:RL:227:HIS:ND1 | 2.41 | 0.45 |
| 41:RO:7:LEU:HD23 | 41:RO:151:LEU:HD21 | 1.97 | 0.45 |
| 41:RP:30:ILE:HD11 | 41:RP:47:ILE:HD11 | 1.98 | 0.45 |
| 41:RP:240:LEU:HB3 | 41:RP:249:ASP:HB3 | 1.98 | 0.45 |
| 40:SA:168:GLU:HB3 | 40:SA:201:ALA:HA | 1.97 | 0.45 |
| 41:SB:382:SER:O | 41:SB:383:GLU:C | 2.54 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SG:320:ARG:HH12 | 40:SG:360:PRO:HB3 | 1.81 | 0.45 |
| 40:SI:433:GLU:HA | 40:SI:436:MET:HG2 | 1.99 | 0.45 |
| 41:SP:323:MET:HB2 | 41:SP:326:VAL:HB | 1.97 | 0.45 |
| 40:UA:69:ASP:N | 40:UA:69:ASP:OD2 | 2.48 | 0.45 |
| 40:UA:288:VAL:HB | 40:UA:327:ASP:HB3 | 1.99 | 0.45 |
| 40:UE:30:ILE:HG22 | 40:UE:36:MET:HB2 | 1.98 | 0.45 |
| 40:UF:100:ALA:HB2 | 41:UM:251:ARG:HD2 | 1.96 | 0.45 |
| 40:UI:224:TYR:CD2 | 41:UP:323:MET:HG3 | 2.49 | 0.45 |
| 41:UP:24:ILE:HD12 | 41:UP:24:ILE:HA | 1.76 | 0.45 |
| 41:UP:86:ARG:HB3 | 41:UP:89:ASN:HB2 | 1.98 | 0.45 |
| 41:VB:120:VAL:HG11 | 41:VB:155:ILE:HD11 | 1.97 | 0.45 |
| 40:VF:89:PRO:HD3 | 40:WE:283:HIS:ND1 | 2.31 | 0.45 |
| 40:VJ:217:LEU:HD21 | 40:VJ:366:ASP:HB3 | 1.98 | 0.45 |
| 41:VN:148:GLY:O | 41:VN:152:ILE:HG12 | 2.16 | 0.45 |
| 40:WA:138:PHE:HZ | 40:WA:235:VAL:HG11 | 1.81 | 0.45 |
| 41:WM:162:ARG:HH11 | 41:WM:162:ARG:HA | 1.81 | 0.45 |
| 41:WM:218:THR:O | 41:WM:220:PRO:HD3 | 2.16 | 0.45 |
| 41:WM:284:LEU:HD12 | 41:WM:284:LEU:HA | 1.81 | 0.45 |
| 41:WN:286:VAL:HB | 41:WN:287:PRO:HD3 | 1.98 | 0.45 |
| 41:WO:290:THR:HB | 41:WO:329:GLN:NE2 | 2.32 | 0.45 |
| 41:WQ:210:ILE:HG12 | 41:WQ:298:ASN:HA | 1.98 | 0.45 |
| 41:WQ:313:VAL:HG12 | 41:WQ:349:VAL:HG23 | 1.97 | 0.45 |
| 8:1X:82:ARG:HH12 | 13:2U:11:LEU:HD12 | 1.81 | 0.45 |
| 8:1X:181:LEU:HD13 | 41:UB:80:PRO:HB3 | 1.98 | 0.45 |
| 10:2G:157:ARG:NH1 | 41:VQ:51:TYR:O | 2.49 | 0.45 |
| 13:2U:79:ILE:HD12 | 13:2U:164:ARG:HB3 | 1.98 | 0.45 |
| 13:2V:22:LEU:HD11 | 13:2V:47:LEU:HG | 1.97 | 0.45 |
| 13:2V:176:GLU:H | 13:2V:176:GLU:HG2 | 1.58 | 0.45 |
| 14:3C:36:GLU:N | 14:3C:36:GLU:OE1 | 2.49 | 0.45 |
| 15:3F:173:LYS:HE2 | 15:3F:173:LYS:HB2 | 1.49 | 0.45 |
| 17:3O:381:SER:O | 17:3O:384:LYS:HG3 | 2.16 | 0.45 |
| 18:3W:186:ILE:HD12 | 18:3W:289:THR:HG23 | 1.98 | 0.45 |
| 22:4J:467:GLU:HG2 | 22:4J:478:GLY:H | 1.81 | 0.45 |
| 24:4O:257:PHE:HB3 | 40:EE:221:ARG:HB3 | 1.99 | 0.45 |
| 23:4Q:216:MET:O | 23:4Q:217:LYS:C | 2.55 | 0.45 |
| 23:4Q:243:LEU:O | 23:4Q:244:PRO:C | 2.55 | 0.45 |
| 28:5B:180:VAL:CG2 | 28:5B:215:LEU:HD22 | 2.46 | 0.45 |
| 29:5D:70:VAL:HG13 | 29:5D:71:HIS:CD2 | 2.51 | 0.45 |
| 31:5I:688:ILE:HA | 31:5I:711:PHE:H | 1.81 | 0.45 |
| 32:5L:66:LEU:HA | 32:5L:69:VAL:HG12 | 1.99 | 0.45 |
| 38:6C:11:GLU:HG3 | 38:6D:281:LYS:HE3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AG:343:PHE:HE2 | 40:AG:350:GLY:HA3 | 1.81 | 0.45 |
| 41:AL:1:MET:HB2 | 41:AL:48:ASN:ND2 | 2.32 | 0.45 |
| 40:BH:3:GLU:HG3 | 40:BH:132:LEU:HD13 | 1.97 | 0.45 |
| 40:BH:367:LEU:HD13 | 40:BH:367:LEU:HA | 1.79 | 0.45 |
| 41:BM:262:ARG:HA | 41:BM:264:HIS:CE1 | 2.51 | 0.45 |
| 41:BM:350:LYS:HD2 | 41:BM:351:THR:H | 1.80 | 0.45 |
| 41:BN:31:ASP:OD1 | 41:BN:35:THR:N | 2.48 | 0.45 |
| 40:CA:401:ARG:HA | 40:CA:401:ARG:HD3 | 1.65 | 0.45 |
| 41:CB:252:LYS:HB2 | 40:CG:100:ALA:HA | 1.97 | 0.45 |
| 41:CB:310:TYR:HA | 41:CB:371:SER:HA | 1.97 | 0.45 |
| 40:CH:63:PRO:HG3 | 40:CH:87:PHE:HA | 1.97 | 0.45 |
| 40:CH:181:VAL:HG12 | 41:CO:347:ASN:O | 2.16 | 0.45 |
| 41:CO:101:TRP:H | 41:CO:184:ASN:ND2 | 2.13 | 0.45 |
| 41:CP:6:HIS:CD2 | 41:CP:21:TRP:HE1 | 2.34 | 0.45 |
| 41:CP:73:MET:HE2 | 41:CP:73:MET:HB2 | 1.71 | 0.45 |
| 41:CP:271:ALA:HB3 | 41:CP:272:PRO:HD3 | 1.98 | 0.45 |
| 40:DA:77:GLU:C | 40:DA:79:ARG:N | 2.70 | 0.45 |
| 40:DF:77:GLU:O | 40:DF:80:THR:N | 2.48 | 0.45 |
| 40:DF:327:ASP:O | 40:DF:328:VAL:C | 2.54 | 0.45 |
| 40:DH:213:CYS:HB3 | 40:DH:222:PRO:HB3 | 1.97 | 0.45 |
| 40:DH:252:LEU:HA | 40:DH:255:PHE:CE2 | 2.50 | 0.45 |
| 40:DH:291:ILE:HB | 40:DH:374:VAL:HG13 | 1.98 | 0.45 |
| 40:DI:287:SER:H | 40:DI:290:GLU:HB2 | 1.81 | 0.45 |
| 41:DL:54:ALA:HB1 | 41:EL:282:ARG:O | 2.17 | 0.45 |
| 41:DM:259:PRO:HG3 | 41:DM:311:LEU:HD11 | 1.98 | 0.45 |
| 41:DM:321:MET:HE3 | 41:DM:321:MET:HB3 | 1.76 | 0.45 |
| 41:DP:239:CYS:C | 41:DP:241:ARG:H | 2.19 | 0.45 |
| 41:DP:330:MET:HE2 | 41:DP:330:MET:HB2 | 1.90 | 0.45 |
| 40:EA:21:TRP:HZ2 | 40:EA:65:ALA:HB2 | 1.80 | 0.45 |
| 40:EA:38:SER:OG | 40:EA:39:ASP:N | 2.48 | 0.45 |
| 41:EB:7:LEU:O | 41:EB:135:LEU:HA | 2.16 | 0.45 |
| 40:EE:271:THR:HB | 40:EE:301:GLN:HA | 1.98 | 0.45 |
| 40:EH:57:GLY:O | 40:EH:58:ALA:HB3 | 2.16 | 0.45 |
| 40:EH:217:LEU:HD21 | 40:EH:367:LEU:HG | 1.97 | 0.45 |
| 40:EH:255:PHE:C | 40:EH:257:THR:H | 2.20 | 0.45 |
| 40:EH:376:MET:SD | 40:EH:378:SER:HB3 | 2.56 | 0.45 |
| 40:EI:288:VAL:HG11 | 40:EI:327:ASP:CB | 2.45 | 0.45 |
| 41:EM:287:PRO:HD3 | 41:EM:325:GLU:HG2 | 1.98 | 0.45 |
| 40:FA:177:VAL:H | 41:FN:331:LEU:HD12 | 1.81 | 0.45 |
| 41:FB:398:TYR:HD1 | 41:FB:408:PHE:HZ | 1.63 | 0.45 |
| 40:FH:11:GLN:HG3 | 40:FH:74:VAL:HG11 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FO:66:VAL:HG21 | 41:FO:151:LEU:HD21 | 1.98 | 0.45 |
| 40:GA:224:TYR:CE2 | 41:GN:323:MET:HG2 | 2.51 | 0.45 |
| 40:GH:194:THR:O | 40:GH:195:LEU:C | 2.55 | 0.45 |
| 40:GI:122:ILE:HD13 | 40:GI:157:LEU:HD11 | 1.98 | 0.45 |
| 40:GI:274:PRO:CB | 40:GI:370:VAL:HG11 | 2.47 | 0.45 |
| 41:GN:58:LYS:HE3 | 41:GN:58:LYS:HB3 | 1.37 | 0.45 |
| 41:GO:189:VAL:O | 41:GO:193:VAL:HG23 | 2.16 | 0.45 |
| 40:HF:134:GLY:HA3 | 40:HF:165:SER:O | 2.15 | 0.45 |
| 40:HH:370:VAL:HG12 | 40:HH:372:ARG:H | 1.81 | 0.45 |
| 40:HI:217:LEU:HB3 | 40:HI:219:ILE:HG22 | 1.98 | 0.45 |
| 41:HP:294:PHE:HE1 | 41:HP:313:VAL:HG11 | 1.80 | 0.45 |
| 41:HQ:372:THR:HG21 | 41:HQ:426:GLY:HA3 | 1.98 | 0.45 |
| 41:IB:235:GLY:HA3 | 41:IB:366:THR:HG21 | 1.98 | 0.45 |
| 40:IG:71:GLU:HB3 | 40:IG:98:ASP:HA | 1.99 | 0.45 |
| 41:IM:221:THR:OG1 | 41:IM:224:ASP:OD1 | 2.23 | 0.45 |
| 40:JA:180:ALA:HB3 | 40:JA:183:GLU:HG3 | 1.98 | 0.45 |
| 41:JB:232:THR:HG22 | 41:JB:270:PHE:HB2 | 1.98 | 0.45 |
| 40:JD:362:VAL:HG21 | 40:JD:369:LYS:HA | 1.98 | 0.45 |
| 40:JF:206:ASN:ND2 | 40:JF:227:LEU:HD21 | 2.31 | 0.45 |
| 40:JG:274:PRO:HG3 | 40:JG:286:LEU:HD12 | 1.98 | 0.45 |
| 40:JH:138:PHE:HZ | 40:JH:235:VAL:HG11 | 1.81 | 0.45 |
| 40:JH:158:SER:OG | 40:JH:166:LYS:NZ | 2.41 | 0.45 |
| 41:JM:21:TRP:CD1 | 41:JM:85:PHE:HE1 | 2.34 | 0.45 |
| 41:JM:188:SER:O | 41:JM:189:VAL:C | 2.54 | 0.45 |
| 41:JN:253:LEU:O | 41:JN:257:MET:HB2 | 2.16 | 0.45 |
| 40:KA:269:LEU:HD13 | 40:KA:303:VAL:HG12 | 1.98 | 0.45 |
| 40:KD:53:PHE:HB3 | 40:KD:61:HIS:HB3 | 1.98 | 0.45 |
| 41:KL:420:ASN:HB2 | 41:KL:421:PRO:HD3 | 1.98 | 0.45 |
| 41:KP:210:ILE:O | 41:KP:214:THR:OG1 | 2.28 | 0.45 |
| 40:LA:209:ILE:HA | 40:LA:212:ILE:HG12 | 1.99 | 0.45 |
| 40:LG:188:ILE:HD12 | 40:LG:424:MET:HG2 | 1.98 | 0.45 |
| 40:MF:157:LEU:HD23 | 40:MF:157:LEU:HA | 1.76 | 0.45 |
| 40:MF:313:MET:HA | 40:MF:344:VAL:HG22 | 1.98 | 0.45 |
| 41:ML:178:THR:HB | 41:ML:181:GLU:HG2 | 1.97 | 0.45 |
| 41:MM:176:SER:OG | 41:MM:178:THR:O | 2.34 | 0.45 |
| 41:MN:293:MET:HG3 | 41:MN:367:PHE:HB2 | 1.98 | 0.45 |
| 41:MN:311:LEU:HD21 | 41:MN:425:ARG:HB3 | 1.99 | 0.45 |
| 40:NA:271:THR:OG1 | 40:NA:376:MET:HB3 | 2.16 | 0.45 |
| 41:NB:170:VAL:HG11 | 41:NB:377:LEU:HD21 | 1.98 | 0.45 |
| 40:ND:253:THR:HG21 | 41:NL:96:GLY:HA3 | 1.96 | 0.45 |
| 40:ND:287:SER:OG | 40:ND:288:VAL:N | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NE:73:THR:HA | 40:NE:76:ASP:HB2 | 1.99 | 0.45 |
| 40:NG:258:ASN:OD1 | 41:NO:99:ASN:ND2 | 2.39 | 0.45 |
| 41:NM:257:MET:O | 41:NM:370:ASN:ND2 | 2.49 | 0.45 |
| 41:NN:226:ASN:N | 43:NN:502:GDP:HN21 | 2.13 | 0.45 |
| 40:OD:213:CYS:O | 40:OD:219:ILE:N | 2.43 | 0.45 |
| 40:OF:107:HIS:CD2 | 40:OF:152:LEU:HB2 | 2.52 | 0.45 |
| 40:OF:262:TYR:HE1 | 41:ON:393:ALA:HA | 1.82 | 0.45 |
| 40:OH:305:CYS:O | 40:OH:306:ASP:C | 2.54 | 0.45 |
| 41:OL:210:ILE:HG12 | 41:OL:298:ASN:HA | 1.98 | 0.45 |
| 41:OM:239:CYS:HB3 | 41:OM:247:ASN:HA | 1.97 | 0.45 |
| 41:OP:64:VAL:HG21 | 41:OP:120:VAL:HG22 | 1.98 | 0.45 |
| 41:OP:211:CYS:HA | 41:OP:215:LEU:HB3 | 1.98 | 0.45 |
| 40:PA:103:TYR:HE1 | 40:PA:148:GLY:HA2 | 1.82 | 0.45 |
| 40:PA:190:THR:O | 40:PA:194:THR:HG23 | 2.16 | 0.45 |
| 41:PB:19:LYS:HG3 | 41:PB:22:GLU:HG3 | 1.96 | 0.45 |
| 40:PD:243:ARG:HG3 | 40:PD:244:PHE:CD2 | 2.52 | 0.45 |
| 40:PF:394:PHE:CD2 | 40:PF:421:ARG:HD3 | 2.51 | 0.45 |
| 40:PG:228:ASN:HA | 40:PG:231:ILE:HD12 | 1.98 | 0.45 |
| 40:PH:242:LEU:H | 40:PH:242:LEU:HD23 | 1.82 | 0.45 |
| 41:PO:19:LYS:O | 41:PO:22:GLU:HB3 | 2.16 | 0.45 |
| 41:PP:234:SER:O | 41:PP:241:ARG:NH2 | 2.49 | 0.45 |
| 41:QB:7:LEU:O | 41:QB:135:LEU:HA | 2.16 | 0.45 |
| 41:QB:154:LYS:HB2 | 41:QB:154:LYS:HE2 | 1.54 | 0.45 |
| 41:QB:251:ARG:O | 41:QB:252:LYS:C | 2.53 | 0.45 |
| 40:QE:31:GLN:NE2 | 40:QE:35:GLN:OE1 | 2.48 | 0.45 |
| 41:QM:293:MET:HE3 | 41:QM:367:PHE:HD1 | 1.82 | 0.45 |
| 41:QN:21:TRP:HZ2 | 41:QN:63:ALA:HB2 | 1.80 | 0.45 |
| 41:QO:139:LEU:HD12 | 41:QO:170:VAL:HG22 | 1.97 | 0.45 |
| 40:RF:185:TYR:HE2 | 40:RF:403:PHE:HB2 | 1.80 | 0.45 |
| 40:RI:229:ARG:NH2 | 40:RI:366:ASP:OD1 | 2.49 | 0.45 |
| 41:RL:310:TYR:HD1 | 41:RL:371:SER:HB2 | 1.79 | 0.45 |
| 41:RM:20:PHE:O | 41:RM:24:ILE:HG12 | 2.16 | 0.45 |
| 41:RP:289:LEU:HD22 | 41:RP:365:ALA:HB2 | 1.97 | 0.45 |
| 40:SA:138:PHE:HE2 | 40:SA:235:VAL:HG21 | 1.82 | 0.45 |
| 41:SB:240:LEU:HD23 | 41:SB:240:LEU:H | 1.81 | 0.45 |
| 40:SE:12:ALA:O | 40:SE:16:ILE:HD12 | 2.16 | 0.45 |
| 41:SP:36:TYR:OH | 41:SP:40:SER:O | 2.33 | 0.45 |
| 40:TA:285:GLN:HB3 | 40:TA:287:SER:HB3 | 1.97 | 0.45 |
| 40:TE:188:ILE:HG13 | 40:TE:420:ALA:HB1 | 1.98 | 0.45 |
| 40:TH:188:ILE:HG22 | 40:TH:420:ALA:HB1 | 1.99 | 0.45 |
| 41:TM:166:THR:HG23 | 41:TM:199:THR:HG23 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TP:60:VAL:HG11 | 41:TP:86:ARG:HH21 | 1.80 | 0.45 |
| 41:TP:226:ASN:ND2 | 43:TP:501:GDP:O6 | 2.49 | 0.45 |
| 40:UA:64:ARG:NH1 | 40:UA:128:GLN:OE1 | 2.46 | 0.45 |
| 40:UA:406:TRP:CE2 | 41:UN:255:VAL:HA | 2.50 | 0.45 |
| 41:UB:331:LEU:HD12 | 40:UG:177:VAL:HA | 1.97 | 0.45 |
| 40:UG:119:LEU:HD22 | 40:UG:156:ARG:HG2 | 1.98 | 0.45 |
| 40:UG:231:ILE:HA | 40:UG:234:ILE:HG22 | 1.98 | 0.45 |
| 40:UI:11:GLN:HA | 40:UI:74:VAL:HG11 | 1.97 | 0.45 |
| 40:UI:72:PRO:HB2 | 40:UI:73:THR:H | 1.55 | 0.45 |
| 41:UN:12:CYS:O | 41:UN:16:ILE:HG12 | 2.17 | 0.45 |
| 41:UO:7:LEU:HD12 | 41:UO:151:LEU:HD21 | 1.98 | 0.45 |
| 41:UP:173:PRO:HB2 | 41:UP:174:LYS:H | 1.64 | 0.45 |
| 41:UP:362:LYS:HE2 | 41:UP:362:LYS:HB2 | 1.43 | 0.45 |
| 41:VB:272:PRO:HG3 | 41:VB:364:SER:HB2 | 1.98 | 0.45 |
| 40:VH:112:LYS:HA | 40:VH:115:ILE:HG22 | 1.98 | 0.45 |
| 40:VH:211:ASP:O | 40:VH:215:ARG:HB2 | 2.16 | 0.45 |
| 41:WB:222:TYR:HD1 | 41:WB:225:LEU:HD12 | 1.80 | 0.45 |
| 41:WB:313:VAL:HB | 41:WB:349:VAL:HG22 | 1.98 | 0.45 |
| 40:WE:255:PHE:CZ | 40:WE:318:LEU:HD21 | 2.52 | 0.45 |
| 40:WG:220:GLU:OE2 | 40:WG:220:GLU:N | 2.49 | 0.45 |
| 40:WH:139:HIS:NE2 | 40:WH:168:GLU:OE2 | 2.49 | 0.45 |
| 40:WI:138:PHE:HZ | 40:WI:235:VAL:HG21 | 1.82 | 0.45 |
| 41:WQ:167:PHE:CE2 | 41:WQ:233:MET:HG2 | 2.51 | 0.45 |
| 7:1S:193:LYS:NZ | 40:VA:58:ALA:HB1 | 2.31 | 0.45 |
| 8:1X:100:LEU:HD22 | 11:2I:250:ILE:HA | 1.98 | 0.45 |
| 11:2I:229:LYS:HB3 | 11:2I:229:LYS:HE3 | 1.75 | 0.45 |
| 11:2J:43:LYS:HG2 | 41:ML:338:SER:HB3 | 1.98 | 0.45 |
| 11:2K:255:LYS:HB3 | 11:2K:255:LYS:HE2 | 1.87 | 0.45 |
| 13:2W:69:LEU:O | 13:2W:71:ILE:HG12 | 2.17 | 0.45 |
| 14:3A:53:VAL:HG22 | 40:MF:440:GLU:HG3 | 1.96 | 0.45 |
| 17:3R:248:ARG:HA | 17:3R:248:ARG:HD2 | 1.83 | 0.45 |
| 18:3T:325:THR:HG23 | 18:3U:71:ARG:NH2 | 2.31 | 0.45 |
| 20:4A:224:GLU:H | 20:4A:224:GLU:HG3 | 1.61 | 0.45 |
| 21:4F:223:TYR:CE2 | 40:BE:46:ASP:HA | 2.52 | 0.45 |
| 22:4J:462:THR:HG21 | 22:4J:483:ARG:HG3 | 1.97 | 0.45 |
| 23:4N:94:TYR:CZ | 23:4N:96:GLY:HA3 | 2.51 | 0.45 |
| 26:4W:5:GLU:OE2 | 26:4W:82:TYR:OH | 2.28 | 0.45 |
| 27:4Y:260:PRO:HA | 27:4Y:263:HIS:ND1 | 2.32 | 0.45 |
| 35:5T:188:ARG:NH2 | 41:KM:74:ASP:OD2 | 2.44 | 0.45 |
| 40:AF:217:LEU:HA | 40:AF:277:SER:HB3 | 1.98 | 0.45 |
| 41:BB:263:LEU:HD22 | 41:BB:422:VAL:HG23 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BE:45:GLY:O | 40:BE:47:ASP:N | 2.49 | 0.45 |
| 40:BE:400:LYS:H | 40:BE:400:LYS:HG2 | 1.59 | 0.45 |
| 40:BF:28:HIS:CE1 | 40:BF:243:ARG:HD2 | 2.52 | 0.45 |
| 40:BH:69:ASP:HB2 | 40:BH:75:ILE:HD12 | 1.98 | 0.45 |
| 41:BL:276:ARG:HE | 41:BL:276:ARG:HB3 | 1.52 | 0.45 |
| 41:BM:372:THR:HA | 41:BM:422:VAL:HG22 | 1.97 | 0.45 |
| 41:BN:100:ASN:HB3 | 41:BN:103:LYS:HB2 | 1.97 | 0.45 |
| 41:BP:201:CYS:O | 41:BP:201:CYS:SG | 2.75 | 0.45 |
| 41:BP:285:THR:O | 41:BP:288:GLU:N | 2.49 | 0.45 |
| 41:BP:402:GLY:O | 41:BP:403:MET:C | 2.53 | 0.45 |
| 41:CB:20:PHE:HA | 41:CB:230:SER:HB3 | 1.98 | 0.45 |
| 40:CE:320:ARG:HH22 | 40:CE:360:PRO:HA | 1.82 | 0.45 |
| 40:CF:264:ARG:NH2 | 40:CF:423:ASP:OD1 | 2.49 | 0.45 |
| 40:CH:237:SER:HB3 | 40:CH:375:CYS:HB3 | 1.98 | 0.45 |
| 40:CI:128:GLN:HE22 | 40:DI:285:GLN:HB3 | 1.81 | 0.45 |
| 41:CP:126:SER:O | 41:CP:128:ASP:N | 2.50 | 0.45 |
| 41:CP:278:SER:HA | 41:CP:281:TYR:HD2 | 1.81 | 0.45 |
| 40:DA:344:VAL:HG22 | 40:DA:345:ASP:H | 1.82 | 0.45 |
| 40:DA:352:LYS:HA | 40:DA:352:LYS:HD2 | 1.55 | 0.45 |
| 41:DB:325:GLU:O | 41:DB:326:VAL:C | 2.54 | 0.45 |
| 40:DE:22:GLU:O | 40:DE:26:LEU:HG | 2.16 | 0.45 |
| 40:DE:256:GLN:HG2 | 40:DE:257:THR:N | 2.31 | 0.45 |
| 40:DF:70:LEU:HD13 | 40:DF:99:ALA:HB2 | 1.98 | 0.45 |
| 40:DF:358:GLN:O | 40:DF:359:PRO:C | 2.55 | 0.45 |
| 40:DH:3:GLU:HB2 | 40:DH:129:CYS:SG | 2.56 | 0.45 |
| 40:DH:24:TYR:HE1 | 40:DH:243:ARG:HH21 | 1.64 | 0.45 |
| 40:DI:273:ALA:O | 40:DI:275:VAL:HG22 | 2.15 | 0.45 |
| 41:DL:321:MET:HE3 | 41:DL:321:MET:HB3 | 1.62 | 0.45 |
| 41:DN:26:ASP:O | 41:DN:27:GLU:C | 2.54 | 0.45 |
| 41:DN:375:GLN:HB2 | 41:DN:422:VAL:HG11 | 1.98 | 0.45 |
| 41:DO:163:ILE:HG21 | 41:DO:250:LEU:HB3 | 1.98 | 0.45 |
| 41:EB:134:GLN:HA | 41:EB:165:ASN:O | 2.16 | 0.45 |
| 40:EE:277:SER:O | 40:EE:279:GLU:N | 2.50 | 0.45 |
| 40:EH:247:ALA:O | 40:EH:249:ASN:N | 2.49 | 0.45 |
| 40:EH:254:GLU:O | 40:EH:257:THR:N | 2.49 | 0.45 |
| 40:EI:104:ALA:O | 40:EI:105:ARG:C | 2.54 | 0.45 |
| 40:EI:133:GLN:NE2 | 40:EI:242:LEU:HD22 | 2.31 | 0.45 |
| 41:EM:132:GLY:HA2 | 41:EM:162:ARG:HB2 | 1.97 | 0.45 |
| 41:EN:286:VAL:HG22 | 41:EN:363:MET:HE3 | 1.97 | 0.45 |
| 41:EO:134:GLN:HG3 | 41:EO:165:ASN:HD22 | 1.81 | 0.45 |
| 40:FA:255:PHE:CZ | 40:FA:318:LEU:HD21 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GA:139:HIS:NE2 | 40:GA:168:GLU:OE2 | 2.50 | 0.45 |
| 40:GA:404:VAL:HG13 | 40:GA:417:PHE:HE2 | 1.82 | 0.45 |
| 40:GE:431:TYR:O | 40:GE:434:VAL:HG22 | 2.16 | 0.45 |
| 40:GF:124:LYS:NZ | 40:HF:284:GLU:OE2 | 2.49 | 0.45 |
| 40:GF:326:LYS:HD2 | 41:GN:208:TYR:CG | 2.52 | 0.45 |
| 40:GH:99:ALA:O | 40:GH:100:ALA:C | 2.54 | 0.45 |
| 41:GP:309:ARG:H | 41:GP:372:THR:HG1 | 1.65 | 0.45 |
| 41:HB:46:ARG:HH21 | 40:HG:73:THR:HA | 1.81 | 0.45 |
| 40:HF:301:GLN:HG2 | 40:HF:303:VAL:HG12 | 1.99 | 0.45 |
| 40:HG:213:CYS:HA | 40:HG:217:LEU:HD23 | 1.97 | 0.45 |
| 40:HH:288:VAL:HB | 40:HH:327:ASP:HB3 | 1.97 | 0.45 |
| 41:HO:2:ARG:HB3 | 41:HO:131:GLN:HE22 | 1.81 | 0.45 |
| 41:IB:91:VAL:HG12 | 41:IB:112:LEU:HD11 | 1.97 | 0.45 |
| 41:IB:100:ASN:HD21 | 41:IB:397:TRP:HB3 | 1.80 | 0.45 |
| 41:IB:255:VAL:HG12 | 40:IG:406:TRP:CD2 | 2.51 | 0.45 |
| 40:IE:79:ARG:NH2 | 40:IE:92:LEU:O | 2.49 | 0.45 |
| 40:IH:247:ALA:O | 41:IP:11:GLN:NE2 | 2.49 | 0.45 |
| 41:IQ:240:LEU:HD23 | 41:IQ:240:LEU:H | 1.81 | 0.45 |
| 40:JD:75:ILE:HD11 | 40:JD:92:LEU:HB3 | 1.99 | 0.45 |
| 40:JG:116:ASP:N | 40:JG:116:ASP:OD1 | 2.48 | 0.45 |
| 41:JM:286:VAL:HB | 41:JM:287:PRO:HD3 | 1.98 | 0.45 |
| 41:KL:35:THR:HB | 41:KL:37:HIS:CE1 | 2.51 | 0.45 |
| 41:KL:269:GLY:HA2 | 41:KL:300:MET:HG3 | 1.99 | 0.45 |
| 41:KM:237:THR:O | 41:KM:241:ARG:NH1 | 2.49 | 0.45 |
| 41:LB:289:LEU:HD11 | 41:LB:363:MET:HG2 | 1.97 | 0.45 |
| 40:LE:258:ASN:ND2 | 41:LM:179:VAL:HG12 | 2.31 | 0.45 |
| 40:LF:209:ILE:HG12 | 40:LF:302:MET:HG3 | 1.97 | 0.45 |
| 40:LG:166:LYS:HE2 | 40:LG:166:LYS:HB2 | 1.57 | 0.45 |
| 40:LG:206:ASN:HD22 | 40:LG:206:ASN:HA | 1.61 | 0.45 |
| 40:LG:246:GLY:HA3 | 40:LG:356:ASN:HA | 1.97 | 0.45 |
| 40:LH:215:ARG:NH2 | 40:LH:299:ALA:O | 2.40 | 0.45 |
| 41:LO:60:VAL:HG11 | 41:LO:86:ARG:HG2 | 1.98 | 0.45 |
| 41:LP:252:LYS:HA | 41:LP:255:VAL:HG12 | 1.98 | 0.45 |
| 40:ME:6:SER:O | 40:ME:65:ALA:HA | 2.17 | 0.45 |
| 40:ME:7:VAL:HG12 | 40:ME:66:VAL:HB | 1.98 | 0.45 |
| 40:MF:175:PRO:HG3 | 40:MF:304:LYS:HG2 | 1.97 | 0.45 |
| 40:MG:175:PRO:HG3 | 40:MG:304:LYS:HB2 | 1.97 | 0.45 |
| 40:MH:75:ILE:HD12 | 40:MH:94:THR:HG23 | 1.97 | 0.45 |
| 40:MH:90:GLU:O | 40:MH:91:GLN:C | 2.55 | 0.45 |
| 40:MH:357:TYR:O | 40:MH:358:GLN:C | 2.55 | 0.45 |
| 41:NB:83:GLN:O | 41:OB:281:TYR:OH | 2.25 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:ND:397:MET:O | 40:ND:398:TYR:C | 2.54 | 0.45 |
| 40:NF:228:ASN:ND2 | 42:NM:501:GTP:HN1 | 2.14 | 0.45 |
| 41:NN:125:GLU:OE2 | 41:ON:291:GLN:NE2 | 2.44 | 0.45 |
| 41:NP:271:ALA:HA | 41:NP:273:LEU:HD23 | 1.98 | 0.45 |
| 41:OB:2:ARG:HH22 | 40:OG:71:GLU:HB2 | 1.81 | 0.45 |
| 40:OE:20:CYS:HA | 40:OE:232:SER:HB2 | 1.98 | 0.45 |
| 40:OG:318:LEU:H | 40:OG:374:VAL:HG23 | 1.81 | 0.45 |
| 41:ON:130:LEU:O | 41:ON:162:ARG:NE | 2.43 | 0.45 |
| 41:ON:377:LEU:HG | 41:ON:380:ARG:NH2 | 2.31 | 0.45 |
| 40:PA:195:LEU:HD11 | 40:PA:427:LEU:HD22 | 1.98 | 0.45 |
| 41:PB:267:MET:HG3 | 41:PB:301:ALA:HB3 | 1.98 | 0.45 |
| 40:PF:122:ILE:HD13 | 40:PF:125:LEU:HD12 | 1.99 | 0.45 |
| 40:PF:180:ALA:HA | 41:PM:256:ASN:HD21 | 1.82 | 0.45 |
| 41:PL:253:LEU:O | 41:PL:257:MET:HB2 | 2.17 | 0.45 |
| 41:PO:3:GLU:OE2 | 41:PO:127:CYS:HB3 | 2.16 | 0.45 |
| 41:PO:257:MET:HB3 | 41:PO:266:PHE:CZ | 2.52 | 0.45 |
| 40:QA:296:PHE:HD2 | 40:QA:341:ILE:HG12 | 1.81 | 0.45 |
| 41:QB:116:VAL:HA | 41:QB:119:VAL:HG22 | 1.98 | 0.45 |
| 41:QB:325:GLU:HG2 | 40:QG:221:ARG:NH1 | 2.29 | 0.45 |
| 40:QF:116:ASP:N | 40:QF:116:ASP:OD1 | 2.47 | 0.45 |
| 41:QN:104:GLY:HA2 | 41:QN:109:GLY:HA3 | 1.98 | 0.45 |
| 41:QP:30:ILE:HG12 | 41:QP:36:TYR:HB3 | 1.98 | 0.45 |
| 41:QP:314:ALA:HB3 | 41:QP:368:ILE:HD12 | 1.98 | 0.45 |
| 41:QP:424:THR:O | 41:QP:428:CYS:HB3 | 2.16 | 0.45 |
| 40:RA:5:ILE:HB | 40:RA:135:PHE:HD1 | 1.81 | 0.45 |
| 40:RF:100:ALA:HB2 | 41:RM:251:ARG:HG3 | 1.97 | 0.45 |
| 41:RL:323:MET:O | 41:RL:326:VAL:HB | 2.17 | 0.45 |
| 41:RO:172:SER:OG | 41:RO:175:VAL:O | 2.34 | 0.45 |
| 41:SB:180:VAL:HB | 41:SB:183:TYR:HB2 | 1.98 | 0.45 |
| 41:SB:325:GLU:HG2 | 40:SG:221:ARG:HH22 | 1.81 | 0.45 |
| 40:SG:258:ASN:HA | 41:SO:179:VAL:HG21 | 1.97 | 0.45 |
| 40:SG:287:SER:OG | 40:SG:290:GLU:OE1 | 2.34 | 0.45 |
| 40:SI:222:PRO:O | 41:SP:322:SER:OG | 2.24 | 0.45 |
| 41:SL:121:ARG:HA | 41:SL:124:ALA:HB3 | 1.97 | 0.45 |
| 41:SM:164:MET:N | 41:SM:164:MET:SD | 2.89 | 0.45 |
| 41:SO:170:VAL:HG21 | 41:SO:377:LEU:HG | 1.98 | 0.45 |
| 41:SO:345:ILE:O | 41:SO:348:ASN:ND2 | 2.49 | 0.45 |
| 41:SP:322:SER:OG | 41:SP:323:MET:N | 2.50 | 0.45 |
| 40:TF:70:LEU:HD12 | 40:TF:145:THR:HG23 | 1.98 | 0.45 |
| 40:TG:121:ARG:O | 40:TG:124:LYS:HG3 | 2.17 | 0.45 |
| 40:UA:60:LYS:HE2 | 40:VA:283:HIS:CD2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UE:270:ALA:HA | 40:UE:376:MET:O | 2.16 | 0.45 |
| 40:UG:102:ASN:ND2 | 40:UG:410:GLU:OE1 | 2.48 | 0.45 |
| 40:UI:211:ASP:O | 40:UI:212:ILE:C | 2.53 | 0.45 |
| 40:UI:306:ASP:HB3 | 40:UI:309:HIS:CG | 2.51 | 0.45 |
| 40:UI:347:CYS:O | 40:UI:348:PRO:C | 2.54 | 0.45 |
| 40:UI:363:VAL:O | 40:UI:364:PRO:C | 2.54 | 0.45 |
| 41:UN:49:VAL:HG11 | 41:UN:241:ARG:HG2 | 1.99 | 0.45 |
| 41:UO:253:LEU:O | 41:UO:257:MET:CB | 2.62 | 0.45 |
| 40:VA:217:LEU:HD12 | 40:VA:366:ASP:HB2 | 1.98 | 0.45 |
| 40:VA:222:PRO:HD2 | 41:VO:324:LYS:HD3 | 1.98 | 0.45 |
| 41:VB:40:SER:HB3 | 41:VB:43:GLN:HB2 | 1.97 | 0.45 |
| 41:VB:310:TYR:HB2 | 41:VB:341:PHE:HD1 | 1.82 | 0.45 |
| 40:VG:205:ASP:OD2 | 40:VG:206:ASN:N | 2.49 | 0.45 |
| 40:VI:419:GLU:HA | 40:VI:422:GLU:HG2 | 1.98 | 0.45 |
| 40:VJ:332:ILE:HD12 | 40:VJ:351:PHE:CD2 | 2.51 | 0.45 |
| 41:VN:6:HIS:O | 41:VN:63:ALA:HA | 2.16 | 0.45 |
| 41:VN:66:VAL:HG12 | 41:VN:91:VAL:HB | 1.98 | 0.45 |
| 40:WE:46:ASP:N | 40:WE:46:ASP:OD1 | 2.47 | 0.45 |
| 40:WG:234:ILE:HD11 | 40:WG:272:TYR:HB2 | 1.99 | 0.45 |
| 40:WG:262:TYR:OH | 41:WO:391:ARG:O | 2.30 | 0.45 |
| 40:WI:185:TYR:HE1 | 40:WI:397:MET:HG2 | 1.82 | 0.45 |
| 41:WM:235:GLY:O | 41:WM:236:VAL:C | 2.54 | 0.45 |
| 41:WN:169:VAL:HA | 41:WN:202:ILE:O | 2.16 | 0.45 |
| 41:WN:303:CYS:O | 41:WN:304:ASP:C | 2.55 | 0.45 |
| 7:1T:174:PHE:CZ | 7:1T:187:LEU:HB2 | 2.51 | 0.45 |
| 7:1T:336:GLU:HG2 | 7:1T:378:HIS:HD2 | 1.82 | 0.45 |
| 11:2I:151:TYR:CE1 | 40:MG:428:GLU:HB3 | 2.51 | 0.45 |
| 11:2I:174:ASN:HA | 11:2I:177:GLN:CD | 2.37 | 0.45 |
| 12:2O:246:TYR:HE1 | 41:AM:261:PRO:HB2 | 1.82 | 0.45 |
| 13:2W:14:LEU:HB3 | 13:2W:165:VAL:HG23 | 1.98 | 0.45 |
| 14:3A:42:ILE:HG12 | 14:3A:49:LEU:HD22 | 1.97 | 0.45 |
| 15:3H:387:GLU:HG2 | 15:3H:388:VAL:HG13 | 1.98 | 0.45 |
| 16:3L:360:GLN:HB3 | 18:3V:237:ASP:HA | 1.99 | 0.45 |
| 17:3P:286:GLY:HA2 | 17:3P:289:ARG:HD2 | 1.98 | 0.45 |
| 17:3R:251:GLN:HE21 | 17:3R:251:GLN:HB3 | 1.53 | 0.45 |
| 18:3T:376:ARG:HG3 | 18:3U:102:LYS:HE3 | 1.99 | 0.45 |
| 18:3W:183:ILE:O | 18:3W:187:GLN:HG2 | 2.16 | 0.45 |
| 21:4D:433:ASP:HA | 21:4D:436:ARG:HG3 | 1.98 | 0.45 |
| 21:4E:260:ARG:NH2 | 21:4E:278:VAL:O | 2.50 | 0.45 |
| 21:4F:477:SER:CB | 21:4F:480:GLU:HB2 | 2.46 | 0.45 |
| 22:4I:543:SER:HA | 22:4I:601:THR:HG21 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4I:591:VAL:O | 22:4I:593:LYS:NZ | 2.50 | 0.45 |
| 22:4I:663:LYS:HD3 | 22:4I:663:LYS:HA | 1.52 | 0.45 |
| 22:4J:358:GLU:HA | 22:4J:361:LYS:HD2 | 1.97 | 0.45 |
| 22:4J:654:PRO:O | 22:4J:655:SER:C | 2.55 | 0.45 |
| 22:4K:579:TYR:OH | 22:4K:607:ARG:NH2 | 2.50 | 0.45 |
| 23:4R:205:LEU:O | 23:4R:206:SER:C | 2.55 | 0.45 |
| 23:4R:259:ARG:HH21 | 40:EI:365:GLY:HA2 | 1.82 | 0.45 |
| 25:4T:429:CYS:O | 25:4T:433:THR:OG1 | 2.34 | 0.45 |
| 27:4Z:86:LEU:HD23 | 27:4Z:244:VAL:HG13 | 1.97 | 0.45 |
| 34:5R:440:ARG:HD3 | 34:5R:440:ARG:HA | 1.35 | 0.45 |
| 39:6K:66:ARG:NH2 | 41:OL:38:GLY:O | 2.50 | 0.45 |
| 39:6K:150:MET:O | 39:6K:154:VAL:HG23 | 2.17 | 0.45 |
| 40:AA:229:ARG:HH11 | 40:AA:363:VAL:HG21 | 1.81 | 0.45 |
| 41:AB:103:LYS:O | 41:AB:107:THR:OG1 | 2.34 | 0.45 |
| 41:AB:281:TYR:CD2 | 41:MB:87:PRO:HD3 | 2.51 | 0.45 |
| 40:AH:318:LEU:O | 40:AH:374:VAL:HA | 2.16 | 0.45 |
| 41:AO:82:GLY:O | 41:AO:84:ILE:N | 2.50 | 0.45 |
| 41:AO:97:ALA:O | 41:AO:100:ASN:N | 2.48 | 0.45 |
| 41:BB:6:HIS:HD2 | 41:BB:134:GLN:HE21 | 1.63 | 0.45 |
| 40:BE:5:ILE:HG21 | 40:BE:122:ILE:HG23 | 1.98 | 0.45 |
| 40:BE:217:LEU:O | 40:BE:219:ILE:HG13 | 2.17 | 0.45 |
| 40:BF:276:ILE:HD12 | 40:BF:281:ALA:HA | 1.99 | 0.45 |
| 40:BH:402:ALA:O | 40:BH:404:VAL:N | 2.50 | 0.45 |
| 40:BI:49:PHE:O | 40:BI:50:ASN:C | 2.55 | 0.45 |
| 41:BL:273:LEU:HD23 | 41:BL:273:LEU:HA | 1.81 | 0.45 |
| 41:BM:318:ARG:H | 41:BM:321:MET:HE3 | 1.82 | 0.45 |
| 41:BO:142:GLY:O | 41:BO:143:THR:C | 2.55 | 0.45 |
| 41:BO:143:THR:HG22 | 41:BO:147:MET:HE2 | 1.98 | 0.45 |
| 40:CA:14:VAL:HG22 | 40:CA:67:PHE:HB3 | 1.97 | 0.45 |
| 41:CB:318:ARG:HA | 41:CB:354:CYS:HB3 | 1.99 | 0.45 |
| 41:CN:101:TRP:O | 41:CN:102:ALA:C | 2.54 | 0.45 |
| 41:CO:1:MET:O | 41:CO:3:GLU:HG2 | 2.16 | 0.45 |
| 41:CO:226:ASN:ND2 | 43:CO:501:GDP:HN1 | 2.15 | 0.45 |
| 41:CP:90:PHE:O | 41:CP:91:VAL:C | 2.53 | 0.45 |
| 40:DA:51:THR:OG1 | 40:DA:52:PHE:N | 2.48 | 0.45 |
| 40:DA:311:LYS:HB2 | 40:DA:311:LYS:HE3 | 1.77 | 0.45 |
| 41:DB:54:ALA:HB1 | 41:EB:282:ARG:O | 2.16 | 0.45 |
| 41:DB:192:LEU:O | 41:DB:193:VAL:C | 2.55 | 0.45 |
| 40:DE:268:PRO:HA | 40:DE:379:ASN:HA | 1.97 | 0.45 |
| 40:DE:319:TYR:O | 40:DE:355:ILE:HA | 2.17 | 0.45 |
| 40:DF:1:GLN:HG2 | 40:DF:2:ARG:N | 2.25 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DF:252:LEU:HA | 40:DF:255:PHE:HE2 | 1.81 | 0.45 |
| 40:DF:349:THR:HG23 | 41:DN:179:VAL:O | 2.17 | 0.45 |
| 41:DL:312:THR:O | 41:DL:370:ASN:N | 2.49 | 0.45 |
| 41:DM:207:LEU:O | 41:DM:210:ILE:N | 2.49 | 0.45 |
| 41:DN:3:GLU:HG2 | 41:DN:49:VAL:HA | 1.98 | 0.45 |
| 41:DN:68:LEU:HD12 | 41:DN:147:MET:HE2 | 1.99 | 0.45 |
| 41:DN:176:SER:OG | 41:DN:177:ASP:N | 2.46 | 0.45 |
| 41:DN:205:GLU:HA | 41:DN:208:TYR:HD2 | 1.80 | 0.45 |
| 41:DP:137:HIS:NE2 | 41:DP:168:SER:HB3 | 2.31 | 0.45 |
| 41:DP:142:GLY:O | 41:DP:144:GLY:N | 2.49 | 0.45 |
| 41:DP:151:LEU:HD13 | 41:DP:151:LEU:HA | 1.80 | 0.45 |
| 41:DP:209:ASP:O | 41:DP:210:ILE:C | 2.53 | 0.45 |
| 41:EB:248:ALA:HA | 41:EB:252:LYS:HG2 | 1.98 | 0.45 |
| 40:EE:262:TYR:CZ | 41:EM:393:ALA:HB2 | 2.52 | 0.45 |
| 40:EH:96:LYS:HB3 | 40:EH:96:LYS:HE3 | 1.33 | 0.45 |
| 40:EH:112:LYS:H | 40:EH:112:LYS:HG3 | 1.42 | 0.45 |
| 40:EH:273:ALA:HB3 | 40:EH:374:VAL:H | 1.80 | 0.45 |
| 40:EI:225:THR:OG1 | 40:EI:226:ASN:N | 2.49 | 0.45 |
| 40:EI:317:LEU:HD12 | 40:EI:374:VAL:HG21 | 1.99 | 0.45 |
| 40:EI:333:ALA:O | 40:EI:336:LYS:N | 2.43 | 0.45 |
| 40:FA:100:ALA:HB2 | 41:FN:251:ARG:HG3 | 1.98 | 0.45 |
| 40:FA:300:ASN:HD22 | 40:FA:300:ASN:HA | 1.56 | 0.45 |
| 40:FI:3:GLU:OE2 | 40:FI:129:CYS:HB3 | 2.16 | 0.45 |
| 41:FN:108:GLU:HA | 41:FN:111:GLU:HB2 | 1.99 | 0.45 |
| 41:FP:58:LYS:HE2 | 41:GP:280:GLN:HE22 | 1.81 | 0.45 |
| 41:FP:222:TYR:HB3 | 43:FP:501:GDP:C6 | 2.52 | 0.45 |
| 40:GA:207:GLU:HA | 40:GA:210:TYR:HB2 | 1.98 | 0.45 |
| 41:GB:138:SER:OG | 43:GB:501:GDP:O1A | 2.34 | 0.45 |
| 40:GH:49:PHE:HE2 | 40:GH:55:GLU:HB2 | 1.80 | 0.45 |
| 40:GH:215:ARG:HD3 | 40:GH:215:ARG:HA | 1.29 | 0.45 |
| 40:GI:115:ILE:HG12 | 40:GI:152:LEU:HG | 1.99 | 0.45 |
| 40:GI:130:THR:OG1 | 40:GI:131:GLY:N | 2.49 | 0.45 |
| 40:GI:235:VAL:O | 40:GI:239:THR:HG22 | 2.17 | 0.45 |
| 40:GI:380:THR:C | 40:GI:382:ALA:H | 2.20 | 0.45 |
| 41:GN:181:GLU:N | 41:GN:182:PRO:HD2 | 2.30 | 0.45 |
| 41:GN:415:MET:HE3 | 41:GN:415:MET:HB3 | 1.80 | 0.45 |
| 40:HA:393:LYS:HD2 | 41:HN:346:PRO:HG3 | 1.99 | 0.45 |
| 41:HB:215:LEU:HB3 | 41:HB:217:LEU:HD23 | 1.97 | 0.45 |
| 40:HI:89:PRO:HD3 | 40:II:283:HIS:ND1 | 2.31 | 0.45 |
| 41:HN:336:LYS:HB3 | 41:HN:336:LYS:HE3 | 1.45 | 0.45 |
| 41:HQ:152:ILE:HD11 | 41:HQ:164:MET:HG2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IE:217:LEU:HD12 | 40:IE:366:ASP:OD2 | 2.17 | 0.45 |
| 41:IO:3:GLU:HA | 41:IO:49:VAL:HA | 1.98 | 0.45 |
| 41:IO:313:VAL:HB | 41:IO:349:VAL:HG22 | 1.97 | 0.45 |
| 40:JE:359:PRO:HA | 40:JE:360:PRO:HD3 | 1.87 | 0.45 |
| 40:JH:3:GLU:HA | 40:JH:51:THR:HA | 1.99 | 0.45 |
| 40:JH:70:LEU:HB2 | 40:JH:145:THR:HG22 | 1.98 | 0.45 |
| 41:JL:67:ASP:HA | 41:JL:143:THR:HG21 | 1.98 | 0.45 |
| 41:JM:288:GLU:HG3 | 41:JM:289:LEU:N | 2.29 | 0.45 |
| 41:JO:205:GLU:OE1 | 41:JO:205:GLU:N | 2.50 | 0.45 |
| 41:KB:313:VAL:O | 41:KB:349:VAL:HA | 2.15 | 0.45 |
| 40:KD:174:ALA:HB3 | 40:KD:178:SER:H | 1.80 | 0.45 |
| 40:KE:206:ASN:OD1 | 42:KE:501:GTP:O2' | 2.33 | 0.45 |
| 40:KG:389:ARG:O | 40:KG:393:LYS:HG2 | 2.17 | 0.45 |
| 41:KL:417:ASP:O | 41:KL:418:LEU:C | 2.55 | 0.45 |
| 41:KL:427:ALA:O | 41:KL:428:CYS:C | 2.54 | 0.45 |
| 41:LL:134:GLN:HE21 | 41:LL:167:PHE:HE2 | 1.62 | 0.45 |
| 41:LL:362:LYS:HD2 | 41:LL:362:LYS:HA | 1.74 | 0.45 |
| 41:LM:7:LEU:HD23 | 41:LM:64:VAL:HB | 1.99 | 0.45 |
| 40:MA:181:VAL:CG1 | 41:MN:348:ASN:HA | 2.46 | 0.45 |
| 41:MB:313:VAL:O | 41:MB:349:VAL:HA | 2.17 | 0.45 |
| 41:MM:304:ASP:OD1 | 41:MM:306:ARG:NH2 | 2.50 | 0.45 |
| 40:OD:30:ILE:HG13 | 40:OD:53:PHE:HE2 | 1.80 | 0.45 |
| 40:OE:68:VAL:HG11 | 40:OE:149:PHE:CZ | 2.52 | 0.45 |
| 40:OH:105:ARG:HE | 40:OH:105:ARG:HB3 | 1.41 | 0.45 |
| 41:OM:131:GLN:HA | 41:OM:162:ARG:HG3 | 1.97 | 0.45 |
| 41:OP:33:THR:HA | 41:OP:83:GLN:HE22 | 1.82 | 0.45 |
| 40:PG:260:VAL:HG13 | 41:PO:397:TRP:HE1 | 1.82 | 0.45 |
| 40:PH:155:GLU:OE1 | 40:PH:197:HIS:NE2 | 2.49 | 0.45 |
| 41:PL:130:LEU:O | 41:PL:162:ARG:NE | 2.49 | 0.45 |
| 41:PM:51:TYR:HE1 | 41:PM:61:PRO:HG3 | 1.80 | 0.45 |
| 41:PM:132:GLY:HA3 | 41:PM:163:ILE:O | 2.16 | 0.45 |
| 40:QA:64:ARG:HA | 40:QA:125:LEU:HD11 | 1.98 | 0.45 |
| 40:QA:100:ALA:HA | 41:QN:252:LYS:HE2 | 1.98 | 0.45 |
| 40:QA:332:ILE:O | 40:QA:336:LYS:HG2 | 2.17 | 0.45 |
| 41:QB:4:ILE:H | 41:QB:62:ARG:NH2 | 2.15 | 0.45 |
| 41:QB:68:LEU:HD12 | 41:QB:143:THR:HG23 | 1.99 | 0.45 |
| 41:QB:271:ALA:O | 41:QB:273:LEU:N | 2.46 | 0.45 |
| 41:QB:318:ARG:HB2 | 41:QB:354:CYS:SG | 2.56 | 0.45 |
| 40:QE:90:GLU:HG3 | 40:RE:280:LYS:NZ | 2.31 | 0.45 |
| 40:QG:139:HIS:CE1 | 40:QG:170:SER:HG | 2.34 | 0.45 |
| 41:QN:31:ASP:OD1 | 41:QN:34:GLY:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QP:183:TYR:HD2 | 41:QP:183:TYR:N | 2.15 | 0.45 |
| 41:QP:368:ILE:H | 41:QP:368:ILE:HG13 | 1.47 | 0.45 |
| 40:RA:291:ILE:HD13 | 40:RA:372:ARG:HG2 | 1.99 | 0.45 |
| 40:RG:56:THR:HA | 40:SG:285:GLN:HB2 | 1.99 | 0.45 |
| 40:RI:88:HIS:HD2 | 40:SI:283:HIS:HB2 | 1.82 | 0.45 |
| 41:RM:313:VAL:O | 41:RM:349:VAL:HA | 2.16 | 0.45 |
| 41:RN:173:PRO:HG3 | 41:RN:380:ARG:HE | 1.81 | 0.45 |
| 41:RO:198:GLU:HG2 | 41:RO:266:PHE:CE2 | 2.50 | 0.45 |
| 41:RO:229:VAL:HG13 | 41:RO:233:MET:HE2 | 1.98 | 0.45 |
| 41:SB:113:VAL:HG22 | 41:SB:117:LEU:HD23 | 1.99 | 0.45 |
| 41:SB:114:ASP:OD1 | 41:SB:115:SER:N | 2.49 | 0.45 |
| 40:SF:3:GLU:O | 40:SF:133:GLN:N | 2.30 | 0.45 |
| 40:SF:325:PRO:HB3 | 40:SF:355:ILE:HG13 | 1.97 | 0.45 |
| 41:SM:207:LEU:HB3 | 41:SM:225:LEU:HD22 | 1.98 | 0.45 |
| 41:SN:207:LEU:HA | 41:SN:210:ILE:HG12 | 1.99 | 0.45 |
| 41:SO:89:ASN:O | 41:SO:91:VAL:N | 2.49 | 0.45 |
| 40:TE:224:TYR:HB3 | 42:TL:501:GTP:N1 | 2.32 | 0.45 |
| 41:TM:25:SER:HG | 41:TM:81:PHE:HE2 | 1.64 | 0.45 |
| 40:UH:134:GLY:HA2 | 40:UH:164:LYS:HG3 | 1.99 | 0.45 |
| 41:UO:140:GLY:HA2 | 41:UO:181:GLU:HG2 | 1.98 | 0.45 |
| 41:UP:68:LEU:HD23 | 41:UP:97:ALA:HB2 | 1.98 | 0.45 |
| 41:UP:190:HIS:HD2 | 41:UP:411:ALA:HA | 1.80 | 0.45 |
| 41:UP:350:LYS:HD2 | 41:UP:350:LYS:HA | 1.71 | 0.45 |
| 40:VI:298:PRO:HG2 | 40:VI:308:ARG:HH21 | 1.82 | 0.45 |
| 40:VI:352:LYS:HD2 | 41:VQ:178:THR:HA | 1.99 | 0.45 |
| 41:VO:317:PHE:HB2 | 41:VO:353:VAL:HG12 | 1.99 | 0.45 |
| 41:VQ:210:ILE:HG12 | 41:VQ:298:ASN:HA | 1.99 | 0.45 |
| 40:WF:291:ILE:HD13 | 40:WF:372:ARG:HB3 | 1.99 | 0.45 |
| 40:WF:346:TRP:HB3 | 41:WN:390:ARG:HH21 | 1.82 | 0.45 |
| 7:1U:440:GLU:HG2 | 7:1U:458:LYS:HG2 | 1.98 | 0.45 |
| 11:2J:75:LYS:HZ1 | 40:LE:418:SER:HB3 | 1.82 | 0.45 |
| 12:2P:212:ASP:OD2 | 12:2P:214:SER:OG | 2.27 | 0.45 |
| 14:3C:14:PHE:HE1 | 41:MO:205:GLU:HG2 | 1.80 | 0.45 |
| 16:3L:103:LEU:HD11 | 16:3L:148:LYS:HG3 | 1.99 | 0.45 |
| 20:4A:11:LYS:H | 20:4A:11:LYS:HG2 | 1.43 | 0.45 |
| 21:4E:517:GLU:H | 21:4E:517:GLU:HG2 | 1.47 | 0.45 |
| 21:4F:122:ILE:HD13 | 21:4F:174:ILE:HD11 | 1.98 | 0.45 |
| 22:4I:121:LYS:NZ | 41:BO:219:THR:OG1 | 2.50 | 0.45 |
| 22:4I:583:ARG:HA | 22:4I:599:LEU:HD11 | 1.98 | 0.45 |
| 22:4I:639:ILE:O | 22:4I:640:ALA:C | 2.54 | 0.45 |
| 23:4N:194:ALA:O | 23:4N:195:ARG:C | 2.54 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:5O:34:LEU:HD21 | 41:KL:174:LYS:HD2 | 1.99 | 0.45 |
| 35:5T:111:LEU:HD13 | 35:5T:114:LEU:HD22 | 1.98 | 0.45 |
| 36:5W:33:PRO:HG2 | 36:5W:57:GLN:HE21 | 1.82 | 0.45 |
| 36:5Y:198:GLN:HA | 36:5Y:201:ILE:HG12 | 1.99 | 0.45 |
| 39:6I:78:LEU:HD23 | 39:6I:81:LEU:HD12 | 1.99 | 0.45 |
| 40:BA:88:HIS:HB3 | 40:BA:91:GLN:HG3 | 1.98 | 0.45 |
| 41:BB:2:ARG:HE | 41:BB:2:ARG:HB2 | 1.56 | 0.45 |
| 41:BB:355:ASP:O | 41:BB:356:ILE:C | 2.54 | 0.45 |
| 40:BE:142:GLY:HA2 | 40:BE:186:ASN:HB2 | 1.99 | 0.45 |
| 41:BL:341:PHE:HB3 | 41:BL:348:ASN:HD21 | 1.81 | 0.45 |
| 41:BM:164:MET:H | 41:BM:164:MET:HG2 | 1.51 | 0.45 |
| 41:BO:87:PRO:CD | 41:CO:281:TYR:CD2 | 2.99 | 0.45 |
| 41:BP:271:ALA:HB3 | 41:BP:272:PRO:HD3 | 1.98 | 0.45 |
| 40:CA:174:ALA:HB3 | 40:CA:177:VAL:CG2 | 2.46 | 0.45 |
| 40:CA:399:ALA:C | 40:CA:401:ARG:H | 2.20 | 0.45 |
| 40:CG:107:HIS:NE2 | 40:CG:155:GLU:OE2 | 2.47 | 0.45 |
| 40:CH:389:ARG:HG2 | 40:CH:390:LEU:N | 2.31 | 0.45 |
| 40:CI:49:PHE:HE2 | 40:CI:55:GLU:HB2 | 1.81 | 0.45 |
| 41:CN:15:GLN:HB3 | 43:CN:501:GDP:O6 | 2.17 | 0.45 |
| 41:CO:375:GLN:NE2 | 41:CO:422:VAL:HB | 2.31 | 0.45 |
| 41:CP:19:LYS:HE2 | 41:CP:19:LYS:HB3 | 1.33 | 0.45 |
| 40:DF:3:GLU:HB2 | 40:DF:129:CYS:SG | 2.55 | 0.45 |
| 40:DG:62:VAL:HA | 40:DG:63:PRO:HD3 | 1.86 | 0.45 |
| 40:DG:141:PHE:HB2 | 40:DG:173:PRO:HD3 | 1.97 | 0.45 |
| 40:DH:132:LEU:O | 40:DH:133:GLN:C | 2.54 | 0.45 |
| 40:DH:209:ILE:O | 40:DH:212:ILE:HG13 | 2.16 | 0.45 |
| 40:DH:276:ILE:H | 40:DH:276:ILE:HG12 | 1.53 | 0.45 |
| 40:DH:335:ILE:HA | 40:DH:338:LYS:HD2 | 1.99 | 0.45 |
| 40:DI:10:GLY:O | 40:DI:13:GLY:N | 2.49 | 0.45 |
| 40:DI:121:ARG:O | 40:DI:122:ILE:C | 2.55 | 0.45 |
| 40:DI:171:ILE:HA | 40:DI:204:VAL:HG12 | 1.98 | 0.45 |
| 41:DM:31:ASP:HB2 | 41:DM:32:PRO:HD2 | 1.99 | 0.45 |
| 41:DN:157:GLU:O | 41:DN:158:GLU:C | 2.54 | 0.45 |
| 41:DO:67:ASP:HA | 41:DO:143:THR:HG21 | 1.99 | 0.45 |
| 41:DO:139:LEU:HD22 | 41:DO:188:SER:HB2 | 1.99 | 0.45 |
| 41:DP:141:GLY:O | 41:DP:184:ASN:ND2 | 2.50 | 0.45 |
| 40:EG:274:PRO:HG3 | 40:EG:286:LEU:HD11 | 1.98 | 0.45 |
| 40:EH:164:LYS:O | 40:EH:166:LYS:N | 2.49 | 0.45 |
| 40:EI:121:ARG:HA | 40:EI:124:LYS:HE2 | 1.98 | 0.45 |
| 40:EI:220:GLU:CD | 40:EI:221:ARG:HG3 | 2.37 | 0.45 |
| 41:EM:5:VAL:HG23 | 41:EM:130:LEU:HD11 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EP:19:LYS:HD3 | 41:EP:19:LYS:HA | 1.51 | 0.45 |
| 41:EP:336:LYS:HE3 | 41:EP:336:LYS:HB3 | 1.65 | 0.45 |
| 41:EP:375:GLN:O | 41:EP:376:GLU:C | 2.55 | 0.45 |
| 40:FA:21:TRP:O | 40:FA:22:GLU:C | 2.55 | 0.45 |
| 40:FH:319:TYR:HE2 | 40:FH:328:VAL:HG23 | 1.82 | 0.45 |
| 40:GA:31:GLN:HB3 | 40:GA:32:PRO:HD2 | 1.98 | 0.45 |
| 41:GB:142:GLY:O | 41:GB:144:GLY:N | 2.50 | 0.45 |
| 40:GG:325:PRO:O | 40:GG:328:VAL:HB | 2.17 | 0.45 |
| 40:GH:340:SER:O | 40:GH:342:GLN:N | 2.49 | 0.45 |
| 40:GI:412:MET:SD | 40:GI:416:GLU:HB3 | 2.57 | 0.45 |
| 41:GN:346:PRO:O | 41:GN:347:ASN:C | 2.54 | 0.45 |
| 41:GP:36:TYR:O | 41:GP:37:HIS:ND1 | 2.49 | 0.45 |
| 41:HB:222:TYR:O | 41:HB:226:ASN:ND2 | 2.49 | 0.45 |
| 41:HN:100:ASN:HD21 | 41:HN:397:TRP:HB3 | 1.81 | 0.45 |
| 41:HQ:107:THR:O | 41:HQ:110:ALA:N | 2.42 | 0.45 |
| 40:IF:133:GLN:NE2 | 40:IF:251:ASP:OD2 | 2.49 | 0.45 |
| 40:JE:385:GLU:OE1 | 40:JE:389:ARG:NH2 | 2.49 | 0.45 |
| 41:JM:388:MET:HG2 | 41:JM:393:ALA:HB3 | 1.99 | 0.45 |
| 40:KF:11:GLN:HG3 | 40:KF:74:VAL:HG21 | 1.98 | 0.45 |
| 40:KG:188:ILE:HG23 | 40:KG:424:MET:HG3 | 1.99 | 0.45 |
| 40:KH:109:THR:OG1 | 40:KH:410:GLU:O | 2.34 | 0.45 |
| 40:KH:175:PRO:HB3 | 40:KH:389:ARG:NE | 2.31 | 0.45 |
| 41:KO:253:LEU:O | 41:KO:257:MET:HB2 | 2.17 | 0.45 |
| 41:KP:8:GLN:OE1 | 41:KP:17:GLY:HA3 | 2.17 | 0.45 |
| 40:LF:182:VAL:HG23 | 40:LF:186:ASN:HD21 | 1.82 | 0.45 |
| 40:LF:332:ILE:HG21 | 41:LN:175:VAL:HG13 | 1.98 | 0.45 |
| 40:LF:333:ALA:O | 40:LF:337:THR:HG23 | 2.16 | 0.45 |
| 40:MA:277:SER:O | 40:MA:279:GLU:N | 2.50 | 0.45 |
| 41:MB:61:PRO:HD3 | 41:MB:84:ILE:HG12 | 1.99 | 0.45 |
| 40:ME:38:SER:OG | 40:ME:39:ASP:N | 2.49 | 0.45 |
| 40:MG:188:ILE:HG12 | 40:MG:390:LEU:HD23 | 1.98 | 0.45 |
| 40:MH:71:GLU:H | 40:MH:71:GLU:HG3 | 1.65 | 0.45 |
| 41:MO:233:MET:HE2 | 41:MO:233:MET:HB2 | 1.82 | 0.45 |
| 41:MO:420:ASN:O | 41:MO:421:PRO:C | 2.55 | 0.45 |
| 41:NB:329:GLN:HA | 41:NB:332:ASN:HD22 | 1.80 | 0.45 |
| 40:ND:185:TYR:O | 40:ND:186:ASN:C | 2.54 | 0.45 |
| 40:NE:214:ARG:HB2 | 41:NL:324:LYS:HE3 | 1.99 | 0.45 |
| 40:NG:328:VAL:HG21 | 40:NG:355:ILE:HD11 | 1.98 | 0.45 |
| 41:NL:20:PHE:O | 41:NL:23:VAL:N | 2.50 | 0.45 |
| 40:OA:3:GLU:OE2 | 40:OA:131:GLY:N | 2.49 | 0.45 |
| 40:OA:70:LEU:HB2 | 40:OA:145:THR:HG22 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OF:116:ASP:OD1 | 40:OF:117:LEU:N | 2.50 | 0.45 |
| 40:OH:209:ILE:HD11 | 40:OH:230:LEU:HB3 | 1.97 | 0.45 |
| 41:PB:263:LEU:HD13 | 41:PB:422:VAL:HG23 | 1.99 | 0.45 |
| 40:PD:133:GLN:HE21 | 40:PD:252:LEU:H | 1.65 | 0.45 |
| 40:PF:9:VAL:HG12 | 40:PF:146:GLY:HA2 | 1.98 | 0.45 |
| 40:PF:75:ILE:O | 40:PF:79:ARG:HG3 | 2.15 | 0.45 |
| 40:PH:320:ARG:HH21 | 40:PH:360:PRO:HB3 | 1.82 | 0.45 |
| 41:PO:232:THR:HG22 | 41:PO:270:PHE:HB2 | 1.99 | 0.45 |
| 41:QB:222:TYR:O | 41:QB:225:LEU:N | 2.50 | 0.45 |
| 41:QB:358:PRO:O | 41:QB:359:ARG:C | 2.54 | 0.45 |
| 40:QG:349:THR:HB | 41:QO:176:SER:HB3 | 1.99 | 0.45 |
| 41:QL:207:LEU:HD21 | 41:QL:229:VAL:HG13 | 1.98 | 0.45 |
| 40:RA:231:ILE:HD13 | 40:RA:231:ILE:HA | 1.80 | 0.45 |
| 41:RB:316:VAL:HA | 41:RB:352:ALA:HB3 | 1.99 | 0.45 |
| 40:RF:102:ASN:OD1 | 40:RF:105:ARG:HB2 | 2.17 | 0.45 |
| 41:RM:311:LEU:HB2 | 41:RM:370:ASN:HB3 | 1.98 | 0.45 |
| 41:RO:54:ALA:HB1 | 41:SO:282:ARG:O | 2.16 | 0.45 |
| 40:SF:25:CYS:O | 40:SF:30:ILE:N | 2.47 | 0.45 |
| 41:SO:150:LEU:HD12 | 41:SO:150:LEU:HA | 1.81 | 0.45 |
| 41:SO:182:PRO:O | 41:SO:183:TYR:C | 2.54 | 0.45 |
| 41:SP:192:LEU:O | 41:SP:264:HIS:NE2 | 2.43 | 0.45 |
| 40:TE:193:THR:O | 40:TE:197:HIS:ND1 | 2.39 | 0.45 |
| 40:TG:140:SER:OG | 42:TG:501:GTP:O1A | 2.25 | 0.45 |
| 40:TG:155:GLU:HA | 40:TG:197:HIS:CD2 | 2.51 | 0.45 |
| 40:TH:175:PRO:HG3 | 40:TH:304:LYS:HB3 | 1.98 | 0.45 |
| 40:TH:276:ILE:HG12 | 40:TH:280:LYS:HB3 | 1.98 | 0.45 |
| 40:UE:20:CYS:O | 40:UE:23:LEU:N | 2.50 | 0.45 |
| 40:UE:101:ASN:HA | 40:UE:144:GLY:H | 1.80 | 0.45 |
| 40:UE:138:PHE:HZ | 40:UE:235:VAL:HG21 | 1.81 | 0.45 |
| 40:UE:292:THR:HG1 | 40:UE:319:TYR:HH | 1.61 | 0.45 |
| 40:UF:195:LEU:HD11 | 40:UF:264:ARG:HD3 | 1.99 | 0.45 |
| 40:UH:187:SER:HA | 40:UH:190:THR:HG22 | 1.99 | 0.45 |
| 40:UH:270:ALA:HB3 | 40:UH:302:MET:HG3 | 1.98 | 0.45 |
| 40:UI:190:THR:O | 40:UI:191:THR:C | 2.54 | 0.45 |
| 41:VB:252:LYS:HA | 41:VB:255:VAL:HG12 | 1.99 | 0.45 |
| 40:VF:260:VAL:HG12 | 40:VF:266:HIS:HA | 1.98 | 0.45 |
| 40:VI:405:HIS:HA | 40:VI:408:VAL:HG12 | 1.98 | 0.45 |
| 41:VN:58:LYS:HA | 41:VN:58:LYS:HD3 | 1.77 | 0.45 |
| 41:VN:207:LEU:HB3 | 41:VN:225:LEU:HG | 1.99 | 0.45 |
| 41:VP:252:LYS:HA | 41:VP:255:VAL:HG12 | 1.99 | 0.45 |
| 41:VP:284:LEU:HA | 41:VP:288:GLU:OE1 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WB:19:LYS:O | 41:WB:22:GLU:HB3 | 2.17 | 0.45 |
| 40:WE:271:THR:HG22 | 40:WE:301:GLN:HA | 1.99 | 0.45 |
| 40:WE:318:LEU:O | 40:WE:374:VAL:HA | 2.16 | 0.45 |
| 40:WG:168:GLU:HB2 | 40:WG:201:ALA:HA | 1.99 | 0.45 |
| 40:WG:274:PRO:HB3 | 40:WG:370:VAL:HG11 | 1.99 | 0.45 |
| 41:WM:191:GLN:O | 41:WM:192:LEU:C | 2.55 | 0.45 |
| 41:WM:202:ILE:HG21 | 41:WM:229:VAL:HG22 | 1.99 | 0.45 |
| 41:WO:3:GLU:HG3 | 41:WO:127:CYS:HB3 | 1.97 | 0.45 |
| 41:WO:173:PRO:HB3 | 41:WO:380:ARG:HD2 | 1.97 | 0.45 |
| 7:1T:43:LEU:HD21 | 7:1T:610:ALA:CB | 2.44 | 0.45 |
| 7:1T:56:GLU:C | 7:1T:57:GLN:HG3 | 2.37 | 0.45 |
| 7:1T:99:LYS:HB3 | 7:1T:99:LYS:HE3 | 1.64 | 0.45 |
| 7:1T:242:THR:OG1 | 7:1T:243:GLY:N | 2.47 | 0.45 |
| 7:1T:347:LEU:HD11 | 11:2J:10:ILE:HD11 | 1.98 | 0.45 |
| 7:1T:560:PHE:HE1 | 7:1T:574:TYR:HA | 1.82 | 0.45 |
| 7:1T:570:LYS:HE2 | 7:1T:570:LYS:HB2 | 1.60 | 0.45 |
| 8:1X:93:LYS:H | 8:1X:93:LYS:HG3 | 1.48 | 0.45 |
| 9:2B:410:GLN:CD | 41:TL:276:ARG:HH21 | 2.20 | 0.45 |
| 12:2P:161:ASN:HB3 | 12:2P:164:VAL:HG12 | 1.99 | 0.45 |
| 12:2R:216:GLN:NE2 | 41:WQ:118:ASP:HB3 | 2.31 | 0.45 |
| 13:2T:47:LEU:HA | 13:2T:47:LEU:HD13 | 1.82 | 0.45 |
| 13:2T:180:GLU:H | 13:2T:180:GLU:HG3 | 1.41 | 0.45 |
| 13:2V:124:ARG:HA | 13:2V:124:ARG:HD2 | 1.72 | 0.45 |
| 17:3P:455:LEU:HA | 17:3P:455:LEU:HD13 | 1.77 | 0.45 |
| 17:3R:127:LEU:O | 17:3R:128:ILE:C | 2.54 | 0.45 |
| 21:4D:474:LYS:HB3 | 21:4D:475:PRO:CD | 2.47 | 0.45 |
| 21:4F:251:ASP:HB3 | 21:4F:257:GLY:HA3 | 1.98 | 0.45 |
| 22:4J:653:LEU:HD23 | 22:4J:653:LEU:HA | 1.84 | 0.45 |
| 22:4K:645:GLN:O | 22:4K:646:ASP:C | 2.55 | 0.45 |
| 22:4K:650:LYS:HE2 | 22:4K:650:LYS:HB3 | 1.52 | 0.45 |
| 23:4M:99:PRO:HB2 | 23:4M:100:GLN:NE2 | 2.31 | 0.45 |
| 23:4M:104:ILE:HG21 | 23:4M:112:VAL:HA | 1.98 | 0.45 |
| 24:4O:201:SER:C | 24:4O:205:LEU:HG | 2.37 | 0.45 |
| 24:4O:217:LYS:HD2 | 24:4O:217:LYS:HA | 1.41 | 0.45 |
| 23:4P:235:THR:HG1 | 23:4P:240:LEU:HA | 1.81 | 0.45 |
| 23:4Q:202:PHE:HB3 | 23:4Q:203:PRO:HD3 | 1.97 | 0.45 |
| 26:4W:361:PRO:O | 26:4W:362:GLU:C | 2.54 | 0.45 |
| 34:5Q:105:LEU:O | 34:5Q:108:GLU:N | 2.50 | 0.45 |
| 36:5W:258:ARG:HG2 | 40:LG:439:VAL:HG11 | 1.99 | 0.45 |
| 36:5X:196:ALA:HA | 36:5X:199:LYS:HE2 | 1.99 | 0.45 |
| 36:5Y:199:LYS:HA | 36:5Y:202:LYS:HE3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AE:73:THR:HA | 40:AE:76:ASP:HB2 | 1.98 | 0.45 |
| 41:AM:313:VAL:HB | 41:AM:349:VAL:HG22 | 1.99 | 0.45 |
| 41:AM:324:LYS:NZ | 41:AM:328:GLU:OE2 | 2.50 | 0.45 |
| 41:BB:151:LEU:HD12 | 41:BB:151:LEU:HA | 1.77 | 0.45 |
| 41:BB:394:PHE:HA | 41:BB:397:TRP:HZ3 | 1.82 | 0.45 |
| 40:BE:57:GLY:C | 40:BE:59:GLY:H | 2.19 | 0.45 |
| 40:BG:228:ASN:ND2 | 42:BG:501:GTP:HN1 | 2.08 | 0.45 |
| 40:BG:292:THR:OG1 | 40:BG:319:TYR:OH | 2.26 | 0.45 |
| 40:BH:20:CYS:HB3 | 40:BH:24:TYR:CE2 | 2.51 | 0.45 |
| 40:BH:288:VAL:HA | 40:BH:291:ILE:HG12 | 1.97 | 0.45 |
| 40:BI:67:PHE:HB3 | 40:BI:75:ILE:HD12 | 1.97 | 0.45 |
| 41:BM:1:MET:O | 41:BM:129:CYS:SG | 2.69 | 0.45 |
| 40:CI:228:ASN:HD21 | 42:CI:501:GTP:HN1 | 1.64 | 0.45 |
| 41:CL:98:GLY:O | 41:CL:99:ASN:C | 2.54 | 0.45 |
| 41:CL:129:CYS:O | 41:CL:131:GLN:N | 2.50 | 0.45 |
| 41:CN:154:LYS:O | 41:CN:157:GLU:HB2 | 2.17 | 0.45 |
| 41:CO:75:SER:O | 41:CO:76:VAL:C | 2.55 | 0.45 |
| 41:CO:330:MET:HB3 | 41:CO:349:VAL:HG11 | 1.98 | 0.45 |
| 41:CP:143:THR:O | 41:CP:144:GLY:C | 2.55 | 0.45 |
| 41:CP:202:ILE:HG22 | 41:CP:207:LEU:HD11 | 1.99 | 0.45 |
| 41:CP:271:ALA:O | 41:CP:273:LEU:N | 2.50 | 0.45 |
| 41:CP:304:ASP:C | 41:CP:306:ARG:H | 2.20 | 0.45 |
| 40:DA:31:GLN:HB2 | 40:DA:35:GLN:O | 2.16 | 0.45 |
| 41:DB:24:ILE:HA | 41:DB:27:GLU:HG3 | 1.98 | 0.45 |
| 41:DB:207:LEU:HB2 | 41:DB:225:LEU:HD23 | 1.98 | 0.45 |
| 40:DE:1:GLN:O | 40:DE:3:GLU:N | 2.50 | 0.45 |
| 40:DE:177:VAL:CG1 | 40:DE:207:GLU:HB2 | 2.46 | 0.45 |
| 40:DE:232:SER:O | 40:DE:235:VAL:N | 2.50 | 0.45 |
| 40:DE:436:MET:O | 41:DM:391:ARG:NH2 | 2.49 | 0.45 |
| 40:DF:121:ARG:HD2 | 40:DF:121:ARG:HA | 1.69 | 0.45 |
| 40:DF:404:VAL:HG22 | 40:DF:417:PHE:CE2 | 2.52 | 0.45 |
| 40:DH:174:ALA:HB1 | 40:DH:207:GLU:HB2 | 1.99 | 0.45 |
| 40:DH:211:ASP:O | 40:DH:215:ARG:HB3 | 2.16 | 0.45 |
| 40:DH:346:TRP:CZ2 | 40:DH:434:VAL:HG13 | 2.49 | 0.45 |
| 40:DI:169:PHE:HA | 40:DI:202:PHE:O | 2.16 | 0.45 |
| 40:DI:326:LYS:HB3 | 40:DI:326:LYS:HE3 | 1.50 | 0.45 |
| 41:DM:109:GLY:HA2 | 41:DM:147:MET:CE | 2.46 | 0.45 |
| 41:DN:190:HIS:CD2 | 41:DN:411:ALA:HA | 2.51 | 0.45 |
| 41:DO:232:THR:HG22 | 41:DO:270:PHE:HB2 | 1.97 | 0.45 |
| 41:DP:418:LEU:O | 41:DP:419:GLY:C | 2.55 | 0.45 |
| 40:EA:319:TYR:HB3 | 40:EA:323:VAL:HG11 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EE:276:ILE:HG23 | 40:EE:280:LYS:HG3 | 1.98 | 0.45 |
| 41:EM:3:GLU:HB3 | 41:EM:62:ARG:HH12 | 1.81 | 0.45 |
| 41:EM:137:HIS:O | 41:EM:168:SER:HA | 2.17 | 0.45 |
| 41:EM:188:SER:O | 41:EM:189:VAL:C | 2.54 | 0.45 |
| 41:EN:313:VAL:HG12 | 41:EN:349:VAL:HG13 | 1.99 | 0.45 |
| 40:FE:2:ARG:HD2 | 40:FE:242:LEU:HB2 | 1.99 | 0.45 |
| 40:FE:235:VAL:O | 40:FE:239:THR:HG22 | 2.17 | 0.45 |
| 40:FE:253:THR:HA | 40:FE:256:GLN:HG2 | 1.98 | 0.45 |
| 40:FF:138:PHE:HZ | 40:FF:235:VAL:HG21 | 1.82 | 0.45 |
| 41:FM:137:HIS:O | 41:FM:168:SER:HA | 2.17 | 0.45 |
| 41:FM:139:LEU:HG | 41:FM:168:SER:HB2 | 1.97 | 0.45 |
| 41:FP:46:ARG:HA | 41:FP:46:ARG:HD3 | 1.70 | 0.45 |
| 40:GA:30:ILE:HG13 | 40:GA:61:HIS:HD2 | 1.81 | 0.45 |
| 40:GE:16:ILE:HG22 | 40:GE:228:ASN:HB3 | 1.99 | 0.45 |
| 40:GF:326:LYS:HB3 | 41:GN:208:TYR:CE1 | 2.51 | 0.45 |
| 40:GI:222:PRO:CD | 41:GP:324:LYS:NZ | 2.80 | 0.45 |
| 41:GN:13:GLY:HA2 | 41:GN:136:THR:HB | 1.97 | 0.45 |
| 41:GN:48:ASN:OD1 | 41:GN:48:ASN:N | 2.46 | 0.45 |
| 41:GN:138:SER:O | 41:GN:139:LEU:C | 2.54 | 0.45 |
| 41:HB:2:ARG:HB3 | 41:HB:131:GLN:HG3 | 1.97 | 0.45 |
| 41:HB:245:GLN:HG3 | 41:HB:353:VAL:HG23 | 1.98 | 0.45 |
| 41:HB:350:LYS:HD2 | 40:HG:180:ALA:HA | 1.97 | 0.45 |
| 40:HE:223:THR:O | 40:HE:226:ASN:ND2 | 2.50 | 0.45 |
| 40:HF:260:VAL:HB | 41:HN:397:TRP:CH2 | 2.52 | 0.45 |
| 40:HG:315:CYS:HA | 40:HG:377:LEU:O | 2.16 | 0.45 |
| 41:HQ:350:LYS:HA | 41:HQ:350:LYS:HD3 | 1.77 | 0.45 |
| 41:IB:16:ILE:HA | 41:IB:226:ASN:HB3 | 1.99 | 0.45 |
| 40:IF:112:LYS:HA | 40:IF:115:ILE:HG22 | 1.97 | 0.45 |
| 40:IG:250:VAL:HG11 | 40:IG:318:LEU:HD11 | 1.97 | 0.45 |
| 40:IH:112:LYS:HA | 40:IH:115:ILE:HG22 | 1.98 | 0.45 |
| 41:JL:193:VAL:HG11 | 41:JL:418:LEU:HD11 | 1.98 | 0.45 |
| 41:JL:253:LEU:O | 41:JL:257:MET:HB2 | 2.17 | 0.45 |
| 41:JN:33:THR:O | 41:JN:58:LYS:NZ | 2.44 | 0.45 |
| 41:KB:7:LEU:HG | 41:KB:135:LEU:HD13 | 1.99 | 0.45 |
| 40:KD:142:GLY:HA2 | 40:KD:183:GLU:HG2 | 1.99 | 0.45 |
| 40:KD:217:LEU:HA | 40:KD:277:SER:HB3 | 1.97 | 0.45 |
| 41:KL:1:MET:HG2 | 41:KL:128:ASP:OD1 | 2.17 | 0.45 |
| 41:KL:380:ARG:HE | 41:KL:380:ARG:HB3 | 1.44 | 0.45 |
| 41:KO:292:GLN:O | 41:KO:298:ASN:ND2 | 2.50 | 0.45 |
| 40:LD:179:THR:OG1 | 40:LD:183:GLU:OE2 | 2.26 | 0.45 |
| 40:LF:172:TYR:CD1 | 40:LF:173:PRO:HD2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:LN:252:LYS:HA | 41:LN:255:VAL:HG12 | 1.98 | 0.45 |
| 41:LP:392:LYS:HB2 | 41:LP:395:LEU:HD13 | 1.98 | 0.45 |
| 40:MA:363:VAL:O | 40:MA:365:GLY:N | 2.49 | 0.45 |
| 41:MB:226:ASN:ND2 | 43:MB:501:GDP:O6 | 2.46 | 0.45 |
| 40:MD:275:VAL:HA | 40:MD:367:LEU:HD22 | 1.98 | 0.45 |
| 40:ME:265:ILE:HG22 | 40:ME:379:ASN:HD21 | 1.82 | 0.45 |
| 40:MH:187:SER:HB2 | 40:MH:390:LEU:CD2 | 2.44 | 0.45 |
| 40:MH:258:ASN:HA | 41:MP:179:VAL:HG22 | 1.98 | 0.45 |
| 41:ML:21:TRP:HA | 41:ML:24:ILE:HG22 | 1.98 | 0.45 |
| 41:NB:404:ASP:OD1 | 41:NB:405:GLU:N | 2.49 | 0.45 |
| 40:ND:288:VAL:HG22 | 40:ND:372:ARG:HD3 | 1.98 | 0.45 |
| 40:ND:333:ALA:O | 40:ND:337:THR:HG23 | 2.17 | 0.45 |
| 40:NE:251:ASP:OD1 | 40:NE:252:LEU:N | 2.47 | 0.45 |
| 41:NL:174:LYS:HG3 | 41:NL:205:GLU:OE2 | 2.16 | 0.45 |
| 41:NM:31:ASP:OD2 | 41:NM:37:HIS:ND1 | 2.50 | 0.45 |
| 41:NO:46:ARG:HD3 | 41:NO:46:ARG:HA | 1.85 | 0.45 |
| 41:NP:183:TYR:OH | 41:NP:393:ALA:O | 2.22 | 0.45 |
| 40:OA:35:GLN:OE1 | 40:OA:35:GLN:N | 2.48 | 0.45 |
| 40:OF:405:HIS:HA | 40:OF:408:VAL:HG12 | 1.98 | 0.45 |
| 40:OG:213:CYS:HA | 40:OG:217:LEU:HB3 | 1.98 | 0.45 |
| 40:OH:72:PRO:O | 40:OH:73:THR:C | 2.55 | 0.45 |
| 41:OO:107:THR:O | 41:OO:110:ALA:N | 2.32 | 0.45 |
| 40:PG:88:HIS:CE1 | 40:PG:90:GLU:HG2 | 2.52 | 0.45 |
| 40:PG:241:SER:OG | 40:PG:250:VAL:O | 2.24 | 0.45 |
| 41:QB:372:THR:O | 41:QB:372:THR:OG1 | 2.34 | 0.45 |
| 41:QB:386:THR:C | 41:QB:388:MET:H | 2.20 | 0.45 |
| 40:QE:14:VAL:HG23 | 40:QE:67:PHE:CG | 2.52 | 0.45 |
| 40:QE:137:ILE:HG21 | 40:QE:154:MET:HE3 | 1.99 | 0.45 |
| 40:QF:228:ASN:HA | 40:QF:231:ILE:HB | 1.98 | 0.45 |
| 41:QL:58:LYS:NZ | 41:RL:281:TYR:HA | 2.32 | 0.45 |
| 41:QL:210:ILE:O | 41:QL:214:THR:OG1 | 2.30 | 0.45 |
| 41:QO:178:THR:HB | 41:QO:181:GLU:HG3 | 1.97 | 0.45 |
| 41:QP:392:LYS:HE2 | 41:QP:392:LYS:HB2 | 1.59 | 0.45 |
| 40:RA:138:PHE:HZ | 40:RA:235:VAL:HG21 | 1.82 | 0.45 |
| 40:RF:75:ILE:HG22 | 40:RF:79:ARG:HH11 | 1.82 | 0.45 |
| 40:RF:224:TYR:O | 40:RF:228:ASN:ND2 | 2.50 | 0.45 |
| 41:RL:31:ASP:OD1 | 41:RL:34:GLY:N | 2.50 | 0.45 |
| 40:SA:88:HIS:CE1 | 40:TA:280:LYS:HE3 | 2.51 | 0.45 |
| 40:SE:188:ILE:HG23 | 40:SE:424:MET:HE3 | 1.97 | 0.45 |
| 40:SF:324:VAL:HB | 40:SF:327:ASP:HB3 | 1.99 | 0.45 |
| 40:SH:167:LEU:HD21 | 40:SH:202:PHE:HD2 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SM:68:LEU:HD23 | 41:SM:112:LEU:HD22 | 1.99 | 0.45 |
| 41:SO:276:ARG:HG2 | 41:SO:277:GLY:N | 2.32 | 0.45 |
| 40:TA:166:LYS:HB3 | 40:TA:199:ASP:HB2 | 1.98 | 0.45 |
| 41:TN:7:LEU:HD12 | 41:TN:151:LEU:HD21 | 1.98 | 0.45 |
| 41:TP:334:GLN:HE22 | 41:TP:347:ASN:HA | 1.82 | 0.45 |
| 40:UA:103:TYR:HD2 | 40:UA:412:MET:HE3 | 1.81 | 0.45 |
| 40:UA:326:LYS:HE3 | 40:UA:329:ASN:HD22 | 1.82 | 0.45 |
| 41:UB:19:LYS:HD2 | 41:UB:19:LYS:HA | 1.80 | 0.45 |
| 40:UF:50:ASN:O | 40:UF:52:PHE:N | 2.45 | 0.45 |
| 40:UG:2:ARG:NE | 40:UG:242:LEU:O | 2.45 | 0.45 |
| 40:UI:62:VAL:HG11 | 40:VJ:283:HIS:CB | 2.46 | 0.45 |
| 41:UM:44:LEU:HA | 41:UM:47:ILE:HG23 | 1.98 | 0.45 |
| 41:UP:13:GLY:O | 41:UP:14:ASN:C | 2.53 | 0.45 |
| 41:UP:33:THR:OG1 | 41:UP:34:GLY:N | 2.49 | 0.45 |
| 41:UP:190:HIS:HB3 | 41:UP:191:GLN:HE21 | 1.81 | 0.45 |
| 41:UP:318:ARG:HB2 | 41:UP:358:PRO:HD3 | 1.98 | 0.45 |
| 41:VB:174:LYS:HG3 | 41:VB:175:VAL:HG22 | 1.98 | 0.45 |
| 40:VI:209:ILE:HB | 40:VI:227:LEU:HD22 | 1.98 | 0.45 |
| 40:VJ:188:ILE:HA | 40:VJ:191:THR:HG22 | 1.99 | 0.45 |
| 41:VN:238:THR:HG21 | 41:VN:318:ARG:HG2 | 1.97 | 0.45 |
| 41:VQ:87:PRO:HD3 | 41:WP:281:TYR:CD1 | 2.51 | 0.45 |
| 40:WA:136:LEU:HD23 | 40:WA:167:LEU:HB2 | 1.99 | 0.45 |
| 40:WE:48:SER:O | 40:WE:51:THR:HG22 | 2.17 | 0.45 |
| 40:WE:186:ASN:OD1 | 40:WE:407:TYR:OH | 2.27 | 0.45 |
| 41:WM:380:ARG:HE | 41:WM:381:ILE:HG13 | 1.81 | 0.45 |
| 41:WN:218:THR:O | 41:WN:220:PRO:HD3 | 2.16 | 0.45 |
| 7:1T:165:VAL:CG1 | 7:1T:211:ILE:HG13 | 2.47 | 0.45 |
| 8:1W:410:LYS:HA | 8:1W:413:GLU:HG3 | 1.99 | 0.45 |
| 8:1X:125:LYS:H | 8:1X:125:LYS:HG3 | 1.48 | 0.45 |
| 8:1X:133:LYS:HE2 | 8:1X:133:LYS:HB2 | 1.35 | 0.45 |
| 8:1X:169:GLU:C | 8:1X:171:ALA:N | 2.68 | 0.45 |
| 11:2I:186:LYS:HG2 | 11:2I:187:ARG:H | 1.81 | 0.45 |
| 12:2P:40:GLU:O | 41:AL:340:TYR:OH | 2.29 | 0.45 |
| 13:2V:81:LYS:HD3 | 13:2V:161:ARG:HD3 | 1.99 | 0.45 |
| 13:2W:42:ILE:HD11 | 13:2W:129:TRP:CD2 | 2.52 | 0.45 |
| 17:3P:211:VAL:O | 17:3P:213:ASP:N | 2.47 | 0.45 |
| 17:3R:331:VAL:O | 17:3R:332:THR:C | 2.55 | 0.45 |
| 21:4E:179:ARG:NH1 | 41:AP:83:GLN:OE1 | 2.39 | 0.45 |
| 21:4F:29:GLN:N | 40:LD:47:ASP:OD1 | 2.49 | 0.45 |
| 21:4F:277:GLU:OE2 | 21:4F:277:GLU:N | 2.49 | 0.45 |
| 22:4H:74:PHE:HB3 | 22:4H:108:LEU:HD12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4I:677:LEU:HD13 | 22:4I:677:LEU:HA | 1.73 | 0.45 |
| 23:4M:170:SER:N | 23:4M:171:PRO:HD2 | 2.31 | 0.45 |
| 23:4M:242:LEU:HD12 | 23:4M:261:TYR:CE2 | 2.52 | 0.45 |
| 23:4P:234:ARG:CG | 41:DN:41:ASP:HB3 | 2.45 | 0.45 |
| 23:4P:241:GLY:HA2 | 23:4P:265:THR:OG1 | 2.17 | 0.45 |
| 23:4Q:216:MET:O | 23:4Q:219:GLN:HG3 | 2.16 | 0.45 |
| 23:4Q:240:LEU:CB | 23:4Q:266:HIS:HA | 2.46 | 0.45 |
| 23:4R:40:THR:O | 23:4R:44:LEU:HG | 2.15 | 0.45 |
| 23:4R:54:PRO:HD2 | 41:BP:41:ASP:HA | 1.98 | 0.45 |
| 26:4W:90:LYS:O | 26:4W:166:ASP:HA | 2.16 | 0.45 |
| 28:5B:207:SER:O | 28:5B:209:ILE:HG13 | 2.17 | 0.45 |
| 34:5R:348:GLN:H | 34:5R:348:GLN:HG3 | 1.53 | 0.45 |
| 34:5R:389:LEU:HD22 | 34:5R:389:LEU:HA | 1.70 | 0.45 |
| 36:5Y:125:ALA:HB1 | 36:5Y:130:LEU:HD22 | 1.99 | 0.45 |
| 41:AB:7:LEU:O | 41:AB:135:LEU:HA | 2.17 | 0.45 |
| 41:AB:149:THR:HB | 41:AB:191:GLN:HB2 | 1.99 | 0.45 |
| 40:AE:62:VAL:HG22 | 40:BE:283:HIS:HD2 | 1.82 | 0.45 |
| 40:AE:181:VAL:HG22 | 41:AL:256:ASN:HD22 | 1.82 | 0.45 |
| 40:AG:287:SER:O | 40:AG:291:ILE:HG12 | 2.17 | 0.45 |
| 40:AH:3:GLU:HA | 40:AH:51:THR:HA | 1.98 | 0.45 |
| 41:AL:103:LYS:NZ | 41:AL:401:GLU:OE2 | 2.33 | 0.45 |
| 41:AM:334:GLN:HE22 | 41:AM:348:ASN:H | 1.64 | 0.45 |
| 41:AO:204:ASN:HD22 | 41:AO:225:LEU:HD23 | 1.81 | 0.45 |
| 41:AP:4:ILE:HA | 41:AP:132:GLY:O | 2.16 | 0.45 |
| 41:BB:260:PHE:HZ | 40:BG:400:LYS:HG3 | 1.81 | 0.45 |
| 40:BG:274:PRO:HB3 | 40:BG:370:VAL:HG11 | 1.99 | 0.45 |
| 41:BL:92:PHE:HE2 | 41:BL:94:GLN:HE22 | 1.65 | 0.45 |
| 41:BM:271:ALA:HB2 | 41:BM:365:ALA:HB3 | 1.97 | 0.45 |
| 41:BO:354:CYS:SG | 41:BO:355:ASP:N | 2.89 | 0.45 |
| 41:BO:421:PRO:C | 41:BO:423:VAL:H | 2.19 | 0.45 |
| 41:BP:293:MET:HG2 | 41:BP:367:PHE:HB2 | 1.99 | 0.45 |
| 40:CA:31:GLN:HB2 | 40:CA:35:GLN:O | 2.16 | 0.45 |
| 40:CH:318:LEU:O | 40:CH:320:ARG:N | 2.50 | 0.45 |
| 40:CI:235:VAL:HA | 40:CI:238:ILE:HG22 | 1.98 | 0.45 |
| 41:CL:97:ALA:O | 41:CL:99:ASN:N | 2.50 | 0.45 |
| 41:CM:55:THR:HG21 | 41:DM:284:LEU:CG | 2.45 | 0.45 |
| 41:CO:183:TYR:O | 41:CO:186:THR:OG1 | 2.32 | 0.45 |
| 40:DA:224:TYR:CE2 | 42:DA:501:GTP:H2' | 2.52 | 0.45 |
| 40:DA:326:LYS:HA | 40:DA:326:LYS:HD3 | 1.48 | 0.45 |
| 41:DB:393:ALA:C | 41:DB:395:LEU:H | 2.20 | 0.45 |
| 40:DE:149:PHE:CE2 | 40:DE:153:LEU:HB2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DF:157:LEU:HD22 | 40:DF:157:LEU:HA | 1.88 | 0.45 |
| 40:DG:268:PRO:HB3 | 40:DG:379:ASN:HB2 | 1.98 | 0.45 |
| 40:DH:225:THR:C | 40:DH:227:LEU:H | 2.20 | 0.45 |
| 40:DI:48:SER:HB2 | 40:DI:243:ARG:O | 2.17 | 0.45 |
| 40:DI:58:ALA:O | 40:DI:59:GLY:C | 2.54 | 0.45 |
| 41:DO:107:THR:O | 41:DO:109:GLY:N | 2.49 | 0.45 |
| 41:DP:41:ASP:O | 41:DP:42:LEU:C | 2.55 | 0.45 |
| 41:DP:135:LEU:O | 41:DP:166:THR:HA | 2.17 | 0.45 |
| 41:DP:237:THR:HA | 41:DP:240:LEU:HD21 | 1.98 | 0.45 |
| 41:EB:139:LEU:HD12 | 41:EB:170:VAL:HG22 | 1.98 | 0.45 |
| 40:EE:5:ILE:HG13 | 40:EE:132:LEU:HD11 | 1.98 | 0.45 |
| 40:EI:105:ARG:CZ | 40:EI:110:ILE:HG12 | 2.47 | 0.45 |
| 40:EI:172:TYR:CG | 40:EI:173:PRO:HD2 | 2.52 | 0.45 |
| 40:EI:414:GLU:HB3 | 40:EI:415:GLY:H | 1.63 | 0.45 |
| 41:EM:303:CYS:O | 41:EM:304:ASP:C | 2.54 | 0.45 |
| 41:EP:87:PRO:O | 41:EP:88:ASP:C | 2.55 | 0.45 |
| 40:FA:255:PHE:HE1 | 40:FA:318:LEU:HD11 | 1.82 | 0.45 |
| 40:FI:88:HIS:NE2 | 40:FI:90:GLU:OE1 | 2.50 | 0.45 |
| 41:FO:33:THR:O | 41:FO:58:LYS:NZ | 2.50 | 0.45 |
| 41:FO:77:ARG:HG3 | 41:FO:90:PHE:HE2 | 1.82 | 0.45 |
| 41:FO:222:TYR:HD1 | 41:FO:225:LEU:HD12 | 1.82 | 0.45 |
| 40:GE:101:ASN:HA | 40:GE:143:GLY:HA2 | 1.99 | 0.45 |
| 40:GH:315:CYS:HB3 | 40:GH:351:PHE:CD1 | 2.51 | 0.45 |
| 40:GI:70:LEU:HD21 | 40:GI:111:GLY:HA2 | 1.98 | 0.45 |
| 40:GI:176:GLN:H | 40:GI:176:GLN:HG3 | 1.47 | 0.45 |
| 41:GN:102:ALA:O | 41:GN:104:GLY:N | 2.45 | 0.45 |
| 41:GO:3:GLU:HA | 41:GO:49:VAL:HG13 | 1.98 | 0.45 |
| 41:GP:137:HIS:O | 41:GP:168:SER:HA | 2.16 | 0.45 |
| 41:HB:142:GLY:O | 41:HB:144:GLY:N | 2.49 | 0.45 |
| 40:HI:238:ILE:HG23 | 40:HI:239:THR:HG23 | 1.98 | 0.45 |
| 41:HM:305:PRO:HB3 | 41:HM:310:TYR:CE1 | 2.50 | 0.45 |
| 41:HO:113:VAL:HG21 | 41:HO:150:LEU:HD23 | 1.98 | 0.45 |
| 41:HO:142:GLY:O | 41:HO:144:GLY:N | 2.50 | 0.45 |
| 41:HP:262:ARG:HA | 41:HP:262:ARG:HD2 | 1.77 | 0.45 |
| 40:IF:97:GLU:OE2 | 41:IM:251:ARG:NH1 | 2.48 | 0.45 |
| 40:IG:288:VAL:HA | 40:IG:291:ILE:HG12 | 1.98 | 0.45 |
| 40:IG:326:LYS:HE3 | 41:IO:225:LEU:HD11 | 1.98 | 0.45 |
| 40:IH:16:ILE:HD12 | 40:IH:171:ILE:HD11 | 1.99 | 0.45 |
| 40:IH:70:LEU:HD23 | 40:IH:114:LEU:HD12 | 1.99 | 0.45 |
| 41:IN:156:ARG:NH2 | 41:IN:197:ASP:OD2 | 2.50 | 0.45 |
| 41:IQ:280:GLN:OE1 | 41:IQ:280:GLN:N | 2.44 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IQ:396:HIS:HA | 41:IQ:399:THR:HG22 | 1.97 | 0.45 |
| 40:JA:7:VAL:HG22 | 40:JA:137:ILE:HA | 1.97 | 0.45 |
| 40:JD:116:ASP:OD1 | 40:JD:117:LEU:N | 2.49 | 0.45 |
| 41:JM:163:ILE:H | 41:JM:163:ILE:HG12 | 1.63 | 0.45 |
| 41:JO:11:GLN:HA | 41:JO:72:THR:HG21 | 1.99 | 0.45 |
| 40:KF:139:HIS:CE1 | 40:KF:150:THR:HG21 | 2.51 | 0.45 |
| 40:KF:276:ILE:HG21 | 40:KF:286:LEU:HD11 | 1.99 | 0.45 |
| 40:LA:177:VAL:HB | 41:LN:331:LEU:HD22 | 1.99 | 0.45 |
| 40:LG:67:PHE:HB2 | 40:LG:92:LEU:HD22 | 1.99 | 0.45 |
| 41:LM:273:LEU:O | 41:LM:292:GLN:NE2 | 2.32 | 0.45 |
| 40:MF:60:LYS:HE3 | 40:MF:60:LYS:HB3 | 1.28 | 0.45 |
| 40:MF:399:ALA:HB3 | 40:MF:400:LYS:HZ2 | 1.81 | 0.45 |
| 40:MG:427:LEU:HD12 | 40:MG:427:LEU:HA | 1.82 | 0.45 |
| 40:MH:271:THR:HA | 40:MH:302:MET:HE3 | 1.99 | 0.45 |
| 40:NA:53:PHE:HA | 40:NA:63:PRO:HA | 1.99 | 0.45 |
| 40:NE:33:ASP:OD2 | 40:NE:34:GLY:N | 2.50 | 0.45 |
| 40:NE:70:LEU:HD23 | 40:NE:114:LEU:HD12 | 1.99 | 0.45 |
| 40:NE:202:PHE:HD1 | 40:NE:268:PRO:HG2 | 1.82 | 0.45 |
| 40:NE:271:THR:OG1 | 40:NE:376:MET:HB3 | 2.17 | 0.45 |
| 40:NF:102:ASN:HB3 | 40:NF:105:ARG:HB2 | 1.99 | 0.45 |
| 40:NG:88:HIS:CE1 | 40:OG:280:LYS:HG3 | 2.51 | 0.45 |
| 40:NH:60:LYS:HZ1 | 40:OH:282:TYR:HB2 | 1.80 | 0.45 |
| 41:NM:46:ARG:HA | 41:NM:46:ARG:HD3 | 1.75 | 0.45 |
| 41:OB:248:ALA:HA | 41:OB:252:LYS:NZ | 2.32 | 0.45 |
| 41:OB:314:ALA:HA | 41:OB:350:LYS:HB3 | 1.98 | 0.45 |
| 40:OD:288:VAL:HA | 40:OD:291:ILE:HG12 | 1.98 | 0.45 |
| 40:OF:122:ILE:HG21 | 40:OF:157:LEU:HD11 | 1.99 | 0.45 |
| 40:OF:234:ILE:HD12 | 40:OF:270:ALA:HB1 | 1.99 | 0.45 |
| 40:OH:101:ASN:HD22 | 41:OO:256:ASN:ND2 | 2.15 | 0.45 |
| 40:OH:304:LYS:HD3 | 40:OH:304:LYS:HA | 1.76 | 0.45 |
| 41:OL:309:ARG:NH1 | 41:OL:341:PHE:O | 2.49 | 0.45 |
| 41:ON:167:PHE:CZ | 41:ON:233:MET:HG3 | 2.51 | 0.45 |
| 41:OO:232:THR:HG23 | 41:OO:366:THR:HG23 | 1.98 | 0.45 |
| 41:OP:7:LEU:HD11 | 41:OP:135:LEU:HD12 | 1.97 | 0.45 |
| 41:PB:30:ILE:HD11 | 41:PB:47:ILE:HD11 | 1.99 | 0.45 |
| 41:PB:323:MET:HE1 | 40:PG:223:THR:HB | 1.99 | 0.45 |
| 40:PD:9:VAL:HG12 | 40:PD:146:GLY:HA2 | 1.98 | 0.45 |
| 40:PD:164:LYS:O | 40:PD:166:LYS:NZ | 2.40 | 0.45 |
| 40:PE:438:SER:OG | 41:PM:390:ARG:NH1 | 2.48 | 0.45 |
| 40:PG:155:GLU:HG3 | 40:PG:197:HIS:HE1 | 1.81 | 0.45 |
| 41:PN:198:GLU:OE1 | 41:PN:200:TYR:OH | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QE:21:TRP:HZ2 | 40:QE:65:ALA:HB2 | 1.81 | 0.45 |
| 40:QE:260:VAL:HG13 | 40:QE:266:HIS:HB3 | 1.99 | 0.45 |
| 40:QH:69:ASP:HA | 40:QH:145:THR:HG21 | 1.97 | 0.45 |
| 41:QO:67:ASP:HA | 41:QO:143:THR:HG21 | 1.99 | 0.45 |
| 40:RH:254:GLU:HG2 | 41:RP:98:GLY:HA2 | 1.97 | 0.45 |
| 41:RL:2:ARG:NH1 | 41:RL:240:LEU:HB2 | 2.30 | 0.45 |
| 41:RL:49:VAL:HG21 | 41:RL:241:ARG:HA | 1.99 | 0.45 |
| 41:RP:202:ILE:HA | 41:RP:300:MET:HG2 | 1.99 | 0.45 |
| 40:SE:118:VAL:O | 40:SE:122:ILE:HG12 | 2.16 | 0.45 |
| 40:SG:46:ASP:OD1 | 40:SG:47:ASP:N | 2.46 | 0.45 |
| 40:SH:437:ASP:OD2 | 40:SH:438:SER:N | 2.49 | 0.45 |
| 40:TA:182:VAL:O | 40:TA:186:ASN:ND2 | 2.50 | 0.45 |
| 41:TB:165:ASN:HB3 | 41:TB:167:PHE:CE1 | 2.52 | 0.45 |
| 40:TF:421:ARG:HH21 | 40:TF:424:MET:HB3 | 1.82 | 0.45 |
| 40:TG:3:GLU:OE2 | 40:TG:130:THR:N | 2.50 | 0.45 |
| 40:TI:202:PHE:HE1 | 40:TI:377:LEU:HD22 | 1.82 | 0.45 |
| 41:TM:232:THR:HG21 | 41:TM:268:PRO:HB2 | 1.98 | 0.45 |
| 41:TN:114:ASP:N | 41:TN:114:ASP:OD1 | 2.50 | 0.45 |
| 41:TO:131:GLN:HE22 | 41:TO:249:ASP:HB2 | 1.82 | 0.45 |
| 40:UF:195:LEU:HA | 40:UF:266:HIS:CE1 | 2.52 | 0.45 |
| 40:UH:101:ASN:ND2 | 41:UO:256:ASN:HD21 | 2.15 | 0.45 |
| 40:UI:156:ARG:HD2 | 40:UI:156:ARG:HA | 1.80 | 0.45 |
| 41:UN:317:PHE:HA | 41:UN:364:SER:O | 2.17 | 0.45 |
| 41:UO:117:LEU:HA | 41:UO:120:VAL:HG12 | 1.97 | 0.45 |
| 41:UO:406:MET:O | 41:UO:409:THR:OG1 | 2.30 | 0.45 |
| 41:UP:294:PHE:CE1 | 41:UP:313:VAL:HG11 | 2.52 | 0.45 |
| 41:UP:372:THR:HA | 41:UP:422:VAL:HG22 | 1.98 | 0.45 |
| 40:VG:51:THR:HG21 | 40:VG:243:ARG:HG2 | 1.99 | 0.45 |
| 40:VG:342:GLN:NE2 | 40:VG:343:PHE:O | 2.49 | 0.45 |
| 41:VQ:67:ASP:HA | 41:VQ:143:THR:HG21 | 1.99 | 0.45 |
| 40:WA:101:ASN:HB2 | 41:WN:255:VAL:HG11 | 1.99 | 0.45 |
| 40:WA:177:VAL:HB | 41:WN:331:LEU:HB2 | 1.99 | 0.45 |
| 40:WA:180:ALA:HA | 41:WN:256:ASN:HD21 | 1.82 | 0.45 |
| 40:WA:184:PRO:O | 40:WA:188:ILE:HB | 2.17 | 0.45 |
| 40:WH:72:PRO:HB2 | 41:WO:46:ARG:HH21 | 1.82 | 0.45 |
| 41:WN:6:HIS:O | 41:WN:63:ALA:HA | 2.17 | 0.45 |
| 41:WO:137:HIS:O | 41:WO:168:SER:HA | 2.17 | 0.45 |
| 41:WQ:404:ASP:N | 41:WQ:404:ASP:OD1 | 2.49 | 0.45 |
| 7:1T:37:GLU:HA | 7:1T:52:ILE:HD12 | 1.99 | 0.45 |
| 7:1T:47:ILE:HB | 7:1T:60:LEU:HD12 | 1.98 | 0.45 |
| 7:1U:457:LEU:HD11 | 7:1U:493:LEU:HD22 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:2B:44:ARG:H | 9:2B:44:ARG:HG3 | 1.55 | 0.45 |
| 11:2I:201:LYS:HA | 11:2I:201:LYS:HD2 | 1.32 | 0.45 |
| 11:2K:245:GLU:O | 11:2K:246:LYS:C | 2.54 | 0.45 |
| 13:2V:86:TYR:O | 13:2V:159:ASN:HB2 | 2.17 | 0.45 |
| 13:2W:38:THR:HA | 13:2W:44:SER:O | 2.17 | 0.45 |
| 13:2X:109:GLN:HE21 | 13:2X:111:THR:HG23 | 1.82 | 0.45 |
| 15:3G:331:ASP:N | 15:3G:331:ASP:OD1 | 2.47 | 0.45 |
| 16:3J:75:LYS:HE3 | 16:3J:180:MET:SD | 2.56 | 0.45 |
| 17:3P:350:ARG:HA | 17:3P:350:ARG:HD2 | 1.30 | 0.45 |
| 17:3Q:355:ALA:O | 17:3Q:356:ASP:C | 2.55 | 0.45 |
| 17:3R:232:ARG:HH21 | 17:3R:328:LEU:CA | 2.14 | 0.45 |
| 18:3V:103:VAL:O | 18:3V:107:LEU:HG | 2.17 | 0.45 |
| 22:4H:89:VAL:HB | 22:4H:98:ARG:HH11 | 1.81 | 0.45 |
| 22:4K:512:LYS:HG3 | 22:4K:519:LEU:HD12 | 1.99 | 0.45 |
| 23:4N:173:SER:HB2 | 23:4N:181:LYS:HZ2 | 1.80 | 0.45 |
| 23:4N:241:GLY:HA2 | 23:4N:265:THR:OG1 | 2.17 | 0.45 |
| 24:4O:240:LEU:CB | 24:4O:266:HIS:HA | 2.46 | 0.45 |
| 26:4V:109:ILE:O | 26:4V:113:ILE:HG12 | 2.17 | 0.45 |
| 34:5R:503:PRO:O | 34:5R:504:MET:C | 2.55 | 0.45 |
| 36:5Y:181:LEU:HD12 | 36:5Y:182:LEU:HD12 | 1.98 | 0.45 |
| 38:6C:47:LEU:HD12 | 38:6C:47:LEU:HA | 1.76 | 0.45 |
| 38:6C:92:LYS:NZ | 41:VB:376:GLU:OE2 | 2.43 | 0.45 |
| 38:6C:199:PRO:HB3 | 41:VQ:329:GLN:HE21 | 1.81 | 0.45 |
| 39:6F:99:LEU:HG | 39:6F:103:LYS:HE2 | 1.97 | 0.45 |
| 41:AB:242:PHE:HB3 | 41:AB:356:ILE:HD13 | 1.98 | 0.45 |
| 40:AG:141:PHE:HB2 | 40:AG:173:PRO:HD3 | 1.99 | 0.45 |
| 40:AG:167:LEU:HD11 | 40:AG:252:LEU:HD22 | 1.99 | 0.45 |
| 41:AN:165:ASN:ND2 | 41:AN:198:GLU:OE2 | 2.49 | 0.45 |
| 41:AN:215:LEU:HD21 | 41:AN:273:LEU:HD22 | 1.99 | 0.45 |
| 40:BA:20:CYS:HA | 40:BA:232:SER:HB2 | 1.99 | 0.45 |
| 40:BE:31:GLN:O | 40:BE:34:GLY:N | 2.48 | 0.45 |
| 40:BE:402:ALA:HB2 | 41:BL:344:TRP:HZ3 | 1.82 | 0.45 |
| 40:BI:100:ALA:O | 40:BI:102:ASN:N | 2.50 | 0.45 |
| 41:BL:120:VAL:HG11 | 41:BL:155:ILE:HD11 | 1.99 | 0.45 |
| 41:BM:77:ARG:HH22 | 41:CM:281:TYR:HE1 | 1.65 | 0.45 |
| 41:BM:226:ASN:HD21 | 43:BM:501:GDP:HN1 | 1.64 | 0.45 |
| 41:BP:117:LEU:HD11 | 41:BP:155:ILE:HG13 | 1.99 | 0.45 |
| 40:CF:20:CYS:HA | 40:CF:232:SER:HB2 | 1.99 | 0.45 |
| 41:CM:321:MET:HE3 | 41:CM:321:MET:HB3 | 1.77 | 0.45 |
| 41:CN:201:CYS:O | 41:CN:268:PRO:HD3 | 2.17 | 0.45 |
| 41:CN:325:GLU:O | 41:CN:329:GLN:HB2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CO:101:TRP:O | 41:CO:102:ALA:C | 2.54 | 0.45 |
| 41:CO:389:PHE:O | 41:CO:390:ARG:C | 2.55 | 0.45 |
| 40:DA:105:ARG:HB3 | 40:DA:110:ILE:CG2 | 2.46 | 0.45 |
| 40:DA:250:VAL:CG2 | 40:DA:354:GLY:HA3 | 2.46 | 0.45 |
| 40:DE:27:GLU:HB3 | 40:DE:244:PHE:HZ | 1.81 | 0.45 |
| 40:DE:213:CYS:C | 40:DE:215:ARG:H | 2.21 | 0.45 |
| 40:DF:349:THR:OG1 | 41:DN:179:VAL:HA | 2.16 | 0.45 |
| 40:DI:240:ALA:HA | 40:DI:243:ARG:HB2 | 1.99 | 0.45 |
| 41:DL:70:PRO:HG3 | 41:DL:94:GLN:HG3 | 1.98 | 0.45 |
| 41:DL:100:ASN:HB3 | 41:DL:103:LYS:HG3 | 1.99 | 0.45 |
| 41:DM:359:ARG:HD2 | 41:DM:359:ARG:HA | 1.82 | 0.45 |
| 41:DN:186:THR:O | 41:DN:187:LEU:C | 2.55 | 0.45 |
| 41:DN:186:THR:OG1 | 41:DN:187:LEU:N | 2.50 | 0.45 |
| 41:EB:16:ILE:HD11 | 41:EB:229:VAL:HG11 | 1.99 | 0.45 |
| 40:EE:210:TYR:HE1 | 40:EE:227:LEU:HD11 | 1.81 | 0.45 |
| 40:EI:333:ALA:O | 40:EI:334:ALA:C | 2.54 | 0.45 |
| 41:EM:289:LEU:HD12 | 41:EM:289:LEU:HA | 1.75 | 0.45 |
| 41:EM:293:MET:HE3 | 41:EM:293:MET:HB3 | 1.76 | 0.45 |
| 41:EO:222:TYR:HD1 | 41:EO:225:LEU:HD12 | 1.82 | 0.45 |
| 41:EP:124:ALA:O | 41:EP:125:GLU:C | 2.54 | 0.45 |
| 41:EP:216:LYS:HA | 41:EP:216:LYS:HD3 | 1.53 | 0.45 |
| 41:EP:270:PHE:HB3 | 41:EP:271:ALA:H | 1.56 | 0.45 |
| 40:FA:119:LEU:HD13 | 40:FA:119:LEU:HA | 1.77 | 0.45 |
| 41:FB:46:ARG:NH2 | 40:FG:76:ASP:OD1 | 2.50 | 0.45 |
| 40:FG:122:ILE:HG21 | 40:FG:157:LEU:HD21 | 1.99 | 0.45 |
| 40:FG:237:SER:HA | 40:FG:320:ARG:HD3 | 1.98 | 0.45 |
| 40:FI:224:TYR:O | 40:FI:228:ASN:ND2 | 2.50 | 0.45 |
| 41:FP:296:ALA:HB1 | 41:FP:305:PRO:HD2 | 1.99 | 0.45 |
| 40:GA:234:ILE:HG13 | 40:GA:375:CYS:SG | 2.57 | 0.45 |
| 40:GE:47:ASP:O | 40:GE:48:SER:C | 2.55 | 0.45 |
| 41:HB:30:ILE:HG22 | 41:HB:36:TYR:HA | 1.99 | 0.45 |
| 40:HI:405:HIS:HA | 40:HI:408:VAL:HG12 | 1.99 | 0.45 |
| 40:IA:7:VAL:HG11 | 40:IA:153:LEU:HD21 | 1.99 | 0.45 |
| 40:IA:228:ASN:ND2 | 42:IA:501:GTP:HN1 | 2.10 | 0.45 |
| 41:IB:284:LEU:HD21 | 41:IB:363:MET:HB2 | 1.99 | 0.45 |
| 40:IE:55:GLU:OE1 | 40:IE:61:HIS:NE2 | 2.49 | 0.45 |
| 40:IF:277:SER:O | 40:IF:279:GLU:N | 2.49 | 0.45 |
| 40:IH:324:VAL:HG11 | 41:IP:219:THR:HB | 1.97 | 0.45 |
| 40:II:236:SER:O | 40:II:243:ARG:NH2 | 2.44 | 0.45 |
| 41:IP:100:ASN:HB3 | 41:IP:103:LYS:HB3 | 1.99 | 0.45 |
| 40:JD:128:GLN:OE1 | 40:KD:290:GLU:HG2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JG:192:HIS:NE2 | 40:JG:419:GLU:OE2 | 2.45 | 0.45 |
| 40:JG:338:LYS:HZ1 | 40:JG:341:ILE:HG12 | 1.82 | 0.45 |
| 41:JM:54:ALA:O | 41:JM:55:THR:C | 2.55 | 0.45 |
| 40:KE:93:ILE:HD13 | 40:KE:118:VAL:HG22 | 1.98 | 0.45 |
| 40:KG:3:GLU:OE2 | 40:KG:129:CYS:HA | 2.16 | 0.45 |
| 40:KG:139:HIS:O | 40:KG:170:SER:HA | 2.17 | 0.45 |
| 41:KL:181:GLU:O | 41:KL:182:PRO:C | 2.56 | 0.45 |
| 41:KL:198:GLU:HB3 | 41:KL:266:PHE:HE2 | 1.82 | 0.45 |
| 41:KN:376:GLU:OE2 | 41:KN:380:ARG:NH2 | 2.49 | 0.45 |
| 41:KO:151:LEU:O | 41:KO:155:ILE:HG13 | 2.16 | 0.45 |
| 41:KP:226:ASN:ND2 | 43:KP:501:GDP:O6 | 2.48 | 0.45 |
| 40:LA:406:TRP:CG | 41:LN:255:VAL:HG23 | 2.52 | 0.45 |
| 40:LG:99:ALA:O | 40:LG:100:ALA:C | 2.55 | 0.45 |
| 41:LL:3:GLU:HA | 41:LL:49:VAL:HA | 1.99 | 0.45 |
| 41:LO:386:THR:HG22 | 41:LO:390:ARG:HD3 | 1.98 | 0.45 |
| 40:MA:79:ARG:HH12 | 40:MA:94:THR:HB | 1.81 | 0.45 |
| 40:MD:248:LEU:HD22 | 40:MD:353:VAL:HG23 | 1.98 | 0.45 |
| 40:MF:164:LYS:HE3 | 40:MF:164:LYS:HB3 | 1.52 | 0.45 |
| 40:MG:255:PHE:HE2 | 40:MG:318:LEU:HD11 | 1.81 | 0.45 |
| 40:MH:30:ILE:HD13 | 40:MH:53:PHE:CD2 | 2.52 | 0.45 |
| 40:MH:282:TYR:HD1 | 40:MH:282:TYR:HA | 1.62 | 0.45 |
| 40:NA:3:GLU:HA | 40:NA:51:THR:HA | 1.98 | 0.45 |
| 40:ND:228:ASN:O | 40:ND:229:ARG:C | 2.56 | 0.45 |
| 40:NH:348:PRO:HG2 | 41:NP:384:GLN:HG2 | 1.99 | 0.45 |
| 41:NN:273:LEU:HD23 | 41:NN:273:LEU:HA | 1.84 | 0.45 |
| 41:NP:107:THR:O | 41:NP:109:GLY:N | 2.50 | 0.45 |
| 40:OA:141:PHE:HB2 | 40:OA:173:PRO:HD3 | 1.99 | 0.45 |
| 40:OD:76:ASP:OD1 | 40:OD:76:ASP:N | 2.50 | 0.45 |
| 40:OD:139:HIS:ND1 | 40:OD:140:SER:O | 2.49 | 0.45 |
| 40:OE:188:ILE:HG23 | 40:OE:424:MET:HG3 | 1.99 | 0.45 |
| 40:OE:391:ASP:HB3 | 40:OE:421:ARG:NH1 | 2.31 | 0.45 |
| 40:OF:165:SER:HA | 40:OF:256:GLN:HE22 | 1.82 | 0.45 |
| 40:OF:383:ILE:HD12 | 40:OF:387:TRP:HE1 | 1.81 | 0.45 |
| 40:OF:394:PHE:HZ | 40:OF:417:PHE:HB3 | 1.81 | 0.45 |
| 41:OL:170:VAL:HB | 41:OL:201:CYS:HB2 | 1.98 | 0.45 |
| 41:ON:44:LEU:HA | 41:ON:47:ILE:HG23 | 1.99 | 0.45 |
| 41:OP:398:TYR:HB3 | 41:OP:403:MET:HB2 | 1.97 | 0.45 |
| 40:PA:3:GLU:HB2 | 40:PA:129:CYS:SG | 2.57 | 0.45 |
| 41:PB:250:LEU:HA | 41:PB:253:LEU:HD12 | 1.99 | 0.45 |
| 40:PD:256:GLN:HG3 | 41:PL:397:TRP:HZ2 | 1.81 | 0.45 |
| 41:PL:3:GLU:OE2 | 41:PL:129:CYS:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PL:271:ALA:HB3 | 41:PL:293:MET:HB3 | 1.97 | 0.45 |
| 41:PN:68:LEU:HD23 | 41:PN:143:THR:HG23 | 1.98 | 0.45 |
| 41:PN:313:VAL:HG23 | 41:PN:349:VAL:HG23 | 1.99 | 0.45 |
| 40:QA:319:TYR:HB2 | 40:QA:355:ILE:HD13 | 1.97 | 0.45 |
| 41:QB:346:PRO:O | 41:QB:347:ASN:C | 2.54 | 0.45 |
| 40:QE:298:PRO:HB3 | 40:QE:307:PRO:HD2 | 1.99 | 0.45 |
| 40:QE:332:ILE:O | 40:QE:336:LYS:HG3 | 2.17 | 0.45 |
| 40:QG:121:ARG:HH11 | 40:QG:124:LYS:HZ1 | 1.65 | 0.45 |
| 40:QH:138:PHE:HE2 | 40:QH:235:VAL:HG21 | 1.81 | 0.45 |
| 41:QP:258:VAL:HG12 | 41:QP:261:PRO:HA | 1.98 | 0.45 |
| 41:QP:417:ASP:O | 41:QP:420:ASN:N | 2.40 | 0.45 |
| 40:RE:238:ILE:HD11 | 40:RE:377:LEU:HD21 | 1.99 | 0.45 |
| 40:RE:242:LEU:H | 40:RE:242:LEU:HD23 | 1.81 | 0.45 |
| 41:RM:7:LEU:HD21 | 41:RM:120:VAL:HG11 | 1.98 | 0.45 |
| 41:RM:18:ALA:HB2 | 41:RM:76:VAL:HG23 | 1.99 | 0.45 |
| 41:RM:271:ALA:HB2 | 41:RM:298:ASN:ND2 | 2.32 | 0.45 |
| 41:RN:33:THR:O | 41:RN:58:LYS:NZ | 2.42 | 0.45 |
| 40:SA:12:ALA:O | 40:SA:16:ILE:HD12 | 2.17 | 0.45 |
| 40:SE:391:ASP:OD1 | 40:SE:421:ARG:NH1 | 2.50 | 0.45 |
| 40:SH:85:GLN:OE1 | 40:TH:283:HIS:NE2 | 2.37 | 0.45 |
| 40:SH:325:PRO:HG2 | 41:SP:221:THR:HA | 1.99 | 0.45 |
| 41:SO:139:LEU:HB2 | 41:SO:169:VAL:O | 2.17 | 0.45 |
| 40:TG:7:VAL:HG11 | 40:TG:153:LEU:HD21 | 1.99 | 0.45 |
| 40:TG:224:TYR:HB3 | 42:TG:501:GTP:N1 | 2.31 | 0.45 |
| 40:TG:405:HIS:HA | 40:TG:408:VAL:HG12 | 1.98 | 0.45 |
| 40:TH:6:SER:O | 40:TH:65:ALA:HA | 2.15 | 0.45 |
| 41:TL:128:ASP:OD2 | 41:TL:129:CYS:N | 2.49 | 0.45 |
| 42:UB:502:GTP:HN1 | 40:UG:228:ASN:HD21 | 1.64 | 0.45 |
| 40:UH:74:VAL:HG13 | 40:UH:75:ILE:HG13 | 1.98 | 0.45 |
| 40:UH:105:ARG:HG2 | 40:UH:410:GLU:HG2 | 1.99 | 0.45 |
| 40:UI:118:VAL:O | 40:UI:122:ILE:HG23 | 2.16 | 0.45 |
| 41:UM:95:SER:OG | 41:UM:96:GLY:N | 2.48 | 0.45 |
| 40:VI:142:GLY:O | 40:VI:186:ASN:ND2 | 2.49 | 0.45 |
| 41:VO:19:LYS:HA | 41:VO:19:LYS:HD3 | 1.69 | 0.45 |
| 40:WE:386:ALA:O | 40:WE:389:ARG:HG2 | 2.17 | 0.45 |
| 40:WF:195:LEU:HD21 | 40:WF:264:ARG:HE | 1.82 | 0.45 |
| 40:WG:51:THR:HG23 | 40:WG:52:PHE:CD2 | 2.51 | 0.45 |
| 40:WH:139:HIS:O | 40:WH:170:SER:HA | 2.17 | 0.45 |
| 41:WM:277:GLY:O | 41:WM:279:GLN:N | 2.47 | 0.45 |
| 41:WN:154:LYS:HA | 41:WN:154:LYS:HD2 | 1.68 | 0.45 |
| 41:WP:375:GLN:NE2 | 41:WP:422:VAL:HG13 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:1W:475:GLU:HG3 | 40:VG:369:LYS:HZ1 | 1.82 | 0.45 |
| 8:1X:105:GLU:O | 8:1X:106:GLU:C | 2.55 | 0.45 |
| 9:2B:51:HIS:HB3 | 11:2K:255:LYS:C | 2.37 | 0.45 |
| 11:2J:130:THR:OG1 | 11:2J:132:ASP:OD2 | 2.34 | 0.45 |
| 12:2P:172:LEU:HD23 | 12:2P:232:PHE:HZ | 1.81 | 0.45 |
| 12:2R:119:MET:HE2 | 12:2R:119:MET:HB2 | 1.85 | 0.45 |
| 14:3A:46:ARG:NH2 | 40:MF:264:ARG:HG3 | 2.32 | 0.45 |
| 14:3B:45:ASP:OD1 | 14:3B:45:ASP:N | 2.50 | 0.45 |
| 17:3O:277:THR:HA | 17:3O:281:ILE:HG13 | 1.98 | 0.45 |
| 17:3Q:354:THR:HG22 | 17:3Q:466:LEU:HD22 | 1.98 | 0.45 |
| 17:3R:156:TRP:HD1 | 17:3R:300:TRP:CZ3 | 2.35 | 0.45 |
| 18:3W:179:GLU:OE1 | 18:3W:296:GLN:HG3 | 2.16 | 0.45 |
| 20:4B:241:LEU:O | 20:4B:242:THR:C | 2.55 | 0.45 |
| 22:4H:304:LEU:HD23 | 22:4H:304:LEU:HA | 1.84 | 0.45 |
| 22:4I:680:LYS:HB3 | 22:4I:681:PHE:HD1 | 1.82 | 0.45 |
| 22:4J:292:VAL:CG2 | 41:CN:359:ARG:HH22 | 2.29 | 0.45 |
| 22:4J:294:GLN:NE2 | 41:CN:361:LEU:HD12 | 2.32 | 0.45 |
| 22:4J:676:ALA:O | 22:4J:679:SER:N | 2.49 | 0.45 |
| 23:4N:189:GLY:CA | 41:CM:46:ARG:HH12 | 2.26 | 0.45 |
| 23:4N:240:LEU:HB2 | 23:4N:241:GLY:H | 1.61 | 0.45 |
| 24:4O:240:LEU:HD13 | 24:4O:266:HIS:CE1 | 2.52 | 0.45 |
| 24:4O:254:LYS:O | 40:EE:221:ARG:NH1 | 2.50 | 0.45 |
| 23:4P:193:ARG:HH12 | 41:CN:55:THR:HA | 1.82 | 0.45 |
| 23:4Q:40:THR:O | 23:4Q:44:LEU:HG | 2.16 | 0.45 |
| 23:4Q:250:VAL:HG13 | 23:4Q:253:TYR:HB2 | 1.99 | 0.45 |
| 25:4T:307:GLY:O | 25:4T:309:LEU:N | 2.49 | 0.45 |
| 31:5I:676:ASP:HB2 | 41:IQ:56:GLY:HA2 | 1.97 | 0.45 |
| 31:5I:750:GLU:OE2 | 31:5I:750:GLU:N | 2.49 | 0.45 |
| 33:5O:54:LYS:HE3 | 33:5O:54:LYS:HB3 | 1.86 | 0.45 |
| 34:5Q:65:GLU:O | 34:5Q:69:HIS:ND1 | 2.48 | 0.45 |
| 34:5R:313:LEU:HA | 34:5R:316:ASN:ND2 | 2.32 | 0.45 |
| 35:5T:81:HIS:O | 35:5T:85:HIS:HB2 | 2.17 | 0.45 |
| 35:5T:146:LEU:HA | 35:5T:149:ARG:HB2 | 1.99 | 0.45 |
| 36:5Y:184:HIS:HA | 41:OP:279:GLN:HE22 | 1.82 | 0.45 |
| 37:6A:113:ARG:HG3 | 40:TH:2:ARG:HH22 | 1.82 | 0.45 |
| 41:AM:7:LEU:HD11 | 41:AM:155:ILE:HD12 | 1.98 | 0.45 |
| 41:AM:253:LEU:O | 41:AM:257:MET:HB2 | 2.17 | 0.45 |
| 41:AO:271:ALA:HB1 | 41:AO:289:LEU:HD22 | 1.99 | 0.45 |
| 41:AP:237:THR:O | 41:AP:241:ARG:NH1 | 2.50 | 0.45 |
| 41:AP:283:ALA:HB2 | 41:MP:54:ALA:HA | 1.99 | 0.45 |
| 40:BA:235:VAL:O | 40:BA:239:THR:HG22 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BF:176:GLN:HG3 | 41:BM:331:LEU:CD1 | 2.47 | 0.45 |
| 40:BI:222:PRO:CG | 41:BP:324:LYS:HE3 | 2.47 | 0.45 |
| 40:BI:383:ILE:HG12 | 40:BI:387:TRP:NE1 | 2.32 | 0.45 |
| 40:BI:430:ASP:O | 40:BI:433:GLU:HG3 | 2.16 | 0.45 |
| 41:BM:2:ARG:HE | 41:BM:2:ARG:HB2 | 1.45 | 0.45 |
| 41:BN:167:PHE:CE2 | 41:BN:233:MET:HG2 | 2.52 | 0.45 |
| 41:BO:241:ARG:H | 41:BO:241:ARG:HG2 | 1.62 | 0.45 |
| 41:BO:303:CYS:SG | 41:BO:374:ILE:HA | 2.57 | 0.45 |
| 41:BP:117:LEU:HB3 | 41:BP:121:ARG:HH22 | 1.81 | 0.45 |
| 41:CB:142:GLY:O | 41:CB:144:GLY:N | 2.50 | 0.45 |
| 40:CE:37:PRO:HB2 | 40:CE:40:LYS:HB2 | 1.98 | 0.45 |
| 40:CE:346:TRP:CD1 | 41:CM:391:ARG:HD3 | 2.52 | 0.45 |
| 40:CH:210:TYR:O | 40:CH:214:ARG:HG3 | 2.17 | 0.45 |
| 40:CH:241:SER:O | 40:CH:243:ARG:N | 2.49 | 0.45 |
| 41:CL:183:TYR:CE1 | 41:CL:388:MET:HB2 | 2.52 | 0.45 |
| 41:CN:285:THR:HB | 41:CN:287:PRO:HD2 | 1.99 | 0.45 |
| 41:CO:200:TYR:CE1 | 41:CO:266:PHE:HD2 | 2.35 | 0.45 |
| 41:CO:254:ALA:O | 41:CO:258:VAL:HG22 | 2.16 | 0.45 |
| 41:CP:58:LYS:O | 41:CP:60:VAL:N | 2.50 | 0.45 |
| 40:DF:6:SER:HB3 | 40:DF:138:PHE:CE1 | 2.51 | 0.45 |
| 40:DF:16:ILE:HG12 | 40:DF:17:GLY:N | 2.32 | 0.45 |
| 40:DF:287:SER:O | 40:DF:288:VAL:C | 2.55 | 0.45 |
| 40:DH:261:PRO:HG3 | 40:DH:313:MET:SD | 2.56 | 0.45 |
| 40:DI:3:GLU:HA | 40:DI:51:THR:HG23 | 1.98 | 0.45 |
| 40:DI:224:TYR:HB3 | 42:DI:501:GTP:C6 | 2.51 | 0.45 |
| 40:DI:390:LEU:HD23 | 40:DI:393:LYS:HD2 | 1.99 | 0.45 |
| 41:DL:176:SER:O | 41:DL:177:ASP:C | 2.55 | 0.45 |
| 41:DL:188:SER:O | 41:DL:189:VAL:C | 2.55 | 0.45 |
| 41:DN:6:HIS:CE1 | 41:DN:8:GLN:HE22 | 2.35 | 0.45 |
| 41:DO:131:GLN:NE2 | 41:DO:250:LEU:H | 2.15 | 0.45 |
| 41:DO:165:ASN:ND2 | 41:DO:198:GLU:OE1 | 2.50 | 0.45 |
| 41:DP:362:LYS:HA | 41:DP:362:LYS:HD2 | 1.83 | 0.45 |
| 41:EB:167:PHE:CZ | 41:EB:233:MET:HG2 | 2.52 | 0.45 |
| 40:EF:366:ASP:OD1 | 40:EF:367:LEU:N | 2.50 | 0.45 |
| 40:EI:100:ALA:O | 40:EI:101:ASN:C | 2.54 | 0.45 |
| 40:EI:287:SER:O | 40:EI:288:VAL:C | 2.55 | 0.45 |
| 41:EL:2:ARG:HH22 | 41:EL:251:ARG:HD3 | 1.82 | 0.45 |
| 41:EM:41:ASP:O | 41:EM:44:LEU:N | 2.49 | 0.45 |
| 41:EN:130:LEU:O | 41:EN:162:ARG:NH1 | 2.49 | 0.45 |
| 41:EP:215:LEU:O | 41:EP:217:LEU:N | 2.50 | 0.45 |
| 40:FA:49:PHE:CE2 | 40:FA:55:GLU:HB2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FE:182:VAL:O | 40:FE:186:ASN:ND2 | 2.49 | 0.45 |
| 40:FI:115:ILE:HA | 40:FI:118:VAL:HG22 | 1.99 | 0.45 |
| 40:GE:191:THR:O | 40:GE:195:LEU:HB2 | 2.16 | 0.45 |
| 40:GE:320:ARG:HH11 | 40:GE:360:PRO:HA | 1.82 | 0.45 |
| 40:GF:20:CYS:HA | 40:GF:232:SER:HB2 | 1.99 | 0.45 |
| 40:GG:1:GLN:N | 40:GG:3:GLU:OE2 | 2.50 | 0.45 |
| 40:GH:88:HIS:O | 40:GH:90:GLU:N | 2.49 | 0.45 |
| 40:GH:304:LYS:HD2 | 40:GH:304:LYS:HA | 1.56 | 0.45 |
| 40:GH:431:TYR:O | 40:GH:434:VAL:HG12 | 2.17 | 0.45 |
| 40:GH:436:MET:HE3 | 40:GH:436:MET:HB3 | 1.76 | 0.45 |
| 40:GI:394:PHE:CD2 | 40:GI:421:ARG:HD3 | 2.49 | 0.45 |
| 41:GN:122:LYS:HD3 | 41:GN:123:GLU:HG2 | 1.99 | 0.45 |
| 41:GN:178:THR:O | 41:GN:181:GLU:N | 2.48 | 0.45 |
| 41:GN:358:PRO:HG3 | 41:GN:364:SER:OG | 2.17 | 0.45 |
| 41:GO:334:GLN:HG2 | 41:GO:341:PHE:HE2 | 1.81 | 0.45 |
| 41:GP:51:TYR:HB3 | 41:GP:59:TYR:HB3 | 1.98 | 0.45 |
| 40:HA:38:SER:OG | 40:HA:39:ASP:N | 2.49 | 0.45 |
| 40:HA:285:GLN:N | 40:HA:285:GLN:OE1 | 2.50 | 0.45 |
| 40:HE:57:GLY:O | 40:HE:58:ALA:C | 2.54 | 0.45 |
| 40:HE:185:TYR:HA | 40:HE:394:PHE:HD1 | 1.82 | 0.45 |
| 40:HE:220:GLU:O | 40:HE:222:PRO:HD3 | 2.17 | 0.45 |
| 40:HI:259:LEU:HD21 | 40:HI:316:CYS:SG | 2.57 | 0.45 |
| 41:HM:215:LEU:HD21 | 41:HM:273:LEU:HD22 | 1.99 | 0.45 |
| 41:HM:305:PRO:HB3 | 41:HM:310:TYR:HE1 | 1.82 | 0.45 |
| 41:HM:316:VAL:HA | 41:HM:352:ALA:O | 2.17 | 0.45 |
| 41:HN:361:LEU:O | 41:HN:363:MET:N | 2.50 | 0.45 |
| 41:HQ:139:LEU:HG | 41:HQ:168:SER:HB2 | 1.99 | 0.45 |
| 40:IA:67:PHE:HB3 | 40:IA:75:ILE:HD12 | 1.99 | 0.45 |
| 41:IO:148:GLY:O | 41:IO:152:ILE:HG12 | 2.17 | 0.45 |
| 40:JD:262:TYR:OH | 41:JL:391:ARG:O | 2.29 | 0.45 |
| 40:JG:265:ILE:HG21 | 40:JG:313:MET:HE1 | 1.99 | 0.45 |
| 41:JM:239:CYS:CB | 41:JM:248:ALA:H | 2.30 | 0.45 |
| 41:JO:100:ASN:HB3 | 41:JO:103:LYS:HB3 | 1.98 | 0.45 |
| 40:KE:150:THR:O | 40:KE:154:MET:HG2 | 2.17 | 0.45 |
| 40:KE:251:ASP:HB3 | 40:KE:254:GLU:HG2 | 1.99 | 0.45 |
| 40:KE:405:HIS:CD2 | 41:KL:261:PRO:HG3 | 2.51 | 0.45 |
| 40:KF:274:PRO:HG3 | 40:KF:286:LEU:HD13 | 1.98 | 0.45 |
| 40:KG:16:ILE:HA | 40:KG:228:ASN:HB3 | 1.99 | 0.45 |
| 40:KH:251:ASP:OD1 | 40:KH:252:LEU:N | 2.48 | 0.45 |
| 41:KL:405:GLU:HA | 41:KL:408:PHE:HD2 | 1.82 | 0.45 |
| 41:KM:91:VAL:HG11 | 41:KM:116:VAL:HG22 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LG:352:LYS:HE3 | 41:LO:179:VAL:CG2 | 2.47 | 0.45 |
| 41:LL:128:ASP:N | 41:LL:128:ASP:OD1 | 2.47 | 0.45 |
| 41:LN:7:LEU:HD23 | 41:LN:64:VAL:HB | 1.98 | 0.45 |
| 40:MG:88:HIS:C | 40:MG:90:GLU:H | 2.20 | 0.45 |
| 40:MH:102:ASN:HD21 | 40:MH:407:TYR:HA | 1.82 | 0.45 |
| 41:ML:273:LEU:HD23 | 41:ML:273:LEU:HA | 1.80 | 0.45 |
| 40:NA:232:SER:HA | 40:NA:235:VAL:HG12 | 1.99 | 0.45 |
| 40:ND:101:ASN:HA | 40:ND:144:GLY:HA3 | 1.98 | 0.45 |
| 41:NL:164:MET:HB2 | 41:NL:196:THR:HA | 1.99 | 0.45 |
| 41:NO:167:PHE:CZ | 41:NO:233:MET:HG3 | 2.51 | 0.45 |
| 41:NP:8:GLN:HE22 | 41:NP:21:TRP:HE1 | 1.65 | 0.45 |
| 41:NP:305:PRO:HB3 | 41:NP:310:TYR:HE1 | 1.82 | 0.45 |
| 40:OD:81:GLY:O | 40:OD:84:ARG:N | 2.35 | 0.45 |
| 40:OD:261:PRO:HB3 | 41:OL:394:PHE:CE2 | 2.52 | 0.45 |
| 40:OD:362:VAL:HG21 | 40:OD:369:LYS:HA | 1.99 | 0.45 |
| 40:OE:101:ASN:HA | 40:OE:144:GLY:H | 1.82 | 0.45 |
| 40:OF:130:THR:OG1 | 40:OF:131:GLY:N | 2.49 | 0.45 |
| 40:OH:254:GLU:O | 40:OH:255:PHE:C | 2.55 | 0.45 |
| 41:OO:8:GLN:HE22 | 41:OO:21:TRP:HE1 | 1.64 | 0.45 |
| 41:PB:143:THR:O | 41:PB:147:MET:N | 2.49 | 0.45 |
| 41:PB:248:ALA:HA | 41:PB:252:LYS:HD2 | 1.98 | 0.45 |
| 41:PB:324:LYS:HE2 | 40:PG:222:PRO:HD2 | 1.99 | 0.45 |
| 40:PD:319:TYR:HB3 | 40:PD:323:VAL:HG11 | 1.99 | 0.45 |
| 40:PE:9:VAL:HG12 | 40:PE:68:VAL:HG23 | 1.98 | 0.45 |
| 40:PF:167:LEU:HA | 40:PF:200:CYS:O | 2.16 | 0.45 |
| 40:PF:258:ASN:HD21 | 41:PN:178:THR:HG23 | 1.81 | 0.45 |
| 41:PL:49:VAL:HG11 | 41:PL:241:ARG:HG2 | 1.99 | 0.45 |
| 41:PM:145:SER:O | 41:PM:149:THR:OG1 | 2.25 | 0.45 |
| 41:PO:210:ILE:HD13 | 41:PO:210:ILE:HA | 1.77 | 0.45 |
| 40:QA:213:CYS:HA | 40:QA:217:LEU:HB2 | 1.98 | 0.45 |
| 41:QB:22:GLU:HA | 41:QB:25:SER:HB2 | 1.99 | 0.45 |
| 41:QB:44:LEU:HD22 | 41:QB:44:LEU:HA | 1.72 | 0.45 |
| 41:QB:118:ASP:HA | 41:QB:121:ARG:HH11 | 1.82 | 0.45 |
| 40:QG:141:PHE:HB2 | 40:QG:173:PRO:HD3 | 1.99 | 0.45 |
| 41:QL:187:LEU:HD11 | 41:QL:408:PHE:HE1 | 1.82 | 0.45 |
| 41:QP:56:GLY:O | 41:QP:57:GLY:C | 2.55 | 0.45 |
| 41:QP:117:LEU:HD12 | 41:QP:117:LEU:HA | 1.88 | 0.45 |
| 41:QP:393:ALA:C | 41:QP:395:LEU:N | 2.70 | 0.45 |
| 40:RG:346:TRP:HB3 | 41:RO:391:ARG:HD3 | 1.98 | 0.45 |
| 40:RH:189:LEU:HD11 | 40:RH:417:PHE:HE1 | 1.82 | 0.45 |
| 41:RL:293:MET:HE3 | 41:RL:367:PHE:HD2 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RM:242:PHE:CD2 | 41:RM:356:ILE:HD13 | 2.52 | 0.45 |
| 41:RN:417:ASP:O | 41:RN:421:PRO:HD3 | 2.17 | 0.45 |
| 41:RP:2:ARG:NH1 | 41:RP:249:ASP:OD2 | 2.50 | 0.45 |
| 41:RP:189:VAL:HA | 41:RP:192:LEU:HB2 | 1.99 | 0.45 |
| 40:SE:135:PHE:HB2 | 40:SE:166:LYS:HG3 | 1.99 | 0.45 |
| 40:SF:221:ARG:NH2 | 41:SM:325:GLU:H | 2.13 | 0.45 |
| 40:SG:119:LEU:HA | 40:SG:122:ILE:HG22 | 1.97 | 0.45 |
| 40:SI:221:ARG:NE | 41:SP:322:SER:HB3 | 2.32 | 0.45 |
| 40:TA:167:LEU:HA | 40:TA:200:CYS:O | 2.16 | 0.45 |
| 40:TA:404:VAL:HG13 | 40:TA:417:PHE:HE2 | 1.82 | 0.45 |
| 40:TE:174:ALA:HB3 | 40:TE:178:SER:HA | 1.99 | 0.45 |
| 40:TH:181:VAL:HG22 | 41:TO:256:ASN:HB2 | 1.98 | 0.45 |
| 40:TH:252:LEU:HA | 40:TH:255:PHE:HD2 | 1.81 | 0.45 |
| 40:TH:255:PHE:CZ | 40:TH:318:LEU:HD21 | 2.52 | 0.45 |
| 40:TI:7:VAL:HG13 | 40:TI:66:VAL:HB | 1.98 | 0.45 |
| 41:TL:293:MET:HA | 41:TL:298:ASN:HD21 | 1.82 | 0.45 |
| 41:TN:269:GLY:HA3 | 41:TN:367:PHE:HB3 | 1.98 | 0.45 |
| 41:TO:180:VAL:HG23 | 41:TO:184:ASN:HD21 | 1.82 | 0.45 |
| 40:UF:33:ASP:OD1 | 40:UF:33:ASP:N | 2.47 | 0.45 |
| 40:UF:114:LEU:HB3 | 40:UF:149:PHE:CZ | 2.52 | 0.45 |
| 40:UF:311:LYS:HE3 | 40:UF:311:LYS:HB3 | 1.80 | 0.45 |
| 40:UI:172:TYR:CE1 | 40:UI:386:ALA:HB1 | 2.52 | 0.45 |
| 40:UI:181:VAL:HA | 41:UP:347:ASN:HD22 | 1.82 | 0.45 |
| 40:UI:274:PRO:HG3 | 40:UI:373:ALA:HB2 | 1.99 | 0.45 |
| 40:UI:275:VAL:HA | 40:UI:367:LEU:HD21 | 1.99 | 0.45 |
| 41:UN:119:VAL:O | 41:UN:122:LYS:HB3 | 2.16 | 0.45 |
| 41:UN:398:TYR:HB3 | 41:UN:403:MET:HG2 | 1.98 | 0.45 |
| 41:VB:183:TYR:OH | 41:VB:393:ALA:O | 2.32 | 0.45 |
| 40:VF:142:GLY:HA2 | 40:VF:183:GLU:HG3 | 1.98 | 0.45 |
| 40:VG:239:THR:HG23 | 40:VG:242:LEU:HD21 | 1.98 | 0.45 |
| 40:VJ:248:LEU:HB2 | 40:VJ:355:ILE:HD12 | 1.98 | 0.45 |
| 41:VP:330:MET:HG3 | 41:VP:351:THR:HG22 | 1.99 | 0.45 |
| 40:WA:141:PHE:HB2 | 40:WA:173:PRO:HD3 | 1.99 | 0.45 |
| 40:WA:178:SER:HB2 | 40:WA:183:GLU:HG3 | 1.99 | 0.45 |
| 41:WB:189:VAL:O | 41:WB:193:VAL:HG23 | 2.17 | 0.45 |
| 40:WE:73:THR:HA | 40:WE:76:ASP:HB2 | 1.98 | 0.45 |
| 40:WG:16:ILE:HA | 40:WG:228:ASN:HB3 | 1.98 | 0.45 |
| 40:WH:18:ASN:O | 40:WH:22:GLU:HB2 | 2.17 | 0.45 |
| 40:WH:90:GLU:OE1 | 40:WH:121:ARG:NE | 2.49 | 0.45 |
| 41:WM:271:ALA:HB3 | 41:WM:272:PRO:HD3 | 1.99 | 0.45 |
| 11:2I:160:LYS:O | 11:2I:163:GLU:HG3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:2I:236:GLN:H | 11:2I:236:GLN:HG3 | 1.66 | 0.45 |
| 12:2R:65:ARG:HB2 | 12:2R:159:LEU:HA | 1.97 | 0.45 |
| 13:2T:53:ASN:HB3 | 13:2T:56:THR:HG22 | 1.98 | 0.45 |
| 13:2T:66:LYS:HB3 | 13:2T:66:LYS:HE3 | 1.68 | 0.45 |
| 15:3E:48:ILE:HD11 | 15:3F:350:ARG:NH1 | 2.32 | 0.45 |
| 15:3E:205:VAL:O | 15:3E:206:ARG:NE | 2.49 | 0.45 |
| 15:3F:129:ARG:HB3 | 15:3F:134:GLN:HE22 | 1.81 | 0.45 |
| 15:3H:105:LEU:HD11 | 15:3H:146:VAL:HG23 | 1.98 | 0.45 |
| 17:3O:360:LYS:HB3 | 17:3O:360:LYS:HE2 | 1.84 | 0.45 |
| 17:3R:147:GLY:O | 17:3R:150:VAL:HB | 2.16 | 0.45 |
| 21:4F:421:ARG:H | 21:4F:421:ARG:HG2 | 1.40 | 0.45 |
| 22:4J:619:VAL:HG12 | 22:4J:677:LEU:HD22 | 1.99 | 0.45 |
| 22:4K:676:ALA:O | 22:4K:677:LEU:C | 2.54 | 0.45 |
| 23:4M:91:ILE:HD11 | 40:AG:79:ARG:CD | 2.43 | 0.45 |
| 23:4M:100:GLN:HB3 | 23:4M:103:PHE:HZ | 1.82 | 0.45 |
| 23:4P:240:LEU:HB2 | 23:4P:241:GLY:H | 1.61 | 0.45 |
| 23:4Q:245:LYS:HA | 23:4Q:245:LYS:HD2 | 1.64 | 0.45 |
| 23:4Q:259:ARG:NH2 | 40:EH:366:ASP:N | 2.65 | 0.45 |
| 27:4Y:6:TYR:HD2 | 27:4Y:10:VAL:HG11 | 1.82 | 0.45 |
| 27:4Y:132:ALA:HB2 | 27:4Y:148:ARG:HB2 | 1.99 | 0.45 |
| 27:4Z:125:ASN:ND2 | 27:4Z:125:ASN:O | 2.50 | 0.45 |
| 34:5R:451:LEU:O | 34:5R:455:ILE:HG13 | 2.17 | 0.45 |
| 36:5X:133:ALA:HA | 36:5X:136:ASN:HB3 | 1.98 | 0.45 |
| 39:6L:127:LEU:O | 39:6L:128:SER:C | 2.55 | 0.45 |
| 40:AF:255:PHE:O | 40:AF:259:LEU:HB2 | 2.16 | 0.45 |
| 40:AG:6:SER:O | 40:AG:65:ALA:HA | 2.17 | 0.45 |
| 40:AH:164:LYS:HD3 | 40:AH:164:LYS:HA | 1.82 | 0.45 |
| 41:AL:25:SER:OG | 41:AL:51:TYR:OH | 2.29 | 0.45 |
| 41:AM:100:ASN:HD21 | 41:AM:397:TRP:HB3 | 1.82 | 0.45 |
| 41:AM:202:ILE:HG21 | 41:AM:229:VAL:HG22 | 1.99 | 0.45 |
| 41:AO:379:LYS:HE2 | 41:AO:379:LYS:HB2 | 1.43 | 0.45 |
| 41:AP:51:TYR:HB3 | 41:AP:59:TYR:HB3 | 1.99 | 0.45 |
| 40:BA:376:MET:SD | 40:BA:378:SER:HB3 | 2.57 | 0.45 |
| 41:BB:101:TRP:HZ3 | 41:BB:106:TYR:HE2 | 1.65 | 0.45 |
| 40:BH:162:GLY:O | 40:BH:164:LYS:N | 2.50 | 0.45 |
| 41:BM:376:GLU:O | 41:BM:377:LEU:C | 2.55 | 0.45 |
| 41:BN:107:THR:O | 41:BN:109:GLY:N | 2.50 | 0.45 |
| 40:CA:416:GLU:H | 40:CA:416:GLU:HG3 | 1.59 | 0.45 |
| 40:CA:429:LYS:HB2 | 40:CA:429:LYS:HE2 | 1.67 | 0.45 |
| 40:CH:236:SER:HA | 40:CH:239:THR:HG22 | 1.99 | 0.45 |
| 40:CH:276:ILE:HB | 40:CH:281:ALA:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CL:4:ILE:HG13 | 41:CL:49:VAL:O | 2.16 | 0.45 |
| 41:CL:257:MET:HA | 41:CL:312:THR:OG1 | 2.17 | 0.45 |
| 41:CM:28:HIS:O | 41:CM:29:GLY:C | 2.55 | 0.45 |
| 41:CO:200:TYR:CE1 | 41:CO:368:ILE:HG13 | 2.52 | 0.45 |
| 40:DA:413:GLU:O | 40:DA:415:GLY:N | 2.49 | 0.45 |
| 41:DB:140:GLY:HA3 | 41:DB:181:GLU:HG3 | 1.99 | 0.45 |
| 40:DE:250:VAL:HG23 | 40:DE:254:GLU:HB3 | 1.99 | 0.45 |
| 40:DF:105:ARG:HD2 | 40:DF:110:ILE:HG22 | 1.99 | 0.45 |
| 40:DG:116:ASP:OD1 | 40:DG:117:LEU:N | 2.50 | 0.45 |
| 40:DI:60:LYS:O | 40:DI:61:HIS:C | 2.55 | 0.45 |
| 40:DI:304:LYS:HA | 40:DI:304:LYS:HD2 | 1.36 | 0.45 |
| 41:DL:117:LEU:HD22 | 41:DL:121:ARG:HH12 | 1.82 | 0.45 |
| 41:DL:238:THR:C | 41:DL:240:LEU:H | 2.20 | 0.45 |
| 41:DM:21:TRP:HZ2 | 41:DM:63:ALA:HB2 | 1.82 | 0.45 |
| 41:DM:130:LEU:O | 41:DM:131:GLN:C | 2.54 | 0.45 |
| 41:DM:172:SER:HB2 | 41:DM:205:GLU:HB2 | 1.99 | 0.45 |
| 41:DM:273:LEU:HD23 | 41:DM:273:LEU:HA | 1.76 | 0.45 |
| 41:DN:68:LEU:HD11 | 41:DN:109:GLY:HA2 | 1.98 | 0.45 |
| 41:DN:375:GLN:HB2 | 41:DN:422:VAL:CG1 | 2.47 | 0.45 |
| 41:DP:139:LEU:O | 41:DP:141:GLY:N | 2.50 | 0.45 |
| 41:DP:183:TYR:O | 41:DP:184:ASN:C | 2.54 | 0.45 |
| 40:EA:112:LYS:HA | 40:EA:115:ILE:HG22 | 1.98 | 0.45 |
| 40:EH:240:ALA:HA | 40:EH:243:ARG:HE | 1.82 | 0.45 |
| 40:EI:166:LYS:HB3 | 40:EI:166:LYS:HE2 | 1.64 | 0.45 |
| 41:EM:125:GLU:O | 41:EM:127:CYS:N | 2.50 | 0.45 |
| 41:EM:127:CYS:SG | 41:EM:127:CYS:O | 2.75 | 0.45 |
| 41:EN:8:GLN:OE1 | 41:EN:14:ASN:HA | 2.17 | 0.45 |
| 41:EO:151:LEU:O | 41:EO:155:ILE:HG12 | 2.16 | 0.45 |
| 40:FA:261:PRO:HD2 | 40:FA:265:ILE:HG13 | 1.99 | 0.45 |
| 40:FE:16:ILE:HA | 40:FE:228:ASN:HB3 | 1.98 | 0.45 |
| 40:FE:88:HIS:ND1 | 40:GE:283:HIS:HB2 | 2.31 | 0.45 |
| 40:FH:260:VAL:HG23 | 40:FH:379:ASN:ND2 | 2.32 | 0.45 |
| 41:FM:293:MET:HG2 | 41:FM:367:PHE:HD1 | 1.82 | 0.45 |
| 41:FP:184:ASN:OD1 | 41:FP:398:TYR:OH | 2.35 | 0.45 |
| 41:FP:234:SER:O | 41:FP:238:THR:HB | 2.17 | 0.45 |
| 40:GG:324:VAL:O | 40:GG:328:VAL:HG23 | 2.17 | 0.45 |
| 41:GM:135:LEU:HD21 | 41:GM:148:GLY:HA2 | 1.98 | 0.45 |
| 41:GM:237:THR:O | 41:GM:241:ARG:NH2 | 2.50 | 0.45 |
| 41:GO:42:LEU:HD11 | 41:GO:243:PRO:HG3 | 1.98 | 0.45 |
| 41:GO:207:LEU:HB3 | 41:GO:225:LEU:HD12 | 1.98 | 0.45 |
| 41:GP:207:LEU:HB3 | 41:GP:225:LEU:HD12 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HE:164:LYS:HA | 40:HE:164:LYS:HD3 | 1.58 | 0.45 |
| 40:HG:188:ILE:HD12 | 40:HG:424:MET:HG3 | 1.99 | 0.45 |
| 40:HH:188:ILE:HG22 | 40:HH:420:ALA:HB1 | 1.99 | 0.45 |
| 40:HI:104:ALA:O | 40:HI:108:TYR:HB2 | 2.17 | 0.45 |
| 41:HQ:218:THR:HG23 | 41:HQ:219:THR:HG22 | 1.98 | 0.45 |
| 40:IE:229:ARG:HD2 | 40:IE:363:VAL:HG11 | 1.99 | 0.45 |
| 40:IG:9:VAL:HG21 | 40:IG:150:THR:HB | 1.98 | 0.45 |
| 40:II:174:ALA:HB3 | 40:II:178:SER:H | 1.81 | 0.45 |
| 41:IM:19:LYS:HA | 41:IM:22:GLU:OE1 | 2.17 | 0.45 |
| 41:IN:165:ASN:HD21 | 41:IN:250:LEU:HD13 | 1.82 | 0.45 |
| 40:JD:172:TYR:OH | 40:JD:386:ALA:O | 2.34 | 0.45 |
| 40:JF:140:SER:OG | 42:JF:501:GTP:O2A | 2.28 | 0.45 |
| 41:JL:274:THR:HG21 | 41:JL:282:ARG:HG3 | 1.98 | 0.45 |
| 40:KA:76:ASP:HA | 40:KA:79:ARG:HG2 | 1.98 | 0.45 |
| 40:KA:400:LYS:HD2 | 41:KN:344:TRP:CE3 | 2.52 | 0.45 |
| 41:KB:282:ARG:HD3 | 41:KB:283:ALA:N | 2.30 | 0.45 |
| 40:KF:376:MET:SD | 40:KF:378:SER:HB3 | 2.57 | 0.45 |
| 40:KG:182:VAL:O | 40:KG:186:ASN:ND2 | 2.48 | 0.45 |
| 40:KH:319:TYR:HB3 | 40:KH:323:VAL:HG21 | 1.99 | 0.45 |
| 41:KL:154:LYS:O | 41:KL:157:GLU:HG3 | 2.16 | 0.45 |
| 41:KO:132:GLY:HA2 | 41:KO:163:ILE:O | 2.17 | 0.45 |
| 41:KP:87:PRO:HD3 | 41:LP:281:TYR:HD2 | 1.82 | 0.45 |
| 40:LD:70:LEU:HD23 | 40:LD:114:LEU:HD12 | 1.99 | 0.45 |
| 40:LE:16:ILE:HG21 | 40:LE:138:PHE:CD1 | 2.52 | 0.45 |
| 40:LG:110:ILE:H | 40:LG:110:ILE:HG12 | 1.49 | 0.45 |
| 40:LH:405:HIS:HA | 40:LH:408:VAL:HG22 | 1.98 | 0.45 |
| 41:LP:211:CYS:HA | 41:LP:215:LEU:HB2 | 1.98 | 0.45 |
| 40:MA:271:THR:HG23 | 40:MA:376:MET:HB3 | 1.98 | 0.45 |
| 40:MA:414:GLU:O | 40:MA:415:GLY:C | 2.54 | 0.45 |
| 40:MD:259:LEU:O | 40:MD:379:ASN:ND2 | 2.44 | 0.45 |
| 40:MG:326:LYS:HD2 | 40:MG:326:LYS:HA | 1.72 | 0.45 |
| 41:MM:26:ASP:HB3 | 41:MM:359:ARG:HH22 | 1.82 | 0.45 |
| 41:MM:401:GLU:N | 41:MM:401:GLU:OE2 | 2.48 | 0.45 |
| 41:MP:178:THR:HG22 | 41:MP:180:VAL:H | 1.82 | 0.45 |
| 40:NA:204:VAL:HG13 | 40:NA:302:MET:HB3 | 1.98 | 0.45 |
| 41:NB:313:VAL:HB | 41:NB:349:VAL:HA | 1.98 | 0.45 |
| 40:NE:107:HIS:CD2 | 40:NE:152:LEU:HB2 | 2.51 | 0.45 |
| 41:NN:385:PHE:HZ | 41:NN:408:PHE:HD2 | 1.65 | 0.45 |
| 40:OD:136:LEU:HD22 | 40:OD:169:PHE:HE2 | 1.80 | 0.45 |
| 40:OG:362:VAL:HG22 | 40:OG:369:LYS:HB3 | 1.97 | 0.45 |
| 40:OH:417:PHE:O | 40:OH:418:SER:C | 2.55 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OL:7:LEU:HD22 | 41:OL:151:LEU:HD21 | 1.97 | 0.45 |
| 41:OO:206:ALA:O | 41:OO:210:ILE:HD12 | 2.16 | 0.45 |
| 40:PA:179:THR:HG21 | 42:PN:501:GTP:H3' | 1.98 | 0.45 |
| 41:PN:137:HIS:O | 41:PN:168:SER:HA | 2.17 | 0.45 |
| 41:QB:262:ARG:HA | 41:QB:264:HIS:CE1 | 2.51 | 0.45 |
| 40:QF:205:ASP:O | 40:QF:209:ILE:HG13 | 2.17 | 0.45 |
| 40:RA:387:TRP:HE3 | 40:RA:424:MET:HE1 | 1.82 | 0.45 |
| 41:RB:193:VAL:HG11 | 41:RB:418:LEU:HG | 1.99 | 0.45 |
| 40:RF:71:GLU:HA | 40:RF:72:PRO:HD3 | 1.85 | 0.45 |
| 40:RG:228:ASN:ND2 | 42:RG:501:GTP:HN1 | 2.09 | 0.45 |
| 40:RH:210:TYR:CD1 | 41:RO:324:LYS:HD3 | 2.51 | 0.45 |
| 41:RM:64:VAL:HG21 | 41:RM:120:VAL:HG12 | 1.99 | 0.45 |
| 41:RM:311:LEU:N | 41:RM:370:ASN:O | 2.49 | 0.45 |
| 41:RN:156:ARG:HH21 | 41:RN:196:THR:HA | 1.81 | 0.45 |
| 41:RO:3:GLU:HA | 41:RO:49:VAL:HG13 | 1.99 | 0.45 |
| 41:RO:58:LYS:HD3 | 41:RO:58:LYS:HA | 1.87 | 0.45 |
| 41:RP:8:GLN:HG2 | 41:RP:65:LEU:HA | 1.99 | 0.45 |
| 41:RP:117:LEU:HA | 41:RP:120:VAL:HG12 | 1.98 | 0.45 |
| 41:SB:322:SER:HB3 | 40:SG:221:ARG:NE | 2.32 | 0.45 |
| 40:SF:145:THR:OG1 | 42:SM:501:GTP:O2B | 2.34 | 0.45 |
| 40:SI:88:HIS:CD2 | 40:SI:121:ARG:HH22 | 2.35 | 0.45 |
| 41:SN:2:ARG:HH21 | 41:SN:240:LEU:HB2 | 1.80 | 0.45 |
| 41:SN:3:GLU:OE1 | 41:SN:3:GLU:N | 2.49 | 0.45 |
| 41:SN:103:LYS:HA | 41:SN:107:THR:OG1 | 2.17 | 0.45 |
| 40:TA:7:VAL:HB | 40:TA:137:ILE:HG13 | 1.99 | 0.45 |
| 40:TA:219:ILE:HD12 | 40:TA:222:PRO:HB3 | 1.98 | 0.45 |
| 40:TF:33:ASP:OD1 | 40:TF:34:GLY:N | 2.50 | 0.45 |
| 40:TI:205:ASP:HB2 | 40:TI:303:VAL:HG22 | 1.99 | 0.45 |
| 40:TI:244:PHE:CG | 40:TI:358:GLN:HG3 | 2.52 | 0.45 |
| 41:TN:104:GLY:HA3 | 41:TN:146:GLY:HA3 | 1.99 | 0.45 |
| 41:UB:189:VAL:O | 41:UB:193:VAL:HG23 | 2.17 | 0.45 |
| 41:UB:236:VAL:HG22 | 41:UB:368:ILE:HD11 | 1.99 | 0.45 |
| 40:UE:224:TYR:O | 40:UE:228:ASN:ND2 | 2.49 | 0.45 |
| 40:UF:182:VAL:O | 40:UF:183:GLU:C | 2.56 | 0.45 |
| 41:UM:375:GLN:HE22 | 41:UM:419:GLY:HA2 | 1.82 | 0.45 |
| 41:UN:132:GLY:HA3 | 41:UN:163:ILE:O | 2.17 | 0.45 |
| 41:UN:317:PHE:O | 41:UN:353:VAL:HA | 2.17 | 0.45 |
| 41:UO:207:LEU:HB3 | 41:UO:225:LEU:HD12 | 1.99 | 0.45 |
| 40:VA:318:LEU:O | 40:VA:374:VAL:HA | 2.17 | 0.45 |
| 40:VG:319:TYR:HB3 | 40:VG:323:VAL:HG11 | 1.99 | 0.45 |
| 40:VJ:139:HIS:ND1 | 40:VJ:140:SER:O | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VJ:240:ALA:HB1 | 40:VJ:356:ASN:HD22 | 1.82 | 0.45 |
| 40:WA:403:PHE:HE2 | 41:WN:345:ILE:HD13 | 1.82 | 0.45 |
| 41:WN:162:ARG:HH22 | 41:WN:251:ARG:HH12 | 1.65 | 0.45 |
| 41:WN:377:LEU:HD13 | 41:WN:380:ARG:HH21 | 1.81 | 0.45 |
| 41:WO:287:PRO:HA | 41:WO:329:GLN:NE2 | 2.32 | 0.45 |
| 41:WP:30:ILE:HD11 | 41:WP:47:ILE:HD11 | 1.98 | 0.45 |
| 10:2F:157:ARG:CZ | 41:VB:51:TYR:HB3 | 2.47 | 0.44 |
| 11:2I:157:TYR:CE1 | 11:2I:158:ILE:HG12 | 2.51 | 0.44 |
| 11:2I:200:LEU:HD11 | 11:2I:244:LEU:HD13 | 1.98 | 0.44 |
| 11:2K:231:GLU:HG3 | 11:2K:232:GLU:N | 2.31 | 0.44 |
| 13:2V:57:THR:HG23 | 13:2V:158:ALA:HB2 | 2.00 | 0.44 |
| 13:2W:67:LYS:HE2 | 13:2W:67:LYS:HB2 | 1.52 | 0.44 |
| 14:3B:8:ASN:HD22 | 41:ML:304:ASP:N | 2.15 | 0.44 |
| 14:3B:56:SER:OG | 14:3B:57:LYS:N | 2.49 | 0.44 |
| 14:3C:52:SER:OG | 14:3C:53:VAL:N | 2.47 | 0.44 |
| 18:3U:96:GLN:NE2 | 18:3U:233:ASN:OD1 | 2.45 | 0.44 |
| 18:3U:278:LEU:O | 18:3U:282:ILE:HG12 | 2.17 | 0.44 |
| 18:3V:127:GLU:OE2 | 18:3V:279:ARG:NE | 2.42 | 0.44 |
| 19:3Y:34:ILE:HD11 | 19:3Z:381:SER:HA | 1.98 | 0.44 |
| 19:3Y:278:TRP:HZ2 | 19:3Y:281:MET:HG2 | 1.80 | 0.44 |
| 20:4A:27:GLN:H | 20:4A:27:GLN:HG3 | 1.56 | 0.44 |
| 21:4D:243:LEU:HD22 | 21:4D:351:THR:HG23 | 1.99 | 0.44 |
| 21:4F:94:LYS:HB3 | 40:AE:42:ILE:HD12 | 1.98 | 0.44 |
| 21:4F:482:PRO:O | 21:4F:483:ILE:C | 2.56 | 0.44 |
| 22:4H:38:GLU:OE1 | 41:AL:276:ARG:NH2 | 2.49 | 0.44 |
| 22:4J:56:LYS:HD2 | 22:4J:56:LYS:HA | 1.69 | 0.44 |
| 22:4K:623:ALA:HB1 | 22:4K:669:PHE:CZ | 2.51 | 0.44 |
| 23:4P:217:LYS:HD2 | 23:4P:217:LYS:HA | 1.55 | 0.44 |
| 23:4Q:262:GLY:C | 23:4Q:264:LEU:H | 2.20 | 0.44 |
| 26:4V:299:MET:HB2 | 26:4V:351:ILE:HD12 | 1.99 | 0.44 |
| 26:4V:370:TYR:HD1 | 26:4V:374:ILE:HB | 1.82 | 0.44 |
| 27:4Z:33:ARG:HA | 27:4Z:38:LEU:HD22 | 1.99 | 0.44 |
| 31:5I:377:ILE:HD11 | 41:IB:217:LEU:HD11 | 1.98 | 0.44 |
| 31:5I:685:GLU:O | 31:5I:713:ILE:HG22 | 2.17 | 0.44 |
| 37:6A:122:LYS:NZ | 40:TH:1:GLN:HG2 | 2.31 | 0.44 |
| 39:6J:26:THR:O | 39:6J:30:ALA:N | 2.43 | 0.44 |
| 40:AA:234:ILE:HD11 | 40:AA:302:MET:SD | 2.57 | 0.44 |
| 40:AA:273:ALA:HB3 | 40:AA:374:VAL:H | 1.82 | 0.44 |
| 41:AB:308:GLY:HA3 | 41:AB:372:THR:HB | 1.99 | 0.44 |
| 40:AF:425:ALA:O | 40:AF:429:LYS:HG2 | 2.17 | 0.44 |
| 40:AG:237:SER:HA | 40:AG:320:ARG:HD2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AM:263:LEU:O | 41:AM:370:ASN:ND2 | 2.48 | 0.44 |
| 41:AO:280:GLN:HB2 | 41:MO:58:LYS:NZ | 2.32 | 0.44 |
| 41:BB:420:ASN:HB2 | 41:BB:421:PRO:HD3 | 1.99 | 0.44 |
| 40:BE:30:ILE:HG21 | 40:BE:61:HIS:HB2 | 1.98 | 0.44 |
| 40:BE:265:ILE:H | 40:BE:265:ILE:HG12 | 1.48 | 0.44 |
| 40:BF:326:LYS:HD2 | 41:BN:220:PRO:HB2 | 1.99 | 0.44 |
| 40:BG:274:PRO:HG3 | 40:BG:286:LEU:HD12 | 1.99 | 0.44 |
| 40:BH:213:CYS:HA | 40:BH:217:LEU:HD23 | 1.99 | 0.44 |
| 40:BH:261:PRO:HB3 | 40:BH:346:TRP:HH2 | 1.81 | 0.44 |
| 40:BI:308:ARG:O | 40:BI:310:GLY:N | 2.51 | 0.44 |
| 41:BL:41:ASP:N | 41:BL:41:ASP:OD1 | 2.50 | 0.44 |
| 41:BM:108:GLU:O | 41:BM:109:GLY:C | 2.55 | 0.44 |
| 41:BN:203:ASP:OD1 | 41:BN:204:ASN:N | 2.50 | 0.44 |
| 41:BP:192:LEU:HD22 | 41:BP:196:THR:HB | 1.98 | 0.44 |
| 40:CA:21:TRP:CD1 | 40:CA:67:PHE:HZ | 2.35 | 0.44 |
| 41:CB:239:CYS:HB2 | 41:CB:248:ALA:H | 1.82 | 0.44 |
| 40:CH:395:ASP:O | 40:CH:397:MET:N | 2.50 | 0.44 |
| 40:CI:238:ILE:HA | 40:CI:318:LEU:HD22 | 1.99 | 0.44 |
| 41:CM:342:VAL:HB | 41:CM:344:TRP:NE1 | 2.32 | 0.44 |
| 41:CN:100:ASN:O | 41:CN:102:ALA:N | 2.50 | 0.44 |
| 41:CO:68:LEU:HD21 | 41:CO:109:GLY:HA2 | 1.98 | 0.44 |
| 40:DA:344:VAL:HG13 | 40:DA:345:ASP:N | 2.32 | 0.44 |
| 40:DF:418:SER:O | 40:DF:419:GLU:C | 2.56 | 0.44 |
| 40:DH:177:VAL:HG13 | 40:DH:178:SER:H | 1.82 | 0.44 |
| 40:DH:185:TYR:O | 40:DH:186:ASN:C | 2.55 | 0.44 |
| 40:DH:220:GLU:O | 40:DH:221:ARG:NE | 2.48 | 0.44 |
| 41:DL:56:GLY:O | 41:DL:57:GLY:C | 2.56 | 0.44 |
| 41:DL:285:THR:O | 41:DL:286:VAL:C | 2.55 | 0.44 |
| 41:DM:41:ASP:C | 41:DM:43:GLN:N | 2.71 | 0.44 |
| 41:DM:162:ARG:HA | 41:DM:162:ARG:HD3 | 1.55 | 0.44 |
| 41:DM:226:ASN:HD22 | 41:DM:226:ASN:HA | 1.48 | 0.44 |
| 41:DM:335:ASN:O | 41:DM:336:LYS:C | 2.55 | 0.44 |
| 41:DN:36:TYR:CE2 | 41:DN:44:LEU:HD22 | 2.52 | 0.44 |
| 41:DN:46:ARG:HA | 41:DN:46:ARG:HD3 | 1.62 | 0.44 |
| 41:DN:75:SER:O | 41:DN:76:VAL:C | 2.55 | 0.44 |
| 40:EA:77:GLU:HA | 40:EA:80:THR:HG22 | 1.99 | 0.44 |
| 41:EB:397:TRP:O | 41:EB:401:GLU:HG2 | 2.16 | 0.44 |
| 40:EF:222:PRO:HD2 | 41:EM:324:LYS:HD2 | 1.99 | 0.44 |
| 40:EH:89:PRO:O | 40:EH:90:GLU:C | 2.55 | 0.44 |
| 40:EI:380:THR:OG1 | 40:EI:381:THR:N | 2.50 | 0.44 |
| 40:EI:414:GLU:O | 40:EI:416:GLU:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EL:313:VAL:HB | 41:EL:349:VAL:HG12 | 1.99 | 0.44 |
| 41:EM:193:VAL:O | 41:EM:195:ASN:N | 2.47 | 0.44 |
| 41:EN:134:GLN:HA | 41:EN:165:ASN:O | 2.17 | 0.44 |
| 40:FA:52:PHE:HE1 | 40:FA:239:THR:HG21 | 1.82 | 0.44 |
| 41:FB:318:ARG:HH11 | 41:FB:358:PRO:HD3 | 1.82 | 0.44 |
| 40:FF:285:GLN:HG3 | 40:FF:287:SER:HB3 | 1.98 | 0.44 |
| 40:FG:191:THR:O | 40:FG:195:LEU:HG | 2.17 | 0.44 |
| 40:GA:224:TYR:HE2 | 41:GN:323:MET:CB | 2.30 | 0.44 |
| 40:GE:114:LEU:O | 40:GE:118:VAL:HG12 | 2.18 | 0.44 |
| 40:GG:132:LEU:O | 40:GG:164:LYS:NZ | 2.48 | 0.44 |
| 40:GG:180:ALA:HB3 | 40:GG:183:GLU:HG3 | 1.99 | 0.44 |
| 40:GG:231:ILE:HA | 40:GG:234:ILE:HG22 | 1.99 | 0.44 |
| 40:GH:107:HIS:HB2 | 40:GH:148:GLY:HA2 | 1.99 | 0.44 |
| 40:GH:344:VAL:HG23 | 40:GH:347:CYS:HB3 | 2.00 | 0.44 |
| 40:GI:221:ARG:CA | 41:GP:324:LYS:NZ | 2.80 | 0.44 |
| 41:GO:109:GLY:O | 41:GO:113:VAL:HG13 | 2.18 | 0.44 |
| 41:GO:139:LEU:HG | 41:GO:168:SER:HB3 | 1.98 | 0.44 |
| 41:GP:289:LEU:O | 41:GP:293:MET:HB2 | 2.17 | 0.44 |
| 40:HE:100:ALA:O | 40:HE:101:ASN:C | 2.55 | 0.44 |
| 40:HF:107:HIS:CE1 | 40:HF:151:SER:HG | 2.35 | 0.44 |
| 41:HM:25:SER:O | 41:HM:30:ILE:N | 2.48 | 0.44 |
| 41:HO:69:GLU:HA | 41:HO:70:PRO:HD3 | 1.86 | 0.44 |
| 41:HQ:108:GLU:HA | 41:HQ:111:GLU:HB3 | 1.99 | 0.44 |
| 41:HQ:319:GLY:HA2 | 41:HQ:357:PRO:HG3 | 1.99 | 0.44 |
| 40:IF:213:CYS:HA | 40:IF:217:LEU:HB3 | 1.99 | 0.44 |
| 40:IH:167:LEU:HA | 40:IH:200:CYS:O | 2.17 | 0.44 |
| 41:IM:323:MET:O | 41:IM:327:ASP:HB2 | 2.17 | 0.44 |
| 41:IO:319:GLY:HA2 | 41:IO:357:PRO:HD3 | 1.98 | 0.44 |
| 41:IP:131:GLN:NE2 | 41:IP:249:ASP:OD2 | 2.43 | 0.44 |
| 40:JD:180:ALA:HB3 | 40:JD:183:GLU:HG3 | 1.98 | 0.44 |
| 40:JE:142:GLY:HA2 | 40:JE:183:GLU:HG2 | 1.99 | 0.44 |
| 40:JE:352:LYS:HZ3 | 41:JM:178:THR:N | 2.15 | 0.44 |
| 41:JL:131:GLN:HE22 | 41:JL:250:LEU:H | 1.64 | 0.44 |
| 41:JM:189:VAL:O | 41:JM:193:VAL:HG13 | 2.17 | 0.44 |
| 41:JM:354:CYS:SG | 41:JM:355:ASP:N | 2.88 | 0.44 |
| 41:JN:8:GLN:N | 41:JN:8:GLN:OE1 | 2.50 | 0.44 |
| 40:KA:72:PRO:HD2 | 41:KN:2:ARG:HH12 | 1.81 | 0.44 |
| 40:KE:6:SER:O | 40:KE:65:ALA:HA | 2.16 | 0.44 |
| 41:KP:107:THR:O | 41:KP:110:ALA:N | 2.50 | 0.44 |
| 40:LE:28:HIS:CE1 | 40:LE:49:PHE:HA | 2.52 | 0.44 |
| 40:LF:230:LEU:HA | 40:LF:230:LEU:HD23 | 1.75 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LG:288:VAL:HG22 | 40:LG:323:VAL:HG12 | 1.99 | 0.44 |
| 40:LG:328:VAL:HG11 | 40:LG:353:VAL:HG11 | 1.99 | 0.44 |
| 40:LH:140:SER:OG | 42:LO:501:GTP:O2A | 2.35 | 0.44 |
| 41:LP:128:ASP:N | 41:LP:128:ASP:OD2 | 2.50 | 0.44 |
| 40:MF:3:GLU:HG3 | 40:MF:129:CYS:HB2 | 1.99 | 0.44 |
| 41:MO:336:LYS:HE3 | 41:MO:336:LYS:HB2 | 1.54 | 0.44 |
| 41:MP:91:VAL:HG11 | 41:MP:116:VAL:HG22 | 1.99 | 0.44 |
| 40:NF:135:PHE:HE2 | 40:NF:157:LEU:HD22 | 1.82 | 0.44 |
| 40:NH:326:LYS:HZ1 | 41:NP:225:LEU:HD11 | 1.82 | 0.44 |
| 41:NM:28:HIS:CE1 | 41:NM:241:ARG:HD3 | 2.52 | 0.44 |
| 41:NM:290:THR:HG21 | 41:NM:329:GLN:HB3 | 1.99 | 0.44 |
| 41:NN:314:ALA:HB3 | 41:NN:368:ILE:HB | 1.99 | 0.44 |
| 40:OA:209:ILE:HA | 40:OA:212:ILE:HG22 | 2.00 | 0.44 |
| 40:OH:123:ARG:O | 40:OH:124:LYS:C | 2.55 | 0.44 |
| 41:OL:215:LEU:HD21 | 41:OL:273:LEU:HD22 | 1.99 | 0.44 |
| 40:PE:116:ASP:N | 40:PE:116:ASP:OD1 | 2.49 | 0.44 |
| 40:PH:135:PHE:HB2 | 40:PH:166:LYS:HB3 | 1.99 | 0.44 |
| 40:PH:325:PRO:HA | 40:PH:328:VAL:HG12 | 1.99 | 0.44 |
| 41:PM:256:ASN:HD22 | 41:PM:350:LYS:HD3 | 1.82 | 0.44 |
| 41:PN:7:LEU:O | 41:PN:135:LEU:HA | 2.17 | 0.44 |
| 41:PP:171:PRO:HB3 | 41:PP:181:GLU:HG2 | 1.98 | 0.44 |
| 41:QB:121:ARG:HG3 | 41:QB:125:GLU:HG3 | 1.99 | 0.44 |
| 41:QN:3:GLU:HG2 | 41:QN:62:ARG:HH12 | 1.82 | 0.44 |
| 41:RB:262:ARG:HB3 | 41:RB:418:LEU:HD11 | 1.98 | 0.44 |
| 40:RE:152:LEU:O | 40:RE:156:ARG:HG2 | 2.17 | 0.44 |
| 40:RG:47:ASP:O | 40:RG:50:ASN:CB | 2.65 | 0.44 |
| 40:RG:79:ARG:HG3 | 40:RG:92:LEU:HD22 | 1.98 | 0.44 |
| 41:RO:230:SER:HA | 41:RO:233:MET:HE3 | 1.99 | 0.44 |
| 40:SA:109:THR:HG21 | 40:SA:410:GLU:OE2 | 2.16 | 0.44 |
| 40:SA:304:LYS:HD2 | 40:SA:304:LYS:HA | 1.73 | 0.44 |
| 40:SE:223:THR:OG1 | 40:SE:224:TYR:N | 2.50 | 0.44 |
| 40:SF:301:GLN:OE1 | 40:SF:301:GLN:N | 2.43 | 0.44 |
| 40:SG:21:TRP:CZ3 | 40:SG:63:PRO:HB3 | 2.52 | 0.44 |
| 40:SG:132:LEU:O | 40:SG:164:LYS:NZ | 2.33 | 0.44 |
| 40:SH:205:ASP:HB3 | 40:SH:303:VAL:HA | 1.99 | 0.44 |
| 40:SH:265:ILE:HG13 | 40:SH:379:ASN:HD21 | 1.82 | 0.44 |
| 40:SH:406:TRP:CH2 | 41:SO:258:VAL:HG13 | 2.48 | 0.44 |
| 40:SI:202:PHE:HE2 | 40:SI:238:ILE:HG12 | 1.82 | 0.44 |
| 41:SL:118:ASP:HA | 41:SL:121:ARG:NH2 | 2.31 | 0.44 |
| 41:SN:211:CYS:HA | 41:SN:215:LEU:HB2 | 2.00 | 0.44 |
| 41:SO:112:LEU:O | 41:SO:115:SER:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:TA:2:ARG:HH21 | 40:TA:50:ASN:HD21 | 1.66 | 0.44 |
| 40:TA:116:ASP:OD1 | 40:TA:117:LEU:N | 2.50 | 0.44 |
| 40:TE:318:LEU:HB2 | 40:TE:375:CYS:HB3 | 1.98 | 0.44 |
| 40:TH:306:ASP:HB3 | 40:TH:309:HIS:NE2 | 2.32 | 0.44 |
| 41:TO:200:TYR:HE2 | 41:TO:368:ILE:HD12 | 1.82 | 0.44 |
| 41:TP:289:LEU:HD13 | 41:TP:363:MET:HG3 | 1.98 | 0.44 |
| 41:TP:309:ARG:H | 41:TP:372:THR:HG1 | 1.60 | 0.44 |
| 40:UA:21:TRP:HA | 40:UA:24:TYR:HD1 | 1.81 | 0.44 |
| 40:UA:28:HIS:O | 40:UA:30:ILE:N | 2.50 | 0.44 |
| 40:UA:221:ARG:NH2 | 41:UN:325:GLU:H | 2.16 | 0.44 |
| 40:UE:7:VAL:HB | 40:UE:137:ILE:HG22 | 1.99 | 0.44 |
| 40:UE:116:ASP:OD1 | 40:UE:117:LEU:N | 2.50 | 0.44 |
| 40:UI:36:MET:HE3 | 40:UI:36:MET:HB3 | 1.70 | 0.44 |
| 40:UI:369:LYS:HB3 | 40:UI:369:LYS:HE3 | 1.59 | 0.44 |
| 41:UP:139:LEU:HD12 | 41:UP:168:SER:HB2 | 1.99 | 0.44 |
| 41:UP:384:GLN:HG2 | 41:UP:384:GLN:H | 1.55 | 0.44 |
| 40:VF:262:TYR:HB2 | 40:VF:265:ILE:HG12 | 1.99 | 0.44 |
| 40:VF:311:LYS:HE2 | 40:VF:311:LYS:HB2 | 1.90 | 0.44 |
| 40:VH:164:LYS:HA | 40:VH:164:LYS:HD3 | 1.73 | 0.44 |
| 40:VJ:172:TYR:HE2 | 40:VJ:386:ALA:HB1 | 1.82 | 0.44 |
| 41:VN:273:LEU:O | 41:VN:292:GLN:NE2 | 2.39 | 0.44 |
| 41:VO:178:THR:HG22 | 41:VO:180:VAL:H | 1.82 | 0.44 |
| 41:VQ:229:VAL:O | 41:VQ:233:MET:HG2 | 2.17 | 0.44 |
| 41:VQ:274:THR:OG1 | 41:VQ:279:GLN:OE1 | 2.26 | 0.44 |
| 41:WB:167:PHE:HD2 | 41:WB:202:ILE:HD11 | 1.83 | 0.44 |
| 40:WE:30:ILE:HG13 | 40:WE:53:PHE:HD2 | 1.81 | 0.44 |
| 40:WE:425:ALA:HB1 | 40:WE:429:LYS:NZ | 2.31 | 0.44 |
| 40:WF:256:GLN:HB3 | 41:WN:397:TRP:CZ2 | 2.52 | 0.44 |
| 41:WP:229:VAL:O | 41:WP:233:MET:HG2 | 2.17 | 0.44 |
| 7:1T:277:ARG:HD3 | 7:1T:277:ARG:HA | 1.53 | 0.44 |
| 8:1X:119:ARG:O | 8:1X:122:LEU:HB2 | 2.17 | 0.44 |
| 11:2I:91:ARG:HA | 40:LA:440:GLU:HG3 | 1.99 | 0.44 |
| 13:2V:119:CYS:O | 13:2V:120:THR:C | 2.55 | 0.44 |
| 14:3A:9:GLN:HE22 | 41:MN:299:MET:HB2 | 1.82 | 0.44 |
| 14:3A:46:ARG:HH21 | 40:MF:264:ARG:HG3 | 1.82 | 0.44 |
| 16:3K:106:LYS:HA | 16:3K:106:LYS:HD3 | 1.81 | 0.44 |
| 17:3O:364:HIS:HB3 | 17:3O:455:LEU:HD11 | 1.99 | 0.44 |
| 17:3O:382:ILE:O | 17:3O:386:ILE:HG13 | 2.17 | 0.44 |
| 17:3P:420:LEU:HD12 | 17:3P:420:LEU:HA | 1.72 | 0.44 |
| 17:3R:292:ALA:O | 17:3R:294:VAL:HG23 | 2.18 | 0.44 |
| 18:3T:168:VAL:HG11 | 18:3U:56:TRP:HB2 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:3T:232:HIS:CD2 | 18:3T:235:SER:HB2 | 2.52 | 0.44 |
| 22:4J:329:ASP:N | 22:4J:329:ASP:OD1 | 2.46 | 0.44 |
| 22:4K:440:LEU:O | 22:4K:512:LYS:NZ | 2.46 | 0.44 |
| 22:4K:555:GLU:HG3 | 22:4K:556:GLU:N | 2.32 | 0.44 |
| 22:4K:679:SER:HA | 22:4K:683:ASP:HB3 | 1.99 | 0.44 |
| 26:4W:52:TYR:CE2 | 26:4W:54:ASP:HB2 | 2.52 | 0.44 |
| 30:5G:85:GLN:HG3 | 40:GA:2:ARG:HH12 | 1.81 | 0.44 |
| 34:5Q:215:ARG:HB3 | 41:GN:276:ARG:HH12 | 1.81 | 0.44 |
| 35:5T:184:VAL:HG23 | 40:KE:46:ASP:HB3 | 2.00 | 0.44 |
| 36:5X:74:SER:OG | 36:5X:75:SER:N | 2.49 | 0.44 |
| 37:6A:81:LYS:HB3 | 37:6A:82:TYR:H | 1.51 | 0.44 |
| 39:6G:55:MET:HB2 | 39:6G:68:LEU:HD22 | 1.98 | 0.44 |
| 40:AA:264:ARG:HA | 40:AA:264:ARG:HD2 | 1.80 | 0.44 |
| 40:AE:223:THR:HG23 | 40:AE:225:THR:HG22 | 1.99 | 0.44 |
| 40:AH:93:ILE:HD13 | 40:AH:93:ILE:HA | 1.83 | 0.44 |
| 41:AL:189:VAL:O | 41:AL:193:VAL:HG23 | 2.18 | 0.44 |
| 41:AM:258:VAL:HG22 | 41:AM:266:PHE:HZ | 1.82 | 0.44 |
| 41:AN:143:THR:O | 41:AN:147:MET:N | 2.47 | 0.44 |
| 41:AO:3:GLU:CD | 41:AO:127:CYS:HB3 | 2.38 | 0.44 |
| 41:AO:236:VAL:HG23 | 41:AO:237:THR:HG23 | 1.99 | 0.44 |
| 41:BB:98:GLY:O | 41:BB:100:ASN:N | 2.50 | 0.44 |
| 41:BB:189:VAL:HG11 | 41:BB:415:MET:HG3 | 1.99 | 0.44 |
| 40:BI:115:ILE:HA | 40:BI:118:VAL:HG22 | 2.00 | 0.44 |
| 40:BI:377:LEU:HA | 40:BI:377:LEU:HD13 | 1.77 | 0.44 |
| 41:BL:19:LYS:HD2 | 41:BL:19:LYS:HA | 1.74 | 0.44 |
| 40:CA:6:SER:HB3 | 40:CA:138:PHE:CE1 | 2.52 | 0.44 |
| 40:CE:4:CYS:SG | 40:CE:136:LEU:HD23 | 2.57 | 0.44 |
| 40:CG:1:GLN:HG3 | 40:CG:2:ARG:HD3 | 1.97 | 0.44 |
| 40:CG:177:VAL:HG23 | 40:CG:178:SER:H | 1.82 | 0.44 |
| 40:CG:234:ILE:HD11 | 40:CG:272:TYR:HB2 | 1.99 | 0.44 |
| 41:CN:162:ARG:HA | 41:CN:162:ARG:HD3 | 1.55 | 0.44 |
| 41:CN:170:VAL:O | 41:CN:171:PRO:C | 2.55 | 0.44 |
| 41:CP:127:CYS:O | 41:CP:128:ASP:C | 2.55 | 0.44 |
| 40:DA:5:ILE:HD12 | 40:DA:132:LEU:HD13 | 1.99 | 0.44 |
| 40:DA:349:THR:O | 41:DB:179:VAL:HG13 | 2.18 | 0.44 |
| 41:DB:131:GLN:HE21 | 41:DB:250:LEU:HB2 | 1.82 | 0.44 |
| 40:DE:111:GLY:O | 40:DE:115:ILE:HG12 | 2.17 | 0.44 |
| 40:DE:240:ALA:O | 40:DE:242:LEU:N | 2.51 | 0.44 |
| 40:DE:324:VAL:HG23 | 40:DE:327:ASP:HB2 | 1.98 | 0.44 |
| 40:DG:383:ILE:HG22 | 40:DG:387:TRP:CD1 | 2.52 | 0.44 |
| 40:DI:109:THR:O | 40:DI:110:ILE:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DL:121:ARG:O | 41:DL:125:GLU:N | 2.49 | 0.44 |
| 41:DL:184:ASN:ND2 | 41:DL:398:TYR:OH | 2.50 | 0.44 |
| 41:DM:324:LYS:HE3 | 41:DM:324:LYS:HB2 | 1.46 | 0.44 |
| 41:DP:253:LEU:HG | 41:DP:257:MET:HE3 | 2.00 | 0.44 |
| 40:EG:15:GLN:HA | 40:EG:18:ASN:HB2 | 1.99 | 0.44 |
| 40:EH:2:ARG:H | 40:EH:2:ARG:HG2 | 1.65 | 0.44 |
| 40:EH:69:ASP:HB3 | 40:EH:74:VAL:HG11 | 1.99 | 0.44 |
| 40:EH:109:THR:O | 40:EH:110:ILE:C | 2.56 | 0.44 |
| 40:EH:242:LEU:HD21 | 40:EH:252:LEU:HD23 | 1.99 | 0.44 |
| 40:EI:332:ILE:HD12 | 40:EI:332:ILE:HA | 1.85 | 0.44 |
| 41:EM:115:SER:O | 41:EM:118:ASP:HB3 | 2.17 | 0.44 |
| 41:EN:170:VAL:HG11 | 41:EN:377:LEU:HD21 | 1.99 | 0.44 |
| 41:EP:68:LEU:HD13 | 41:EP:68:LEU:HA | 1.74 | 0.44 |
| 41:EP:418:LEU:O | 41:EP:422:VAL:HG12 | 2.17 | 0.44 |
| 41:FB:87:PRO:HA | 41:FB:90:PHE:HD2 | 1.81 | 0.44 |
| 40:FI:317:LEU:HG | 40:FI:376:MET:HG2 | 1.99 | 0.44 |
| 41:FN:285:THR:HB | 41:FN:287:PRO:HD2 | 1.99 | 0.44 |
| 41:FO:288:GLU:HA | 41:FO:291:GLN:HG3 | 1.98 | 0.44 |
| 40:GE:182:VAL:O | 40:GE:183:GLU:C | 2.56 | 0.44 |
| 40:GG:255:PHE:HZ | 40:GG:318:LEU:HD21 | 1.81 | 0.44 |
| 40:GH:211:ASP:HA | 40:GH:214:ARG:HD3 | 1.99 | 0.44 |
| 40:GI:75:ILE:HB | 40:GI:94:THR:HG23 | 2.00 | 0.44 |
| 40:GI:217:LEU:C | 40:GI:219:ILE:H | 2.19 | 0.44 |
| 41:GN:409:THR:OG1 | 41:GN:410:GLU:N | 2.49 | 0.44 |
| 40:HA:213:CYS:HA | 40:HA:217:LEU:HD23 | 1.98 | 0.44 |
| 40:HA:238:ILE:HD12 | 40:HA:377:LEU:HD21 | 1.99 | 0.44 |
| 40:HE:129:CYS:SG | 40:HE:132:LEU:HB2 | 2.57 | 0.44 |
| 40:HF:259:LEU:HD21 | 40:HF:377:LEU:HB3 | 1.98 | 0.44 |
| 40:HH:70:LEU:HD12 | 40:HH:110:ILE:HG13 | 1.99 | 0.44 |
| 40:HI:123:ARG:HH22 | 40:II:338:LYS:HE3 | 1.82 | 0.44 |
| 41:HO:122:LYS:HA | 41:HO:122:LYS:HD3 | 1.75 | 0.44 |
| 41:IM:150:LEU:HD11 | 41:IM:154:LYS:HE2 | 2.00 | 0.44 |
| 41:IO:7:LEU:HD23 | 41:IO:64:VAL:HB | 1.99 | 0.44 |
| 41:JB:290:THR:HA | 41:JB:293:MET:HE3 | 1.99 | 0.44 |
| 40:JD:228:ASN:HA | 40:JD:231:ILE:HB | 1.99 | 0.44 |
| 40:JH:105:ARG:HG2 | 40:JH:410:GLU:HG2 | 1.99 | 0.44 |
| 41:JL:107:THR:O | 41:JL:110:ALA:N | 2.37 | 0.44 |
| 41:JM:7:LEU:HD21 | 41:JM:133:PHE:HB3 | 1.98 | 0.44 |
| 41:JM:51:TYR:HE2 | 41:JM:61:PRO:HG3 | 1.82 | 0.44 |
| 41:JM:202:ILE:HG21 | 41:JM:229:VAL:HG22 | 1.99 | 0.44 |
| 40:KA:88:HIS:HB3 | 40:KA:91:GLN:HG3 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KD:98:ASP:O | 40:KD:105:ARG:NH2 | 2.48 | 0.44 |
| 40:KG:326:LYS:HZ1 | 41:KO:225:LEU:HD21 | 1.82 | 0.44 |
| 40:LA:130:THR:OG1 | 40:LA:131:GLY:N | 2.50 | 0.44 |
| 40:LF:191:THR:O | 40:LF:195:LEU:HB2 | 2.17 | 0.44 |
| 40:LF:209:ILE:HG12 | 40:LF:302:MET:CG | 2.48 | 0.44 |
| 40:LF:271:THR:HA | 40:LF:302:MET:HE2 | 1.98 | 0.44 |
| 40:LH:104:ALA:HB2 | 40:LH:412:MET:HG2 | 1.99 | 0.44 |
| 40:LH:192:HIS:NE2 | 40:LH:419:GLU:OE1 | 2.50 | 0.44 |
| 41:LM:172:SER:HB2 | 41:LM:205:GLU:HG3 | 1.99 | 0.44 |
| 41:LM:418:LEU:O | 41:LM:421:PRO:HD2 | 2.17 | 0.44 |
| 41:LN:210:ILE:HG12 | 41:LN:298:ASN:HA | 1.98 | 0.44 |
| 41:LO:149:THR:HA | 41:LO:152:ILE:HD12 | 1.99 | 0.44 |
| 41:LP:107:THR:HG22 | 41:LP:108:GLU:H | 1.83 | 0.44 |
| 41:MB:17:GLY:HA2 | 41:MB:20:PHE:HB3 | 1.99 | 0.44 |
| 40:MG:225:THR:O | 40:MG:226:ASN:C | 2.56 | 0.44 |
| 40:MH:139:HIS:CD2 | 40:MH:139:HIS:H | 2.34 | 0.44 |
| 41:MN:108:GLU:HA | 41:MN:111:GLU:HG2 | 1.99 | 0.44 |
| 40:NA:141:PHE:HB2 | 40:NA:173:PRO:HD3 | 1.98 | 0.44 |
| 41:NB:46:ARG:HD3 | 41:NB:46:ARG:HA | 1.85 | 0.44 |
| 40:ND:228:ASN:OD1 | 42:ND:501:GTP:N2 | 2.49 | 0.44 |
| 40:NF:116:ASP:N | 40:NF:116:ASP:OD1 | 2.50 | 0.44 |
| 40:NG:306:ASP:OD2 | 40:NG:309:HIS:ND1 | 2.50 | 0.44 |
| 41:NN:293:MET:HE2 | 41:NN:367:PHE:HB2 | 2.00 | 0.44 |
| 40:OD:89:PRO:HD2 | 40:PD:280:LYS:HZ2 | 1.82 | 0.44 |
| 40:OH:63:PRO:HG2 | 40:OH:91:GLN:OE1 | 2.17 | 0.44 |
| 40:OH:172:TYR:HB3 | 40:OH:204:VAL:O | 2.18 | 0.44 |
| 41:OM:12:CYS:SG | 41:OM:13:GLY:N | 2.90 | 0.44 |
| 41:ON:99:ASN:HD22 | 41:ON:99:ASN:C | 2.20 | 0.44 |
| 41:PB:86:ARG:HA | 41:QB:281:TYR:CD1 | 2.51 | 0.44 |
| 40:PD:276:ILE:HG23 | 40:PD:280:LYS:HB3 | 1.98 | 0.44 |
| 40:PG:88:HIS:ND1 | 40:PG:90:GLU:HG2 | 2.32 | 0.44 |
| 40:PH:72:PRO:HD2 | 41:PO:2:ARG:NH2 | 2.32 | 0.44 |
| 41:PM:19:LYS:HD3 | 41:PM:22:GLU:HB2 | 1.99 | 0.44 |
| 41:PM:425:ARG:HA | 41:PM:425:ARG:HD2 | 1.63 | 0.44 |
| 40:QG:247:ALA:O | 41:QO:11:GLN:NE2 | 2.49 | 0.44 |
| 40:QH:150:THR:O | 40:QH:154:MET:HG2 | 2.16 | 0.44 |
| 41:QO:268:PRO:HA | 41:QO:368:ILE:HD13 | 1.99 | 0.44 |
| 41:QO:385:PHE:HZ | 41:QO:408:PHE:HB3 | 1.81 | 0.44 |
| 41:QP:390:ARG:HB2 | 41:QP:390:ARG:CZ | 2.47 | 0.44 |
| 40:RA:302:MET:HE3 | 40:RA:303:VAL:HG23 | 1.99 | 0.44 |
| 40:RI:91:GLN:HA | 40:RI:121:ARG:NH2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RI:204:VAL:HG23 | 40:RI:302:MET:HB3 | 1.98 | 0.44 |
| 41:RL:382:SER:OG | 41:RL:412:GLU:OE2 | 2.31 | 0.44 |
| 41:RP:306:ARG:HG3 | 41:RP:340:TYR:HE2 | 1.81 | 0.44 |
| 40:SH:271:THR:OG1 | 40:SH:300:ASN:O | 2.25 | 0.44 |
| 41:SO:30:ILE:HG23 | 41:SO:34:GLY:HA2 | 1.99 | 0.44 |
| 41:SO:154:LYS:HE2 | 41:SO:154:LYS:HB2 | 1.50 | 0.44 |
| 41:SO:358:PRO:HB2 | 41:SO:361:LEU:HB2 | 1.98 | 0.44 |
| 40:TE:287:SER:OG | 40:TE:290:GLU:OE1 | 2.34 | 0.44 |
| 40:TF:11:GLN:HA | 40:TF:14:VAL:HG12 | 1.99 | 0.44 |
| 40:TH:181:VAL:HG23 | 40:TH:182:VAL:HG13 | 1.97 | 0.44 |
| 40:TI:398:TYR:OH | 40:TI:414:GLU:OE2 | 2.24 | 0.44 |
| 41:TM:21:TRP:CZ2 | 41:TM:63:ALA:HB2 | 2.52 | 0.44 |
| 41:TO:6:HIS:HE1 | 41:TO:136:THR:HG23 | 1.81 | 0.44 |
| 40:UA:137:ILE:HD11 | 40:UA:168:GLU:HG2 | 1.98 | 0.44 |
| 41:UB:210:ILE:HG12 | 41:UB:298:ASN:HA | 1.98 | 0.44 |
| 40:UF:62:VAL:HG11 | 40:VG:283:HIS:HA | 1.99 | 0.44 |
| 41:UM:210:ILE:O | 41:UM:214:THR:OG1 | 2.31 | 0.44 |
| 41:UP:6:HIS:CD2 | 41:UP:134:GLN:HE21 | 2.35 | 0.44 |
| 40:VI:255:PHE:HZ | 40:VI:318:LEU:HD21 | 1.81 | 0.44 |
| 41:VN:292:GLN:HG2 | 41:VN:298:ASN:ND2 | 2.33 | 0.44 |
| 41:VO:64:VAL:HG12 | 41:VO:66:VAL:HG23 | 1.99 | 0.44 |
| 40:WA:318:LEU:O | 40:WA:374:VAL:HA | 2.17 | 0.44 |
| 41:WB:314:ALA:HA | 41:WB:350:LYS:HB3 | 1.98 | 0.44 |
| 41:WM:20:PHE:CE1 | 41:WM:24:ILE:HG13 | 2.52 | 0.44 |
| 41:WN:180:VAL:O | 41:WN:181:GLU:C | 2.55 | 0.44 |
| 41:WP:63:ALA:O | 41:WP:89:ASN:ND2 | 2.50 | 0.44 |
| 7:1S:147:ALA:HB3 | 40:VA:42:ILE:HD12 | 1.98 | 0.44 |
| 7:1S:530:GLU:HB2 | 7:1S:537:ILE:HD11 | 2.00 | 0.44 |
| 7:1U:12:ALA:HB3 | 7:1U:581:HIS:CD2 | 2.53 | 0.44 |
| 9:2B:356:ALA:O | 9:2B:360:LYS:HG2 | 2.18 | 0.44 |
| 10:2G:157:ARG:NH2 | 41:VQ:51:TYR:HB3 | 2.32 | 0.44 |
| 14:3C:9:GLN:HG3 | 14:3C:10:TYR:CD1 | 2.52 | 0.44 |
| 14:3C:85:THR:HG22 | 36:5W:248:ASP:HB2 | 1.99 | 0.44 |
| 17:3O:437:ARG:HH21 | 17:3R:123:ASP:HB3 | 1.81 | 0.44 |
| 17:3P:264:ALA:HB2 | 17:3Q:410:GLU:HG2 | 1.99 | 0.44 |
| 17:3R:182:GLU:HG3 | 17:3R:237:LEU:HD21 | 1.98 | 0.44 |
| 17:3R:335:GLU:O | 17:3R:338:ASN:HB2 | 2.18 | 0.44 |
| 17:3R:342:LYS:HE3 | 17:3R:342:LYS:HB2 | 1.55 | 0.44 |
| 18:3T:370:ARG:HA | 18:3T:370:ARG:HD3 | 1.76 | 0.44 |
| 20:4A:71:VAL:HA | 20:4A:74:ASP:OD1 | 2.18 | 0.44 |
| 20:4B:253:LEU:O | 41:MP:276:ARG:HD2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4H:248:GLU:OE2 | 22:4H:379:LYS:NZ | 2.48 | 0.44 |
| 22:4H:276:SER:HB2 | 41:CL:74:ASP:HB3 | 1.99 | 0.44 |
| 22:4J:139:PRO:HA | 22:4J:140:PRO:HD3 | 1.74 | 0.44 |
| 22:4J:663:LYS:O | 22:4J:666:ARG:N | 2.49 | 0.44 |
| 23:4N:94:TYR:C | 23:4N:96:GLY:H | 2.20 | 0.44 |
| 23:4N:240:LEU:HD13 | 23:4N:266:HIS:ND1 | 2.33 | 0.44 |
| 23:4P:202:PHE:HA | 23:4P:205:LEU:HB3 | 1.98 | 0.44 |
| 23:4P:240:LEU:HD13 | 23:4P:266:HIS:ND1 | 2.33 | 0.44 |
| 23:4Q:198:PHE:HE1 | 40:DH:223:THR:N | 2.16 | 0.44 |
| 31:5I:550:GLU:OE2 | 31:5I:550:GLU:N | 2.40 | 0.44 |
| 36:5W:93:GLY:HA2 | 41:ON:217:LEU:HD11 | 1.99 | 0.44 |
| 36:5Y:110:CYS:HB2 | 36:5Y:112:HIS:CE1 | 2.53 | 0.44 |
| 39:6H:70:MET:O | 39:6H:74:ILE:HG12 | 2.17 | 0.44 |
| 40:AA:182:VAL:O | 40:AA:186:ASN:ND2 | 2.50 | 0.44 |
| 41:AB:202:ILE:HG21 | 41:AB:229:VAL:HG22 | 1.99 | 0.44 |
| 40:AG:20:CYS:HB3 | 40:AG:24:TYR:HE1 | 1.82 | 0.44 |
| 40:AG:136:LEU:HD23 | 40:AG:167:LEU:HB2 | 1.98 | 0.44 |
| 41:AN:226:ASN:ND2 | 43:AN:501:GDP:O6 | 2.41 | 0.44 |
| 41:BB:400:GLY:O | 41:BB:401:GLU:C | 2.56 | 0.44 |
| 40:BE:38:SER:O | 40:BE:39:ASP:C | 2.56 | 0.44 |
| 40:BF:141:PHE:HB2 | 40:BF:173:PRO:HD3 | 2.00 | 0.44 |
| 40:BF:177:VAL:HB | 41:BM:327:ASP:OD2 | 2.17 | 0.44 |
| 40:BH:113:GLU:H | 40:BH:113:GLU:HG3 | 1.44 | 0.44 |
| 41:BM:396:HIS:HB3 | 41:BM:397:TRP:CZ3 | 2.52 | 0.44 |
| 41:BN:131:GLN:HE22 | 41:BN:240:LEU:HD22 | 1.81 | 0.44 |
| 41:BN:226:ASN:ND2 | 43:BN:501:GDP:O6 | 2.38 | 0.44 |
| 41:BO:46:ARG:CB | 41:BO:241:ARG:HA | 2.43 | 0.44 |
| 41:BO:294:PHE:CE2 | 41:BO:313:VAL:HG11 | 2.51 | 0.44 |
| 41:BO:311:LEU:HD12 | 41:BO:342:VAL:HG11 | 2.00 | 0.44 |
| 41:BP:42:LEU:CG | 41:BP:45:GLU:HB2 | 2.40 | 0.44 |
| 41:BP:61:PRO:HG2 | 41:BP:84:ILE:HG23 | 2.00 | 0.44 |
| 40:CA:56:THR:OG1 | 40:CA:57:GLY:N | 2.50 | 0.44 |
| 40:CA:100:ALA:O | 40:CA:101:ASN:C | 2.55 | 0.44 |
| 41:CB:22:GLU:HA | 41:CB:81:PHE:CD2 | 2.52 | 0.44 |
| 41:CM:394:PHE:HD1 | 41:CM:397:TRP:HH2 | 1.65 | 0.44 |
| 40:DA:276:ILE:CG2 | 40:DA:281:ALA:HB2 | 2.48 | 0.44 |
| 40:DA:344:VAL:HG13 | 40:DA:345:ASP:H | 1.82 | 0.44 |
| 41:DB:123:GLU:O | 41:DB:126:SER:N | 2.49 | 0.44 |
| 41:DB:173:PRO:HD2 | 41:DB:205:GLU:HB2 | 1.99 | 0.44 |
| 41:DB:240:LEU:HD22 | 41:DB:249:ASP:HB2 | 1.99 | 0.44 |
| 40:DE:273:ALA:O | 40:DE:275:VAL:HG22 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DF:68:VAL:HG21 | 40:DF:149:PHE:HE2 | 1.83 | 0.44 |
| 40:DF:311:LYS:H | 40:DF:381:THR:HG22 | 1.81 | 0.44 |
| 40:DG:101:ASN:HA | 40:DG:144:GLY:N | 2.32 | 0.44 |
| 40:DH:101:ASN:O | 41:DO:255:VAL:HG11 | 2.16 | 0.44 |
| 40:DI:125:LEU:O | 40:DI:126:ALA:C | 2.55 | 0.44 |
| 40:DI:270:ALA:HB1 | 40:DI:376:MET:O | 2.17 | 0.44 |
| 41:DL:73:MET:O | 41:DL:74:ASP:C | 2.55 | 0.44 |
| 41:DL:228:LEU:H | 41:DL:228:LEU:HG | 1.50 | 0.44 |
| 41:DM:15:GLN:O | 41:DM:16:ILE:C | 2.54 | 0.44 |
| 41:DM:284:LEU:HG | 41:DM:284:LEU:H | 1.67 | 0.44 |
| 41:DO:208:TYR:CE1 | 41:DO:212:PHE:HB2 | 2.52 | 0.44 |
| 41:DP:68:LEU:HB2 | 41:DP:143:THR:HG23 | 1.98 | 0.44 |
| 41:DP:292:GLN:HE21 | 41:DP:292:GLN:HB3 | 1.57 | 0.44 |
| 40:EF:209:ILE:HG23 | 40:EF:230:LEU:HD23 | 1.99 | 0.44 |
| 40:EF:383:ILE:HG12 | 40:EF:387:TRP:CD1 | 2.53 | 0.44 |
| 40:EH:179:THR:OG1 | 40:EH:180:ALA:N | 2.50 | 0.44 |
| 40:EI:333:ALA:HA | 40:EI:336:LYS:HD2 | 1.99 | 0.44 |
| 40:FA:11:GLN:O | 40:FA:12:ALA:C | 2.54 | 0.44 |
| 40:FA:258:ASN:ND2 | 40:FA:352:LYS:HG3 | 2.33 | 0.44 |
| 40:FA:367:LEU:HD22 | 40:FA:367:LEU:HA | 1.72 | 0.44 |
| 40:FE:240:ALA:HA | 40:FE:243:ARG:HB3 | 1.98 | 0.44 |
| 40:FF:93:ILE:HD13 | 40:FF:118:VAL:HG12 | 1.99 | 0.44 |
| 40:FG:233:GLN:HG3 | 40:FG:367:LEU:HD13 | 1.99 | 0.44 |
| 40:FI:139:HIS:CG | 40:FI:150:THR:HG21 | 2.52 | 0.44 |
| 41:FM:41:ASP:OD1 | 41:FM:41:ASP:N | 2.48 | 0.44 |
| 41:FM:240:LEU:H | 41:FM:240:LEU:HD23 | 1.82 | 0.44 |
| 41:FN:39:ASP:N | 41:FN:39:ASP:OD1 | 2.49 | 0.44 |
| 41:FN:149:THR:HG21 | 41:FN:188:SER:HA | 1.98 | 0.44 |
| 41:GB:101:TRP:HB2 | 41:GB:184:ASN:HD22 | 1.83 | 0.44 |
| 40:GE:81:GLY:O | 40:GE:84:ARG:HB3 | 2.18 | 0.44 |
| 40:GE:277:SER:O | 40:GE:279:GLU:N | 2.50 | 0.44 |
| 40:GH:30:ILE:H | 40:GH:30:ILE:HG12 | 1.48 | 0.44 |
| 40:GI:177:VAL:CG2 | 40:GI:207:GLU:HB2 | 2.47 | 0.44 |
| 41:GN:2:ARG:HE | 41:GN:2:ARG:HB2 | 1.68 | 0.44 |
| 41:GN:201:CYS:SG | 41:GN:201:CYS:O | 2.75 | 0.44 |
| 40:HA:88:HIS:ND1 | 40:HA:89:PRO:HD2 | 2.31 | 0.44 |
| 40:HE:37:PRO:O | 40:HE:38:SER:C | 2.56 | 0.44 |
| 40:HE:263:PRO:O | 40:HE:264:ARG:C | 2.55 | 0.44 |
| 40:HI:185:TYR:OH | 40:HI:402:ALA:O | 2.20 | 0.44 |
| 41:HM:313:VAL:HG13 | 41:HM:367:PHE:CE1 | 2.52 | 0.44 |
| 41:HO:152:ILE:HG23 | 41:HO:164:MET:SD | 2.57 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:IA:270:ALA:HA | 40:IA:376:MET:O | 2.17 | 0.44 |
| 40:IF:88:HIS:CD2 | 40:IF:89:PRO:HD2 | 2.53 | 0.44 |
| 40:IF:115:ILE:HG13 | 40:IF:119:LEU:HD23 | 1.98 | 0.44 |
| 40:IF:229:ARG:HD3 | 40:IF:363:VAL:HG11 | 1.99 | 0.44 |
| 40:IF:253:THR:HG22 | 41:IN:98:GLY:HA3 | 1.97 | 0.44 |
| 40:IG:209:ILE:HG23 | 40:IG:230:LEU:HD23 | 1.99 | 0.44 |
| 41:IM:46:ARG:HA | 41:IM:46:ARG:HD3 | 1.85 | 0.44 |
| 41:IO:362:LYS:HD2 | 41:IO:363:MET:HG2 | 2.00 | 0.44 |
| 40:JA:21:TRP:CH2 | 40:JA:52:PHE:HB3 | 2.51 | 0.44 |
| 41:JM:137:HIS:HE1 | 41:JM:192:LEU:HD11 | 1.82 | 0.44 |
| 41:JM:143:THR:O | 41:JM:144:GLY:C | 2.56 | 0.44 |
| 40:KH:255:PHE:HE1 | 40:KH:318:LEU:HD21 | 1.83 | 0.44 |
| 40:KH:317:LEU:HB3 | 40:KH:319:TYR:CE1 | 2.53 | 0.44 |
| 41:KL:193:VAL:HA | 41:KL:264:HIS:NE2 | 2.31 | 0.44 |
| 40:LD:53:PHE:O | 40:LD:64:ARG:NH1 | 2.49 | 0.44 |
| 40:LE:296:PHE:CE2 | 40:LE:335:ILE:HG21 | 2.52 | 0.44 |
| 40:LG:390:LEU:HD23 | 40:LG:390:LEU:HA | 1.81 | 0.44 |
| 40:LG:396:LEU:HD12 | 40:LG:396:LEU:HA | 1.85 | 0.44 |
| 41:MB:200:TYR:HE2 | 41:MB:368:ILE:HD12 | 1.82 | 0.44 |
| 40:MF:5:ILE:HG12 | 40:MF:132:LEU:HD11 | 1.98 | 0.44 |
| 41:MM:226:ASN:ND2 | 43:MM:502:GDP:O6 | 2.49 | 0.44 |
| 42:MM:501:GTP:HO2' | 42:MM:501:GTP:HO3' | 1.52 | 0.44 |
| 41:MN:3:GLU:HA | 41:MN:49:VAL:HG13 | 1.99 | 0.44 |
| 41:MN:321:MET:HE2 | 41:MN:363:MET:HG3 | 1.99 | 0.44 |
| 40:ND:112:LYS:N | 40:ND:112:LYS:CD | 2.80 | 0.44 |
| 40:NE:139:HIS:O | 40:NE:170:SER:HA | 2.17 | 0.44 |
| 41:OB:22:GLU:HG2 | 41:OB:81:PHE:HB2 | 2.00 | 0.44 |
| 40:OG:217:LEU:HA | 40:OG:277:SER:HB3 | 1.99 | 0.44 |
| 40:OH:110:ILE:O | 40:OH:113:GLU:HB3 | 2.17 | 0.44 |
| 40:PA:169:PHE:HA | 40:PA:202:PHE:O | 2.17 | 0.44 |
| 41:PB:119:VAL:O | 41:PB:122:LYS:HB2 | 2.17 | 0.44 |
| 41:PB:152:ILE:HA | 41:PB:164:MET:HE3 | 1.99 | 0.44 |
| 41:PB:350:LYS:NZ | 40:PG:181:VAL:HG13 | 2.32 | 0.44 |
| 40:PE:56:THR:HB | 40:PE:60:LYS:HB3 | 1.99 | 0.44 |
| 40:PF:404:VAL:HG12 | 40:PF:417:PHE:HE2 | 1.82 | 0.44 |
| 40:PG:239:THR:OG1 | 40:PG:243:ARG:NH2 | 2.50 | 0.44 |
| 40:PH:88:HIS:CD2 | 40:QH:283:HIS:HB3 | 2.53 | 0.44 |
| 40:PH:111:GLY:O | 40:PH:115:ILE:HG12 | 2.17 | 0.44 |
| 40:PH:139:HIS:CD2 | 40:PH:150:THR:HG21 | 2.52 | 0.44 |
| 41:PO:318:ARG:O | 41:PO:363:MET:HA | 2.18 | 0.44 |
| 41:QB:399:THR:O | 41:QB:401:GLU:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QF:64:ARG:NH2 | 40:QF:129:CYS:HB3 | 2.33 | 0.44 |
| 41:QL:67:ASP:OD1 | 41:QL:69:GLU:N | 2.47 | 0.44 |
| 41:QL:139:LEU:HG | 41:QL:168:SER:HB2 | 1.98 | 0.44 |
| 41:QM:232:THR:HG21 | 41:QM:300:MET:HE1 | 1.99 | 0.44 |
| 41:QM:237:THR:HB | 41:QM:250:LEU:HD21 | 1.99 | 0.44 |
| 41:QP:262:ARG:HH12 | 41:QP:417:ASP:HB3 | 1.82 | 0.44 |
| 41:QP:271:ALA:HB2 | 41:QP:367:PHE:CE1 | 2.51 | 0.44 |
| 40:RF:224:TYR:HD2 | 41:RM:245:GLN:HG3 | 1.82 | 0.44 |
| 40:RG:353:VAL:HG22 | 41:RO:177:ASP:HA | 1.99 | 0.44 |
| 41:RL:176:SER:OG | 41:RL:178:THR:O | 2.34 | 0.44 |
| 41:RM:355:ASP:HB2 | 41:RM:356:ILE:HD12 | 1.99 | 0.44 |
| 41:RN:282:ARG:HH22 | 41:RN:291:GLN:NE2 | 2.15 | 0.44 |
| 41:RO:178:THR:N | 41:RO:181:GLU:OE2 | 2.50 | 0.44 |
| 41:RP:237:THR:HG23 | 41:RP:241:ARG:HH21 | 1.83 | 0.44 |
| 40:SA:316:CYS:HA | 40:SA:352:LYS:HB2 | 1.99 | 0.44 |
| 40:SA:391:ASP:OD2 | 40:SA:421:ARG:NH2 | 2.49 | 0.44 |
| 40:SA:398:TYR:OH | 40:SA:414:GLU:OE2 | 2.35 | 0.44 |
| 41:SB:164:MET:SD | 41:SB:164:MET:N | 2.90 | 0.44 |
| 40:SE:47:ASP:O | 40:SE:50:ASN:HB2 | 2.18 | 0.44 |
| 40:SE:71:GLU:HG3 | 40:SE:98:ASP:HA | 1.99 | 0.44 |
| 40:SF:181:VAL:HG23 | 40:SF:182:VAL:HG13 | 1.99 | 0.44 |
| 41:SL:66:VAL:HG11 | 41:SL:116:VAL:HG22 | 1.98 | 0.44 |
| 41:SL:70:PRO:HB3 | 41:SL:92:PHE:HB2 | 1.98 | 0.44 |
| 41:SN:271:ALA:HB1 | 41:SN:292:GLN:HB3 | 2.00 | 0.44 |
| 41:SO:107:THR:HB | 41:SO:108:GLU:H | 1.50 | 0.44 |
| 40:TI:90:GLU:OE2 | 40:UI:280:LYS:HD3 | 2.17 | 0.44 |
| 40:TI:209:ILE:HA | 40:TI:212:ILE:HB | 1.99 | 0.44 |
| 41:TM:51:TYR:HA | 41:TM:60:VAL:O | 2.17 | 0.44 |
| 41:TN:290:THR:HA | 41:TN:293:MET:HG2 | 1.98 | 0.44 |
| 41:TO:217:LEU:HD23 | 41:TO:217:LEU:HA | 1.88 | 0.44 |
| 40:UF:232:SER:O | 40:UF:233:GLN:C | 2.55 | 0.44 |
| 40:UF:274:PRO:HD3 | 40:UF:373:ALA:HA | 2.00 | 0.44 |
| 40:UH:407:TYR:O | 40:UH:412:MET:HB3 | 2.18 | 0.44 |
| 40:UI:311:LYS:HB3 | 40:UI:344:VAL:HG12 | 1.99 | 0.44 |
| 41:UP:69:GLU:CB | 41:UP:96:GLY:HA2 | 2.46 | 0.44 |
| 41:UP:84:ILE:HA | 41:VQ:281:TYR:OH | 2.18 | 0.44 |
| 41:UP:155:ILE:HD12 | 41:UP:155:ILE:HA | 1.76 | 0.44 |
| 40:VA:104:ALA:HB2 | 40:VA:412:MET:HB2 | 1.99 | 0.44 |
| 40:VF:301:GLN:HG2 | 40:VF:303:VAL:H | 1.82 | 0.44 |
| 40:VH:115:ILE:HA | 40:VH:118:VAL:HG12 | 1.99 | 0.44 |
| 40:VI:72:PRO:HD2 | 41:VP:2:ARG:HH12 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VP:226:ASN:ND2 | 43:VP:502:GDP:O6 | 2.43 | 0.44 |
| 40:WF:258:ASN:CG | 40:WF:352:LYS:HD2 | 2.38 | 0.44 |
| 40:WH:265:ILE:HG22 | 40:WH:379:ASN:HD21 | 1.82 | 0.44 |
| 40:WI:269:LEU:HD22 | 40:WI:303:VAL:HG12 | 1.98 | 0.44 |
| 41:WM:112:LEU:O | 41:WM:116:VAL:HG23 | 2.17 | 0.44 |
| 41:WM:175:VAL:HG13 | 41:WM:205:GLU:HG3 | 1.99 | 0.44 |
| 41:WN:121:ARG:O | 41:WN:125:GLU:HG2 | 2.17 | 0.44 |
| 41:WQ:303:CYS:SG | 41:WQ:377:LEU:HB2 | 2.58 | 0.44 |
| 7:1T:282:LYS:HA | 7:1T:282:LYS:HD3 | 1.75 | 0.44 |
| 8:1X:112:TRP:O | 8:1X:114:SER:N | 2.45 | 0.44 |
| 8:1X:166:VAL:O | 8:1X:170:ARG:N | 2.50 | 0.44 |
| 10:2E:78:ALA:HB3 | 40:AE:308:ARG:HH12 | 1.82 | 0.44 |
| 11:2I:72:LEU:HD22 | 40:LA:401:ARG:HH21 | 1.82 | 0.44 |
| 11:2I:119:LYS:HZ3 | 40:LG:410:GLU:N | 2.15 | 0.44 |
| 13:2U:112:THR:HG23 | 13:2U:121:MET:HA | 1.99 | 0.44 |
| 13:2X:125:LEU:HD23 | 13:2X:132:ILE:HD11 | 1.98 | 0.44 |
| 15:3F:239:LYS:HB2 | 15:3F:239:LYS:HE3 | 1.64 | 0.44 |
| 16:3K:390:CYS:O | 16:3K:394:ARG:HB2 | 2.18 | 0.44 |
| 16:3L:126:ILE:HG21 | 16:3M:20:ASN:HD22 | 1.83 | 0.44 |
| 17:3O:283:TYR:HB3 | 17:3P:394:LYS:NZ | 2.33 | 0.44 |
| 17:3R:321:LEU:HD13 | 17:3R:321:LEU:HA | 1.80 | 0.44 |
| 18:3W:138:LEU:HD22 | 18:3W:286:LEU:HD11 | 1.98 | 0.44 |
| 19:3Y:179:ARG:HB3 | 19:3Y:183:LYS:HZ1 | 1.79 | 0.44 |
| 20:4A:84:GLN:HE22 | 22:4J:14:ASN:H | 1.65 | 0.44 |
| 21:4D:509:ASP:O | 21:4D:510:ASP:C | 2.56 | 0.44 |
| 21:4E:334:PRO:HA | 21:4E:343:PHE:HA | 1.99 | 0.44 |
| 21:4E:477:SER:HB3 | 21:4E:480:GLU:O | 2.17 | 0.44 |
| 22:4H:236:TRP:CZ2 | 22:4H:349:ARG:HD3 | 2.52 | 0.44 |
| 22:4I:651:LYS:HD3 | 22:4I:651:LYS:HA | 1.34 | 0.44 |
| 22:4J:689:ASN:HB3 | 22:4J:692:SER:HB3 | 1.98 | 0.44 |
| 22:4K:562:LEU:HB3 | 22:4K:566:PHE:CZ | 2.53 | 0.44 |
| 23:4M:89:SER:O | 40:AG:84:ARG:CD | 2.64 | 0.44 |
| 23:4M:106:ALA:O | 23:4M:107:LYS:HG3 | 2.17 | 0.44 |
| 23:4N:202:PHE:HB3 | 23:4N:203:PRO:HD3 | 1.98 | 0.44 |
| 26:4W:233:THR:OG1 | 26:4W:312:GLU:OE1 | 2.34 | 0.44 |
| 26:4W:298:GLU:HA | 26:4W:301:THR:HG22 | 2.00 | 0.44 |
| 31:5I:453:GLU:OE2 | 31:5I:453:GLU:N | 2.51 | 0.44 |
| 35:5T:73:ARG:NH1 | 40:JD:322:ASP:OD1 | 2.36 | 0.44 |
| 40:AA:210:TYR:O | 40:AA:214:ARG:HG3 | 2.18 | 0.44 |
| 41:AB:164:MET:O | 41:AB:196:THR:OG1 | 2.36 | 0.44 |
| 40:AE:88:HIS:NE2 | 40:BE:280:LYS:HG2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AG:209:ILE:HB | 40:AG:227:LEU:HD22 | 1.99 | 0.44 |
| 41:AO:61:PRO:HD2 | 41:AO:84:ILE:O | 2.17 | 0.44 |
| 41:AO:107:THR:HB | 41:AO:108:GLU:H | 1.65 | 0.44 |
| 41:AO:260:PHE:HB3 | 41:AO:261:PRO:HD2 | 2.00 | 0.44 |
| 41:BB:105:HIS:CD2 | 41:BB:149:THR:HG22 | 2.53 | 0.44 |
| 40:BE:12:ALA:O | 40:BE:13:GLY:C | 2.54 | 0.44 |
| 40:BE:260:VAL:CG1 | 40:BE:266:HIS:HB3 | 2.48 | 0.44 |
| 40:BI:97:GLU:HB3 | 40:BI:110:ILE:HG12 | 1.99 | 0.44 |
| 40:BI:213:CYS:HB3 | 40:BI:219:ILE:HG13 | 1.99 | 0.44 |
| 41:BL:200:TYR:HE1 | 41:BL:368:ILE:HD12 | 1.83 | 0.44 |
| 41:BP:119:VAL:O | 41:BP:123:GLU:HG2 | 2.18 | 0.44 |
| 40:CA:90:GLU:O | 40:CA:91:GLN:C | 2.56 | 0.44 |
| 40:CA:167:LEU:HD22 | 40:CA:200:CYS:HB3 | 2.00 | 0.44 |
| 40:CA:223:THR:HG23 | 41:CN:322:SER:HA | 1.99 | 0.44 |
| 41:CB:318:ARG:O | 41:CB:363:MET:HA | 2.17 | 0.44 |
| 40:CE:396:LEU:HD11 | 41:CL:343:GLU:O | 2.17 | 0.44 |
| 40:CF:180:ALA:O | 41:CM:347:ASN:ND2 | 2.50 | 0.44 |
| 40:CH:204:VAL:HG12 | 40:CH:302:MET:HB2 | 1.99 | 0.44 |
| 40:CH:400:LYS:HB2 | 40:CH:400:LYS:HE3 | 1.83 | 0.44 |
| 41:CL:323:MET:CE | 41:CL:353:VAL:HG21 | 2.47 | 0.44 |
| 41:CO:46:ARG:HD3 | 41:CO:46:ARG:HA | 1.73 | 0.44 |
| 40:DA:271:THR:HG1 | 40:DA:301:GLN:HA | 1.82 | 0.44 |
| 41:DB:31:ASP:C | 41:DB:33:THR:H | 2.20 | 0.44 |
| 41:DB:161:ASP:O | 41:DB:162:ARG:NH1 | 2.50 | 0.44 |
| 40:DE:83:TYR:O | 40:DE:85:GLN:N | 2.50 | 0.44 |
| 40:DE:264:ARG:HA | 40:DE:264:ARG:HD3 | 1.62 | 0.44 |
| 40:DF:103:TYR:HB3 | 40:DF:407:TYR:HE2 | 1.83 | 0.44 |
| 40:DF:421:ARG:HA | 40:DF:421:ARG:HD2 | 1.45 | 0.44 |
| 40:DG:288:VAL:HA | 40:DG:291:ILE:HG12 | 2.00 | 0.44 |
| 40:DH:139:HIS:CD2 | 40:DH:170:SER:HB2 | 2.51 | 0.44 |
| 40:DI:311:LYS:HE3 | 40:DI:311:LYS:HB3 | 1.48 | 0.44 |
| 41:DL:26:ASP:O | 41:DL:27:GLU:C | 2.55 | 0.44 |
| 41:DL:283:ALA:O | 41:DL:285:THR:N | 2.50 | 0.44 |
| 41:DN:12:CYS:SG | 41:DN:169:VAL:HG21 | 2.58 | 0.44 |
| 41:DN:321:MET:HE3 | 41:DN:321:MET:HB3 | 1.75 | 0.44 |
| 41:DO:167:PHE:CE2 | 41:DO:233:MET:HB2 | 2.52 | 0.44 |
| 40:EG:213:CYS:HB3 | 40:EG:219:ILE:HB | 2.00 | 0.44 |
| 40:EG:329:ASN:OD1 | 41:EO:175:VAL:HG11 | 2.17 | 0.44 |
| 40:EI:10:GLY:O | 40:EI:13:GLY:N | 2.50 | 0.44 |
| 40:EI:285:GLN:O | 40:EI:286:LEU:C | 2.55 | 0.44 |
| 40:EI:344:VAL:O | 40:EI:345:ASP:C | 2.55 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EI:427:LEU:HD12 | 40:EI:427:LEU:HA | 1.84 | 0.44 |
| 41:EM:7:LEU:O | 41:EM:135:LEU:HA | 2.17 | 0.44 |
| 41:EM:374:ILE:HG23 | 41:EM:378:PHE:HE2 | 1.82 | 0.44 |
| 41:EO:101:TRP:CD1 | 41:EO:146:GLY:HA2 | 2.53 | 0.44 |
| 41:EP:267:MET:HE3 | 41:EP:267:MET:HB3 | 1.69 | 0.44 |
| 40:FA:258:ASN:HD21 | 41:FB:178:THR:HA | 1.82 | 0.44 |
| 41:FB:54:ALA:HB3 | 41:FB:58:LYS:O | 2.16 | 0.44 |
| 40:FI:280:LYS:HB3 | 40:FI:280:LYS:HE2 | 1.73 | 0.44 |
| 41:FM:36:TYR:OH | 41:FM:43:GLN:OE1 | 2.31 | 0.44 |
| 40:GE:27:GLU:HG3 | 40:GE:361:THR:HG21 | 2.00 | 0.44 |
| 40:GE:153:LEU:O | 40:GE:154:MET:C | 2.54 | 0.44 |
| 40:GF:167:LEU:HA | 40:GF:200:CYS:O | 2.17 | 0.44 |
| 40:GG:136:LEU:HB3 | 40:GG:138:PHE:HE1 | 1.83 | 0.44 |
| 40:GH:86:LEU:HB3 | 40:GH:87:PHE:H | 1.69 | 0.44 |
| 40:GI:254:GLU:O | 40:GI:255:PHE:C | 2.56 | 0.44 |
| 41:HO:86:ARG:NH1 | 41:HO:123:GLU:OE1 | 2.50 | 0.44 |
| 41:HP:107:THR:O | 41:HP:109:GLY:N | 2.51 | 0.44 |
| 40:IF:224:TYR:CD1 | 40:IF:227:LEU:HD22 | 2.52 | 0.44 |
| 40:IH:248:LEU:HA | 41:IP:11:GLN:HE22 | 1.81 | 0.44 |
| 41:IO:180:VAL:HG23 | 41:IO:184:ASN:HD21 | 1.82 | 0.44 |
| 42:JB:502:GTP:N1 | 40:JG:224:TYR:HB3 | 2.33 | 0.44 |
| 40:JD:320:ARG:HA | 40:JD:356:ASN:O | 2.17 | 0.44 |
| 40:JF:254:GLU:OE2 | 40:JF:352:LYS:NZ | 2.44 | 0.44 |
| 41:JM:215:LEU:O | 41:JM:216:LYS:C | 2.55 | 0.44 |
| 40:KF:6:SER:O | 40:KF:65:ALA:HA | 2.17 | 0.44 |
| 41:KL:7:LEU:HD21 | 41:KL:120:VAL:HG22 | 1.99 | 0.44 |
| 41:LB:3:GLU:HA | 41:LB:49:VAL:HA | 1.98 | 0.44 |
| 41:LB:180:VAL:O | 41:LB:184:ASN:ND2 | 2.51 | 0.44 |
| 41:LB:303:CYS:SG | 41:LB:377:LEU:HB2 | 2.56 | 0.44 |
| 40:LD:262:TYR:HB2 | 40:LD:265:ILE:HD12 | 1.99 | 0.44 |
| 40:LE:164:LYS:HA | 40:LE:164:LYS:HD3 | 1.82 | 0.44 |
| 40:LF:396:LEU:HD23 | 40:LF:396:LEU:HA | 1.88 | 0.44 |
| 40:LG:34:GLY:O | 40:LG:35:GLN:C | 2.55 | 0.44 |
| 41:LO:330:MET:HA | 41:LO:333:VAL:HG12 | 1.99 | 0.44 |
| 40:MA:430:ASP:C | 40:MA:432:GLU:H | 2.21 | 0.44 |
| 41:MB:178:THR:OG1 | 41:MB:181:GLU:HB2 | 2.18 | 0.44 |
| 40:ME:31:GLN:HG2 | 40:ME:35:GLN:O | 2.18 | 0.44 |
| 40:MF:418:SER:O | 40:MF:419:GLU:C | 2.56 | 0.44 |
| 41:MO:112:LEU:O | 41:MO:116:VAL:HG23 | 2.18 | 0.44 |
| 41:MP:180:VAL:HG23 | 41:MP:184:ASN:HD21 | 1.81 | 0.44 |
| 41:MP:309:ARG:N | 41:MP:372:THR:HG1 | 2.15 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NA:164:LYS:HA | 40:NA:164:LYS:HD2 | 1.63 | 0.44 |
| 40:NE:318:LEU:O | 40:NE:374:VAL:HA | 2.17 | 0.44 |
| 40:NF:139:HIS:HE1 | 40:NF:168:GLU:HG3 | 1.83 | 0.44 |
| 40:NF:326:LYS:NZ | 41:NN:208:TYR:HB2 | 2.32 | 0.44 |
| 40:NH:142:GLY:HA2 | 40:NH:183:GLU:HG2 | 1.99 | 0.44 |
| 41:NN:8:GLN:HA | 41:NN:135:LEU:HD12 | 2.00 | 0.44 |
| 41:OB:11:GLN:HA | 41:OB:72:THR:HG21 | 1.98 | 0.44 |
| 40:OD:89:PRO:HG2 | 40:PD:283:HIS:ND1 | 2.30 | 0.44 |
| 40:OH:20:CYS:SG | 40:OH:21:TRP:N | 2.90 | 0.44 |
| 40:OH:221:ARG:N | 40:OH:222:PRO:CD | 2.80 | 0.44 |
| 41:ON:42:LEU:HD22 | 41:ON:356:ILE:HD11 | 1.99 | 0.44 |
| 41:OO:36:TYR:CZ | 41:OO:44:LEU:HB2 | 2.52 | 0.44 |
| 41:OO:275:SER:O | 41:OO:279:GLN:HB2 | 2.17 | 0.44 |
| 41:OP:174:LYS:HG3 | 41:OP:175:VAL:HG13 | 1.99 | 0.44 |
| 40:PA:234:ILE:O | 40:PA:238:ILE:HG12 | 2.17 | 0.44 |
| 40:PD:251:ASP:OD1 | 40:PD:252:LEU:N | 2.50 | 0.44 |
| 40:PE:190:THR:O | 40:PE:194:THR:OG1 | 2.29 | 0.44 |
| 40:PE:217:LEU:HA | 40:PE:277:SER:HB2 | 1.99 | 0.44 |
| 40:PE:350:GLY:HA2 | 41:PM:179:VAL:HG12 | 2.00 | 0.44 |
| 40:PG:405:HIS:HA | 40:PG:408:VAL:HG22 | 2.00 | 0.44 |
| 41:PN:64:VAL:HG21 | 41:PN:120:VAL:HG22 | 1.99 | 0.44 |
| 40:QA:255:PHE:HE1 | 40:QA:318:LEU:HD11 | 1.83 | 0.44 |
| 41:QB:73:MET:HB3 | 41:QB:77:ARG:NH2 | 2.33 | 0.44 |
| 41:QB:178:THR:HB | 41:QB:181:GLU:HB2 | 1.98 | 0.44 |
| 41:QB:304:ASP:HB3 | 41:QB:306:ARG:HH21 | 1.83 | 0.44 |
| 40:QE:12:ALA:O | 40:QE:16:ILE:HD12 | 2.17 | 0.44 |
| 41:QL:135:LEU:HG | 41:QL:137:HIS:ND1 | 2.33 | 0.44 |
| 41:QL:342:VAL:HG23 | 41:QL:345:ILE:HG22 | 1.99 | 0.44 |
| 41:QM:24:ILE:HD12 | 41:QM:241:ARG:NH2 | 2.31 | 0.44 |
| 41:QM:167:PHE:HD2 | 41:QM:202:ILE:HD11 | 1.83 | 0.44 |
| 41:QO:199:THR:OG1 | 41:QO:265:PHE:HA | 2.17 | 0.44 |
| 41:QO:207:LEU:HD22 | 41:QO:300:MET:HB2 | 1.98 | 0.44 |
| 41:QP:89:ASN:O | 41:QP:90:PHE:C | 2.55 | 0.44 |
| 41:QP:263:LEU:HD13 | 41:QP:263:LEU:HA | 1.73 | 0.44 |
| 40:RA:315:CYS:HA | 40:RA:377:LEU:O | 2.17 | 0.44 |
| 40:RH:142:GLY:HA2 | 40:RH:183:GLU:HG2 | 2.00 | 0.44 |
| 40:RI:175:PRO:HD2 | 40:RI:304:LYS:HE2 | 1.99 | 0.44 |
| 41:RL:324:LYS:HA | 41:RL:327:ASP:OD2 | 2.18 | 0.44 |
| 41:RN:145:SER:O | 41:RN:149:THR:HG23 | 2.17 | 0.44 |
| 41:RO:20:PHE:O | 41:RO:24:ILE:HG12 | 2.17 | 0.44 |
| 41:RP:86:ARG:HH12 | 41:SP:282:ARG:CZ | 2.31 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SA:101:ASN:HB3 | 40:SA:182:VAL:HG11 | 1.99 | 0.44 |
| 41:SB:334:GLN:HE21 | 41:SB:349:VAL:HG23 | 1.82 | 0.44 |
| 41:SB:403:MET:HG3 | 41:SB:408:PHE:CZ | 2.51 | 0.44 |
| 41:SM:285:THR:HG22 | 41:SM:287:PRO:HD2 | 1.99 | 0.44 |
| 41:SO:70:PRO:HA | 41:SO:73:MET:HG2 | 2.00 | 0.44 |
| 41:SO:380:ARG:O | 41:SO:384:GLN:HG2 | 2.17 | 0.44 |
| 40:TA:311:LYS:H | 40:TA:381:THR:HG1 | 1.63 | 0.44 |
| 40:TE:213:CYS:HA | 40:TE:217:LEU:HB2 | 1.98 | 0.44 |
| 40:TG:273:ALA:HB3 | 40:TG:374:VAL:H | 1.82 | 0.44 |
| 40:TI:219:ILE:HG22 | 40:TI:222:PRO:HD3 | 1.99 | 0.44 |
| 40:TI:297:GLU:HA | 40:TI:298:PRO:HD3 | 1.80 | 0.44 |
| 41:TM:285:THR:HB | 41:TM:287:PRO:HD2 | 2.00 | 0.44 |
| 40:UF:3:GLU:CG | 40:UF:129:CYS:HB2 | 2.40 | 0.44 |
| 40:UG:219:ILE:HD12 | 40:UG:222:PRO:HB3 | 2.00 | 0.44 |
| 40:UI:94:THR:OG1 | 40:UI:95:GLY:N | 2.48 | 0.44 |
| 41:UM:130:LEU:O | 41:UM:162:ARG:NH1 | 2.50 | 0.44 |
| 41:UO:52:ASN:OD1 | 41:UO:62:ARG:NH2 | 2.50 | 0.44 |
| 41:UP:214:THR:OG1 | 41:UP:215:LEU:N | 2.50 | 0.44 |
| 40:VA:105:ARG:HD2 | 41:VO:251:ARG:NH2 | 2.32 | 0.44 |
| 40:VF:260:VAL:HG23 | 41:VN:397:TRP:HZ2 | 1.82 | 0.44 |
| 40:VI:89:PRO:HD3 | 40:WH:283:HIS:CD2 | 2.52 | 0.44 |
| 40:VI:217:LEU:HA | 40:VI:277:SER:HB3 | 1.98 | 0.44 |
| 40:VI:319:TYR:HB3 | 40:VI:323:VAL:HG21 | 1.98 | 0.44 |
| 40:VI:371:GLN:H | 40:VI:371:GLN:HG2 | 1.64 | 0.44 |
| 41:VQ:316:VAL:HG23 | 41:VQ:352:ALA:HB3 | 2.00 | 0.44 |
| 40:WA:76:ASP:O | 40:WA:80:THR:HB | 2.16 | 0.44 |
| 40:WA:234:ILE:HD13 | 40:WA:272:TYR:HD2 | 1.82 | 0.44 |
| 40:WG:228:ASN:ND2 | 42:WG:501:GTP:HN1 | 2.11 | 0.44 |
| 41:WQ:385:PHE:O | 41:WQ:389:PHE:HB2 | 2.18 | 0.44 |
| 5:1M:141:LYS:HD2 | 41:GB:107:THR:HG22 | 1.99 | 0.44 |
| 7:1T:211:ILE:HD12 | 7:1T:212:SER:H | 1.82 | 0.44 |
| 8:1Y:162:ASP:N | 8:1Y:162:ASP:OD1 | 2.50 | 0.44 |
| 8:1Z:441:ARG:NH1 | 37:6A:64:ASP:OD2 | 2.50 | 0.44 |
| 10:2E:141:HIS:CG | 41:WM:357:PRO:HD2 | 2.52 | 0.44 |
| 10:2F:58:ARG:HA | 40:MA:163:LYS:HD3 | 1.98 | 0.44 |
| 10:2G:160:SER:O | 10:2G:161:ARG:HD2 | 2.17 | 0.44 |
| 12:2Q:216:GLN:H | 12:2Q:216:GLN:HG3 | 1.55 | 0.44 |
| 13:2T:115:LYS:O | 13:2T:116:PRO:C | 2.56 | 0.44 |
| 14:3A:25:ALA:HB1 | 40:MF:337:THR:O | 2.17 | 0.44 |
| 14:3B:9:GLN:NE2 | 41:ML:305:PRO:HD2 | 2.32 | 0.44 |
| 15:3E:201:SER:HB2 | 15:3F:314:HIS:HB3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:3P:228:CYS:SG | 17:3P:229:CYS:N | 2.91 | 0.44 |
| 17:3P:253:GLU:HA | 17:3P:256:LYS:HD2 | 2.00 | 0.44 |
| 18:3U:344:LYS:HA | 18:3U:344:LYS:HD3 | 1.80 | 0.44 |
| 19:3Y:218:VAL:HG22 | 40:LF:369:LYS:HD3 | 1.99 | 0.44 |
| 21:4D:225:THR:OG1 | 40:BA:38:SER:O | 2.25 | 0.44 |
| 21:4E:108:PRO:HD3 | 41:BP:280:GLN:HG3 | 1.98 | 0.44 |
| 21:4E:290:LEU:HB3 | 41:CP:77:ARG:HH21 | 1.82 | 0.44 |
| 21:4E:465:LYS:HB2 | 21:4E:465:LYS:HE3 | 1.41 | 0.44 |
| 21:4E:467:LEU:HD11 | 21:4E:499:PHE:HB2 | 1.99 | 0.44 |
| 21:4E:498:VAL:O | 21:4E:500:GLY:N | 2.50 | 0.44 |
| 22:4H:365:LYS:HZ1 | 22:4H:371:GLU:HB2 | 1.82 | 0.44 |
| 22:4J:689:ASN:HD22 | 22:4J:692:SER:HB3 | 1.83 | 0.44 |
| 23:4M:20:PRO:HG3 | 40:CG:279:GLU:OE1 | 2.18 | 0.44 |
| 24:4O:240:LEU:HB2 | 24:4O:266:HIS:ND1 | 2.32 | 0.44 |
| 23:4R:236:TYR:CD1 | 23:4R:267:ASP:HB3 | 2.50 | 0.44 |
| 23:4R:261:TYR:CE1 | 23:4R:265:THR:HG21 | 2.52 | 0.44 |
| 26:4V:32:ASP:OD1 | 26:4V:32:ASP:N | 2.50 | 0.44 |
| 27:4Z:89:ASP:HB3 | 27:4Z:119:LYS:HZ1 | 1.82 | 0.44 |
| 31:5I:344:ARG:NH2 | 41:HN:48:ASN:HB3 | 2.32 | 0.44 |
| 34:5R:366:LYS:HA | 34:5R:369:GLU:HG3 | 1.99 | 0.44 |
| 36:5W:245:PRO:CA | 40:LG:429:LYS:HD2 | 2.47 | 0.44 |
| 39:6F:119:TYR:HA | 39:6F:120:PRO:HA | 1.81 | 0.44 |
| 40:AA:139:HIS:ND1 | 40:AA:146:GLY:O | 2.50 | 0.44 |
| 40:AA:255:PHE:HE1 | 40:AA:377:LEU:HD12 | 1.81 | 0.44 |
| 40:AE:318:LEU:O | 40:AE:374:VAL:HA | 2.17 | 0.44 |
| 40:AH:167:LEU:HD22 | 40:AH:200:CYS:HB3 | 1.98 | 0.44 |
| 41:AM:173:PRO:HB3 | 41:AM:380:ARG:HD2 | 2.00 | 0.44 |
| 41:BB:152:ILE:HD13 | 41:BB:192:LEU:HD21 | 1.99 | 0.44 |
| 41:BB:313:VAL:HG12 | 41:BB:349:VAL:HG13 | 1.98 | 0.44 |
| 40:BF:320:ARG:HD3 | 40:BF:360:PRO:HG3 | 2.00 | 0.44 |
| 40:BF:402:ALA:HB2 | 41:BM:344:TRP:HZ3 | 1.83 | 0.44 |
| 40:BH:29:GLY:O | 40:BH:30:ILE:C | 2.55 | 0.44 |
| 40:BH:140:SER:O | 40:BH:142:GLY:N | 2.51 | 0.44 |
| 41:BL:7:LEU:O | 41:BL:135:LEU:HA | 2.18 | 0.44 |
| 41:BM:323:MET:HB3 | 41:BM:323:MET:HE2 | 1.88 | 0.44 |
| 41:BO:137:HIS:NE2 | 41:BO:168:SER:HB3 | 2.33 | 0.44 |
| 41:BP:213:ARG:HH21 | 41:BP:297:LYS:HD3 | 1.81 | 0.44 |
| 40:CE:132:LEU:HD21 | 40:CE:135:PHE:HE2 | 1.82 | 0.44 |
| 40:CE:228:ASN:ND2 | 42:CE:501:GTP:HN1 | 2.06 | 0.44 |
| 40:CF:155:GLU:HA | 40:CF:197:HIS:CE1 | 2.53 | 0.44 |
| 40:CH:177:VAL:HG11 | 41:CO:327:ASP:HB3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CN:31:ASP:O | 41:CN:33:THR:N | 2.46 | 0.44 |
| 41:CO:246:LEU:HD12 | 41:CO:246:LEU:HA | 1.82 | 0.44 |
| 41:CP:45:GLU:HG2 | 41:CP:46:ARG:HG2 | 1.98 | 0.44 |
| 40:DA:77:GLU:C | 40:DA:79:ARG:H | 2.19 | 0.44 |
| 40:DA:221:ARG:HB2 | 41:DN:322:SER:CB | 2.47 | 0.44 |
| 41:DB:311:LEU:HD12 | 41:DB:311:LEU:HA | 1.79 | 0.44 |
| 40:DE:277:SER:O | 40:DE:278:ALA:C | 2.55 | 0.44 |
| 40:DG:101:ASN:HA | 40:DG:144:GLY:H | 1.81 | 0.44 |
| 40:DG:258:ASN:HD21 | 40:DG:352:LYS:HE3 | 1.83 | 0.44 |
| 40:DI:14:VAL:O | 40:DI:16:ILE:N | 2.50 | 0.44 |
| 40:DI:183:GLU:O | 40:DI:184:PRO:C | 2.56 | 0.44 |
| 40:DI:225:THR:O | 40:DI:228:ASN:N | 2.50 | 0.44 |
| 41:DL:378:PHE:HA | 41:DL:381:ILE:HD12 | 1.99 | 0.44 |
| 41:DN:153:SER:OG | 41:DN:154:LYS:N | 2.50 | 0.44 |
| 41:DN:393:ALA:C | 41:DN:395:LEU:H | 2.19 | 0.44 |
| 41:DP:36:TYR:OH | 41:DP:38:GLY:HA3 | 2.17 | 0.44 |
| 40:EA:64:ARG:HH12 | 40:EA:128:GLN:HG2 | 1.83 | 0.44 |
| 40:EE:3:GLU:HG2 | 40:EE:64:ARG:HH22 | 1.82 | 0.44 |
| 40:EE:235:VAL:HA | 40:EE:238:ILE:HG22 | 1.98 | 0.44 |
| 40:EI:213:CYS:O | 40:EI:214:ARG:C | 2.56 | 0.44 |
| 40:EI:312:TYR:HA | 40:EI:380:THR:HB | 1.99 | 0.44 |
| 40:FA:274:PRO:CB | 40:FA:370:VAL:HG11 | 2.47 | 0.44 |
| 41:FB:3:GLU:HA | 41:FB:49:VAL:HG23 | 1.98 | 0.44 |
| 40:FG:238:ILE:HD12 | 40:FG:377:LEU:HD11 | 1.99 | 0.44 |
| 40:FH:317:LEU:HD23 | 40:FH:376:MET:HG2 | 1.98 | 0.44 |
| 41:FN:40:SER:HB3 | 41:FN:43:GLN:HG3 | 2.00 | 0.44 |
| 41:FN:101:TRP:HB2 | 41:FN:184:ASN:HD22 | 1.83 | 0.44 |
| 41:FO:140:GLY:HA2 | 41:FO:181:GLU:HB2 | 1.99 | 0.44 |
| 41:FP:163:ILE:HD11 | 41:FP:251:ARG:HB2 | 2.00 | 0.44 |
| 40:GA:35:GLN:HA | 40:GA:59:GLY:O | 2.17 | 0.44 |
| 40:GA:181:VAL:HG12 | 41:GN:347:ASN:O | 2.17 | 0.44 |
| 40:GE:119:LEU:HD13 | 40:GE:119:LEU:HA | 1.76 | 0.44 |
| 40:GE:333:ALA:O | 40:GE:337:THR:HG23 | 2.18 | 0.44 |
| 40:GF:73:THR:OG1 | 41:GM:46:ARG:NE | 2.50 | 0.44 |
| 40:GG:117:LEU:O | 40:GG:121:ARG:HG2 | 2.18 | 0.44 |
| 40:GH:17:GLY:O | 40:GH:18:ASN:C | 2.55 | 0.44 |
| 40:GI:119:LEU:HD11 | 40:GI:157:LEU:HD12 | 1.99 | 0.44 |
| 41:GN:192:LEU:HD23 | 41:GN:192:LEU:HA | 1.74 | 0.44 |
| 41:GN:249:ASP:HB2 | 41:GN:250:LEU:H | 1.66 | 0.44 |
| 41:GN:316:VAL:HA | 41:GN:352:ALA:HB3 | 2.00 | 0.44 |
| 41:GP:109:GLY:O | 41:GP:113:VAL:HG23 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HA:137:ILE:HD11 | 40:HA:168:GLU:HG2 | 1.98 | 0.44 |
| 41:HB:270:PHE:HD1 | 41:HB:366:THR:HG22 | 1.82 | 0.44 |
| 40:HE:326:LYS:HA | 40:HE:326:LYS:HD2 | 1.61 | 0.44 |
| 40:HE:326:LYS:HG3 | 41:HM:208:TYR:CD1 | 2.53 | 0.44 |
| 40:HF:177:VAL:HG22 | 41:HM:327:ASP:OD2 | 2.18 | 0.44 |
| 40:HG:60:LYS:HD3 | 40:IG:283:HIS:CD2 | 2.52 | 0.44 |
| 40:HH:154:MET:HG3 | 40:HH:194:THR:HG23 | 1.98 | 0.44 |
| 40:HI:8:HIS:ND1 | 40:HI:17:GLY:HA3 | 2.33 | 0.44 |
| 41:HM:19:LYS:HG3 | 41:HM:226:ASN:HB2 | 1.99 | 0.44 |
| 41:HP:7:LEU:O | 41:HP:135:LEU:HA | 2.18 | 0.44 |
| 40:IA:212:ILE:HD12 | 40:IA:212:ILE:HA | 1.85 | 0.44 |
| 41:IB:313:VAL:HB | 41:IB:349:VAL:HG23 | 1.99 | 0.44 |
| 40:IF:195:LEU:HD12 | 40:IF:266:HIS:CE1 | 2.49 | 0.44 |
| 40:IH:189:LEU:HD11 | 40:IH:417:PHE:HE1 | 1.83 | 0.44 |
| 40:IH:332:ILE:HG21 | 41:IP:175:VAL:HG23 | 1.99 | 0.44 |
| 41:IP:208:TYR:HD1 | 41:IP:225:LEU:HD21 | 1.82 | 0.44 |
| 40:JA:51:THR:HG21 | 40:JA:243:ARG:HG2 | 2.00 | 0.44 |
| 41:JB:156:ARG:NH1 | 41:JB:195:ASN:O | 2.51 | 0.44 |
| 40:JF:288:VAL:HA | 40:JF:291:ILE:HG12 | 1.98 | 0.44 |
| 40:JG:251:ASP:OD1 | 40:JG:252:LEU:N | 2.49 | 0.44 |
| 40:JH:102:ASN:HB3 | 40:JH:105:ARG:HG3 | 2.00 | 0.44 |
| 41:JL:330:MET:HA | 41:JL:333:VAL:HG12 | 1.99 | 0.44 |
| 41:JM:3:GLU:HA | 41:JM:49:VAL:HA | 2.00 | 0.44 |
| 41:JM:183:TYR:O | 41:JM:186:THR:OG1 | 2.33 | 0.44 |
| 41:JM:216:LYS:HE3 | 41:JM:216:LYS:HB3 | 1.50 | 0.44 |
| 41:JN:21:TRP:CZ3 | 41:JN:24:ILE:HD11 | 2.53 | 0.44 |
| 40:KE:400:LYS:HZ3 | 41:KL:344:TRP:CB | 2.31 | 0.44 |
| 41:KL:101:TRP:CD1 | 41:KL:145:SER:HB3 | 2.52 | 0.44 |
| 41:KL:285:THR:OG1 | 41:KL:287:PRO:HD2 | 2.17 | 0.44 |
| 41:KN:392:LYS:NZ | 41:KN:405:GLU:OE2 | 2.36 | 0.44 |
| 41:KO:242:PHE:HB3 | 41:KO:356:ILE:HD13 | 1.99 | 0.44 |
| 40:LD:325:PRO:HA | 40:LD:328:VAL:HG12 | 2.00 | 0.44 |
| 40:LF:30:ILE:H | 40:LF:30:ILE:HG12 | 1.41 | 0.44 |
| 40:LF:76:ASP:HA | 40:LF:79:ARG:CG | 2.47 | 0.44 |
| 40:LF:85:GLN:O | 40:LF:86:LEU:C | 2.56 | 0.44 |
| 40:LF:296:PHE:CZ | 40:LF:351:PHE:HE2 | 2.34 | 0.44 |
| 40:LF:326:LYS:CG | 41:LN:220:PRO:HG2 | 2.47 | 0.44 |
| 40:LG:29:GLY:O | 40:LG:30:ILE:C | 2.56 | 0.44 |
| 40:LG:304:LYS:HE2 | 40:LG:304:LYS:HB3 | 1.31 | 0.44 |
| 40:LH:138:PHE:HZ | 40:LH:235:VAL:HG21 | 1.82 | 0.44 |
| 41:LL:282:ARG:NH1 | 41:LL:288:GLU:OE2 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MA:5:ILE:H | 40:MA:132:LEU:HD11 | 1.82 | 0.44 |
| 40:MA:319:TYR:N | 40:MA:354:GLY:O | 2.50 | 0.44 |
| 41:MB:91:VAL:HG11 | 41:MB:116:VAL:HG22 | 2.00 | 0.44 |
| 40:MF:217:LEU:HD21 | 40:MF:275:VAL:HG12 | 1.99 | 0.44 |
| 40:MH:139:HIS:HB2 | 40:MH:140:SER:H | 1.61 | 0.44 |
| 41:MN:128:ASP:OD1 | 41:MN:128:ASP:N | 2.50 | 0.44 |
| 41:MO:290:THR:HG21 | 41:MO:329:GLN:HB3 | 1.99 | 0.44 |
| 41:MO:383:GLU:O | 41:MO:386:THR:HG22 | 2.17 | 0.44 |
| 40:NA:258:ASN:HD22 | 40:NA:352:LYS:HE3 | 1.81 | 0.44 |
| 41:NB:253:LEU:HD22 | 41:NB:257:MET:HE1 | 2.00 | 0.44 |
| 40:ND:276:ILE:H | 40:ND:276:ILE:HG12 | 1.38 | 0.44 |
| 40:ND:297:GLU:OE2 | 40:ND:299:ALA:HB3 | 2.17 | 0.44 |
| 40:ND:308:ARG:H | 40:ND:308:ARG:HG3 | 1.55 | 0.44 |
| 40:OA:324:VAL:HA | 40:OA:325:PRO:HD3 | 1.85 | 0.44 |
| 40:OE:210:TYR:HE1 | 40:OE:227:LEU:HD21 | 1.81 | 0.44 |
| 40:OH:21:TRP:CZ2 | 40:OH:65:ALA:HB2 | 2.53 | 0.44 |
| 40:OH:135:PHE:HB2 | 40:OH:165:SER:O | 2.17 | 0.44 |
| 40:PG:103:TYR:H | 40:PG:407:TYR:HE1 | 1.65 | 0.44 |
| 40:PH:393:LYS:O | 40:PH:397:MET:HB2 | 2.18 | 0.44 |
| 41:PM:190:HIS:NE2 | 41:PM:194:GLU:OE2 | 2.51 | 0.44 |
| 41:PN:263:LEU:HD13 | 41:PN:311:LEU:HD21 | 2.00 | 0.44 |
| 40:QA:208:ALA:O | 40:QA:212:ILE:HG12 | 2.18 | 0.44 |
| 41:QM:285:THR:HG22 | 41:QM:287:PRO:HD2 | 1.99 | 0.44 |
| 41:QN:22:GLU:HG2 | 41:QN:81:PHE:CD2 | 2.52 | 0.44 |
| 41:QN:286:VAL:HB | 41:QN:325:GLU:HG2 | 1.99 | 0.44 |
| 41:QP:150:LEU:O | 41:QP:154:LYS:N | 2.43 | 0.44 |
| 41:RB:243:PRO:HB3 | 40:RG:73:THR:HB | 1.99 | 0.44 |
| 40:RE:97:GLU:HG2 | 41:RL:251:ARG:HH21 | 1.81 | 0.44 |
| 40:RF:88:HIS:ND1 | 40:RF:91:GLN:HB2 | 2.33 | 0.44 |
| 40:RG:133:GLN:O | 40:RG:165:SER:HB2 | 2.17 | 0.44 |
| 41:RM:176:SER:OG | 41:RM:181:GLU:OE1 | 2.36 | 0.44 |
| 41:RP:315:ALA:HB1 | 41:RP:317:PHE:CE1 | 2.52 | 0.44 |
| 40:SA:400:LYS:HD2 | 41:SN:425:ARG:NH1 | 2.32 | 0.44 |
| 40:SI:255:PHE:HZ | 40:SI:318:LEU:HD21 | 1.82 | 0.44 |
| 41:SN:114:ASP:OD1 | 41:SN:115:SER:N | 2.50 | 0.44 |
| 41:SO:142:GLY:O | 41:SO:144:GLY:N | 2.51 | 0.44 |
| 41:SP:305:PRO:HB3 | 41:SP:310:TYR:HE1 | 1.82 | 0.44 |
| 40:TH:7:VAL:HG23 | 40:TH:66:VAL:HB | 1.99 | 0.44 |
| 40:TI:206:ASN:ND2 | 42:TI:501:GTP:O2' | 2.36 | 0.44 |
| 40:TI:258:ASN:OD1 | 40:TI:259:LEU:N | 2.51 | 0.44 |
| 41:TN:176:SER:OG | 41:TN:178:THR:O | 2.34 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TN:313:VAL:O | 41:TN:349:VAL:HA | 2.18 | 0.44 |
| 41:TP:133:PHE:HB2 | 41:TP:164:MET:SD | 2.57 | 0.44 |
| 41:TP:272:PRO:HG3 | 41:TP:364:SER:HA | 2.00 | 0.44 |
| 40:UA:107:HIS:ND1 | 40:UA:152:LEU:HB2 | 2.33 | 0.44 |
| 41:UB:282:ARG:HH22 | 41:UB:288:GLU:HB2 | 1.82 | 0.44 |
| 40:UF:167:LEU:HD22 | 40:UF:252:LEU:HG | 2.00 | 0.44 |
| 40:UF:215:ARG:HE | 40:UF:215:ARG:HB3 | 1.68 | 0.44 |
| 41:UO:142:GLY:O | 41:UO:144:GLY:N | 2.50 | 0.44 |
| 41:UP:105:HIS:HA | 41:UP:150:LEU:HD22 | 1.99 | 0.44 |
| 40:VA:12:ALA:HB1 | 40:VA:171:ILE:HD12 | 2.00 | 0.44 |
| 41:VP:137:HIS:NE2 | 41:VP:166:THR:OG1 | 2.47 | 0.44 |
| 40:WA:319:TYR:HB3 | 40:WA:323:VAL:HG21 | 1.99 | 0.44 |
| 40:WG:223:THR:HG23 | 40:WG:225:THR:H | 1.83 | 0.44 |
| 40:WI:206:ASN:OD1 | 42:WI:501:GTP:O2' | 2.23 | 0.44 |
| 40:WI:416:GLU:HA | 40:WI:419:GLU:HG2 | 1.98 | 0.44 |
| 41:WM:17:GLY:HA2 | 41:WM:20:PHE:HB3 | 1.98 | 0.44 |
| 41:WN:74:ASP:N | 41:WN:74:ASP:OD1 | 2.50 | 0.44 |
| 41:WN:105:HIS:HB2 | 41:WN:146:GLY:HA2 | 2.00 | 0.44 |
| 41:WP:150:LEU:O | 41:WP:154:LYS:HG2 | 2.18 | 0.44 |
| 9:2B:154:PHE:CD1 | 9:2C:475:ARG:HD3 | 2.52 | 0.44 |
| 11:2K:55:GLU:O | 41:LO:154:LYS:NZ | 2.36 | 0.44 |
| 12:2M:188:PRO:O | 12:2M:191:ARG:NH2 | 2.50 | 0.44 |
| 13:2U:86:TYR:O | 13:2U:159:ASN:HB2 | 2.17 | 0.44 |
| 13:2V:47:LEU:HD13 | 13:2V:47:LEU:HA | 1.80 | 0.44 |
| 13:2W:54:VAL:HG12 | 13:2W:158:ALA:HB3 | 2.00 | 0.44 |
| 14:3A:45:ASP:OD1 | 41:MN:392:LYS:NZ | 2.41 | 0.44 |
| 14:3A:114:LEU:HD23 | 14:3A:114:LEU:HA | 1.86 | 0.44 |
| 16:3J:200:SER:OG | 16:3J:201:LEU:N | 2.50 | 0.44 |
| 16:3K:92:LEU:HD23 | 16:3K:162:LEU:HG | 2.00 | 0.44 |
| 17:3O:149:ARG:NH2 | 17:3P:412:CYS:SG | 2.91 | 0.44 |
| 21:4D:428:SER:OG | 21:4D:433:ASP:HB3 | 2.18 | 0.44 |
| 22:4H:236:TRP:NE1 | 22:4H:238:ASP:OD2 | 2.51 | 0.44 |
| 22:4I:329:ASP:N | 22:4I:329:ASP:OD1 | 2.50 | 0.44 |
| 22:4I:673:LEU:HD13 | 22:4I:673:LEU:HA | 1.88 | 0.44 |
| 22:4K:616:THR:OG1 | 22:4K:617:CYS:N | 2.49 | 0.44 |
| 23:4P:174:MET:HB2 | 23:4P:178:ASP:OD2 | 2.16 | 0.44 |
| 23:4Q:261:TYR:O | 23:4Q:265:THR:N | 2.42 | 0.44 |
| 23:4R:91:ILE:HD12 | 23:4R:93:GLY:H | 1.82 | 0.44 |
| 23:4R:200:SER:O | 40:DI:219:ILE:HG23 | 2.17 | 0.44 |
| 26:4W:42:ASN:O | 26:4W:42:ASN:ND2 | 2.46 | 0.44 |
| 26:4W:248:HIS:CG | 26:4W:352:GLN:HB3 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:5W:219:SER:O | 36:5W:223:ARG:HB3 | 2.17 | 0.44 |
| 40:AA:76:ASP:OD1 | 40:AA:79:ARG:NH2 | 2.50 | 0.44 |
| 40:AA:134:GLY:HA2 | 40:AA:164:LYS:HG3 | 2.00 | 0.44 |
| 41:AB:221:THR:OG1 | 41:AB:222:TYR:N | 2.51 | 0.44 |
| 40:AG:71:GLU:HG3 | 40:AG:98:ASP:HB2 | 1.99 | 0.44 |
| 40:AG:291:ILE:HG22 | 40:AG:374:VAL:HG12 | 2.00 | 0.44 |
| 41:AO:104:GLY:O | 41:AO:147:MET:N | 2.51 | 0.44 |
| 41:AP:240:LEU:HD21 | 41:AP:250:LEU:HD13 | 1.99 | 0.44 |
| 40:BE:239:THR:O | 40:BE:239:THR:OG1 | 2.34 | 0.44 |
| 40:BH:187:SER:O | 40:BH:190:THR:HG22 | 2.17 | 0.44 |
| 40:BH:301:GLN:HG3 | 40:BH:307:PRO:CG | 2.47 | 0.44 |
| 41:BL:117:LEU:HA | 41:BL:120:VAL:HG12 | 1.99 | 0.44 |
| 41:BL:240:LEU:HD11 | 41:BL:249:ASP:HA | 2.00 | 0.44 |
| 41:BO:139:LEU:HD12 | 41:BO:139:LEU:HA | 1.71 | 0.44 |
| 41:BP:7:LEU:HD13 | 41:BP:151:LEU:HD21 | 2.00 | 0.44 |
| 41:BP:383:GLU:H | 41:BP:383:GLU:HG3 | 1.64 | 0.44 |
| 40:CA:180:ALA:HB3 | 40:CA:183:GLU:HG3 | 1.98 | 0.44 |
| 40:CA:276:ILE:H | 40:CA:276:ILE:HG12 | 1.70 | 0.44 |
| 40:CA:383:ILE:O | 40:CA:386:ALA:HB3 | 2.17 | 0.44 |
| 40:CI:188:ILE:HG21 | 40:CI:394:PHE:CD1 | 2.52 | 0.44 |
| 41:CL:101:TRP:HZ2 | 41:CL:191:GLN:NE2 | 2.16 | 0.44 |
| 41:CL:319:GLY:O | 41:CL:321:MET:N | 2.51 | 0.44 |
| 41:CM:257:MET:HE3 | 41:CM:314:ALA:HB2 | 1.98 | 0.44 |
| 41:CN:236:VAL:HG23 | 41:CN:366:THR:HG21 | 2.00 | 0.44 |
| 41:CO:77:ARG:HA | 41:CO:77:ARG:HD2 | 1.34 | 0.44 |
| 41:CP:263:LEU:HD21 | 41:CP:421:PRO:HB2 | 2.00 | 0.44 |
| 40:DA:69:ASP:HA | 40:DA:145:THR:HG21 | 2.00 | 0.44 |
| 40:DA:250:VAL:HG22 | 40:DA:354:GLY:HA3 | 1.98 | 0.44 |
| 40:DA:281:ALA:O | 40:DA:282:TYR:C | 2.56 | 0.44 |
| 41:DB:5:VAL:HG23 | 41:DB:130:LEU:HD11 | 2.00 | 0.44 |
| 40:DG:273:ALA:HB1 | 40:DG:274:PRO:HD2 | 2.00 | 0.44 |
| 40:DH:103:TYR:O | 40:DH:106:GLY:N | 2.51 | 0.44 |
| 40:DH:109:THR:OG1 | 40:DH:110:ILE:N | 2.50 | 0.44 |
| 40:DI:68:VAL:HG12 | 40:DI:93:ILE:HG13 | 1.99 | 0.44 |
| 40:DI:400:LYS:O | 40:DI:401:ARG:C | 2.56 | 0.44 |
| 41:DM:101:TRP:O | 41:DM:104:GLY:N | 2.50 | 0.44 |
| 41:DP:5:VAL:HB | 41:DP:133:PHE:HD1 | 1.82 | 0.44 |
| 41:DP:36:TYR:CZ | 41:DP:38:GLY:HA3 | 2.53 | 0.44 |
| 41:DP:128:ASP:O | 41:DP:130:LEU:N | 2.50 | 0.44 |
| 40:EG:70:LEU:HD22 | 40:EG:110:ILE:HG22 | 1.99 | 0.44 |
| 40:EH:288:VAL:O | 40:EH:291:ILE:HG12 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EH:311:LYS:HE2 | 40:EH:311:LYS:HB2 | 1.63 | 0.44 |
| 40:EI:211:ASP:O | 40:EI:214:ARG:HG3 | 2.18 | 0.44 |
| 41:EM:135:LEU:O | 41:EM:166:THR:HA | 2.17 | 0.44 |
| 41:EM:250:LEU:O | 41:EM:251:ARG:C | 2.55 | 0.44 |
| 41:EO:248:ALA:HA | 41:EO:252:LYS:HG2 | 1.99 | 0.44 |
| 41:EP:362:LYS:HE2 | 41:EP:362:LYS:HB2 | 1.31 | 0.44 |
| 40:FA:407:TYR:HB2 | 40:FA:417:PHE:HZ | 1.83 | 0.44 |
| 41:FM:107:THR:O | 41:FM:109:GLY:N | 2.51 | 0.44 |
| 41:GB:255:VAL:HG23 | 40:GG:406:TRP:CG | 2.53 | 0.44 |
| 40:GE:201:ALA:O | 40:GE:268:PRO:HD2 | 2.17 | 0.44 |
| 40:GH:23:LEU:HA | 40:GH:26:LEU:HD11 | 1.99 | 0.44 |
| 40:GH:52:PHE:HZ | 40:GH:136:LEU:HD12 | 1.82 | 0.44 |
| 40:GH:295:CYS:SG | 40:GH:376:MET:HB2 | 2.58 | 0.44 |
| 40:GI:311:LYS:N | 40:GI:381:THR:OG1 | 2.50 | 0.44 |
| 40:GI:344:VAL:CG2 | 40:GI:347:CYS:HB2 | 2.47 | 0.44 |
| 41:GN:61:PRO:CD | 41:GN:84:ILE:HG12 | 2.44 | 0.44 |
| 41:GO:318:ARG:HG2 | 41:GO:354:CYS:HB3 | 2.00 | 0.44 |
| 41:GP:268:PRO:HG2 | 41:GP:300:MET:HB2 | 2.00 | 0.44 |
| 40:HF:309:HIS:ND1 | 40:HF:385:GLU:OE1 | 2.41 | 0.44 |
| 40:HH:251:ASP:OD1 | 40:HH:252:LEU:N | 2.47 | 0.44 |
| 41:HN:65:LEU:HD13 | 41:HN:90:PHE:HE1 | 1.82 | 0.44 |
| 40:IF:191:THR:O | 40:IF:195:LEU:HB2 | 2.17 | 0.44 |
| 40:IF:320:ARG:HG2 | 40:IF:360:PRO:HG3 | 1.99 | 0.44 |
| 40:IF:376:MET:SD | 40:IF:378:SER:HB3 | 2.57 | 0.44 |
| 40:IH:164:LYS:O | 40:IH:166:LYS:NZ | 2.50 | 0.44 |
| 40:II:226:ASN:ND2 | 40:II:366:ASP:OD2 | 2.50 | 0.44 |
| 41:IO:99:ASN:HD22 | 41:IO:178:THR:HG21 | 1.80 | 0.44 |
| 41:IP:203:ASP:N | 41:IP:300:MET:O | 2.49 | 0.44 |
| 41:IQ:64:VAL:HG22 | 41:IQ:89:ASN:HD22 | 1.83 | 0.44 |
| 41:JB:137:HIS:ND1 | 41:JB:144:GLY:O | 2.51 | 0.44 |
| 41:JB:202:ILE:HD13 | 41:JB:229:VAL:HG13 | 1.98 | 0.44 |
| 41:JB:258:VAL:HG23 | 40:JG:406:TRP:HE1 | 1.83 | 0.44 |
| 40:JD:326:LYS:HD2 | 41:JL:208:TYR:CD1 | 2.53 | 0.44 |
| 40:JF:234:ILE:HD11 | 40:JF:272:TYR:HB2 | 1.99 | 0.44 |
| 41:JM:244:GLY:HA2 | 41:JM:355:ASP:HB2 | 1.99 | 0.44 |
| 41:JM:271:ALA:HB2 | 41:JM:293:MET:HG3 | 2.00 | 0.44 |
| 41:JM:358:PRO:HG2 | 41:JM:361:LEU:HD12 | 1.99 | 0.44 |
| 41:JN:7:LEU:O | 41:JN:135:LEU:HA | 2.18 | 0.44 |
| 41:JN:8:GLN:NE2 | 41:JN:65:LEU:HG | 2.31 | 0.44 |
| 41:JN:107:THR:O | 41:JN:110:ALA:N | 2.50 | 0.44 |
| 41:JO:257:MET:HB3 | 41:JO:266:PHE:CZ | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KG:326:LYS:HZ3 | 41:KO:208:TYR:HB2 | 1.82 | 0.44 |
| 40:KH:319:TYR:HB2 | 40:KH:355:ILE:HD13 | 2.00 | 0.44 |
| 41:KL:252:LYS:HE2 | 41:KL:252:LYS:HB3 | 1.54 | 0.44 |
| 41:KM:60:VAL:HG11 | 41:KM:86:ARG:HG2 | 1.99 | 0.44 |
| 41:KN:273:LEU:O | 41:KN:292:GLN:NE2 | 2.49 | 0.44 |
| 41:LB:14:ASN:HD21 | 41:LB:67:ASP:HB2 | 1.83 | 0.44 |
| 41:LB:108:GLU:HA | 41:LB:111:GLU:HB2 | 2.00 | 0.44 |
| 40:LG:223:THR:OG1 | 40:LG:224:TYR:N | 2.50 | 0.44 |
| 40:LG:265:ILE:H | 40:LG:265:ILE:HG12 | 1.50 | 0.44 |
| 40:LH:88:HIS:CE1 | 40:LH:90:GLU:HB2 | 2.52 | 0.44 |
| 40:LH:278:ALA:H | 40:LH:368:ALA:HB2 | 1.83 | 0.44 |
| 41:LP:138:SER:OG | 43:LP:501:GDP:O1A | 2.35 | 0.44 |
| 41:MB:240:LEU:HD23 | 41:MB:249:ASP:HB2 | 1.99 | 0.44 |
| 40:MD:70:LEU:HD23 | 40:MD:114:LEU:HD22 | 1.99 | 0.44 |
| 40:MF:333:ALA:O | 40:MF:337:THR:HG23 | 2.18 | 0.44 |
| 40:MG:9:VAL:HG22 | 40:MG:68:VAL:HG13 | 1.99 | 0.44 |
| 40:MH:280:LYS:C | 40:MH:282:TYR:H | 2.21 | 0.44 |
| 41:MN:21:TRP:CZ3 | 41:MN:50:TYR:HB3 | 2.53 | 0.44 |
| 40:NA:265:ILE:HG13 | 40:NA:431:TYR:HE1 | 1.83 | 0.44 |
| 40:ND:162:GLY:O | 40:ND:164:LYS:N | 2.45 | 0.44 |
| 40:ND:164:LYS:HD2 | 40:ND:164:LYS:HA | 1.70 | 0.44 |
| 40:NE:145:THR:OG1 | 42:NE:501:GTP:O2B | 2.36 | 0.44 |
| 40:NF:16:ILE:HD13 | 40:NF:228:ASN:HB3 | 1.98 | 0.44 |
| 40:NG:56:THR:OG1 | 40:NG:57:GLY:N | 2.51 | 0.44 |
| 40:NH:332:ILE:O | 40:NH:336:LYS:HG2 | 2.18 | 0.44 |
| 41:NL:309:ARG:NH2 | 41:NL:341:PHE:O | 2.50 | 0.44 |
| 41:NL:323:MET:HA | 41:NL:326:VAL:HG12 | 1.99 | 0.44 |
| 41:NM:330:MET:HA | 41:NM:333:VAL:HG12 | 2.00 | 0.44 |
| 41:NN:284:LEU:HD11 | 41:NN:362:LYS:HB2 | 2.00 | 0.44 |
| 40:OA:221:ARG:NH2 | 41:ON:328:GLU:OE1 | 2.51 | 0.44 |
| 40:OE:166:LYS:HG2 | 40:OE:199:ASP:HB2 | 1.99 | 0.44 |
| 40:OF:104:ALA:O | 40:OF:108:TYR:HB2 | 2.18 | 0.44 |
| 40:OF:152:LEU:O | 40:OF:156:ARG:HG2 | 2.18 | 0.44 |
| 40:OG:25:CYS:SG | 40:OG:86:LEU:HD11 | 2.58 | 0.44 |
| 40:OG:73:THR:HA | 40:OG:76:ASP:HB2 | 1.99 | 0.44 |
| 41:OL:149:THR:HG21 | 41:OL:188:SER:HA | 1.99 | 0.44 |
| 41:OL:236:VAL:HG23 | 41:OL:237:THR:HG23 | 1.98 | 0.44 |
| 41:OM:286:VAL:HG11 | 41:OM:326:VAL:HG22 | 2.00 | 0.44 |
| 40:PG:139:HIS:ND1 | 40:PG:140:SER:O | 2.49 | 0.44 |
| 40:PH:209:ILE:HD11 | 40:PH:230:LEU:HB2 | 1.99 | 0.44 |
| 41:PL:60:VAL:HG21 | 41:PL:86:ARG:HE | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QB:379:LYS:HA | 41:QB:379:LYS:HD3 | 1.46 | 0.44 |
| 40:QE:21:TRP:CD1 | 40:QE:67:PHE:HZ | 2.35 | 0.44 |
| 40:QF:251:ASP:H | 40:QF:254:GLU:HB2 | 1.83 | 0.44 |
| 41:QM:156:ARG:NH2 | 41:QM:196:THR:HA | 2.32 | 0.44 |
| 41:QN:19:LYS:HD2 | 41:QN:19:LYS:HA | 1.79 | 0.44 |
| 41:QP:124:ALA:O | 41:QP:126:SER:N | 2.50 | 0.44 |
| 41:QP:161:ASP:O | 41:QP:162:ARG:C | 2.56 | 0.44 |
| 41:QP:327:ASP:O | 41:QP:331:LEU:HB2 | 2.17 | 0.44 |
| 41:QP:425:ARG:H | 41:QP:425:ARG:HG3 | 1.41 | 0.44 |
| 40:RA:26:LEU:HD12 | 40:RA:363:VAL:HG22 | 2.00 | 0.44 |
| 40:RA:234:ILE:O | 40:RA:238:ILE:HG12 | 2.18 | 0.44 |
| 40:RF:97:GLU:CD | 40:RF:105:ARG:HH22 | 2.20 | 0.44 |
| 40:RH:315:CYS:HA | 40:RH:377:LEU:O | 2.17 | 0.44 |
| 41:RM:237:THR:HB | 41:RM:240:LEU:HD21 | 2.00 | 0.44 |
| 41:RO:156:ARG:HA | 41:RO:156:ARG:HD3 | 1.86 | 0.44 |
| 41:RP:334:GLN:HA | 41:RP:341:PHE:HE2 | 1.82 | 0.44 |
| 40:SA:56:THR:OG1 | 40:SA:57:GLY:N | 2.50 | 0.44 |
| 40:SE:265:ILE:HD11 | 40:SE:430:ASP:HB3 | 2.00 | 0.44 |
| 40:SF:205:ASP:HB3 | 40:SF:303:VAL:HA | 1.99 | 0.44 |
| 40:SH:236:SER:HB2 | 40:SH:243:ARG:HH12 | 1.82 | 0.44 |
| 41:SO:241:ARG:O | 41:SO:242:PHE:C | 2.55 | 0.44 |
| 40:TA:405:HIS:CD2 | 41:TN:261:PRO:HG3 | 2.53 | 0.44 |
| 40:TF:177:VAL:HA | 41:TM:331:LEU:HD12 | 2.00 | 0.44 |
| 40:TH:11:GLN:HG3 | 40:TH:74:VAL:HG21 | 2.00 | 0.44 |
| 40:TI:336:LYS:HG2 | 40:TI:343:PHE:HE2 | 1.82 | 0.44 |
| 41:TM:68:LEU:HB2 | 41:TM:97:ALA:HB2 | 1.98 | 0.44 |
| 41:TN:341:PHE:HB3 | 41:TN:348:ASN:HD21 | 1.81 | 0.44 |
| 40:UF:16:ILE:HA | 40:UF:228:ASN:ND2 | 2.32 | 0.44 |
| 40:UG:421:ARG:HD2 | 40:UG:421:ARG:HA | 1.76 | 0.44 |
| 40:UI:47:ASP:HA | 40:UI:49:PHE:CE1 | 2.53 | 0.44 |
| 40:UI:163:LYS:H | 40:UI:163:LYS:HG3 | 1.32 | 0.44 |
| 41:UM:234:SER:OG | 41:UM:241:ARG:NH2 | 2.49 | 0.44 |
| 41:UO:16:ILE:HD11 | 41:UO:136:THR:HB | 1.99 | 0.44 |
| 41:UO:210:ILE:HG21 | 41:UO:273:LEU:HD13 | 1.99 | 0.44 |
| 41:UP:21:TRP:CZ2 | 41:UP:63:ALA:HB2 | 2.53 | 0.44 |
| 41:UP:143:THR:O | 41:UP:145:SER:N | 2.51 | 0.44 |
| 41:UP:282:ARG:HA | 41:UP:282:ARG:HD2 | 1.44 | 0.44 |
| 41:UP:310:TYR:HA | 41:UP:371:SER:HA | 2.00 | 0.44 |
| 40:VF:105:ARG:HG2 | 40:VF:410:GLU:HG2 | 1.99 | 0.44 |
| 40:VF:109:THR:HG21 | 40:VF:410:GLU:HG3 | 1.99 | 0.44 |
| 40:VF:326:LYS:NZ | 41:VN:208:TYR:HB2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VG:239:THR:O | 40:VG:243:ARG:NE | 2.41 | 0.44 |
| 41:VN:286:VAL:HA | 41:VN:289:LEU:HD12 | 2.00 | 0.44 |
| 41:VP:269:GLY:N | 41:VP:367:PHE:O | 2.50 | 0.44 |
| 40:WF:406:TRP:NE1 | 41:WM:258:VAL:HG23 | 2.32 | 0.44 |
| 40:WG:2:ARG:O | 40:WG:51:THR:OG1 | 2.36 | 0.44 |
| 40:WH:112:LYS:HA | 40:WH:115:ILE:HG22 | 2.00 | 0.44 |
| 40:WH:155:GLU:HA | 40:WH:197:HIS:CE1 | 2.53 | 0.44 |
| 41:WM:5:VAL:HG23 | 41:WM:130:LEU:HD21 | 1.99 | 0.44 |
| 41:WM:151:LEU:HD12 | 41:WM:155:ILE:HD12 | 1.98 | 0.44 |
| 7:1S:204:MET:HA | 41:WB:78:SER:HB3 | 1.99 | 0.44 |
| 7:1T:53:LYS:HE3 | 7:1T:53:LYS:HB2 | 1.75 | 0.44 |
| 7:1U:72:ILE:HG22 | 7:1U:79:ILE:HG12 | 1.99 | 0.44 |
| 8:1X:77:ILE:HG12 | 8:1X:90:ILE:HD12 | 1.99 | 0.44 |
| 8:1X:234:ARG:CZ | 41:UN:280:GLN:HE22 | 2.31 | 0.44 |
| 9:2C:421:ARG:NH1 | 9:2C:422:LYS:HG3 | 2.32 | 0.44 |
| 11:2I:246:LYS:HB3 | 11:2I:246:LYS:HE3 | 1.44 | 0.44 |
| 11:2J:185:MET:O | 11:2J:186:LYS:HG2 | 2.18 | 0.44 |
| 13:2X:20:LYS:HE2 | 13:2X:20:LYS:HB3 | 1.59 | 0.44 |
| 15:3F:68:GLU:OE1 | 16:3L:270:ARG:NH2 | 2.49 | 0.44 |
| 17:3P:248:ARG:HA | 17:3P:248:ARG:HD2 | 1.34 | 0.44 |
| 17:3P:452:LYS:HE2 | 17:3P:452:LYS:HB2 | 1.34 | 0.44 |
| 17:3R:167:MET:HG2 | 17:3R:251:GLN:HG2 | 2.00 | 0.44 |
| 17:3R:248:ARG:NH1 | 17:3R:251:GLN:HB2 | 2.32 | 0.44 |
| 17:3R:315:ARG:O | 17:3R:318:SER:HB3 | 2.18 | 0.44 |
| 19:3Y:179:ARG:HB3 | 19:3Y:183:LYS:HZ3 | 1.81 | 0.44 |
| 21:4D:277:GLU:N | 21:4D:277:GLU:OE2 | 2.51 | 0.44 |
| 21:4D:461:ILE:H | 21:4D:461:ILE:HG12 | 1.42 | 0.44 |
| 21:4D:528:LEU:O | 21:4D:533:ASN:N | 2.49 | 0.44 |
| 21:4F:514:LYS:HD3 | 21:4F:514:LYS:HA | 1.68 | 0.44 |
| 23:4M:92:PRO:CG | 40:AG:89:PRO:HB2 | 2.42 | 0.44 |
| 23:4Q:170:SER:N | 23:4Q:171:PRO:HD2 | 2.33 | 0.44 |
| 23:4Q:183:PHE:O | 23:4Q:184:MET:C | 2.54 | 0.44 |
| 26:4V:281:ASN:ND2 | 26:4V:375:LEU:HD21 | 2.33 | 0.44 |
| 29:5E:107:ILE:HA | 40:GE:96:LYS:HD2 | 2.00 | 0.44 |
| 31:5I:340:PHE:CE1 | 41:HN:45:GLU:HA | 2.53 | 0.44 |
| 33:5N:220:VAL:HG11 | 41:HP:280:GLN:NE2 | 2.32 | 0.44 |
| 33:5N:447:GLU:O | 33:5N:450:LYS:HG3 | 2.18 | 0.44 |
| 34:5R:410:LYS:HZ1 | 34:5R:414:GLU:HB2 | 1.79 | 0.44 |
| 34:5R:434:GLN:O | 34:5R:435:GLU:C | 2.56 | 0.44 |
| 38:6C:195:LEU:HD21 | 41:VQ:295:ASP:HB3 | 1.99 | 0.44 |
| 41:AL:378:PHE:HD1 | 41:AL:415:MET:HG3 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AN:22:GLU:HG2 | 41:AN:81:PHE:HB2 | 2.00 | 0.44 |
| 40:BE:324:VAL:HG21 | 41:BM:219:THR:HB | 2.00 | 0.44 |
| 40:BE:346:TRP:NE1 | 40:BE:434:VAL:O | 2.50 | 0.44 |
| 40:BG:177:VAL:HG23 | 40:BG:178:SER:H | 1.83 | 0.44 |
| 40:BG:289:ALA:O | 40:BG:293:ASN:ND2 | 2.41 | 0.44 |
| 40:BH:174:ALA:HB1 | 40:BH:175:PRO:HD2 | 2.00 | 0.44 |
| 41:BN:1:MET:HB2 | 41:BN:48:ASN:HD21 | 1.82 | 0.44 |
| 41:BP:189:VAL:O | 41:BP:190:HIS:C | 2.56 | 0.44 |
| 40:CA:182:VAL:O | 40:CA:183:GLU:C | 2.54 | 0.44 |
| 40:CE:262:TYR:HE2 | 41:CM:393:ALA:HA | 1.83 | 0.44 |
| 40:CF:2:ARG:HH22 | 40:CF:47:ASP:HB3 | 1.82 | 0.44 |
| 40:CG:207:GLU:HA | 40:CG:210:TYR:CD2 | 2.53 | 0.44 |
| 40:CH:123:ARG:HD3 | 40:CH:123:ARG:HA | 1.83 | 0.44 |
| 41:CL:97:ALA:O | 41:CL:98:GLY:C | 2.55 | 0.44 |
| 41:CL:101:TRP:N | 41:CL:184:ASN:OD1 | 2.51 | 0.44 |
| 41:CL:185:ALA:O | 41:CL:188:SER:N | 2.51 | 0.44 |
| 41:CL:233:MET:C | 41:CL:235:GLY:H | 2.21 | 0.44 |
| 41:CL:313:VAL:HB | 41:CL:341:PHE:CZ | 2.51 | 0.44 |
| 41:CM:67:ASP:O | 41:CM:68:LEU:C | 2.56 | 0.44 |
| 41:CO:11:GLN:H | 43:CO:501:GDP:PB | 2.41 | 0.44 |
| 41:CO:65:LEU:HD11 | 41:CO:85:PHE:CD1 | 2.52 | 0.44 |
| 40:DA:96:LYS:HE2 | 40:DA:96:LYS:HB3 | 1.40 | 0.44 |
| 40:DA:177:VAL:CG1 | 40:DA:207:GLU:HB2 | 2.48 | 0.44 |
| 40:DA:336:LYS:HE3 | 40:DA:336:LYS:HB3 | 1.63 | 0.44 |
| 40:DE:262:TYR:CE2 | 40:DE:434:VAL:HG13 | 2.52 | 0.44 |
| 40:DE:335:ILE:HD11 | 40:DE:351:PHE:CZ | 2.53 | 0.44 |
| 40:DF:333:ALA:O | 40:DF:337:THR:HG23 | 2.18 | 0.44 |
| 40:DG:19:ALA:HB1 | 40:DG:229:ARG:HD3 | 1.99 | 0.44 |
| 40:DH:200:CYS:HB3 | 40:DH:202:PHE:CE2 | 2.52 | 0.44 |
| 40:DH:415:GLY:O | 40:DH:416:GLU:C | 2.56 | 0.44 |
| 40:DI:83:TYR:O | 40:DI:85:GLN:N | 2.51 | 0.44 |
| 40:DI:286:LEU:O | 40:DI:372:ARG:NH2 | 2.50 | 0.44 |
| 41:DL:113:VAL:HG23 | 41:DL:151:LEU:HD23 | 2.00 | 0.44 |
| 41:DL:117:LEU:O | 41:DL:121:ARG:HG2 | 2.18 | 0.44 |
| 41:DM:245:GLN:HB2 | 41:DM:246:LEU:H | 1.63 | 0.44 |
| 41:DM:311:LEU:HD22 | 41:DM:370:ASN:HB3 | 2.00 | 0.44 |
| 41:DN:101:TRP:CD2 | 41:DN:105:HIS:HD2 | 2.36 | 0.44 |
| 41:DN:127:CYS:SG | 41:DN:128:ASP:N | 2.90 | 0.44 |
| 40:EF:66:VAL:HG12 | 40:EF:68:VAL:HG13 | 1.99 | 0.44 |
| 40:EF:206:ASN:OD1 | 42:EF:501:GTP:O2' | 2.35 | 0.44 |
| 40:EH:102:ASN:HD21 | 40:EH:105:ARG:HD2 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EM:6:HIS:HB2 | 41:EM:21:TRP:HZ2 | 1.83 | 0.44 |
| 41:EM:64:VAL:O | 41:EM:65:LEU:C | 2.55 | 0.44 |
| 41:EM:103:LYS:HA | 41:EM:107:THR:HG23 | 2.00 | 0.44 |
| 41:EM:237:THR:HG23 | 41:EM:240:LEU:HD21 | 1.99 | 0.44 |
| 41:EN:417:ASP:O | 41:EN:421:PRO:HD3 | 2.17 | 0.44 |
| 41:EP:316:VAL:HA | 41:EP:352:ALA:HB3 | 1.99 | 0.44 |
| 40:FA:3:GLU:HB3 | 40:FA:132:LEU:HD22 | 1.99 | 0.44 |
| 40:FA:205:ASP:H | 40:FA:303:VAL:HG22 | 1.82 | 0.44 |
| 40:FA:207:GLU:O | 40:FA:210:TYR:HB2 | 2.17 | 0.44 |
| 40:FA:348:PRO:CB | 41:FB:384:GLN:HG2 | 2.48 | 0.44 |
| 40:FG:248:LEU:HB2 | 40:FG:355:ILE:H | 1.81 | 0.44 |
| 41:FM:54:ALA:HA | 41:GM:283:ALA:HB2 | 2.00 | 0.44 |
| 40:GA:98:ASP:O | 40:GA:105:ARG:NH1 | 2.51 | 0.44 |
| 40:GE:387:TRP:O | 40:GE:388:ALA:C | 2.55 | 0.44 |
| 40:GG:141:PHE:HB2 | 40:GG:173:PRO:HD3 | 2.00 | 0.44 |
| 40:GI:85:GLN:O | 40:GI:86:LEU:C | 2.56 | 0.44 |
| 40:GI:184:PRO:O | 40:GI:185:TYR:C | 2.56 | 0.44 |
| 41:GN:206:ALA:O | 41:GN:207:LEU:C | 2.55 | 0.44 |
| 40:HE:88:HIS:CD2 | 40:IE:283:HIS:CB | 2.99 | 0.44 |
| 40:HE:213:CYS:HA | 40:HE:217:LEU:HD12 | 2.00 | 0.44 |
| 40:HI:217:LEU:HA | 40:HI:277:SER:HB3 | 1.98 | 0.44 |
| 41:HN:124:ALA:O | 41:HN:125:GLU:C | 2.55 | 0.44 |
| 41:HP:341:PHE:HB3 | 41:HP:348:ASN:HD21 | 1.83 | 0.44 |
| 41:HQ:68:LEU:HB2 | 41:HQ:143:THR:HG22 | 2.00 | 0.44 |
| 40:IF:103:TYR:HH | 40:IF:107:HIS:CE1 | 2.36 | 0.44 |
| 40:IG:139:HIS:NE2 | 40:IG:168:GLU:OE1 | 2.45 | 0.44 |
| 40:IG:141:PHE:HB3 | 40:IG:187:SER:HB2 | 2.00 | 0.44 |
| 41:IM:186:THR:HG21 | 41:IM:385:PHE:CD2 | 2.53 | 0.44 |
| 40:JA:188:ILE:HG22 | 40:JA:420:ALA:HB1 | 1.98 | 0.44 |
| 40:JD:154:MET:HG3 | 40:JD:194:THR:HG22 | 2.00 | 0.44 |
| 41:JN:272:PRO:HG3 | 41:JN:364:SER:HA | 1.99 | 0.44 |
| 41:JO:7:LEU:HD12 | 41:JO:135:LEU:HD13 | 1.99 | 0.44 |
| 40:KE:248:LEU:HD22 | 40:KE:353:VAL:HG13 | 2.00 | 0.44 |
| 40:KF:20:CYS:HA | 40:KF:232:SER:HB2 | 2.00 | 0.44 |
| 40:KF:269:LEU:HD22 | 40:KF:303:VAL:HG21 | 1.98 | 0.44 |
| 41:KL:102:ALA:C | 41:KL:104:GLY:N | 2.71 | 0.44 |
| 41:KL:210:ILE:O | 41:KL:211:CYS:C | 2.56 | 0.44 |
| 41:KM:293:MET:HG3 | 41:KM:367:PHE:HB2 | 1.99 | 0.44 |
| 41:KP:262:ARG:HD3 | 41:KP:418:LEU:HD12 | 1.99 | 0.44 |
| 41:KP:383:GLU:HA | 41:KP:386:THR:HG22 | 2.00 | 0.44 |
| 40:LE:70:LEU:HD22 | 40:LE:110:ILE:HG22 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LE:210:TYR:HB3 | 41:LL:324:LYS:HE2 | 1.99 | 0.44 |
| 40:LG:60:LYS:HD2 | 40:MG:282:TYR:CE1 | 2.53 | 0.44 |
| 40:LH:112:LYS:HA | 40:LH:115:ILE:HG22 | 2.00 | 0.44 |
| 40:MA:269:LEU:CD2 | 40:MA:380:THR:HG22 | 2.47 | 0.44 |
| 40:MD:167:LEU:HD22 | 40:MD:252:LEU:HD22 | 2.00 | 0.44 |
| 40:MF:76:ASP:HA | 40:MF:79:ARG:HG2 | 1.99 | 0.44 |
| 40:MF:191:THR:O | 40:MF:195:LEU:HB2 | 2.18 | 0.44 |
| 40:MF:436:MET:HE3 | 40:MF:436:MET:HB3 | 1.87 | 0.44 |
| 40:MH:416:GLU:O | 40:MH:417:PHE:C | 2.56 | 0.44 |
| 41:MN:31:ASP:OD1 | 41:MN:35:THR:N | 2.50 | 0.44 |
| 40:NA:221:ARG:NH1 | 41:NN:325:GLU:OE1 | 2.51 | 0.44 |
| 40:ND:273:ALA:CB | 40:ND:274:PRO:HD2 | 2.33 | 0.44 |
| 40:NE:142:GLY:HA2 | 40:NE:183:GLU:HG2 | 1.99 | 0.44 |
| 40:NH:250:VAL:HG23 | 40:NH:255:PHE:HE1 | 1.83 | 0.44 |
| 41:NL:159:TYR:HB3 | 41:NL:162:ARG:HD3 | 2.00 | 0.44 |
| 40:OA:191:THR:HA | 40:OA:194:THR:OG1 | 2.18 | 0.44 |
| 41:OB:107:THR:O | 41:OB:109:GLY:N | 2.51 | 0.44 |
| 40:OH:16:ILE:HA | 40:OH:228:ASN:CB | 2.48 | 0.44 |
| 40:OH:84:ARG:HG3 | 40:OH:85:GLN:N | 2.33 | 0.44 |
| 40:OH:406:TRP:CZ2 | 41:OO:254:ALA:HB1 | 2.52 | 0.44 |
| 41:OM:86:ARG:HG2 | 41:OM:88:ASP:H | 1.82 | 0.44 |
| 41:OM:317:PHE:O | 41:OM:353:VAL:HA | 2.18 | 0.44 |
| 41:OO:309:ARG:HD3 | 41:OO:342:VAL:HA | 2.00 | 0.44 |
| 40:PA:142:GLY:HA2 | 40:PA:183:GLU:OE2 | 2.17 | 0.44 |
| 40:PF:264:ARG:NH1 | 40:PF:430:ASP:OD2 | 2.51 | 0.44 |
| 40:PG:8:HIS:HD2 | 40:PG:67:PHE:HE1 | 1.65 | 0.44 |
| 40:PH:101:ASN:HB2 | 41:PO:252:LYS:NZ | 2.33 | 0.44 |
| 40:PH:180:ALA:HB3 | 40:PH:183:GLU:HG3 | 1.98 | 0.44 |
| 41:PL:52:ASN:OD1 | 41:PL:62:ARG:NH1 | 2.50 | 0.44 |
| 41:PL:406:MET:O | 41:PL:409:THR:OG1 | 2.29 | 0.44 |
| 41:PM:355:ASP:HB3 | 41:PM:356:ILE:HD12 | 2.00 | 0.44 |
| 41:PP:204:ASN:HA | 41:PP:207:LEU:HD12 | 1.98 | 0.44 |
| 40:QF:50:ASN:N | 40:QF:50:ASN:OD1 | 2.50 | 0.44 |
| 40:QF:101:ASN:HA | 40:QF:144:GLY:N | 2.33 | 0.44 |
| 40:QF:296:PHE:CD2 | 40:QF:335:ILE:HG12 | 2.52 | 0.44 |
| 41:QO:100:ASN:ND2 | 41:QO:103:LYS:HG3 | 2.32 | 0.44 |
| 41:QP:21:TRP:HZ2 | 41:QP:63:ALA:HB2 | 1.83 | 0.44 |
| 41:QP:87:PRO:O | 41:QP:88:ASP:C | 2.56 | 0.44 |
| 41:QP:155:ILE:C | 41:QP:157:GLU:H | 2.20 | 0.44 |
| 40:RE:311:LYS:N | 40:RE:381:THR:OG1 | 2.46 | 0.44 |
| 40:RH:5:ILE:O | 40:RH:135:PHE:HA | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RI:27:GLU:HG2 | 40:RI:361:THR:HB | 2.00 | 0.44 |
| 41:RM:263:LEU:HD23 | 41:RM:263:LEU:HA | 1.80 | 0.44 |
| 41:RN:267:MET:HG2 | 41:RN:301:ALA:HB3 | 1.99 | 0.44 |
| 41:RN:309:ARG:NH1 | 41:RN:339:SER:O | 2.51 | 0.44 |
| 41:RO:143:THR:OG1 | 43:RO:502:GDP:O1B | 2.29 | 0.44 |
| 40:SE:168:GLU:OE1 | 40:SE:198:SER:OG | 2.24 | 0.44 |
| 40:SF:234:ILE:HG13 | 40:SF:272:TYR:HB2 | 1.99 | 0.44 |
| 40:SH:238:ILE:HG23 | 40:SH:255:PHE:CE1 | 2.53 | 0.44 |
| 41:SN:240:LEU:HD13 | 41:SN:249:ASP:HB2 | 1.99 | 0.44 |
| 41:SO:16:ILE:HD13 | 41:SO:229:VAL:HG11 | 1.98 | 0.44 |
| 41:SO:152:ILE:O | 41:SO:153:SER:C | 2.56 | 0.44 |
| 41:SP:243:PRO:HD2 | 41:SP:356:ILE:HD13 | 2.00 | 0.44 |
| 41:SP:244:GLY:HA3 | 41:SP:354:CYS:HA | 1.99 | 0.44 |
| 41:TB:116:VAL:HA | 41:TB:119:VAL:HG12 | 1.99 | 0.44 |
| 41:TB:285:THR:O | 41:TB:288:GLU:HG3 | 2.18 | 0.44 |
| 40:TF:112:LYS:HA | 40:TF:115:ILE:HG22 | 1.97 | 0.44 |
| 41:TN:7:LEU:HB3 | 41:TN:135:LEU:HD13 | 2.00 | 0.44 |
| 41:UB:46:ARG:HE | 40:UG:73:THR:HB | 1.83 | 0.44 |
| 40:UE:64:ARG:NH1 | 40:UE:128:GLN:O | 2.47 | 0.44 |
| 40:UE:352:LYS:HZ3 | 41:UM:178:THR:N | 2.15 | 0.44 |
| 40:UF:55:GLU:HB2 | 40:UF:61:HIS:CD2 | 2.53 | 0.44 |
| 40:UF:195:LEU:HA | 40:UF:266:HIS:HE1 | 1.82 | 0.44 |
| 40:UH:258:ASN:HB2 | 40:UH:352:LYS:HE2 | 1.99 | 0.44 |
| 40:UI:88:HIS:O | 40:UI:90:GLU:N | 2.50 | 0.44 |
| 41:UN:222:TYR:HD1 | 41:UN:225:LEU:HD12 | 1.83 | 0.44 |
| 41:VB:292:GLN:HG2 | 41:VB:298:ASN:HD22 | 1.82 | 0.44 |
| 40:VI:100:ALA:O | 41:VP:255:VAL:HG11 | 2.17 | 0.44 |
| 41:VO:268:PRO:HG2 | 41:VO:300:MET:HB2 | 1.99 | 0.44 |
| 40:WF:136:LEU:HD22 | 40:WF:169:PHE:CZ | 2.53 | 0.44 |
| 40:WH:136:LEU:HD23 | 40:WH:167:LEU:HB2 | 1.99 | 0.44 |
| 41:WM:63:ALA:O | 41:WM:89:ASN:HB3 | 2.18 | 0.44 |
| 41:WM:100:ASN:HB3 | 41:WM:103:LYS:HG3 | 1.98 | 0.44 |
| 41:WM:317:PHE:HB3 | 41:WM:321:MET:SD | 2.58 | 0.44 |
| 41:WN:212:PHE:O | 41:WN:216:LYS:HA | 2.18 | 0.44 |
| 7:1S:459:GLU:HB3 | 7:1S:486:ILE:HD13 | 2.00 | 0.44 |
| 7:1T:390:ILE:HG23 | 7:1T:398:ILE:HG22 | 1.99 | 0.44 |
| 7:1T:397:LYS:HB3 | 7:1T:399:ARG:HG2 | 1.99 | 0.44 |
| 8:1X:174:LEU:HD23 | 8:1X:174:LEU:HA | 1.82 | 0.44 |
| 12:2M:78:ARG:HD2 | 13:2T:72:LYS:HE2 | 1.99 | 0.44 |
| 13:2T:137:SER:O | 13:2T:140:THR:HG22 | 2.17 | 0.44 |
| 13:2X:86:TYR:HB3 | 13:2X:108:TYR:CE2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:3F:132:VAL:HG13 | 15:3F:264:PHE:CE1 | 2.53 | 0.44 |
| 16:3J:350:ALA:O | 16:3J:353:LYS:N | 2.50 | 0.44 |
| 17:3P:218:GLU:HB3 | 17:3P:343:VAL:HG22 | 1.99 | 0.44 |
| 17:3R:285:ARG:HD3 | 17:3R:285:ARG:HA | 1.51 | 0.44 |
| 19:3Y:335:GLN:OE1 | 21:4F:20:SER:OG | 2.35 | 0.44 |
| 20:4A:233:HIS:HA | 20:4A:236:GLN:OE1 | 2.18 | 0.44 |
| 22:4H:250:ILE:HB | 22:4H:263:LYS:HG2 | 2.00 | 0.44 |
| 22:4J:662:CYS:O | 22:4J:667:LEU:HB2 | 2.17 | 0.44 |
| 22:4K:503:LYS:HE2 | 22:4K:503:LYS:HB2 | 1.89 | 0.44 |
| 23:4P:174:MET:HE3 | 23:4P:174:MET:HB3 | 1.89 | 0.44 |
| 23:4Q:171:PRO:HD3 | 41:CO:44:LEU:HD23 | 1.99 | 0.44 |
| 23:4Q:217:LYS:HA | 23:4Q:217:LYS:HD2 | 1.33 | 0.44 |
| 23:4R:173:SER:C | 23:4R:175:ASP:H | 2.20 | 0.44 |
| 23:4R:205:LEU:O | 23:4R:208:GLN:N | 2.51 | 0.44 |
| 25:4T:432:SER:OG | 41:LB:94:GLN:NE2 | 2.51 | 0.44 |
| 26:4V:139:ASP:OD1 | 26:4V:139:ASP:N | 2.51 | 0.44 |
| 26:4W:370:TYR:HA | 26:4W:374:ILE:HG12 | 2.00 | 0.44 |
| 33:5O:106:LYS:HZ1 | 41:HM:33:THR:H | 1.65 | 0.44 |
| 34:5R:344:GLN:O | 34:5R:347:ALA:HB3 | 2.18 | 0.44 |
| 35:5T:71:LYS:HA | 35:5T:74:VAL:HG22 | 2.00 | 0.44 |
| 35:5T:162:MET:CE | 41:KL:320:ARG:HG3 | 2.48 | 0.44 |
| 38:6C:127:GLN:HB3 | 40:VH:339:ARG:HD3 | 1.98 | 0.44 |
| 40:AA:4:CYS:HB2 | 40:AA:52:PHE:HE2 | 1.82 | 0.44 |
| 41:AB:100:ASN:HD22 | 41:AB:103:LYS:HE2 | 1.83 | 0.44 |
| 40:AH:288:VAL:HA | 40:AH:291:ILE:HG12 | 2.00 | 0.44 |
| 41:AN:106:TYR:HE2 | 41:AN:403:MET:HG2 | 1.82 | 0.44 |
| 41:AO:6:HIS:HE1 | 41:AO:17:GLY:HA2 | 1.83 | 0.44 |
| 41:AP:20:PHE:HA | 41:AP:230:SER:HB2 | 2.00 | 0.44 |
| 40:BA:101:ASN:ND2 | 40:BA:143:GLY:HA2 | 2.33 | 0.44 |
| 40:BA:276:ILE:HD12 | 40:BA:281:ALA:HA | 2.00 | 0.44 |
| 40:BG:128:GLN:HE21 | 40:BG:128:GLN:HB3 | 1.58 | 0.44 |
| 40:BH:88:HIS:HB3 | 40:BH:91:GLN:HB3 | 2.00 | 0.44 |
| 40:BH:228:ASN:HA | 40:BH:231:ILE:HD12 | 1.98 | 0.44 |
| 40:BI:56:THR:HG22 | 40:BI:62:VAL:HG12 | 2.00 | 0.44 |
| 40:BI:190:THR:O | 40:BI:193:THR:HG23 | 2.17 | 0.44 |
| 41:BO:360:GLY:O | 41:BO:361:LEU:C | 2.56 | 0.44 |
| 40:CA:12:ALA:O | 40:CA:13:GLY:C | 2.54 | 0.44 |
| 41:CB:150:LEU:O | 41:CB:154:LYS:HG2 | 2.17 | 0.44 |
| 40:CE:181:VAL:HG23 | 40:CE:182:VAL:HG13 | 1.99 | 0.44 |
| 40:CF:62:VAL:HG11 | 40:DF:283:HIS:HB3 | 2.00 | 0.44 |
| 40:CF:88:HIS:HB3 | 40:CF:91:GLN:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CH:114:LEU:HD23 | 40:CH:114:LEU:HA | 1.77 | 0.44 |
| 41:CL:107:THR:O | 41:CL:108:GLU:C | 2.56 | 0.44 |
| 41:CL:320:ARG:HA | 41:CL:320:ARG:HD2 | 1.49 | 0.44 |
| 41:CL:325:GLU:H | 41:CL:325:GLU:HG3 | 1.49 | 0.44 |
| 41:CN:142:GLY:O | 41:CN:143:THR:C | 2.56 | 0.44 |
| 41:CO:49:VAL:O | 41:CO:62:ARG:NH2 | 2.50 | 0.44 |
| 41:CP:56:GLY:O | 41:CP:58:LYS:N | 2.42 | 0.44 |
| 41:CP:56:GLY:C | 41:CP:58:LYS:H | 2.20 | 0.44 |
| 41:CP:226:ASN:ND2 | 43:CP:501:GDP:N1 | 2.66 | 0.44 |
| 40:DA:283:HIS:H | 40:DA:283:HIS:CD2 | 2.36 | 0.44 |
| 40:DA:301:GLN:N | 40:DA:301:GLN:OE1 | 2.51 | 0.44 |
| 40:DA:326:LYS:NZ | 41:DB:208:TYR:HB2 | 2.33 | 0.44 |
| 40:DA:335:ILE:HD13 | 40:DA:335:ILE:HA | 1.77 | 0.44 |
| 40:DA:384:ALA:O | 40:DA:385:GLU:C | 2.55 | 0.44 |
| 40:DA:405:HIS:NE2 | 41:DN:259:PRO:O | 2.50 | 0.44 |
| 40:DE:138:PHE:HD2 | 40:DE:169:PHE:HB2 | 1.83 | 0.44 |
| 40:DF:174:ALA:HB1 | 40:DF:207:GLU:HB3 | 1.99 | 0.44 |
| 40:DH:71:GLU:H | 40:DH:71:GLU:HG3 | 1.41 | 0.44 |
| 40:DI:14:VAL:C | 40:DI:16:ILE:H | 2.22 | 0.44 |
| 40:DI:88:HIS:O | 40:DI:90:GLU:N | 2.50 | 0.44 |
| 40:DI:112:LYS:O | 40:DI:114:LEU:N | 2.50 | 0.44 |
| 41:DL:293:MET:O | 41:DL:294:PHE:C | 2.56 | 0.44 |
| 41:DM:146:GLY:O | 41:DM:147:MET:C | 2.56 | 0.44 |
| 41:DM:289:LEU:HD11 | 41:DM:363:MET:HG2 | 2.00 | 0.44 |
| 41:DM:309:ARG:N | 41:DM:372:THR:HG22 | 2.33 | 0.44 |
| 41:DM:313:VAL:HA | 41:DM:369:GLY:HA3 | 1.99 | 0.44 |
| 41:DM:336:LYS:HB3 | 41:DM:336:LYS:HE2 | 1.26 | 0.44 |
| 41:DN:54:ALA:HB1 | 41:EN:282:ARG:O | 2.17 | 0.44 |
| 41:DN:97:ALA:O | 41:DN:99:ASN:N | 2.51 | 0.44 |
| 41:DN:418:LEU:HD23 | 41:DN:418:LEU:HA | 1.89 | 0.44 |
| 41:DO:131:GLN:HE22 | 41:DO:250:LEU:H | 1.64 | 0.44 |
| 41:DP:21:TRP:HZ2 | 41:DP:63:ALA:HB2 | 1.81 | 0.44 |
| 41:DP:49:VAL:HG21 | 41:DP:240:LEU:O | 2.16 | 0.44 |
| 40:EA:209:ILE:HG23 | 40:EA:230:LEU:HD23 | 2.00 | 0.44 |
| 41:EB:222:TYR:O | 41:EB:226:ASN:ND2 | 2.51 | 0.44 |
| 40:EG:259:LEU:O | 40:EG:379:ASN:ND2 | 2.38 | 0.44 |
| 40:EI:63:PRO:HG2 | 40:EI:87:PHE:CD1 | 2.52 | 0.44 |
| 40:EI:100:ALA:HA | 41:EP:252:LYS:HG3 | 2.00 | 0.44 |
| 40:EI:336:LYS:HE3 | 40:EI:336:LYS:HB3 | 1.26 | 0.44 |
| 41:EL:46:ARG:HH12 | 41:EL:243:PRO:HG3 | 1.82 | 0.44 |
| 41:EM:16:ILE:HA | 41:EM:226:ASN:OD1 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EM:417:ASP:O | 41:EM:421:PRO:HG2 | 2.18 | 0.44 |
| 41:EP:191:GLN:HG3 | 41:EP:195:ASN:HD22 | 1.83 | 0.44 |
| 41:EP:383:GLU:HG2 | 41:EP:384:GLN:N | 2.32 | 0.44 |
| 40:FA:172:TYR:CE2 | 40:FA:386:ALA:HB1 | 2.53 | 0.44 |
| 40:FF:88:HIS:HD2 | 40:GF:283:HIS:HB2 | 1.82 | 0.44 |
| 41:FM:7:LEU:HD21 | 41:FM:120:VAL:HG21 | 1.99 | 0.44 |
| 40:GA:182:VAL:O | 40:GA:186:ASN:ND2 | 2.51 | 0.44 |
| 40:GF:326:LYS:HZ3 | 41:GN:208:TYR:HB2 | 1.82 | 0.44 |
| 40:GI:406:TRP:HB3 | 41:GP:255:VAL:HG13 | 1.99 | 0.44 |
| 41:GM:7:LEU:HB3 | 41:GM:135:LEU:HD13 | 2.00 | 0.44 |
| 41:GM:107:THR:O | 41:GM:109:GLY:N | 2.51 | 0.44 |
| 41:GN:107:THR:O | 41:GN:108:GLU:C | 2.56 | 0.44 |
| 41:GN:178:THR:O | 41:GN:181:GLU:HB2 | 2.17 | 0.44 |
| 41:GN:363:MET:HE3 | 41:GN:363:MET:HB3 | 1.88 | 0.44 |
| 41:GO:323:MET:HA | 41:GO:326:VAL:HG12 | 1.99 | 0.44 |
| 41:HB:256:ASN:HD21 | 40:HG:101:ASN:HD22 | 1.65 | 0.44 |
| 40:HE:380:THR:O | 40:HE:381:THR:C | 2.57 | 0.44 |
| 40:HI:332:ILE:HG22 | 40:HI:336:LYS:HD2 | 1.99 | 0.44 |
| 40:IE:307:PRO:HB3 | 40:IE:312:TYR:HE1 | 1.82 | 0.44 |
| 41:IN:205:GLU:O | 41:IN:208:TYR:HB3 | 2.18 | 0.44 |
| 41:IN:266:PHE:HE1 | 41:IN:370:ASN:HD22 | 1.65 | 0.44 |
| 40:JE:238:ILE:HG22 | 40:JE:318:LEU:HD22 | 1.99 | 0.44 |
| 40:JF:150:THR:O | 40:JF:154:MET:HG2 | 2.17 | 0.44 |
| 41:JM:403:MET:HE2 | 41:JM:403:MET:HB2 | 1.88 | 0.44 |
| 41:KB:309:ARG:NH2 | 41:KB:339:SER:O | 2.50 | 0.44 |
| 40:KF:141:PHE:HB2 | 40:KF:173:PRO:HD3 | 2.00 | 0.44 |
| 40:KG:6:SER:O | 40:KG:65:ALA:HA | 2.18 | 0.44 |
| 40:KG:204:VAL:HG11 | 40:KG:231:ILE:HG12 | 1.99 | 0.44 |
| 40:KG:271:THR:HB | 40:KG:301:GLN:HA | 2.00 | 0.44 |
| 41:KL:271:ALA:HB3 | 41:KL:272:PRO:HD3 | 2.00 | 0.44 |
| 40:LA:319:TYR:HB3 | 40:LA:323:VAL:HG21 | 2.00 | 0.44 |
| 40:LA:394:PHE:HE2 | 40:LA:421:ARG:HB2 | 1.83 | 0.44 |
| 40:LD:217:LEU:HA | 40:LD:277:SER:HB3 | 2.00 | 0.44 |
| 40:MA:278:ALA:H | 40:MA:368:ALA:HB2 | 1.82 | 0.44 |
| 40:MD:288:VAL:HA | 40:MD:291:ILE:HG12 | 2.00 | 0.44 |
| 40:MF:22:GLU:O | 40:MF:26:LEU:HG | 2.18 | 0.44 |
| 40:MF:418:SER:OG | 40:MF:419:GLU:N | 2.51 | 0.44 |
| 40:MG:206:ASN:HA | 40:MG:209:ILE:HD12 | 1.99 | 0.44 |
| 41:ML:25:SER:OG | 41:ML:51:TYR:OH | 2.33 | 0.44 |
| 41:ML:162:ARG:HD3 | 41:ML:162:ARG:HA | 1.75 | 0.44 |
| 41:MN:166:THR:HG23 | 41:MN:199:THR:HG23 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:MN:226:ASN:ND2 | 43:MN:502:GDP:O6 | 2.48 | 0.44 |
| 41:MP:191:GLN:O | 41:MP:195:ASN:ND2 | 2.40 | 0.44 |
| 41:NB:86:ARG:HB2 | 41:NB:89:ASN:HB2 | 1.99 | 0.44 |
| 41:NB:276:ARG:O | 41:NB:276:ARG:NE | 2.37 | 0.44 |
| 40:ND:172:TYR:HD2 | 40:ND:205:ASP:HB2 | 1.82 | 0.44 |
| 40:NE:250:VAL:HB | 40:NE:352:LYS:HZ1 | 1.83 | 0.44 |
| 40:NH:31:GLN:HE22 | 40:NH:37:PRO:HG3 | 1.81 | 0.44 |
| 41:NL:143:THR:O | 41:NL:147:MET:N | 2.43 | 0.44 |
| 41:NN:238:THR:HG21 | 41:NN:318:ARG:HD3 | 2.00 | 0.44 |
| 41:NO:4:ILE:HD11 | 41:NO:131:GLN:HB2 | 2.00 | 0.44 |
| 41:OB:178:THR:HG22 | 41:OB:180:VAL:H | 1.83 | 0.44 |
| 41:OB:202:ILE:HG22 | 41:OB:207:LEU:HD11 | 1.99 | 0.44 |
| 40:OD:240:ALA:HA | 40:OD:243:ARG:NH1 | 2.32 | 0.44 |
| 40:OE:240:ALA:HA | 40:OE:243:ARG:NH1 | 2.33 | 0.44 |
| 40:OE:332:ILE:O | 40:OE:336:LYS:HG2 | 2.18 | 0.44 |
| 40:OF:265:ILE:HG22 | 40:OF:379:ASN:HD21 | 1.83 | 0.44 |
| 40:OG:31:GLN:OE1 | 40:OG:31:GLN:N | 2.51 | 0.44 |
| 40:OG:343:PHE:HZ | 40:OG:351:PHE:HE1 | 1.65 | 0.44 |
| 40:OH:435:GLY:O | 40:OH:436:MET:C | 2.56 | 0.44 |
| 41:OL:268:PRO:HG2 | 41:OL:300:MET:HB2 | 1.99 | 0.44 |
| 41:OM:240:LEU:HD13 | 41:OM:249:ASP:HB2 | 1.99 | 0.44 |
| 40:PA:8:HIS:CE1 | 40:PA:67:PHE:HA | 2.53 | 0.44 |
| 40:PA:402:ALA:HB2 | 41:PN:344:TRP:HZ3 | 1.83 | 0.44 |
| 41:PB:134:GLN:HB2 | 41:PB:165:ASN:HB2 | 1.99 | 0.44 |
| 40:PF:51:THR:HG23 | 40:PF:52:PHE:HD2 | 1.83 | 0.44 |
| 40:PF:210:TYR:HE1 | 40:PF:227:LEU:HD11 | 1.83 | 0.44 |
| 40:PG:232:SER:HA | 40:PG:235:VAL:HG22 | 2.00 | 0.44 |
| 40:PH:318:LEU:O | 40:PH:374:VAL:HA | 2.18 | 0.44 |
| 41:PO:68:LEU:HD21 | 41:PO:109:GLY:HA2 | 2.00 | 0.44 |
| 41:PP:319:GLY:HA2 | 41:PP:357:PRO:HG3 | 2.00 | 0.44 |
| 41:QB:225:LEU:HA | 41:QB:228:LEU:HD12 | 2.00 | 0.44 |
| 41:QB:321:MET:HE3 | 41:QB:321:MET:HB3 | 1.83 | 0.44 |
| 41:QB:414:ASN:O | 41:QB:417:ASP:HB2 | 2.18 | 0.44 |
| 41:QB:425:ARG:HE | 41:QB:425:ARG:HB3 | 1.70 | 0.44 |
| 40:QH:20:CYS:HA | 40:QH:232:SER:HB2 | 2.00 | 0.44 |
| 40:QH:407:TYR:HD2 | 40:QH:417:PHE:HZ | 1.66 | 0.44 |
| 41:QM:36:TYR:O | 41:QM:37:HIS:ND1 | 2.50 | 0.44 |
| 41:QN:67:ASP:HA | 41:QN:143:THR:HG21 | 2.00 | 0.44 |
| 41:QP:19:LYS:HA | 41:QP:19:LYS:HD2 | 1.60 | 0.44 |
| 41:QP:19:LYS:HZ3 | 41:QP:227:HIS:HB2 | 1.83 | 0.44 |
| 41:QP:108:GLU:O | 41:QP:111:GLU:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QP:279:GLN:H | 41:QP:279:GLN:HG2 | 1.56 | 0.44 |
| 41:RB:73:MET:HB3 | 41:RB:90:PHE:CE2 | 2.53 | 0.44 |
| 41:RB:172:SER:OG | 41:RB:175:VAL:O | 2.33 | 0.44 |
| 40:RE:322:ASP:O | 40:RE:372:ARG:NE | 2.50 | 0.44 |
| 41:RL:243:PRO:O | 41:RL:355:ASP:HB2 | 2.17 | 0.44 |
| 41:RL:272:PRO:HG3 | 41:RL:364:SER:HB2 | 2.00 | 0.44 |
| 41:RO:342:VAL:HB | 41:RO:344:TRP:CD1 | 2.53 | 0.44 |
| 40:SG:145:THR:OG1 | 40:SG:146:GLY:N | 2.50 | 0.44 |
| 41:SO:391:ARG:O | 41:SO:392:LYS:C | 2.56 | 0.44 |
| 41:SO:394:PHE:HD1 | 41:SO:397:TRP:HH2 | 1.64 | 0.44 |
| 40:TE:81:GLY:O | 40:TE:84:ARG:NH1 | 2.51 | 0.44 |
| 40:TE:248:LEU:HG | 40:TE:353:VAL:HG23 | 1.99 | 0.44 |
| 41:TM:189:VAL:HA | 41:TM:192:LEU:HB2 | 2.00 | 0.44 |
| 41:TM:290:THR:HG21 | 41:TM:329:GLN:HB3 | 2.00 | 0.44 |
| 41:TO:238:THR:HG21 | 41:TO:318:ARG:NE | 2.33 | 0.44 |
| 41:TO:313:VAL:HB | 41:TO:349:VAL:HG22 | 2.00 | 0.44 |
| 41:TP:86:ARG:HG3 | 41:TP:88:ASP:H | 1.82 | 0.44 |
| 40:UF:221:ARG:H | 40:UF:221:ARG:HG3 | 1.63 | 0.44 |
| 40:UG:177:VAL:HG23 | 40:UG:178:SER:H | 1.83 | 0.44 |
| 40:UI:119:LEU:O | 40:UI:122:ILE:HG12 | 2.18 | 0.44 |
| 40:UI:259:LEU:HD22 | 40:UI:316:CYS:HB3 | 1.99 | 0.44 |
| 40:UI:383:ILE:H | 40:UI:383:ILE:HG13 | 1.64 | 0.44 |
| 41:UM:131:GLN:HE22 | 41:UM:240:LEU:HD22 | 1.81 | 0.44 |
| 41:UP:36:TYR:CZ | 41:UP:38:GLY:HA3 | 2.53 | 0.44 |
| 40:VA:326:LYS:HD3 | 41:VB:208:TYR:CE1 | 2.52 | 0.44 |
| 40:VH:16:ILE:HD11 | 40:VH:171:ILE:HD11 | 1.99 | 0.44 |
| 40:VH:116:ASP:OD1 | 40:VH:117:LEU:N | 2.51 | 0.44 |
| 41:VP:323:MET:HE2 | 41:VP:323:MET:HB3 | 1.89 | 0.44 |
| 41:VQ:237:THR:HG23 | 41:VQ:241:ARG:HH21 | 1.83 | 0.44 |
| 41:WB:253:LEU:O | 41:WB:257:MET:HB2 | 2.18 | 0.44 |
| 40:WE:51:THR:HG21 | 40:WE:243:ARG:HG2 | 2.00 | 0.44 |
| 41:WM:263:LEU:HD22 | 41:WM:263:LEU:HA | 1.86 | 0.44 |
| 41:WQ:105:HIS:CD2 | 41:WQ:150:LEU:HB2 | 2.53 | 0.44 |
| 7:1U:129:LEU:HD11 | 7:1U:161:ALA:HB3 | 2.00 | 0.44 |
| 9:2B:330:ASN:O | 9:2B:334:LYS:NZ | 2.41 | 0.44 |
| 9:2B:359:GLU:O | 9:2B:363:ARG:HG2 | 2.17 | 0.44 |
| 9:2B:365:LYS:HZ1 | 40:TE:371:GLN:HE21 | 1.66 | 0.44 |
| 10:2E:46:ARG:NH1 | 40:ME:430:ASP:OD1 | 2.49 | 0.44 |
| 10:2E:164:ASP:HB3 | 40:VG:117:LEU:HD22 | 1.99 | 0.44 |
| 11:2I:166:LYS:HD3 | 11:2I:166:LYS:HA | 1.49 | 0.44 |
| 12:2Q:158:ASN:HD22 | 12:2Q:158:ASN:HA | 1.59 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2U:59:ILE:HG13 | 13:2U:156:ILE:O | 2.18 | 0.44 |
| 13:2W:173:SER:O | 13:2W:175:ASP:N | 2.51 | 0.44 |
| 14:3B:2:ALA:HA | 40:MD:348:PRO:HA | 2.00 | 0.44 |
| 17:3O:434:LEU:HD23 | 17:3O:434:LEU:HA | 1.82 | 0.44 |
| 17:3P:451:THR:HG23 | 17:3P:455:LEU:HD23 | 1.99 | 0.44 |
| 17:3R:157:LYS:HE3 | 17:3R:157:LYS:HB2 | 1.63 | 0.44 |
| 18:3U:376:ARG:HD2 | 18:3U:376:ARG:HA | 1.82 | 0.44 |
| 20:4A:169:GLN:C | 20:4A:171:GLN:N | 2.71 | 0.44 |
| 20:4B:228:ARG:HB3 | 20:4B:229:GLN:H | 1.51 | 0.44 |
| 21:4D:517:GLU:O | 21:4D:518:SER:C | 2.55 | 0.44 |
| 21:4E:50:ASP:N | 21:4E:50:ASP:OD1 | 2.50 | 0.44 |
| 22:4H:276:SER:OG | 22:4H:277:LEU:N | 2.49 | 0.44 |
| 22:4I:696:ALA:O | 22:4I:697:LEU:C | 2.56 | 0.44 |
| 22:4J:461:ASP:N | 22:4J:461:ASP:OD1 | 2.48 | 0.44 |
| 23:4M:216:MET:O | 23:4M:217:LYS:C | 2.57 | 0.44 |
| 23:4N:27:PRO:HG2 | 41:BM:44:LEU:HD13 | 1.99 | 0.44 |
| 23:4P:195:ARG:HA | 23:4P:195:ARG:HD3 | 1.47 | 0.44 |
| 27:4Y:136:VAL:HG23 | 27:4Y:138:GLY:H | 1.81 | 0.44 |
| 31:5I:560:PHE:HB3 | 40:II:370:VAL:HG12 | 2.00 | 0.44 |
| 31:5I:599:HIS:O | 31:5I:603:LYS:HG2 | 2.17 | 0.44 |
| 31:5J:784:SER:HB2 | 31:5J:786:ARG:HH22 | 1.83 | 0.44 |
| 34:5R:426:LEU:HD12 | 34:5R:426:LEU:HA | 1.76 | 0.44 |
| 36:5X:217:THR:O | 36:5X:221:GLN:NE2 | 2.51 | 0.44 |
| 38:6C:144:ASN:HB2 | 41:VP:336:LYS:NZ | 2.33 | 0.44 |
| 40:AA:20:CYS:HA | 40:AA:232:SER:HB2 | 2.00 | 0.44 |
| 40:AE:182:VAL:HG22 | 41:AL:256:ASN:HD21 | 1.83 | 0.44 |
| 40:AG:164:LYS:HD3 | 40:AG:164:LYS:HA | 1.77 | 0.44 |
| 40:AG:317:LEU:HG | 40:AG:376:MET:HG2 | 1.98 | 0.44 |
| 41:AL:139:LEU:HD12 | 41:AL:170:VAL:HG22 | 1.99 | 0.44 |
| 41:AM:73:MET:HG3 | 41:AM:92:PHE:HD2 | 1.83 | 0.44 |
| 40:BA:213:CYS:HB3 | 40:BA:222:PRO:HG3 | 1.98 | 0.44 |
| 40:BG:7:VAL:HG11 | 40:BG:153:LEU:HD11 | 2.00 | 0.44 |
| 40:BG:238:ILE:HG23 | 40:BG:255:PHE:HE2 | 1.83 | 0.44 |
| 40:BI:84:ARG:HG2 | 40:BI:85:GLN:N | 2.33 | 0.44 |
| 40:BI:205:ASP:HB2 | 40:BI:303:VAL:HA | 1.99 | 0.44 |
| 41:BN:171:PRO:O | 41:BN:380:ARG:NH2 | 2.51 | 0.44 |
| 41:BO:101:TRP:HZ3 | 41:BO:106:TYR:CE2 | 2.36 | 0.44 |
| 41:BP:58:LYS:HA | 41:BP:58:LYS:HD2 | 1.59 | 0.44 |
| 40:CA:210:TYR:CD1 | 40:CA:222:PRO:HG2 | 2.52 | 0.44 |
| 40:CG:182:VAL:HG23 | 40:CG:186:ASN:HD21 | 1.83 | 0.44 |
| 40:CH:9:VAL:HA | 40:CH:68:VAL:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CH:11:GLN:HA | 40:CH:74:VAL:HG21 | 2.00 | 0.44 |
| 40:CH:136:LEU:HD13 | 40:CH:136:LEU:HA | 1.85 | 0.44 |
| 40:CI:352:LYS:HD3 | 40:CI:352:LYS:HA | 1.76 | 0.44 |
| 41:CM:123:GLU:O | 41:CM:124:ALA:C | 2.56 | 0.44 |
| 41:CN:297:LYS:HE3 | 41:CN:297:LYS:HB2 | 1.59 | 0.44 |
| 41:CO:100:ASN:O | 41:CO:101:TRP:C | 2.56 | 0.44 |
| 41:CP:42:LEU:HD12 | 41:CP:42:LEU:HA | 1.78 | 0.44 |
| 40:DA:15:GLN:HE22 | 40:DA:16:ILE:HG12 | 1.83 | 0.44 |
| 41:DB:192:LEU:O | 41:DB:196:THR:HG22 | 2.18 | 0.44 |
| 40:DE:406:TRP:O | 40:DE:407:TYR:C | 2.56 | 0.44 |
| 40:DF:12:ALA:O | 40:DF:16:ILE:HG23 | 2.18 | 0.44 |
| 40:DF:236:SER:O | 40:DF:240:ALA:N | 2.51 | 0.44 |
| 40:DH:14:VAL:HG21 | 40:DH:75:ILE:HG12 | 2.00 | 0.44 |
| 40:DH:213:CYS:HB2 | 40:DH:222:PRO:CB | 2.47 | 0.44 |
| 40:DI:186:ASN:ND2 | 40:DI:407:TYR:OH | 2.50 | 0.44 |
| 40:DI:262:TYR:O | 40:DI:263:PRO:C | 2.56 | 0.44 |
| 40:DI:322:ASP:O | 40:DI:323:VAL:C | 2.57 | 0.44 |
| 40:DI:333:ALA:O | 40:DI:337:THR:HG23 | 2.18 | 0.44 |
| 41:DM:46:ARG:HA | 41:DM:46:ARG:HD3 | 1.40 | 0.44 |
| 41:DN:218:THR:C | 41:DN:220:PRO:HD3 | 2.38 | 0.44 |
| 41:EB:226:ASN:ND2 | 43:EB:501:GDP:O6 | 2.49 | 0.44 |
| 40:EF:262:TYR:HB2 | 40:EF:265:ILE:HG22 | 2.00 | 0.44 |
| 40:EI:31:GLN:HB3 | 40:EI:32:PRO:HD2 | 2.00 | 0.44 |
| 41:EM:151:LEU:HD22 | 41:EM:151:LEU:HA | 1.86 | 0.44 |
| 41:EO:404:ASP:OD1 | 41:EO:405:GLU:N | 2.50 | 0.44 |
| 41:EP:89:ASN:O | 41:EP:90:PHE:C | 2.57 | 0.44 |
| 41:EP:280:GLN:H | 41:EP:280:GLN:HG2 | 1.62 | 0.44 |
| 40:FA:104:ALA:O | 40:FA:105:ARG:C | 2.57 | 0.44 |
| 41:FB:214:THR:OG1 | 41:FB:215:LEU:N | 2.51 | 0.44 |
| 40:FE:70:LEU:HA | 40:FE:95:GLY:HA3 | 2.00 | 0.44 |
| 40:FE:225:THR:HG22 | 40:FE:229:ARG:HH21 | 1.83 | 0.44 |
| 40:FF:318:LEU:O | 40:FF:374:VAL:HA | 2.18 | 0.44 |
| 40:GE:20:CYS:HA | 40:GE:232:SER:HB2 | 1.99 | 0.44 |
| 40:GE:170:SER:HB3 | 40:GE:203:MET:SD | 2.58 | 0.44 |
| 40:GG:356:ASN:OD1 | 40:GG:357:TYR:N | 2.51 | 0.44 |
| 40:GH:109:THR:HB | 40:GH:110:ILE:H | 1.61 | 0.44 |
| 40:GH:260:VAL:O | 40:GH:261:PRO:C | 2.56 | 0.44 |
| 41:GN:107:THR:HB | 41:GN:108:GLU:H | 1.64 | 0.44 |
| 41:GN:117:LEU:HD11 | 41:GN:154:LYS:HB3 | 1.99 | 0.44 |
| 41:GP:236:VAL:HG13 | 41:GP:237:THR:HG23 | 2.00 | 0.44 |
| 40:HE:380:THR:C | 40:HE:382:ALA:N | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HF:132:LEU:HD23 | 40:HF:164:LYS:HZ2 | 1.81 | 0.44 |
| 40:HF:136:LEU:HD23 | 40:HF:167:LEU:HB2 | 2.00 | 0.44 |
| 40:HF:221:ARG:NH1 | 41:HM:325:GLU:OE1 | 2.50 | 0.44 |
| 40:HF:234:ILE:HD12 | 40:HF:270:ALA:HB1 | 2.00 | 0.44 |
| 40:HG:326:LYS:HG2 | 40:HG:329:ASN:HB2 | 1.99 | 0.44 |
| 40:HI:16:ILE:HA | 40:HI:228:ASN:HB3 | 1.98 | 0.44 |
| 40:HI:206:ASN:HD22 | 40:HI:227:LEU:HD12 | 1.82 | 0.44 |
| 41:HN:67:ASP:C | 41:HN:69:GLU:H | 2.21 | 0.44 |
| 41:HO:214:THR:OG1 | 41:HO:297:LYS:NZ | 2.32 | 0.44 |
| 41:HO:330:MET:HA | 41:HO:333:VAL:HG12 | 1.98 | 0.44 |
| 41:HQ:266:PHE:HB3 | 41:HQ:368:ILE:HD11 | 2.00 | 0.44 |
| 40:IG:96:LYS:HE3 | 40:IG:96:LYS:HB2 | 1.81 | 0.44 |
| 41:IN:86:ARG:HB3 | 41:IN:89:ASN:HB2 | 2.00 | 0.44 |
| 41:IP:42:LEU:HD21 | 41:IP:243:PRO:HD2 | 1.99 | 0.44 |
| 40:JD:254:GLU:HG3 | 41:JL:99:ASN:HB2 | 2.00 | 0.44 |
| 40:JE:11:GLN:HG3 | 40:JE:74:VAL:HG21 | 2.00 | 0.44 |
| 40:JF:324:VAL:HG12 | 40:JF:327:ASP:H | 1.82 | 0.44 |
| 40:JH:172:TYR:OH | 40:JH:386:ALA:O | 2.30 | 0.44 |
| 41:JM:289:LEU:HD23 | 41:JM:289:LEU:HA | 1.72 | 0.44 |
| 41:KB:385:PHE:HE1 | 41:KB:412:GLU:HB2 | 1.83 | 0.44 |
| 40:KE:288:VAL:HA | 40:KE:291:ILE:HG12 | 1.98 | 0.44 |
| 40:KF:88:HIS:HB3 | 40:KF:91:GLN:HG3 | 2.00 | 0.44 |
| 40:KG:224:TYR:O | 40:KG:228:ASN:ND2 | 2.51 | 0.44 |
| 41:KL:142:GLY:O | 41:KL:143:THR:C | 2.55 | 0.44 |
| 41:KP:309:ARG:H | 41:KP:372:THR:HG1 | 1.62 | 0.44 |
| 40:LA:178:SER:OG | 40:LA:179:THR:N | 2.51 | 0.44 |
| 41:LB:198:GLU:HG2 | 41:LB:266:PHE:HE2 | 1.83 | 0.44 |
| 40:LD:238:ILE:HG23 | 40:LD:255:PHE:CE2 | 2.53 | 0.44 |
| 41:LP:274:THR:HG22 | 41:LP:282:ARG:HH11 | 1.82 | 0.44 |
| 40:MF:320:ARG:HG2 | 40:MF:360:PRO:HG3 | 1.99 | 0.44 |
| 40:MG:119:LEU:HD23 | 40:MG:122:ILE:HD12 | 2.00 | 0.44 |
| 40:MG:313:MET:HE2 | 40:MG:434:VAL:HG23 | 2.00 | 0.44 |
| 40:MH:139:HIS:HE2 | 40:MH:168:GLU:HG3 | 1.82 | 0.44 |
| 41:MM:36:TYR:OH | 41:MM:40:SER:O | 2.30 | 0.44 |
| 41:MM:183:TYR:HE2 | 41:MM:394:PHE:HB2 | 1.83 | 0.44 |
| 41:MO:49:VAL:HG21 | 41:MO:240:LEU:O | 2.17 | 0.44 |
| 41:MO:420:ASN:O | 41:MO:423:VAL:N | 2.51 | 0.44 |
| 40:NA:200:CYS:HA | 40:NA:266:HIS:HB2 | 2.00 | 0.44 |
| 40:NA:256:GLN:HG2 | 41:NB:397:TRP:HZ2 | 1.80 | 0.44 |
| 40:NE:205:ASP:HB2 | 40:NE:303:VAL:HG22 | 2.00 | 0.44 |
| 40:NG:141:PHE:HB2 | 40:NG:173:PRO:HD3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NG:196:GLU:HG2 | 40:NG:197:HIS:CD2 | 2.53 | 0.44 |
| 40:NG:276:ILE:HD13 | 40:NG:286:LEU:HD11 | 2.00 | 0.44 |
| 41:NL:107:THR:O | 41:NL:109:GLY:N | 2.50 | 0.44 |
| 40:OA:242:LEU:H | 40:OA:242:LEU:HD23 | 1.83 | 0.44 |
| 40:OD:114:LEU:HD23 | 40:OD:117:LEU:HD21 | 2.00 | 0.44 |
| 40:OE:221:ARG:NE | 41:OL:322:SER:OG | 2.32 | 0.44 |
| 40:OH:222:PRO:CD | 41:OO:324:LYS:HD3 | 2.48 | 0.44 |
| 41:OL:331:LEU:O | 41:OL:335:ASN:ND2 | 2.50 | 0.44 |
| 41:OP:139:LEU:HD13 | 41:OP:170:VAL:HG12 | 2.00 | 0.44 |
| 40:PG:345:ASP:OD1 | 40:PG:345:ASP:N | 2.45 | 0.44 |
| 40:PH:138:PHE:HD1 | 40:PH:169:PHE:HB2 | 1.83 | 0.44 |
| 40:PH:234:ILE:O | 40:PH:238:ILE:HG23 | 2.18 | 0.44 |
| 41:PP:19:LYS:HG3 | 41:PP:226:ASN:HB2 | 2.00 | 0.44 |
| 41:PP:107:THR:HG22 | 41:PP:108:GLU:H | 1.83 | 0.44 |
| 41:PP:285:THR:N | 41:PP:288:GLU:OE2 | 2.48 | 0.44 |
| 41:QB:400:GLY:O | 41:QB:401:GLU:C | 2.56 | 0.44 |
| 40:QG:150:THR:O | 40:QG:154:MET:HG2 | 2.18 | 0.44 |
| 40:QH:238:ILE:HA | 40:QH:318:LEU:HD22 | 2.00 | 0.44 |
| 41:QL:111:GLU:OE2 | 41:QL:111:GLU:N | 2.48 | 0.44 |
| 41:QL:232:THR:HG22 | 41:QL:270:PHE:HB2 | 2.00 | 0.44 |
| 41:QM:31:ASP:OD1 | 41:QM:34:GLY:N | 2.49 | 0.44 |
| 41:QN:139:LEU:HG | 41:QN:168:SER:HB2 | 2.00 | 0.44 |
| 41:QO:134:GLN:NE2 | 41:QO:233:MET:SD | 2.87 | 0.44 |
| 41:QO:139:LEU:HG | 41:QO:168:SER:HB2 | 1.98 | 0.44 |
| 41:QP:245:GLN:O | 41:QP:246:LEU:C | 2.55 | 0.44 |
| 41:RB:258:VAL:HB | 40:RG:406:TRP:CH2 | 2.53 | 0.44 |
| 40:RE:164:LYS:O | 40:RE:166:LYS:NZ | 2.51 | 0.44 |
| 41:RO:107:THR:O | 41:RO:110:ALA:N | 2.35 | 0.44 |
| 40:SA:177:VAL:HG23 | 40:SA:178:SER:H | 1.81 | 0.44 |
| 41:SB:391:ARG:O | 41:SB:392:LYS:C | 2.56 | 0.44 |
| 40:SG:326:LYS:HD3 | 41:SO:208:TYR:CD2 | 2.53 | 0.44 |
| 41:SL:282:ARG:HD2 | 41:SL:283:ALA:N | 2.31 | 0.44 |
| 41:SO:211:CYS:SG | 41:SO:212:PHE:N | 2.91 | 0.44 |
| 41:TB:282:ARG:HA | 41:TB:282:ARG:HD2 | 1.78 | 0.44 |
| 40:TE:209:ILE:HG22 | 40:TE:227:LEU:HD22 | 1.98 | 0.44 |
| 40:TG:273:ALA:HB1 | 40:TG:291:ILE:HB | 1.98 | 0.44 |
| 41:TL:240:LEU:HD23 | 41:TL:240:LEU:H | 1.83 | 0.44 |
| 41:TN:262:ARG:HH11 | 41:TN:418:LEU:HD13 | 1.83 | 0.44 |
| 41:TO:375:GLN:NE2 | 41:TO:419:GLY:HA2 | 2.33 | 0.44 |
| 41:TP:207:LEU:HA | 41:TP:210:ILE:HG22 | 2.00 | 0.44 |
| 40:UF:280:LYS:HB3 | 40:UF:280:LYS:HE3 | 1.76 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UF:325:PRO:HB3 | 41:UN:222:TYR:OH | 2.17 | 0.44 |
| 40:UF:346:TRP:HZ2 | 40:UF:434:VAL:HG13 | 1.81 | 0.44 |
| 40:UF:346:TRP:CB | 41:UN:391:ARG:HD3 | 2.44 | 0.44 |
| 40:UF:399:ALA:C | 40:UF:401:ARG:H | 2.21 | 0.44 |
| 40:UG:259:LEU:HD23 | 40:UG:259:LEU:HA | 1.84 | 0.44 |
| 41:UO:134:GLN:HB3 | 41:UO:167:PHE:HE2 | 1.82 | 0.44 |
| 41:UP:55:THR:HG22 | 41:VQ:282:ARG:O | 2.18 | 0.44 |
| 41:UP:289:LEU:HD23 | 41:UP:289:LEU:HA | 1.83 | 0.44 |
| 40:VH:231:ILE:O | 40:VH:235:VAL:HG23 | 2.18 | 0.44 |
| 40:VH:306:ASP:HB3 | 40:VH:309:HIS:HB2 | 1.99 | 0.44 |
| 40:WA:288:VAL:HA | 40:WA:291:ILE:HG12 | 1.99 | 0.44 |
| 41:WM:88:ASP:C | 41:WM:90:PHE:H | 2.21 | 0.44 |
| 41:WM:178:THR:HB | 41:WM:181:GLU:HG2 | 2.00 | 0.44 |
| 41:WP:22:GLU:OE2 | 41:WP:81:PHE:HB2 | 2.18 | 0.44 |
| 8:1X:160:LEU:HD11 | 8:1X:168:LYS:HD3 | 1.99 | 0.43 |
| 11:2I:119:LYS:NZ | 40:LG:409:GLY:C | 2.70 | 0.43 |
| 12:2Q:246:TYR:CE1 | 41:AO:261:PRO:HB3 | 2.53 | 0.43 |
| 13:2T:36:ARG:HG2 | 13:2T:47:LEU:HD13 | 2.00 | 0.43 |
| 13:2T:37:ILE:HD12 | 13:2T:37:ILE:HA | 1.76 | 0.43 |
| 13:2V:80:ILE:CG2 | 13:2V:160:CYS:HB2 | 2.48 | 0.43 |
| 13:2X:10:PHE:CZ | 13:2X:178:PRO:HD3 | 2.53 | 0.43 |
| 13:2X:13:ILE:HD12 | 13:2X:154:VAL:HG11 | 1.99 | 0.43 |
| 17:3P:100:TYR:HA | 17:3P:103:ASN:HB2 | 2.00 | 0.43 |
| 17:3P:164:LEU:HD12 | 17:3P:164:LEU:HA | 1.82 | 0.43 |
| 17:3P:337:TRP:CZ3 | 17:3P:480:PHE:HB2 | 2.53 | 0.43 |
| 17:3P:434:LEU:HD13 | 17:3P:434:LEU:HA | 1.79 | 0.43 |
| 17:3R:118:GLU:HB2 | 17:3R:119:ARG:HH21 | 1.83 | 0.43 |
| 17:3R:182:GLU:O | 17:3R:186:MET:HG3 | 2.18 | 0.43 |
| 17:3R:197:GLU:O | 17:3R:198:CYS:C | 2.56 | 0.43 |
| 17:3R:345:LEU:HA | 17:3R:345:LEU:HD22 | 1.76 | 0.43 |
| 18:3T:88:THR:HG21 | 18:3W:391:LEU:HD11 | 2.00 | 0.43 |
| 19:3Z:369:PRO:O | 41:LP:279:GLN:NE2 | 2.51 | 0.43 |
| 20:4B:250:SER:O | 20:4B:254:THR:HB | 2.18 | 0.43 |
| 20:4B:351:LYS:HA | 20:4B:354:HIS:CD2 | 2.53 | 0.43 |
| 21:4D:514:LYS:HA | 21:4D:514:LYS:HD3 | 1.86 | 0.43 |
| 21:4E:98:LYS:HD2 | 40:AH:41:THR:HG23 | 1.99 | 0.43 |
| 21:4E:348:ASP:OD1 | 21:4E:348:ASP:N | 2.50 | 0.43 |
| 21:4E:497:GLU:HB3 | 21:4E:502:ARG:HB2 | 2.00 | 0.43 |
| 21:4F:263:ILE:HB | 21:4F:276:LEU:HB2 | 2.00 | 0.43 |
| 21:4F:513:LEU:O | 21:4F:514:LYS:C | 2.56 | 0.43 |
| 22:4I:63:GLU:HG3 | 22:4I:181:ILE:HD13 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4I:233:PHE:HB2 | 22:4I:355:ASP:HB3 | 2.00 | 0.43 |
| 22:4J:358:GLU:HB2 | 40:CF:39:ASP:OD1 | 2.18 | 0.43 |
| 22:4J:654:PRO:O | 22:4J:657:ASP:N | 2.50 | 0.43 |
| 22:4K:656:LYS:HB2 | 22:4K:656:LYS:HE2 | 1.35 | 0.43 |
| 23:4N:243:LEU:O | 23:4N:246:TYR:HB3 | 2.18 | 0.43 |
| 23:4P:193:ARG:HH22 | 41:CN:56:GLY:H | 1.64 | 0.43 |
| 23:4P:243:LEU:O | 23:4P:246:TYR:HB3 | 2.18 | 0.43 |
| 23:4R:233:SER:HB2 | 23:4R:234:ARG:H | 1.63 | 0.43 |
| 26:4W:233:THR:HA | 26:4W:271:ALA:HB2 | 1.99 | 0.43 |
| 28:5B:102:LEU:HD12 | 28:5B:103:ASN:HB2 | 1.99 | 0.43 |
| 31:5J:763:HIS:NE2 | 40:IE:369:LYS:HB2 | 2.32 | 0.43 |
| 34:5R:312:LYS:HE2 | 34:5R:313:LEU:N | 2.32 | 0.43 |
| 36:5W:110:CYS:HG | 36:5W:112:HIS:HD1 | 1.62 | 0.43 |
| 36:5W:118:TYR:HD2 | 36:5W:121:MET:HG3 | 1.83 | 0.43 |
| 38:6C:63:ASP:HB3 | 40:VA:304:LYS:NZ | 2.33 | 0.43 |
| 39:6F:44:PRO:HB3 | 39:6F:135:HIS:HA | 2.00 | 0.43 |
| 41:AB:421:PRO:O | 41:AB:425:ARG:HG2 | 2.19 | 0.43 |
| 41:AM:170:VAL:HG11 | 41:AM:377:LEU:HD21 | 2.00 | 0.43 |
| 41:AO:191:GLN:H | 41:AO:191:GLN:HG2 | 1.57 | 0.43 |
| 40:BA:177:VAL:HG23 | 40:BA:178:SER:H | 1.82 | 0.43 |
| 40:BE:119:LEU:HD13 | 40:BE:119:LEU:HA | 1.72 | 0.43 |
| 41:BM:110:ALA:C | 41:BM:112:LEU:H | 2.21 | 0.43 |
| 41:BO:101:TRP:HZ3 | 41:BO:106:TYR:HE2 | 1.65 | 0.43 |
| 41:BP:70:PRO:O | 41:BP:71:GLY:C | 2.56 | 0.43 |
| 41:BP:371:SER:C | 41:BP:373:ALA:N | 2.72 | 0.43 |
| 40:CA:99:ALA:O | 40:CA:100:ALA:C | 2.56 | 0.43 |
| 40:CA:296:PHE:HE1 | 40:CA:317:LEU:HD21 | 1.83 | 0.43 |
| 40:CA:326:LYS:O | 40:CA:327:ASP:C | 2.57 | 0.43 |
| 41:CB:296:ALA:HB1 | 41:CB:305:PRO:HD2 | 2.00 | 0.43 |
| 40:CE:400:LYS:HD2 | 41:CL:344:TRP:CG | 2.53 | 0.43 |
| 40:CH:88:HIS:C | 40:CH:90:GLU:H | 2.21 | 0.43 |
| 40:CH:429:LYS:HB2 | 40:CH:429:LYS:HE3 | 1.61 | 0.43 |
| 41:CL:251:ARG:O | 41:CL:254:ALA:N | 2.51 | 0.43 |
| 41:CM:101:TRP:O | 41:CM:102:ALA:C | 2.57 | 0.43 |
| 40:DA:7:VAL:HG13 | 40:DA:137:ILE:HA | 2.00 | 0.43 |
| 40:DA:31:GLN:C | 40:DA:33:ASP:N | 2.71 | 0.43 |
| 41:DB:273:LEU:HD23 | 41:DB:273:LEU:HA | 1.82 | 0.43 |
| 40:DE:403:PHE:HZ | 41:DL:312:THR:HG21 | 1.82 | 0.43 |
| 41:DL:279:GLN:HG3 | 41:DL:280:GLN:H | 1.83 | 0.43 |
| 41:DM:147:MET:HE2 | 41:DM:147:MET:HB2 | 1.49 | 0.43 |
| 41:DN:15:GLN:O | 41:DN:16:ILE:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DN:222:TYR:O | 41:DN:226:ASN:N | 2.50 | 0.43 |
| 41:DO:39:ASP:OD1 | 41:DO:39:ASP:N | 2.49 | 0.43 |
| 41:DP:12:CYS:HB2 | 43:DP:501:GDP:C8 | 2.53 | 0.43 |
| 40:EA:71:GLU:OE2 | 41:EN:2:ARG:NH1 | 2.51 | 0.43 |
| 40:EF:122:ILE:HG22 | 40:EF:161:TYR:HE2 | 1.83 | 0.43 |
| 40:EF:234:ILE:HD13 | 40:EF:272:TYR:HD2 | 1.83 | 0.43 |
| 40:EI:187:SER:O | 40:EI:191:THR:HG23 | 2.18 | 0.43 |
| 40:EI:230:LEU:HD13 | 40:EI:230:LEU:HA | 1.78 | 0.43 |
| 40:EI:317:LEU:HD13 | 40:EI:317:LEU:HA | 1.80 | 0.43 |
| 41:EM:19:LYS:HB2 | 41:EM:226:ASN:ND2 | 2.34 | 0.43 |
| 41:EN:103:LYS:HG2 | 41:EN:107:THR:HG21 | 2.00 | 0.43 |
| 40:FA:31:GLN:O | 40:FA:32:PRO:C | 2.56 | 0.43 |
| 40:FA:91:GLN:HG3 | 40:FA:121:ARG:HH21 | 1.82 | 0.43 |
| 40:FA:219:ILE:HB | 40:FA:222:PRO:HG3 | 2.00 | 0.43 |
| 40:FA:219:ILE:H | 40:FA:219:ILE:HG12 | 1.58 | 0.43 |
| 40:FA:273:ALA:HB2 | 40:FA:374:VAL:CG1 | 2.48 | 0.43 |
| 40:FA:398:TYR:CZ | 40:FA:417:PHE:HB2 | 2.52 | 0.43 |
| 40:FF:235:VAL:O | 40:FF:239:THR:HG22 | 2.18 | 0.43 |
| 41:FP:10:GLY:HA2 | 41:FP:143:THR:HG22 | 2.00 | 0.43 |
| 40:GE:126:ALA:HA | 40:GE:132:LEU:HD21 | 2.00 | 0.43 |
| 40:GE:211:ASP:O | 40:GE:212:ILE:C | 2.56 | 0.43 |
| 40:GE:315:CYS:SG | 40:GE:316:CYS:N | 2.90 | 0.43 |
| 40:GE:406:TRP:HA | 40:GE:406:TRP:CE3 | 2.53 | 0.43 |
| 40:GF:260:VAL:HG12 | 40:GF:266:HIS:HA | 1.99 | 0.43 |
| 40:GF:371:GLN:N | 40:GF:371:GLN:OE1 | 2.51 | 0.43 |
| 40:GI:48:SER:O | 40:GI:49:PHE:C | 2.56 | 0.43 |
| 40:GI:421:ARG:HD2 | 40:GI:421:ARG:HA | 1.51 | 0.43 |
| 41:GN:20:PHE:CE1 | 41:GN:233:MET:HB3 | 2.53 | 0.43 |
| 41:GN:226:ASN:O | 41:GN:229:VAL:N | 2.51 | 0.43 |
| 41:GO:240:LEU:HD12 | 41:GO:241:ARG:HG3 | 1.99 | 0.43 |
| 41:GO:342:VAL:HG21 | 41:GO:345:ILE:HD12 | 2.00 | 0.43 |
| 41:GP:316:VAL:HA | 41:GP:352:ALA:O | 2.18 | 0.43 |
| 40:HE:252:LEU:HA | 40:HE:255:PHE:CD2 | 2.53 | 0.43 |
| 40:HF:383:ILE:HA | 40:HF:386:ALA:HB3 | 1.99 | 0.43 |
| 40:HH:89:PRO:HD3 | 40:IH:283:HIS:ND1 | 2.33 | 0.43 |
| 41:HM:102:ALA:HB1 | 41:HM:401:GLU:HB2 | 1.99 | 0.43 |
| 40:IA:115:ILE:HA | 40:IA:118:VAL:HG12 | 1.99 | 0.43 |
| 40:IE:318:LEU:O | 40:IE:374:VAL:HA | 2.18 | 0.43 |
| 40:IF:416:GLU:HA | 40:IF:419:GLU:HG3 | 2.00 | 0.43 |
| 40:IG:115:ILE:HA | 40:IG:118:VAL:HG12 | 2.00 | 0.43 |
| 40:IG:224:TYR:HA | 40:IG:227:LEU:HD12 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IM:8:GLN:NE2 | 41:IM:14:ASN:OD1 | 2.51 | 0.43 |
| 41:IM:142:GLY:O | 41:IM:144:GLY:N | 2.51 | 0.43 |
| 41:IM:216:LYS:HE2 | 41:IM:216:LYS:HB2 | 1.77 | 0.43 |
| 41:IQ:312:THR:OG1 | 41:IQ:370:ASN:OD1 | 2.36 | 0.43 |
| 40:JD:10:GLY:HA2 | 40:JD:145:THR:HG22 | 2.00 | 0.43 |
| 40:JH:276:ILE:HG22 | 40:JH:277:SER:H | 1.82 | 0.43 |
| 41:JL:213:ARG:HE | 41:JL:297:LYS:HZ1 | 1.66 | 0.43 |
| 41:JM:138:SER:O | 41:JM:139:LEU:C | 2.56 | 0.43 |
| 41:JM:154:LYS:HE2 | 41:JM:154:LYS:HB2 | 1.93 | 0.43 |
| 41:KB:237:THR:HG22 | 41:KB:250:LEU:HD21 | 2.00 | 0.43 |
| 41:KB:284:LEU:HD11 | 41:KB:362:LYS:HB3 | 1.99 | 0.43 |
| 40:KD:323:VAL:HG22 | 40:KD:372:ARG:HG2 | 2.00 | 0.43 |
| 40:KF:229:ARG:HD2 | 40:KF:363:VAL:HG11 | 2.00 | 0.43 |
| 40:KH:137:ILE:HG13 | 40:KH:154:MET:HE1 | 2.00 | 0.43 |
| 41:KL:16:ILE:HG13 | 41:KL:229:VAL:HG13 | 1.99 | 0.43 |
| 41:KL:156:ARG:HA | 41:KL:156:ARG:HD2 | 1.44 | 0.43 |
| 41:KL:350:LYS:HE2 | 41:KL:350:LYS:HB2 | 1.53 | 0.43 |
| 41:KN:226:ASN:ND2 | 43:KN:502:GDP:O6 | 2.44 | 0.43 |
| 41:KN:284:LEU:HD21 | 41:KN:363:MET:HB2 | 2.00 | 0.43 |
| 40:LA:164:LYS:HA | 40:LA:164:LYS:HD3 | 1.82 | 0.43 |
| 41:LB:240:LEU:H | 41:LB:240:LEU:HD23 | 1.82 | 0.43 |
| 40:LD:168:GLU:HB2 | 40:LD:201:ALA:HA | 1.99 | 0.43 |
| 40:LG:35:GLN:H | 40:LG:35:GLN:HG2 | 1.48 | 0.43 |
| 40:LH:185:TYR:HE1 | 40:LH:397:MET:HB3 | 1.82 | 0.43 |
| 40:LH:328:VAL:HG21 | 40:LH:355:ILE:HD11 | 2.00 | 0.43 |
| 40:MA:397:MET:C | 40:MA:399:ALA:H | 2.20 | 0.43 |
| 40:MF:102:ASN:O | 40:MF:103:TYR:C | 2.56 | 0.43 |
| 40:MH:258:ASN:HD22 | 41:MP:179:VAL:HG22 | 1.82 | 0.43 |
| 41:ML:7:LEU:O | 41:ML:135:LEU:HA | 2.18 | 0.43 |
| 41:MM:101:TRP:HZ2 | 41:MM:191:GLN:HG3 | 1.82 | 0.43 |
| 41:MN:262:ARG:NH2 | 41:MN:414:ASN:OD1 | 2.51 | 0.43 |
| 40:NA:318:LEU:O | 40:NA:374:VAL:HA | 2.18 | 0.43 |
| 40:NA:400:LYS:HE3 | 41:NN:425:ARG:HH21 | 1.83 | 0.43 |
| 41:NL:289:LEU:HD23 | 41:NL:289:LEU:HA | 1.91 | 0.43 |
| 40:OA:217:LEU:HB3 | 40:OA:219:ILE:HG12 | 2.00 | 0.43 |
| 41:OB:120:VAL:HG11 | 41:OB:155:ILE:HD11 | 1.99 | 0.43 |
| 41:OB:358:PRO:HG2 | 41:OB:361:LEU:HG | 1.99 | 0.43 |
| 40:OD:53:PHE:HB3 | 40:OD:61:HIS:HB3 | 2.00 | 0.43 |
| 40:OD:88:HIS:HB3 | 40:OD:91:GLN:HG3 | 2.00 | 0.43 |
| 40:OF:269:LEU:O | 40:OF:377:LEU:HA | 2.17 | 0.43 |
| 40:OG:142:GLY:HA2 | 40:OG:183:GLU:OE2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OM:28:HIS:CE1 | 41:OM:241:ARG:HD2 | 2.53 | 0.43 |
| 41:OO:289:LEU:HD11 | 41:OO:363:MET:HG2 | 2.00 | 0.43 |
| 41:OO:319:GLY:HA2 | 41:OO:357:PRO:HD3 | 2.00 | 0.43 |
| 40:PA:274:PRO:HD3 | 40:PA:291:ILE:HD11 | 2.00 | 0.43 |
| 40:PF:208:ALA:HB2 | 40:PF:304:LYS:HG2 | 2.00 | 0.43 |
| 40:PH:213:CYS:SG | 40:PH:217:LEU:HD23 | 2.58 | 0.43 |
| 41:PP:104:GLY:HA2 | 41:PP:109:GLY:HA3 | 2.00 | 0.43 |
| 41:QB:48:ASN:O | 41:QB:49:VAL:C | 2.56 | 0.43 |
| 40:QE:5:ILE:O | 40:QE:135:PHE:HA | 2.17 | 0.43 |
| 40:QG:228:ASN:O | 40:QG:232:SER:HB3 | 2.18 | 0.43 |
| 40:QH:271:THR:HG22 | 40:QH:376:MET:HB3 | 1.99 | 0.43 |
| 41:QN:303:CYS:SG | 41:QN:377:LEU:HB2 | 2.58 | 0.43 |
| 41:QP:296:ALA:HA | 41:QP:299:MET:HG2 | 2.00 | 0.43 |
| 41:QP:350:LYS:HA | 41:QP:350:LYS:HD3 | 1.43 | 0.43 |
| 40:RE:234:ILE:O | 40:RE:238:ILE:HG12 | 2.18 | 0.43 |
| 40:RG:189:LEU:HD11 | 40:RG:417:PHE:HE1 | 1.83 | 0.43 |
| 41:RN:49:VAL:HB | 41:RN:241:ARG:NH1 | 2.32 | 0.43 |
| 41:RP:53:GLU:HG2 | 41:RP:59:TYR:HE1 | 1.83 | 0.43 |
| 41:RP:309:ARG:N | 41:RP:372:THR:HG1 | 2.16 | 0.43 |
| 41:SB:386:THR:C | 41:SB:388:MET:H | 2.22 | 0.43 |
| 40:SE:311:LYS:NZ | 40:SE:435:GLY:O | 2.38 | 0.43 |
| 40:SF:127:ASP:OD1 | 40:SF:128:GLN:N | 2.51 | 0.43 |
| 40:SG:238:ILE:HA | 40:SG:318:LEU:HD22 | 1.98 | 0.43 |
| 40:SH:88:HIS:HB3 | 40:SH:91:GLN:HG2 | 2.00 | 0.43 |
| 41:SM:156:ARG:NH1 | 41:SM:164:MET:HE1 | 2.33 | 0.43 |
| 41:SM:293:MET:SD | 41:SM:367:PHE:HB2 | 2.58 | 0.43 |
| 41:SN:240:LEU:H | 41:SN:240:LEU:HD23 | 1.83 | 0.43 |
| 41:SO:263:LEU:HB3 | 41:SO:370:ASN:HD21 | 1.82 | 0.43 |
| 41:TB:41:ASP:N | 41:TB:41:ASP:OD1 | 2.48 | 0.43 |
| 40:TH:285:GLN:HB3 | 40:TH:287:SER:HB3 | 2.01 | 0.43 |
| 40:TI:247:ALA:HB3 | 40:TI:355:ILE:HB | 1.99 | 0.43 |
| 41:TL:32:PRO:HG3 | 41:TL:81:PHE:CE2 | 2.52 | 0.43 |
| 41:TO:107:THR:O | 41:TO:110:ALA:N | 2.51 | 0.43 |
| 40:UE:16:ILE:HD13 | 40:UE:171:ILE:HD11 | 2.00 | 0.43 |
| 40:UF:332:ILE:HG23 | 40:UF:351:PHE:CD2 | 2.50 | 0.43 |
| 40:UG:212:ILE:HD11 | 40:UG:300:ASN:HA | 1.99 | 0.43 |
| 40:UI:211:ASP:HA | 40:UI:214:ARG:CD | 2.43 | 0.43 |
| 41:UO:87:PRO:HA | 41:UO:90:PHE:HD2 | 1.83 | 0.43 |
| 41:UP:194:GLU:H | 41:UP:194:GLU:HG2 | 1.73 | 0.43 |
| 41:VB:117:LEU:HA | 41:VB:120:VAL:HG12 | 2.00 | 0.43 |
| 40:VJ:142:GLY:HA2 | 40:VJ:183:GLU:HG2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VJ:190:THR:O | 40:VJ:194:THR:CB | 2.66 | 0.43 |
| 40:WA:50:ASN:O | 40:WA:51:THR:OG1 | 2.35 | 0.43 |
| 40:WI:253:THR:HG22 | 41:WQ:98:GLY:HA2 | 2.00 | 0.43 |
| 41:WM:19:LYS:HE2 | 41:WM:19:LYS:HB2 | 1.40 | 0.43 |
| 41:WM:28:HIS:O | 41:WM:43:GLN:HB3 | 2.18 | 0.43 |
| 41:WM:202:ILE:HD13 | 41:WM:229:VAL:HG11 | 1.99 | 0.43 |
| 41:WN:12:CYS:O | 41:WN:13:GLY:C | 2.55 | 0.43 |
| 41:WP:210:ILE:O | 41:WP:214:THR:OG1 | 2.35 | 0.43 |
| 7:1T:115:GLU:CD | 7:1T:131:GLY:HA2 | 2.39 | 0.43 |
| 7:1T:256:ILE:HD11 | 7:1T:264:LEU:HG | 1.99 | 0.43 |
| 7:1T:260:LYS:HE3 | 7:1T:260:LYS:HB3 | 1.31 | 0.43 |
| 8:1X:148:LYS:HD3 | 8:1X:149:GLN:HE21 | 1.82 | 0.43 |
| 8:1X:189:LEU:HD21 | 8:1Z:515:ILE:HG23 | 2.00 | 0.43 |
| 10:2E:69:LYS:HA | 10:2E:69:LYS:HD2 | 1.83 | 0.43 |
| 13:2V:90:GLU:HB2 | 13:2V:104:ARG:HD3 | 2.00 | 0.43 |
| 13:2W:89:PHE:CE2 | 13:2W:105:ALA:HB3 | 2.53 | 0.43 |
| 13:2W:133:GLN:HE21 | 13:2W:133:GLN:HB2 | 1.60 | 0.43 |
| 16:3J:140:GLU:HA | 16:3J:257:GLN:HG2 | 2.00 | 0.43 |
| 16:3L:319:GLU:HG2 | 16:3M:202:LYS:HD2 | 1.99 | 0.43 |
| 17:3R:330:VAL:O | 17:3R:331:VAL:C | 2.56 | 0.43 |
| 22:4H:253:TYR:HE2 | 22:4H:255:LEU:HG | 1.82 | 0.43 |
| 22:4J:457:PHE:O | 22:4J:461:ASP:HA | 2.18 | 0.43 |
| 23:4N:50:GLY:O | 23:4N:51:LEU:C | 2.57 | 0.43 |
| 23:4P:170:SER:CB | 23:4P:192:PRO:HD2 | 2.48 | 0.43 |
| 23:4P:195:ARG:HD3 | 40:DA:221:ARG:HH12 | 1.83 | 0.43 |
| 23:4P:260:THR:CB | 40:EA:219:ILE:CD1 | 2.97 | 0.43 |
| 23:4Q:254:LYS:HB3 | 23:4Q:254:LYS:HE2 | 1.38 | 0.43 |
| 23:4R:18:TYR:CD1 | 23:4R:60:LEU:HD21 | 2.53 | 0.43 |
| 23:4R:99:PRO:O | 23:4R:100:GLN:HB2 | 2.19 | 0.43 |
| 23:4R:186:GLY:O | 40:CI:79:ARG:NH1 | 2.51 | 0.43 |
| 26:4W:109:ILE:HA | 26:4W:112:ILE:HG22 | 1.99 | 0.43 |
| 27:4Y:77:HIS:HB2 | 27:4Y:85:PHE:HZ | 1.82 | 0.43 |
| 27:4Z:214:ASN:ND2 | 27:4Z:267:VAL:HA | 2.33 | 0.43 |
| 29:5D:29:ARG:HH11 | 34:5R:330:GLN:HE21 | 1.66 | 0.43 |
| 34:5Q:104:LEU:O | 34:5Q:107:SER:OG | 2.32 | 0.43 |
| 36:5Y:218:ARG:NE | 41:KP:157:GLU:OE2 | 2.37 | 0.43 |
| 39:6I:61:ASN:HA | 41:ON:56:GLY:HA2 | 1.99 | 0.43 |
| 39:6I:131:GLU:O | 39:6I:136:TYR:N | 2.51 | 0.43 |
| 40:AA:79:ARG:HH22 | 40:AA:94:THR:HG21 | 1.83 | 0.43 |
| 40:AG:255:PHE:CZ | 40:AG:318:LEU:HD21 | 2.53 | 0.43 |
| 41:AL:128:ASP:OD1 | 41:AL:129:CYS:N | 2.50 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AO:112:LEU:O | 41:AO:116:VAL:HG23 | 2.18 | 0.43 |
| 40:BE:3:GLU:HA | 40:BE:51:THR:HA | 2.00 | 0.43 |
| 40:BE:189:LEU:HD11 | 40:BE:417:PHE:HE1 | 1.83 | 0.43 |
| 40:BE:191:THR:O | 40:BE:195:LEU:HB3 | 2.18 | 0.43 |
| 40:BE:340:SER:O | 40:BE:342:GLN:N | 2.50 | 0.43 |
| 41:BM:2:ARG:HB3 | 41:BM:131:GLN:NE2 | 2.33 | 0.43 |
| 41:BM:65:LEU:HB3 | 41:BM:73:MET:SD | 2.58 | 0.43 |
| 40:CF:121:ARG:HA | 40:CF:121:ARG:HD2 | 1.73 | 0.43 |
| 40:CF:234:ILE:HD11 | 40:CF:272:TYR:HB2 | 2.00 | 0.43 |
| 40:CG:260:VAL:HG13 | 41:CO:397:TRP:HH2 | 1.82 | 0.43 |
| 40:CI:8:HIS:HE1 | 40:CI:21:TRP:HE1 | 1.66 | 0.43 |
| 41:CL:260:PHE:HD2 | 41:CL:263:LEU:HD12 | 1.83 | 0.43 |
| 41:CM:46:ARG:HD3 | 41:CM:46:ARG:HA | 1.84 | 0.43 |
| 41:CM:355:ASP:O | 41:CM:356:ILE:C | 2.55 | 0.43 |
| 41:CO:181:GLU:O | 41:CO:182:PRO:C | 2.56 | 0.43 |
| 41:CP:181:GLU:O | 41:CP:182:PRO:C | 2.55 | 0.43 |
| 40:DA:3:GLU:HG2 | 40:DA:132:LEU:HA | 2.01 | 0.43 |
| 40:DA:9:VAL:O | 40:DA:13:GLY:HA3 | 2.18 | 0.43 |
| 40:DA:104:ALA:O | 40:DA:105:ARG:C | 2.57 | 0.43 |
| 41:DB:67:ASP:HB3 | 41:DB:73:MET:SD | 2.58 | 0.43 |
| 41:DB:142:GLY:O | 41:DB:143:THR:C | 2.57 | 0.43 |
| 40:DE:190:THR:O | 40:DE:191:THR:C | 2.56 | 0.43 |
| 40:DE:191:THR:HA | 40:DE:194:THR:OG1 | 2.18 | 0.43 |
| 40:DE:326:LYS:HB2 | 40:DE:326:LYS:HE3 | 1.61 | 0.43 |
| 40:DF:104:ALA:O | 40:DF:105:ARG:C | 2.56 | 0.43 |
| 40:DG:284:GLU:N | 40:DG:284:GLU:OE2 | 2.51 | 0.43 |
| 40:DH:5:ILE:HG13 | 40:DH:132:LEU:HD23 | 2.00 | 0.43 |
| 40:DH:96:LYS:NZ | 41:DO:1:MET:O | 2.51 | 0.43 |
| 40:DH:174:ALA:HB3 | 40:DH:177:VAL:HG13 | 2.01 | 0.43 |
| 40:DH:182:VAL:O | 40:DH:183:GLU:C | 2.56 | 0.43 |
| 40:DH:267:PHE:CE2 | 40:DH:427:LEU:HD11 | 2.53 | 0.43 |
| 41:DL:191:GLN:O | 41:DL:192:LEU:C | 2.56 | 0.43 |
| 41:DM:73:MET:N | 41:DM:73:MET:SD | 2.91 | 0.43 |
| 41:DM:308:GLY:HA3 | 41:DM:373:ALA:HB2 | 2.00 | 0.43 |
| 41:DN:211:CYS:O | 41:DN:212:PHE:C | 2.55 | 0.43 |
| 41:DP:218:THR:C | 41:DP:220:PRO:HD3 | 2.38 | 0.43 |
| 40:EG:103:TYR:HD2 | 40:EG:189:LEU:HD13 | 1.83 | 0.43 |
| 40:EG:118:VAL:HG12 | 40:EG:119:LEU:HD23 | 2.00 | 0.43 |
| 40:EG:288:VAL:HA | 40:EG:291:ILE:HG12 | 2.00 | 0.43 |
| 40:EH:69:ASP:N | 40:EH:75:ILE:HD11 | 2.33 | 0.43 |
| 40:EI:100:ALA:O | 40:EI:102:ASN:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EI:164:LYS:O | 40:EI:165:SER:C | 2.55 | 0.43 |
| 40:EI:172:TYR:HE1 | 40:EI:191:THR:HG21 | 1.82 | 0.43 |
| 41:EM:143:THR:O | 41:EM:147:MET:N | 2.50 | 0.43 |
| 41:EO:334:GLN:HE22 | 41:EO:349:VAL:HG23 | 1.83 | 0.43 |
| 40:FA:104:ALA:O | 40:FA:108:TYR:HB2 | 2.18 | 0.43 |
| 40:FE:167:LEU:HA | 40:FE:200:CYS:O | 2.17 | 0.43 |
| 40:FF:405:HIS:HA | 40:FF:408:VAL:HG22 | 1.99 | 0.43 |
| 41:FP:22:GLU:HA | 41:FP:81:PHE:HD2 | 1.83 | 0.43 |
| 40:GE:400:LYS:HA | 40:GE:400:LYS:HD3 | 1.64 | 0.43 |
| 40:GG:102:ASN:HB2 | 40:GG:105:ARG:HB2 | 2.00 | 0.43 |
| 40:GG:269:LEU:HD21 | 40:GG:383:ILE:HD13 | 2.00 | 0.43 |
| 40:GH:183:GLU:N | 40:GH:184:PRO:HD2 | 2.32 | 0.43 |
| 41:HB:273:LEU:O | 41:HB:292:GLN:NE2 | 2.38 | 0.43 |
| 41:HB:341:PHE:HB3 | 41:HB:348:ASN:HD21 | 1.82 | 0.43 |
| 40:HE:53:PHE:HE2 | 40:HE:86:LEU:HD21 | 1.82 | 0.43 |
| 40:HE:329:ASN:HB2 | 41:HM:175:VAL:HG21 | 2.00 | 0.43 |
| 40:HF:79:ARG:HH21 | 40:HF:92:LEU:HB2 | 1.83 | 0.43 |
| 40:HI:332:ILE:HD12 | 40:HI:351:PHE:CD2 | 2.53 | 0.43 |
| 41:HM:18:ALA:O | 41:HM:22:GLU:HG3 | 2.18 | 0.43 |
| 41:HM:117:LEU:HA | 41:HM:120:VAL:HG12 | 2.00 | 0.43 |
| 41:HN:130:LEU:HD23 | 41:HN:162:ARG:HG3 | 2.00 | 0.43 |
| 41:HN:305:PRO:O | 41:HN:306:ARG:C | 2.56 | 0.43 |
| 40:IA:121:ARG:NH1 | 40:IA:124:LYS:HE3 | 2.31 | 0.43 |
| 41:IB:267:MET:HE1 | 41:IB:373:ALA:HB3 | 2.00 | 0.43 |
| 40:II:115:ILE:HA | 40:II:118:VAL:HG12 | 2.00 | 0.43 |
| 41:IO:240:LEU:HD12 | 41:IO:249:ASP:HB2 | 2.00 | 0.43 |
| 41:IQ:184:ASN:OD1 | 41:IQ:398:TYR:OH | 2.36 | 0.43 |
| 41:JB:132:GLY:HA2 | 41:JB:162:ARG:HB3 | 2.00 | 0.43 |
| 40:JD:190:THR:HA | 40:JD:193:THR:HG22 | 1.98 | 0.43 |
| 40:JE:98:ASP:O | 40:JE:105:ARG:NH2 | 2.37 | 0.43 |
| 41:JL:358:PRO:HG2 | 41:JL:361:LEU:HD12 | 1.99 | 0.43 |
| 41:JM:140:GLY:HA2 | 41:JM:181:GLU:HG2 | 2.00 | 0.43 |
| 41:JN:130:LEU:O | 41:JN:162:ARG:NE | 2.50 | 0.43 |
| 41:JO:345:ILE:HG22 | 41:JO:348:ASN:HB3 | 2.00 | 0.43 |
| 40:KD:3:GLU:HG3 | 40:KD:129:CYS:SG | 2.58 | 0.43 |
| 40:KE:209:ILE:HG23 | 40:KE:230:LEU:HD23 | 2.01 | 0.43 |
| 40:KG:71:GLU:HB3 | 40:KG:98:ASP:HA | 2.00 | 0.43 |
| 41:KN:8:GLN:OE1 | 41:KN:17:GLY:HA3 | 2.19 | 0.43 |
| 41:KN:165:ASN:HD22 | 41:KN:198:GLU:HB2 | 1.82 | 0.43 |
| 41:KN:238:THR:HG21 | 41:KN:318:ARG:HD2 | 1.99 | 0.43 |
| 41:KN:240:LEU:H | 41:KN:240:LEU:HD23 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KO:203:ASP:OD2 | 41:KO:302:ALA:N | 2.48 | 0.43 |
| 41:KP:3:GLU:OE2 | 41:KP:127:CYS:HB3 | 2.17 | 0.43 |
| 40:LA:239:THR:O | 40:LA:243:ARG:NE | 2.52 | 0.43 |
| 41:LB:165:ASN:HA | 41:LB:198:GLU:O | 2.18 | 0.43 |
| 40:LD:298:PRO:HB3 | 40:LD:307:PRO:HD2 | 1.99 | 0.43 |
| 41:LL:317:PHE:HB2 | 41:LL:353:VAL:HG22 | 2.00 | 0.43 |
| 40:MA:178:SER:CB | 41:MN:347:ASN:HD22 | 2.31 | 0.43 |
| 40:MA:273:ALA:HB2 | 40:MA:295:CYS:SG | 2.58 | 0.43 |
| 41:MB:65:LEU:HD22 | 41:MB:90:PHE:CE1 | 2.53 | 0.43 |
| 41:MB:256:ASN:HD21 | 40:MG:182:VAL:HG22 | 1.84 | 0.43 |
| 40:MD:71:GLU:HB3 | 40:MD:98:ASP:HA | 1.99 | 0.43 |
| 40:ME:320:ARG:HG2 | 40:ME:356:ASN:HB2 | 2.00 | 0.43 |
| 40:MF:69:ASP:OD2 | 40:MF:74:VAL:HG11 | 2.18 | 0.43 |
| 40:MF:182:VAL:HG22 | 41:MM:256:ASN:ND2 | 2.33 | 0.43 |
| 40:MG:252:LEU:HA | 40:MG:255:PHE:HD1 | 1.83 | 0.43 |
| 41:ML:226:ASN:ND2 | 43:ML:502:GDP:O6 | 2.50 | 0.43 |
| 40:NA:376:MET:SD | 40:NA:378:SER:HB3 | 2.58 | 0.43 |
| 40:NE:167:LEU:HA | 40:NE:200:CYS:O | 2.17 | 0.43 |
| 40:NH:139:HIS:CD2 | 40:NH:150:THR:HG21 | 2.53 | 0.43 |
| 41:NM:19:LYS:HA | 41:NM:19:LYS:HD3 | 1.80 | 0.43 |
| 41:NM:163:ILE:HG23 | 41:NM:197:ASP:HB2 | 2.00 | 0.43 |
| 41:NM:189:VAL:O | 41:NM:193:VAL:HG23 | 2.18 | 0.43 |
| 41:NM:381:ILE:HD13 | 41:NM:381:ILE:HA | 1.81 | 0.43 |
| 41:NN:189:VAL:O | 41:NN:193:VAL:HG23 | 2.18 | 0.43 |
| 40:OA:21:TRP:CZ2 | 40:OA:65:ALA:HB2 | 2.53 | 0.43 |
| 40:OD:238:ILE:HG12 | 40:OD:377:LEU:HD11 | 1.99 | 0.43 |
| 40:OD:260:VAL:HG23 | 41:OL:397:TRP:HZ2 | 1.83 | 0.43 |
| 40:OE:331:ALA:O | 40:OE:335:ILE:HG12 | 2.19 | 0.43 |
| 40:OF:62:VAL:HG21 | 40:OF:88:HIS:HB2 | 1.99 | 0.43 |
| 40:OH:205:ASP:HB3 | 40:OH:303:VAL:HA | 1.99 | 0.43 |
| 41:OL:63:ALA:O | 41:OL:89:ASN:ND2 | 2.50 | 0.43 |
| 41:OL:285:THR:HB | 41:OL:287:PRO:HD2 | 2.00 | 0.43 |
| 41:ON:285:THR:HB | 41:ON:287:PRO:HD2 | 2.00 | 0.43 |
| 41:OO:290:THR:HG21 | 41:OO:329:GLN:HB3 | 2.00 | 0.43 |
| 40:PA:273:ALA:HB3 | 40:PA:374:VAL:H | 1.83 | 0.43 |
| 40:PD:255:PHE:CZ | 40:PD:318:LEU:HD21 | 2.53 | 0.43 |
| 40:PH:224:TYR:O | 40:PH:228:ASN:ND2 | 2.51 | 0.43 |
| 41:PL:226:ASN:ND2 | 43:PL:501:GDP:O6 | 2.48 | 0.43 |
| 41:PM:68:LEU:HB2 | 41:PM:97:ALA:HB2 | 1.99 | 0.43 |
| 41:PM:152:ILE:O | 41:PM:156:ARG:HB2 | 2.18 | 0.43 |
| 41:PO:236:VAL:HG12 | 41:PO:368:ILE:HD11 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PP:70:PRO:HB3 | 41:PP:92:PHE:HB2 | 2.01 | 0.43 |
| 41:QB:101:TRP:CZ2 | 41:QB:187:LEU:HB3 | 2.53 | 0.43 |
| 41:QB:199:THR:HB | 41:QB:264:HIS:O | 2.18 | 0.43 |
| 41:QB:217:LEU:O | 41:QB:218:THR:C | 2.55 | 0.43 |
| 41:QB:225:LEU:O | 41:QB:226:ASN:C | 2.56 | 0.43 |
| 40:QE:68:VAL:HG12 | 40:QE:93:ILE:HB | 1.99 | 0.43 |
| 40:QE:188:ILE:HG23 | 40:QE:424:MET:HG3 | 2.00 | 0.43 |
| 41:QM:108:GLU:N | 41:QM:108:GLU:OE2 | 2.51 | 0.43 |
| 41:QN:140:GLY:HA3 | 41:QN:181:GLU:HG2 | 2.00 | 0.43 |
| 41:QO:226:ASN:ND2 | 43:QO:502:GDP:O6 | 2.47 | 0.43 |
| 41:QP:183:TYR:N | 41:QP:183:TYR:CD2 | 2.85 | 0.43 |
| 40:RA:247:ALA:HB3 | 40:RA:355:ILE:HB | 2.00 | 0.43 |
| 41:RB:252:LYS:HE3 | 41:RB:350:LYS:HE3 | 1.98 | 0.43 |
| 40:RE:250:VAL:HG23 | 40:RE:352:LYS:HZ3 | 1.83 | 0.43 |
| 40:RH:298:PRO:HB3 | 40:RH:307:PRO:HD2 | 2.00 | 0.43 |
| 41:RM:221:THR:HG23 | 41:RM:223:GLY:H | 1.82 | 0.43 |
| 41:RN:113:VAL:HA | 41:RN:116:VAL:HG12 | 2.00 | 0.43 |
| 41:RN:297:LYS:HA | 41:RN:297:LYS:HD3 | 1.79 | 0.43 |
| 40:SA:219:ILE:HG13 | 40:SA:222:PRO:HD3 | 2.00 | 0.43 |
| 40:SA:224:TYR:HA | 40:SA:227:LEU:HB2 | 2.00 | 0.43 |
| 41:SB:31:ASP:OD1 | 41:SB:34:GLY:N | 2.51 | 0.43 |
| 40:SG:115:ILE:HG13 | 40:SG:119:LEU:HD23 | 2.00 | 0.43 |
| 40:SH:306:ASP:OD2 | 40:SH:308:ARG:NH2 | 2.52 | 0.43 |
| 40:SH:387:TRP:HZ3 | 40:SH:431:TYR:HE2 | 1.66 | 0.43 |
| 40:SI:190:THR:O | 40:SI:194:THR:OG1 | 2.22 | 0.43 |
| 41:SN:24:ILE:HA | 41:SN:27:GLU:HB2 | 1.99 | 0.43 |
| 41:SP:321:MET:HB3 | 41:SP:321:MET:HE2 | 1.83 | 0.43 |
| 41:TM:137:HIS:O | 41:TM:168:SER:HA | 2.19 | 0.43 |
| 41:TN:39:ASP:N | 41:TN:39:ASP:OD1 | 2.50 | 0.43 |
| 41:TP:142:GLY:O | 41:TP:144:GLY:N | 2.51 | 0.43 |
| 41:TP:230:SER:HA | 41:TP:233:MET:HG2 | 1.99 | 0.43 |
| 40:UF:50:ASN:C | 40:UF:52:PHE:H | 2.22 | 0.43 |
| 40:UF:68:VAL:HG21 | 40:UF:118:VAL:HG22 | 2.00 | 0.43 |
| 40:UH:191:THR:HG21 | 40:UH:387:TRP:HH2 | 1.82 | 0.43 |
| 40:UH:238:ILE:HG23 | 40:UH:239:THR:HG23 | 1.99 | 0.43 |
| 40:UI:49:PHE:CG | 40:UI:50:ASN:N | 2.84 | 0.43 |
| 40:UI:344:VAL:CG2 | 40:UI:347:CYS:HB2 | 2.48 | 0.43 |
| 41:UO:165:ASN:HD22 | 41:UO:198:GLU:HB2 | 1.82 | 0.43 |
| 41:UP:47:ILE:H | 41:UP:47:ILE:HG13 | 1.67 | 0.43 |
| 41:VB:170:VAL:HG21 | 41:VB:377:LEU:HD13 | 1.99 | 0.43 |
| 41:VB:285:THR:H | 41:VB:288:GLU:HG3 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VI:115:ILE:HA | 40:VI:118:VAL:HG12 | 1.99 | 0.43 |
| 41:VN:171:PRO:HG3 | 41:VN:181:GLU:HB3 | 2.00 | 0.43 |
| 41:VO:107:THR:O | 41:VO:110:ALA:N | 2.35 | 0.43 |
| 41:VO:151:LEU:O | 41:VO:155:ILE:HG12 | 2.18 | 0.43 |
| 40:WA:326:LYS:HD2 | 41:WB:208:TYR:CD1 | 2.53 | 0.43 |
| 40:WH:66:VAL:HG12 | 40:WH:68:VAL:HG23 | 1.98 | 0.43 |
| 40:WH:395:ASP:OD2 | 40:WH:421:ARG:NH2 | 2.45 | 0.43 |
| 40:WI:155:GLU:O | 40:WI:159:VAL:HG23 | 2.17 | 0.43 |
| 41:WM:286:VAL:HB | 41:WM:287:PRO:HD3 | 2.00 | 0.43 |
| 41:WM:389:PHE:CE1 | 41:WM:395:LEU:HD21 | 2.53 | 0.43 |
| 41:WN:98:GLY:O | 41:WN:99:ASN:C | 2.56 | 0.43 |
| 41:WN:336:LYS:HB3 | 41:WN:336:LYS:HE3 | 1.58 | 0.43 |
| 41:WO:259:PRO:HG2 | 41:WO:311:LEU:HD23 | 1.99 | 0.43 |
| 5:1M:182:LEU:HD11 | 40:HG:308:ARG:HB3 | 2.00 | 0.43 |
| 6:1Q:236:VAL:HG11 | 7:1U:320:THR:HG21 | 2.00 | 0.43 |
| 7:1T:368:LEU:HD12 | 7:1T:368:LEU:HA | 1.72 | 0.43 |
| 7:1T:461:LYS:H | 7:1T:461:LYS:HG2 | 1.65 | 0.43 |
| 7:1U:103:LEU:HD11 | 7:1U:106:ARG:HH21 | 1.83 | 0.43 |
| 11:2K:211:PHE:C | 11:2K:213:SER:H | 2.22 | 0.43 |
| 12:2N:161:ASN:HB3 | 12:2N:164:VAL:HB | 1.99 | 0.43 |
| 12:2Q:245:LYS:HE3 | 12:2Q:245:LYS:HB3 | 1.88 | 0.43 |
| 13:2W:85:LYS:HB3 | 13:2W:159:ASN:ND2 | 2.33 | 0.43 |
| 17:3R:196:ARG:HE | 17:3R:223:VAL:HB | 1.82 | 0.43 |
| 17:3R:295:SER:OG | 17:3R:296:VAL:N | 2.51 | 0.43 |
| 18:3T:376:ARG:HA | 18:3T:376:ARG:HD2 | 1.76 | 0.43 |
| 20:4B:353:GLN:H | 20:4B:353:GLN:HG3 | 1.51 | 0.43 |
| 21:4D:34:ARG:NH2 | 21:4D:37:TYR:HB2 | 2.33 | 0.43 |
| 22:4I:228:LYS:HE3 | 22:4I:359:PHE:HZ | 1.83 | 0.43 |
| 22:4I:649:LYS:HA | 22:4I:649:LYS:HD3 | 1.45 | 0.43 |
| 22:4I:700:ARG:HA | 22:4I:700:ARG:HD2 | 1.53 | 0.43 |
| 22:4K:509:VAL:HG12 | 22:4K:596:ASP:HB3 | 2.01 | 0.43 |
| 24:4O:245:LYS:HB3 | 24:4O:245:LYS:HE3 | 1.49 | 0.43 |
| 23:4P:210:LEU:HD13 | 23:4P:210:LEU:HA | 1.74 | 0.43 |
| 26:4V:91:LYS:HB3 | 26:4V:164:LEU:HD12 | 1.99 | 0.43 |
| 26:4V:130:ARG:HA | 26:4V:130:ARG:NH1 | 2.32 | 0.43 |
| 26:4V:173:LYS:HA | 26:4V:173:LYS:HD3 | 1.81 | 0.43 |
| 28:5B:68:GLU:O | 28:5B:71:LYS:NZ | 2.50 | 0.43 |
| 31:5I:514:LEU:HD22 | 41:IP:280:GLN:HB3 | 2.01 | 0.43 |
| 34:5R:368:LYS:HA | 34:5R:371:LYS:HE2 | 1.99 | 0.43 |
| 34:5R:458:ARG:HB3 | 34:5R:462:ARG:HH12 | 1.84 | 0.43 |
| 39:6H:61:ASN:O | 39:6H:63:THR:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AB:232:THR:HG21 | 41:AB:268:PRO:HB2 | 1.99 | 0.43 |
| 41:AB:281:TYR:O | 41:MB:86:ARG:NH1 | 2.50 | 0.43 |
| 41:AM:100:ASN:HB3 | 41:AM:103:LYS:HB2 | 1.99 | 0.43 |
| 41:AO:241:ARG:HE | 41:AO:241:ARG:HB3 | 1.47 | 0.43 |
| 41:AO:260:PHE:HE2 | 41:AO:344:TRP:CH2 | 2.36 | 0.43 |
| 40:BE:121:ARG:HH12 | 40:BE:125:LEU:HG | 1.83 | 0.43 |
| 40:BE:311:LYS:H | 40:BE:311:LYS:HG2 | 1.50 | 0.43 |
| 40:BH:222:PRO:HD2 | 41:BO:324:LYS:HD2 | 2.00 | 0.43 |
| 40:BI:112:LYS:HA | 40:BI:112:LYS:HD2 | 1.87 | 0.43 |
| 40:BI:311:LYS:HE2 | 40:BI:311:LYS:HB2 | 1.60 | 0.43 |
| 41:BM:185:ALA:O | 41:BM:186:THR:C | 2.56 | 0.43 |
| 41:BN:95:SER:OG | 41:BN:96:GLY:N | 2.50 | 0.43 |
| 41:BN:313:VAL:HB | 41:BN:349:VAL:HG22 | 2.00 | 0.43 |
| 41:BP:51:TYR:CD1 | 41:BP:61:PRO:HA | 2.54 | 0.43 |
| 41:BP:207:LEU:HB3 | 41:BP:225:LEU:HD12 | 2.00 | 0.43 |
| 40:CA:40:LYS:HB3 | 40:CA:40:LYS:HE2 | 1.35 | 0.43 |
| 40:CA:191:THR:HB | 40:CA:424:MET:CE | 2.48 | 0.43 |
| 41:CB:172:SER:OG | 41:CB:175:VAL:O | 2.36 | 0.43 |
| 41:CL:251:ARG:O | 41:CL:252:LYS:C | 2.56 | 0.43 |
| 41:CN:21:TRP:CE3 | 41:CN:24:ILE:HD11 | 2.53 | 0.43 |
| 41:CN:245:GLN:O | 41:CN:246:LEU:C | 2.56 | 0.43 |
| 41:CN:272:PRO:HG2 | 41:CN:361:LEU:HD13 | 1.99 | 0.43 |
| 40:DA:59:GLY:O | 40:DA:61:HIS:N | 2.51 | 0.43 |
| 40:DA:86:LEU:O | 40:DA:87:PHE:C | 2.56 | 0.43 |
| 40:DA:126:ALA:O | 40:DA:129:CYS:HB2 | 2.18 | 0.43 |
| 40:DA:437:ASP:O | 40:DA:439:VAL:N | 2.49 | 0.43 |
| 41:DB:150:LEU:HD23 | 41:DB:150:LEU:HA | 1.76 | 0.43 |
| 40:DF:114:LEU:HB3 | 40:DF:149:PHE:CZ | 2.53 | 0.43 |
| 40:DH:54:SER:HB3 | 40:DH:64:ARG:HG3 | 2.01 | 0.43 |
| 40:DH:79:ARG:HE | 40:DH:79:ARG:HB3 | 1.67 | 0.43 |
| 40:DH:92:LEU:H | 40:DH:92:LEU:HG | 1.35 | 0.43 |
| 40:DH:99:ALA:O | 40:DH:100:ALA:HB3 | 2.18 | 0.43 |
| 40:DH:258:ASN:HD21 | 41:DP:99:ASN:HD21 | 1.66 | 0.43 |
| 40:DI:11:GLN:HB3 | 42:DI:501:GTP:O1B | 2.19 | 0.43 |
| 40:DI:195:LEU:HD13 | 40:DI:195:LEU:HA | 1.85 | 0.43 |
| 40:DI:387:TRP:CE3 | 40:DI:424:MET:HE1 | 2.53 | 0.43 |
| 41:DM:41:ASP:CG | 41:DM:44:LEU:HD21 | 2.39 | 0.43 |
| 41:DM:123:GLU:O | 41:DM:124:ALA:C | 2.56 | 0.43 |
| 41:DM:257:MET:SD | 41:DM:314:ALA:N | 2.91 | 0.43 |
| 41:DM:319:GLY:O | 41:DM:320:ARG:C | 2.57 | 0.43 |
| 41:DN:290:THR:O | 41:DN:291:GLN:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DP:108:GLU:O | 41:DP:109:GLY:C | 2.56 | 0.43 |
| 40:EA:27:GLU:OE2 | 40:EA:243:ARG:NH2 | 2.44 | 0.43 |
| 40:EH:332:ILE:HG23 | 40:EH:351:PHE:CD1 | 2.54 | 0.43 |
| 40:EH:338:LYS:HE2 | 40:EH:338:LYS:HB3 | 1.52 | 0.43 |
| 41:EL:74:ASP:HA | 41:EL:77:ARG:HH12 | 1.83 | 0.43 |
| 41:EL:193:VAL:HA | 41:EL:264:HIS:HE1 | 1.83 | 0.43 |
| 41:EM:193:VAL:HG11 | 41:EM:418:LEU:HD21 | 2.00 | 0.43 |
| 41:EP:25:SER:O | 41:EP:26:ASP:C | 2.56 | 0.43 |
| 41:EP:50:TYR:O | 41:EP:62:ARG:HB3 | 2.19 | 0.43 |
| 41:EP:358:PRO:O | 41:EP:359:ARG:C | 2.56 | 0.43 |
| 40:FA:222:PRO:N | 41:FN:324:LYS:NZ | 2.65 | 0.43 |
| 41:FM:25:SER:OG | 41:FM:30:ILE:O | 2.35 | 0.43 |
| 41:FM:178:THR:O | 41:FM:181:GLU:HG3 | 2.17 | 0.43 |
| 40:GA:16:ILE:CG1 | 40:GA:228:ASN:HD22 | 2.30 | 0.43 |
| 40:GE:49:PHE:CE2 | 40:GE:55:GLU:HB2 | 2.53 | 0.43 |
| 40:HE:401:ARG:HD2 | 40:HE:404:VAL:HG21 | 2.00 | 0.43 |
| 40:HG:105:ARG:HG2 | 40:HG:410:GLU:HG3 | 2.00 | 0.43 |
| 40:HI:221:ARG:HH12 | 41:HP:325:GLU:HB2 | 1.82 | 0.43 |
| 41:HM:171:PRO:HB3 | 41:HM:181:GLU:HG2 | 1.99 | 0.43 |
| 41:HM:263:LEU:HD21 | 41:HM:421:PRO:HB2 | 2.00 | 0.43 |
| 41:HN:244:GLY:HA2 | 41:HN:355:ASP:HB2 | 2.01 | 0.43 |
| 40:IG:7:VAL:HB | 40:IG:137:ILE:HG13 | 1.99 | 0.43 |
| 40:II:48:SER:O | 40:II:51:THR:HG22 | 2.18 | 0.43 |
| 41:IM:21:TRP:CZ3 | 41:IM:24:ILE:HD11 | 2.52 | 0.43 |
| 41:IN:107:THR:O | 41:IN:109:GLY:N | 2.51 | 0.43 |
| 41:JB:16:ILE:HD11 | 41:JB:229:VAL:HB | 1.99 | 0.43 |
| 40:JF:207:GLU:HA | 40:JF:210:TYR:CD1 | 2.54 | 0.43 |
| 40:JF:228:ASN:HD21 | 42:JF:501:GTP:HN1 | 1.66 | 0.43 |
| 41:JL:9:ALA:HA | 41:JL:66:VAL:O | 2.18 | 0.43 |
| 41:JL:135:LEU:O | 41:JL:166:THR:HA | 2.17 | 0.43 |
| 41:JM:1:MET:HB3 | 41:JM:3:GLU:CD | 2.39 | 0.43 |
| 41:JM:47:ILE:O | 41:JM:48:ASN:C | 2.57 | 0.43 |
| 41:JO:16:ILE:HG12 | 41:JO:226:ASN:HB3 | 2.00 | 0.43 |
| 41:JO:139:LEU:HG | 41:JO:168:SER:HB3 | 2.01 | 0.43 |
| 41:JO:241:ARG:HH21 | 41:JO:242:PHE:HE2 | 1.66 | 0.43 |
| 40:KA:298:PRO:HB3 | 40:KA:307:PRO:HD2 | 2.00 | 0.43 |
| 40:KE:100:ALA:HA | 41:KL:252:LYS:HG2 | 2.00 | 0.43 |
| 40:KF:97:GLU:OE2 | 41:KM:251:ARG:NH2 | 2.47 | 0.43 |
| 40:KH:433:GLU:O | 41:KP:391:ARG:NH2 | 2.52 | 0.43 |
| 41:KL:348:ASN:OD1 | 41:KL:348:ASN:N | 2.49 | 0.43 |
| 40:LA:71:GLU:HG3 | 40:LA:98:ASP:HB2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:LB:51:TYR:HB3 | 41:LB:59:TYR:HB3 | 1.99 | 0.43 |
| 41:LB:246:LEU:HD21 | 40:LG:179:THR:HB | 2.00 | 0.43 |
| 40:LH:177:VAL:HB | 41:LO:331:LEU:HD22 | 2.00 | 0.43 |
| 41:LN:51:TYR:HE1 | 41:LN:61:PRO:HG3 | 1.83 | 0.43 |
| 41:LO:204:ASN:OD1 | 43:LO:502:GDP:O2' | 2.35 | 0.43 |
| 41:MB:39:ASP:N | 41:MB:39:ASP:OD1 | 2.50 | 0.43 |
| 41:MB:293:MET:HE3 | 41:MB:367:PHE:HB2 | 2.00 | 0.43 |
| 40:MF:140:SER:O | 40:MF:141:PHE:C | 2.57 | 0.43 |
| 40:MG:63:PRO:HG2 | 40:MG:87:PHE:CD1 | 2.52 | 0.43 |
| 40:MG:160:ASP:HB2 | 40:MG:161:TYR:H | 1.69 | 0.43 |
| 40:MH:266:HIS:O | 40:MH:268:PRO:HD3 | 2.19 | 0.43 |
| 41:ML:189:VAL:O | 41:ML:193:VAL:HG23 | 2.19 | 0.43 |
| 41:MM:271:ALA:HB3 | 41:MM:293:MET:HG3 | 1.98 | 0.43 |
| 41:MO:296:ALA:HB1 | 41:MO:305:PRO:HD2 | 1.99 | 0.43 |
| 40:ND:129:CYS:SG | 40:ND:130:THR:N | 2.91 | 0.43 |
| 40:ND:162:GLY:C | 40:ND:164:LYS:H | 2.20 | 0.43 |
| 40:ND:383:ILE:O | 40:ND:386:ALA:N | 2.51 | 0.43 |
| 40:NE:141:PHE:HB2 | 40:NE:173:PRO:HD3 | 2.00 | 0.43 |
| 41:NL:22:GLU:HG3 | 41:NL:81:PHE:CD2 | 2.53 | 0.43 |
| 41:NL:167:PHE:CE1 | 41:NL:233:MET:HG2 | 2.54 | 0.43 |
| 41:NP:388:MET:HB2 | 41:NP:393:ALA:HB3 | 2.00 | 0.43 |
| 41:OB:267:MET:HG3 | 41:OB:374:ILE:HD11 | 2.01 | 0.43 |
| 40:OE:8:HIS:HD2 | 40:OE:138:PHE:HB2 | 1.83 | 0.43 |
| 40:OE:244:PHE:HB2 | 40:OE:356:ASN:HD21 | 1.83 | 0.43 |
| 40:OE:247:ALA:HB3 | 40:OE:355:ILE:HB | 1.99 | 0.43 |
| 40:OF:120:ASP:O | 40:OF:124:LYS:HG2 | 2.19 | 0.43 |
| 40:OF:352:LYS:HE2 | 41:ON:178:THR:HA | 2.00 | 0.43 |
| 40:OH:107:HIS:NE2 | 40:OH:152:LEU:HD13 | 2.33 | 0.43 |
| 40:OH:114:LEU:HD23 | 40:OH:114:LEU:HA | 1.80 | 0.43 |
| 41:OO:18:ALA:O | 41:OO:22:GLU:HG2 | 2.19 | 0.43 |
| 41:OO:341:PHE:HB3 | 41:OO:348:ASN:HD21 | 1.83 | 0.43 |
| 41:OP:199:THR:O | 41:OP:266:PHE:HB2 | 2.18 | 0.43 |
| 41:PB:36:TYR:OH | 41:PB:40:SER:O | 2.29 | 0.43 |
| 40:PD:175:PRO:HD2 | 40:PD:207:GLU:OE2 | 2.18 | 0.43 |
| 40:PE:346:TRP:HB3 | 41:PM:391:ARG:HH11 | 1.83 | 0.43 |
| 40:PF:1:GLN:N | 40:PF:3:GLU:OE2 | 2.35 | 0.43 |
| 41:PM:209:ASP:OD1 | 41:PM:213:ARG:NH2 | 2.51 | 0.43 |
| 41:PO:238:THR:HG21 | 41:PO:318:ARG:HD2 | 2.00 | 0.43 |
| 41:PP:286:VAL:HG11 | 41:PP:325:GLU:HG3 | 2.00 | 0.43 |
| 40:QE:405:HIS:HA | 40:QE:408:VAL:HG12 | 1.99 | 0.43 |
| 40:QH:211:ASP:HA | 40:QH:214:ARG:NH1 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QP:31:ASP:C | 41:QP:33:THR:H | 2.22 | 0.43 |
| 41:QP:143:THR:O | 41:QP:144:GLY:C | 2.56 | 0.43 |
| 41:QP:271:ALA:N | 41:QP:272:PRO:CD | 2.81 | 0.43 |
| 40:RA:322:ASP:O | 40:RA:372:ARG:NE | 2.40 | 0.43 |
| 41:RB:324:LYS:HE3 | 40:RG:222:PRO:HD2 | 2.01 | 0.43 |
| 40:RE:70:LEU:HD23 | 40:RE:114:LEU:HD12 | 2.00 | 0.43 |
| 40:RH:76:ASP:HA | 40:RH:79:ARG:HG2 | 2.00 | 0.43 |
| 40:RI:237:SER:HB3 | 40:RI:375:CYS:HB2 | 1.99 | 0.43 |
| 41:RM:142:GLY:O | 41:RM:144:GLY:N | 2.52 | 0.43 |
| 41:RM:200:TYR:CD1 | 41:RM:266:PHE:HB2 | 2.53 | 0.43 |
| 41:RN:407:GLU:OE2 | 41:RN:407:GLU:N | 2.48 | 0.43 |
| 41:RO:31:ASP:OD2 | 41:RO:34:GLY:N | 2.51 | 0.43 |
| 41:RO:136:THR:HG22 | 41:RO:167:PHE:HB2 | 2.00 | 0.43 |
| 41:RO:171:PRO:HB3 | 41:RO:181:GLU:HB3 | 2.01 | 0.43 |
| 41:RO:215:LEU:HB3 | 41:RO:217:LEU:HD13 | 2.00 | 0.43 |
| 41:RP:41:ASP:OD1 | 41:RP:41:ASP:N | 2.50 | 0.43 |
| 40:SA:224:TYR:HB3 | 42:SN:501:GTP:C2 | 2.52 | 0.43 |
| 40:SF:139:HIS:CG | 40:SF:150:THR:HG21 | 2.53 | 0.43 |
| 40:SH:329:ASN:ND2 | 41:SP:175:VAL:HG21 | 2.33 | 0.43 |
| 40:SI:49:PHE:HB3 | 40:SI:53:PHE:HB2 | 1.99 | 0.43 |
| 40:SI:97:GLU:HG2 | 41:SP:251:ARG:HH22 | 1.83 | 0.43 |
| 41:SL:268:PRO:HG2 | 41:SL:300:MET:HE3 | 2.01 | 0.43 |
| 41:SM:100:ASN:HB2 | 41:SM:103:LYS:HB2 | 2.00 | 0.43 |
| 41:SO:32:PRO:HA | 41:SO:84:ILE:HD11 | 2.01 | 0.43 |
| 41:SO:76:VAL:O | 41:SO:77:ARG:C | 2.57 | 0.43 |
| 41:SO:261:PRO:O | 41:SO:262:ARG:C | 2.57 | 0.43 |
| 41:SO:268:PRO:HA | 41:SO:367:PHE:O | 2.18 | 0.43 |
| 41:SO:296:ALA:O | 41:SO:299:MET:HB2 | 2.18 | 0.43 |
| 41:SP:26:ASP:O | 41:SP:359:ARG:NH2 | 2.51 | 0.43 |
| 41:SP:113:VAL:HA | 41:SP:116:VAL:HB | 2.00 | 0.43 |
| 41:SP:309:ARG:H | 41:SP:372:THR:HG1 | 1.59 | 0.43 |
| 40:TA:304:LYS:HD2 | 40:TA:304:LYS:HA | 1.85 | 0.43 |
| 41:TB:318:ARG:HH12 | 41:TB:358:PRO:HB3 | 1.84 | 0.43 |
| 40:TF:21:TRP:CZ2 | 40:TF:65:ALA:HB2 | 2.53 | 0.43 |
| 40:TF:55:GLU:HG2 | 40:TF:61:HIS:HE1 | 1.82 | 0.43 |
| 40:TF:76:ASP:HA | 40:TF:79:ARG:HB2 | 1.98 | 0.43 |
| 40:TF:207:GLU:HA | 40:TF:210:TYR:CD2 | 2.53 | 0.43 |
| 40:TG:3:GLU:HG3 | 40:TG:129:CYS:SG | 2.58 | 0.43 |
| 40:TI:255:PHE:HZ | 40:TI:318:LEU:HD21 | 1.82 | 0.43 |
| 41:TM:95:SER:OG | 41:TM:96:GLY:N | 2.52 | 0.43 |
| 40:UA:16:ILE:HD11 | 40:UA:171:ILE:HD11 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 42:UB:502:GTP:O2A | 40:UG:140:SER:OG | 2.36 | 0.43 |
| 40:UE:254:GLU:OE1 | 41:UM:99:ASN:ND2 | 2.51 | 0.43 |
| 40:UF:250:VAL:HG21 | 40:UF:318:LEU:HD22 | 2.00 | 0.43 |
| 40:UF:421:ARG:HH11 | 40:UF:425:ALA:HB2 | 1.82 | 0.43 |
| 40:UG:352:LYS:NZ | 41:UO:176:SER:O | 2.44 | 0.43 |
| 40:UI:194:THR:O | 40:UI:195:LEU:C | 2.57 | 0.43 |
| 41:UO:398:TYR:HD2 | 41:UO:408:PHE:HZ | 1.66 | 0.43 |
| 41:UP:19:LYS:HA | 41:UP:19:LYS:HD2 | 1.38 | 0.43 |
| 41:UP:337:ASN:C | 41:UP:339:SER:H | 2.21 | 0.43 |
| 41:VQ:139:LEU:HG | 41:VQ:168:SER:HB2 | 1.99 | 0.43 |
| 40:WA:181:VAL:HB | 41:WN:345:ILE:HD11 | 2.00 | 0.43 |
| 40:WF:260:VAL:HG12 | 41:WN:396:HIS:HE1 | 1.83 | 0.43 |
| 40:WG:112:LYS:HA | 40:WG:115:ILE:HG22 | 2.00 | 0.43 |
| 41:WO:3:GLU:OE2 | 41:WO:62:ARG:NH2 | 2.51 | 0.43 |
| 41:WQ:113:VAL:HG22 | 41:WQ:117:LEU:HD23 | 2.00 | 0.43 |
| 7:1U:495:ARG:HD2 | 7:1U:498:MET:HB2 | 2.00 | 0.43 |
| 9:2B:181:ASP:OD1 | 9:2B:184:TRP:HB2 | 2.17 | 0.43 |
| 9:2C:420:LYS:HA | 9:2C:420:LYS:HD3 | 1.78 | 0.43 |
| 10:2E:74:PHE:CD1 | 10:2E:94:LEU:HD21 | 2.53 | 0.43 |
| 12:2R:166:CYS:O | 12:2R:170:LYS:HG2 | 2.17 | 0.43 |
| 13:2U:71:ILE:HD13 | 13:2U:71:ILE:HA | 1.78 | 0.43 |
| 16:3L:79:ASP:OD1 | 16:3L:176:HIS:NE2 | 2.51 | 0.43 |
| 17:3O:205:ARG:HE | 17:3O:205:ARG:HB2 | 1.72 | 0.43 |
| 17:3P:355:ALA:O | 17:3P:356:ASP:C | 2.57 | 0.43 |
| 17:3R:168:ILE:HG22 | 17:3R:172:ASN:HD21 | 1.83 | 0.43 |
| 17:3R:202:ARG:HD2 | 17:3R:347:PHE:CZ | 2.53 | 0.43 |
| 18:3W:163:GLN:HB3 | 18:3W:418:VAL:HG13 | 2.00 | 0.43 |
| 19:3Z:362:LYS:HE3 | 19:3Z:362:LYS:HB3 | 1.90 | 0.43 |
| 19:3Z:364:ILE:HG23 | 41:LP:320:ARG:HH12 | 1.82 | 0.43 |
| 20:4B:345:GLN:O | 20:4B:346:LEU:C | 2.57 | 0.43 |
| 21:4F:408:ASP:O | 21:4F:409:VAL:C | 2.56 | 0.43 |
| 22:4H:284:LEU:HD22 | 22:4H:333:TYR:CD2 | 2.54 | 0.43 |
| 22:4J:61:PRO:HG2 | 22:4J:63:GLU:HG2 | 2.00 | 0.43 |
| 22:4J:94:GLN:HG2 | 22:4J:196:TYR:CG | 2.53 | 0.43 |
| 22:4K:470:GLU:N | 22:4K:470:GLU:OE1 | 2.51 | 0.43 |
| 22:4K:679:SER:HA | 22:4K:683:ASP:CB | 2.48 | 0.43 |
| 23:4N:238:HIS:CE1 | 23:4N:239:ASN:HD22 | 2.37 | 0.43 |
| 23:4P:238:HIS:CE1 | 23:4P:239:ASN:HD22 | 2.37 | 0.43 |
| 25:4T:284:ASN:HB3 | 25:4T:288:GLN:HB3 | 2.00 | 0.43 |
| 29:5D:28:TYR:OH | 34:5R:342:TYR:HB2 | 2.19 | 0.43 |
| 33:5N:453:LYS:HD3 | 33:5N:475:ASP:HB3 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:5W:186:TYR:HE2 | 41:OB:280:GLN:HB2 | 1.83 | 0.43 |
| 39:6G:129:CYS:HA | 40:OG:85:GLN:HE22 | 1.82 | 0.43 |
| 40:AE:262:TYR:OH | 41:AM:391:ARG:O | 2.29 | 0.43 |
| 40:AF:68:VAL:HG11 | 40:AF:149:PHE:HE1 | 1.82 | 0.43 |
| 40:AG:175:PRO:HB3 | 40:AG:389:ARG:NH1 | 2.33 | 0.43 |
| 41:AO:156:ARG:O | 41:AO:157:GLU:C | 2.56 | 0.43 |
| 41:AO:361:LEU:H | 41:AO:361:LEU:HG | 1.57 | 0.43 |
| 41:AP:86:ARG:NH2 | 41:BP:281:TYR:O | 2.44 | 0.43 |
| 40:BA:205:ASP:HB3 | 40:BA:303:VAL:HA | 1.99 | 0.43 |
| 40:BE:415:GLY:O | 40:BE:416:GLU:C | 2.57 | 0.43 |
| 40:BH:211:ASP:HA | 40:BH:214:ARG:HD2 | 2.00 | 0.43 |
| 41:BM:149:THR:HG21 | 41:BM:188:SER:HA | 2.00 | 0.43 |
| 40:CA:131:GLY:O | 40:CA:133:GLN:N | 2.51 | 0.43 |
| 40:CE:116:ASP:N | 40:CE:116:ASP:OD1 | 2.52 | 0.43 |
| 40:CE:260:VAL:O | 41:CM:396:HIS:HE1 | 2.02 | 0.43 |
| 40:CI:164:LYS:O | 40:CI:166:LYS:NZ | 2.40 | 0.43 |
| 40:CI:221:ARG:HG2 | 41:CP:322:SER:CB | 2.47 | 0.43 |
| 41:CL:107:THR:HB | 41:CL:108:GLU:H | 1.61 | 0.43 |
| 41:CM:135:LEU:HD23 | 41:CM:152:ILE:HD11 | 2.00 | 0.43 |
| 41:CM:163:ILE:HD13 | 41:CM:163:ILE:HA | 1.91 | 0.43 |
| 41:CM:295:ASP:HB3 | 41:CM:296:ALA:H | 1.63 | 0.43 |
| 41:CP:21:TRP:CZ2 | 41:CP:63:ALA:HB2 | 2.53 | 0.43 |
| 41:CP:57:GLY:O | 41:CP:58:LYS:C | 2.56 | 0.43 |
| 40:DA:317:LEU:HD13 | 40:DA:351:PHE:HD2 | 1.83 | 0.43 |
| 40:DA:320:ARG:HB3 | 40:DA:356:ASN:HB2 | 2.01 | 0.43 |
| 41:DB:40:SER:HB2 | 41:DB:42:LEU:HG | 2.00 | 0.43 |
| 41:DB:123:GLU:H | 41:DB:123:GLU:HG2 | 1.66 | 0.43 |
| 40:DE:96:LYS:HA | 40:DE:96:LYS:HD3 | 1.91 | 0.43 |
| 40:DE:322:ASP:OD2 | 40:DE:371:GLN:HB2 | 2.17 | 0.43 |
| 40:DF:36:MET:HE2 | 40:DF:36:MET:HB2 | 1.77 | 0.43 |
| 40:DG:398:TYR:O | 40:DG:401:ARG:NH1 | 2.50 | 0.43 |
| 40:DH:218:ASP:OD1 | 40:DH:280:LYS:HB2 | 2.19 | 0.43 |
| 40:DI:27:GLU:HB2 | 40:DI:244:PHE:HE2 | 1.82 | 0.43 |
| 40:DI:50:ASN:O | 40:DI:64:ARG:NH2 | 2.52 | 0.43 |
| 41:DL:254:ALA:O | 41:DL:255:VAL:C | 2.57 | 0.43 |
| 41:DL:338:SER:O | 41:DL:339:SER:C | 2.56 | 0.43 |
| 41:DM:153:SER:OG | 41:DM:154:LYS:N | 2.50 | 0.43 |
| 41:DN:24:ILE:HA | 41:DN:27:GLU:HB2 | 2.00 | 0.43 |
| 41:DN:247:ASN:HD22 | 41:DN:247:ASN:HA | 1.63 | 0.43 |
| 41:DN:367:PHE:C | 41:DN:368:ILE:HG13 | 2.38 | 0.43 |
| 41:DP:211:CYS:O | 41:DP:212:PHE:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EE:102:ASN:ND2 | 40:EE:410:GLU:OE2 | 2.52 | 0.43 |
| 40:EE:137:ILE:HB | 40:EE:168:GLU:HG3 | 2.00 | 0.43 |
| 40:EE:228:ASN:ND2 | 42:EL:501:GTP:HN1 | 2.12 | 0.43 |
| 40:EE:276:ILE:HD13 | 40:EE:286:LEU:HD11 | 2.00 | 0.43 |
| 40:EI:179:THR:HG23 | 40:EI:180:ALA:H | 1.83 | 0.43 |
| 41:EL:20:PHE:O | 41:EL:24:ILE:HG12 | 2.17 | 0.43 |
| 41:EM:142:GLY:O | 41:EM:144:GLY:N | 2.51 | 0.43 |
| 41:EM:358:PRO:O | 41:EM:359:ARG:C | 2.56 | 0.43 |
| 41:EO:232:THR:HG23 | 41:EO:270:PHE:HB2 | 2.00 | 0.43 |
| 41:EO:272:PRO:HG3 | 41:EO:364:SER:HB2 | 2.00 | 0.43 |
| 41:EP:15:GLN:C | 41:EP:226:ASN:HD21 | 2.21 | 0.43 |
| 41:EP:28:HIS:O | 41:EP:43:GLN:HB3 | 2.18 | 0.43 |
| 41:EP:419:GLY:O | 41:EP:423:VAL:HB | 2.18 | 0.43 |
| 40:FA:2:ARG:O | 40:FA:51:THR:HA | 2.19 | 0.43 |
| 40:FA:12:ALA:HB3 | 40:FA:140:SER:HB3 | 1.99 | 0.43 |
| 40:FA:222:PRO:HG2 | 41:FN:324:LYS:HZ3 | 1.83 | 0.43 |
| 40:FA:258:ASN:ND2 | 41:FB:178:THR:HG23 | 2.34 | 0.43 |
| 40:FA:262:TYR:HH | 41:FB:391:ARG:HB3 | 1.83 | 0.43 |
| 40:FA:278:ALA:O | 40:FA:280:LYS:N | 2.51 | 0.43 |
| 41:FB:385:PHE:HZ | 41:FB:408:PHE:HB3 | 1.83 | 0.43 |
| 40:FI:306:ASP:OD1 | 40:FI:308:ARG:HG2 | 2.19 | 0.43 |
| 41:FM:7:LEU:HD22 | 41:FM:151:LEU:HD21 | 2.01 | 0.43 |
| 40:GA:79:ARG:NH2 | 40:GA:94:THR:OG1 | 2.52 | 0.43 |
| 40:GA:184:PRO:HG3 | 40:GA:393:LYS:HG3 | 2.01 | 0.43 |
| 41:GB:255:VAL:HG21 | 40:GG:102:ASN:OD1 | 2.19 | 0.43 |
| 40:GE:32:PRO:O | 40:GE:33:ASP:C | 2.57 | 0.43 |
| 40:GE:50:ASN:O | 40:GE:52:PHE:N | 2.52 | 0.43 |
| 40:GE:207:GLU:O | 40:GE:210:TYR:HB2 | 2.18 | 0.43 |
| 40:GE:291:ILE:H | 40:GE:291:ILE:HG12 | 1.41 | 0.43 |
| 40:GE:338:LYS:HB2 | 40:GE:341:ILE:HD11 | 2.00 | 0.43 |
| 40:GG:255:PHE:CZ | 40:GG:318:LEU:HD21 | 2.53 | 0.43 |
| 40:GH:173:PRO:HG2 | 40:GH:187:SER:HB3 | 1.99 | 0.43 |
| 40:GH:284:GLU:H | 40:GH:284:GLU:HG2 | 1.69 | 0.43 |
| 40:GH:311:LYS:N | 40:GH:381:THR:HG22 | 2.30 | 0.43 |
| 40:GI:2:ARG:O | 40:GI:3:GLU:HG3 | 2.17 | 0.43 |
| 40:GI:96:LYS:HB3 | 40:GI:97:GLU:H | 1.65 | 0.43 |
| 40:GI:246:GLY:HA2 | 40:GI:357:TYR:CE2 | 2.53 | 0.43 |
| 40:GI:261:PRO:HD2 | 40:GI:265:ILE:O | 2.18 | 0.43 |
| 41:GN:335:ASN:O | 41:GN:336:LYS:C | 2.57 | 0.43 |
| 41:GN:354:CYS:O | 41:GN:355:ASP:C | 2.57 | 0.43 |
| 41:GO:149:THR:O | 41:GO:152:ILE:HB | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HE:414:GLU:O | 40:HE:415:GLY:C | 2.56 | 0.43 |
| 41:HM:184:ASN:OD1 | 41:HM:398:TYR:OH | 2.25 | 0.43 |
| 41:HN:238:THR:HG21 | 41:HN:318:ARG:HD2 | 2.01 | 0.43 |
| 41:HN:263:LEU:HD13 | 41:HN:263:LEU:HA | 1.86 | 0.43 |
| 41:HQ:132:GLY:HA3 | 41:HQ:163:ILE:O | 2.18 | 0.43 |
| 40:IF:79:ARG:HH21 | 40:IF:92:LEU:HB2 | 1.83 | 0.43 |
| 40:IH:105:ARG:HA | 40:IH:109:THR:HG22 | 1.99 | 0.43 |
| 40:II:239:THR:O | 40:II:243:ARG:HG3 | 2.18 | 0.43 |
| 40:II:276:ILE:HG22 | 40:II:277:SER:H | 1.84 | 0.43 |
| 40:II:320:ARG:HD3 | 40:II:360:PRO:HG3 | 2.01 | 0.43 |
| 41:IP:240:LEU:H | 41:IP:240:LEU:HD23 | 1.82 | 0.43 |
| 41:JB:139:LEU:HG | 41:JB:168:SER:HB2 | 2.01 | 0.43 |
| 41:JB:324:LYS:HE2 | 40:JG:222:PRO:HG2 | 2.01 | 0.43 |
| 41:JL:109:GLY:O | 41:JL:113:VAL:HG13 | 2.17 | 0.43 |
| 41:JM:394:PHE:HD1 | 41:JM:397:TRP:HZ3 | 1.66 | 0.43 |
| 41:JN:207:LEU:HB3 | 41:JN:225:LEU:HD22 | 2.00 | 0.43 |
| 40:KA:222:PRO:HD2 | 41:KN:324:LYS:HB2 | 2.00 | 0.43 |
| 40:KD:116:ASP:N | 40:KD:116:ASP:OD1 | 2.48 | 0.43 |
| 41:KP:27:GLU:OE2 | 41:KP:318:ARG:NH2 | 2.36 | 0.43 |
| 40:LF:285:GLN:O | 40:LF:286:LEU:C | 2.57 | 0.43 |
| 40:LF:400:LYS:H | 40:LF:400:LYS:HG2 | 1.49 | 0.43 |
| 41:LP:16:ILE:HA | 41:LP:226:ASN:HB3 | 2.00 | 0.43 |
| 40:MF:88:HIS:HB3 | 40:MF:91:GLN:HG2 | 2.00 | 0.43 |
| 40:MF:266:HIS:C | 40:MF:268:PRO:HD3 | 2.39 | 0.43 |
| 40:MG:319:TYR:HD2 | 40:MG:323:VAL:HG11 | 1.84 | 0.43 |
| 40:MH:431:TYR:O | 40:MH:432:GLU:C | 2.56 | 0.43 |
| 41:MN:210:ILE:HG12 | 41:MN:298:ASN:HA | 2.00 | 0.43 |
| 41:NB:176:SER:OG | 41:NB:181:GLU:OE1 | 2.30 | 0.43 |
| 40:ND:7:VAL:HG13 | 40:ND:66:VAL:HG13 | 2.00 | 0.43 |
| 40:NF:358:GLN:HA | 40:NF:359:PRO:HD3 | 1.87 | 0.43 |
| 40:NH:104:ALA:O | 40:NH:108:TYR:HB2 | 2.19 | 0.43 |
| 41:NP:288:GLU:HA | 41:NP:291:GLN:HE21 | 1.82 | 0.43 |
| 40:OA:238:ILE:HD13 | 40:OA:377:LEU:HD11 | 2.00 | 0.43 |
| 40:OD:112:LYS:HA | 40:OD:115:ILE:HG22 | 2.00 | 0.43 |
| 40:OD:144:GLY:N | 42:OD:501:GTP:O2G | 2.51 | 0.43 |
| 40:OD:236:SER:O | 40:OD:320:ARG:NH1 | 2.51 | 0.43 |
| 40:OD:343:PHE:HZ | 40:OD:351:PHE:CE1 | 2.36 | 0.43 |
| 40:OG:319:TYR:HE2 | 40:OG:328:VAL:HG13 | 1.83 | 0.43 |
| 41:OO:180:VAL:HG22 | 41:OO:183:TYR:HB2 | 2.00 | 0.43 |
| 41:OO:286:VAL:HG11 | 41:OO:326:VAL:HG22 | 1.99 | 0.43 |
| 40:PA:315:CYS:HA | 40:PA:377:LEU:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PB:132:GLY:HA2 | 41:PB:162:ARG:HB3 | 2.01 | 0.43 |
| 41:PB:226:ASN:ND2 | 43:PB:501:GDP:O6 | 2.50 | 0.43 |
| 40:PD:30:ILE:HD13 | 40:PD:53:PHE:HD2 | 1.82 | 0.43 |
| 40:PD:140:SER:HB2 | 40:PD:171:ILE:HB | 2.01 | 0.43 |
| 41:PM:19:LYS:NZ | 41:PM:223:GLY:O | 2.50 | 0.43 |
| 41:PP:292:GLN:O | 41:PP:298:ASN:ND2 | 2.46 | 0.43 |
| 41:QL:100:ASN:HB3 | 41:QL:103:LYS:HB2 | 2.00 | 0.43 |
| 41:QL:228:LEU:O | 41:QL:232:THR:HG23 | 2.18 | 0.43 |
| 41:QM:139:LEU:O | 41:QM:145:SER:OG | 2.30 | 0.43 |
| 41:QN:119:VAL:O | 41:QN:122:LYS:HB3 | 2.18 | 0.43 |
| 41:QN:137:HIS:HE1 | 41:QN:139:LEU:HD21 | 1.83 | 0.43 |
| 41:QP:14:ASN:HD21 | 41:QP:67:ASP:HB2 | 1.82 | 0.43 |
| 41:QP:187:LEU:O | 41:QP:188:SER:C | 2.56 | 0.43 |
| 40:RA:217:LEU:HA | 40:RA:277:SER:HB2 | 2.01 | 0.43 |
| 41:RB:22:GLU:HG3 | 41:RB:81:PHE:CD2 | 2.51 | 0.43 |
| 40:RE:30:ILE:HG13 | 40:RE:53:PHE:HE2 | 1.84 | 0.43 |
| 40:RI:234:ILE:O | 40:RI:238:ILE:HD12 | 2.18 | 0.43 |
| 41:RM:19:LYS:HD3 | 41:RM:19:LYS:HA | 1.87 | 0.43 |
| 41:RO:310:TYR:CD1 | 41:RO:371:SER:HB2 | 2.54 | 0.43 |
| 41:RO:407:GLU:HA | 41:RO:410:GLU:HG3 | 2.00 | 0.43 |
| 40:SA:391:ASP:HA | 40:SA:421:ARG:HH12 | 1.83 | 0.43 |
| 41:SB:100:ASN:OD1 | 41:SB:100:ASN:N | 2.51 | 0.43 |
| 40:SF:195:LEU:HD21 | 40:SF:264:ARG:HE | 1.84 | 0.43 |
| 40:SG:63:PRO:HG2 | 40:SG:87:PHE:HA | 2.00 | 0.43 |
| 40:SH:21:TRP:CZ2 | 40:SH:65:ALA:HB2 | 2.53 | 0.43 |
| 41:SO:73:MET:HE2 | 41:SO:73:MET:HB2 | 1.87 | 0.43 |
| 41:SO:87:PRO:O | 41:SO:90:PHE:HB2 | 2.18 | 0.43 |
| 40:TA:107:HIS:CD2 | 40:TA:152:LEU:HB2 | 2.53 | 0.43 |
| 40:TA:140:SER:HA | 40:TA:171:ILE:HB | 2.00 | 0.43 |
| 40:TA:271:THR:HB | 40:TA:376:MET:HB2 | 2.00 | 0.43 |
| 41:TB:113:VAL:HG21 | 41:TB:154:LYS:HE3 | 2.00 | 0.43 |
| 40:TE:237:SER:OG | 40:TE:375:CYS:SG | 2.69 | 0.43 |
| 40:TF:195:LEU:HD22 | 40:TF:427:LEU:HD21 | 2.00 | 0.43 |
| 40:TG:73:THR:HA | 40:TG:76:ASP:HB2 | 1.99 | 0.43 |
| 40:TH:121:ARG:HA | 40:TH:121:ARG:HD3 | 1.78 | 0.43 |
| 40:TI:238:ILE:HA | 40:TI:318:LEU:HD22 | 1.99 | 0.43 |
| 41:TM:311:LEU:N | 41:TM:370:ASN:O | 2.52 | 0.43 |
| 41:TN:238:THR:HG21 | 41:TN:318:ARG:CZ | 2.49 | 0.43 |
| 40:UA:223:THR:HB | 41:UN:322:SER:HB2 | 1.99 | 0.43 |
| 41:UB:137:HIS:O | 41:UB:168:SER:HA | 2.18 | 0.43 |
| 41:UB:255:VAL:HG11 | 40:UG:100:ALA:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UE:438:SER:HB3 | 41:UM:391:ARG:HH21 | 1.83 | 0.43 |
| 40:UF:406:TRP:CD1 | 41:UM:255:VAL:HG23 | 2.53 | 0.43 |
| 40:UF:414:GLU:O | 40:UF:415:GLY:C | 2.57 | 0.43 |
| 40:UH:316:CYS:SG | 40:UH:377:LEU:HB2 | 2.58 | 0.43 |
| 40:UI:199:ASP:O | 40:UI:266:HIS:HB2 | 2.18 | 0.43 |
| 40:UI:221:ARG:N | 40:UI:222:PRO:CD | 2.82 | 0.43 |
| 40:UI:338:LYS:HB2 | 40:UI:341:ILE:HG13 | 2.00 | 0.43 |
| 40:UI:401:ARG:HA | 40:UI:401:ARG:HD3 | 1.35 | 0.43 |
| 40:UI:421:ARG:HA | 40:UI:421:ARG:HD2 | 1.35 | 0.43 |
| 41:UM:290:THR:HA | 41:UM:293:MET:HB3 | 2.00 | 0.43 |
| 41:UM:299:MET:SD | 41:UM:299:MET:N | 2.91 | 0.43 |
| 41:UP:75:SER:O | 41:UP:79:GLY:N | 2.51 | 0.43 |
| 41:UP:190:HIS:CD2 | 41:UP:411:ALA:HA | 2.53 | 0.43 |
| 41:UP:404:ASP:HB3 | 41:UP:407:GLU:HG3 | 1.98 | 0.43 |
| 40:VG:167:LEU:HD11 | 40:VG:256:GLN:NE2 | 2.33 | 0.43 |
| 40:VI:11:GLN:HG2 | 40:VI:74:VAL:HG21 | 2.01 | 0.43 |
| 40:VI:118:VAL:O | 40:VI:122:ILE:HG12 | 2.18 | 0.43 |
| 41:VP:2:ARG:HD2 | 41:VP:131:GLN:HE21 | 1.83 | 0.43 |
| 40:WA:21:TRP:CH2 | 40:WA:52:PHE:HB3 | 2.53 | 0.43 |
| 40:WF:400:LYS:NZ | 41:WM:344:TRP:HB2 | 2.34 | 0.43 |
| 40:WI:228:ASN:ND2 | 42:WI:501:GTP:HN1 | 2.14 | 0.43 |
| 41:WM:338:SER:O | 41:WM:339:SER:C | 2.57 | 0.43 |
| 7:1S:418:ILE:HD12 | 10:2F:148:VAL:HG12 | 2.00 | 0.43 |
| 8:1X:118:THR:O | 8:1X:119:ARG:C | 2.57 | 0.43 |
| 9:2B:90:LYS:HD3 | 9:2B:90:LYS:HA | 1.78 | 0.43 |
| 10:2E:43:PRO:HA | 40:ME:433:GLU:OE2 | 2.19 | 0.43 |
| 11:2I:210:GLU:HB2 | 11:2I:230:LEU:HD21 | 2.00 | 0.43 |
| 13:2U:101:ARG:H | 13:2U:101:ARG:HG2 | 1.70 | 0.43 |
| 13:2W:17:ILE:HG23 | 41:WN:125:GLU:HA | 2.01 | 0.43 |
| 15:3E:38:VAL:HA | 15:3F:295:ASN:HD22 | 1.82 | 0.43 |
| 15:3F:282:LEU:HA | 15:3F:372:LEU:HD13 | 2.00 | 0.43 |
| 15:3G:375:GLU:O | 15:3G:379:LYS:HG2 | 2.18 | 0.43 |
| 16:3K:209:PRO:O | 16:3K:212:SER:OG | 2.36 | 0.43 |
| 16:3K:368:LYS:HA | 16:3K:368:LYS:HD3 | 1.80 | 0.43 |
| 17:3R:179:LYS:HB3 | 17:3R:179:LYS:HE2 | 1.69 | 0.43 |
| 17:3R:192:LEU:HD12 | 17:3R:192:LEU:HA | 1.76 | 0.43 |
| 17:3R:209:ASP:OD1 | 17:3R:210:LEU:HD22 | 2.18 | 0.43 |
| 17:3R:320:LYS:O | 17:3R:321:LEU:C | 2.57 | 0.43 |
| 21:4E:263:ILE:HB | 21:4E:276:LEU:HB2 | 2.01 | 0.43 |
| 21:4F:452:PHE:CE2 | 40:EE:46:ASP:HB3 | 2.53 | 0.43 |
| 22:4H:19:LYS:HG2 | 22:4H:44:GLY:HA2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:4O:240:LEU:HB2 | 24:4O:266:HIS:HA | 2.01 | 0.43 |
| 25:4T:289:VAL:H | 25:4T:290:PRO:HD3 | 1.84 | 0.43 |
| 25:4T:418:ILE:HG12 | 25:4T:424:PRO:HB3 | 2.00 | 0.43 |
| 26:4V:279:ARG:HG3 | 26:4V:304:TYR:CE1 | 2.53 | 0.43 |
| 27:4Y:86:LEU:HB2 | 27:4Y:235:PHE:HE1 | 1.82 | 0.43 |
| 31:5I:489:HIS:O | 31:5I:494:TYR:OH | 2.28 | 0.43 |
| 31:5I:492:ASN:HB2 | 31:5I:494:TYR:CZ | 2.53 | 0.43 |
| 33:5N:473:ASP:O | 33:5N:477:LEU:HA | 2.17 | 0.43 |
| 36:5W:66:LEU:HB3 | 40:OF:221:ARG:CZ | 2.49 | 0.43 |
| 39:6F:152:GLU:HG3 | 39:6F:156:HIS:CE1 | 2.53 | 0.43 |
| 39:6K:77:GLU:HA | 39:6K:80:LYS:HE2 | 1.99 | 0.43 |
| 40:AF:68:VAL:HG22 | 40:AF:93:ILE:HB | 2.00 | 0.43 |
| 40:AF:405:HIS:HA | 40:AF:408:VAL:HG22 | 2.00 | 0.43 |
| 40:AG:36:MET:HG3 | 40:AG:61:HIS:CE1 | 2.54 | 0.43 |
| 40:AG:323:VAL:HG22 | 40:AG:372:ARG:HG2 | 1.99 | 0.43 |
| 40:AH:335:ILE:HA | 40:AH:338:LYS:HD2 | 2.01 | 0.43 |
| 41:AM:199:THR:HG23 | 41:AM:264:HIS:HD2 | 1.83 | 0.43 |
| 41:AO:69:GLU:HG2 | 41:AO:96:GLY:HA2 | 1.99 | 0.43 |
| 41:AP:309:ARG:NH1 | 41:AP:339:SER:O | 2.51 | 0.43 |
| 41:BB:362:LYS:HE2 | 41:BB:362:LYS:HB2 | 1.39 | 0.43 |
| 40:BH:257:THR:OG1 | 41:BP:99:ASN:ND2 | 2.51 | 0.43 |
| 40:BH:348:PRO:HG2 | 41:BP:384:GLN:HA | 2.01 | 0.43 |
| 40:BI:413:GLU:O | 40:BI:414:GLU:C | 2.55 | 0.43 |
| 41:BL:89:ASN:HA | 41:BL:119:VAL:HG21 | 2.00 | 0.43 |
| 41:BL:149:THR:HB | 41:BL:191:GLN:HG3 | 2.00 | 0.43 |
| 41:BL:328:GLU:O | 41:BL:332:ASN:HB2 | 2.19 | 0.43 |
| 41:BM:341:PHE:HB3 | 41:BM:348:ASN:OD1 | 2.18 | 0.43 |
| 41:BO:19:LYS:HG3 | 41:BO:230:SER:HB3 | 2.01 | 0.43 |
| 41:BP:200:TYR:HE1 | 41:BP:368:ILE:HG12 | 1.82 | 0.43 |
| 41:BP:321:MET:H | 41:BP:321:MET:HG2 | 1.68 | 0.43 |
| 40:CA:132:LEU:HB3 | 40:CA:164:LYS:HE2 | 2.00 | 0.43 |
| 40:CA:346:TRP:CB | 41:CB:391:ARG:HD3 | 2.38 | 0.43 |
| 40:CG:112:LYS:HA | 40:CG:115:ILE:HG22 | 2.00 | 0.43 |
| 40:CG:115:ILE:HG13 | 40:CG:119:LEU:HD13 | 1.99 | 0.43 |
| 40:CH:258:ASN:HA | 41:CP:179:VAL:CG1 | 2.47 | 0.43 |
| 40:CI:96:LYS:NZ | 41:CP:1:MET:HB2 | 2.31 | 0.43 |
| 41:CL:311:LEU:HG | 41:CL:342:VAL:HG11 | 2.00 | 0.43 |
| 41:CL:420:ASN:N | 41:CL:421:PRO:HD2 | 2.34 | 0.43 |
| 41:CN:248:ALA:HB2 | 41:CN:352:ALA:HB2 | 2.01 | 0.43 |
| 41:CN:309:ARG:O | 41:CN:310:TYR:C | 2.57 | 0.43 |
| 41:CN:310:TYR:HA | 41:CN:371:SER:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CO:376:GLU:H | 41:CO:376:GLU:HG2 | 1.56 | 0.43 |
| 40:DA:256:GLN:HG3 | 41:DB:397:TRP:CZ2 | 2.49 | 0.43 |
| 41:DB:86:ARG:HD3 | 41:DB:89:ASN:HB2 | 2.00 | 0.43 |
| 40:DE:330:ALA:O | 40:DE:333:ALA:HB3 | 2.18 | 0.43 |
| 40:DF:400:LYS:O | 40:DF:401:ARG:C | 2.57 | 0.43 |
| 40:DG:319:TYR:HB2 | 40:DG:355:ILE:HG12 | 2.01 | 0.43 |
| 40:DH:128:GLN:HE22 | 40:EH:290:GLU:HB2 | 1.83 | 0.43 |
| 40:DI:152:LEU:HD12 | 40:DI:152:LEU:HA | 1.75 | 0.43 |
| 41:DL:273:LEU:HD13 | 41:DL:273:LEU:HA | 1.72 | 0.43 |
| 41:DL:324:LYS:HA | 41:DL:327:ASP:HB2 | 1.99 | 0.43 |
| 41:DM:131:GLN:HE22 | 41:DM:250:LEU:H | 1.65 | 0.43 |
| 41:DN:399:THR:C | 41:DN:401:GLU:H | 2.22 | 0.43 |
| 41:DO:20:PHE:HA | 41:DO:230:SER:OG | 2.18 | 0.43 |
| 41:DP:31:ASP:OD1 | 41:DP:35:THR:N | 2.51 | 0.43 |
| 41:DP:80:PRO:O | 41:DP:82:GLY:N | 2.51 | 0.43 |
| 41:DP:393:ALA:O | 41:DP:394:PHE:C | 2.57 | 0.43 |
| 41:EB:19:LYS:O | 41:EB:22:GLU:HG3 | 2.18 | 0.43 |
| 40:EF:209:ILE:HA | 40:EF:212:ILE:HG22 | 2.00 | 0.43 |
| 40:EF:264:ARG:NH2 | 40:EF:423:ASP:OD1 | 2.51 | 0.43 |
| 40:EF:347:CYS:HA | 41:EN:388:MET:HE2 | 2.00 | 0.43 |
| 40:EI:259:LEU:O | 40:EI:261:PRO:HD3 | 2.18 | 0.43 |
| 40:EI:312:TYR:CD1 | 40:EI:380:THR:HB | 2.54 | 0.43 |
| 41:EM:119:VAL:O | 41:EM:120:VAL:C | 2.55 | 0.43 |
| 41:EM:321:MET:H | 41:EM:321:MET:HG2 | 1.59 | 0.43 |
| 41:EN:247:ASN:OD1 | 41:EN:247:ASN:N | 2.52 | 0.43 |
| 40:FA:139:HIS:O | 40:FA:170:SER:HA | 2.19 | 0.43 |
| 41:FB:31:ASP:OD2 | 41:FB:37:HIS:ND1 | 2.36 | 0.43 |
| 40:FF:262:TYR:OH | 41:FN:391:ARG:O | 2.36 | 0.43 |
| 41:FM:190:HIS:CD2 | 41:FM:411:ALA:HA | 2.54 | 0.43 |
| 41:FO:232:THR:HG22 | 41:FO:270:PHE:HB2 | 2.00 | 0.43 |
| 41:FO:306:ARG:HA | 41:FO:340:TYR:CE2 | 2.53 | 0.43 |
| 41:FP:11:GLN:HA | 41:FP:72:THR:HG21 | 2.00 | 0.43 |
| 40:GA:243:ARG:HD2 | 40:GA:244:PHE:CZ | 2.53 | 0.43 |
| 40:GA:252:LEU:HA | 40:GA:255:PHE:HD2 | 1.83 | 0.43 |
| 41:GB:254:ALA:O | 41:GB:258:VAL:HG12 | 2.18 | 0.43 |
| 40:GE:91:GLN:HE21 | 40:GE:91:GLN:HB2 | 1.64 | 0.43 |
| 40:GF:142:GLY:HA2 | 40:GF:183:GLU:HG2 | 2.01 | 0.43 |
| 40:GG:271:THR:HB | 40:GG:376:MET:HB3 | 1.99 | 0.43 |
| 40:GI:2:ARG:H | 40:GI:2:ARG:HG2 | 1.31 | 0.43 |
| 41:GM:216:LYS:HB3 | 41:GM:216:LYS:HE2 | 1.79 | 0.43 |
| 41:GN:193:VAL:O | 41:GN:264:HIS:HE1 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HB:132:GLY:HA3 | 41:HB:163:ILE:O | 2.18 | 0.43 |
| 40:HE:136:LEU:HB3 | 40:HE:138:PHE:CZ | 2.54 | 0.43 |
| 40:HI:182:VAL:O | 40:HI:186:ASN:ND2 | 2.52 | 0.43 |
| 41:HM:173:PRO:HB3 | 41:HM:380:ARG:NE | 2.33 | 0.43 |
| 41:HN:1:MET:SD | 41:HN:48:ASN:ND2 | 2.91 | 0.43 |
| 41:HO:31:ASP:OD2 | 41:HO:35:THR:OG1 | 2.37 | 0.43 |
| 41:HO:139:LEU:HD11 | 41:HO:189:VAL:HG23 | 2.01 | 0.43 |
| 40:IA:298:PRO:HG2 | 40:IA:308:ARG:HH11 | 1.84 | 0.43 |
| 40:II:177:VAL:HG22 | 40:II:207:GLU:OE2 | 2.18 | 0.43 |
| 41:IQ:137:HIS:NE2 | 41:IQ:166:THR:OG1 | 2.50 | 0.43 |
| 40:JH:304:LYS:O | 40:JH:389:ARG:NH2 | 2.50 | 0.43 |
| 41:JL:190:HIS:ND1 | 41:JL:411:ALA:HA | 2.33 | 0.43 |
| 40:KA:188:ILE:HG13 | 40:KA:394:PHE:CG | 2.54 | 0.43 |
| 40:KD:11:GLN:HG3 | 40:KD:74:VAL:HG21 | 2.00 | 0.43 |
| 40:KE:3:GLU:HA | 40:KE:51:THR:HA | 2.01 | 0.43 |
| 40:KG:20:CYS:HA | 40:KG:232:SER:HB2 | 2.00 | 0.43 |
| 41:KL:216:LYS:HA | 41:KL:216:LYS:HD3 | 1.67 | 0.43 |
| 41:KL:245:GLN:O | 41:KL:246:LEU:C | 2.56 | 0.43 |
| 41:KL:270:PHE:HB3 | 41:KL:273:LEU:HD21 | 1.99 | 0.43 |
| 41:KN:263:LEU:HD21 | 41:KN:421:PRO:HB2 | 2.01 | 0.43 |
| 41:KN:296:ALA:HB3 | 41:KN:306:ARG:HH12 | 1.83 | 0.43 |
| 41:LB:202:ILE:HG21 | 41:LB:229:VAL:HG22 | 2.00 | 0.43 |
| 40:LD:76:ASP:HA | 40:LD:79:ARG:HG2 | 2.00 | 0.43 |
| 40:LF:56:THR:O | 40:LF:57:GLY:C | 2.57 | 0.43 |
| 40:LG:11:GLN:O | 40:LG:12:ALA:C | 2.57 | 0.43 |
| 41:LM:118:ASP:O | 41:LM:122:LYS:HG2 | 2.19 | 0.43 |
| 41:LM:178:THR:HG22 | 41:LM:180:VAL:H | 1.84 | 0.43 |
| 40:MA:191:THR:C | 40:MA:193:THR:H | 2.22 | 0.43 |
| 40:ME:402:ALA:HB2 | 41:ML:344:TRP:HZ3 | 1.83 | 0.43 |
| 40:MF:79:ARG:HE | 40:MF:79:ARG:HB3 | 1.57 | 0.43 |
| 40:MF:132:LEU:HD12 | 40:MF:132:LEU:HA | 1.93 | 0.43 |
| 40:MH:400:LYS:O | 40:MH:401:ARG:C | 2.56 | 0.43 |
| 41:MO:1:MET:O | 41:MO:2:ARG:C | 2.56 | 0.43 |
| 41:MO:262:ARG:O | 41:MO:264:HIS:N | 2.52 | 0.43 |
| 40:ND:398:TYR:O | 40:ND:399:ALA:C | 2.56 | 0.43 |
| 40:NF:195:LEU:HD21 | 40:NF:264:ARG:HE | 1.82 | 0.43 |
| 40:NH:22:GLU:OE1 | 40:NH:83:TYR:OH | 2.35 | 0.43 |
| 41:NM:43:GLN:HA | 41:NM:242:PHE:HE1 | 1.84 | 0.43 |
| 41:NN:28:HIS:C | 41:NN:43:GLN:HE21 | 2.22 | 0.43 |
| 41:NP:330:MET:HB3 | 41:NP:349:VAL:HG21 | 2.00 | 0.43 |
| 41:OB:289:LEU:O | 41:OB:293:MET:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OG:155:GLU:OE2 | 40:OG:156:ARG:NH1 | 2.52 | 0.43 |
| 40:OH:3:GLU:CD | 40:OH:3:GLU:H | 2.21 | 0.43 |
| 40:OH:129:CYS:SG | 40:OH:130:THR:N | 2.88 | 0.43 |
| 40:OH:208:ALA:O | 40:OH:209:ILE:C | 2.57 | 0.43 |
| 40:OH:326:LYS:HD3 | 40:OH:326:LYS:HA | 1.53 | 0.43 |
| 40:OH:406:TRP:HE1 | 41:OO:258:VAL:HG23 | 1.83 | 0.43 |
| 41:OM:211:CYS:HA | 41:OM:215:LEU:HB2 | 1.99 | 0.43 |
| 41:ON:239:CYS:HB3 | 41:ON:248:ALA:H | 1.83 | 0.43 |
| 41:OP:207:LEU:HD13 | 41:OP:225:LEU:HB3 | 2.00 | 0.43 |
| 40:PA:83:TYR:HB3 | 40:PA:87:PHE:HE2 | 1.82 | 0.43 |
| 41:PB:7:LEU:H | 41:PB:7:LEU:HG | 1.66 | 0.43 |
| 41:PB:324:LYS:CE | 40:PG:222:PRO:HD2 | 2.48 | 0.43 |
| 40:PD:235:VAL:O | 40:PD:239:THR:HG22 | 2.18 | 0.43 |
| 40:PE:130:THR:OG1 | 40:PE:131:GLY:N | 2.51 | 0.43 |
| 40:PE:222:PRO:HD2 | 41:PL:324:LYS:HB3 | 2.00 | 0.43 |
| 40:PF:400:LYS:HD3 | 41:PM:425:ARG:NH2 | 2.34 | 0.43 |
| 40:PG:297:GLU:O | 40:PG:301:GLN:NE2 | 2.47 | 0.43 |
| 40:PH:68:VAL:HG11 | 40:PH:149:PHE:CE1 | 2.54 | 0.43 |
| 40:PH:395:ASP:OD1 | 40:PH:421:ARG:NE | 2.41 | 0.43 |
| 41:PM:313:VAL:O | 41:PM:349:VAL:HA | 2.18 | 0.43 |
| 41:PN:207:LEU:HB3 | 41:PN:225:LEU:HD22 | 2.00 | 0.43 |
| 41:PP:7:LEU:HD12 | 41:PP:135:LEU:HB2 | 1.99 | 0.43 |
| 40:QA:278:ALA:HB2 | 40:QA:368:ALA:HB2 | 2.00 | 0.43 |
| 41:QB:343:GLU:C | 41:QB:345:ILE:H | 2.22 | 0.43 |
| 40:QF:238:ILE:HD12 | 40:QF:377:LEU:HD11 | 2.00 | 0.43 |
| 40:QG:217:LEU:HA | 40:QG:277:SER:HB2 | 2.01 | 0.43 |
| 41:QP:207:LEU:O | 41:QP:208:TYR:C | 2.57 | 0.43 |
| 41:QP:209:ASP:O | 41:QP:213:ARG:HB2 | 2.19 | 0.43 |
| 41:QP:347:ASN:O | 41:QP:348:ASN:C | 2.57 | 0.43 |
| 40:RF:11:GLN:HG3 | 40:RF:74:VAL:HG21 | 2.01 | 0.43 |
| 40:RG:370:VAL:HG22 | 40:RG:372:ARG:H | 1.83 | 0.43 |
| 40:RI:297:GLU:HA | 40:RI:298:PRO:HD3 | 1.89 | 0.43 |
| 41:RL:178:THR:HG22 | 41:RL:179:VAL:H | 1.84 | 0.43 |
| 41:RM:316:VAL:HA | 41:RM:352:ALA:HB3 | 2.01 | 0.43 |
| 41:RO:33:THR:O | 41:RO:58:LYS:NZ | 2.46 | 0.43 |
| 41:RO:199:THR:HB | 41:RO:265:PHE:CD1 | 2.53 | 0.43 |
| 41:RP:33:THR:O | 41:RP:58:LYS:NZ | 2.50 | 0.43 |
| 41:RP:325:GLU:OE2 | 41:RP:325:GLU:N | 2.51 | 0.43 |
| 40:SA:204:VAL:HG13 | 40:SA:302:MET:HB3 | 1.99 | 0.43 |
| 41:SB:7:LEU:HD13 | 41:SB:151:LEU:HD21 | 2.01 | 0.43 |
| 41:SB:261:PRO:HG3 | 40:SG:405:HIS:CD2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SF:401:ARG:HD3 | 40:SF:401:ARG:HA | 1.77 | 0.43 |
| 40:SG:271:THR:H | 40:SG:376:MET:HB3 | 1.83 | 0.43 |
| 40:SH:326:LYS:HD3 | 41:SP:208:TYR:HB2 | 2.00 | 0.43 |
| 40:SH:397:MET:HE2 | 41:SO:345:ILE:HG23 | 2.01 | 0.43 |
| 41:SL:25:SER:OG | 41:SL:51:TYR:OH | 2.29 | 0.43 |
| 41:SL:382:SER:OG | 41:SL:412:GLU:OE2 | 2.33 | 0.43 |
| 41:SN:179:VAL:HG11 | 41:SN:394:PHE:CZ | 2.54 | 0.43 |
| 41:SO:183:TYR:CE1 | 41:SO:395:LEU:HD13 | 2.53 | 0.43 |
| 41:SO:333:VAL:O | 41:SO:334:GLN:C | 2.56 | 0.43 |
| 40:TA:112:LYS:HA | 40:TA:115:ILE:HG22 | 2.01 | 0.43 |
| 40:TA:311:LYS:NZ | 40:TA:342:GLN:OE1 | 2.45 | 0.43 |
| 41:TB:134:GLN:HG3 | 41:TB:165:ASN:HB2 | 1.99 | 0.43 |
| 40:TF:242:LEU:HD11 | 40:TF:252:LEU:HG | 2.00 | 0.43 |
| 40:TG:107:HIS:HD2 | 40:TG:152:LEU:HD12 | 1.84 | 0.43 |
| 40:TH:386:ALA:HA | 40:TH:389:ARG:HG2 | 2.01 | 0.43 |
| 40:TH:405:HIS:HA | 40:TH:408:VAL:HG12 | 2.00 | 0.43 |
| 40:TI:35:GLN:NE2 | 40:TI:59:GLY:O | 2.51 | 0.43 |
| 40:TI:304:LYS:HE2 | 40:TI:304:LYS:HB2 | 1.69 | 0.43 |
| 41:TM:20:PHE:HA | 41:TM:230:SER:HB2 | 2.01 | 0.43 |
| 41:TO:12:CYS:HB3 | 41:TO:138:SER:HB3 | 2.01 | 0.43 |
| 40:UA:121:ARG:HA | 40:UA:121:ARG:HD3 | 1.63 | 0.43 |
| 40:UE:16:ILE:HD11 | 40:UE:138:PHE:HB3 | 2.00 | 0.43 |
| 40:UE:39:ASP:N | 40:UE:39:ASP:OD1 | 2.52 | 0.43 |
| 40:UF:56:THR:HA | 40:VG:285:GLN:OE1 | 2.18 | 0.43 |
| 40:UF:285:GLN:O | 40:UF:286:LEU:C | 2.56 | 0.43 |
| 40:UI:13:GLY:O | 40:UI:14:VAL:C | 2.57 | 0.43 |
| 41:UM:150:LEU:O | 41:UM:154:LYS:HG2 | 2.18 | 0.43 |
| 41:UO:66:VAL:HG21 | 41:UO:116:VAL:HG13 | 2.00 | 0.43 |
| 41:UP:104:GLY:HA3 | 41:UP:146:GLY:CA | 2.38 | 0.43 |
| 40:VI:169:PHE:HE2 | 40:VI:235:VAL:HG13 | 1.83 | 0.43 |
| 40:VI:180:ALA:HB1 | 41:VP:256:ASN:HD21 | 1.84 | 0.43 |
| 41:VN:6:HIS:NE2 | 41:VN:8:GLN:OE1 | 2.36 | 0.43 |
| 40:WA:71:GLU:OE1 | 40:WA:71:GLU:N | 2.43 | 0.43 |
| 40:WA:226:ASN:HA | 40:WA:229:ARG:HB2 | 2.00 | 0.43 |
| 40:WE:24:TYR:HE1 | 40:WE:236:SER:HB2 | 1.83 | 0.43 |
| 40:WI:141:PHE:HB2 | 40:WI:173:PRO:HD3 | 1.99 | 0.43 |
| 41:WM:82:GLY:C | 41:WM:84:ILE:H | 2.22 | 0.43 |
| 41:WM:129:CYS:O | 41:WM:130:LEU:C | 2.56 | 0.43 |
| 41:WN:113:VAL:HG21 | 41:WN:150:LEU:HG | 2.00 | 0.43 |
| 41:WN:320:ARG:HD2 | 41:WN:320:ARG:HA | 1.35 | 0.43 |
| 41:WO:245:GLN:NE2 | 41:WO:323:MET:SD | 2.92 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1T:21:GLY:HA2 | 7:1T:330:CYS:CB | 2.48 | 0.43 |
| 7:1T:445:GLN:HB3 | 7:1T:452:LYS:HE2 | 2.01 | 0.43 |
| 9:2B:168:ASP:HA | 9:2B:171:ILE:HG22 | 2.00 | 0.43 |
| 9:2B:213:LEU:HD21 | 40:TG:371:GLN:HE22 | 1.82 | 0.43 |
| 10:2F:157:ARG:HG2 | 41:VB:53:GLU:HA | 1.99 | 0.43 |
| 12:2M:105:TYR:HD2 | 12:2M:141:LYS:HB3 | 1.83 | 0.43 |
| 12:2M:220:ASN:ND2 | 12:2M:223:ASP:OD2 | 2.52 | 0.43 |
| 12:2Q:76:TYR:OH | 40:WH:127:ASP:OD2 | 2.35 | 0.43 |
| 13:2T:173:SER:O | 13:2T:175:ASP:N | 2.45 | 0.43 |
| 13:2V:115:LYS:HB3 | 40:AH:264:ARG:HH21 | 1.84 | 0.43 |
| 13:2W:15:TYR:HA | 13:2W:163:ARG:O | 2.19 | 0.43 |
| 13:2X:1:MET:O | 13:2X:2:PHE:C | 2.57 | 0.43 |
| 17:3Q:345:LEU:HD22 | 17:3Q:345:LEU:HA | 1.81 | 0.43 |
| 17:3R:148:GLU:HA | 17:3R:151:ASN:ND2 | 2.34 | 0.43 |
| 17:3R:261:LYS:HA | 17:3R:261:LYS:HD3 | 1.40 | 0.43 |
| 17:3R:348:THR:OG1 | 17:3R:349:ASN:N | 2.52 | 0.43 |
| 21:4E:448:MET:HG2 | 21:4E:471:LYS:HG2 | 2.00 | 0.43 |
| 21:4F:471:LYS:HB3 | 21:4F:471:LYS:HE2 | 1.34 | 0.43 |
| 22:4H:79:LEU:HG | 22:4H:108:LEU:HD23 | 2.01 | 0.43 |
| 22:4I:656:LYS:HE2 | 22:4I:656:LYS:HB2 | 1.45 | 0.43 |
| 22:4J:615:ASP:O | 22:4J:616:THR:C | 2.57 | 0.43 |
| 22:4K:663:LYS:HD3 | 22:4K:663:LYS:HA | 1.35 | 0.43 |
| 23:4N:104:ILE:H | 23:4N:104:ILE:HG12 | 1.37 | 0.43 |
| 24:4O:201:SER:O | 24:4O:202:PHE:C | 2.56 | 0.43 |
| 23:4Q:22:TYR:HB3 | 23:4Q:37:TYR:CE2 | 2.54 | 0.43 |
| 23:4Q:256:GLN:HB3 | 23:4Q:264:LEU:HD22 | 2.01 | 0.43 |
| 23:4R:254:LYS:HB2 | 23:4R:254:LYS:HE2 | 1.49 | 0.43 |
| 26:4W:286:TYR:HB3 | 26:4W:296:TYR:HE1 | 1.84 | 0.43 |
| 26:4W:363:ASP:HB2 | 34:5Q:97:ARG:NH1 | 2.34 | 0.43 |
| 27:4Y:47:LYS:HE3 | 27:4Y:47:LYS:HB2 | 1.61 | 0.43 |
| 31:5J:768:VAL:O | 40:IE:372:ARG:NH2 | 2.52 | 0.43 |
| 32:5L:26:TRP:O | 32:5L:30:HIS:HB2 | 2.18 | 0.43 |
| 33:5N:463:LEU:HD22 | 33:5N:467:VAL:HG11 | 1.99 | 0.43 |
| 40:AA:121:ARG:HA | 40:AA:121:ARG:HD2 | 1.79 | 0.43 |
| 40:AF:138:PHE:HZ | 40:AF:235:VAL:HG11 | 1.83 | 0.43 |
| 40:AH:51:THR:HG21 | 40:AH:243:ARG:HG2 | 2.01 | 0.43 |
| 41:AO:272:PRO:HD3 | 41:AO:364:SER:HA | 1.99 | 0.43 |
| 41:AP:313:VAL:O | 41:AP:349:VAL:HA | 2.18 | 0.43 |
| 41:BB:20:PHE:HA | 41:BB:230:SER:OG | 2.19 | 0.43 |
| 40:BE:263:PRO:HG3 | 41:BM:396:HIS:CD2 | 2.53 | 0.43 |
| 40:BF:180:ALA:HB3 | 40:BF:183:GLU:HG3 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BG:287:SER:OG | 40:BG:290:GLU:OE2 | 2.28 | 0.43 |
| 40:BH:21:TRP:HZ2 | 40:BH:65:ALA:HB2 | 1.83 | 0.43 |
| 40:BI:222:PRO:HD2 | 41:BP:324:LYS:HE3 | 2.01 | 0.43 |
| 41:BM:359:ARG:H | 41:BM:359:ARG:HG2 | 1.42 | 0.43 |
| 41:BP:217:LEU:HD13 | 41:BP:217:LEU:HA | 1.71 | 0.43 |
| 40:CA:20:CYS:CA | 40:CA:232:SER:HB2 | 2.47 | 0.43 |
| 41:CB:131:GLN:HG2 | 41:CB:163:ILE:HG22 | 2.01 | 0.43 |
| 40:CE:265:ILE:HG23 | 40:CE:431:TYR:CZ | 2.54 | 0.43 |
| 40:CG:217:LEU:HA | 40:CG:277:SER:HB3 | 1.99 | 0.43 |
| 40:CG:262:TYR:CE1 | 41:CO:393:ALA:HA | 2.43 | 0.43 |
| 40:CG:288:VAL:HG13 | 40:CG:319:TYR:HE2 | 1.83 | 0.43 |
| 40:CI:360:PRO:HG3 | 40:CI:373:ALA:HB2 | 2.00 | 0.43 |
| 41:CM:201:CYS:O | 41:CM:268:PRO:HD3 | 2.19 | 0.43 |
| 41:CM:362:LYS:HA | 41:CM:362:LYS:HD3 | 1.74 | 0.43 |
| 41:CN:21:TRP:CZ3 | 41:CN:24:ILE:HD11 | 2.53 | 0.43 |
| 41:CP:152:ILE:HD13 | 41:CP:192:LEU:HD21 | 2.01 | 0.43 |
| 41:CP:420:ASN:HD22 | 41:CP:420:ASN:HA | 1.61 | 0.43 |
| 40:DA:19:ALA:O | 40:DA:22:GLU:HB3 | 2.19 | 0.43 |
| 40:DA:114:LEU:HB3 | 40:DA:149:PHE:CE1 | 2.53 | 0.43 |
| 41:DB:256:ASN:ND2 | 40:DG:101:ASN:HD21 | 2.17 | 0.43 |
| 41:DB:268:PRO:O | 41:DB:299:MET:HA | 2.18 | 0.43 |
| 40:DE:137:ILE:O | 40:DE:168:GLU:HA | 2.19 | 0.43 |
| 40:DF:311:LYS:HB3 | 40:DF:311:LYS:HE2 | 1.91 | 0.43 |
| 40:DH:121:ARG:HD2 | 40:DH:121:ARG:HA | 1.47 | 0.43 |
| 40:DH:331:ALA:O | 40:DH:332:ILE:C | 2.56 | 0.43 |
| 40:DI:207:GLU:HG3 | 40:DI:208:ALA:N | 2.33 | 0.43 |
| 41:DL:204:ASN:HA | 41:DL:207:LEU:HD12 | 1.99 | 0.43 |
| 41:DL:284:LEU:HD23 | 41:DL:284:LEU:HA | 1.74 | 0.43 |
| 41:DN:121:ARG:O | 41:DN:122:LYS:C | 2.56 | 0.43 |
| 41:DN:198:GLU:HB2 | 41:DN:266:PHE:CE2 | 2.54 | 0.43 |
| 41:DP:28:HIS:NE2 | 41:DP:241:ARG:HG2 | 2.32 | 0.43 |
| 41:DP:116:VAL:HG11 | 41:DP:151:LEU:HD21 | 2.01 | 0.43 |
| 41:DP:142:GLY:HA2 | 41:DP:145:SER:OG | 2.19 | 0.43 |
| 41:DP:155:ILE:HG21 | 41:DP:164:MET:SD | 2.58 | 0.43 |
| 40:EE:49:PHE:O | 40:EE:51:THR:N | 2.49 | 0.43 |
| 40:EH:28:HIS:ND1 | 40:EH:49:PHE:HA | 2.33 | 0.43 |
| 40:EI:288:VAL:O | 40:EI:291:ILE:HG12 | 2.18 | 0.43 |
| 41:EL:4:ILE:HD12 | 41:EL:134:GLN:HB2 | 2.00 | 0.43 |
| 41:FB:67:ASP:OD2 | 41:FB:72:THR:OG1 | 2.26 | 0.43 |
| 40:FF:188:ILE:HG22 | 40:FF:420:ALA:HB1 | 2.00 | 0.43 |
| 40:FG:88:HIS:HE1 | 40:GG:280:LYS:HG2 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FH:172:TYR:OH | 40:FH:386:ALA:O | 2.31 | 0.43 |
| 40:FI:376:MET:SD | 40:FI:378:SER:HB3 | 2.59 | 0.43 |
| 41:FN:309:ARG:H | 41:FN:372:THR:HG1 | 1.61 | 0.43 |
| 40:GA:105:ARG:HA | 40:GA:109:THR:HG22 | 2.01 | 0.43 |
| 41:GB:87:PRO:HA | 41:GB:90:PHE:HD2 | 1.84 | 0.43 |
| 40:GG:71:GLU:HB3 | 40:GG:98:ASP:HA | 2.01 | 0.43 |
| 40:GI:246:GLY:HA2 | 40:GI:357:TYR:CD2 | 2.53 | 0.43 |
| 41:GN:112:LEU:O | 41:GN:116:VAL:HG23 | 2.18 | 0.43 |
| 40:HE:49:PHE:O | 40:HE:50:ASN:C | 2.57 | 0.43 |
| 40:HG:286:LEU:HD12 | 40:HG:286:LEU:HA | 1.88 | 0.43 |
| 40:HI:79:ARG:HG2 | 40:HI:92:LEU:HD13 | 2.01 | 0.43 |
| 41:HM:134:GLN:HG2 | 41:HM:165:ASN:HB2 | 2.01 | 0.43 |
| 41:HQ:47:ILE:HG21 | 41:HQ:59:TYR:CD1 | 2.54 | 0.43 |
| 41:HQ:253:LEU:O | 41:HQ:257:MET:HB3 | 2.18 | 0.43 |
| 40:IG:111:GLY:O | 40:IG:115:ILE:HB | 2.18 | 0.43 |
| 40:IG:172:TYR:HD1 | 40:IG:203:MET:HE2 | 1.83 | 0.43 |
| 40:II:116:ASP:N | 40:II:116:ASP:OD1 | 2.50 | 0.43 |
| 41:IQ:424:THR:OG1 | 41:IQ:425:ARG:NH1 | 2.51 | 0.43 |
| 40:JA:102:ASN:HB3 | 40:JA:105:ARG:HB2 | 2.00 | 0.43 |
| 40:JD:212:ILE:HD11 | 40:JD:300:ASN:HA | 1.99 | 0.43 |
| 40:JD:270:ALA:HB3 | 40:JD:302:MET:HG3 | 2.01 | 0.43 |
| 40:JG:138:PHE:HZ | 40:JG:235:VAL:HG21 | 1.84 | 0.43 |
| 41:JM:151:LEU:O | 41:JM:152:ILE:C | 2.57 | 0.43 |
| 41:JM:393:ALA:O | 41:JM:394:PHE:C | 2.56 | 0.43 |
| 40:KD:205:ASP:HB3 | 40:KD:303:VAL:HA | 1.99 | 0.43 |
| 40:KD:254:GLU:HB3 | 40:KD:352:LYS:HE2 | 2.00 | 0.43 |
| 40:KH:209:ILE:HG23 | 40:KH:230:LEU:HD12 | 1.99 | 0.43 |
| 40:KH:405:HIS:HA | 40:KH:408:VAL:HG12 | 1.99 | 0.43 |
| 41:KM:165:ASN:HD22 | 41:KM:198:GLU:HB2 | 1.82 | 0.43 |
| 41:KO:385:PHE:HE2 | 41:KO:412:GLU:HB2 | 1.84 | 0.43 |
| 40:LD:36:MET:HG3 | 40:LD:61:HIS:NE2 | 2.32 | 0.43 |
| 40:LD:51:THR:HG23 | 40:LD:52:PHE:HD1 | 1.83 | 0.43 |
| 40:LF:305:CYS:O | 40:LF:305:CYS:SG | 2.77 | 0.43 |
| 40:LG:236:SER:O | 40:LG:240:ALA:N | 2.51 | 0.43 |
| 40:LH:167:LEU:HA | 40:LH:200:CYS:O | 2.18 | 0.43 |
| 40:LH:277:SER:O | 40:LH:279:GLU:N | 2.51 | 0.43 |
| 41:LL:73:MET:HB3 | 41:LL:90:PHE:CZ | 2.54 | 0.43 |
| 41:LN:249:ASP:OD1 | 41:LN:249:ASP:N | 2.43 | 0.43 |
| 41:LO:31:ASP:OD1 | 41:LO:35:THR:N | 2.44 | 0.43 |
| 41:LO:87:PRO:HA | 41:LO:90:PHE:HD2 | 1.84 | 0.43 |
| 41:LP:421:PRO:O | 41:LP:425:ARG:HG2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MG:315:CYS:HA | 40:MG:378:SER:HA | 2.01 | 0.43 |
| 40:MG:419:GLU:H | 40:MG:419:GLU:HG3 | 1.61 | 0.43 |
| 40:MH:100:ALA:O | 40:MH:101:ASN:C | 2.56 | 0.43 |
| 40:MH:136:LEU:CD2 | 40:MH:167:LEU:HB2 | 2.49 | 0.43 |
| 40:MH:223:THR:OG1 | 40:MH:224:TYR:N | 2.50 | 0.43 |
| 41:MO:69:GLU:O | 41:MO:71:GLY:N | 2.52 | 0.43 |
| 41:MO:223:GLY:HA2 | 41:MO:226:ASN:HD22 | 1.82 | 0.43 |
| 40:NA:322:ASP:O | 40:NA:372:ARG:NE | 2.52 | 0.43 |
| 40:NF:137:ILE:HG21 | 40:NF:154:MET:HE3 | 2.00 | 0.43 |
| 40:NH:398:TYR:OH | 40:NH:414:GLU:OE2 | 2.37 | 0.43 |
| 41:NN:133:PHE:HB2 | 41:NN:164:MET:SD | 2.58 | 0.43 |
| 41:NO:95:SER:OG | 41:NO:96:GLY:N | 2.51 | 0.43 |
| 41:NO:105:HIS:HD2 | 41:NO:106:TYR:CE1 | 2.37 | 0.43 |
| 41:NP:34:GLY:HA3 | 41:NP:58:LYS:HE3 | 2.00 | 0.43 |
| 41:NP:273:LEU:HB2 | 41:NP:292:GLN:HE22 | 1.84 | 0.43 |
| 40:OH:96:LYS:HD3 | 40:OH:96:LYS:HA | 1.43 | 0.43 |
| 40:OH:108:TYR:HB2 | 40:OH:412:MET:HE3 | 2.01 | 0.43 |
| 41:OM:273:LEU:HA | 41:OM:273:LEU:HD23 | 1.76 | 0.43 |
| 41:OO:21:TRP:HZ2 | 41:OO:63:ALA:HB2 | 1.83 | 0.43 |
| 40:PA:105:ARG:HG3 | 40:PA:410:GLU:HG2 | 2.01 | 0.43 |
| 40:PA:320:ARG:HE | 40:PA:373:ALA:HB3 | 1.83 | 0.43 |
| 41:PB:6:HIS:O | 41:PB:63:ALA:HA | 2.18 | 0.43 |
| 41:PB:260:PHE:HB2 | 41:PB:263:LEU:HG | 2.00 | 0.43 |
| 40:PD:175:PRO:HA | 40:PD:393:LYS:NZ | 2.33 | 0.43 |
| 40:PE:16:ILE:HG13 | 40:PE:228:ASN:HB3 | 1.99 | 0.43 |
| 40:PF:124:LYS:HA | 40:PF:127:ASP:HB2 | 2.01 | 0.43 |
| 40:PF:140:SER:HA | 40:PF:171:ILE:HB | 2.01 | 0.43 |
| 40:PG:3:GLU:OE2 | 40:PG:131:GLY:N | 2.51 | 0.43 |
| 41:PL:21:TRP:CZ3 | 41:PL:24:ILE:HD11 | 2.53 | 0.43 |
| 41:PO:6:HIS:CD2 | 41:PO:8:GLN:HE21 | 2.36 | 0.43 |
| 41:QB:5:VAL:HG23 | 41:QB:130:LEU:HD11 | 1.99 | 0.43 |
| 41:QB:101:TRP:O | 41:QB:103:LYS:HG2 | 2.19 | 0.43 |
| 41:QB:245:GLN:NE2 | 40:QG:224:TYR:HD2 | 2.15 | 0.43 |
| 40:QG:352:LYS:HZ2 | 41:QO:179:VAL:HA | 1.83 | 0.43 |
| 41:QL:271:ALA:HB3 | 41:QL:293:MET:SD | 2.59 | 0.43 |
| 41:QO:74:ASP:OD1 | 41:QO:77:ARG:NH1 | 2.35 | 0.43 |
| 41:QP:101:TRP:HE1 | 41:QP:149:THR:HG21 | 1.83 | 0.43 |
| 41:QP:230:SER:O | 41:QP:233:MET:HB2 | 2.19 | 0.43 |
| 41:QP:286:VAL:N | 41:QP:287:PRO:HD2 | 2.33 | 0.43 |
| 41:QP:362:LYS:HB2 | 41:QP:362:LYS:HE3 | 1.48 | 0.43 |
| 41:QP:420:ASN:O | 41:QP:421:PRO:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RA:391:ASP:OD1 | 40:RA:421:ARG:NH2 | 2.52 | 0.43 |
| 40:RE:188:ILE:HG23 | 40:RE:424:MET:HG3 | 2.01 | 0.43 |
| 40:RF:305:CYS:HB3 | 40:RF:386:ALA:HB2 | 1.99 | 0.43 |
| 40:RG:88:HIS:HA | 40:RG:89:PRO:HD3 | 1.83 | 0.43 |
| 40:RH:21:TRP:CZ2 | 40:RH:65:ALA:HB2 | 2.54 | 0.43 |
| 40:RI:126:ALA:HA | 40:RI:129:CYS:HB2 | 1.99 | 0.43 |
| 41:RN:193:VAL:HG21 | 41:RN:418:LEU:HG | 2.00 | 0.43 |
| 41:RO:309:ARG:NH1 | 41:RO:339:SER:O | 2.51 | 0.43 |
| 41:SB:309:ARG:NH1 | 41:SB:339:SER:O | 2.49 | 0.43 |
| 41:SB:323:MET:SD | 41:SB:323:MET:N | 2.85 | 0.43 |
| 40:SE:49:PHE:HE2 | 40:SE:55:GLU:HB2 | 1.83 | 0.43 |
| 40:SE:140:SER:HA | 40:SE:171:ILE:H | 1.83 | 0.43 |
| 40:SG:112:LYS:HA | 40:SG:115:ILE:HG22 | 2.01 | 0.43 |
| 41:SL:22:GLU:HG2 | 41:SL:81:PHE:CD2 | 2.53 | 0.43 |
| 41:SO:272:PRO:HD3 | 41:SO:364:SER:HA | 2.01 | 0.43 |
| 40:TF:101:ASN:HA | 40:TF:101:ASN:HD22 | 1.57 | 0.43 |
| 40:TG:326:LYS:NZ | 41:TO:220:PRO:HD2 | 2.33 | 0.43 |
| 40:TI:185:TYR:HE2 | 40:TI:403:PHE:HB2 | 1.84 | 0.43 |
| 40:TI:273:ALA:HB3 | 40:TI:374:VAL:H | 1.83 | 0.43 |
| 41:TM:325:GLU:HA | 41:TM:328:GLU:HG3 | 1.99 | 0.43 |
| 41:UB:100:ASN:HB3 | 41:UB:103:LYS:HB2 | 2.01 | 0.43 |
| 41:UB:330:MET:HB3 | 41:UB:349:VAL:HG11 | 2.00 | 0.43 |
| 40:UE:11:GLN:NE2 | 42:UE:501:GTP:O3G | 2.51 | 0.43 |
| 40:UF:232:SER:O | 40:UF:235:VAL:N | 2.52 | 0.43 |
| 40:UF:376:MET:SD | 40:UF:378:SER:HB2 | 2.58 | 0.43 |
| 40:UH:141:PHE:HB2 | 40:UH:173:PRO:HD3 | 2.01 | 0.43 |
| 40:UH:298:PRO:HB3 | 40:UH:307:PRO:HD2 | 2.00 | 0.43 |
| 40:UI:51:THR:HG21 | 40:UI:243:ARG:HG2 | 2.00 | 0.43 |
| 40:UI:96:LYS:HD2 | 41:UP:1:MET:N | 2.33 | 0.43 |
| 41:UM:344:TRP:CD1 | 41:UM:345:ILE:HG13 | 2.54 | 0.43 |
| 41:UN:284:LEU:HB3 | 41:UN:363:MET:HE1 | 2.00 | 0.43 |
| 41:UO:240:LEU:HD21 | 41:UO:249:ASP:HB3 | 2.00 | 0.43 |
| 41:UP:58:LYS:O | 41:UP:60:VAL:N | 2.51 | 0.43 |
| 41:UP:296:ALA:HB1 | 41:UP:305:PRO:HD2 | 2.00 | 0.43 |
| 41:VB:383:GLU:HA | 41:VB:386:THR:HG22 | 1.99 | 0.43 |
| 41:VN:171:PRO:HB3 | 41:VN:181:GLU:HG2 | 2.00 | 0.43 |
| 41:VQ:20:PHE:HA | 41:VQ:230:SER:HB2 | 2.01 | 0.43 |
| 40:WA:70:LEU:HB2 | 40:WA:145:THR:HG22 | 2.00 | 0.43 |
| 40:WF:5:ILE:HD13 | 40:WF:64:ARG:HB3 | 2.00 | 0.43 |
| 40:WF:102:ASN:HB3 | 40:WF:105:ARG:HG3 | 2.01 | 0.43 |
| 41:WM:68:LEU:HG | 41:WM:147:MET:HE2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WM:199:THR:HG23 | 41:WM:265:PHE:HA | 2.00 | 0.43 |
| 41:WQ:6:HIS:O | 41:WQ:63:ALA:HA | 2.19 | 0.43 |
| 7:1T:13:LYS:HE2 | 7:1T:584:VAL:H | 1.83 | 0.43 |
| 7:1U:19:VAL:HG12 | 7:1U:57:GLN:HG3 | 2.01 | 0.43 |
| 7:1U:340:PHE:CE1 | 7:1U:348:PHE:HB3 | 2.54 | 0.43 |
| 8:1W:445:GLU:HB3 | 8:1W:449:ARG:HH12 | 1.83 | 0.43 |
| 10:2E:55:SER:HA | 10:2E:58:ARG:HG2 | 1.99 | 0.43 |
| 11:2I:186:LYS:HG2 | 11:2I:251:TYR:HB3 | 2.00 | 0.43 |
| 11:2I:228:GLN:O | 11:2I:229:LYS:C | 2.57 | 0.43 |
| 11:2K:248:LYS:HA | 11:2K:248:LYS:HD2 | 1.91 | 0.43 |
| 13:2V:163:ARG:HG3 | 13:2V:164:ARG:N | 2.34 | 0.43 |
| 14:3C:46:ARG:HH21 | 40:MG:264:ARG:HH12 | 1.66 | 0.43 |
| 15:3E:384:TYR:HB2 | 17:3P:467:TYR:CZ | 2.53 | 0.43 |
| 16:3J:24:LEU:HD23 | 16:3K:373:LEU:HD23 | 2.01 | 0.43 |
| 17:3P:280:GLY:O | 17:3P:281:ILE:C | 2.56 | 0.43 |
| 17:3Q:384:LYS:HB3 | 17:3Q:384:LYS:HE3 | 1.47 | 0.43 |
| 18:3U:321:HIS:O | 18:3U:325:THR:OG1 | 2.27 | 0.43 |
| 18:3U:324:LYS:HB2 | 18:3U:324:LYS:HE3 | 1.82 | 0.43 |
| 20:4A:86:GLU:HA | 20:4A:89:ARG:HE | 1.84 | 0.43 |
| 20:4A:199:MET:N | 20:4A:199:MET:SD | 2.91 | 0.43 |
| 20:4A:200:ALA:HB2 | 41:ML:276:ARG:HH11 | 1.84 | 0.43 |
| 21:4F:510:ASP:HA | 21:4F:513:LEU:HD21 | 2.01 | 0.43 |
| 22:4I:263:LYS:HZ3 | 40:CG:46:ASP:N | 2.16 | 0.43 |
| 22:4J:87:ASP:OD1 | 22:4J:87:ASP:N | 2.52 | 0.43 |
| 22:4K:680:LYS:HB3 | 22:4K:681:PHE:CD1 | 2.54 | 0.43 |
| 23:4M:90:MET:O | 23:4M:91:ILE:HG23 | 2.18 | 0.43 |
| 23:4M:243:LEU:HD22 | 40:DG:79:ARG:HG2 | 2.00 | 0.43 |
| 23:4M:246:TYR:OH | 41:DB:45:GLU:HG3 | 2.19 | 0.43 |
| 23:4R:110:ASN:HD21 | 40:BI:279:GLU:CG | 2.32 | 0.43 |
| 26:4V:246:LYS:HG3 | 26:4V:353:ASN:O | 2.18 | 0.43 |
| 26:4W:328:PRO:HD2 | 26:4W:334:ALA:HB2 | 2.01 | 0.43 |
| 27:4Z:39:LEU:N | 32:5L:58:GLU:OE2 | 2.52 | 0.43 |
| 31:5I:728:LYS:HG3 | 31:5I:729:THR:HG23 | 2.00 | 0.43 |
| 31:5J:805:GLY:HA2 | 31:5J:810:PHE:HE1 | 1.83 | 0.43 |
| 34:5R:380:ARG:HD2 | 34:5R:380:ARG:HA | 1.66 | 0.43 |
| 39:6F:117:ALA:HB1 | 39:6F:121:HIS:CD2 | 2.54 | 0.43 |
| 39:6G:129:CYS:SG | 39:6G:133:ARG:NH2 | 2.80 | 0.43 |
| 40:AA:169:PHE:CD2 | 40:AA:235:VAL:HG22 | 2.52 | 0.43 |
| 41:AB:334:GLN:HE21 | 41:AB:349:VAL:HG23 | 1.84 | 0.43 |
| 40:AF:332:ILE:HD12 | 40:AF:351:PHE:HB3 | 2.01 | 0.43 |
| 40:AH:169:PHE:CE2 | 40:AH:235:VAL:HG22 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AL:113:VAL:HA | 41:AL:116:VAL:HG12 | 2.01 | 0.43 |
| 41:AL:237:THR:HB | 41:AL:240:LEU:HD11 | 1.99 | 0.43 |
| 41:AO:271:ALA:HB3 | 41:AO:272:PRO:CD | 2.48 | 0.43 |
| 41:AP:103:LYS:HG3 | 41:AP:401:GLU:HG3 | 2.01 | 0.43 |
| 41:BM:287:PRO:HA | 41:BM:329:GLN:HG3 | 2.01 | 0.43 |
| 41:BO:324:LYS:HB2 | 41:BO:324:LYS:HE2 | 1.45 | 0.43 |
| 41:BP:19:LYS:HD3 | 41:BP:19:LYS:HA | 1.83 | 0.43 |
| 41:BP:24:ILE:HD13 | 41:BP:24:ILE:HA | 1.75 | 0.43 |
| 41:CB:16:ILE:HA | 41:CB:226:ASN:HB3 | 2.01 | 0.43 |
| 40:CE:143:GLY:N | 42:CE:501:GTP:O2A | 2.40 | 0.43 |
| 40:CF:175:PRO:HB3 | 40:CF:389:ARG:CZ | 2.49 | 0.43 |
| 40:CH:288:VAL:HG21 | 40:CH:327:ASP:CG | 2.39 | 0.43 |
| 41:CL:147:MET:O | 41:CL:151:LEU:HG | 2.18 | 0.43 |
| 41:CM:208:TYR:O | 41:CM:209:ASP:C | 2.57 | 0.43 |
| 41:CM:394:PHE:HB3 | 41:CM:397:TRP:CZ3 | 2.47 | 0.43 |
| 41:CN:139:LEU:O | 41:CN:140:GLY:C | 2.56 | 0.43 |
| 41:CO:8:GLN:HE21 | 41:CO:14:ASN:HA | 1.84 | 0.43 |
| 41:CO:48:ASN:O | 41:CO:49:VAL:C | 2.57 | 0.43 |
| 41:CP:123:GLU:O | 41:CP:124:ALA:C | 2.56 | 0.43 |
| 41:DB:9:ALA:HB1 | 41:DB:66:VAL:HG22 | 2.00 | 0.43 |
| 41:DB:390:ARG:HA | 41:DB:390:ARG:HD3 | 1.78 | 0.43 |
| 40:DF:294:ALA:O | 40:DF:295:CYS:C | 2.57 | 0.43 |
| 40:DF:326:LYS:NZ | 41:DN:208:TYR:O | 2.40 | 0.43 |
| 40:DH:3:GLU:HB3 | 40:DH:64:ARG:HH12 | 1.83 | 0.43 |
| 40:DH:6:SER:HB2 | 40:DH:52:PHE:CZ | 2.54 | 0.43 |
| 40:DH:8:HIS:CD2 | 40:DH:8:HIS:H | 2.35 | 0.43 |
| 40:DH:82:THR:O | 40:DH:84:ARG:N | 2.51 | 0.43 |
| 40:DI:212:ILE:HD11 | 40:DI:300:ASN:HA | 2.00 | 0.43 |
| 40:DI:303:VAL:O | 40:DI:305:CYS:N | 2.51 | 0.43 |
| 41:DL:73:MET:HB3 | 41:DL:90:PHE:CZ | 2.53 | 0.43 |
| 41:DL:210:ILE:O | 41:DL:214:THR:N | 2.50 | 0.43 |
| 41:DM:405:GLU:O | 41:DM:409:THR:HG23 | 2.19 | 0.43 |
| 41:DN:12:CYS:HA | 41:DN:15:GLN:HE21 | 1.84 | 0.43 |
| 41:DN:250:LEU:H | 41:DN:250:LEU:HG | 1.61 | 0.43 |
| 41:DO:171:PRO:HG3 | 41:DO:181:GLU:HG2 | 2.01 | 0.43 |
| 41:DO:398:TYR:HD2 | 41:DO:408:PHE:HZ | 1.67 | 0.43 |
| 41:DP:74:ASP:HA | 41:DP:77:ARG:NH1 | 2.31 | 0.43 |
| 41:DP:99:ASN:O | 41:DP:180:VAL:HG21 | 2.19 | 0.43 |
| 41:DP:393:ALA:O | 41:DP:395:LEU:N | 2.51 | 0.43 |
| 40:EA:137:ILE:HG21 | 40:EA:154:MET:HE3 | 2.00 | 0.43 |
| 40:EA:366:ASP:OD1 | 40:EA:367:LEU:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EI:20:CYS:HA | 40:EI:232:SER:OG | 2.19 | 0.43 |
| 41:EM:135:LEU:HB3 | 41:EM:166:THR:HG22 | 2.01 | 0.43 |
| 41:EM:420:ASN:HB2 | 41:EM:421:PRO:HD3 | 2.01 | 0.43 |
| 41:EN:398:TYR:HB3 | 41:EN:408:PHE:HZ | 1.83 | 0.43 |
| 41:EO:170:VAL:HG11 | 41:EO:377:LEU:HD21 | 1.99 | 0.43 |
| 41:EP:226:ASN:CG | 43:EP:501:GDP:HN1 | 2.22 | 0.43 |
| 41:EP:401:GLU:OE1 | 41:EP:401:GLU:N | 2.51 | 0.43 |
| 41:FB:257:MET:HE3 | 41:FB:314:ALA:HB2 | 2.01 | 0.43 |
| 40:FG:71:GLU:HB3 | 40:FG:98:ASP:HA | 1.99 | 0.43 |
| 40:FG:238:ILE:HA | 40:FG:318:LEU:HD22 | 2.01 | 0.43 |
| 40:FH:125:LEU:HD23 | 40:FH:125:LEU:HA | 1.87 | 0.43 |
| 41:FP:27:GLU:OE1 | 41:FP:318:ARG:NH1 | 2.51 | 0.43 |
| 40:GA:139:HIS:CD2 | 40:GA:150:THR:HG21 | 2.54 | 0.43 |
| 40:GE:348:PRO:HB2 | 41:GM:384:GLN:NE2 | 2.34 | 0.43 |
| 40:GF:239:THR:HG22 | 40:GF:252:LEU:HD21 | 2.01 | 0.43 |
| 40:GG:273:ALA:HA | 40:GG:275:VAL:HG22 | 2.00 | 0.43 |
| 40:GI:96:LYS:HD3 | 40:GI:96:LYS:HA | 1.81 | 0.43 |
| 40:GI:136:LEU:HB3 | 40:GI:169:PHE:HE1 | 1.83 | 0.43 |
| 40:GI:177:VAL:O | 41:GP:347:ASN:ND2 | 2.52 | 0.43 |
| 41:GO:85:PHE:HB2 | 41:GO:90:PHE:HE1 | 1.83 | 0.43 |
| 40:HA:171:ILE:HG21 | 42:HA:501:GTP:H1' | 2.00 | 0.43 |
| 41:HB:113:VAL:HG22 | 41:HB:117:LEU:HD23 | 2.01 | 0.43 |
| 40:HH:134:GLY:HA3 | 40:HH:165:SER:O | 2.19 | 0.43 |
| 40:HH:191:THR:O | 40:HH:195:LEU:HB2 | 2.17 | 0.43 |
| 41:HN:87:PRO:HD3 | 41:IN:281:TYR:HD2 | 1.74 | 0.43 |
| 41:HQ:189:VAL:O | 41:HQ:193:VAL:HG23 | 2.18 | 0.43 |
| 41:IB:121:ARG:NH1 | 41:IB:158:GLU:OE1 | 2.52 | 0.43 |
| 40:IE:239:THR:O | 40:IE:243:ARG:NE | 2.52 | 0.43 |
| 41:IM:58:LYS:HD3 | 41:IM:58:LYS:HA | 1.89 | 0.43 |
| 40:JG:262:TYR:OH | 41:JO:391:ARG:O | 2.35 | 0.43 |
| 40:JH:167:LEU:HD22 | 40:JH:200:CYS:HB3 | 2.01 | 0.43 |
| 41:JM:29:GLY:O | 41:JM:30:ILE:C | 2.56 | 0.43 |
| 41:JM:102:ALA:O | 41:JM:103:LYS:C | 2.56 | 0.43 |
| 41:JM:344:TRP:CE3 | 41:JM:345:ILE:HG23 | 2.53 | 0.43 |
| 40:KE:88:HIS:CE1 | 40:KE:90:GLU:HG3 | 2.54 | 0.43 |
| 40:KE:263:PRO:HG3 | 41:KM:396:HIS:CG | 2.53 | 0.43 |
| 40:KF:7:VAL:HG13 | 40:KF:66:VAL:HG13 | 2.01 | 0.43 |
| 40:KG:88:HIS:HB3 | 40:KG:91:GLN:HG3 | 2.01 | 0.43 |
| 40:KH:70:LEU:HD23 | 40:KH:114:LEU:HD12 | 1.99 | 0.43 |
| 40:KH:73:THR:HA | 41:KO:46:ARG:HH21 | 1.83 | 0.43 |
| 41:KL:268:PRO:HA | 41:KL:367:PHE:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KL:284:LEU:HA | 41:KL:284:LEU:HD12 | 1.74 | 0.43 |
| 41:KM:313:VAL:HG12 | 41:KM:349:VAL:HG23 | 2.00 | 0.43 |
| 41:KO:170:VAL:HG11 | 41:KO:377:LEU:HD21 | 2.01 | 0.43 |
| 40:LD:22:GLU:OE2 | 40:LD:229:ARG:NH1 | 2.51 | 0.43 |
| 40:LD:205:ASP:HB3 | 40:LD:303:VAL:HA | 2.00 | 0.43 |
| 40:MA:228:ASN:HD22 | 42:MN:501:GTP:HN21 | 1.67 | 0.43 |
| 40:MA:288:VAL:HG13 | 40:MA:319:TYR:CE2 | 2.54 | 0.43 |
| 40:MA:304:LYS:HB3 | 40:MA:304:LYS:HE3 | 1.64 | 0.43 |
| 40:MD:136:LEU:HB3 | 40:MD:138:PHE:CE2 | 2.54 | 0.43 |
| 40:MF:144:GLY:O | 40:MF:148:GLY:N | 2.47 | 0.43 |
| 40:MG:88:HIS:ND1 | 40:MG:89:PRO:HD2 | 2.33 | 0.43 |
| 40:MG:363:VAL:O | 40:MG:365:GLY:N | 2.52 | 0.43 |
| 40:MH:315:CYS:HA | 40:MH:378:SER:HA | 2.00 | 0.43 |
| 40:MH:326:LYS:HG3 | 40:MH:327:ASP:H | 1.82 | 0.43 |
| 40:MH:341:ILE:H | 40:MH:341:ILE:HG12 | 1.43 | 0.43 |
| 41:MN:271:ALA:HA | 41:MN:273:LEU:HD13 | 2.01 | 0.43 |
| 41:MP:256:ASN:HD22 | 41:MP:350:LYS:HG3 | 1.83 | 0.43 |
| 41:MP:391:ARG:HA | 41:MP:391:ARG:HD3 | 1.74 | 0.43 |
| 41:NB:145:SER:HB2 | 41:NB:188:SER:HB2 | 2.00 | 0.43 |
| 40:ND:51:THR:OG1 | 40:ND:243:ARG:HG3 | 2.19 | 0.43 |
| 40:NE:71:GLU:HB3 | 40:NE:98:ASP:HA | 2.00 | 0.43 |
| 40:NF:104:ALA:O | 40:NF:108:TYR:HB2 | 2.18 | 0.43 |
| 41:NL:198:GLU:HB2 | 41:NL:266:PHE:HE2 | 1.83 | 0.43 |
| 41:NL:282:ARG:NH2 | 41:NL:292:GLN:OE1 | 2.51 | 0.43 |
| 41:NL:392:LYS:HD2 | 41:NL:395:LEU:HD23 | 2.00 | 0.43 |
| 41:NP:242:PHE:HB3 | 41:NP:356:ILE:HD12 | 2.00 | 0.43 |
| 41:OB:261:PRO:HG3 | 40:OG:405:HIS:CG | 2.54 | 0.43 |
| 40:OE:257:THR:HG21 | 41:OM:98:GLY:O | 2.19 | 0.43 |
| 40:OF:73:THR:OG1 | 41:OM:46:ARG:NH1 | 2.43 | 0.43 |
| 40:OF:230:LEU:HD12 | 40:OF:230:LEU:HA | 1.87 | 0.43 |
| 40:OH:3:GLU:HG2 | 40:OH:132:LEU:HA | 2.00 | 0.43 |
| 40:OH:294:ALA:O | 40:OH:297:GLU:HB2 | 2.19 | 0.43 |
| 41:OL:7:LEU:O | 41:OL:135:LEU:HA | 2.19 | 0.43 |
| 41:PB:188:SER:HA | 41:PB:191:GLN:NE2 | 2.33 | 0.43 |
| 41:PB:273:LEU:N | 41:PB:292:GLN:OE1 | 2.43 | 0.43 |
| 40:PE:326:LYS:HE3 | 41:PM:220:PRO:HG2 | 2.00 | 0.43 |
| 40:PG:324:VAL:HG12 | 40:PG:326:LYS:H | 1.84 | 0.43 |
| 41:PM:11:GLN:HA | 41:PM:72:THR:HG21 | 2.00 | 0.43 |
| 41:PP:74:ASP:HA | 41:PP:77:ARG:HG2 | 2.01 | 0.43 |
| 40:QA:11:GLN:HE22 | 41:QN:247:ASN:H | 1.66 | 0.43 |
| 41:QB:1:MET:H2 | 41:QB:2:ARG:NH1 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QE:276:ILE:HG23 | 40:QE:280:LYS:HG3 | 2.01 | 0.43 |
| 41:QP:149:THR:HA | 41:QP:152:ILE:HD12 | 1.99 | 0.43 |
| 41:QP:271:ALA:O | 41:QP:273:LEU:N | 2.48 | 0.43 |
| 41:RB:205:GLU:HA | 41:RB:208:TYR:HB2 | 2.01 | 0.43 |
| 40:RF:217:LEU:HA | 40:RF:277:SER:HB2 | 2.01 | 0.43 |
| 40:RF:228:ASN:ND2 | 42:RF:501:GTP:HN1 | 2.05 | 0.43 |
| 40:RF:236:SER:O | 40:RF:240:ALA:HB2 | 2.19 | 0.43 |
| 40:RG:169:PHE:HE2 | 40:RG:235:VAL:HG13 | 1.84 | 0.43 |
| 40:RG:320:ARG:HH12 | 40:RG:360:PRO:HA | 1.83 | 0.43 |
| 40:RG:325:PRO:HG3 | 40:RG:355:ILE:HD13 | 2.01 | 0.43 |
| 40:RH:172:TYR:OH | 40:RH:386:ALA:O | 2.35 | 0.43 |
| 40:RI:65:ALA:O | 40:RI:91:GLN:NE2 | 2.52 | 0.43 |
| 40:RI:116:ASP:N | 40:RI:116:ASP:OD1 | 2.52 | 0.43 |
| 40:RI:172:TYR:N | 40:RI:204:VAL:O | 2.42 | 0.43 |
| 40:SA:342:GLN:NE2 | 40:SA:343:PHE:O | 2.52 | 0.43 |
| 40:SE:284:GLU:HB3 | 40:SE:285:GLN:H | 1.65 | 0.43 |
| 40:SG:326:LYS:NZ | 41:SO:208:TYR:CB | 2.82 | 0.43 |
| 40:SI:251:ASP:OD1 | 40:SI:252:LEU:N | 2.49 | 0.43 |
| 41:SM:311:LEU:H | 41:SM:371:SER:HA | 1.84 | 0.43 |
| 41:SN:334:GLN:HE22 | 41:SN:347:ASN:HA | 1.84 | 0.43 |
| 41:SO:162:ARG:HD3 | 41:SO:162:ARG:HA | 1.74 | 0.43 |
| 41:TB:109:GLY:O | 41:TB:113:VAL:HG13 | 2.19 | 0.43 |
| 40:TE:177:VAL:HG12 | 41:TL:331:LEU:HB2 | 2.01 | 0.43 |
| 40:TI:217:LEU:HD11 | 40:TI:366:ASP:HB3 | 1.99 | 0.43 |
| 41:TL:273:LEU:O | 41:TL:292:GLN:NE2 | 2.52 | 0.43 |
| 40:UA:21:TRP:CZ2 | 40:UA:65:ALA:HB2 | 2.54 | 0.43 |
| 41:UB:348:ASN:HA | 40:UG:181:VAL:HG12 | 2.00 | 0.43 |
| 40:UF:99:ALA:O | 40:UF:100:ALA:C | 2.56 | 0.43 |
| 40:UF:308:ARG:O | 40:UF:310:GLY:N | 2.51 | 0.43 |
| 41:UM:62:ARG:NH1 | 41:UM:127:CYS:SG | 2.92 | 0.43 |
| 41:UN:404:ASP:OD1 | 41:UN:405:GLU:N | 2.48 | 0.43 |
| 40:VA:64:ARG:NH2 | 40:VA:129:CYS:SG | 2.92 | 0.43 |
| 40:VF:3:GLU:HA | 40:VF:51:THR:HG23 | 2.00 | 0.43 |
| 40:VH:298:PRO:HB3 | 40:VH:307:PRO:HD2 | 2.00 | 0.43 |
| 40:VJ:205:ASP:HB2 | 40:VJ:303:VAL:HG23 | 2.00 | 0.43 |
| 41:WB:31:ASP:OD2 | 41:WB:35:THR:N | 2.52 | 0.43 |
| 40:WF:169:PHE:HE1 | 40:WF:202:PHE:HD1 | 1.65 | 0.43 |
| 40:WF:215:ARG:NH2 | 40:WF:299:ALA:O | 2.51 | 0.43 |
| 40:WG:242:LEU:H | 40:WG:242:LEU:HD23 | 1.84 | 0.43 |
| 40:WI:205:ASP:O | 40:WI:209:ILE:HG13 | 2.19 | 0.43 |
| 41:WM:358:PRO:O | 41:WM:359:ARG:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WN:420:ASN:H | 41:WN:421:PRO:HD2 | 1.83 | 0.43 |
| 41:WO:19:LYS:HG2 | 41:WO:226:ASN:HB2 | 2.01 | 0.43 |
| 8:1Y:107:PHE:CB | 11:2J:252:ILE:HG21 | 2.49 | 0.43 |
| 12:2M:113:PHE:HA | 12:2M:131:ILE:HD11 | 2.00 | 0.43 |
| 12:2O:146:ILE:O | 12:2O:147:PRO:C | 2.57 | 0.43 |
| 13:2T:24:ILE:HG12 | 13:2T:25:TRP:CD1 | 2.53 | 0.43 |
| 13:2T:67:LYS:HB3 | 13:2T:67:LYS:HE3 | 1.65 | 0.43 |
| 13:2V:178:PRO:O | 13:2V:179:ALA:C | 2.57 | 0.43 |
| 16:3L:126:ILE:HD12 | 16:3M:12:PHE:CG | 2.54 | 0.43 |
| 16:3L:131:ASP:HB3 | 16:3L:133:VAL:HG12 | 2.01 | 0.43 |
| 16:3L:171:GLN:HB3 | 16:3L:228:ARG:NH2 | 2.33 | 0.43 |
| 16:3L:261:THR:OG1 | 16:3L:394:ARG:NH1 | 2.52 | 0.43 |
| 17:3R:324:ASP:O | 17:3R:325:ILE:C | 2.57 | 0.43 |
| 18:3T:252:SER:OG | 18:3W:366:VAL:O | 2.37 | 0.43 |
| 20:4B:293:ARG:HD2 | 40:MH:282:TYR:CE2 | 2.54 | 0.43 |
| 22:4J:293:TYR:HB3 | 22:4J:297:GLN:HB2 | 2.01 | 0.43 |
| 22:4K:642:CYS:HB3 | 22:4K:690:TYR:CZ | 2.54 | 0.43 |
| 23:4M:187:PHE:HB3 | 23:4M:202:PHE:HE2 | 1.83 | 0.43 |
| 23:4Q:250:VAL:HG21 | 23:4Q:265:THR:CG2 | 2.49 | 0.43 |
| 23:4R:86:LEU:HD22 | 23:4R:86:LEU:HA | 1.86 | 0.43 |
| 30:5G:101:THR:HA | 41:HB:295:ASP:HA | 2.01 | 0.43 |
| 33:5O:134:ASN:ND2 | 40:GE:58:ALA:HB1 | 2.34 | 0.43 |
| 36:5X:237:MET:HG3 | 40:LF:395:ASP:HB3 | 1.99 | 0.43 |
| 36:5Y:101:TRP:HZ2 | 41:OO:282:ARG:HG2 | 1.82 | 0.43 |
| 38:6C:45:GLN:NE2 | 41:VO:296:ALA:H | 2.17 | 0.43 |
| 38:6C:204:ASP:O | 38:6C:206:ASN:N | 2.52 | 0.43 |
| 39:6H:48:ILE:HD12 | 39:6H:108:HIS:HA | 2.01 | 0.43 |
| 39:6J:4:ASN:OD1 | 39:6J:5:GLU:N | 2.52 | 0.43 |
| 39:6L:116:ARG:HD3 | 39:6L:116:ARG:HA | 1.77 | 0.43 |
| 41:AO:232:THR:HG21 | 41:AO:268:PRO:CB | 2.49 | 0.43 |
| 41:BB:282:ARG:NH2 | 41:BB:292:GLN:OE1 | 2.51 | 0.43 |
| 40:BE:400:LYS:O | 40:BE:402:ALA:N | 2.52 | 0.43 |
| 40:BH:69:ASP:HB2 | 40:BH:75:ILE:CD1 | 2.49 | 0.43 |
| 40:BH:326:LYS:O | 40:BH:327:ASP:C | 2.57 | 0.43 |
| 40:BI:82:THR:C | 40:BI:84:ARG:H | 2.21 | 0.43 |
| 41:BM:237:THR:O | 41:BM:241:ARG:NE | 2.52 | 0.43 |
| 41:BP:44:LEU:HD22 | 41:BP:59:TYR:CZ | 2.53 | 0.43 |
| 41:BP:378:PHE:HB3 | 41:BP:415:MET:HE2 | 2.01 | 0.43 |
| 40:CA:88:HIS:O | 40:CA:89:PRO:C | 2.57 | 0.43 |
| 40:CA:164:LYS:H | 40:CA:164:LYS:HG2 | 1.37 | 0.43 |
| 40:CA:296:PHE:HB2 | 40:CA:335:ILE:HD11 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CA:432:GLU:H | 40:CA:432:GLU:HG3 | 1.68 | 0.43 |
| 40:CF:1:GLN:HG3 | 40:CF:2:ARG:HG3 | 2.00 | 0.43 |
| 40:CG:318:LEU:O | 40:CG:374:VAL:HA | 2.19 | 0.43 |
| 40:CH:68:VAL:HG11 | 40:CH:118:VAL:HG21 | 2.01 | 0.43 |
| 40:CH:360:PRO:HG3 | 40:CH:373:ALA:HB2 | 2.01 | 0.43 |
| 40:CH:393:LYS:O | 40:CH:394:PHE:C | 2.57 | 0.43 |
| 41:CL:210:ILE:HD11 | 41:CL:300:MET:HA | 2.01 | 0.43 |
| 41:CN:125:GLU:H | 41:CN:125:GLU:HG2 | 1.58 | 0.43 |
| 41:CN:146:GLY:O | 41:CN:147:MET:C | 2.56 | 0.43 |
| 41:CP:96:GLY:O | 41:CP:98:GLY:N | 2.52 | 0.43 |
| 41:CP:356:ILE:H | 41:CP:356:ILE:HG12 | 1.39 | 0.43 |
| 41:CP:364:SER:OG | 41:CP:365:ALA:N | 2.52 | 0.43 |
| 40:DA:9:VAL:O | 40:DA:139:HIS:HA | 2.19 | 0.43 |
| 40:DA:100:ALA:HA | 41:DN:252:LYS:NZ | 2.31 | 0.43 |
| 40:DA:141:PHE:O | 40:DA:142:GLY:C | 2.56 | 0.43 |
| 41:DB:77:ARG:HG3 | 41:DB:83:GLN:HE22 | 1.84 | 0.43 |
| 41:DB:337:ASN:O | 41:DB:339:SER:N | 2.50 | 0.43 |
| 40:DE:71:GLU:HB2 | 40:DE:74:VAL:HG23 | 2.01 | 0.43 |
| 40:DF:93:ILE:HG21 | 40:DF:118:VAL:HG22 | 2.01 | 0.43 |
| 40:DH:145:THR:O | 40:DH:150:THR:HG23 | 2.18 | 0.43 |
| 41:DM:28:HIS:CE1 | 41:DM:47:ILE:HA | 2.53 | 0.43 |
| 41:DM:251:ARG:O | 41:DM:255:VAL:HG13 | 2.18 | 0.43 |
| 41:DN:75:SER:OG | 41:DN:76:VAL:N | 2.52 | 0.43 |
| 41:DN:209:ASP:O | 41:DN:213:ARG:HB2 | 2.18 | 0.43 |
| 41:DP:313:VAL:HB | 41:DP:367:PHE:HE2 | 1.84 | 0.43 |
| 40:EA:182:VAL:HG22 | 41:EN:256:ASN:HD21 | 1.84 | 0.43 |
| 41:EB:36:TYR:OH | 41:EB:40:SER:O | 2.33 | 0.43 |
| 41:EB:309:ARG:H | 41:EB:372:THR:HG22 | 1.83 | 0.43 |
| 40:EH:85:GLN:O | 40:EH:86:LEU:C | 2.57 | 0.43 |
| 40:EH:170:SER:C | 40:EH:171:ILE:HG12 | 2.39 | 0.43 |
| 40:EI:164:LYS:HD3 | 40:EI:164:LYS:HA | 1.55 | 0.43 |
| 41:EL:311:LEU:N | 41:EL:370:ASN:O | 2.43 | 0.43 |
| 41:EN:267:MET:HE1 | 41:EN:305:PRO:HG3 | 2.00 | 0.43 |
| 41:EO:117:LEU:HA | 41:EO:120:VAL:HG22 | 2.01 | 0.43 |
| 41:EO:189:VAL:O | 41:EO:193:VAL:HG23 | 2.18 | 0.43 |
| 40:FF:151:SER:HB3 | 40:FF:193:THR:HG21 | 2.00 | 0.43 |
| 40:FH:169:PHE:HZ | 40:FH:238:ILE:HG21 | 1.84 | 0.43 |
| 41:FM:334:GLN:HE22 | 41:FM:348:ASN:N | 2.17 | 0.43 |
| 40:GA:16:ILE:CA | 40:GA:228:ASN:ND2 | 2.81 | 0.43 |
| 41:GB:230:SER:HA | 41:GB:233:MET:HB3 | 2.01 | 0.43 |
| 40:GE:8:HIS:HB3 | 40:GE:13:GLY:C | 2.39 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:GE:360:PRO:O | 40:GE:361:THR:C | 2.57 | 0.43 |
| 40:GI:166:LYS:HE2 | 40:GI:166:LYS:HB2 | 1.58 | 0.43 |
| 40:GI:278:ALA:O | 40:GI:281:ALA:N | 2.36 | 0.43 |
| 41:GM:65:LEU:HD12 | 41:GM:90:PHE:HE2 | 1.82 | 0.43 |
| 41:GN:69:GLU:O | 41:GN:71:GLY:N | 2.52 | 0.43 |
| 41:GN:323:MET:HE3 | 41:GN:323:MET:HB2 | 1.65 | 0.43 |
| 40:HE:20:CYS:HA | 40:HE:232:SER:HB2 | 2.01 | 0.43 |
| 40:HE:23:LEU:O | 40:HE:24:TYR:C | 2.57 | 0.43 |
| 40:HE:169:PHE:HZ | 40:HE:238:ILE:HG13 | 1.83 | 0.43 |
| 40:HF:278:ALA:H | 40:HF:368:ALA:HB2 | 1.84 | 0.43 |
| 40:HH:265:ILE:HG22 | 40:HH:379:ASN:HD21 | 1.83 | 0.43 |
| 41:HN:189:VAL:O | 41:HN:193:VAL:HG13 | 2.18 | 0.43 |
| 41:HN:380:ARG:HE | 41:HN:380:ARG:HB2 | 1.58 | 0.43 |
| 41:HO:202:ILE:HD13 | 41:HO:229:VAL:HG13 | 2.00 | 0.43 |
| 41:HP:203:ASP:N | 41:HP:300:MET:O | 2.43 | 0.43 |
| 40:IE:269:LEU:HD21 | 40:IE:302:MET:H | 1.84 | 0.43 |
| 40:IH:276:ILE:HG23 | 40:IH:280:LYS:HB2 | 2.00 | 0.43 |
| 40:JA:143:GLY:N | 42:JA:501:GTP:O2A | 2.37 | 0.43 |
| 41:JB:190:HIS:ND1 | 41:JB:411:ALA:HA | 2.34 | 0.43 |
| 41:JB:200:TYR:O | 41:JB:202:ILE:HG13 | 2.19 | 0.43 |
| 40:JE:100:ALA:O | 41:JL:255:VAL:HG11 | 2.19 | 0.43 |
| 40:JF:405:HIS:CD2 | 41:JM:261:PRO:HG3 | 2.53 | 0.43 |
| 40:JG:71:GLU:HB3 | 40:JG:98:ASP:HA | 2.01 | 0.43 |
| 41:JM:46:ARG:HA | 41:JM:46:ARG:HD3 | 1.38 | 0.43 |
| 41:JN:323:MET:HA | 41:JN:326:VAL:HB | 2.01 | 0.43 |
| 41:JO:210:ILE:O | 41:JO:214:THR:OG1 | 2.27 | 0.43 |
| 40:KG:11:GLN:HG3 | 40:KG:74:VAL:HG11 | 2.01 | 0.43 |
| 40:KG:429:LYS:O | 40:KG:433:GLU:HG2 | 2.19 | 0.43 |
| 41:KL:153:SER:OG | 41:KL:154:LYS:N | 2.52 | 0.43 |
| 41:KL:189:VAL:O | 41:KL:193:VAL:HG23 | 2.19 | 0.43 |
| 41:KL:362:LYS:HB3 | 41:KL:362:LYS:HE2 | 1.70 | 0.43 |
| 41:KO:240:LEU:H | 41:KO:240:LEU:HD23 | 1.84 | 0.43 |
| 41:KO:274:THR:HB | 41:KO:282:ARG:NH1 | 2.33 | 0.43 |
| 40:LA:292:THR:OG1 | 40:LA:319:TYR:OH | 2.32 | 0.43 |
| 41:LB:176:SER:OG | 41:LB:178:THR:O | 2.36 | 0.43 |
| 40:LF:228:ASN:HD21 | 42:LM:501:GTP:HN1 | 1.67 | 0.43 |
| 41:LM:230:SER:HA | 41:LM:233:MET:HB2 | 2.01 | 0.43 |
| 41:LM:358:PRO:HG2 | 41:LM:361:LEU:HD12 | 2.00 | 0.43 |
| 40:MF:117:LEU:H | 40:MF:117:LEU:HG | 1.53 | 0.43 |
| 40:MG:166:LYS:HE2 | 40:MG:166:LYS:HB2 | 1.43 | 0.43 |
| 41:MO:30:ILE:HG23 | 41:MO:34:GLY:HA2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:MP:313:VAL:HB | 41:MP:349:VAL:HG22 | 2.01 | 0.43 |
| 40:NA:400:LYS:HE2 | 41:NN:344:TRP:CD2 | 2.54 | 0.43 |
| 41:NB:324:LYS:NZ | 40:NG:222:PRO:HG2 | 2.34 | 0.43 |
| 40:ND:153:LEU:O | 40:ND:157:LEU:HB2 | 2.18 | 0.43 |
| 40:ND:352:LYS:HB2 | 40:ND:352:LYS:HE3 | 1.75 | 0.43 |
| 40:NF:256:GLN:HG3 | 41:NN:397:TRP:CZ2 | 2.54 | 0.43 |
| 40:NF:326:LYS:HD3 | 40:NF:329:ASN:HD22 | 1.84 | 0.43 |
| 40:NG:247:ALA:HB3 | 40:NG:355:ILE:HB | 1.99 | 0.43 |
| 40:NH:142:GLY:HA3 | 42:NO:501:GTP:H5' | 2.00 | 0.43 |
| 41:NM:137:HIS:NE2 | 41:NM:166:THR:OG1 | 2.47 | 0.43 |
| 41:NP:350:LYS:HD3 | 41:NP:350:LYS:HA | 1.81 | 0.43 |
| 40:OD:125:LEU:HA | 40:OD:128:GLN:HG2 | 2.00 | 0.43 |
| 40:OH:139:HIS:CG | 40:OH:150:THR:HG21 | 2.54 | 0.43 |
| 40:OH:222:PRO:CB | 41:OO:324:LYS:HD3 | 2.48 | 0.43 |
| 40:OH:262:TYR:O | 40:OH:263:PRO:C | 2.57 | 0.43 |
| 40:OH:383:ILE:H | 40:OH:383:ILE:HG12 | 1.31 | 0.43 |
| 41:OM:7:LEU:HD23 | 41:OM:151:LEU:HD21 | 2.01 | 0.43 |
| 41:OM:154:LYS:HB2 | 41:OM:154:LYS:HE2 | 1.81 | 0.43 |
| 41:ON:133:PHE:HB2 | 41:ON:164:MET:CB | 2.48 | 0.43 |
| 40:PA:209:ILE:HG23 | 40:PA:227:LEU:HD22 | 2.00 | 0.43 |
| 41:PB:323:MET:SD | 41:PB:323:MET:N | 2.76 | 0.43 |
| 40:PE:3:GLU:N | 40:PE:3:GLU:OE2 | 2.52 | 0.43 |
| 40:PF:70:LEU:HA | 40:PF:95:GLY:HA3 | 2.01 | 0.43 |
| 40:PH:341:ILE:HD12 | 40:PH:341:ILE:HA | 1.95 | 0.43 |
| 41:PM:185:ALA:O | 41:PM:189:VAL:HG23 | 2.18 | 0.43 |
| 40:QA:70:LEU:HD23 | 40:QA:114:LEU:HD12 | 2.00 | 0.43 |
| 41:QB:137:HIS:CD2 | 41:QB:137:HIS:H | 2.37 | 0.43 |
| 41:QB:324:LYS:HE2 | 41:QB:324:LYS:HB2 | 1.81 | 0.43 |
| 40:QG:189:LEU:HD11 | 40:QG:417:PHE:HE2 | 1.83 | 0.43 |
| 41:QM:269:GLY:HA3 | 41:QM:367:PHE:HB3 | 2.00 | 0.43 |
| 41:QO:131:GLN:HE22 | 41:QO:250:LEU:H | 1.66 | 0.43 |
| 41:QP:51:TYR:HB3 | 41:QP:59:TYR:HB3 | 2.01 | 0.43 |
| 41:QP:377:LEU:HA | 41:QP:377:LEU:HD12 | 1.81 | 0.43 |
| 40:RF:262:TYR:HB2 | 40:RF:265:ILE:HG22 | 2.01 | 0.43 |
| 40:RH:188:ILE:HD12 | 40:RH:424:MET:SD | 2.59 | 0.43 |
| 40:RH:366:ASP:OD1 | 40:RH:367:LEU:N | 2.52 | 0.43 |
| 40:RI:89:PRO:HD3 | 40:SI:283:HIS:CD2 | 2.53 | 0.43 |
| 41:RL:173:PRO:HD2 | 41:RL:205:GLU:OE1 | 2.18 | 0.43 |
| 41:RL:206:ALA:O | 41:RL:210:ILE:HD12 | 2.19 | 0.43 |
| 41:RL:320:ARG:NH1 | 41:RL:320:ARG:HA | 2.34 | 0.43 |
| 41:RM:262:ARG:NH2 | 41:RM:417:ASP:O | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RO:139:LEU:HG | 41:RO:168:SER:HB3 | 2.00 | 0.43 |
| 40:SA:254:GLU:O | 40:SA:255:PHE:C | 2.57 | 0.43 |
| 40:SF:101:ASN:HD22 | 40:SF:143:GLY:HA2 | 1.84 | 0.43 |
| 40:SG:3:GLU:N | 40:SG:133:GLN:OE1 | 2.52 | 0.43 |
| 41:SL:138:SER:HA | 41:SL:169:VAL:H | 1.83 | 0.43 |
| 41:SL:229:VAL:O | 41:SL:233:MET:HG2 | 2.18 | 0.43 |
| 41:SN:267:MET:HE3 | 41:SN:371:SER:HB3 | 2.01 | 0.43 |
| 41:SO:25:SER:O | 41:SO:26:ASP:C | 2.57 | 0.43 |
| 41:TB:166:THR:HG21 | 41:TB:192:LEU:HD22 | 2.00 | 0.43 |
| 41:TB:296:ALA:HB2 | 41:TB:305:PRO:HD3 | 2.01 | 0.43 |
| 40:TE:140:SER:HA | 40:TE:171:ILE:H | 1.84 | 0.43 |
| 40:TH:229:ARG:NH2 | 40:TH:364:PRO:O | 2.51 | 0.43 |
| 40:TH:244:PHE:HB2 | 40:TH:356:ASN:HD21 | 1.83 | 0.43 |
| 41:TL:7:LEU:HD22 | 41:TL:151:LEU:HD21 | 2.01 | 0.43 |
| 41:TO:211:CYS:SG | 41:TO:225:LEU:HD21 | 2.59 | 0.43 |
| 41:TP:27:GLU:HA | 41:TP:359:ARG:NH1 | 2.22 | 0.43 |
| 40:UA:115:ILE:HD13 | 40:UA:152:LEU:HD21 | 2.00 | 0.43 |
| 41:UB:20:PHE:HA | 41:UB:230:SER:HB2 | 2.00 | 0.43 |
| 41:UB:73:MET:HB2 | 41:UB:90:PHE:CE1 | 2.54 | 0.43 |
| 40:UF:31:GLN:HE21 | 40:UF:31:GLN:HB3 | 1.61 | 0.43 |
| 40:UF:121:ARG:HD2 | 40:UF:121:ARG:HA | 1.84 | 0.43 |
| 40:UF:261:PRO:HB2 | 40:UF:262:TYR:H | 1.57 | 0.43 |
| 40:UF:269:LEU:N | 40:UF:378:SER:O | 2.42 | 0.43 |
| 40:UF:376:MET:O | 40:UF:377:LEU:C | 2.57 | 0.43 |
| 40:UI:137:ILE:HG21 | 40:UI:154:MET:SD | 2.59 | 0.43 |
| 40:UI:144:GLY:O | 40:UI:147:SER:N | 2.52 | 0.43 |
| 40:UI:166:LYS:HE3 | 40:UI:166:LYS:HB2 | 1.40 | 0.43 |
| 40:UI:195:LEU:HD11 | 40:UI:264:ARG:HG2 | 2.00 | 0.43 |
| 40:UI:259:LEU:HD12 | 40:UI:259:LEU:HA | 1.81 | 0.43 |
| 40:UI:354:GLY:O | 40:UI:356:ASN:N | 2.52 | 0.43 |
| 40:UI:396:LEU:O | 40:UI:397:MET:C | 2.56 | 0.43 |
| 41:UP:305:PRO:HB3 | 41:UP:310:TYR:CZ | 2.54 | 0.43 |
| 40:VA:10:GLY:HA2 | 40:VA:145:THR:HG23 | 2.00 | 0.43 |
| 41:VB:34:GLY:O | 41:VB:59:TYR:N | 2.51 | 0.43 |
| 41:VB:121:ARG:NH2 | 41:VB:158:GLU:OE2 | 2.52 | 0.43 |
| 40:VF:304:LYS:O | 40:VF:389:ARG:NH2 | 2.52 | 0.43 |
| 40:VI:172:TYR:OH | 40:VI:390:LEU:HD13 | 2.19 | 0.43 |
| 41:VN:28:HIS:HE1 | 41:VN:47:ILE:HA | 1.83 | 0.43 |
| 41:VO:192:LEU:HD23 | 41:VO:196:THR:HG21 | 2.01 | 0.43 |
| 41:WB:202:ILE:HG23 | 41:WB:300:MET:HB3 | 2.01 | 0.43 |
| 40:WG:103:TYR:CD1 | 40:WG:189:LEU:HD23 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WM:207:LEU:HD13 | 41:WM:207:LEU:HA | 1.81 | 0.43 |
| 41:WQ:170:VAL:HG21 | 41:WQ:201:CYS:HB3 | 2.00 | 0.43 |
| 8:1W:250:GLU:HA | 8:1W:253:ILE:HG22 | 2.00 | 0.43 |
| 8:1W:338:VAL:HA | 8:1W:341:PHE:CD1 | 2.54 | 0.43 |
| 8:1X:164:GLU:O | 8:1X:165:GLU:C | 2.57 | 0.43 |
| 9:2B:134:LYS:HA | 9:2B:137:ILE:HG22 | 2.00 | 0.43 |
| 11:2I:47:LYS:HD3 | 41:MN:336:LYS:HD2 | 2.01 | 0.43 |
| 13:2T:61:CYS:HB3 | 13:2T:62:PRO:HD3 | 2.01 | 0.43 |
| 15:3E:59:VAL:HG22 | 15:3F:336:ARG:HG3 | 2.00 | 0.43 |
| 17:3R:139:GLN:O | 17:3R:142:SER:OG | 2.36 | 0.43 |
| 17:3R:165:ASP:O | 17:3R:168:ILE:N | 2.52 | 0.43 |
| 18:3T:318:LEU:HD12 | 18:3U:64:TYR:HE1 | 1.84 | 0.43 |
| 18:3T:367:GLU:OE1 | 18:3U:217:ASP:HB3 | 2.19 | 0.43 |
| 18:3U:187:GLN:HB3 | 18:3U:191:LYS:HZ1 | 1.84 | 0.43 |
| 18:3W:127:GLU:OE2 | 18:3W:279:ARG:NH1 | 2.50 | 0.43 |
| 19:3Z:377:PHE:HD1 | 41:LP:224:ASP:OD1 | 2.01 | 0.43 |
| 20:4A:160:PHE:O | 20:4A:161:ARG:C | 2.57 | 0.43 |
| 21:4D:240:LYS:HZ3 | 40:CA:42:ILE:HB | 1.84 | 0.43 |
| 21:4D:478:SER:O | 21:4D:479:MET:C | 2.57 | 0.43 |
| 21:4E:416:ASP:O | 21:4E:417:ASN:C | 2.56 | 0.43 |
| 21:4F:154:LEU:HD13 | 21:4F:176:ILE:HD13 | 2.01 | 0.43 |
| 22:4I:113:ILE:HB | 22:4I:136:ILE:HD12 | 2.00 | 0.43 |
| 22:4J:131:ILE:HG21 | 22:4J:136:ILE:HD11 | 2.01 | 0.43 |
| 23:4N:54:PRO:HB2 | 41:BM:41:ASP:HA | 2.01 | 0.43 |
| 23:4Q:191:VAL:HG11 | 23:4Q:206:SER:HB3 | 2.00 | 0.43 |
| 27:4Y:39:LEU:HD13 | 27:4Y:102:TYR:HE1 | 1.83 | 0.43 |
| 31:5I:611:THR:OG1 | 31:5I:612:LEU:N | 2.51 | 0.43 |
| 34:5R:327:LYS:HB2 | 34:5R:327:LYS:HE2 | 1.69 | 0.43 |
| 36:5X:30:PRO:HB3 | 36:5X:77:PRO:HA | 2.00 | 0.43 |
| 39:6F:93:PRO:HA | 39:6F:96:ASN:HB2 | 2.01 | 0.43 |
| 40:AA:217:LEU:HD23 | 40:AA:277:SER:HB3 | 2.01 | 0.43 |
| 41:AB:334:GLN:HE22 | 41:AB:347:ASN:HA | 1.83 | 0.43 |
| 40:AE:49:PHE:HB2 | 40:AE:53:PHE:HB2 | 2.01 | 0.43 |
| 40:AE:202:PHE:CE2 | 40:AE:238:ILE:HD13 | 2.54 | 0.43 |
| 41:AO:83:GLN:HE21 | 41:AO:83:GLN:HB3 | 1.66 | 0.43 |
| 41:AO:121:ARG:O | 41:AO:125:GLU:HG2 | 2.19 | 0.43 |
| 41:AO:132:GLY:HA3 | 41:AO:163:ILE:O | 2.18 | 0.43 |
| 41:AO:258:VAL:HG22 | 41:AO:266:PHE:HZ | 1.83 | 0.43 |
| 41:AO:268:PRO:HG2 | 41:AO:300:MET:HB2 | 2.00 | 0.43 |
| 40:BA:332:ILE:O | 40:BA:336:LYS:HG3 | 2.18 | 0.43 |
| 41:BB:271:ALA:HB1 | 41:BB:289:LEU:HD22 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BE:145:THR:OG1 | 40:BE:146:GLY:N | 2.52 | 0.43 |
| 40:BF:27:GLU:HG2 | 40:BF:243:ARG:HH12 | 1.83 | 0.43 |
| 41:BL:316:VAL:HA | 41:BL:352:ALA:O | 2.18 | 0.43 |
| 41:BM:122:LYS:HZ3 | 41:BM:122:LYS:HG3 | 1.53 | 0.43 |
| 41:BM:130:LEU:HD22 | 41:BM:130:LEU:HA | 1.79 | 0.43 |
| 41:BP:16:ILE:HG12 | 41:BP:226:ASN:OD1 | 2.19 | 0.43 |
| 41:BP:256:ASN:O | 41:BP:312:THR:HG21 | 2.18 | 0.43 |
| 40:CH:224:TYR:O | 40:CH:225:THR:C | 2.57 | 0.43 |
| 40:CI:216:ASN:ND2 | 40:CI:300:ASN:OD1 | 2.47 | 0.43 |
| 41:CL:123:GLU:O | 41:CL:126:SER:N | 2.52 | 0.43 |
| 41:CL:317:PHE:HB3 | 41:CL:321:MET:SD | 2.59 | 0.43 |
| 41:CN:102:ALA:O | 41:CN:107:THR:HG22 | 2.18 | 0.43 |
| 41:CO:143:THR:O | 41:CO:144:GLY:C | 2.57 | 0.43 |
| 41:CO:186:THR:HG21 | 41:CO:385:PHE:HB2 | 2.00 | 0.43 |
| 41:CO:214:THR:C | 41:CO:216:LYS:H | 2.21 | 0.43 |
| 41:CP:271:ALA:HB2 | 41:CP:293:MET:HG3 | 2.01 | 0.43 |
| 40:DA:66:VAL:HG21 | 40:DA:122:ILE:HG12 | 2.00 | 0.43 |
| 41:DB:6:HIS:CD2 | 41:DB:134:GLN:HE21 | 2.36 | 0.43 |
| 41:DB:380:ARG:O | 41:DB:384:GLN:HG2 | 2.19 | 0.43 |
| 40:DE:131:GLY:O | 40:DE:132:LEU:C | 2.56 | 0.43 |
| 40:DE:250:VAL:HG11 | 40:DE:318:LEU:HD23 | 2.00 | 0.43 |
| 40:DF:123:ARG:HH22 | 40:DF:161:TYR:HB2 | 1.84 | 0.43 |
| 40:DF:304:LYS:HA | 40:DF:304:LYS:HD3 | 1.86 | 0.43 |
| 40:DH:318:LEU:HD13 | 40:DH:318:LEU:HA | 1.88 | 0.43 |
| 40:DI:228:ASN:HA | 40:DI:231:ILE:HD12 | 2.01 | 0.43 |
| 40:DI:400:LYS:HB3 | 40:DI:400:LYS:HE2 | 1.40 | 0.43 |
| 41:DL:8:GLN:HG2 | 41:DL:13:GLY:O | 2.19 | 0.43 |
| 41:DL:248:ALA:HB1 | 41:DL:252:LYS:HG2 | 1.99 | 0.43 |
| 41:DM:313:VAL:O | 41:DM:349:VAL:HA | 2.18 | 0.43 |
| 41:DN:379:LYS:HB3 | 41:DN:379:LYS:HE3 | 1.57 | 0.43 |
| 41:DP:22:GLU:HG3 | 41:DP:81:PHE:CD2 | 2.53 | 0.43 |
| 40:EF:235:VAL:HA | 40:EF:238:ILE:HG22 | 1.99 | 0.43 |
| 40:EF:242:LEU:H | 40:EF:242:LEU:HD23 | 1.83 | 0.43 |
| 40:EG:102:ASN:ND2 | 40:EG:105:ARG:HG3 | 2.33 | 0.43 |
| 41:EL:240:LEU:H | 41:EL:240:LEU:HD23 | 1.83 | 0.43 |
| 41:EM:216:LYS:HB2 | 41:EM:275:SER:HB2 | 2.00 | 0.43 |
| 41:EP:9:ALA:O | 41:EP:13:GLY:HA3 | 2.18 | 0.43 |
| 41:EP:99:ASN:O | 41:EP:180:VAL:HG21 | 2.19 | 0.43 |
| 41:EP:313:VAL:O | 41:EP:349:VAL:HA | 2.19 | 0.43 |
| 41:EP:314:ALA:HB3 | 41:EP:368:ILE:HB | 2.00 | 0.43 |
| 40:FA:352:LYS:HE3 | 41:FB:179:VAL:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FB:239:CYS:HB3 | 41:FB:247:ASN:HB2 | 2.00 | 0.43 |
| 40:FE:147:SER:HB2 | 40:FE:190:THR:HG21 | 2.00 | 0.43 |
| 40:FH:295:CYS:HB3 | 40:FH:376:MET:HG3 | 2.00 | 0.43 |
| 40:FI:255:PHE:O | 40:FI:259:LEU:HB2 | 2.19 | 0.43 |
| 41:FM:359:ARG:HA | 41:FM:359:ARG:HD2 | 1.88 | 0.43 |
| 41:FO:236:VAL:HG22 | 41:FO:368:ILE:HD11 | 2.01 | 0.43 |
| 41:GB:67:ASP:OD1 | 41:GB:68:LEU:N | 2.51 | 0.43 |
| 41:GB:404:ASP:OD1 | 41:GB:405:GLU:N | 2.52 | 0.43 |
| 40:GE:101:ASN:HA | 40:GE:144:GLY:H | 1.84 | 0.43 |
| 40:GG:352:LYS:HG3 | 41:GO:177:ASP:O | 2.18 | 0.43 |
| 40:GH:104:ALA:O | 40:GH:108:TYR:N | 2.52 | 0.43 |
| 40:GH:339:ARG:H | 40:GH:339:ARG:HG2 | 1.62 | 0.43 |
| 40:GI:156:ARG:C | 40:GI:158:SER:H | 2.22 | 0.43 |
| 40:GI:183:GLU:N | 40:GI:184:PRO:HD2 | 2.34 | 0.43 |
| 40:GI:422:GLU:H | 40:GI:422:GLU:HG3 | 1.63 | 0.43 |
| 41:GM:286:VAL:HA | 41:GM:289:LEU:HB2 | 2.01 | 0.43 |
| 41:GO:237:THR:O | 41:GO:241:ARG:NE | 2.45 | 0.43 |
| 40:HE:149:PHE:HD1 | 40:HE:149:PHE:HA | 1.76 | 0.43 |
| 40:HE:169:PHE:CZ | 40:HE:238:ILE:HG13 | 2.54 | 0.43 |
| 40:HE:383:ILE:H | 40:HE:383:ILE:HG13 | 1.35 | 0.43 |
| 40:HF:172:TYR:CD1 | 40:HF:173:PRO:HD2 | 2.54 | 0.43 |
| 40:HF:352:LYS:HE2 | 41:HN:99:ASN:ND2 | 2.33 | 0.43 |
| 40:HH:101:ASN:HB2 | 41:HO:252:LYS:NZ | 2.34 | 0.43 |
| 40:IE:26:LEU:HD23 | 40:IE:26:LEU:HA | 1.90 | 0.43 |
| 40:IG:164:LYS:HE2 | 40:IG:164:LYS:HB2 | 1.88 | 0.43 |
| 40:II:318:LEU:O | 40:II:374:VAL:HA | 2.19 | 0.43 |
| 41:IN:172:SER:OG | 41:IN:175:VAL:O | 2.34 | 0.43 |
| 41:IQ:417:ASP:O | 41:IQ:421:PRO:HD3 | 2.18 | 0.43 |
| 40:JA:85:GLN:O | 40:KA:283:HIS:NE2 | 2.45 | 0.43 |
| 41:JB:249:ASP:OD1 | 41:JB:249:ASP:N | 2.47 | 0.43 |
| 40:JE:7:VAL:HG23 | 40:JE:66:VAL:HG23 | 2.00 | 0.43 |
| 40:JF:222:PRO:HD2 | 41:JM:324:LYS:HB3 | 2.01 | 0.43 |
| 40:JG:234:ILE:O | 40:JG:238:ILE:HG12 | 2.19 | 0.43 |
| 40:JH:93:ILE:HD11 | 40:JH:121:ARG:HG3 | 2.00 | 0.43 |
| 40:JH:270:ALA:HA | 40:JH:377:LEU:HD23 | 2.01 | 0.43 |
| 40:JH:345:ASP:N | 40:JH:345:ASP:OD1 | 2.51 | 0.43 |
| 41:JL:67:ASP:OD1 | 41:JL:68:LEU:N | 2.52 | 0.43 |
| 41:JM:306:ARG:HA | 41:JM:306:ARG:HD3 | 1.85 | 0.43 |
| 41:JO:249:ASP:H | 41:JO:252:LYS:HB3 | 1.84 | 0.43 |
| 40:KE:141:PHE:HD2 | 40:KE:172:TYR:HA | 1.82 | 0.43 |
| 40:KE:205:ASP:HB2 | 40:KE:303:VAL:HG23 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KE:207:GLU:HA | 40:KE:210:TYR:HD2 | 1.82 | 0.43 |
| 40:KF:4:CYS:HB3 | 40:KF:133:GLN:HB2 | 2.00 | 0.43 |
| 40:KF:153:LEU:O | 40:KF:157:LEU:HB2 | 2.19 | 0.43 |
| 41:LB:101:TRP:HD1 | 41:LB:145:SER:HB2 | 1.84 | 0.43 |
| 40:LF:90:GLU:O | 40:LF:91:GLN:C | 2.57 | 0.43 |
| 40:LF:259:LEU:HD21 | 40:LF:377:LEU:CB | 2.47 | 0.43 |
| 40:LF:273:ALA:HB2 | 40:LF:374:VAL:HG13 | 2.00 | 0.43 |
| 40:MD:20:CYS:HA | 40:MD:232:SER:HB2 | 2.01 | 0.43 |
| 40:ME:104:ALA:O | 40:ME:108:TYR:HB2 | 2.18 | 0.43 |
| 40:MG:100:ALA:O | 40:MG:101:ASN:C | 2.58 | 0.43 |
| 41:ML:6:HIS:O | 41:ML:63:ALA:HA | 2.19 | 0.43 |
| 41:ML:152:ILE:HG12 | 41:ML:164:MET:HE1 | 2.01 | 0.43 |
| 41:MM:317:PHE:HB2 | 41:MM:353:VAL:HG22 | 1.99 | 0.43 |
| 41:MO:103:LYS:HB2 | 41:MO:103:LYS:HE3 | 1.32 | 0.43 |
| 41:MP:354:CYS:SG | 41:MP:355:ASP:N | 2.91 | 0.43 |
| 41:NB:250:LEU:HD23 | 41:NB:250:LEU:HA | 1.87 | 0.43 |
| 41:NB:310:TYR:HE1 | 41:NB:367:PHE:HZ | 1.67 | 0.43 |
| 41:NL:58:LYS:HZ3 | 41:OL:281:TYR:HE1 | 1.67 | 0.43 |
| 41:NN:240:LEU:H | 41:NN:240:LEU:HD23 | 1.83 | 0.43 |
| 40:OD:328:VAL:O | 40:OD:332:ILE:HG12 | 2.18 | 0.43 |
| 40:OE:240:ALA:HA | 40:OE:243:ARG:HH12 | 1.83 | 0.43 |
| 40:OG:88:HIS:HB3 | 40:OG:91:GLN:OE1 | 2.19 | 0.43 |
| 40:OG:107:HIS:CD2 | 40:OG:152:LEU:HB2 | 2.54 | 0.43 |
| 41:OO:385:PHE:O | 41:OO:389:PHE:HB2 | 2.19 | 0.43 |
| 40:PA:15:GLN:HB3 | 40:PA:228:ASN:HD21 | 1.84 | 0.43 |
| 40:PA:169:PHE:HB3 | 40:PA:202:PHE:HB2 | 2.01 | 0.43 |
| 41:PB:86:ARG:NH1 | 41:QB:281:TYR:O | 2.50 | 0.43 |
| 41:PB:237:THR:HB | 41:PB:240:LEU:HD21 | 2.01 | 0.43 |
| 40:PD:276:ILE:HG21 | 40:PD:281:ALA:HA | 1.99 | 0.43 |
| 40:PE:185:TYR:HE2 | 40:PE:403:PHE:HB2 | 1.84 | 0.43 |
| 41:PN:210:ILE:O | 41:PN:214:THR:OG1 | 2.27 | 0.43 |
| 41:PO:130:LEU:HD21 | 41:PO:133:PHE:CE1 | 2.54 | 0.43 |
| 41:PP:21:TRP:CZ3 | 41:PP:24:ILE:HD11 | 2.54 | 0.43 |
| 40:QA:193:THR:HG23 | 40:QA:194:THR:HG23 | 2.00 | 0.43 |
| 41:QB:19:LYS:O | 41:QB:20:PHE:C | 2.57 | 0.43 |
| 41:QB:283:ALA:O | 41:QB:285:THR:N | 2.49 | 0.43 |
| 41:QB:326:VAL:HG12 | 41:QB:330:MET:SD | 2.58 | 0.43 |
| 40:QE:56:THR:OG1 | 40:QE:57:GLY:N | 2.51 | 0.43 |
| 40:QE:115:ILE:HD13 | 40:QE:152:LEU:HD21 | 2.01 | 0.43 |
| 40:QF:214:ARG:HB3 | 41:QM:324:LYS:NZ | 2.34 | 0.43 |
| 41:QM:21:TRP:CZ2 | 41:QM:63:ALA:HB2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QM:342:VAL:HG23 | 41:QM:345:ILE:HG22 | 2.01 | 0.43 |
| 41:QN:342:VAL:HG23 | 41:QN:345:ILE:HG22 | 2.01 | 0.43 |
| 41:QP:61:PRO:O | 41:QP:62:ARG:C | 2.56 | 0.43 |
| 41:QP:153:SER:O | 41:QP:154:LYS:C | 2.57 | 0.43 |
| 40:RA:48:SER:O | 40:RA:51:THR:HG22 | 2.19 | 0.43 |
| 41:RB:31:ASP:OD1 | 41:RB:34:GLY:N | 2.52 | 0.43 |
| 40:RE:26:LEU:HD13 | 40:RE:363:VAL:HG13 | 2.00 | 0.43 |
| 40:RE:161:TYR:O | 40:RE:164:LYS:HG2 | 2.19 | 0.43 |
| 40:RE:274:PRO:HA | 40:RE:276:ILE:HG12 | 1.99 | 0.43 |
| 40:RE:313:MET:HB2 | 40:RE:346:TRP:HH2 | 1.84 | 0.43 |
| 40:RF:179:THR:OG1 | 40:RF:183:GLU:OE2 | 2.34 | 0.43 |
| 40:RF:274:PRO:HA | 40:RF:276:ILE:HD12 | 2.00 | 0.43 |
| 40:RG:153:LEU:HG | 40:RG:157:LEU:HD13 | 2.01 | 0.43 |
| 40:RH:247:ALA:HB3 | 40:RH:355:ILE:HB | 2.01 | 0.43 |
| 40:RI:123:ARG:NH2 | 40:RI:124:LYS:HZ3 | 2.17 | 0.43 |
| 41:RL:11:GLN:N | 43:RL:501:GDP:O2B | 2.46 | 0.43 |
| 40:SE:254:GLU:HA | 40:SE:257:THR:HG22 | 2.00 | 0.43 |
| 40:SG:385:GLU:O | 40:SG:389:ARG:NH1 | 2.51 | 0.43 |
| 41:SN:189:VAL:O | 41:SN:193:VAL:HG23 | 2.19 | 0.43 |
| 41:SO:260:PHE:O | 41:SO:261:PRO:C | 2.57 | 0.43 |
| 41:SO:283:ALA:C | 41:SO:285:THR:H | 2.22 | 0.43 |
| 41:SO:320:ARG:N | 41:SO:354:CYS:O | 2.51 | 0.43 |
| 41:SP:354:CYS:SG | 41:SP:355:ASP:N | 2.92 | 0.43 |
| 41:TB:398:TYR:HB3 | 41:TB:403:MET:HG3 | 2.01 | 0.43 |
| 41:TL:156:ARG:NH1 | 41:TL:162:ARG:O | 2.52 | 0.43 |
| 41:TN:103:LYS:O | 41:TN:107:THR:OG1 | 2.37 | 0.43 |
| 41:TN:204:ASN:OD1 | 43:TN:502:GDP:O2' | 2.37 | 0.43 |
| 41:TO:290:THR:HA | 41:TO:293:MET:HG2 | 2.00 | 0.43 |
| 40:UA:54:SER:O | 40:UA:61:HIS:HA | 2.19 | 0.43 |
| 40:UE:7:VAL:HG13 | 40:UE:66:VAL:HG23 | 2.00 | 0.43 |
| 40:UE:185:TYR:HE2 | 40:UE:403:PHE:HB2 | 1.83 | 0.43 |
| 40:UF:58:ALA:O | 40:UF:59:GLY:C | 2.57 | 0.43 |
| 40:UF:190:THR:O | 40:UF:191:THR:C | 2.57 | 0.43 |
| 40:UH:329:ASN:CB | 41:UP:175:VAL:HG21 | 2.46 | 0.43 |
| 40:UI:75:ILE:HG21 | 40:UI:94:THR:HG22 | 2.00 | 0.43 |
| 41:UO:21:TRP:HZ3 | 41:UO:50:TYR:HB3 | 1.83 | 0.43 |
| 41:UP:250:LEU:HA | 41:UP:253:LEU:HD12 | 2.01 | 0.43 |
| 40:VA:88:HIS:NE2 | 40:VA:90:GLU:HB2 | 2.34 | 0.43 |
| 40:VI:27:GLU:HA | 40:VI:361:THR:HG21 | 2.01 | 0.43 |
| 40:VJ:285:GLN:HB2 | 40:VJ:290:GLU:OE1 | 2.19 | 0.43 |
| 41:VO:237:THR:HG22 | 41:VO:250:LEU:HD21 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VO:316:VAL:O | 41:VO:365:ALA:HA | 2.19 | 0.43 |
| 41:WB:31:ASP:OD2 | 41:WB:31:ASP:N | 2.51 | 0.43 |
| 40:WF:210:TYR:CE1 | 41:WM:324:LYS:HE3 | 2.53 | 0.43 |
| 40:WH:72:PRO:HB2 | 41:WO:46:ARG:NH2 | 2.34 | 0.43 |
| 40:WH:236:SER:O | 40:WH:320:ARG:NH2 | 2.52 | 0.43 |
| 41:WM:66:VAL:HG21 | 41:WM:116:VAL:CG1 | 2.41 | 0.43 |
| 41:WN:161:ASP:N | 41:WN:161:ASP:OD1 | 2.52 | 0.43 |
| 41:WN:226:ASN:OD1 | 41:WN:226:ASN:N | 2.50 | 0.43 |
| 5:1M:182:LEU:HD22 | 40:HG:308:ARG:HH11 | 1.82 | 0.43 |
| 7:1T:51:ALA:O | 7:1T:55:GLN:NE2 | 2.52 | 0.43 |
| 7:1T:467:ILE:HG23 | 7:1T:478:THR:HG22 | 2.01 | 0.43 |
| 7:1U:235:ARG:H | 7:1U:235:ARG:HG3 | 1.63 | 0.43 |
| 11:2I:224:LYS:HB3 | 11:2I:224:LYS:HE2 | 1.60 | 0.43 |
| 11:2K:32:LYS:HB2 | 11:2K:32:LYS:HE2 | 1.78 | 0.43 |
| 11:2K:221:ILE:CG2 | 11:2K:222:PRO:CD | 2.89 | 0.43 |
| 13:2X:174:GLU:O | 13:2X:175:ASP:C | 2.57 | 0.43 |
| 16:3K:243:ILE:O | 16:3K:247:ILE:HG12 | 2.19 | 0.43 |
| 16:3L:100:GLU:CD | 18:3U:161:ARG:HH22 | 2.22 | 0.43 |
| 17:3O:192:LEU:HD12 | 17:3O:196:ARG:NH1 | 2.34 | 0.43 |
| 17:3Q:462:LYS:HA | 17:3Q:462:LYS:HD3 | 1.52 | 0.43 |
| 18:3U:379:SER:HA | 18:3U:382:GLU:HG2 | 2.01 | 0.43 |
| 20:4B:228:ARG:O | 20:4B:229:GLN:C | 2.57 | 0.43 |
| 21:4E:412:MET:HE2 | 21:4E:412:MET:HB2 | 1.72 | 0.43 |
| 21:4E:478:SER:O | 21:4E:479:MET:C | 2.56 | 0.43 |
| 21:4F:435:GLY:O | 21:4F:437:ARG:N | 2.51 | 0.43 |
| 21:4F:457:ARG:O | 21:4F:458:ASN:C | 2.56 | 0.43 |
| 22:4H:19:LYS:HE3 | 22:4H:19:LYS:HB2 | 1.67 | 0.43 |
| 22:4I:616:THR:OG1 | 22:4I:617:CYS:N | 2.51 | 0.43 |
| 22:4I:678:LEU:HD23 | 22:4I:678:LEU:HA | 1.80 | 0.43 |
| 22:4J:25:HIS:HB3 | 41:MN:77:ARG:HH11 | 1.84 | 0.43 |
| 22:4J:34:MET:HG3 | 22:4J:36:VAL:N | 2.34 | 0.43 |
| 22:4J:292:VAL:HG22 | 41:CN:359:ARG:HH22 | 1.83 | 0.43 |
| 22:4J:677:LEU:HD13 | 22:4J:677:LEU:HA | 1.73 | 0.43 |
| 23:4N:253:TYR:OH | 40:EF:220:GLU:HG2 | 2.19 | 0.43 |
| 24:4O:198:PHE:HA | 40:DE:221:ARG:HG3 | 2.00 | 0.43 |
| 23:4Q:184:MET:HE2 | 23:4Q:184:MET:HB2 | 1.84 | 0.43 |
| 28:5B:47:LEU:HD13 | 28:5B:51:TRP:CD2 | 2.54 | 0.43 |
| 31:5I:442:LEU:O | 31:5I:446:VAL:HG12 | 2.19 | 0.43 |
| 31:5I:571:ALA:O | 31:5I:575:ILE:HG12 | 2.19 | 0.43 |
| 34:5Q:66:TRP:HH2 | 41:JN:73:MET:HB2 | 1.84 | 0.43 |
| 34:5Q:234:LEU:HD22 | 40:GF:282:TYR:CE1 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:5Q:292:LEU:HD21 | 40:GE:279:GLU:CA | 2.48 | 0.43 |
| 36:5W:118:TYR:CD1 | 41:KN:421:PRO:HG3 | 2.53 | 0.43 |
| 36:5W:256:ARG:HE | 36:5W:256:ARG:HB2 | 1.62 | 0.43 |
| 36:5Z:236:HIS:ND1 | 40:LD:391:ASP:OD2 | 2.51 | 0.43 |
| 41:AB:314:ALA:HA | 41:AB:350:LYS:O | 2.19 | 0.43 |
| 40:AE:121:ARG:HD2 | 40:AE:121:ARG:HA | 1.89 | 0.43 |
| 40:AH:283:HIS:HB3 | 40:MH:62:VAL:HG21 | 1.99 | 0.43 |
| 41:AO:273:LEU:HB2 | 41:AO:292:GLN:HE22 | 1.84 | 0.43 |
| 41:AP:86:ARG:HG2 | 41:AP:88:ASP:H | 1.84 | 0.43 |
| 41:BB:30:ILE:HG12 | 41:BB:59:TYR:HB2 | 2.01 | 0.43 |
| 40:BF:203:MET:HB2 | 40:BF:268:PRO:O | 2.18 | 0.43 |
| 40:BH:265:ILE:HG13 | 40:BH:434:VAL:HG21 | 2.01 | 0.43 |
| 40:BI:273:ALA:HB3 | 40:BI:374:VAL:H | 1.83 | 0.43 |
| 40:CA:110:ILE:H | 40:CA:110:ILE:HG12 | 1.51 | 0.43 |
| 40:CE:29:GLY:N | 40:CE:42:ILE:HD13 | 2.33 | 0.43 |
| 40:CE:224:TYR:CE2 | 41:CL:323:MET:HG2 | 2.54 | 0.43 |
| 40:CG:328:VAL:O | 40:CG:332:ILE:HG12 | 2.19 | 0.43 |
| 40:CH:20:CYS:SG | 40:CH:21:TRP:N | 2.91 | 0.43 |
| 40:CH:86:LEU:O | 40:CH:87:PHE:C | 2.57 | 0.43 |
| 40:CH:99:ALA:HA | 40:CH:105:ARG:HH11 | 1.83 | 0.43 |
| 40:CH:121:ARG:HA | 40:CH:121:ARG:HD2 | 1.26 | 0.43 |
| 40:CI:319:TYR:HB3 | 40:CI:323:VAL:HG21 | 2.00 | 0.43 |
| 41:CL:392:LYS:HB2 | 41:CL:392:LYS:HE3 | 1.57 | 0.43 |
| 41:CM:12:CYS:HB2 | 43:CM:501:GDP:C8 | 2.53 | 0.43 |
| 41:CM:313:VAL:O | 41:CM:349:VAL:HA | 2.19 | 0.43 |
| 41:CN:317:PHE:HB3 | 41:CN:321:MET:HE1 | 2.01 | 0.43 |
| 41:CP:19:LYS:HA | 41:CP:22:GLU:HB2 | 2.01 | 0.43 |
| 40:DA:186:ASN:ND2 | 40:DA:407:TYR:OH | 2.52 | 0.43 |
| 40:DA:324:VAL:O | 40:DA:325:PRO:C | 2.57 | 0.43 |
| 40:DA:402:ALA:C | 40:DA:404:VAL:N | 2.72 | 0.43 |
| 41:DB:67:ASP:HB3 | 41:DB:73:MET:CE | 2.49 | 0.43 |
| 41:DB:251:ARG:O | 41:DB:252:LYS:C | 2.57 | 0.43 |
| 40:DF:217:LEU:HD23 | 40:DF:366:ASP:HB2 | 1.99 | 0.43 |
| 40:DG:241:SER:OG | 40:DG:249:ASN:OD1 | 2.34 | 0.43 |
| 40:DH:342:GLN:H | 40:DH:342:GLN:HG2 | 1.50 | 0.43 |
| 40:DH:405:HIS:HA | 40:DH:408:VAL:HG12 | 2.00 | 0.43 |
| 40:DI:101:ASN:OD1 | 41:DP:252:LYS:HD3 | 2.19 | 0.43 |
| 40:DI:142:GLY:O | 40:DI:143:GLY:C | 2.56 | 0.43 |
| 40:DI:230:LEU:O | 40:DI:234:ILE:HG23 | 2.19 | 0.43 |
| 41:DM:350:LYS:HA | 41:DM:350:LYS:HD2 | 1.63 | 0.43 |
| 41:DN:346:PRO:O | 41:DN:347:ASN:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EF:258:ASN:ND2 | 40:EF:316:CYS:SG | 2.92 | 0.43 |
| 41:EM:210:ILE:O | 41:EM:214:THR:HB | 2.19 | 0.43 |
| 41:EM:258:VAL:HG22 | 41:EM:266:PHE:CZ | 2.50 | 0.43 |
| 41:EP:13:GLY:O | 41:EP:16:ILE:HG12 | 2.18 | 0.43 |
| 41:EP:88:ASP:O | 41:EP:89:ASN:C | 2.58 | 0.43 |
| 41:EP:200:TYR:N | 41:EP:200:TYR:CD2 | 2.86 | 0.43 |
| 41:EP:299:MET:C | 41:EP:301:ALA:H | 2.21 | 0.43 |
| 41:EP:367:PHE:CE1 | 41:EP:369:GLY:HA3 | 2.53 | 0.43 |
| 40:FA:256:GLN:O | 40:FA:260:VAL:HG13 | 2.19 | 0.43 |
| 40:FA:400:LYS:O | 40:FA:402:ALA:N | 2.51 | 0.43 |
| 40:FF:405:HIS:ND1 | 41:FM:261:PRO:HG3 | 2.33 | 0.43 |
| 40:FI:57:GLY:C | 40:FI:59:GLY:H | 2.22 | 0.43 |
| 40:FI:138:PHE:HZ | 40:FI:235:VAL:HG11 | 1.83 | 0.43 |
| 41:FM:237:THR:HG23 | 41:FM:240:LEU:HD21 | 2.01 | 0.43 |
| 40:GA:143:GLY:H | 42:GA:501:GTP:PA | 2.42 | 0.43 |
| 40:GE:358:GLN:HE21 | 40:GE:358:GLN:HB2 | 1.54 | 0.43 |
| 40:GF:6:SER:O | 40:GF:65:ALA:HA | 2.19 | 0.43 |
| 40:GG:53:PHE:HE2 | 40:GG:86:LEU:HD11 | 1.84 | 0.43 |
| 40:GH:63:PRO:HD3 | 40:GH:86:LEU:HG | 2.01 | 0.43 |
| 40:GH:141:PHE:CE1 | 40:GH:191:THR:HB | 2.54 | 0.43 |
| 40:GI:72:PRO:O | 40:GI:74:VAL:N | 2.52 | 0.43 |
| 40:GI:140:SER:C | 40:GI:142:GLY:H | 2.23 | 0.43 |
| 40:GI:372:ARG:HE | 40:GI:372:ARG:HB2 | 1.53 | 0.43 |
| 41:GM:65:LEU:HD12 | 41:GM:90:PHE:CE2 | 2.53 | 0.43 |
| 41:GP:107:THR:O | 41:GP:110:ALA:N | 2.47 | 0.43 |
| 40:HA:143:GLY:HA3 | 42:HA:501:GTP:O3B | 2.19 | 0.43 |
| 40:HE:55:GLU:HG3 | 40:HE:56:THR:N | 2.33 | 0.43 |
| 40:HE:90:GLU:HB3 | 40:IE:280:LYS:NZ | 2.34 | 0.43 |
| 40:HE:188:ILE:HG22 | 40:HE:420:ALA:HB1 | 2.00 | 0.43 |
| 40:HE:278:ALA:O | 40:HE:280:LYS:N | 2.52 | 0.43 |
| 40:HE:308:ARG:HE | 40:HE:308:ARG:HB2 | 1.41 | 0.43 |
| 40:HF:115:ILE:HG12 | 40:HF:152:LEU:HD22 | 2.00 | 0.43 |
| 40:HH:60:LYS:HZ1 | 40:IH:283:HIS:HD2 | 1.66 | 0.43 |
| 40:HI:329:ASN:HB3 | 41:HQ:175:VAL:HG11 | 2.01 | 0.43 |
| 41:HP:163:ILE:HD11 | 41:HP:251:ARG:HB2 | 2.01 | 0.43 |
| 40:IH:213:CYS:HA | 40:IH:217:LEU:HB2 | 2.01 | 0.43 |
| 40:JA:113:GLU:HG2 | 40:JA:114:LEU:HG | 2.00 | 0.43 |
| 40:JD:191:THR:O | 40:JD:195:LEU:HB2 | 2.18 | 0.43 |
| 41:JL:178:THR:HB | 41:JL:181:GLU:HG3 | 2.01 | 0.43 |
| 41:JM:375:GLN:NE2 | 41:JM:419:GLY:O | 2.52 | 0.43 |
| 40:KA:139:HIS:ND1 | 40:KA:146:GLY:O | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KE:251:ASP:OD1 | 40:KE:252:LEU:N | 2.49 | 0.43 |
| 40:KG:271:THR:HA | 40:KG:302:MET:HG2 | 2.01 | 0.43 |
| 40:KG:289:ALA:O | 40:KG:293:ASN:ND2 | 2.52 | 0.43 |
| 41:KL:12:CYS:O | 41:KL:16:ILE:HG22 | 2.18 | 0.43 |
| 41:KN:316:VAL:HB | 41:KN:366:THR:HG22 | 2.01 | 0.43 |
| 40:LA:140:SER:HA | 40:LA:171:ILE:H | 1.84 | 0.43 |
| 40:LA:141:PHE:HB2 | 40:LA:173:PRO:HD3 | 2.00 | 0.43 |
| 40:LD:2:ARG:NH2 | 41:LL:70:PRO:O | 2.51 | 0.43 |
| 40:LG:16:ILE:HG12 | 40:LG:228:ASN:OD1 | 2.18 | 0.43 |
| 40:LG:301:GLN:HG3 | 40:LG:307:PRO:HG2 | 2.01 | 0.43 |
| 41:LL:16:ILE:HG12 | 41:LL:226:ASN:ND2 | 2.34 | 0.43 |
| 41:LM:132:GLY:HA3 | 41:LM:163:ILE:O | 2.19 | 0.43 |
| 41:LN:16:ILE:HA | 41:LN:226:ASN:HB3 | 2.00 | 0.43 |
| 41:LP:135:LEU:HB3 | 41:LP:166:THR:HG22 | 2.01 | 0.43 |
| 40:MA:209:ILE:H | 40:MA:209:ILE:HG12 | 1.47 | 0.43 |
| 40:MF:187:SER:O | 40:MF:190:THR:HG22 | 2.18 | 0.43 |
| 40:MG:111:GLY:H | 40:MG:113:GLU:HG2 | 1.84 | 0.43 |
| 41:MP:176:SER:OG | 41:MP:178:THR:O | 2.36 | 0.43 |
| 40:ND:273:ALA:CB | 40:ND:374:VAL:HG12 | 2.49 | 0.43 |
| 40:NE:137:ILE:HD11 | 40:NE:168:GLU:HG2 | 2.00 | 0.43 |
| 40:NE:140:SER:OG | 40:NE:141:PHE:N | 2.52 | 0.43 |
| 41:NM:105:HIS:HE1 | 41:NM:150:LEU:HD13 | 1.83 | 0.43 |
| 41:NN:179:VAL:HG12 | 41:NN:394:PHE:HE2 | 1.84 | 0.43 |
| 40:OA:79:ARG:O | 40:OA:84:ARG:HD2 | 2.19 | 0.43 |
| 40:OA:147:SER:HB2 | 40:OA:190:THR:HB | 2.00 | 0.43 |
| 40:OF:109:THR:OG1 | 40:OF:410:GLU:OE2 | 2.25 | 0.43 |
| 40:OG:260:VAL:HG21 | 40:OG:266:HIS:HB3 | 2.01 | 0.43 |
| 40:OH:72:PRO:HD2 | 41:OO:2:ARG:NH1 | 2.34 | 0.43 |
| 41:OL:225:LEU:HD13 | 41:OL:225:LEU:HA | 1.80 | 0.43 |
| 41:OM:42:LEU:HD11 | 41:OM:243:PRO:HG3 | 2.00 | 0.43 |
| 40:PA:103:TYR:CE1 | 40:PA:148:GLY:HA2 | 2.54 | 0.43 |
| 40:PE:139:HIS:CE1 | 40:PE:150:THR:HG21 | 2.54 | 0.43 |
| 40:PG:56:THR:HG22 | 40:QG:285:GLN:HA | 2.01 | 0.43 |
| 41:PL:36:TYR:OH | 41:PL:43:GLN:HB2 | 2.19 | 0.43 |
| 41:PO:31:ASP:OD1 | 41:PO:34:GLY:N | 2.52 | 0.43 |
| 41:PO:42:LEU:HD12 | 41:PO:243:PRO:HG3 | 2.01 | 0.43 |
| 40:QA:110:ILE:HG13 | 40:QA:113:GLU:OE2 | 2.18 | 0.43 |
| 40:QA:421:ARG:HA | 40:QA:421:ARG:HD2 | 1.82 | 0.43 |
| 41:QB:190:HIS:O | 41:QB:191:GLN:C | 2.57 | 0.43 |
| 40:QE:104:ALA:HA | 40:QE:108:TYR:HD2 | 1.83 | 0.43 |
| 40:QE:248:LEU:HD11 | 43:QM:501:GDP:H5” | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QF:287:SER:OG | 40:QF:290:GLU:OE1 | 2.24 | 0.43 |
| 41:QP:121:ARG:O | 41:QP:124:ALA:N | 2.48 | 0.43 |
| 41:RB:119:VAL:HA | 41:RB:122:LYS:HG3 | 2.01 | 0.43 |
| 40:RE:265:ILE:HG22 | 40:RE:379:ASN:HD21 | 1.84 | 0.43 |
| 40:RE:286:LEU:HD21 | 40:RE:372:ARG:H | 1.84 | 0.43 |
| 40:RG:332:ILE:HG23 | 40:RG:351:PHE:CD2 | 2.53 | 0.43 |
| 40:RI:21:TRP:CH2 | 40:RI:52:PHE:HB3 | 2.54 | 0.43 |
| 41:RN:252:LYS:HG2 | 41:RN:350:LYS:HZ1 | 1.84 | 0.43 |
| 41:RO:131:GLN:HA | 41:RO:162:ARG:HH11 | 1.83 | 0.43 |
| 41:RO:143:THR:OG1 | 41:RO:144:GLY:N | 2.51 | 0.43 |
| 41:RP:263:LEU:HD21 | 41:RP:421:PRO:HB2 | 2.00 | 0.43 |
| 41:RP:286:VAL:HA | 41:RP:289:LEU:HB2 | 2.01 | 0.43 |
| 41:RP:309:ARG:N | 41:RP:372:THR:OG1 | 2.52 | 0.43 |
| 41:SB:375:GLN:HG2 | 41:SB:376:GLU:N | 2.34 | 0.43 |
| 40:SF:118:VAL:O | 40:SF:122:ILE:HG12 | 2.19 | 0.43 |
| 40:SG:336:LYS:HA | 40:SG:336:LYS:HD3 | 1.86 | 0.43 |
| 40:SH:259:LEU:HD21 | 40:SH:316:CYS:HB2 | 2.01 | 0.43 |
| 40:SH:390:LEU:HD23 | 40:SH:390:LEU:HA | 1.85 | 0.43 |
| 41:SO:171:PRO:HG2 | 41:SO:185:ALA:HB2 | 2.00 | 0.43 |
| 41:SO:285:THR:O | 41:SO:286:VAL:C | 2.57 | 0.43 |
| 41:SO:423:VAL:O | 41:SO:424:THR:C | 2.57 | 0.43 |
| 41:TM:6:HIS:ND1 | 41:TM:134:GLN:NE2 | 2.61 | 0.43 |
| 41:TP:109:GLY:O | 41:TP:113:VAL:HG23 | 2.19 | 0.43 |
| 40:UF:112:LYS:HA | 40:UF:112:LYS:HD3 | 1.77 | 0.43 |
| 40:UF:252:LEU:HA | 40:UF:255:PHE:CD2 | 2.54 | 0.43 |
| 40:UF:291:ILE:HG13 | 40:UF:374:VAL:HB | 2.00 | 0.43 |
| 40:UF:339:ARG:H | 40:UF:339:ARG:HG3 | 1.53 | 0.43 |
| 40:UF:390:LEU:HD23 | 40:UF:390:LEU:HA | 1.92 | 0.43 |
| 40:UI:115:ILE:HD11 | 40:UI:156:ARG:HG2 | 2.01 | 0.43 |
| 40:UI:195:LEU:HA | 40:UI:266:HIS:NE2 | 2.34 | 0.43 |
| 40:UI:318:LEU:HD22 | 40:UI:318:LEU:HA | 1.75 | 0.43 |
| 41:UM:183:TYR:OH | 41:UM:388:MET:O | 2.36 | 0.43 |
| 41:UN:19:LYS:HG3 | 41:UN:226:ASN:HB2 | 2.00 | 0.43 |
| 41:UO:21:TRP:CZ3 | 41:UO:50:TYR:HB3 | 2.54 | 0.43 |
| 41:UP:144:GLY:O | 41:UP:148:GLY:HA3 | 2.18 | 0.43 |
| 41:UP:191:GLN:C | 41:UP:193:VAL:H | 2.23 | 0.43 |
| 42:VB:502:GTP:O2' | 40:VH:206:ASN:OD1 | 2.28 | 0.43 |
| 40:VJ:7:VAL:HG13 | 40:VJ:66:VAL:HG23 | 2.00 | 0.43 |
| 41:VN:25:SER:HB3 | 41:VN:81:PHE:HE2 | 1.83 | 0.43 |
| 41:VO:204:ASN:OD1 | 43:VO:501:GDP:O2' | 2.26 | 0.43 |
| 40:WH:311:LYS:H | 40:WH:381:THR:HG22 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:WI:169:PHE:HZ | 40:WI:238:ILE:HG21 | 1.84 | 0.43 |
| 41:WN:30:ILE:H | 41:WN:30:ILE:HG12 | 1.46 | 0.43 |
| 7:1T:522:THR:C | 7:1T:524:ARG:H | 2.21 | 0.42 |
| 7:1T:523:ASP:C | 7:1T:524:ARG:HG3 | 2.37 | 0.42 |
| 9:2B:47:THR:HG21 | 11:2K:246:LYS:HG3 | 2.01 | 0.42 |
| 11:2I:90:LEU:HD21 | 40:LA:439:VAL:HG22 | 2.01 | 0.42 |
| 11:2I:189:SER:O | 11:2I:192:GLU:HB2 | 2.19 | 0.42 |
| 11:2J:88:VAL:HG21 | 41:LM:392:LYS:HB2 | 2.00 | 0.42 |
| 13:2U:102:ARG:HE | 13:2U:102:ARG:HB2 | 1.65 | 0.42 |
| 13:2W:37:ILE:HD13 | 13:2W:37:ILE:HA | 1.87 | 0.42 |
| 13:2X:144:TYR:O | 13:2X:146:THR:N | 2.52 | 0.42 |
| 16:3J:326:ASN:OD1 | 16:3J:327:VAL:N | 2.51 | 0.42 |
| 16:3J:369:HIS:CD2 | 16:3L:31:GLN:HG2 | 2.53 | 0.42 |
| 16:3L:331:ARG:HB3 | 16:3L:336:PHE:HE1 | 1.84 | 0.42 |
| 16:3M:36:HIS:HA | 16:3M:39:ARG:NH1 | 2.34 | 0.42 |
| 20:4A:95:VAL:HA | 20:4A:98:PHE:CD2 | 2.54 | 0.42 |
| 20:4A:174:ALA:HA | 20:4A:177:ASP:OD2 | 2.18 | 0.42 |
| 21:4D:505:ILE:H | 21:4D:505:ILE:HG12 | 1.59 | 0.42 |
| 21:4D:513:LEU:HB3 | 21:4D:514:LYS:HZ2 | 1.84 | 0.42 |
| 21:4E:474:LYS:HD3 | 21:4E:485:TYR:OH | 2.19 | 0.42 |
| 22:4H:120:LEU:H | 22:4H:127:LYS:HE3 | 1.84 | 0.42 |
| 22:4I:654:PRO:HB2 | 22:4I:656:LYS:HG3 | 2.01 | 0.42 |
| 22:4J:297:GLN:OE1 | 41:CN:276:ARG:HA | 2.19 | 0.42 |
| 24:4O:173:SER:C | 24:4O:175:ASP:H | 2.22 | 0.42 |
| 23:4Q:19:ILE:HD11 | 40:BH:79:ARG:HB3 | 2.00 | 0.42 |
| 38:6C:189:LYS:HB3 | 38:6C:189:LYS:HE3 | 1.66 | 0.42 |
| 39:6L:92:THR:HG23 | 39:6L:95:THR:H | 1.84 | 0.42 |
| 41:AB:22:GLU:HG2 | 41:AB:81:PHE:HB2 | 2.01 | 0.42 |
| 41:AL:41:ASP:N | 41:AL:41:ASP:OD1 | 2.52 | 0.42 |
| 41:AN:52:ASN:HD22 | 41:AN:86:ARG:NH2 | 2.17 | 0.42 |
| 40:BE:140:SER:OG | 40:BE:141:PHE:N | 2.52 | 0.42 |
| 40:BE:245:ASP:HA | 40:BE:249:ASN:HD21 | 1.83 | 0.42 |
| 40:BH:128:GLN:NE2 | 40:CH:285:GLN:HB2 | 2.34 | 0.42 |
| 40:BI:300:ASN:HD22 | 40:BI:300:ASN:HA | 1.56 | 0.42 |
| 41:BM:32:PRO:C | 41:BM:34:GLY:H | 2.23 | 0.42 |
| 40:CA:97:GLU:CD | 41:CN:251:ARG:HH21 | 2.22 | 0.42 |
| 40:CE:256:GLN:HE21 | 40:CE:256:GLN:HB2 | 1.72 | 0.42 |
| 40:CE:260:VAL:O | 41:CM:397:TRP:CZ2 | 2.72 | 0.42 |
| 40:CF:185:TYR:O | 40:CF:188:ILE:HG22 | 2.19 | 0.42 |
| 40:CI:101:ASN:HA | 40:CI:144:GLY:N | 2.34 | 0.42 |
| 41:CN:17:GLY:O | 41:CN:18:ALA:C | 2.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CN:136:THR:HG23 | 41:CN:136:THR:O | 2.18 | 0.42 |
| 41:CN:190:HIS:HB2 | 41:CN:411:ALA:HA | 2.01 | 0.42 |
| 41:CN:373:ALA:C | 41:CN:375:GLN:N | 2.72 | 0.42 |
| 41:CO:103:LYS:HB3 | 41:CO:103:LYS:HE3 | 1.85 | 0.42 |
| 41:CO:271:ALA:HB2 | 41:CO:365:ALA:HB3 | 2.00 | 0.42 |
| 41:CO:325:GLU:O | 41:CO:326:VAL:C | 2.57 | 0.42 |
| 41:CO:372:THR:HG22 | 41:CO:422:VAL:HG12 | 2.01 | 0.42 |
| 41:CP:182:PRO:HB3 | 41:CP:384:GLN:CB | 2.49 | 0.42 |
| 40:DA:8:HIS:H | 40:DA:8:HIS:CD2 | 2.37 | 0.42 |
| 41:DB:211:CYS:O | 41:DB:212:PHE:C | 2.57 | 0.42 |
| 41:DB:239:CYS:C | 41:DB:241:ARG:N | 2.73 | 0.42 |
| 40:DF:172:TYR:CD1 | 40:DF:173:PRO:HD2 | 2.53 | 0.42 |
| 40:DF:390:LEU:HD23 | 40:DF:390:LEU:HA | 1.84 | 0.42 |
| 40:DF:429:LYS:HE2 | 40:DF:429:LYS:HB2 | 1.67 | 0.42 |
| 40:DH:107:HIS:CD2 | 40:DH:151:SER:HB2 | 2.54 | 0.42 |
| 40:DH:108:TYR:CE2 | 40:DH:412:MET:HG3 | 2.53 | 0.42 |
| 40:DH:132:LEU:HB3 | 40:DH:164:LYS:HZ3 | 1.84 | 0.42 |
| 40:DH:142:GLY:HA3 | 40:DH:183:GLU:HG3 | 2.01 | 0.42 |
| 40:DH:144:GLY:O | 40:DH:145:THR:C | 2.58 | 0.42 |
| 40:DH:153:LEU:O | 40:DH:154:MET:C | 2.57 | 0.42 |
| 40:DH:172:TYR:CZ | 40:DH:390:LEU:HD12 | 2.54 | 0.42 |
| 40:DI:248:LEU:HB3 | 40:DI:355:ILE:HG13 | 2.01 | 0.42 |
| 40:DI:406:TRP:CE3 | 40:DI:406:TRP:HA | 2.53 | 0.42 |
| 41:DL:102:ALA:HA | 41:DL:106:TYR:CD2 | 2.53 | 0.42 |
| 41:DL:277:GLY:C | 41:DL:279:GLN:H | 2.22 | 0.42 |
| 41:DL:336:LYS:HB2 | 41:DL:336:LYS:HE3 | 1.85 | 0.42 |
| 41:DM:167:PHE:CE2 | 41:DM:233:MET:HA | 2.54 | 0.42 |
| 41:DM:218:THR:C | 41:DM:220:PRO:HD3 | 2.39 | 0.42 |
| 41:DN:186:THR:HG21 | 41:DN:385:PHE:HB2 | 2.02 | 0.42 |
| 41:DP:297:LYS:HE2 | 41:DP:297:LYS:HB2 | 1.45 | 0.42 |
| 41:EB:256:ASN:HD21 | 40:EG:101:ASN:ND2 | 2.16 | 0.42 |
| 40:EE:258:ASN:ND2 | 40:EE:352:LYS:HD2 | 2.34 | 0.42 |
| 40:EG:21:TRP:CH2 | 40:EG:52:PHE:HB3 | 2.49 | 0.42 |
| 40:EH:28:HIS:CE1 | 40:EH:49:PHE:HA | 2.54 | 0.42 |
| 40:EH:305:CYS:HB2 | 40:EH:382:ALA:O | 2.20 | 0.42 |
| 40:EI:154:MET:HA | 40:EI:154:MET:CE | 2.49 | 0.42 |
| 41:EM:390:ARG:HD2 | 41:EM:390:ARG:HA | 1.66 | 0.42 |
| 41:EO:135:LEU:O | 41:EO:166:THR:HA | 2.19 | 0.42 |
| 41:EP:16:ILE:CD1 | 41:EP:136:THR:HB | 2.49 | 0.42 |
| 40:FI:205:ASP:O | 40:FI:209:ILE:HG12 | 2.19 | 0.42 |
| 41:FM:313:VAL:HG13 | 41:FM:349:VAL:HG23 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FN:87:PRO:HD3 | 41:GN:281:TYR:HD2 | 1.83 | 0.42 |
| 41:FN:257:MET:HB3 | 41:FN:266:PHE:CZ | 2.54 | 0.42 |
| 40:GA:244:PHE:CZ | 40:GA:358:GLN:HG2 | 2.53 | 0.42 |
| 40:GA:405:HIS:CD2 | 41:GN:261:PRO:HD3 | 2.54 | 0.42 |
| 40:GE:21:TRP:CD1 | 40:GE:67:PHE:HZ | 2.37 | 0.42 |
| 40:GF:274:PRO:HB3 | 40:GF:370:VAL:HG11 | 2.01 | 0.42 |
| 40:GF:405:HIS:HA | 40:GF:408:VAL:HG12 | 2.01 | 0.42 |
| 40:GG:138:PHE:CZ | 40:GG:235:VAL:HG21 | 2.52 | 0.42 |
| 40:GI:9:VAL:HG12 | 40:GI:68:VAL:HB | 2.01 | 0.42 |
| 41:GN:309:ARG:HE | 41:GN:309:ARG:HB3 | 1.73 | 0.42 |
| 41:GN:355:ASP:HB3 | 41:GN:356:ILE:H | 1.64 | 0.42 |
| 41:GO:21:TRP:CZ3 | 41:GO:61:PRO:HB3 | 2.54 | 0.42 |
| 40:HA:177:VAL:HG23 | 40:HA:178:SER:H | 1.84 | 0.42 |
| 40:HE:104:ALA:HB1 | 40:HE:410:GLU:HB2 | 2.01 | 0.42 |
| 40:HE:175:PRO:HB2 | 40:HE:176:GLN:OE1 | 2.19 | 0.42 |
| 40:HH:213:CYS:HA | 40:HH:217:LEU:HB2 | 2.00 | 0.42 |
| 41:HM:73:MET:N | 41:HM:73:MET:SD | 2.92 | 0.42 |
| 41:HN:122:LYS:NZ | 41:IN:291:GLN:HB3 | 2.33 | 0.42 |
| 41:HO:149:THR:HB | 41:HO:191:GLN:HB2 | 2.01 | 0.42 |
| 41:HP:210:ILE:HG12 | 41:HP:298:ASN:HA | 2.00 | 0.42 |
| 41:HQ:70:PRO:HG3 | 41:HQ:94:GLN:HA | 2.00 | 0.42 |
| 40:IA:27:GLU:HG2 | 40:IA:243:ARG:NH2 | 2.34 | 0.42 |
| 41:IB:34:GLY:HA3 | 41:IB:58:LYS:HG3 | 2.00 | 0.42 |
| 41:IB:183:TYR:OH | 41:IB:388:MET:O | 2.34 | 0.42 |
| 41:IB:252:LYS:HB2 | 40:IG:100:ALA:HA | 2.00 | 0.42 |
| 40:IE:138:PHE:HZ | 40:IE:235:VAL:HG11 | 1.84 | 0.42 |
| 40:II:260:VAL:HB | 41:IQ:397:TRP:CZ3 | 2.54 | 0.42 |
| 40:II:391:ASP:OD2 | 40:II:421:ARG:NH1 | 2.52 | 0.42 |
| 41:IM:189:VAL:HG21 | 41:IM:378:PHE:HE1 | 1.84 | 0.42 |
| 41:IP:121:ARG:NH1 | 41:IP:158:GLU:OE2 | 2.52 | 0.42 |
| 40:JA:16:ILE:HD11 | 40:JA:138:PHE:HB3 | 2.00 | 0.42 |
| 40:JA:210:TYR:O | 40:JA:214:ARG:HG2 | 2.19 | 0.42 |
| 41:JB:313:VAL:HG13 | 41:JB:367:PHE:CE2 | 2.54 | 0.42 |
| 40:JD:234:ILE:HD11 | 40:JD:272:TYR:HB2 | 2.01 | 0.42 |
| 41:JL:7:LEU:HG | 41:JL:135:LEU:HD13 | 2.01 | 0.42 |
| 41:JM:165:ASN:N | 41:JM:165:ASN:OD1 | 2.51 | 0.42 |
| 41:JM:420:ASN:H | 41:JM:421:PRO:HD2 | 1.84 | 0.42 |
| 41:JN:354:CYS:SG | 41:JN:355:ASP:N | 2.92 | 0.42 |
| 41:KB:392:LYS:HE3 | 41:KB:405:GLU:OE2 | 2.18 | 0.42 |
| 40:KE:228:ASN:ND2 | 42:KE:501:GTP:HN1 | 2.16 | 0.42 |
| 40:LA:53:PHE:HB3 | 40:LA:61:HIS:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LA:260:VAL:HG12 | 40:LA:266:HIS:HA | 2.00 | 0.42 |
| 40:LA:274:PRO:HG3 | 40:LA:286:LEU:HD22 | 2.00 | 0.42 |
| 40:LG:114:LEU:HA | 40:LG:114:LEU:HD23 | 1.76 | 0.42 |
| 40:LH:217:LEU:HD23 | 40:LH:366:ASP:HB3 | 2.00 | 0.42 |
| 41:LN:385:PHE:HZ | 41:LN:408:PHE:HB3 | 1.84 | 0.42 |
| 41:LP:51:TYR:HB3 | 41:LP:59:TYR:HB3 | 2.01 | 0.42 |
| 40:MA:70:LEU:HD21 | 40:MA:111:GLY:HA2 | 2.01 | 0.42 |
| 40:MA:407:TYR:O | 40:MA:408:VAL:C | 2.58 | 0.42 |
| 40:MD:56:THR:OG1 | 40:MD:57:GLY:N | 2.52 | 0.42 |
| 40:MD:116:ASP:OD1 | 40:MD:117:LEU:N | 2.52 | 0.42 |
| 40:MG:185:TYR:HA | 40:MG:394:PHE:HD1 | 1.83 | 0.42 |
| 40:MG:195:LEU:HD13 | 40:MG:267:PHE:CZ | 2.54 | 0.42 |
| 40:MG:304:LYS:HE3 | 40:MG:304:LYS:HB3 | 1.36 | 0.42 |
| 40:MH:105:ARG:HA | 40:MH:109:THR:OG1 | 2.18 | 0.42 |
| 40:MH:244:PHE:HB2 | 40:MH:356:ASN:OD1 | 2.19 | 0.42 |
| 41:MO:213:ARG:HE | 41:MO:213:ARG:HB2 | 1.61 | 0.42 |
| 41:MP:2:ARG:HB2 | 41:MP:240:LEU:HD11 | 2.01 | 0.42 |
| 41:MP:116:VAL:HG11 | 41:MP:151:LEU:HD11 | 1.99 | 0.42 |
| 41:NB:200:TYR:CD1 | 41:NB:266:PHE:HB2 | 2.54 | 0.42 |
| 40:NF:88:HIS:HB3 | 40:NF:91:GLN:HG2 | 2.01 | 0.42 |
| 40:NF:156:ARG:HD3 | 40:NF:156:ARG:HA | 1.92 | 0.42 |
| 40:NF:222:PRO:HB2 | 40:NF:226:ASN:HB3 | 2.01 | 0.42 |
| 40:NG:98:ASP:OD1 | 40:NG:99:ALA:N | 2.51 | 0.42 |
| 41:NL:89:ASN:HA | 41:NL:119:VAL:HG21 | 2.01 | 0.42 |
| 40:OA:32:PRO:HB3 | 40:OA:83:TYR:HE1 | 1.83 | 0.42 |
| 40:OA:237:SER:HA | 40:OA:320:ARG:HH11 | 1.83 | 0.42 |
| 40:OA:259:LEU:HD11 | 40:OA:377:LEU:HD23 | 2.01 | 0.42 |
| 40:OD:234:ILE:HD12 | 40:OD:270:ALA:HB1 | 2.01 | 0.42 |
| 40:OE:276:ILE:HG23 | 40:OE:280:LYS:HB2 | 2.00 | 0.42 |
| 40:OG:284:GLU:HB2 | 40:OG:286:LEU:HD12 | 2.00 | 0.42 |
| 40:OH:26:LEU:H | 40:OH:26:LEU:HG | 1.66 | 0.42 |
| 40:OH:140:SER:O | 40:OH:142:GLY:N | 2.47 | 0.42 |
| 40:OH:156:ARG:HD2 | 40:OH:156:ARG:HA | 1.56 | 0.42 |
| 40:OH:224:TYR:OH | 42:OO:501:GTP:H2' | 2.19 | 0.42 |
| 40:OH:426:ALA:O | 40:OH:427:LEU:C | 2.56 | 0.42 |
| 41:OL:31:ASP:OD1 | 41:OL:35:THR:N | 2.51 | 0.42 |
| 41:OM:287:PRO:HD3 | 41:OM:325:GLU:HG2 | 2.01 | 0.42 |
| 40:PE:322:ASP:N | 40:PE:322:ASP:OD1 | 2.52 | 0.42 |
| 41:PN:169:VAL:HG22 | 41:PN:202:ILE:HD11 | 1.99 | 0.42 |
| 41:PP:421:PRO:HB3 | 41:PP:425:ARG:HH22 | 1.84 | 0.42 |
| 41:QB:102:ALA:O | 41:QB:103:LYS:C | 2.56 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QE:147:SER:O | 40:QE:150:THR:OG1 | 2.31 | 0.42 |
| 40:QE:286:LEU:HD12 | 40:QE:370:VAL:HG21 | 2.00 | 0.42 |
| 40:QF:287:SER:N | 40:QF:290:GLU:OE2 | 2.51 | 0.42 |
| 40:QG:35:GLN:OE1 | 40:QG:35:GLN:N | 2.52 | 0.42 |
| 40:QH:234:ILE:HD11 | 40:QH:272:TYR:HB2 | 2.01 | 0.42 |
| 41:QL:142:GLY:O | 41:QL:144:GLY:N | 2.52 | 0.42 |
| 40:RG:273:ALA:HB2 | 40:RG:295:CYS:SG | 2.59 | 0.42 |
| 40:RG:346:TRP:HZ3 | 41:RO:393:ALA:HA | 1.84 | 0.42 |
| 40:RI:68:VAL:HG21 | 40:RI:118:VAL:HG11 | 2.00 | 0.42 |
| 41:RO:21:TRP:CH2 | 41:RO:61:PRO:HB3 | 2.54 | 0.42 |
| 41:RO:87:PRO:HG2 | 41:SO:277:GLY:O | 2.19 | 0.42 |
| 40:SA:247:ALA:HB2 | 40:SA:357:TYR:OH | 2.19 | 0.42 |
| 41:SO:27:GLU:O | 41:SO:28:HIS:C | 2.56 | 0.42 |
| 41:SO:60:VAL:HG21 | 41:SO:86:ARG:CZ | 2.48 | 0.42 |
| 41:SO:309:ARG:N | 41:SO:372:THR:OG1 | 2.52 | 0.42 |
| 41:SO:341:PHE:O | 41:SO:343:GLU:N | 2.52 | 0.42 |
| 41:SO:361:LEU:HD23 | 41:SO:361:LEU:HA | 1.91 | 0.42 |
| 41:TB:86:ARG:HG2 | 41:TB:88:ASP:H | 1.83 | 0.42 |
| 40:TE:257:THR:HG23 | 41:TM:397:TRP:HZ3 | 1.83 | 0.42 |
| 40:TH:318:LEU:HB2 | 40:TH:375:CYS:SG | 2.59 | 0.42 |
| 40:UF:258:ASN:OD1 | 41:UN:99:ASN:ND2 | 2.52 | 0.42 |
| 40:UF:271:THR:CG2 | 40:UF:295:CYS:HA | 2.49 | 0.42 |
| 40:UF:366:ASP:O | 40:UF:367:LEU:C | 2.57 | 0.42 |
| 40:UG:288:VAL:HA | 40:UG:291:ILE:HG12 | 2.00 | 0.42 |
| 40:UH:206:ASN:OD1 | 42:UO:501:GTP:O2' | 2.35 | 0.42 |
| 40:UI:256:GLN:H | 40:UI:256:GLN:HG2 | 1.48 | 0.42 |
| 41:UM:36:TYR:OH | 41:UM:43:GLN:NE2 | 2.52 | 0.42 |
| 41:UN:309:ARG:O | 41:UN:372:THR:OG1 | 2.28 | 0.42 |
| 41:UO:258:VAL:HG21 | 41:UO:264:HIS:HB3 | 2.01 | 0.42 |
| 41:UP:354:CYS:O | 41:UP:355:ASP:C | 2.57 | 0.42 |
| 41:VB:117:LEU:O | 41:VB:121:ARG:HG3 | 2.19 | 0.42 |
| 40:VG:212:ILE:HD11 | 40:VG:300:ASN:HA | 2.00 | 0.42 |
| 40:VG:254:GLU:O | 40:VG:258:ASN:ND2 | 2.52 | 0.42 |
| 41:VN:100:ASN:HB3 | 41:VN:103:LYS:HB3 | 2.01 | 0.42 |
| 41:VQ:280:GLN:HG3 | 41:VQ:281:TYR:CD1 | 2.54 | 0.42 |
| 41:VQ:322:SER:OG | 41:VQ:325:GLU:OE1 | 2.26 | 0.42 |
| 40:WA:195:LEU:HD22 | 40:WA:427:LEU:HD11 | 2.00 | 0.42 |
| 40:WE:254:GLU:HA | 40:WE:257:THR:HG22 | 2.01 | 0.42 |
| 40:WI:204:VAL:HG11 | 40:WI:231:ILE:HG12 | 2.00 | 0.42 |
| 41:WN:56:GLY:O | 41:WN:57:GLY:C | 2.57 | 0.42 |
| 41:WN:135:LEU:HD23 | 41:WN:152:ILE:HG13 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WN:217:LEU:HD12 | 41:WN:217:LEU:HA | 1.76 | 0.42 |
| 41:WN:375:GLN:HB2 | 41:WN:422:VAL:HG11 | 2.00 | 0.42 |
| 41:WO:303:CYS:SG | 41:WO:377:LEU:HB2 | 2.59 | 0.42 |
| 11:2I:215:SER:OG | 11:2I:216:VAL:N | 2.52 | 0.42 |
| 12:2M:254:CYS:SG | 13:2U:84:LYS:HG3 | 2.58 | 0.42 |
| 12:2R:47:MET:HG3 | 41:AP:336:LYS:HG3 | 2.00 | 0.42 |
| 12:2R:65:ARG:HA | 12:2R:65:ARG:HD3 | 1.85 | 0.42 |
| 13:2T:125:LEU:H | 13:2T:125:LEU:HD12 | 1.84 | 0.42 |
| 13:2V:100:ARG:HG3 | 13:2V:152:LEU:HD12 | 2.01 | 0.42 |
| 13:2W:97:LYS:HB3 | 41:AN:392:LYS:HZ1 | 1.84 | 0.42 |
| 13:2W:102:ARG:HB3 | 13:2W:118:ILE:HD12 | 2.01 | 0.42 |
| 13:2X:139:PHE:HA | 13:2X:142:ARG:HG3 | 2.01 | 0.42 |
| 14:3A:48:HIS:HE1 | 40:MF:429:LYS:HG3 | 1.83 | 0.42 |
| 16:3J:350:ALA:O | 16:3J:352:LEU:N | 2.52 | 0.42 |
| 16:3L:321:ARG:NH2 | 16:3L:332:ASP:OD2 | 2.52 | 0.42 |
| 17:3O:351:ILE:HG12 | 17:3O:469:ASP:HB3 | 2.01 | 0.42 |
| 17:3O:364:HIS:HD2 | 17:3R:110:SER:HB3 | 1.84 | 0.42 |
| 17:3P:204:LYS:HE2 | 17:3P:204:LYS:HB2 | 1.52 | 0.42 |
| 17:3P:384:LYS:HG3 | 17:3P:385:ALA:N | 2.34 | 0.42 |
| 17:3Q:438:LEU:HD13 | 17:3Q:438:LEU:HA | 1.89 | 0.42 |
| 17:3R:140:ALA:O | 17:3R:141:ASP:C | 2.58 | 0.42 |
| 19:3Y:74:MET:HE2 | 41:LO:361:LEU:HA | 2.01 | 0.42 |
| 19:3Y:340:ARG:HG3 | 40:KD:58:ALA:HB2 | 2.02 | 0.42 |
| 21:4E:330:ILE:HG13 | 21:4E:355:TYR:HE2 | 1.83 | 0.42 |
| 21:4E:460:GLY:C | 21:4E:461:ILE:HG12 | 2.39 | 0.42 |
| 22:4H:236:TRP:CH2 | 22:4H:349:ARG:HD3 | 2.54 | 0.42 |
| 22:4I:642:CYS:HB3 | 22:4I:690:TYR:CD2 | 2.54 | 0.42 |
| 22:4K:555:GLU:O | 22:4K:556:GLU:C | 2.58 | 0.42 |
| 22:4K:630:HIS:ND1 | 22:4K:668:PRO:HB2 | 2.33 | 0.42 |
| 23:4M:235:THR:OG1 | 23:4M:239:ASN:O | 2.36 | 0.42 |
| 23:4P:184:MET:O | 23:4P:186:GLY:N | 2.52 | 0.42 |
| 23:4P:196:PHE:HZ | 41:CN:53:GLU:HB3 | 1.84 | 0.42 |
| 23:4Q:107:LYS:HB2 | 23:4Q:107:LYS:HE3 | 1.68 | 0.42 |
| 25:4T:400:GLN:O | 25:4T:401:PRO:C | 2.58 | 0.42 |
| 31:5I:589:ARG:HH12 | 31:5I:593:LEU:HD22 | 1.83 | 0.42 |
| 31:5I:646:LYS:O | 31:5I:650:GLN:HG3 | 2.18 | 0.42 |
| 34:5Q:194:LYS:HA | 34:5Q:194:LYS:HD2 | 1.85 | 0.42 |
| 35:5T:146:LEU:HD13 | 35:5T:149:ARG:HD2 | 2.00 | 0.42 |
| 36:5W:146:ARG:O | 36:5W:147:ILE:HD13 | 2.19 | 0.42 |
| 40:AF:167:LEU:HD22 | 40:AF:200:CYS:HB3 | 2.01 | 0.42 |
| 40:AF:217:LEU:HD11 | 40:AF:366:ASP:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AG:138:PHE:HE2 | 40:AG:235:VAL:HG21 | 1.84 | 0.42 |
| 41:AL:61:PRO:HD3 | 41:AL:84:ILE:HG12 | 2.01 | 0.42 |
| 41:AM:332:ASN:O | 41:AM:336:LYS:HG3 | 2.19 | 0.42 |
| 41:AN:113:VAL:HG22 | 41:AN:117:LEU:HD23 | 2.00 | 0.42 |
| 41:BB:258:VAL:HG22 | 41:BB:266:PHE:HZ | 1.84 | 0.42 |
| 40:BE:138:PHE:HE2 | 40:BE:235:VAL:HG21 | 1.84 | 0.42 |
| 40:BF:3:GLU:HA | 40:BF:51:THR:HA | 2.01 | 0.42 |
| 40:BG:52:PHE:HZ | 40:BG:239:THR:HG21 | 1.84 | 0.42 |
| 40:BH:115:ILE:HD12 | 40:BH:115:ILE:HA | 1.92 | 0.42 |
| 40:BH:177:VAL:HG22 | 40:BH:178:SER:N | 2.34 | 0.42 |
| 40:BH:316:CYS:O | 40:BH:316:CYS:SG | 2.77 | 0.42 |
| 40:BI:131:GLY:O | 40:BI:132:LEU:C | 2.57 | 0.42 |
| 40:BI:147:SER:OG | 40:BI:148:GLY:N | 2.53 | 0.42 |
| 40:BI:229:ARG:HE | 40:BI:229:ARG:HB2 | 1.76 | 0.42 |
| 41:BL:228:LEU:HD11 | 41:BL:273:LEU:HD11 | 2.01 | 0.42 |
| 41:BM:198:GLU:HB3 | 41:BM:200:TYR:HE1 | 1.82 | 0.42 |
| 41:BM:202:ILE:HD13 | 41:BM:268:PRO:HG3 | 2.01 | 0.42 |
| 41:BP:73:MET:SD | 41:BP:90:PHE:HD1 | 2.43 | 0.42 |
| 41:CB:137:HIS:O | 41:CB:168:SER:HA | 2.19 | 0.42 |
| 40:CE:313:MET:HB2 | 40:CE:379:ASN:HB3 | 2.01 | 0.42 |
| 40:CF:178:SER:OG | 41:CM:347:ASN:ND2 | 2.52 | 0.42 |
| 40:CF:333:ALA:HB2 | 41:CN:174:LYS:HE3 | 2.01 | 0.42 |
| 40:CG:12:ALA:O | 40:CG:16:ILE:HG12 | 2.19 | 0.42 |
| 40:CH:248:LEU:HD12 | 40:CH:248:LEU:HA | 1.80 | 0.42 |
| 40:CH:352:LYS:HD2 | 41:CP:178:THR:HA | 2.00 | 0.42 |
| 40:CH:395:ASP:O | 40:CH:396:LEU:C | 2.56 | 0.42 |
| 41:CM:9:ALA:HA | 41:CM:66:VAL:O | 2.19 | 0.42 |
| 41:CM:87:PRO:HD3 | 41:DM:281:TYR:HD2 | 1.84 | 0.42 |
| 41:CN:101:TRP:H | 41:CN:184:ASN:ND2 | 2.17 | 0.42 |
| 41:CO:109:GLY:O | 41:CO:110:ALA:C | 2.57 | 0.42 |
| 41:CO:191:GLN:HE21 | 41:CO:191:GLN:HB3 | 1.51 | 0.42 |
| 41:CO:256:ASN:HD22 | 41:CO:350:LYS:HD3 | 1.84 | 0.42 |
| 41:CP:42:LEU:HG | 41:CP:243:PRO:HG3 | 2.01 | 0.42 |
| 40:DA:206:ASN:HA | 40:DA:209:ILE:HD12 | 2.01 | 0.42 |
| 40:DA:400:LYS:O | 40:DA:402:ALA:N | 2.52 | 0.42 |
| 40:DF:24:TYR:HB3 | 40:DF:53:PHE:CE2 | 2.54 | 0.42 |
| 40:DF:208:ALA:O | 40:DF:212:ILE:HG23 | 2.19 | 0.42 |
| 40:DF:210:TYR:CD1 | 41:DM:324:LYS:HE2 | 2.54 | 0.42 |
| 40:DH:123:ARG:O | 40:DH:124:LYS:C | 2.56 | 0.42 |
| 40:DI:271:THR:HG21 | 40:DI:295:CYS:O | 2.18 | 0.42 |
| 40:DI:281:ALA:O | 40:DI:283:HIS:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DI:387:TRP:HE1 | 40:DI:431:TYR:HH | 1.65 | 0.42 |
| 41:DL:322:SER:OG | 41:DL:323:MET:N | 2.51 | 0.42 |
| 41:DL:350:LYS:HD2 | 41:DL:350:LYS:HA | 1.55 | 0.42 |
| 41:DM:325:GLU:HA | 41:DM:328:GLU:HB3 | 2.00 | 0.42 |
| 41:DN:30:ILE:HD11 | 41:DN:47:ILE:HD11 | 2.01 | 0.42 |
| 41:DO:134:GLN:HA | 41:DO:165:ASN:O | 2.19 | 0.42 |
| 41:DP:48:ASN:O | 41:DP:50:TYR:N | 2.52 | 0.42 |
| 41:DP:380:ARG:O | 41:DP:384:GLN:HG2 | 2.19 | 0.42 |
| 40:EA:98:ASP:N | 40:EA:98:ASP:OD1 | 2.52 | 0.42 |
| 40:EI:366:ASP:O | 40:EI:367:LEU:C | 2.58 | 0.42 |
| 41:EM:290:THR:HG21 | 41:EM:329:GLN:HB3 | 2.00 | 0.42 |
| 40:FA:34:GLY:O | 40:FA:35:GLN:C | 2.57 | 0.42 |
| 40:FA:105:ARG:HA | 40:FA:109:THR:CG2 | 2.49 | 0.42 |
| 40:FA:224:TYR:O | 40:FA:225:THR:C | 2.56 | 0.42 |
| 40:FE:22:GLU:HG2 | 40:FE:83:TYR:CE1 | 2.54 | 0.42 |
| 41:FO:176:SER:OG | 41:FO:177:ASP:N | 2.52 | 0.42 |
| 41:FO:303:CYS:SG | 41:FO:377:LEU:HB2 | 2.59 | 0.42 |
| 41:FO:330:MET:HA | 41:FO:333:VAL:HG12 | 2.00 | 0.42 |
| 41:FP:179:VAL:HG23 | 41:FP:180:VAL:HG23 | 2.01 | 0.42 |
| 40:GA:166:LYS:HE2 | 40:GA:166:LYS:HB2 | 1.78 | 0.42 |
| 40:GA:258:ASN:HA | 41:GB:394:PHE:HE1 | 1.84 | 0.42 |
| 40:GA:273:ALA:HB3 | 40:GA:374:VAL:H | 1.84 | 0.42 |
| 40:GF:105:ARG:CD | 41:GM:251:ARG:HH12 | 2.32 | 0.42 |
| 40:GG:238:ILE:HA | 40:GG:318:LEU:HD22 | 2.01 | 0.42 |
| 40:GH:164:LYS:HA | 40:GH:164:LYS:HD3 | 1.70 | 0.42 |
| 40:GH:256:GLN:HG2 | 40:GH:257:THR:N | 2.34 | 0.42 |
| 40:GH:288:VAL:O | 40:GH:291:ILE:HG12 | 2.19 | 0.42 |
| 40:GH:392:HIS:CE1 | 40:GH:396:LEU:HD21 | 2.54 | 0.42 |
| 41:GN:23:VAL:HG22 | 41:GN:227:HIS:CE1 | 2.53 | 0.42 |
| 40:HA:69:ASP:N | 40:HA:69:ASP:OD2 | 2.50 | 0.42 |
| 40:HA:311:LYS:NZ | 40:HA:435:GLY:O | 2.51 | 0.42 |
| 41:HB:21:TRP:HZ2 | 41:HB:63:ALA:HB2 | 1.84 | 0.42 |
| 40:HE:21:TRP:CZ2 | 40:HE:65:ALA:HB2 | 2.54 | 0.42 |
| 40:HE:103:TYR:HE1 | 40:HE:151:SER:HB2 | 1.84 | 0.42 |
| 40:HF:217:LEU:HA | 40:HF:277:SER:HB2 | 2.02 | 0.42 |
| 40:HI:88:HIS:HB3 | 40:HI:91:GLN:HG2 | 2.01 | 0.42 |
| 41:HO:316:VAL:HG12 | 41:HO:352:ALA:HB3 | 2.00 | 0.42 |
| 40:IG:90:GLU:N | 40:IG:90:GLU:OE1 | 2.51 | 0.42 |
| 41:IO:180:VAL:O | 41:IO:184:ASN:ND2 | 2.52 | 0.42 |
| 41:IO:228:LEU:HD23 | 41:IO:228:LEU:HA | 1.87 | 0.42 |
| 41:IQ:153:SER:HA | 41:IQ:195:ASN:HD21 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JL:285:THR:HG22 | 41:JL:287:PRO:HD2 | 2.00 | 0.42 |
| 41:JM:155:ILE:HD12 | 41:JM:155:ILE:HA | 1.82 | 0.42 |
| 41:JO:170:VAL:HG11 | 41:JO:377:LEU:HD21 | 2.01 | 0.42 |
| 40:KD:138:PHE:HE2 | 40:KD:235:VAL:HG21 | 1.83 | 0.42 |
| 41:KL:109:GLY:O | 41:KL:113:VAL:N | 2.51 | 0.42 |
| 41:KO:181:GLU:HG2 | 41:KO:182:PRO:HD3 | 2.02 | 0.42 |
| 40:LA:101:ASN:ND2 | 40:LA:143:GLY:HA2 | 2.34 | 0.42 |
| 40:LD:306:ASP:N | 40:LD:306:ASP:OD1 | 2.52 | 0.42 |
| 40:LE:116:ASP:OD1 | 40:LE:117:LEU:N | 2.52 | 0.42 |
| 40:LG:100:ALA:O | 40:LG:102:ASN:N | 2.52 | 0.42 |
| 40:LG:104:ALA:HB1 | 40:LG:410:GLU:HB3 | 2.00 | 0.42 |
| 40:MA:428:GLU:O | 40:MA:432:GLU:HB2 | 2.18 | 0.42 |
| 40:ME:298:PRO:HB3 | 40:ME:307:PRO:HD2 | 2.01 | 0.42 |
| 40:MF:326:LYS:O | 40:MF:328:VAL:N | 2.52 | 0.42 |
| 41:MP:131:GLN:HE22 | 41:MP:249:ASP:HB2 | 1.85 | 0.42 |
| 41:MP:198:GLU:HG2 | 41:MP:266:PHE:HE2 | 1.83 | 0.42 |
| 41:NB:398:TYR:HB3 | 41:NB:403:MET:HE2 | 2.01 | 0.42 |
| 40:ND:110:ILE:H | 40:ND:110:ILE:HG12 | 1.51 | 0.42 |
| 40:ND:140:SER:HA | 40:ND:171:ILE:H | 1.84 | 0.42 |
| 40:NE:240:ALA:HA | 40:NE:243:ARG:HB2 | 2.02 | 0.42 |
| 40:NF:178:SER:OG | 40:NF:183:GLU:OE2 | 2.33 | 0.42 |
| 40:NF:210:TYR:CD1 | 41:NM:324:LYS:HG3 | 2.54 | 0.42 |
| 40:NH:2:ARG:HH22 | 41:NP:71:GLY:HA2 | 1.84 | 0.42 |
| 41:NM:189:VAL:HA | 41:NM:192:LEU:HB2 | 2.01 | 0.42 |
| 41:OB:133:PHE:O | 41:OB:164:MET:HB2 | 2.19 | 0.42 |
| 41:OB:173:PRO:HB3 | 41:OB:380:ARG:HD2 | 2.00 | 0.42 |
| 41:OB:258:VAL:HG22 | 41:OB:266:PHE:HZ | 1.84 | 0.42 |
| 40:OD:93:ILE:HG23 | 40:OD:117:LEU:HD11 | 2.00 | 0.42 |
| 40:OH:172:TYR:CD1 | 40:OH:173:PRO:HD2 | 2.55 | 0.42 |
| 41:OL:32:PRO:HG3 | 41:OL:81:PHE:CE1 | 2.54 | 0.42 |
| 41:ON:215:LEU:HD21 | 41:ON:273:LEU:HD22 | 2.01 | 0.42 |
| 41:ON:242:PHE:CG | 41:ON:356:ILE:HD12 | 2.54 | 0.42 |
| 40:PA:9:VAL:HG23 | 40:PA:146:GLY:HA2 | 2.01 | 0.42 |
| 41:PB:139:LEU:HB3 | 41:PB:185:ALA:HA | 2.00 | 0.42 |
| 40:PG:311:LYS:NZ | 40:PG:344:VAL:HA | 2.35 | 0.42 |
| 40:PH:2:ARG:HH21 | 41:PP:71:GLY:HA3 | 1.83 | 0.42 |
| 40:QA:223:THR:OG1 | 40:QA:226:ASN:OD1 | 2.34 | 0.42 |
| 40:QA:274:PRO:HB3 | 40:QA:276:ILE:HG12 | 2.00 | 0.42 |
| 41:QB:144:GLY:O | 41:QB:148:GLY:HA3 | 2.19 | 0.42 |
| 41:QB:174:LYS:HE2 | 41:QB:174:LYS:HB2 | 1.34 | 0.42 |
| 40:QH:248:LEU:HD11 | 43:QP:501:GDP:H5” | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QL:246:LEU:HG | 41:QL:352:ALA:HA | 2.00 | 0.42 |
| 41:QN:378:PHE:HA | 41:QN:381:ILE:HG22 | 2.00 | 0.42 |
| 41:QP:216:LYS:HA | 41:QP:216:LYS:HD2 | 1.51 | 0.42 |
| 41:QP:305:PRO:O | 41:QP:306:ARG:C | 2.57 | 0.42 |
| 40:RA:5:ILE:HD12 | 40:RA:125:LEU:HD23 | 2.00 | 0.42 |
| 40:RE:14:VAL:HG22 | 40:RE:67:PHE:HD2 | 1.84 | 0.42 |
| 40:RG:394:PHE:CD1 | 40:RG:421:ARG:HD3 | 2.54 | 0.42 |
| 40:RI:318:LEU:O | 40:RI:374:VAL:HA | 2.19 | 0.42 |
| 41:RL:88:ASP:OD2 | 41:RL:88:ASP:N | 2.50 | 0.42 |
| 41:RM:151:LEU:O | 41:RM:155:ILE:HG12 | 2.19 | 0.42 |
| 41:RM:257:MET:HG3 | 41:RM:266:PHE:CE1 | 2.54 | 0.42 |
| 41:RO:310:TYR:HD1 | 41:RO:371:SER:HB2 | 1.84 | 0.42 |
| 40:SA:255:PHE:CE2 | 40:SA:318:LEU:HD21 | 2.54 | 0.42 |
| 40:SA:328:VAL:HG11 | 40:SA:355:ILE:HD11 | 2.01 | 0.42 |
| 41:SB:51:TYR:HA | 41:SB:60:VAL:O | 2.19 | 0.42 |
| 40:SH:250:VAL:HG13 | 40:SH:255:PHE:HE2 | 1.84 | 0.42 |
| 40:SI:204:VAL:HG22 | 40:SI:302:MET:SD | 2.59 | 0.42 |
| 41:SL:128:ASP:OD1 | 41:SL:129:CYS:N | 2.51 | 0.42 |
| 41:SO:106:TYR:HE2 | 41:SO:403:MET:HE2 | 1.83 | 0.42 |
| 41:SP:14:ASN:ND2 | 41:SP:65:LEU:HG | 2.33 | 0.42 |
| 40:TE:116:ASP:OD1 | 40:TE:117:LEU:N | 2.52 | 0.42 |
| 40:TG:224:TYR:HB3 | 42:TG:501:GTP:C6 | 2.55 | 0.42 |
| 40:TH:49:PHE:O | 40:TH:53:PHE:N | 2.50 | 0.42 |
| 40:TH:101:ASN:HD21 | 40:TH:180:ALA:HB1 | 1.84 | 0.42 |
| 40:TI:32:PRO:HB3 | 40:TI:83:TYR:CE1 | 2.54 | 0.42 |
| 41:TM:69:GLU:O | 41:TM:71:GLY:N | 2.46 | 0.42 |
| 41:UB:210:ILE:O | 41:UB:214:THR:OG1 | 2.32 | 0.42 |
| 40:UF:162:GLY:O | 40:UF:163:LYS:C | 2.56 | 0.42 |
| 40:UH:256:GLN:NE2 | 41:UP:397:TRP:CE2 | 2.87 | 0.42 |
| 40:UI:102:ASN:HB3 | 40:UI:105:ARG:HG3 | 2.01 | 0.42 |
| 41:UN:293:MET:SD | 41:UN:367:PHE:HB2 | 2.59 | 0.42 |
| 41:UP:50:TYR:HE2 | 41:UP:241:ARG:HH11 | 1.68 | 0.42 |
| 41:UP:193:VAL:HG23 | 41:UP:265:PHE:HE1 | 1.84 | 0.42 |
| 40:VF:258:ASN:HD22 | 40:VF:352:LYS:NZ | 2.18 | 0.42 |
| 40:VG:88:HIS:HB2 | 40:WF:283:HIS:HB3 | 2.00 | 0.42 |
| 40:VH:139:HIS:ND1 | 40:VH:140:SER:O | 2.52 | 0.42 |
| 40:VH:224:TYR:HA | 40:VH:227:LEU:HB2 | 2.02 | 0.42 |
| 40:VJ:269:LEU:HD23 | 40:VJ:383:ILE:HD11 | 2.00 | 0.42 |
| 41:VO:272:PRO:HG2 | 41:VO:361:LEU:HD23 | 2.02 | 0.42 |
| 41:VQ:2:ARG:HE | 41:VQ:240:LEU:HD23 | 1.84 | 0.42 |
| 41:WM:137:HIS:NE2 | 41:WM:166:THR:HB | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WN:252:LYS:HG2 | 41:WN:350:LYS:HZ1 | 1.84 | 0.42 |
| 41:WO:254:ALA:O | 41:WO:258:VAL:HG22 | 2.19 | 0.42 |
| 41:WO:263:LEU:HD23 | 41:WO:263:LEU:HA | 1.90 | 0.42 |
| 41:WO:376:GLU:HA | 41:WO:379:LYS:HZ2 | 1.83 | 0.42 |
| 41:WQ:92:PHE:HE2 | 41:WQ:94:GLN:HE22 | 1.67 | 0.42 |
| 7:1S:460:HIS:CE1 | 7:1S:486:ILE:HD12 | 2.54 | 0.42 |
| 7:1T:286:LYS:HE3 | 7:1T:286:LYS:HB2 | 1.50 | 0.42 |
| 7:1T:576:GLU:H | 7:1T:576:GLU:HG2 | 1.62 | 0.42 |
| 11:2K:197:LEU:HD21 | 11:2K:244:LEU:O | 2.18 | 0.42 |
| 12:2O:113:PHE:HB3 | 12:2O:152:PRO:CB | 2.48 | 0.42 |
| 12:2R:97:LYS:HE2 | 12:2R:97:LYS:HB3 | 1.76 | 0.42 |
| 13:2T:28:LYS:O | 13:2T:57:THR:HA | 2.19 | 0.42 |
| 13:2T:83:LEU:HD21 | 13:2T:161:ARG:HD2 | 2.01 | 0.42 |
| 15:3E:171:LEU:HD11 | 15:3E:228:ALA:HB2 | 2.01 | 0.42 |
| 16:3J:74:TRP:HB3 | 16:3J:179:LYS:HE3 | 2.01 | 0.42 |
| 16:3L:328:GLU:HG3 | 16:3M:182:THR:OG1 | 2.19 | 0.42 |
| 17:3O:261:LYS:HD3 | 17:3O:261:LYS:HA | 1.76 | 0.42 |
| 18:3T:197:ALA:O | 18:3T:201:ILE:HG12 | 2.20 | 0.42 |
| 19:3Y:40:ARG:NH1 | 40:LH:327:ASP:OD2 | 2.53 | 0.42 |
| 21:4F:334:PRO:HA | 21:4F:343:PHE:HA | 2.02 | 0.42 |
| 22:4H:336:SER:OG | 22:4H:368:TYR:OH | 2.26 | 0.42 |
| 22:4I:36:VAL:HG13 | 22:4I:37:SER:H | 1.84 | 0.42 |
| 23:4M:263:HIS:HA | 23:4M:266:HIS:NE2 | 2.35 | 0.42 |
| 23:4N:173:SER:HB3 | 23:4N:181:LYS:HA | 2.01 | 0.42 |
| 26:4W:286:TYR:HE2 | 26:4W:299:MET:HB3 | 1.85 | 0.42 |
| 26:4W:375:LEU:HD23 | 26:4W:375:LEU:HA | 1.90 | 0.42 |
| 27:4Y:4:ASN:ND2 | 41:IM:126:SER:O | 2.51 | 0.42 |
| 28:5B:76:SER:OG | 28:5B:78:TYR:O | 2.33 | 0.42 |
| 29:5E:112:ASP:OD1 | 29:5E:112:ASP:N | 2.47 | 0.42 |
| 34:5R:377:LYS:HA | 34:5R:377:LYS:HD3 | 1.81 | 0.42 |
| 35:5T:107:TYR:CD2 | 35:5T:134:LEU:HD22 | 2.53 | 0.42 |
| 38:6C:67:VAL:HG22 | 40:VA:308:ARG:HH22 | 1.83 | 0.42 |
| 39:6K:50:GLN:HG2 | 39:6K:54:TYR:CE2 | 2.54 | 0.42 |
| 40:AA:376:MET:HE3 | 40:AA:378:SER:HB3 | 2.02 | 0.42 |
| 40:AE:217:LEU:HD21 | 40:AE:367:LEU:HD12 | 2.00 | 0.42 |
| 40:AG:26:LEU:HD11 | 40:AG:363:VAL:HG12 | 2.01 | 0.42 |
| 41:AL:121:ARG:NH1 | 41:AL:158:GLU:OE1 | 2.52 | 0.42 |
| 41:AL:281:TYR:O | 41:ML:86:ARG:NH1 | 2.52 | 0.42 |
| 41:AN:309:ARG:NH1 | 41:AN:426:GLY:O | 2.52 | 0.42 |
| 40:BA:261:PRO:HG2 | 40:BA:313:MET:HE3 | 2.01 | 0.42 |
| 41:BB:192:LEU:O | 41:BB:264:HIS:NE2 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BE:20:CYS:HB3 | 40:BE:24:TYR:CE2 | 2.54 | 0.42 |
| 40:BE:143:GLY:O | 40:BE:144:GLY:C | 2.57 | 0.42 |
| 40:BF:356:ASN:OD1 | 40:BF:357:TYR:N | 2.52 | 0.42 |
| 40:BH:6:SER:O | 40:BH:65:ALA:HA | 2.19 | 0.42 |
| 40:BH:306:ASP:O | 40:BH:307:PRO:C | 2.57 | 0.42 |
| 40:BI:3:GLU:HA | 40:BI:51:THR:O | 2.20 | 0.42 |
| 41:BM:343:GLU:H | 41:BM:343:GLU:HG3 | 1.58 | 0.42 |
| 41:BO:200:TYR:CE2 | 41:BO:266:PHE:HD2 | 2.38 | 0.42 |
| 41:BP:90:PHE:O | 41:BP:92:PHE:N | 2.53 | 0.42 |
| 40:CA:103:TYR:CD2 | 40:CA:189:LEU:HB3 | 2.54 | 0.42 |
| 40:CE:101:ASN:HB2 | 41:CL:252:LYS:HD2 | 2.00 | 0.42 |
| 40:CE:133:GLN:HG2 | 40:CE:242:LEU:HD11 | 2.01 | 0.42 |
| 40:CE:150:THR:O | 40:CE:154:MET:HG2 | 2.18 | 0.42 |
| 40:CF:79:ARG:HH12 | 40:CF:94:THR:HG21 | 1.85 | 0.42 |
| 40:CG:274:PRO:HG3 | 40:CG:286:LEU:HD23 | 2.02 | 0.42 |
| 40:CH:75:ILE:HD12 | 40:CH:94:THR:HB | 2.01 | 0.42 |
| 40:CH:255:PHE:CE1 | 40:CH:318:LEU:HD11 | 2.54 | 0.42 |
| 40:CI:387:TRP:CD1 | 40:CI:431:TYR:HE2 | 2.36 | 0.42 |
| 41:CL:80:PRO:HB2 | 41:CL:81:PHE:H | 1.62 | 0.42 |
| 41:CM:54:ALA:O | 41:CM:56:GLY:N | 2.53 | 0.42 |
| 41:CM:97:ALA:O | 41:CM:98:GLY:C | 2.57 | 0.42 |
| 41:CM:344:TRP:CZ2 | 41:CM:425:ARG:HB3 | 2.53 | 0.42 |
| 41:CM:392:LYS:HD3 | 41:CM:392:LYS:HA | 1.59 | 0.42 |
| 41:CN:286:VAL:HA | 41:CN:363:MET:HE1 | 2.01 | 0.42 |
| 41:CN:389:PHE:O | 41:CN:390:ARG:C | 2.57 | 0.42 |
| 41:CP:46:ARG:HB2 | 41:CP:241:ARG:O | 2.20 | 0.42 |
| 41:CP:65:LEU:HD11 | 41:CP:85:PHE:HB3 | 2.00 | 0.42 |
| 41:CP:222:TYR:HA | 41:CP:225:LEU:HD12 | 2.02 | 0.42 |
| 41:CP:257:MET:SD | 41:CP:312:THR:HB | 2.59 | 0.42 |
| 40:DA:31:GLN:O | 40:DA:33:ASP:N | 2.52 | 0.42 |
| 40:DA:162:GLY:O | 40:DA:163:LYS:C | 2.57 | 0.42 |
| 40:DA:397:MET:O | 40:DA:398:TYR:C | 2.58 | 0.42 |
| 41:DB:130:LEU:O | 41:DB:131:GLN:C | 2.57 | 0.42 |
| 40:DE:123:ARG:HA | 40:DE:123:ARG:HD2 | 1.71 | 0.42 |
| 40:DE:225:THR:HA | 40:DE:228:ASN:ND2 | 2.35 | 0.42 |
| 40:DF:159:VAL:O | 40:DF:161:TYR:N | 2.52 | 0.42 |
| 40:DG:169:PHE:CE1 | 40:DG:202:PHE:HD1 | 2.37 | 0.42 |
| 40:DG:273:ALA:HB3 | 40:DG:374:VAL:H | 1.84 | 0.42 |
| 40:DG:326:LYS:HG2 | 41:DO:208:TYR:CD1 | 2.54 | 0.42 |
| 40:DI:240:ALA:O | 40:DI:243:ARG:N | 2.52 | 0.42 |
| 41:DL:80:PRO:C | 41:DL:82:GLY:H | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DL:143:THR:O | 41:DL:146:GLY:N | 2.48 | 0.42 |
| 41:DL:189:VAL:O | 41:DL:190:HIS:C | 2.57 | 0.42 |
| 41:DM:101:TRP:O | 41:DM:102:ALA:C | 2.57 | 0.42 |
| 41:DM:137:HIS:CE1 | 41:DM:192:LEU:HD11 | 2.54 | 0.42 |
| 41:DM:142:GLY:O | 41:DM:145:SER:N | 2.52 | 0.42 |
| 41:DM:414:ASN:O | 41:DM:417:ASP:HB2 | 2.19 | 0.42 |
| 41:DN:257:MET:HA | 41:DN:312:THR:HB | 2.00 | 0.42 |
| 41:DN:285:THR:O | 41:DN:286:VAL:C | 2.58 | 0.42 |
| 41:DP:137:HIS:CE1 | 41:DP:166:THR:HB | 2.52 | 0.42 |
| 41:DP:218:THR:OG1 | 41:DP:219:THR:N | 2.52 | 0.42 |
| 41:DP:389:PHE:O | 41:DP:392:LYS:N | 2.51 | 0.42 |
| 41:DP:420:ASN:O | 41:DP:423:VAL:N | 2.43 | 0.42 |
| 40:EA:205:ASP:HB2 | 40:EA:303:VAL:HG22 | 2.01 | 0.42 |
| 40:EG:2:ARG:HH22 | 40:EG:249:ASN:HD21 | 1.65 | 0.42 |
| 40:EG:264:ARG:HE | 40:EG:264:ARG:HB2 | 1.71 | 0.42 |
| 41:EN:119:VAL:HA | 41:EN:122:LYS:HB2 | 2.01 | 0.42 |
| 41:EO:252:LYS:HG3 | 41:EO:350:LYS:NZ | 2.34 | 0.42 |
| 41:EP:180:VAL:O | 41:EP:181:GLU:C | 2.57 | 0.42 |
| 40:FA:29:GLY:O | 40:FA:30:ILE:C | 2.58 | 0.42 |
| 40:FA:288:VAL:HG11 | 40:FA:327:ASP:HB3 | 2.01 | 0.42 |
| 40:FF:336:LYS:HE3 | 40:FF:351:PHE:CE1 | 2.55 | 0.42 |
| 40:FG:269:LEU:HD21 | 40:FG:383:ILE:HD13 | 2.00 | 0.42 |
| 41:FM:240:LEU:HD13 | 41:FM:249:ASP:HB2 | 2.00 | 0.42 |
| 41:FN:228:LEU:HD11 | 41:FN:273:LEU:HD11 | 2.01 | 0.42 |
| 41:FN:242:PHE:HD1 | 41:FN:356:ILE:HB | 1.84 | 0.42 |
| 41:FP:16:ILE:HA | 41:FP:226:ASN:HD22 | 1.84 | 0.42 |
| 40:GE:2:ARG:O | 40:GE:51:THR:HA | 2.19 | 0.42 |
| 40:GE:88:HIS:C | 40:GE:90:GLU:N | 2.72 | 0.42 |
| 40:GG:278:ALA:CA | 40:GG:368:ALA:HB2 | 2.50 | 0.42 |
| 40:GG:352:LYS:HE3 | 41:GO:178:THR:HG22 | 2.01 | 0.42 |
| 40:GH:72:PRO:O | 40:GH:74:VAL:N | 2.52 | 0.42 |
| 40:GI:318:LEU:HD22 | 40:GI:318:LEU:HA | 1.78 | 0.42 |
| 41:GM:11:GLN:HA | 41:GM:72:THR:HG21 | 2.01 | 0.42 |
| 41:GN:21:TRP:CZ2 | 41:GN:63:ALA:HB2 | 2.54 | 0.42 |
| 41:GN:174:LYS:HE2 | 41:GN:174:LYS:HB3 | 1.71 | 0.42 |
| 41:GP:148:GLY:O | 41:GP:152:ILE:HG12 | 2.18 | 0.42 |
| 41:GP:392:LYS:NZ | 41:GP:405:GLU:OE2 | 2.33 | 0.42 |
| 40:HE:31:GLN:HG2 | 40:HE:31:GLN:H | 1.61 | 0.42 |
| 40:HE:104:ALA:HB1 | 40:HE:410:GLU:CB | 2.50 | 0.42 |
| 40:HE:323:VAL:HB | 40:HE:355:ILE:HG23 | 2.01 | 0.42 |
| 40:HH:88:HIS:ND1 | 40:IH:283:HIS:HB2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HM:296:ALA:HB1 | 41:HM:305:PRO:HD2 | 2.01 | 0.42 |
| 41:HM:379:LYS:O | 41:HM:382:SER:OG | 2.24 | 0.42 |
| 41:HP:7:LEU:HG | 41:HP:64:VAL:HB | 2.01 | 0.42 |
| 41:HP:189:VAL:O | 41:HP:193:VAL:HG23 | 2.19 | 0.42 |
| 41:HQ:24:ILE:HA | 41:HQ:27:GLU:HB2 | 2.00 | 0.42 |
| 41:IB:21:TRP:CE3 | 41:IB:24:ILE:HD11 | 2.55 | 0.42 |
| 41:IB:74:ASP:OD2 | 41:IB:74:ASP:N | 2.53 | 0.42 |
| 41:IB:238:THR:HG21 | 41:IB:318:ARG:HD2 | 2.01 | 0.42 |
| 40:IG:241:SER:OG | 40:IG:250:VAL:O | 2.32 | 0.42 |
| 40:II:67:PHE:CE1 | 40:II:78:VAL:HG11 | 2.54 | 0.42 |
| 41:IM:68:LEU:HD22 | 41:IM:97:ALA:HB2 | 2.01 | 0.42 |
| 41:IO:155:ILE:HD13 | 41:IO:155:ILE:HA | 1.91 | 0.42 |
| 40:JH:31:GLN:HG3 | 40:JH:37:PRO:HD3 | 2.01 | 0.42 |
| 41:JM:109:GLY:O | 41:JM:112:LEU:N | 2.52 | 0.42 |
| 41:JM:159:TYR:HB3 | 41:JM:162:ARG:HD2 | 2.01 | 0.42 |
| 41:JN:7:LEU:HD12 | 41:JN:135:LEU:HD13 | 2.00 | 0.42 |
| 41:JO:163:ILE:HG13 | 41:JO:251:ARG:HB2 | 2.00 | 0.42 |
| 41:KB:236:VAL:HG22 | 41:KB:368:ILE:HD11 | 2.01 | 0.42 |
| 40:KD:288:VAL:HA | 40:KD:291:ILE:HG12 | 2.01 | 0.42 |
| 40:KF:150:THR:O | 40:KF:154:MET:HG2 | 2.19 | 0.42 |
| 40:KG:167:LEU:HD22 | 40:KG:200:CYS:HB3 | 2.01 | 0.42 |
| 41:KN:341:PHE:HB3 | 41:KN:348:ASN:HD21 | 1.84 | 0.42 |
| 41:LN:21:TRP:CZ3 | 41:LN:50:TYR:HB3 | 2.54 | 0.42 |
| 41:LN:204:ASN:HD22 | 41:LN:207:LEU:HD12 | 1.84 | 0.42 |
| 40:MD:215:ARG:NH2 | 40:MD:299:ALA:O | 2.53 | 0.42 |
| 40:MG:79:ARG:HE | 40:MG:79:ARG:HB3 | 1.55 | 0.42 |
| 40:MH:30:ILE:HG12 | 40:MH:61:HIS:HB3 | 2.02 | 0.42 |
| 41:MN:86:ARG:HG3 | 41:MN:88:ASP:H | 1.84 | 0.42 |
| 41:MN:178:THR:HB | 41:MN:181:GLU:HB3 | 2.01 | 0.42 |
| 40:NF:276:ILE:HG13 | 40:NF:368:ALA:HB3 | 2.01 | 0.42 |
| 40:NG:328:VAL:O | 40:NG:332:ILE:HG12 | 2.19 | 0.42 |
| 41:NN:87:PRO:HA | 41:NN:90:PHE:HD2 | 1.84 | 0.42 |
| 40:OA:223:THR:HG22 | 41:ON:322:SER:HA | 2.01 | 0.42 |
| 41:OB:385:PHE:O | 41:OB:389:PHE:HB3 | 2.19 | 0.42 |
| 40:OD:326:LYS:HB2 | 40:OD:329:ASN:HB2 | 2.00 | 0.42 |
| 40:OF:12:ALA:HB1 | 40:OF:171:ILE:HD12 | 2.01 | 0.42 |
| 40:OH:75:ILE:H | 40:OH:75:ILE:HG12 | 1.69 | 0.42 |
| 40:OH:213:CYS:CB | 40:OH:222:PRO:HG3 | 2.48 | 0.42 |
| 41:OL:325:GLU:OE2 | 41:OL:325:GLU:N | 2.52 | 0.42 |
| 41:OM:64:VAL:HG21 | 41:OM:120:VAL:HG22 | 2.01 | 0.42 |
| 41:PB:20:PHE:HA | 41:PB:23:VAL:HG12 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:PD:316:CYS:HB3 | 40:PD:377:LEU:HB2 | 2.01 | 0.42 |
| 40:PG:20:CYS:HA | 40:PG:232:SER:HB2 | 2.01 | 0.42 |
| 41:PL:4:ILE:HD11 | 41:PL:50:TYR:CZ | 2.55 | 0.42 |
| 41:PN:225:LEU:HD23 | 41:PN:225:LEU:HA | 1.91 | 0.42 |
| 41:QB:306:ARG:HG3 | 41:QB:340:TYR:CE2 | 2.55 | 0.42 |
| 40:QE:119:LEU:HA | 40:QE:122:ILE:HG22 | 2.00 | 0.42 |
| 40:QF:210:TYR:CE1 | 40:QF:227:LEU:HD11 | 2.53 | 0.42 |
| 40:QG:187:SER:O | 40:QG:191:THR:OG1 | 2.28 | 0.42 |
| 41:QL:11:GLN:HG3 | 41:QL:72:THR:HB | 2.00 | 0.42 |
| 41:QP:100:ASN:HB3 | 41:QP:103:LYS:HG2 | 2.01 | 0.42 |
| 41:QP:143:THR:HG22 | 41:QP:144:GLY:N | 2.34 | 0.42 |
| 41:QP:252:LYS:HA | 41:QP:252:LYS:HD2 | 1.64 | 0.42 |
| 41:QP:299:MET:O | 41:QP:300:MET:C | 2.57 | 0.42 |
| 41:QP:313:VAL:CG1 | 41:QP:369:GLY:HA3 | 2.49 | 0.42 |
| 41:QP:424:THR:OG1 | 41:QP:425:ARG:N | 2.50 | 0.42 |
| 40:RA:178:SER:OG | 40:RA:179:THR:N | 2.53 | 0.42 |
| 40:RE:319:TYR:HB3 | 40:RE:323:VAL:HG11 | 2.01 | 0.42 |
| 40:RF:318:LEU:O | 40:RF:374:VAL:HA | 2.19 | 0.42 |
| 40:RG:208:ALA:O | 40:RG:212:ILE:HG12 | 2.18 | 0.42 |
| 40:RG:278:ALA:C | 40:RG:280:LYS:H | 2.21 | 0.42 |
| 40:RI:405:HIS:CD2 | 41:RP:261:PRO:HG3 | 2.54 | 0.42 |
| 41:RM:134:GLN:HA | 41:RM:165:ASN:O | 2.19 | 0.42 |
| 41:RM:204:ASN:O | 41:RM:208:TYR:HB2 | 2.19 | 0.42 |
| 41:RN:21:TRP:CZ3 | 41:RN:61:PRO:HB3 | 2.55 | 0.42 |
| 41:RO:107:THR:O | 41:RO:109:GLY:N | 2.53 | 0.42 |
| 40:SA:150:THR:O | 40:SA:154:MET:HG2 | 2.19 | 0.42 |
| 40:SE:20:CYS:HA | 40:SE:232:SER:HB2 | 2.00 | 0.42 |
| 40:SF:311:LYS:NZ | 40:SF:435:GLY:O | 2.44 | 0.42 |
| 40:SH:33:ASP:OD2 | 40:SH:34:GLY:N | 2.51 | 0.42 |
| 40:SH:36:MET:HG3 | 40:SH:61:HIS:NE2 | 2.34 | 0.42 |
| 40:SH:88:HIS:HB2 | 40:TH:283:HIS:HB3 | 2.01 | 0.42 |
| 40:SH:99:ALA:O | 40:SH:105:ARG:NH1 | 2.52 | 0.42 |
| 40:SH:317:LEU:HD12 | 40:SH:353:VAL:HG12 | 2.02 | 0.42 |
| 40:SI:54:SER:HB2 | 40:SI:64:ARG:HE | 1.84 | 0.42 |
| 40:SI:101:ASN:ND2 | 41:SP:256:ASN:HD21 | 2.17 | 0.42 |
| 40:SI:118:VAL:O | 40:SI:122:ILE:HG12 | 2.19 | 0.42 |
| 40:SI:248:LEU:H | 40:SI:355:ILE:HB | 1.82 | 0.42 |
| 40:SI:297:GLU:O | 40:SI:301:GLN:NE2 | 2.40 | 0.42 |
| 41:SL:14:ASN:ND2 | 41:SL:67:ASP:OD2 | 2.50 | 0.42 |
| 41:SN:334:GLN:HG2 | 41:SN:341:PHE:CE2 | 2.54 | 0.42 |
| 40:TA:2:ARG:O | 40:TA:51:THR:OG1 | 2.31 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TB:19:LYS:HD3 | 41:TB:19:LYS:HA | 1.73 | 0.42 |
| 41:TB:20:PHE:CD1 | 41:TB:233:MET:HE2 | 2.54 | 0.42 |
| 40:TE:284:GLU:HB2 | 40:TE:286:LEU:HD22 | 2.01 | 0.42 |
| 40:TG:31:GLN:N | 40:TG:31:GLN:OE1 | 2.51 | 0.42 |
| 40:TH:260:VAL:HG12 | 40:TH:266:HIS:HA | 2.02 | 0.42 |
| 41:TN:359:ARG:HH11 | 41:TN:360:GLY:HA3 | 1.84 | 0.42 |
| 41:TO:313:VAL:O | 41:TO:349:VAL:HA | 2.19 | 0.42 |
| 41:TP:309:ARG:N | 41:TP:372:THR:OG1 | 2.47 | 0.42 |
| 40:UF:104:ALA:HB1 | 40:UF:410:GLU:HB2 | 2.01 | 0.42 |
| 40:UF:250:VAL:HB | 40:UF:255:PHE:CE1 | 2.54 | 0.42 |
| 40:UH:117:LEU:O | 40:UH:121:ARG:HG2 | 2.20 | 0.42 |
| 40:UH:177:VAL:HB | 41:UO:331:LEU:HD22 | 2.01 | 0.42 |
| 41:UM:204:ASN:ND2 | 43:UM:502:GDP:O2' | 2.50 | 0.42 |
| 41:UP:396:HIS:ND1 | 41:UP:396:HIS:N | 2.65 | 0.42 |
| 40:VA:116:ASP:OD1 | 40:VA:117:LEU:N | 2.52 | 0.42 |
| 41:VB:139:LEU:HG | 41:VB:168:SER:HB2 | 2.01 | 0.42 |
| 40:VG:167:LEU:HG | 40:VG:200:CYS:HB3 | 2.00 | 0.42 |
| 40:VG:210:TYR:HE1 | 40:VG:227:LEU:HD21 | 1.84 | 0.42 |
| 41:VP:99:ASN:HA | 41:VP:142:GLY:N | 2.34 | 0.42 |
| 40:WA:51:THR:HG21 | 40:WA:243:ARG:HG2 | 2.01 | 0.42 |
| 40:WA:109:THR:OG1 | 40:WA:410:GLU:O | 2.35 | 0.42 |
| 40:WH:67:PHE:HD2 | 40:WH:92:LEU:HD22 | 1.83 | 0.42 |
| 40:WI:311:LYS:HD3 | 40:WI:344:VAL:HG22 | 2.00 | 0.42 |
| 41:WN:389:PHE:O | 41:WN:390:ARG:C | 2.57 | 0.42 |
| 41:WP:180:VAL:HG23 | 41:WP:184:ASN:HD21 | 1.85 | 0.42 |
| 7:1U:159:GLY:HA3 | 7:1U:179:ASN:HB3 | 2.00 | 0.42 |
| 7:1U:412:ILE:HG22 | 7:1U:415:ALA:HB2 | 2.01 | 0.42 |
| 10:2F:164:ASP:HB2 | 40:VH:117:LEU:HD11 | 2.01 | 0.42 |
| 10:2G:157:ARG:NH2 | 41:VQ:52:ASN:O | 2.38 | 0.42 |
| 12:2Q:105:TYR:OH | 12:2Q:137:HIS:O | 2.27 | 0.42 |
| 12:2R:241:PHE:CE1 | 12:2R:253:SER:HB2 | 2.53 | 0.42 |
| 13:2X:32:GLY:HA2 | 13:2X:51:GLY:HA2 | 2.02 | 0.42 |
| 14:3C:102:LEU:HG | 14:3C:109:LEU:HB2 | 2.01 | 0.42 |
| 15:3H:109:LEU:HB2 | 15:3H:143:ILE:HG21 | 2.01 | 0.42 |
| 15:3H:203:ASN:O | 15:3H:205:VAL:N | 2.53 | 0.42 |
| 16:3J:341:GLU:CG | 16:3L:56:ASP:HB3 | 2.50 | 0.42 |
| 18:3T:328:GLU:HB3 | 18:3U:71:ARG:HE | 1.84 | 0.42 |
| 20:4A:29:ARG:NH2 | 40:MA:322:ASP:OD1 | 2.52 | 0.42 |
| 20:4A:53:LYS:HB2 | 20:4A:53:LYS:HE2 | 1.88 | 0.42 |
| 21:4D:436:ARG:HE | 21:4D:436:ARG:HB3 | 1.75 | 0.42 |
| 21:4D:511:TYR:O | 21:4D:514:LYS:HB2 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4E:407:LYS:HD2 | 40:DH:58:ALA:H | 1.84 | 0.42 |
| 21:4F:413:LEU:HD23 | 21:4F:413:LEU:HA | 1.80 | 0.42 |
| 22:4I:457:PHE:O | 22:4I:459:SER:N | 2.51 | 0.42 |
| 22:4J:276:SER:OG | 22:4J:277:LEU:N | 2.52 | 0.42 |
| 22:4K:652:VAL:CG2 | 22:4K:687:GLN:HB3 | 2.49 | 0.42 |
| 23:4M:27:PRO:HG3 | 41:BB:44:LEU:HD13 | 2.00 | 0.42 |
| 23:4R:27:PRO:O | 23:4R:28:LEU:C | 2.57 | 0.42 |
| 23:4R:184:MET:SD | 40:CI:79:ARG:HD3 | 2.60 | 0.42 |
| 25:4T:329:PRO:HA | 25:4T:330:PRO:HD3 | 1.91 | 0.42 |
| 26:4V:283:GLU:O | 26:4V:287:GLU:HB2 | 2.19 | 0.42 |
| 27:4Y:92:LEU:HD11 | 27:4Y:246:VAL:HG11 | 2.02 | 0.42 |
| 31:5I:344:ARG:HH21 | 41:HN:48:ASN:HB3 | 1.84 | 0.42 |
| 31:5I:386:GLN:NE2 | 41:IB:360:GLY:O | 2.52 | 0.42 |
| 31:5I:677:LYS:HG2 | 41:IQ:56:GLY:HA3 | 2.01 | 0.42 |
| 31:5J:798:LEU:HD23 | 31:5J:798:LEU:HA | 1.90 | 0.42 |
| 31:5J:823:ILE:HD13 | 31:5J:826:ILE:HG13 | 2.01 | 0.42 |
| 33:5N:373:GLU:O | 33:5N:377:LYS:HG2 | 2.18 | 0.42 |
| 36:5Y:77:PRO:HD2 | 40:OG:282:TYR:CE2 | 2.54 | 0.42 |
| 39:6J:99:LEU:HG | 39:6J:103:LYS:HE2 | 2.01 | 0.42 |
| 40:AA:334:ALA:O | 40:AA:338:LYS:HG3 | 2.18 | 0.42 |
| 40:AA:433:GLU:HA | 40:AA:436:MET:HG2 | 2.01 | 0.42 |
| 41:AB:117:LEU:HD11 | 41:AB:154:LYS:HD3 | 2.02 | 0.42 |
| 41:AM:2:ARG:NH1 | 41:AM:249:ASP:OD2 | 2.52 | 0.42 |
| 41:AM:316:VAL:HB | 41:AM:366:THR:HG22 | 2.01 | 0.42 |
| 41:AO:61:PRO:HG2 | 41:AO:84:ILE:HG23 | 2.01 | 0.42 |
| 41:AO:427:ALA:O | 41:AO:428:CYS:C | 2.57 | 0.42 |
| 41:AP:307:HIS:ND1 | 41:AP:376:GLU:OE2 | 2.50 | 0.42 |
| 40:BF:33:ASP:OD2 | 40:BF:34:GLY:N | 2.52 | 0.42 |
| 40:BF:101:ASN:HD22 | 41:BM:256:ASN:ND2 | 2.17 | 0.42 |
| 40:BF:171:ILE:HG21 | 42:BF:501:GTP:H1' | 2.01 | 0.42 |
| 41:BN:318:ARG:HE | 41:BN:358:PRO:HD3 | 1.84 | 0.42 |
| 40:CA:252:LEU:HD12 | 40:CA:252:LEU:HA | 1.75 | 0.42 |
| 40:CI:88:HIS:HB3 | 40:CI:91:GLN:OE1 | 2.19 | 0.42 |
| 41:CM:218:THR:C | 41:CM:220:PRO:HD3 | 2.39 | 0.42 |
| 40:DA:177:VAL:O | 40:DA:178:SER:C | 2.57 | 0.42 |
| 40:DA:190:THR:O | 40:DA:193:THR:N | 2.51 | 0.42 |
| 41:DB:7:LEU:HB3 | 41:DB:135:LEU:HG | 2.01 | 0.42 |
| 41:DB:285:THR:O | 41:DB:286:VAL:C | 2.57 | 0.42 |
| 40:DF:21:TRP:HA | 40:DF:24:TYR:CD2 | 2.55 | 0.42 |
| 40:DH:180:ALA:HB3 | 40:DH:183:GLU:HB2 | 2.02 | 0.42 |
| 40:DH:259:LEU:HD11 | 40:DH:377:LEU:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DH:416:GLU:O | 40:DH:417:PHE:C | 2.58 | 0.42 |
| 40:DI:168:GLU:OE2 | 40:DI:198:SER:HB2 | 2.18 | 0.42 |
| 40:DI:324:VAL:HG13 | 40:DI:327:ASP:HB2 | 2.00 | 0.42 |
| 41:DL:154:LYS:HA | 41:DL:154:LYS:HD2 | 1.71 | 0.42 |
| 41:DN:123:GLU:O | 41:DN:125:GLU:N | 2.52 | 0.42 |
| 41:DO:15:GLN:HE22 | 41:DO:226:ASN:HD22 | 1.68 | 0.42 |
| 41:DP:350:LYS:HA | 41:DP:350:LYS:HD2 | 1.71 | 0.42 |
| 40:EF:395:ASP:OD1 | 40:EF:421:ARG:NE | 2.40 | 0.42 |
| 40:EH:236:SER:O | 40:EH:237:SER:C | 2.57 | 0.42 |
| 40:EI:114:LEU:O | 40:EI:115:ILE:C | 2.56 | 0.42 |
| 41:EL:289:LEU:HD13 | 41:EL:365:ALA:HB2 | 2.01 | 0.42 |
| 41:EM:58:LYS:HA | 41:EM:58:LYS:HD2 | 1.64 | 0.42 |
| 41:EM:186:THR:HG21 | 41:EM:385:PHE:CD2 | 2.54 | 0.42 |
| 41:EO:176:SER:OG | 41:EO:178:THR:O | 2.38 | 0.42 |
| 41:EP:11:GLN:O | 41:EP:12:CYS:C | 2.58 | 0.42 |
| 41:EP:95:SER:OG | 41:EP:96:GLY:N | 2.51 | 0.42 |
| 41:EP:295:ASP:C | 41:EP:297:LYS:H | 2.21 | 0.42 |
| 40:FA:217:LEU:HG | 40:FA:219:ILE:HD11 | 2.01 | 0.42 |
| 40:FA:311:LYS:N | 40:FA:381:THR:OG1 | 2.40 | 0.42 |
| 40:FA:319:TYR:N | 40:FA:354:GLY:O | 2.51 | 0.42 |
| 40:FI:297:GLU:HA | 40:FI:298:PRO:HD3 | 1.78 | 0.42 |
| 41:FM:273:LEU:HD23 | 41:FM:273:LEU:HA | 1.85 | 0.42 |
| 41:FP:134:GLN:HA | 41:FP:165:ASN:O | 2.20 | 0.42 |
| 40:GE:115:ILE:HG21 | 40:GE:156:ARG:HH22 | 1.84 | 0.42 |
| 40:GE:133:GLN:HG3 | 40:GE:242:LEU:HD11 | 2.01 | 0.42 |
| 40:GE:401:ARG:HD3 | 40:GE:401:ARG:HA | 1.74 | 0.42 |
| 40:GH:6:SER:O | 40:GH:65:ALA:HA | 2.19 | 0.42 |
| 40:GH:118:VAL:O | 40:GH:122:ILE:HG13 | 2.20 | 0.42 |
| 40:GI:104:ALA:O | 40:GI:106:GLY:N | 2.49 | 0.42 |
| 41:GM:316:VAL:HB | 41:GM:366:THR:HB | 2.02 | 0.42 |
| 41:GO:314:ALA:HA | 41:GO:350:LYS:HB3 | 2.01 | 0.42 |
| 40:HE:188:ILE:HD12 | 40:HE:424:MET:HG2 | 2.00 | 0.42 |
| 40:HF:356:ASN:OD1 | 40:HF:357:TYR:N | 2.53 | 0.42 |
| 40:HG:269:LEU:HD22 | 40:HG:303:VAL:HG11 | 2.01 | 0.42 |
| 41:HM:21:TRP:HA | 41:HM:24:ILE:HG22 | 2.01 | 0.42 |
| 41:HM:99:ASN:HB2 | 41:HM:141:GLY:HA2 | 2.00 | 0.42 |
| 41:HM:376:GLU:O | 41:HM:380:ARG:HG3 | 2.19 | 0.42 |
| 41:HM:404:ASP:N | 41:HM:404:ASP:OD1 | 2.52 | 0.42 |
| 41:HN:106:TYR:HD2 | 41:HN:403:MET:HG2 | 1.84 | 0.42 |
| 41:HN:292:GLN:O | 41:HN:295:ASP:HB2 | 2.19 | 0.42 |
| 41:HN:376:GLU:O | 41:HN:380:ARG:HG3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HO:362:LYS:HE2 | 41:HO:362:LYS:HB2 | 1.90 | 0.42 |
| 41:HP:362:LYS:HD2 | 41:HP:363:MET:HB2 | 2.01 | 0.42 |
| 41:IM:107:THR:O | 41:IM:109:GLY:N | 2.52 | 0.42 |
| 41:IM:183:TYR:OH | 41:IM:388:MET:O | 2.33 | 0.42 |
| 41:IQ:87:PRO:HB2 | 40:JH:280:LYS:NZ | 2.35 | 0.42 |
| 41:IQ:362:LYS:HA | 41:IQ:362:LYS:HD3 | 1.74 | 0.42 |
| 41:JB:101:TRP:HZ3 | 41:JB:106:TYR:HE2 | 1.67 | 0.42 |
| 41:JB:190:HIS:HE1 | 41:JB:410:GLU:HG2 | 1.85 | 0.42 |
| 40:JD:174:ALA:HB3 | 40:JD:178:SER:H | 1.85 | 0.42 |
| 40:JE:271:THR:OG1 | 40:JE:301:GLN:OE1 | 2.37 | 0.42 |
| 40:JE:326:LYS:HA | 40:JE:326:LYS:HD3 | 1.78 | 0.42 |
| 40:JF:429:LYS:O | 40:JF:432:GLU:HG2 | 2.20 | 0.42 |
| 40:JH:312:TYR:HD1 | 40:JH:341:ILE:HG23 | 1.84 | 0.42 |
| 41:JL:142:GLY:O | 41:JL:144:GLY:N | 2.52 | 0.42 |
| 40:KA:385:GLU:O | 40:KA:389:ARG:HG2 | 2.20 | 0.42 |
| 40:KF:405:HIS:HA | 40:KF:408:VAL:HG12 | 1.99 | 0.42 |
| 40:KG:261:PRO:O | 41:KO:396:HIS:NE2 | 2.47 | 0.42 |
| 40:KG:320:ARG:HG2 | 40:KG:356:ASN:HB2 | 2.01 | 0.42 |
| 40:KH:252:LEU:HA | 40:KH:255:PHE:HD2 | 1.83 | 0.42 |
| 41:KL:29:GLY:O | 41:KL:30:ILE:C | 2.56 | 0.42 |
| 41:KL:36:TYR:CE1 | 41:KL:38:GLY:HA3 | 2.54 | 0.42 |
| 41:KL:152:ILE:H | 41:KL:152:ILE:HG13 | 1.61 | 0.42 |
| 41:KL:418:LEU:HD12 | 41:KL:418:LEU:HA | 1.80 | 0.42 |
| 40:LA:188:ILE:HG22 | 40:LA:420:ALA:HB1 | 2.00 | 0.42 |
| 40:LH:274:PRO:HG3 | 40:LH:286:LEU:HD23 | 2.01 | 0.42 |
| 40:LH:404:VAL:HA | 40:LH:407:TYR:HD1 | 1.83 | 0.42 |
| 41:LL:207:LEU:HB3 | 41:LL:225:LEU:HG | 2.01 | 0.42 |
| 41:LM:139:LEU:HD12 | 41:LM:170:VAL:HG22 | 2.02 | 0.42 |
| 41:LN:263:LEU:HD21 | 41:LN:421:PRO:HB2 | 2.01 | 0.42 |
| 40:MA:287:SER:O | 40:MA:291:ILE:HG23 | 2.20 | 0.42 |
| 40:MA:348:PRO:CB | 41:MB:384:GLN:HG2 | 2.49 | 0.42 |
| 40:MD:169:PHE:CE2 | 40:MD:235:VAL:HG22 | 2.54 | 0.42 |
| 40:MF:127:ASP:C | 40:MF:129:CYS:H | 2.23 | 0.42 |
| 40:MF:228:ASN:CB | 42:MM:501:GTP:HN21 | 2.32 | 0.42 |
| 40:MF:424:MET:HE2 | 40:MF:424:MET:HB3 | 1.94 | 0.42 |
| 40:MH:206:ASN:ND2 | 42:MH:501:GTP:O2' | 2.53 | 0.42 |
| 41:MO:196:THR:HG21 | 41:MO:199:THR:OG1 | 2.19 | 0.42 |
| 41:MO:222:TYR:O | 41:MO:226:ASN:ND2 | 2.53 | 0.42 |
| 41:MO:393:ALA:O | 41:MO:394:PHE:C | 2.57 | 0.42 |
| 40:ND:383:ILE:O | 40:ND:384:ALA:C | 2.57 | 0.42 |
| 40:NF:67:PHE:HB3 | 40:NF:75:ILE:HD12 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NF:333:ALA:O | 40:NF:337:THR:HG23 | 2.19 | 0.42 |
| 40:NG:88:HIS:HA | 40:NG:89:PRO:HD3 | 1.85 | 0.42 |
| 40:NH:96:LYS:HA | 40:NH:96:LYS:HD2 | 1.79 | 0.42 |
| 41:NL:257:MET:HA | 41:NL:312:THR:HG21 | 2.00 | 0.42 |
| 41:NN:148:GLY:O | 41:NN:152:ILE:HG12 | 2.19 | 0.42 |
| 41:NN:309:ARG:N | 41:NN:372:THR:OG1 | 2.43 | 0.42 |
| 41:NP:191:GLN:O | 41:NP:195:ASN:CB | 2.58 | 0.42 |
| 41:NP:331:LEU:HA | 41:NP:334:GLN:HE21 | 1.85 | 0.42 |
| 41:OB:388:MET:HE2 | 41:OB:388:MET:HB3 | 1.96 | 0.42 |
| 40:OE:320:ARG:NH2 | 40:OE:360:PRO:HA | 2.34 | 0.42 |
| 40:OH:209:ILE:HG12 | 40:OH:227:LEU:HB3 | 2.00 | 0.42 |
| 41:ON:202:ILE:HD13 | 41:ON:229:VAL:HG13 | 2.00 | 0.42 |
| 41:PB:286:VAL:HG23 | 41:PB:287:PRO:HD3 | 2.00 | 0.42 |
| 40:PD:31:GLN:HA | 40:PD:32:PRO:HD3 | 1.79 | 0.42 |
| 40:PG:8:HIS:HD2 | 40:PG:67:PHE:CE1 | 2.38 | 0.42 |
| 40:PG:108:TYR:O | 40:PG:112:LYS:NZ | 2.47 | 0.42 |
| 40:PH:73:THR:HA | 40:PH:76:ASP:HB3 | 2.02 | 0.42 |
| 41:PP:50:TYR:OH | 41:PP:237:THR:OG1 | 2.36 | 0.42 |
| 41:PP:105:HIS:HA | 41:PP:150:LEU:HD22 | 2.01 | 0.42 |
| 41:PP:208:TYR:CE1 | 41:PP:225:LEU:HD21 | 2.54 | 0.42 |
| 41:PP:228:LEU:O | 41:PP:232:THR:HG23 | 2.19 | 0.42 |
| 40:QA:391:ASP:HB3 | 40:QA:421:ARG:NH2 | 2.34 | 0.42 |
| 41:QB:5:VAL:HG13 | 41:QB:63:ALA:HA | 2.00 | 0.42 |
| 41:QB:265:PHE:CB | 41:QB:374:ILE:HG12 | 2.49 | 0.42 |
| 41:QB:280:GLN:H | 41:QB:280:GLN:HG3 | 1.48 | 0.42 |
| 41:QB:284:LEU:HD12 | 41:QB:284:LEU:HA | 1.87 | 0.42 |
| 41:QB:421:PRO:O | 41:QB:425:ARG:HG2 | 2.20 | 0.42 |
| 40:QF:118:VAL:O | 40:QF:122:ILE:HG12 | 2.19 | 0.42 |
| 40:QF:405:HIS:CG | 41:QM:261:PRO:HG3 | 2.54 | 0.42 |
| 40:QF:416:GLU:OE2 | 40:QF:416:GLU:N | 2.46 | 0.42 |
| 40:QG:133:GLN:HB3 | 40:QG:252:LEU:HD12 | 2.02 | 0.42 |
| 40:QG:210:TYR:CE1 | 40:QG:227:LEU:HD11 | 2.53 | 0.42 |
| 41:QP:98:GLY:O | 41:QP:99:ASN:C | 2.58 | 0.42 |
| 41:QP:286:VAL:HB | 41:QP:325:GLU:HG2 | 2.00 | 0.42 |
| 41:QP:415:MET:H | 41:QP:415:MET:HG2 | 1.72 | 0.42 |
| 40:RE:21:TRP:CZ3 | 40:RE:63:PRO:HB3 | 2.55 | 0.42 |
| 40:RE:223:THR:OG1 | 40:RE:224:TYR:N | 2.52 | 0.42 |
| 40:RG:323:VAL:HA | 40:RG:372:ARG:NH2 | 2.34 | 0.42 |
| 40:RI:255:PHE:HZ | 40:RI:318:LEU:HD21 | 1.84 | 0.42 |
| 41:RP:239:CYS:HB3 | 41:RP:248:ALA:H | 1.83 | 0.42 |
| 40:SA:225:THR:O | 40:SA:229:ARG:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SA:258:ASN:HD21 | 41:SB:99:ASN:HB2 | 1.84 | 0.42 |
| 41:SN:226:ASN:ND2 | 43:SN:502:GDP:O6 | 2.52 | 0.42 |
| 41:SO:81:PHE:HD1 | 41:SO:84:ILE:HG12 | 1.83 | 0.42 |
| 41:SO:339:SER:O | 41:SO:341:PHE:N | 2.46 | 0.42 |
| 41:SO:397:TRP:O | 41:SO:398:TYR:C | 2.57 | 0.42 |
| 40:TA:234:ILE:HD11 | 40:TA:272:TYR:HB2 | 2.02 | 0.42 |
| 40:TE:185:TYR:HE2 | 40:TE:403:PHE:HB2 | 1.84 | 0.42 |
| 40:TF:71:GLU:HA | 40:TF:72:PRO:HD3 | 1.86 | 0.42 |
| 40:TF:231:ILE:HA | 40:TF:234:ILE:HG22 | 2.01 | 0.42 |
| 40:TG:401:ARG:HD3 | 40:TG:404:VAL:HG11 | 2.02 | 0.42 |
| 40:TH:69:ASP:OD2 | 40:TH:70:LEU:N | 2.52 | 0.42 |
| 40:TH:421:ARG:HH12 | 40:TH:425:ALA:HB2 | 1.83 | 0.42 |
| 41:TP:287:PRO:HA | 41:TP:329:GLN:OE1 | 2.19 | 0.42 |
| 40:UE:276:ILE:H | 40:UE:276:ILE:HG12 | 1.62 | 0.42 |
| 40:VA:231:ILE:O | 40:VA:235:VAL:HG23 | 2.19 | 0.42 |
| 41:VB:183:TYR:OH | 41:VB:388:MET:O | 2.38 | 0.42 |
| 41:VB:304:ASP:HA | 41:VB:305:PRO:HD3 | 1.93 | 0.42 |
| 40:VF:276:ILE:HG23 | 40:VF:280:LYS:HE3 | 2.01 | 0.42 |
| 40:VG:76:ASP:HA | 40:VG:79:ARG:HG2 | 2.01 | 0.42 |
| 40:VG:139:HIS:ND1 | 40:VG:146:GLY:O | 2.49 | 0.42 |
| 40:VI:2:ARG:HE | 40:VI:2:ARG:HB2 | 1.72 | 0.42 |
| 40:VJ:316:CYS:SG | 40:VJ:377:LEU:HB2 | 2.60 | 0.42 |
| 41:VQ:139:LEU:HD21 | 41:VQ:192:LEU:HD11 | 2.02 | 0.42 |
| 41:WB:20:PHE:HA | 41:WB:230:SER:OG | 2.19 | 0.42 |
| 41:WB:209:ASP:HA | 41:WB:213:ARG:NH2 | 2.34 | 0.42 |
| 40:WE:425:ALA:HB1 | 40:WE:429:LYS:HZ1 | 1.83 | 0.42 |
| 40:WG:68:VAL:HG11 | 40:WG:149:PHE:CE2 | 2.54 | 0.42 |
| 40:WG:141:PHE:CE2 | 40:WG:191:THR:HB | 2.54 | 0.42 |
| 40:WI:402:ALA:HB2 | 41:WP:344:TRP:HZ3 | 1.84 | 0.42 |
| 41:WQ:204:ASN:OD1 | 43:WQ:501:GDP:O2' | 2.35 | 0.42 |
| 7:1T:72:ILE:HG22 | 7:1T:79:ILE:HG13 | 2.01 | 0.42 |
| 7:1U:185:TRP:CZ3 | 7:1U:196:PRO:HB3 | 2.55 | 0.42 |
| 11:2I:177:GLN:HG2 | 11:2I:178:GLU:N | 2.33 | 0.42 |
| 12:2N:109:LEU:HD23 | 12:2N:145:VAL:HG11 | 2.01 | 0.42 |
| 12:2P:183:GLY:O | 12:2P:187:VAL:HG23 | 2.20 | 0.42 |
| 13:2V:37:ILE:HG22 | 13:2V:161:ARG:HH22 | 1.85 | 0.42 |
| 13:2V:51:GLY:HA3 | 13:2V:57:THR:HG21 | 2.00 | 0.42 |
| 13:2V:129:TRP:HB3 | 13:2V:183:LEU:HD21 | 2.01 | 0.42 |
| 15:3F:188:CYS:SG | 15:3G:320:ARG:HG3 | 2.60 | 0.42 |
| 16:3J:122:CYS:O | 16:3J:124:ARG:NH1 | 2.53 | 0.42 |
| 16:3J:145:GLU:HA | 16:3J:148:LYS:HD3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:3P:337:TRP:HZ3 | 17:3P:480:PHE:HB2 | 1.85 | 0.42 |
| 17:3R:97:ASP:O | 17:3R:100:TYR:N | 2.51 | 0.42 |
| 17:3R:188:THR:O | 17:3R:191:PRO:HD2 | 2.20 | 0.42 |
| 17:3R:339:GLN:OE1 | 17:3R:339:GLN:HA | 2.19 | 0.42 |
| 18:3T:236:THR:OG1 | 18:3T:237:ASP:N | 2.52 | 0.42 |
| 18:3T:307:ARG:NH1 | 18:3T:310:GLU:OE2 | 2.52 | 0.42 |
| 18:3T:311:LEU:HD23 | 18:3T:423:LEU:HD23 | 2.01 | 0.42 |
| 18:3U:120:HIS:CE1 | 18:3U:265:LEU:HG | 2.55 | 0.42 |
| 18:3U:168:VAL:HG11 | 18:3V:56:TRP:HB2 | 2.00 | 0.42 |
| 21:4D:288:PHE:CD2 | 41:CB:77:ARG:HG3 | 2.54 | 0.42 |
| 21:4D:410:ILE:H | 21:4D:410:ILE:HG12 | 1.44 | 0.42 |
| 21:4E:477:SER:O | 21:4E:478:SER:C | 2.58 | 0.42 |
| 21:4F:87:PRO:HB3 | 40:ME:58:ALA:HB2 | 2.01 | 0.42 |
| 21:4F:134:ILE:HD12 | 21:4F:147:LYS:HA | 2.02 | 0.42 |
| 22:4I:79:LEU:HB3 | 22:4I:174:THR:HG23 | 2.02 | 0.42 |
| 22:4J:282:ARG:HH22 | 41:CN:80:PRO:CD | 2.33 | 0.42 |
| 22:4J:558:LYS:HB3 | 22:4J:561:GLU:OE1 | 2.19 | 0.42 |
| 23:4M:186:GLY:O | 23:4M:188:THR:N | 2.52 | 0.42 |
| 23:4P:253:TYR:O | 23:4P:254:LYS:C | 2.58 | 0.42 |
| 23:4Q:193:ARG:HH11 | 41:CO:56:GLY:H | 1.67 | 0.42 |
| 23:4R:173:SER:HB2 | 23:4R:181:LYS:CA | 2.45 | 0.42 |
| 26:4V:61:PHE:HE1 | 26:4V:93:LYS:HZ1 | 1.66 | 0.42 |
| 26:4V:369:GLN:O | 26:4V:374:ILE:HG12 | 2.18 | 0.42 |
| 26:4W:181:SER:HB2 | 26:4W:203:ASN:HB3 | 2.02 | 0.42 |
| 26:4W:311:MET:HE3 | 26:4W:311:MET:HB2 | 1.90 | 0.42 |
| 33:5N:302:LEU:HD12 | 33:5N:302:LEU:HA | 1.93 | 0.42 |
| 34:5R:403:GLU:O | 34:5R:406:GLN:HG3 | 2.19 | 0.42 |
| 38:6C:124:PHE:HD1 | 40:VH:308:ARG:HD3 | 1.84 | 0.42 |
| 39:6F:131:GLU:O | 39:6F:136:TYR:N | 2.53 | 0.42 |
| 41:AB:325:GLU:OE1 | 40:AG:221:ARG:NH1 | 2.40 | 0.42 |
| 40:AF:112:LYS:HA | 40:AF:115:ILE:HG22 | 2.01 | 0.42 |
| 40:AF:346:TRP:CD1 | 41:AN:391:ARG:HD3 | 2.54 | 0.42 |
| 40:AH:228:ASN:OD1 | 42:AH:501:GTP:N1 | 2.48 | 0.42 |
| 41:AL:316:VAL:HG23 | 41:AL:366:THR:HB | 2.00 | 0.42 |
| 41:AN:34:GLY:C | 41:AN:58:LYS:HD3 | 2.39 | 0.42 |
| 41:AN:137:HIS:O | 41:AN:168:SER:HA | 2.19 | 0.42 |
| 40:BE:40:LYS:HB3 | 40:BE:40:LYS:HE2 | 1.50 | 0.42 |
| 40:BE:118:VAL:O | 40:BE:122:ILE:HG13 | 2.19 | 0.42 |
| 40:BE:279:GLU:H | 40:BE:279:GLU:HG2 | 1.45 | 0.42 |
| 40:BG:11:GLN:HA | 40:BG:74:VAL:HG11 | 2.01 | 0.42 |
| 40:BG:102:ASN:HB3 | 40:BG:105:ARG:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BG:175:PRO:HG3 | 40:BG:304:LYS:HB2 | 2.01 | 0.42 |
| 40:BH:215:ARG:HE | 40:BH:215:ARG:HB2 | 1.44 | 0.42 |
| 41:BL:139:LEU:N | 41:BL:169:VAL:O | 2.49 | 0.42 |
| 41:BN:383:GLU:HA | 41:BN:386:THR:HG22 | 2.02 | 0.42 |
| 41:BO:358:PRO:CG | 41:BO:364:SER:HB3 | 2.40 | 0.42 |
| 41:BP:153:SER:OG | 41:BP:154:LYS:N | 2.52 | 0.42 |
| 40:CA:240:ALA:HA | 40:CA:243:ARG:HH11 | 1.84 | 0.42 |
| 40:CA:431:TYR:HA | 40:CA:434:VAL:HG12 | 2.01 | 0.42 |
| 40:CF:398:TYR:OH | 40:CF:414:GLU:OE2 | 2.33 | 0.42 |
| 41:CL:162:ARG:HD3 | 41:CL:162:ARG:HA | 1.36 | 0.42 |
| 41:CL:239:CYS:C | 41:CL:241:ARG:H | 2.23 | 0.42 |
| 41:CM:53:GLU:HG3 | 41:CM:59:TYR:CZ | 2.55 | 0.42 |
| 41:CM:101:TRP:CE3 | 41:CM:187:LEU:HB3 | 2.55 | 0.42 |
| 41:CN:398:TYR:C | 41:CN:400:GLY:H | 2.21 | 0.42 |
| 41:CO:167:PHE:CE1 | 41:CO:233:MET:HG2 | 2.55 | 0.42 |
| 41:CP:273:LEU:HD12 | 41:CP:273:LEU:HA | 1.71 | 0.42 |
| 40:DA:324:VAL:HG21 | 41:DB:219:THR:HG22 | 2.00 | 0.42 |
| 41:DB:200:TYR:O | 41:DB:201:CYS:C | 2.57 | 0.42 |
| 41:DB:276:ARG:HE | 41:DB:276:ARG:HB2 | 1.62 | 0.42 |
| 40:DE:185:TYR:HA | 40:DE:394:PHE:CE1 | 2.55 | 0.42 |
| 40:DF:3:GLU:HB3 | 40:DF:4:CYS:H | 1.63 | 0.42 |
| 40:DF:70:LEU:H | 40:DF:145:THR:HG21 | 1.85 | 0.42 |
| 40:DF:337:THR:O | 40:DF:339:ARG:N | 2.52 | 0.42 |
| 40:DF:403:PHE:HZ | 41:DM:312:THR:HG21 | 1.84 | 0.42 |
| 40:DG:21:TRP:CH2 | 40:DG:52:PHE:HB3 | 2.54 | 0.42 |
| 40:DH:51:THR:OG1 | 40:DH:243:ARG:HD3 | 2.20 | 0.42 |
| 40:DH:101:ASN:ND2 | 40:DH:142:GLY:O | 2.52 | 0.42 |
| 40:DI:23:LEU:O | 40:DI:27:GLU:HG2 | 2.18 | 0.42 |
| 40:DI:337:THR:O | 40:DI:339:ARG:N | 2.52 | 0.42 |
| 40:DI:421:ARG:HD2 | 40:DI:421:ARG:HA | 1.32 | 0.42 |
| 41:DL:183:TYR:HB2 | 41:DL:398:TYR:CZ | 2.54 | 0.42 |
| 41:DL:216:LYS:HD2 | 41:DL:216:LYS:HA | 1.37 | 0.42 |
| 41:DM:73:MET:O | 41:DM:74:ASP:C | 2.57 | 0.42 |
| 41:DM:130:LEU:O | 41:DM:162:ARG:HD2 | 2.19 | 0.42 |
| 41:DM:257:MET:HA | 41:DM:312:THR:HB | 2.00 | 0.42 |
| 41:DN:193:VAL:HA | 41:DN:264:HIS:CE1 | 2.55 | 0.42 |
| 40:EA:185:TYR:OH | 40:EA:397:MET:O | 2.36 | 0.42 |
| 40:EH:104:ALA:O | 40:EH:105:ARG:C | 2.58 | 0.42 |
| 40:EI:21:TRP:CZ3 | 40:EI:52:PHE:HB3 | 2.55 | 0.42 |
| 40:EI:109:THR:O | 40:EI:110:ILE:C | 2.56 | 0.42 |
| 40:EI:116:ASP:OD1 | 40:EI:116:ASP:N | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EI:210:TYR:CE1 | 41:EP:324:LYS:HG2 | 2.55 | 0.42 |
| 41:EM:61:PRO:HD2 | 41:EM:84:ILE:O | 2.19 | 0.42 |
| 41:EM:254:ALA:O | 41:EM:256:ASN:N | 2.52 | 0.42 |
| 41:EP:295:ASP:N | 41:EP:295:ASP:OD1 | 2.51 | 0.42 |
| 40:FA:117:LEU:O | 40:FA:118:VAL:C | 2.55 | 0.42 |
| 40:FF:255:PHE:CZ | 40:FF:318:LEU:HD21 | 2.55 | 0.42 |
| 40:FI:181:VAL:HG23 | 40:FI:182:VAL:HG13 | 2.02 | 0.42 |
| 41:FM:240:LEU:HD22 | 41:FM:249:ASP:HA | 2.02 | 0.42 |
| 41:FP:421:PRO:O | 41:FP:425:ARG:HG2 | 2.20 | 0.42 |
| 40:GF:139:HIS:HE1 | 40:GF:168:GLU:HB3 | 1.84 | 0.42 |
| 40:GG:276:ILE:HD12 | 40:GG:276:ILE:HA | 1.77 | 0.42 |
| 40:GH:94:THR:HB | 40:GH:95:GLY:H | 1.58 | 0.42 |
| 40:GH:152:LEU:HD12 | 40:GH:152:LEU:HA | 1.77 | 0.42 |
| 40:GH:168:GLU:HG2 | 40:GH:169:PHE:N | 2.35 | 0.42 |
| 40:GH:285:GLN:O | 40:GH:285:GLN:HG3 | 2.20 | 0.42 |
| 40:HE:269:LEU:HB3 | 40:HE:270:ALA:H | 1.74 | 0.42 |
| 40:HE:281:ALA:O | 40:HE:282:TYR:C | 2.58 | 0.42 |
| 40:HE:429:LYS:HD2 | 40:HE:429:LYS:HA | 1.64 | 0.42 |
| 40:HF:254:GLU:HG3 | 41:HN:98:GLY:HA2 | 2.01 | 0.42 |
| 40:HG:105:ARG:HE | 40:HG:105:ARG:HB3 | 1.49 | 0.42 |
| 41:HN:51:TYR:CZ | 41:HN:61:PRO:HG3 | 2.54 | 0.42 |
| 41:HN:143:THR:O | 41:HN:144:GLY:C | 2.57 | 0.42 |
| 41:HN:226:ASN:ND2 | 43:HN:501:GDP:HN1 | 2.18 | 0.42 |
| 41:HP:77:ARG:NH2 | 41:HP:83:GLN:OE1 | 2.53 | 0.42 |
| 41:HQ:238:THR:HG21 | 41:HQ:318:ARG:HD2 | 2.01 | 0.42 |
| 40:IF:260:VAL:HG12 | 40:IF:266:HIS:HA | 2.01 | 0.42 |
| 40:IH:288:VAL:HG22 | 40:IH:372:ARG:HD3 | 2.00 | 0.42 |
| 40:II:269:LEU:HD22 | 40:II:303:VAL:HG22 | 2.01 | 0.42 |
| 40:II:319:TYR:CD2 | 40:II:323:VAL:HG11 | 2.55 | 0.42 |
| 41:IM:139:LEU:HG | 41:IM:168:SER:HB3 | 2.02 | 0.42 |
| 41:IO:21:TRP:CZ3 | 41:IO:24:ILE:HD11 | 2.54 | 0.42 |
| 41:IQ:257:MET:HE3 | 41:IQ:266:PHE:CE1 | 2.54 | 0.42 |
| 40:JA:291:ILE:HG22 | 40:JA:374:VAL:HG12 | 2.00 | 0.42 |
| 40:JD:153:LEU:HG | 40:JD:157:LEU:HD23 | 2.01 | 0.42 |
| 40:JF:205:ASP:HB3 | 40:JF:303:VAL:HA | 2.00 | 0.42 |
| 40:JF:282:TYR:OH | 40:JF:369:LYS:HB2 | 2.19 | 0.42 |
| 40:JG:26:LEU:HD21 | 40:JG:363:VAL:HG12 | 2.01 | 0.42 |
| 40:JH:71:GLU:HG2 | 40:JH:98:ASP:OD1 | 2.20 | 0.42 |
| 41:JL:311:LEU:HD23 | 41:JL:311:LEU:HA | 1.91 | 0.42 |
| 41:KB:191:GLN:O | 41:KB:195:ASN:ND2 | 2.51 | 0.42 |
| 41:KB:256:ASN:ND2 | 41:KB:350:LYS:HD3 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KB:313:VAL:HB | 41:KB:349:VAL:HG22 | 1.99 | 0.42 |
| 40:KD:276:ILE:HG23 | 40:KD:281:ALA:HB2 | 2.01 | 0.42 |
| 40:KE:179:THR:HA | 41:KL:351:THR:HG23 | 2.01 | 0.42 |
| 40:KE:231:ILE:HA | 40:KE:234:ILE:HD12 | 2.01 | 0.42 |
| 40:KG:204:VAL:HG12 | 40:KG:209:ILE:HD11 | 2.01 | 0.42 |
| 41:KL:335:ASN:O | 41:KL:338:SER:HB2 | 2.20 | 0.42 |
| 41:KP:232:THR:HG21 | 41:KP:268:PRO:HB2 | 2.02 | 0.42 |
| 40:LE:177:VAL:HG22 | 41:LL:331:LEU:HD22 | 2.01 | 0.42 |
| 40:LG:180:ALA:HB3 | 40:LG:183:GLU:HG3 | 2.01 | 0.42 |
| 40:MA:192:HIS:O | 40:MA:192:HIS:CG | 2.72 | 0.42 |
| 40:MA:252:LEU:HD23 | 40:MA:255:PHE:CE2 | 2.53 | 0.42 |
| 40:MF:101:ASN:O | 40:MF:182:VAL:HG21 | 2.20 | 0.42 |
| 40:MG:376:MET:HB2 | 40:MG:376:MET:HE3 | 1.65 | 0.42 |
| 40:MH:203:MET:HE1 | 40:MH:267:PHE:HB3 | 2.01 | 0.42 |
| 40:MH:327:ASP:OD1 | 40:MH:328:VAL:N | 2.52 | 0.42 |
| 41:MO:260:PHE:O | 41:MO:261:PRO:C | 2.58 | 0.42 |
| 41:MP:125:GLU:HA | 41:MP:127:CYS:HB2 | 2.01 | 0.42 |
| 40:NA:265:ILE:HG21 | 40:NA:313:MET:HE1 | 2.01 | 0.42 |
| 40:ND:140:SER:C | 40:ND:142:GLY:H | 2.21 | 0.42 |
| 40:NE:297:GLU:HA | 40:NE:298:PRO:HD3 | 1.84 | 0.42 |
| 40:NH:177:VAL:HB | 41:NO:327:ASP:HB3 | 2.01 | 0.42 |
| 41:NM:174:LYS:HB2 | 41:NM:205:GLU:OE1 | 2.19 | 0.42 |
| 41:NP:143:THR:OG1 | 41:NP:144:GLY:N | 2.52 | 0.42 |
| 40:OA:258:ASN:ND2 | 40:OA:352:LYS:HE3 | 2.33 | 0.42 |
| 42:OB:502:GTP:O2B | 40:OG:145:THR:OG1 | 2.27 | 0.42 |
| 40:OE:370:VAL:HG23 | 40:OE:372:ARG:H | 1.84 | 0.42 |
| 40:OF:188:ILE:HG13 | 40:OF:420:ALA:HB1 | 2.01 | 0.42 |
| 40:OH:224:TYR:HD1 | 40:OH:227:LEU:HD12 | 1.83 | 0.42 |
| 40:OH:369:LYS:H | 40:OH:369:LYS:HG3 | 1.71 | 0.42 |
| 40:PA:15:GLN:HB3 | 40:PA:228:ASN:ND2 | 2.35 | 0.42 |
| 40:PA:194:THR:O | 40:PA:198:SER:OG | 2.30 | 0.42 |
| 41:PB:9:ALA:HA | 41:PB:66:VAL:O | 2.19 | 0.42 |
| 41:PB:142:GLY:O | 41:PB:144:GLY:N | 2.53 | 0.42 |
| 41:PB:221:THR:HG23 | 41:PB:224:ASP:H | 1.84 | 0.42 |
| 41:PB:362:LYS:HG3 | 41:PB:363:MET:HE3 | 2.00 | 0.42 |
| 40:PH:79:ARG:HG2 | 40:PH:92:LEU:HD13 | 1.99 | 0.42 |
| 40:PH:139:HIS:NE2 | 40:PH:168:GLU:OE1 | 2.46 | 0.42 |
| 41:PN:21:TRP:CE3 | 41:PN:24:ILE:HD11 | 2.55 | 0.42 |
| 41:PN:318:ARG:O | 41:PN:363:MET:HA | 2.20 | 0.42 |
| 41:PP:95:SER:OG | 41:PP:96:GLY:N | 2.52 | 0.42 |
| 41:PP:183:TYR:HD2 | 41:PP:398:TYR:HE2 | 1.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QA:263:PRO:HA | 41:QB:396:HIS:CE1 | 2.54 | 0.42 |
| 41:QB:142:GLY:O | 41:QB:145:SER:N | 2.52 | 0.42 |
| 41:QB:202:ILE:CG2 | 41:QB:229:VAL:HG11 | 2.46 | 0.42 |
| 40:QE:70:LEU:H | 40:QE:145:THR:HG21 | 1.85 | 0.42 |
| 40:QH:210:TYR:CZ | 40:QH:227:LEU:HD11 | 2.54 | 0.42 |
| 41:QL:313:VAL:HA | 41:QL:368:ILE:O | 2.20 | 0.42 |
| 41:QN:263:LEU:HD23 | 41:QN:263:LEU:HA | 1.91 | 0.42 |
| 40:RA:329:ASN:ND2 | 41:RB:175:VAL:HG21 | 2.35 | 0.42 |
| 41:RB:232:THR:HG21 | 41:RB:300:MET:HE1 | 2.01 | 0.42 |
| 41:RB:291:GLN:NE2 | 41:RB:292:GLN:OE1 | 2.43 | 0.42 |
| 40:RE:75:ILE:HG22 | 40:RE:79:ARG:HH11 | 1.84 | 0.42 |
| 40:RE:255:PHE:HZ | 40:RE:318:LEU:HD21 | 1.84 | 0.42 |
| 40:RH:232:SER:HA | 40:RH:235:VAL:HG12 | 2.00 | 0.42 |
| 40:RI:89:PRO:HD3 | 40:SI:283:HIS:HD2 | 1.84 | 0.42 |
| 40:RI:229:ARG:HH22 | 40:RI:365:GLY:HA3 | 1.85 | 0.42 |
| 41:RL:5:VAL:HB | 41:RL:133:PHE:CD1 | 2.54 | 0.42 |
| 41:RL:345:ILE:HB | 41:RL:348:ASN:HB3 | 2.01 | 0.42 |
| 41:RO:12:CYS:SG | 41:RO:138:SER:HB3 | 2.59 | 0.42 |
| 40:SF:36:MET:N | 40:SF:36:MET:SD | 2.92 | 0.42 |
| 40:SF:121:ARG:HD3 | 40:SF:125:LEU:HG | 2.01 | 0.42 |
| 40:SG:5:ILE:O | 40:SG:135:PHE:HA | 2.19 | 0.42 |
| 40:SG:36:MET:HG2 | 40:SG:61:HIS:NE2 | 2.34 | 0.42 |
| 40:SH:221:ARG:CZ | 41:SO:325:GLU:HB2 | 2.49 | 0.42 |
| 40:SI:209:ILE:HG23 | 40:SI:230:LEU:HD23 | 2.02 | 0.42 |
| 41:SL:158:GLU:HG3 | 41:SL:159:TYR:CD2 | 2.54 | 0.42 |
| 41:SL:196:THR:OG1 | 41:SL:197:ASP:N | 2.53 | 0.42 |
| 41:SN:314:ALA:HA | 41:SN:350:LYS:O | 2.19 | 0.42 |
| 41:SO:165:ASN:ND2 | 41:SO:200:TYR:OH | 2.52 | 0.42 |
| 41:SO:172:SER:HA | 41:SO:203:ASP:OD1 | 2.19 | 0.42 |
| 41:SO:173:PRO:HB3 | 41:SO:380:ARG:HD2 | 2.02 | 0.42 |
| 41:SO:403:MET:HE2 | 41:SO:403:MET:HB2 | 1.86 | 0.42 |
| 41:TB:12:CYS:O | 41:TB:16:ILE:HG22 | 2.20 | 0.42 |
| 40:TH:21:TRP:CZ3 | 40:TH:52:PHE:HB3 | 2.55 | 0.42 |
| 41:TN:87:PRO:HD3 | 41:UN:281:TYR:CD2 | 2.54 | 0.42 |
| 41:TO:379:LYS:O | 41:TO:382:SER:N | 2.52 | 0.42 |
| 40:UA:101:ASN:HD22 | 41:UN:256:ASN:HD21 | 1.65 | 0.42 |
| 40:UA:136:LEU:HD23 | 40:UA:167:LEU:HB2 | 2.01 | 0.42 |
| 40:UF:305:CYS:O | 40:UF:307:PRO:HD3 | 2.19 | 0.42 |
| 40:UH:320:ARG:HG3 | 40:UH:360:PRO:HD3 | 2.00 | 0.42 |
| 40:UI:5:ILE:HD13 | 40:UI:125:LEU:HB3 | 2.00 | 0.42 |
| 40:UI:11:GLN:HE21 | 40:UI:15:GLN:HE21 | 1.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UI:27:GLU:H | 40:UI:27:GLU:HG3 | 1.69 | 0.42 |
| 40:UI:162:GLY:O | 40:UI:164:LYS:N | 2.52 | 0.42 |
| 41:UP:40:SER:O | 41:UP:42:LEU:N | 2.52 | 0.42 |
| 41:UP:313:VAL:HG13 | 41:UP:367:PHE:HD1 | 1.85 | 0.42 |
| 40:VA:177:VAL:HG13 | 40:VA:178:SER:H | 1.83 | 0.42 |
| 40:VF:121:ARG:HE | 40:VF:121:ARG:HB3 | 1.60 | 0.42 |
| 40:VI:239:THR:HB | 40:VI:242:LEU:HD11 | 2.01 | 0.42 |
| 40:VI:320:ARG:HH21 | 40:VI:360:PRO:HA | 1.83 | 0.42 |
| 40:VJ:175:PRO:HG3 | 40:VJ:304:LYS:HG2 | 2.01 | 0.42 |
| 41:VO:11:GLN:HA | 41:VO:72:THR:HG21 | 2.01 | 0.42 |
| 41:VP:134:GLN:HA | 41:VP:165:ASN:O | 2.20 | 0.42 |
| 41:VP:262:ARG:HE | 41:VP:262:ARG:HB3 | 1.71 | 0.42 |
| 41:VQ:189:VAL:HA | 41:VQ:192:LEU:HB2 | 2.01 | 0.42 |
| 41:VQ:226:ASN:ND2 | 43:VQ:502:GDP:O6 | 2.40 | 0.42 |
| 41:VQ:271:ALA:HB1 | 41:VQ:292:GLN:HB3 | 2.01 | 0.42 |
| 41:WB:8:GLN:HG3 | 41:WB:14:ASN:HA | 2.01 | 0.42 |
| 40:WF:100:ALA:O | 41:WM:255:VAL:HG11 | 2.20 | 0.42 |
| 40:WH:119:LEU:HD11 | 40:WH:156:ARG:HB3 | 2.01 | 0.42 |
| 40:WH:258:ASN:HD22 | 40:WH:352:LYS:HB2 | 1.85 | 0.42 |
| 41:WM:398:TYR:C | 41:WM:400:GLY:H | 2.22 | 0.42 |
| 41:WO:138:SER:OG | 43:WO:502:GDP:O1A | 2.35 | 0.42 |
| 2:1D:22:ARG:NH2 | 40:GH:405:HIS:O | 2.51 | 0.42 |
| 7:1S:453:LEU:HD21 | 7:1S:456:ALA:HB2 | 2.02 | 0.42 |
| 7:1S:474:GLU:O | 7:1S:490:LEU:N | 2.51 | 0.42 |
| 7:1S:586:HIS:NE2 | 7:1S:612:LEU:HB2 | 2.34 | 0.42 |
| 7:1T:124:LEU:HD13 | 7:1T:124:LEU:HA | 1.77 | 0.42 |
| 7:1T:136:SER:HB2 | 40:VF:41:THR:HG21 | 2.02 | 0.42 |
| 7:1U:257:LYS:HG2 | 7:1U:298:LEU:HD21 | 2.00 | 0.42 |
| 7:1U:548:ILE:HA | 7:1U:564:GLY:HA3 | 2.01 | 0.42 |
| 10:2E:75:ARG:NH2 | 40:AE:340:SER:OG | 2.43 | 0.42 |
| 12:2M:73:ARG:NH2 | 12:2M:118:GLU:OE2 | 2.52 | 0.42 |
| 12:2O:49:LYS:HB3 | 12:2O:50:ASN:H | 1.63 | 0.42 |
| 12:2O:135:LEU:HD23 | 12:2O:135:LEU:HA | 1.91 | 0.42 |
| 12:2R:254:CYS:SG | 12:2R:255:LEU:N | 2.89 | 0.42 |
| 13:2U:15:TYR:HD2 | 13:2U:164:ARG:HB2 | 1.83 | 0.42 |
| 13:2U:69:LEU:HD11 | 13:2U:151:THR:HG22 | 2.02 | 0.42 |
| 13:2W:183:LEU:HD12 | 13:2W:183:LEU:HA | 1.83 | 0.42 |
| 13:2X:170:ARG:HB2 | 13:2X:171:LEU:H | 1.66 | 0.42 |
| 14:3A:59:SER:OG | 14:3A:61:TRP:O | 2.28 | 0.42 |
| 15:3F:111:ILE:HD12 | 15:3F:393:MET:HG2 | 2.02 | 0.42 |
| 15:3H:392:HIS:CD2 | 17:3Q:459:LEU:HB3 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:3J:131:ASP:OD2 | 16:3J:268:ARG:NE | 2.52 | 0.42 |
| 17:3R:204:LYS:HE2 | 17:3R:204:LYS:HB2 | 1.76 | 0.42 |
| 19:3Y:193:ARG:HH22 | 41:KN:55:THR:HG21 | 1.83 | 0.42 |
| 21:4D:34:ARG:O | 21:4D:36:GLY:N | 2.50 | 0.42 |
| 21:4D:426:LEU:HB2 | 21:4D:438:PHE:CE2 | 2.52 | 0.42 |
| 21:4D:435:GLY:O | 21:4D:437:ARG:N | 2.53 | 0.42 |
| 21:4E:243:LEU:O | 21:4E:265:HIS:HA | 2.20 | 0.42 |
| 21:4F:474:LYS:HD3 | 21:4F:497:GLU:HB2 | 2.01 | 0.42 |
| 22:4I:125:LEU:HD23 | 41:BO:277:GLY:HA2 | 2.01 | 0.42 |
| 22:4I:619:VAL:HG21 | 22:4I:680:LYS:HG3 | 2.00 | 0.42 |
| 22:4I:629:LYS:HG3 | 22:4I:629:LYS:H | 1.54 | 0.42 |
| 22:4I:653:LEU:HD23 | 22:4I:653:LEU:HA | 1.91 | 0.42 |
| 22:4J:621:ALA:O | 22:4J:622:GLN:C | 2.58 | 0.42 |
| 23:4M:91:ILE:O | 23:4M:92:PRO:C | 2.58 | 0.42 |
| 23:4M:196:PHE:CE2 | 41:CB:53:GLU:HG3 | 2.55 | 0.42 |
| 23:4M:215:GLN:HE21 | 23:4M:216:MET:HB3 | 1.85 | 0.42 |
| 23:4N:253:TYR:O | 23:4N:254:LYS:C | 2.58 | 0.42 |
| 23:4R:190:TYR:HB2 | 41:CP:48:ASN:HD22 | 1.84 | 0.42 |
| 34:5Q:204:LEU:HD21 | 41:GN:360:GLY:HA2 | 2.01 | 0.42 |
| 34:5R:361:ASP:C | 34:5R:363:ILE:N | 2.73 | 0.42 |
| 34:5R:418:GLU:H | 34:5R:418:GLU:HG3 | 1.63 | 0.42 |
| 34:5R:432:GLU:O | 34:5R:435:GLU:HB2 | 2.19 | 0.42 |
| 36:5Y:72:ARG:HD3 | 36:5Y:76:LEU:HD12 | 2.02 | 0.42 |
| 36:5Y:176:THR:HG23 | 36:5Y:178:PHE:H | 1.82 | 0.42 |
| 39:6G:78:LEU:HD13 | 39:6G:146:VAL:HG11 | 2.02 | 0.42 |
| 40:AA:295:CYS:O | 40:AA:301:GLN:NE2 | 2.50 | 0.42 |
| 40:AH:7:VAL:O | 40:AH:137:ILE:HA | 2.19 | 0.42 |
| 41:AL:303:CYS:SG | 41:AL:380:ARG:NH2 | 2.93 | 0.42 |
| 41:AM:311:LEU:HD21 | 41:AM:425:ARG:HB3 | 2.00 | 0.42 |
| 41:AM:375:GLN:HB3 | 41:AM:422:VAL:HG23 | 2.00 | 0.42 |
| 41:AO:149:THR:HB | 41:AO:191:GLN:HE21 | 1.84 | 0.42 |
| 40:BE:344:VAL:HG23 | 40:BE:347:CYS:HB3 | 2.01 | 0.42 |
| 40:BH:129:CYS:O | 40:BH:129:CYS:SG | 2.78 | 0.42 |
| 40:BI:210:TYR:CE2 | 41:BP:324:LYS:HG2 | 2.55 | 0.42 |
| 40:BI:273:ALA:HB3 | 40:BI:374:VAL:N | 2.35 | 0.42 |
| 41:BM:318:ARG:N | 41:BM:321:MET:HE3 | 2.35 | 0.42 |
| 41:BP:270:PHE:HB3 | 41:BP:273:LEU:HD11 | 2.02 | 0.42 |
| 40:CE:206:ASN:OD1 | 42:CE:501:GTP:O2' | 2.23 | 0.42 |
| 40:CE:245:ASP:OD2 | 40:CE:245:ASP:N | 2.52 | 0.42 |
| 40:CG:210:TYR:HD1 | 40:CG:222:PRO:HG2 | 1.84 | 0.42 |
| 40:CH:33:ASP:O | 40:CH:35:GLN:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CH:260:VAL:HG22 | 41:CP:396:HIS:CE1 | 2.54 | 0.42 |
| 40:CH:274:PRO:HG2 | 40:CH:372:ARG:O | 2.19 | 0.42 |
| 40:CH:390:LEU:HD12 | 40:CH:390:LEU:HA | 1.88 | 0.42 |
| 40:CI:241:SER:HB3 | 40:CI:249:ASN:HD22 | 1.84 | 0.42 |
| 41:CL:174:LYS:HB3 | 41:CL:174:LYS:HE2 | 1.57 | 0.42 |
| 41:CN:86:ARG:HG2 | 41:CN:89:ASN:H | 1.85 | 0.42 |
| 41:CN:249:ASP:H | 41:CN:252:LYS:HB3 | 1.83 | 0.42 |
| 41:CO:412:GLU:HG3 | 41:CO:416:ASN:HD21 | 1.85 | 0.42 |
| 41:CP:270:PHE:H | 41:CP:300:MET:HE3 | 1.85 | 0.42 |
| 41:CP:358:PRO:HD3 | 41:CP:364:SER:CB | 2.48 | 0.42 |
| 40:DE:28:HIS:CE1 | 40:DE:243:ARG:HD2 | 2.54 | 0.42 |
| 40:DE:128:GLN:H | 40:DE:128:GLN:HG2 | 1.44 | 0.42 |
| 40:DF:11:GLN:HB3 | 42:DF:501:GTP:O1B | 2.20 | 0.42 |
| 40:DF:53:PHE:HB3 | 40:DF:61:HIS:HB3 | 2.01 | 0.42 |
| 40:DF:405:HIS:NE2 | 41:DM:259:PRO:O | 2.52 | 0.42 |
| 40:DF:415:GLY:O | 40:DF:416:GLU:C | 2.58 | 0.42 |
| 41:DL:238:THR:O | 41:DL:240:LEU:N | 2.52 | 0.42 |
| 41:DL:272:PRO:HG3 | 41:DL:364:SER:CB | 2.49 | 0.42 |
| 41:DL:293:MET:HA | 41:DL:298:ASN:ND2 | 2.35 | 0.42 |
| 41:DM:115:SER:O | 41:DM:118:ASP:HB2 | 2.19 | 0.42 |
| 41:DM:418:LEU:O | 41:DM:419:GLY:C | 2.57 | 0.42 |
| 41:DN:6:HIS:O | 41:DN:64:VAL:HG22 | 2.20 | 0.42 |
| 41:DN:119:VAL:O | 41:DN:120:VAL:C | 2.58 | 0.42 |
| 41:DN:388:MET:O | 41:DN:389:PHE:C | 2.57 | 0.42 |
| 40:EE:332:ILE:O | 40:EE:336:LYS:HG3 | 2.19 | 0.42 |
| 40:EE:371:GLN:HG2 | 40:EE:372:ARG:NE | 2.34 | 0.42 |
| 40:EF:90:GLU:HG2 | 40:EF:121:ARG:NH2 | 2.35 | 0.42 |
| 40:EG:23:LEU:HD11 | 40:EG:233:GLN:NE2 | 2.34 | 0.42 |
| 40:EH:14:VAL:HG13 | 40:EH:67:PHE:CD2 | 2.53 | 0.42 |
| 40:EH:407:TYR:O | 40:EH:408:VAL:C | 2.56 | 0.42 |
| 40:EH:429:LYS:HE2 | 40:EH:429:LYS:HB3 | 1.58 | 0.42 |
| 40:EI:424:MET:O | 40:EI:428:GLU:HG2 | 2.20 | 0.42 |
| 41:EM:150:LEU:HD22 | 41:EM:150:LEU:HA | 1.84 | 0.42 |
| 41:EM:193:VAL:HG22 | 41:EM:265:PHE:CZ | 2.54 | 0.42 |
| 41:EM:233:MET:O | 41:EM:236:VAL:HG12 | 2.20 | 0.42 |
| 41:EM:272:PRO:HG3 | 41:EM:364:SER:CB | 2.49 | 0.42 |
| 41:EM:296:ALA:O | 41:EM:297:LYS:C | 2.57 | 0.42 |
| 41:EP:21:TRP:CD2 | 41:EP:61:PRO:HB3 | 2.55 | 0.42 |
| 41:EP:54:ALA:HA | 41:FP:283:ALA:HA | 2.01 | 0.42 |
| 40:FA:101:ASN:HB3 | 40:FA:182:VAL:CG2 | 2.50 | 0.42 |
| 40:FA:115:ILE:HG12 | 40:FA:152:LEU:HG | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FA:188:ILE:H | 40:FA:188:ILE:HG12 | 1.64 | 0.42 |
| 40:FE:376:MET:SD | 40:FE:378:SER:HB3 | 2.59 | 0.42 |
| 40:FG:274:PRO:HB3 | 40:FG:370:VAL:HG11 | 2.02 | 0.42 |
| 40:FH:176:GLN:N | 40:FH:176:GLN:OE1 | 2.53 | 0.42 |
| 40:FH:288:VAL:HA | 40:FH:291:ILE:HG12 | 2.00 | 0.42 |
| 41:FP:60:VAL:HG11 | 41:FP:86:ARG:HH21 | 1.85 | 0.42 |
| 41:FP:227:HIS:O | 41:FP:230:SER:OG | 2.37 | 0.42 |
| 40:GE:37:PRO:O | 40:GE:39:ASP:N | 2.52 | 0.42 |
| 40:GE:104:ALA:HB1 | 40:GE:411:GLY:H | 1.83 | 0.42 |
| 40:GE:274:PRO:HG3 | 40:GE:291:ILE:HG21 | 2.00 | 0.42 |
| 40:GG:136:LEU:HD23 | 40:GG:167:LEU:HB2 | 2.02 | 0.42 |
| 40:GH:206:ASN:O | 40:GH:207:GLU:C | 2.58 | 0.42 |
| 40:GI:390:LEU:HD12 | 40:GI:390:LEU:HA | 1.74 | 0.42 |
| 41:GM:5:VAL:HB | 41:GM:133:PHE:CD1 | 2.55 | 0.42 |
| 41:GN:189:VAL:O | 41:GN:193:VAL:HG23 | 2.20 | 0.42 |
| 41:GN:202:ILE:H | 41:GN:202:ILE:HG13 | 1.64 | 0.42 |
| 41:GN:357:PRO:HB2 | 41:GN:358:PRO:HD2 | 2.02 | 0.42 |
| 41:GO:296:ALA:O | 41:GO:297:LYS:HD3 | 2.18 | 0.42 |
| 41:HB:87:PRO:HA | 41:HB:90:PHE:HD2 | 1.85 | 0.42 |
| 40:HE:108:TYR:CD2 | 40:HE:412:MET:HG2 | 2.55 | 0.42 |
| 40:HE:194:THR:HA | 40:HE:197:HIS:HD2 | 1.85 | 0.42 |
| 40:HH:12:ALA:O | 40:HH:16:ILE:HG12 | 2.20 | 0.42 |
| 41:HM:36:TYR:CZ | 41:HM:44:LEU:HB2 | 2.55 | 0.42 |
| 41:HO:316:VAL:HA | 41:HO:352:ALA:O | 2.20 | 0.42 |
| 41:HP:207:LEU:HB3 | 41:HP:225:LEU:HD12 | 2.01 | 0.42 |
| 41:HQ:26:ASP:N | 41:HQ:26:ASP:OD1 | 2.52 | 0.42 |
| 41:HQ:156:ARG:HH11 | 41:HQ:164:MET:HE1 | 1.85 | 0.42 |
| 41:HQ:407:GLU:OE2 | 41:HQ:407:GLU:N | 2.52 | 0.42 |
| 41:IB:27:GLU:OE1 | 41:IB:234:SER:OG | 2.37 | 0.42 |
| 40:IE:228:ASN:ND2 | 42:IE:501:GTP:HN1 | 2.12 | 0.42 |
| 40:IF:228:ASN:ND2 | 42:IF:501:GTP:HN1 | 2.11 | 0.42 |
| 40:II:65:ALA:O | 40:II:91:GLN:HG3 | 2.20 | 0.42 |
| 41:IM:171:PRO:HB3 | 41:IM:181:GLU:HB3 | 2.02 | 0.42 |
| 41:IQ:167:PHE:CD1 | 41:IQ:233:MET:HE3 | 2.54 | 0.42 |
| 41:IQ:206:ALA:O | 41:IQ:210:ILE:HG12 | 2.19 | 0.42 |
| 41:JB:318:ARG:HG2 | 41:JB:354:CYS:HB3 | 2.00 | 0.42 |
| 40:JH:20:CYS:HA | 40:JH:232:SER:HB2 | 2.01 | 0.42 |
| 40:JH:153:LEU:HA | 40:JH:153:LEU:HD12 | 1.81 | 0.42 |
| 41:JM:140:GLY:CA | 41:JM:181:GLU:HG2 | 2.49 | 0.42 |
| 41:JM:261:PRO:O | 41:JM:262:ARG:C | 2.58 | 0.42 |
| 41:JM:289:LEU:HD11 | 41:JM:364:SER:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:JM:350:LYS:HA | 41:JM:350:LYS:HD2 | 1.76 | 0.42 |
| 41:KB:285:THR:OG1 | 41:KB:288:GLU:OE2 | 2.37 | 0.42 |
| 41:KB:286:VAL:H | 41:KB:286:VAL:HG22 | 1.61 | 0.42 |
| 41:KB:326:VAL:O | 41:KB:330:MET:HG3 | 2.19 | 0.42 |
| 40:KE:332:ILE:HA | 40:KE:335:ILE:HG22 | 2.01 | 0.42 |
| 40:KF:2:ARG:NH2 | 41:KN:69:GLU:HB3 | 2.31 | 0.42 |
| 40:KG:166:LYS:HB3 | 40:KG:166:LYS:HE3 | 1.86 | 0.42 |
| 40:KG:180:ALA:HB3 | 40:KG:183:GLU:HB2 | 2.00 | 0.42 |
| 40:KH:6:SER:O | 40:KH:65:ALA:HA | 2.20 | 0.42 |
| 40:KH:125:LEU:HD23 | 40:KH:125:LEU:HA | 1.87 | 0.42 |
| 40:KH:254:GLU:HG2 | 41:KP:98:GLY:HA2 | 2.01 | 0.42 |
| 41:KL:30:ILE:HG23 | 41:KL:34:GLY:HA2 | 2.02 | 0.42 |
| 41:KL:297:LYS:HE2 | 41:KL:297:LYS:HB3 | 1.38 | 0.42 |
| 40:LF:102:ASN:O | 40:LF:104:ALA:N | 2.53 | 0.42 |
| 40:LF:228:ASN:CG | 42:LM:501:GTP:HN21 | 2.23 | 0.42 |
| 40:LF:271:THR:HG23 | 40:LF:376:MET:HB3 | 2.01 | 0.42 |
| 40:LH:298:PRO:HB3 | 40:LH:307:PRO:HD2 | 2.01 | 0.42 |
| 41:LN:19:LYS:HD2 | 41:LN:227:HIS:HD2 | 1.84 | 0.42 |
| 41:LN:334:GLN:HE21 | 41:LN:349:VAL:HG23 | 1.85 | 0.42 |
| 41:LO:262:ARG:NH2 | 41:LO:414:ASN:OD1 | 2.52 | 0.42 |
| 40:MA:248:LEU:HD22 | 40:MA:248:LEU:HA | 1.73 | 0.42 |
| 40:MG:411:GLY:O | 40:MG:413:GLU:N | 2.52 | 0.42 |
| 40:MH:264:ARG:HE | 40:MH:264:ARG:HB3 | 1.56 | 0.42 |
| 40:MH:348:PRO:HD2 | 41:MP:388:MET:CG | 2.49 | 0.42 |
| 41:ML:318:ARG:HG2 | 41:ML:354:CYS:HB3 | 2.01 | 0.42 |
| 41:MN:230:SER:HA | 41:MN:233:MET:HB2 | 2.01 | 0.42 |
| 41:MO:158:GLU:O | 41:MO:160:PRO:HD3 | 2.20 | 0.42 |
| 40:NE:27:GLU:HA | 40:NE:361:THR:HG21 | 2.01 | 0.42 |
| 40:NF:180:ALA:N | 40:NF:183:GLU:OE2 | 2.51 | 0.42 |
| 40:NG:319:TYR:HB3 | 40:NG:323:VAL:HG11 | 2.02 | 0.42 |
| 41:NM:296:ALA:HB1 | 41:NM:305:PRO:HD2 | 2.01 | 0.42 |
| 41:OB:139:LEU:HD13 | 41:OB:170:VAL:HG22 | 2.02 | 0.42 |
| 40:OE:97:GLU:HB3 | 41:OL:129:CYS:SG | 2.59 | 0.42 |
| 40:OF:205:ASP:HB3 | 40:OF:303:VAL:HA | 2.01 | 0.42 |
| 40:OH:206:ASN:O | 40:OH:209:ILE:HG22 | 2.19 | 0.42 |
| 41:OM:392:LYS:HG3 | 41:OM:395:LEU:HD13 | 2.00 | 0.42 |
| 41:ON:309:ARG:N | 41:ON:372:THR:OG1 | 2.52 | 0.42 |
| 41:OO:152:ILE:HD13 | 41:OO:192:LEU:HD21 | 2.01 | 0.42 |
| 40:PA:69:ASP:N | 40:PA:69:ASP:OD1 | 2.52 | 0.42 |
| 40:PE:134:GLY:HA2 | 40:PE:165:SER:O | 2.20 | 0.42 |
| 40:PF:329:ASN:ND2 | 41:PN:175:VAL:HG11 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:PG:4:CYS:SG | 40:PG:136:LEU:HD23 | 2.59 | 0.42 |
| 40:PH:352:LYS:NZ | 41:PP:178:THR:O | 2.49 | 0.42 |
| 41:PL:2:ARG:HE | 41:PL:131:GLN:HB2 | 1.84 | 0.42 |
| 41:PL:379:LYS:O | 41:PL:383:GLU:HG2 | 2.20 | 0.42 |
| 41:PM:73:MET:HA | 41:PM:76:VAL:HG12 | 2.00 | 0.42 |
| 41:PO:209:ASP:O | 41:PO:213:ARG:HB2 | 2.19 | 0.42 |
| 41:PP:113:VAL:HA | 41:PP:116:VAL:HB | 2.02 | 0.42 |
| 41:PP:208:TYR:HE1 | 41:PP:225:LEU:HD21 | 1.85 | 0.42 |
| 41:QB:14:ASN:HD21 | 41:QB:65:LEU:HG | 1.83 | 0.42 |
| 40:QE:322:ASP:OD1 | 40:QE:322:ASP:N | 2.51 | 0.42 |
| 40:QE:404:VAL:HG13 | 40:QE:417:PHE:HE2 | 1.84 | 0.42 |
| 40:QF:73:THR:HA | 40:QF:76:ASP:HB3 | 2.02 | 0.42 |
| 40:QF:318:LEU:O | 40:QF:374:VAL:HA | 2.19 | 0.42 |
| 41:QN:134:GLN:HE22 | 41:QN:233:MET:HG3 | 1.85 | 0.42 |
| 41:QO:3:GLU:HG2 | 41:QO:62:ARG:HH12 | 1.85 | 0.42 |
| 41:QP:31:ASP:O | 41:QP:33:THR:N | 2.53 | 0.42 |
| 41:QP:46:ARG:HA | 41:QP:46:ARG:HD3 | 1.37 | 0.42 |
| 41:QP:114:ASP:OD1 | 41:QP:115:SER:N | 2.47 | 0.42 |
| 41:QP:296:ALA:O | 41:QP:297:LYS:C | 2.58 | 0.42 |
| 41:RB:34:GLY:HA3 | 41:RB:58:LYS:HZ3 | 1.85 | 0.42 |
| 41:RB:137:HIS:HE1 | 41:RB:139:LEU:HD23 | 1.85 | 0.42 |
| 40:RF:421:ARG:NH1 | 40:RF:421:ARG:O | 2.52 | 0.42 |
| 40:RF:440:GLU:HB2 | 41:RN:390:ARG:HH12 | 1.85 | 0.42 |
| 40:RH:75:ILE:HD11 | 40:RH:92:LEU:HB3 | 2.02 | 0.42 |
| 40:RH:235:VAL:O | 40:RH:239:THR:HG22 | 2.19 | 0.42 |
| 40:RI:20:CYS:HA | 40:RI:232:SER:HB2 | 2.01 | 0.42 |
| 41:RO:14:ASN:HD21 | 41:RO:67:ASP:HB2 | 1.83 | 0.42 |
| 41:SB:50:TYR:O | 41:SB:62:ARG:HG2 | 2.19 | 0.42 |
| 40:SF:172:TYR:CD1 | 40:SF:173:PRO:HD2 | 2.55 | 0.42 |
| 40:SG:33:ASP:O | 40:SG:60:LYS:NZ | 2.41 | 0.42 |
| 40:SI:177:VAL:HG22 | 41:SP:331:LEU:HB2 | 2.01 | 0.42 |
| 40:SI:225:THR:O | 40:SI:229:ARG:CB | 2.67 | 0.42 |
| 41:SO:202:ILE:O | 41:SO:203:ASP:C | 2.57 | 0.42 |
| 41:SO:323:MET:O | 41:SO:324:LYS:C | 2.58 | 0.42 |
| 40:TA:101:ASN:HA | 40:TA:144:GLY:H | 1.84 | 0.42 |
| 40:TG:238:ILE:HA | 40:TG:318:LEU:HD22 | 2.01 | 0.42 |
| 40:TH:287:SER:O | 40:TH:291:ILE:HG12 | 2.20 | 0.42 |
| 40:TI:167:LEU:HD13 | 40:TI:200:CYS:HB3 | 2.00 | 0.42 |
| 41:TN:73:MET:HG3 | 41:TN:90:PHE:CZ | 2.55 | 0.42 |
| 41:TN:109:GLY:O | 41:TN:113:VAL:HG13 | 2.20 | 0.42 |
| 41:TO:173:PRO:HA | 41:TO:380:ARG:NH2 | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UA:88:HIS:HB3 | 40:UA:91:GLN:OE1 | 2.19 | 0.42 |
| 40:UF:25:CYS:SG | 40:UF:30:ILE:HB | 2.60 | 0.42 |
| 40:UF:203:MET:HE2 | 40:UF:203:MET:HB3 | 1.91 | 0.42 |
| 40:UG:242:LEU:HD23 | 40:UG:242:LEU:H | 1.85 | 0.42 |
| 40:UG:429:LYS:HD2 | 40:UG:429:LYS:HA | 1.84 | 0.42 |
| 40:UI:201:ALA:O | 40:UI:203:MET:N | 2.52 | 0.42 |
| 41:UM:396:HIS:HA | 41:UM:399:THR:HG22 | 2.01 | 0.42 |
| 41:UO:25:SER:HB3 | 41:UO:81:PHE:HE2 | 1.84 | 0.42 |
| 41:UO:112:LEU:O | 41:UO:116:VAL:HG23 | 2.20 | 0.42 |
| 41:UP:332:ASN:O | 41:UP:333:VAL:C | 2.58 | 0.42 |
| 40:VA:34:GLY:O | 40:VA:61:HIS:N | 2.46 | 0.42 |
| 40:VA:359:PRO:HA | 40:VA:360:PRO:HD3 | 1.92 | 0.42 |
| 40:VF:245:ASP:OD2 | 40:VF:245:ASP:N | 2.52 | 0.42 |
| 40:VF:269:LEU:HD23 | 40:VF:383:ILE:HD11 | 2.01 | 0.42 |
| 40:VI:102:ASN:HB3 | 40:VI:105:ARG:HB2 | 2.01 | 0.42 |
| 40:VJ:277:SER:O | 40:VJ:279:GLU:N | 2.52 | 0.42 |
| 40:WA:98:ASP:OD2 | 41:WN:252:LYS:HE2 | 2.20 | 0.42 |
| 40:WE:50:ASN:O | 40:WE:64:ARG:NH1 | 2.53 | 0.42 |
| 40:WF:324:VAL:O | 40:WF:328:VAL:HG23 | 2.19 | 0.42 |
| 40:WF:349:THR:O | 41:WN:179:VAL:HA | 2.19 | 0.42 |
| 40:WH:181:VAL:HG22 | 41:WO:256:ASN:OD1 | 2.20 | 0.42 |
| 41:WM:138:SER:O | 41:WM:139:LEU:C | 2.58 | 0.42 |
| 41:WM:293:MET:HG2 | 41:WM:367:PHE:HB2 | 2.00 | 0.42 |
| 41:WN:252:LYS:HE2 | 41:WN:252:LYS:HB2 | 1.73 | 0.42 |
| 41:WN:267:MET:HE2 | 41:WN:301:ALA:HB3 | 2.01 | 0.42 |
| 41:WN:398:TYR:C | 41:WN:400:GLY:H | 2.23 | 0.42 |
| 41:WP:58:LYS:HA | 41:WP:58:LYS:HD2 | 1.94 | 0.42 |
| 7:1T:374:ASN:ND2 | 41:WM:39:ASP:O | 2.52 | 0.42 |
| 7:1T:460:HIS:CD2 | 7:1T:486:ILE:HG13 | 2.55 | 0.42 |
| 7:1U:231:LYS:HB3 | 7:1U:231:LYS:HE2 | 1.70 | 0.42 |
| 8:1X:117:PRO:O | 8:1X:118:THR:C | 2.56 | 0.42 |
| 8:1X:278:GLU:O | 8:1X:281:LYS:HB2 | 2.19 | 0.42 |
| 12:2Q:212:ASP:HB2 | 13:2V:37:ILE:HD11 | 2.01 | 0.42 |
| 13:2U:2:PHE:CZ | 13:2U:11:LEU:HD11 | 2.53 | 0.42 |
| 13:2U:183:LEU:HB3 | 13:2U:184:TYR:H | 1.55 | 0.42 |
| 14:3C:80:THR:HA | 14:3C:114:LEU:O | 2.20 | 0.42 |
| 16:3J:200:SER:OG | 18:3T:212:GLU:OE1 | 2.34 | 0.42 |
| 16:3L:286:THR:HG23 | 16:3L:366:LEU:HD12 | 2.00 | 0.42 |
| 16:3L:315:HIS:CE1 | 16:3M:205:PRO:HG3 | 2.55 | 0.42 |
| 17:3P:197:GLU:O | 17:3P:200:PHE:HB3 | 2.19 | 0.42 |
| 21:4D:501:HIS:C | 21:4D:502:ARG:HG3 | 2.39 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4E:103:PHE:HB3 | 21:4E:181:PHE:HD1 | 1.84 | 0.42 |
| 21:4F:407:LYS:HZ3 | 21:4F:407:LYS:HG2 | 1.66 | 0.42 |
| 22:4H:232:PHE:HE2 | 22:4H:360:THR:HG21 | 1.85 | 0.42 |
| 22:4I:658:ILE:H | 22:4I:658:ILE:HG12 | 1.39 | 0.42 |
| 22:4J:286:LYS:HB2 | 22:4J:331:GLU:HG2 | 2.00 | 0.42 |
| 22:4K:670:ASN:O | 22:4K:673:LEU:N | 2.53 | 0.42 |
| 23:4N:253:TYR:O | 23:4N:255:PHE:N | 2.53 | 0.42 |
| 23:4Q:260:THR:O | 23:4Q:261:TYR:C | 2.57 | 0.42 |
| 23:4R:97:PHE:CE2 | 41:AP:59:TYR:HE1 | 2.37 | 0.42 |
| 23:4R:108:ASN:HD21 | 23:4R:110:ASN:HB2 | 1.85 | 0.42 |
| 25:4T:344:MET:CE | 26:4W:374:ILE:HB | 2.49 | 0.42 |
| 26:4V:118:PHE:HD1 | 26:4V:165:ARG:HB2 | 1.84 | 0.42 |
| 26:4W:22:ARG:HB3 | 26:4W:24:TYR:HE1 | 1.85 | 0.42 |
| 31:5I:482:LYS:HE3 | 31:5I:482:LYS:HA | 2.02 | 0.42 |
| 31:5I:613:LEU:O | 31:5I:617:ARG:HG2 | 2.20 | 0.42 |
| 39:6K:25:PHE:HD2 | 39:6K:28:ILE:HD12 | 1.85 | 0.42 |
| 40:AE:154:MET:HE3 | 40:AE:197:HIS:HB2 | 2.02 | 0.42 |
| 40:AE:376:MET:SD | 40:AE:378:SER:HB3 | 2.59 | 0.42 |
| 41:AL:139:LEU:HG | 41:AL:168:SER:HB2 | 2.02 | 0.42 |
| 41:AN:6:HIS:O | 41:AN:63:ALA:HA | 2.19 | 0.42 |
| 41:AO:245:GLN:O | 41:AO:246:LEU:C | 2.57 | 0.42 |
| 41:AO:294:PHE:CZ | 41:AO:313:VAL:HG11 | 2.55 | 0.42 |
| 41:AP:242:PHE:HB3 | 41:AP:356:ILE:HD13 | 2.00 | 0.42 |
| 41:BB:93:GLY:O | 41:BB:95:SER:N | 2.53 | 0.42 |
| 41:BB:379:LYS:HB3 | 41:BB:379:LYS:HE2 | 1.79 | 0.42 |
| 41:BM:102:ALA:HB1 | 41:BM:401:GLU:HB2 | 2.01 | 0.42 |
| 41:BM:321:MET:HE1 | 41:BM:363:MET:HG2 | 2.00 | 0.42 |
| 41:BN:87:PRO:HD3 | 41:CN:281:TYR:HD1 | 1.84 | 0.42 |
| 41:BN:372:THR:HA | 41:BN:422:VAL:HG22 | 2.01 | 0.42 |
| 41:BO:3:GLU:H | 41:BO:3:GLU:HG2 | 1.49 | 0.42 |
| 41:BO:206:ALA:O | 41:BO:210:ILE:HG13 | 2.20 | 0.42 |
| 41:BP:262:ARG:O | 41:BP:264:HIS:N | 2.53 | 0.42 |
| 40:CA:102:ASN:HB3 | 40:CA:105:ARG:HG3 | 2.01 | 0.42 |
| 40:CA:239:THR:O | 40:CA:243:ARG:NH1 | 2.52 | 0.42 |
| 40:CA:248:LEU:HD23 | 40:CA:248:LEU:HA | 1.82 | 0.42 |
| 40:CF:14:VAL:HG11 | 40:CF:74:VAL:HB | 2.01 | 0.42 |
| 40:CG:319:TYR:CE2 | 40:CG:328:VAL:HG22 | 2.54 | 0.42 |
| 40:CH:156:ARG:HD2 | 40:CH:156:ARG:HA | 1.77 | 0.42 |
| 40:CI:103:TYR:CE2 | 40:CI:189:LEU:HB3 | 2.55 | 0.42 |
| 41:CL:425:ARG:H | 41:CL:425:ARG:HG2 | 1.63 | 0.42 |
| 41:CM:7:LEU:O | 41:CM:135:LEU:HD12 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CM:372:THR:HA | 41:CM:422:VAL:HG12 | 2.02 | 0.42 |
| 41:CM:418:LEU:O | 41:CM:422:VAL:HG23 | 2.20 | 0.42 |
| 41:CO:244:GLY:HA3 | 41:CO:354:CYS:HA | 2.01 | 0.42 |
| 41:CO:415:MET:HE2 | 41:CO:415:MET:HB3 | 1.84 | 0.42 |
| 40:DA:12:ALA:HB2 | 42:DA:501:GTP:C8 | 2.54 | 0.42 |
| 40:DA:63:PRO:HD3 | 40:DA:86:LEU:HG | 2.01 | 0.42 |
| 40:DA:186:ASN:H | 40:DA:186:ASN:HD22 | 1.68 | 0.42 |
| 40:DA:224:TYR:HB3 | 42:DA:501:GTP:C6 | 2.55 | 0.42 |
| 40:DA:263:PRO:O | 40:DA:264:ARG:C | 2.57 | 0.42 |
| 40:DE:57:GLY:O | 40:DE:58:ALA:HB3 | 2.19 | 0.42 |
| 40:DE:405:HIS:ND1 | 40:DE:405:HIS:N | 2.67 | 0.42 |
| 40:DF:98:ASP:HB3 | 40:DF:99:ALA:H | 1.51 | 0.42 |
| 40:DH:3:GLU:HB3 | 40:DH:64:ARG:NH1 | 2.35 | 0.42 |
| 40:DH:74:VAL:O | 40:DH:75:ILE:C | 2.58 | 0.42 |
| 40:DH:139:HIS:ND1 | 40:DH:140:SER:O | 2.53 | 0.42 |
| 40:DI:189:LEU:HD22 | 40:DI:416:GLU:HG2 | 2.02 | 0.42 |
| 40:DI:236:SER:HA | 40:DI:243:ARG:NH2 | 2.34 | 0.42 |
| 41:DL:5:VAL:HG12 | 41:DL:64:VAL:HG22 | 2.02 | 0.42 |
| 41:DL:92:PHE:HB2 | 41:DL:93:GLY:H | 1.64 | 0.42 |
| 41:DN:163:ILE:H | 41:DN:163:ILE:HG13 | 1.65 | 0.42 |
| 41:DO:210:ILE:HG12 | 41:DO:298:ASN:HA | 2.02 | 0.42 |
| 41:DP:252:LYS:O | 41:DP:255:VAL:HG12 | 2.20 | 0.42 |
| 40:EF:341:ILE:HD12 | 40:EF:341:ILE:HA | 1.94 | 0.42 |
| 40:EH:25:CYS:HA | 40:EH:30:ILE:HG13 | 2.01 | 0.42 |
| 40:EH:63:PRO:CG | 40:EH:86:LEU:HG | 2.50 | 0.42 |
| 40:EI:232:SER:O | 40:EI:236:SER:N | 2.42 | 0.42 |
| 41:EN:7:LEU:HD23 | 41:EN:64:VAL:HB | 2.02 | 0.42 |
| 40:FA:387:TRP:CE3 | 40:FA:387:TRP:HA | 2.55 | 0.42 |
| 42:FB:502:GTP:O2' | 40:FG:206:ASN:ND2 | 2.52 | 0.42 |
| 40:FH:105:ARG:HH21 | 40:FH:110:ILE:HG13 | 1.84 | 0.42 |
| 40:FI:5:ILE:O | 40:FI:135:PHE:HA | 2.20 | 0.42 |
| 40:FI:56:THR:HB | 40:GI:283:HIS:O | 2.20 | 0.42 |
| 41:FP:245:GLN:N | 41:FP:245:GLN:OE1 | 2.52 | 0.42 |
| 41:GB:324:LYS:HA | 40:GG:210:TYR:CE1 | 2.54 | 0.42 |
| 40:GE:49:PHE:O | 40:GE:53:PHE:N | 2.53 | 0.42 |
| 40:GG:90:GLU:HG2 | 40:GG:121:ARG:NH1 | 2.35 | 0.42 |
| 40:GH:29:GLY:O | 40:GH:30:ILE:C | 2.58 | 0.42 |
| 40:GH:73:THR:O | 40:GH:74:VAL:C | 2.58 | 0.42 |
| 40:GH:260:VAL:HG23 | 41:GP:397:TRP:HZ2 | 1.83 | 0.42 |
| 40:GH:307:PRO:C | 40:GH:309:HIS:H | 2.23 | 0.42 |
| 41:GM:69:GLU:HA | 41:GM:70:PRO:HD3 | 1.88 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GN:147:MET:O | 41:GN:148:GLY:C | 2.57 | 0.42 |
| 41:GN:169:VAL:HA | 41:GN:202:ILE:O | 2.20 | 0.42 |
| 41:GN:191:GLN:O | 41:GN:192:LEU:C | 2.57 | 0.42 |
| 40:HA:100:ALA:HA | 41:HN:252:LYS:HG3 | 2.02 | 0.42 |
| 41:HB:127:CYS:SG | 41:HB:128:ASP:N | 2.93 | 0.42 |
| 40:HE:118:VAL:O | 40:HE:119:LEU:C | 2.58 | 0.42 |
| 41:HM:5:VAL:HG22 | 41:HM:62:ARG:HD3 | 2.02 | 0.42 |
| 41:HM:107:THR:O | 41:HM:109:GLY:N | 2.52 | 0.42 |
| 41:HN:62:ARG:H | 41:HN:62:ARG:HG3 | 1.62 | 0.42 |
| 41:HQ:299:MET:HE2 | 41:HQ:305:PRO:HG2 | 2.01 | 0.42 |
| 40:IA:173:PRO:HB3 | 40:IA:183:GLU:HB3 | 2.00 | 0.42 |
| 41:IB:167:PHE:CE2 | 41:IB:233:MET:HG2 | 2.54 | 0.42 |
| 41:IM:130:LEU:HD21 | 41:IM:133:PHE:CZ | 2.55 | 0.42 |
| 41:IM:131:GLN:HE22 | 41:IM:249:ASP:HB2 | 1.84 | 0.42 |
| 41:IO:170:VAL:HG21 | 41:IO:377:LEU:HD11 | 2.02 | 0.42 |
| 41:IP:43:GLN:OE1 | 41:IP:359:ARG:NH2 | 2.52 | 0.42 |
| 41:IP:53:GLU:N | 41:IP:53:GLU:OE1 | 2.53 | 0.42 |
| 40:JA:119:LEU:HD11 | 40:JA:156:ARG:HG2 | 2.02 | 0.42 |
| 40:JA:207:GLU:HA | 40:JA:210:TYR:CD2 | 2.54 | 0.42 |
| 40:JE:298:PRO:HB3 | 40:JE:307:PRO:HD2 | 2.01 | 0.42 |
| 40:JH:113:GLU:HG2 | 40:JH:114:LEU:HD12 | 2.02 | 0.42 |
| 41:JL:74:ASP:O | 41:JL:78:SER:HB3 | 2.19 | 0.42 |
| 41:JM:131:GLN:HE21 | 41:JM:131:GLN:HB3 | 1.54 | 0.42 |
| 41:JM:357:PRO:HB3 | 41:JM:362:LYS:O | 2.20 | 0.42 |
| 40:KA:16:ILE:HG12 | 40:KA:228:ASN:HD22 | 1.85 | 0.42 |
| 40:KH:271:THR:HG22 | 40:KH:301:GLN:HA | 2.00 | 0.42 |
| 40:KH:277:SER:O | 40:KH:279:GLU:N | 2.52 | 0.42 |
| 41:KL:267:MET:HE2 | 41:KL:267:MET:HB2 | 1.86 | 0.42 |
| 41:KL:393:ALA:O | 41:KL:395:LEU:N | 2.53 | 0.42 |
| 41:KO:77:ARG:HB2 | 41:KO:90:PHE:HE2 | 1.84 | 0.42 |
| 41:KO:165:ASN:HA | 41:KO:198:GLU:O | 2.18 | 0.42 |
| 41:KP:7:LEU:HG | 41:KP:135:LEU:HD13 | 2.02 | 0.42 |
| 40:LA:3:GLU:HA | 40:LA:51:THR:HA | 2.02 | 0.42 |
| 40:LA:273:ALA:HB1 | 40:LA:291:ILE:HB | 2.01 | 0.42 |
| 41:LB:10:GLY:O | 41:LB:14:ASN:ND2 | 2.53 | 0.42 |
| 40:LD:310:GLY:HA3 | 40:LD:382:ALA:HB2 | 2.02 | 0.42 |
| 40:LE:331:ALA:O | 40:LE:335:ILE:HG12 | 2.20 | 0.42 |
| 40:LF:274:PRO:HG3 | 40:LF:373:ALA:HA | 2.01 | 0.42 |
| 40:LG:337:THR:O | 40:LG:338:LYS:C | 2.58 | 0.42 |
| 41:MB:246:LEU:HD21 | 42:MB:502:GTP:H5" | 2.01 | 0.42 |
| 40:ME:172:TYR:CE2 | 40:ME:386:ALA:HB1 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MF:248:LEU:HD21 | 43:MN:502:GDP:H2' | 2.01 | 0.42 |
| 40:MF:252:LEU:HA | 40:MF:255:PHE:CD2 | 2.54 | 0.42 |
| 40:MG:71:GLU:O | 40:MG:94:THR:HG22 | 2.19 | 0.42 |
| 40:MG:76:ASP:HA | 40:MG:79:ARG:HD2 | 2.02 | 0.42 |
| 40:MG:157:LEU:HD12 | 40:MG:157:LEU:HA | 1.91 | 0.42 |
| 40:MG:397:MET:C | 40:MG:399:ALA:N | 2.73 | 0.42 |
| 40:MH:96:LYS:HB3 | 40:MH:96:LYS:HE3 | 1.68 | 0.42 |
| 40:MH:337:THR:O | 40:MH:338:LYS:C | 2.58 | 0.42 |
| 41:ML:383:GLU:HA | 41:ML:386:THR:HG22 | 2.02 | 0.42 |
| 41:MN:279:GLN:NE2 | 41:MN:279:GLN:O | 2.53 | 0.42 |
| 41:MO:296:ALA:CB | 41:MO:305:PRO:HD2 | 2.50 | 0.42 |
| 40:NA:190:THR:O | 40:NA:194:THR:CB | 2.67 | 0.42 |
| 40:ND:152:LEU:HD12 | 40:ND:152:LEU:HA | 1.78 | 0.42 |
| 40:ND:338:LYS:HB3 | 40:ND:338:LYS:HE3 | 1.60 | 0.42 |
| 40:NG:177:VAL:HG23 | 40:NG:178:SER:H | 1.85 | 0.42 |
| 41:NM:42:LEU:HA | 41:NM:45:GLU:HB2 | 2.00 | 0.42 |
| 41:NO:132:GLY:HA3 | 41:NO:163:ILE:O | 2.20 | 0.42 |
| 41:NO:149:THR:HG21 | 41:NO:188:SER:HA | 2.01 | 0.42 |
| 41:NP:189:VAL:HA | 41:NP:192:LEU:HB2 | 2.00 | 0.42 |
| 41:NP:209:ASP:O | 41:NP:213:ARG:HB3 | 2.20 | 0.42 |
| 40:OG:88:HIS:HA | 40:OG:89:PRO:HD3 | 1.90 | 0.42 |
| 40:OH:105:ARG:HA | 40:OH:109:THR:HB | 2.01 | 0.42 |
| 40:OH:118:VAL:HG11 | 40:OH:153:LEU:HD11 | 2.01 | 0.42 |
| 40:OH:144:GLY:O | 40:OH:145:THR:C | 2.58 | 0.42 |
| 41:OL:204:ASN:OD1 | 43:OL:502:GDP:O2' | 2.38 | 0.42 |
| 41:OP:44:LEU:HD12 | 41:OP:47:ILE:HG21 | 2.01 | 0.42 |
| 41:OP:143:THR:O | 41:OP:147:MET:N | 2.52 | 0.42 |
| 40:PE:329:ASN:ND2 | 41:PM:175:VAL:HG21 | 2.34 | 0.42 |
| 41:PO:31:ASP:OD1 | 41:PO:35:THR:N | 2.52 | 0.42 |
| 41:PO:183:TYR:HD2 | 41:PO:398:TYR:HE2 | 1.66 | 0.42 |
| 40:QA:68:VAL:HG12 | 40:QA:93:ILE:HB | 2.01 | 0.42 |
| 40:QA:404:VAL:HG12 | 40:QA:417:PHE:HE2 | 1.84 | 0.42 |
| 41:QB:42:LEU:H | 41:QB:42:LEU:HG | 1.50 | 0.42 |
| 41:QB:251:ARG:HB3 | 40:QG:100:ALA:HB2 | 2.01 | 0.42 |
| 41:QB:289:LEU:HD22 | 41:QB:364:SER:HA | 2.02 | 0.42 |
| 41:QB:350:LYS:HZ3 | 40:QG:180:ALA:HB1 | 1.84 | 0.42 |
| 41:QB:424:THR:C | 41:QB:426:GLY:H | 2.22 | 0.42 |
| 40:QF:49:PHE:HE2 | 40:QF:55:GLU:HB2 | 1.85 | 0.42 |
| 40:QF:143:GLY:N | 42:QF:501:GTP:O2A | 2.37 | 0.42 |
| 40:QH:401:ARG:NH2 | 40:QH:414:GLU:OE2 | 2.52 | 0.42 |
| 41:QN:137:HIS:HE1 | 41:QN:139:LEU:CD2 | 2.32 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QN:139:LEU:HD21 | 41:QN:192:LEU:HD11 | 2.02 | 0.42 |
| 41:QP:142:GLY:O | 41:QP:144:GLY:N | 2.53 | 0.42 |
| 40:RE:427:LEU:HG | 40:RE:431:TYR:CE2 | 2.55 | 0.42 |
| 40:RH:326:LYS:HG2 | 41:RP:208:TYR:CE1 | 2.55 | 0.42 |
| 41:RL:122:LYS:HE3 | 41:SL:291:GLN:HE22 | 1.85 | 0.42 |
| 41:RO:326:VAL:O | 41:RO:330:MET:HB2 | 2.20 | 0.42 |
| 41:RP:4:ILE:HG13 | 41:RP:131:GLN:HE21 | 1.85 | 0.42 |
| 41:SB:417:ASP:O | 41:SB:420:ASN:N | 2.48 | 0.42 |
| 40:SE:16:ILE:O | 40:SE:20:CYS:CB | 2.64 | 0.42 |
| 40:SF:100:ALA:O | 41:SM:255:VAL:HG11 | 2.19 | 0.42 |
| 40:SF:212:ILE:HD13 | 40:SF:300:ASN:HA | 2.01 | 0.42 |
| 41:SN:280:GLN:OE1 | 41:SN:280:GLN:N | 2.45 | 0.42 |
| 41:SO:297:LYS:O | 41:SO:298:ASN:C | 2.57 | 0.42 |
| 41:SP:180:VAL:HG23 | 41:SP:184:ASN:HD21 | 1.85 | 0.42 |
| 41:TB:100:ASN:HD22 | 41:TB:398:TYR:HE2 | 1.67 | 0.42 |
| 41:TB:149:THR:HB | 41:TB:191:GLN:HG2 | 2.01 | 0.42 |
| 40:TF:238:ILE:HG23 | 40:TF:255:PHE:CE2 | 2.55 | 0.42 |
| 40:TI:386:ALA:HA | 40:TI:389:ARG:HG2 | 2.01 | 0.42 |
| 41:TM:21:TRP:CZ3 | 41:TM:24:ILE:HD11 | 2.55 | 0.42 |
| 41:TO:6:HIS:HD2 | 41:TO:21:TRP:HE1 | 1.67 | 0.42 |
| 41:TO:210:ILE:O | 41:TO:214:THR:OG1 | 2.35 | 0.42 |
| 41:TO:342:VAL:HB | 41:TO:344:TRP:CD1 | 2.54 | 0.42 |
| 41:TP:165:ASN:HA | 41:TP:198:GLU:O | 2.19 | 0.42 |
| 41:TP:198:GLU:HG2 | 41:TP:266:PHE:HE2 | 1.85 | 0.42 |
| 41:TP:210:ILE:HD12 | 41:TP:298:ASN:HA | 2.02 | 0.42 |
| 40:UA:9:VAL:HG22 | 40:UA:68:VAL:HB | 2.01 | 0.42 |
| 40:UA:228:ASN:ND2 | 42:UA:501:GTP:C2 | 2.85 | 0.42 |
| 41:UB:193:VAL:HG11 | 41:UB:262:ARG:HH21 | 1.84 | 0.42 |
| 40:UF:101:ASN:O | 40:UF:182:VAL:HG21 | 2.20 | 0.42 |
| 40:UI:35:GLN:HE21 | 40:UI:35:GLN:HB2 | 1.53 | 0.42 |
| 40:UI:71:GLU:HB2 | 40:UI:98:ASP:CA | 2.48 | 0.42 |
| 40:UI:281:ALA:O | 40:UI:282:TYR:C | 2.58 | 0.42 |
| 40:UI:312:TYR:O | 40:UI:343:PHE:HA | 2.19 | 0.42 |
| 41:UM:173:PRO:HA | 41:UM:380:ARG:NH1 | 2.34 | 0.42 |
| 41:UN:248:ALA:HA | 41:UN:252:LYS:HD3 | 2.02 | 0.42 |
| 41:UP:143:THR:HB | 41:UP:144:GLY:H | 1.63 | 0.42 |
| 40:VF:390:LEU:HD23 | 40:VF:390:LEU:HA | 1.89 | 0.42 |
| 40:VH:68:VAL:HG22 | 40:VH:93:ILE:HB | 2.01 | 0.42 |
| 40:VI:326:LYS:HZ1 | 41:VQ:225:LEU:HD21 | 1.83 | 0.42 |
| 41:VN:268:PRO:HG2 | 41:VN:300:MET:HB2 | 2.02 | 0.42 |
| 41:VN:330:MET:HB3 | 41:VN:349:VAL:HG11 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VO:1:MET:SD | 41:VO:48:ASN:ND2 | 2.90 | 0.42 |
| 41:VP:27:GLU:CD | 41:VP:241:ARG:HH12 | 2.23 | 0.42 |
| 41:VP:77:ARG:HD2 | 41:VP:90:PHE:HE2 | 1.85 | 0.42 |
| 40:WA:3:GLU:N | 40:WA:3:GLU:OE2 | 2.51 | 0.42 |
| 40:WA:217:LEU:HA | 40:WA:277:SER:HB3 | 2.02 | 0.42 |
| 41:WB:318:ARG:CZ | 41:WB:358:PRO:HD3 | 2.50 | 0.42 |
| 40:WH:362:VAL:HG11 | 40:WH:369:LYS:HA | 2.02 | 0.42 |
| 41:WM:42:LEU:HD22 | 41:WM:243:PRO:HG3 | 2.01 | 0.42 |
| 41:WM:61:PRO:HD2 | 41:WM:84:ILE:O | 2.20 | 0.42 |
| 41:WM:107:THR:HB | 41:WM:108:GLU:H | 1.62 | 0.42 |
| 41:WM:183:TYR:CZ | 41:WM:388:MET:HB3 | 2.54 | 0.42 |
| 41:WN:273:LEU:H | 41:WN:292:GLN:NE2 | 2.05 | 0.42 |
| 41:WN:290:THR:HG22 | 41:WN:317:PHE:CZ | 2.55 | 0.42 |
| 41:WN:317:PHE:HB3 | 41:WN:321:MET:SD | 2.60 | 0.42 |
| 41:WN:418:LEU:C | 41:WN:420:ASN:H | 2.23 | 0.42 |
| 7:1T:95:LEU:O | 7:1T:96:TRP:C | 2.58 | 0.42 |
| 7:1U:569:VAL:CG2 | 7:1U:586:HIS:HE1 | 2.32 | 0.42 |
| 12:2Q:65:ARG:HA | 12:2Q:65:ARG:HD3 | 1.90 | 0.42 |
| 12:2R:105:TYR:CD1 | 12:2R:141:LYS:HG2 | 2.55 | 0.42 |
| 13:2T:6:PHE:CE2 | 13:2T:8:SER:HB3 | 2.55 | 0.42 |
| 13:2V:94:LEU:HB2 | 13:2V:152:LEU:HD11 | 2.02 | 0.42 |
| 13:2W:7:GLN:NE2 | 13:2W:70:GLY:O | 2.42 | 0.42 |
| 13:2W:101:ARG:H | 13:2W:101:ARG:HG2 | 1.55 | 0.42 |
| 15:3H:398:PRO:HA | 15:3H:399:PRO:HD3 | 1.94 | 0.42 |
| 16:3K:349:ILE:HG22 | 16:3K:353:LYS:NZ | 2.35 | 0.42 |
| 16:3L:123:ARG:NH1 | 16:3L:131:ASP:OD2 | 2.49 | 0.42 |
| 17:3O:222:GLU:O | 17:3O:226:ILE:HG12 | 2.20 | 0.42 |
| 20:4A:225:VAL:HG12 | 20:4A:229:GLN:HE21 | 1.85 | 0.42 |
| 22:4J:91:ASP:H | 41:BN:281:TYR:N | 2.01 | 0.42 |
| 22:4J:626:GLN:H | 22:4J:626:GLN:HG2 | 1.60 | 0.42 |
| 22:4K:560:ARG:O | 22:4K:563:LYS:N | 2.53 | 0.42 |
| 23:4P:253:TYR:O | 23:4P:255:PHE:N | 2.53 | 0.42 |
| 23:4Q:235:THR:HG21 | 23:4Q:242:LEU:HD23 | 2.02 | 0.42 |
| 23:4R:60:LEU:H | 23:4R:60:LEU:HG | 1.54 | 0.42 |
| 23:4R:244:PRO:HD2 | 40:DI:89:PRO:CG | 2.49 | 0.42 |
| 27:4Z:236:LEU:HD23 | 27:4Z:245:GLU:HB3 | 2.01 | 0.42 |
| 31:5I:498:THR:OG1 | 40:IH:322:ASP:OD2 | 2.31 | 0.42 |
| 33:5N:405:LYS:HE3 | 40:GF:59:GLY:HA3 | 2.02 | 0.42 |
| 36:5X:164:PRO:O | 36:5X:166:MET:HG2 | 2.20 | 0.42 |
| 36:5X:218:ARG:HA | 36:5X:221:GLN:HG2 | 2.02 | 0.42 |
| 39:6J:117:ALA:HB1 | 39:6J:121:HIS:HD2 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:6L:118:LYS:HG2 | 39:6L:121:HIS:CG | 2.55 | 0.42 |
| 39:6L:135:HIS:O | 39:6L:137:GLY:N | 2.52 | 0.42 |
| 40:AA:112:LYS:HA | 40:AA:115:ILE:HG22 | 2.01 | 0.42 |
| 40:AE:88:HIS:HE2 | 40:BE:280:LYS:HG2 | 1.83 | 0.42 |
| 40:AF:239:THR:O | 40:AF:243:ARG:NE | 2.41 | 0.42 |
| 40:AG:203:MET:HE3 | 40:AG:267:PHE:HB3 | 2.02 | 0.42 |
| 40:AH:78:VAL:HG23 | 40:AH:92:LEU:HD13 | 2.01 | 0.42 |
| 41:AM:107:THR:O | 41:AM:109:GLY:N | 2.53 | 0.42 |
| 41:AO:11:GLN:HA | 41:AO:72:THR:HG21 | 2.02 | 0.42 |
| 41:AO:89:ASN:HA | 41:AO:119:VAL:HG11 | 2.01 | 0.42 |
| 40:BA:245:ASP:OD1 | 40:BA:245:ASP:N | 2.50 | 0.42 |
| 41:BB:21:TRP:O | 41:BB:25:SER:HB2 | 2.20 | 0.42 |
| 41:BB:143:THR:HB | 41:BB:144:GLY:H | 1.70 | 0.42 |
| 40:BE:167:LEU:HD12 | 40:BE:167:LEU:H | 1.84 | 0.42 |
| 40:BF:175:PRO:HB3 | 40:BF:389:ARG:CZ | 2.49 | 0.42 |
| 40:BH:31:GLN:O | 40:BH:34:GLY:N | 2.48 | 0.42 |
| 40:BH:75:ILE:CG2 | 40:BH:94:THR:HG23 | 2.50 | 0.42 |
| 40:BH:183:GLU:HB3 | 40:BH:184:PRO:HD3 | 2.01 | 0.42 |
| 40:BH:258:ASN:HA | 41:BP:179:VAL:HG22 | 2.02 | 0.42 |
| 40:BH:266:HIS:ND1 | 40:BH:266:HIS:O | 2.52 | 0.42 |
| 41:BM:425:ARG:C | 41:BM:427:ALA:H | 2.23 | 0.42 |
| 41:BN:207:LEU:HB3 | 41:BN:225:LEU:HD22 | 2.00 | 0.42 |
| 41:BN:282:ARG:HB3 | 41:BN:283:ALA:H | 1.52 | 0.42 |
| 41:BO:382:SER:O | 41:BO:386:THR:HG23 | 2.20 | 0.42 |
| 41:BP:263:LEU:H | 41:BP:263:LEU:HG | 1.64 | 0.42 |
| 40:CA:36:MET:O | 40:CA:37:PRO:C | 2.58 | 0.42 |
| 41:CB:11:GLN:HA | 41:CB:72:THR:HG21 | 2.01 | 0.42 |
| 40:CE:397:MET:CG | 41:CL:346:PRO:HD2 | 2.50 | 0.42 |
| 40:CH:299:ALA:O | 40:CH:301:GLN:N | 2.52 | 0.42 |
| 40:CH:319:TYR:O | 40:CH:355:ILE:HA | 2.20 | 0.42 |
| 40:CH:326:LYS:NZ | 41:CP:208:TYR:HB2 | 2.35 | 0.42 |
| 40:CH:377:LEU:H | 40:CH:377:LEU:HG | 1.61 | 0.42 |
| 40:CI:205:ASP:HB2 | 40:CI:303:VAL:HA | 2.01 | 0.42 |
| 41:CL:273:LEU:HD23 | 41:CL:273:LEU:HA | 1.79 | 0.42 |
| 41:CN:101:TRP:CE3 | 41:CN:145:SER:HB3 | 2.55 | 0.42 |
| 41:CN:245:GLN:NE2 | 41:CN:323:MET:SD | 2.93 | 0.42 |
| 41:CO:12:CYS:HB2 | 43:CO:501:GDP:C8 | 2.55 | 0.42 |
| 41:CP:280:GLN:H | 41:CP:280:GLN:HG2 | 1.67 | 0.42 |
| 41:CP:316:VAL:HG23 | 41:CP:366:THR:O | 2.20 | 0.42 |
| 41:CP:328:GLU:O | 41:CP:329:GLN:C | 2.58 | 0.42 |
| 40:DA:2:ARG:HA | 40:DA:133:GLN:HG3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DA:103:TYR:CD1 | 40:DA:190:THR:HG22 | 2.55 | 0.42 |
| 41:DB:290:THR:C | 41:DB:292:GLN:H | 2.23 | 0.42 |
| 40:DE:261:PRO:HD2 | 40:DE:265:ILE:HG23 | 2.01 | 0.42 |
| 40:DE:440:GLU:H | 40:DE:440:GLU:HG2 | 1.61 | 0.42 |
| 40:DG:230:LEU:HA | 40:DG:230:LEU:HD12 | 1.84 | 0.42 |
| 40:DG:270:ALA:HB3 | 40:DG:302:MET:HG3 | 2.00 | 0.42 |
| 40:DG:326:LYS:HD3 | 40:DG:326:LYS:HA | 1.84 | 0.42 |
| 40:DI:294:ALA:O | 40:DI:297:GLU:HB3 | 2.20 | 0.42 |
| 41:DM:420:ASN:HB2 | 41:DM:421:PRO:HD3 | 2.02 | 0.42 |
| 41:DN:222:TYR:HA | 41:DN:225:LEU:HD12 | 2.01 | 0.42 |
| 41:DO:139:LEU:HG | 41:DO:168:SER:HB2 | 2.01 | 0.42 |
| 41:DP:80:PRO:HB2 | 41:DP:81:PHE:H | 1.66 | 0.42 |
| 41:DP:326:VAL:O | 41:DP:327:ASP:C | 2.58 | 0.42 |
| 40:EG:401:ARG:HB3 | 40:EG:404:VAL:HG11 | 2.02 | 0.42 |
| 40:EH:300:ASN:O | 40:EH:301:GLN:C | 2.58 | 0.42 |
| 40:EH:312:TYR:CG | 40:EH:341:ILE:HD11 | 2.55 | 0.42 |
| 40:EI:398:TYR:HE1 | 40:EI:417:PHE:HB3 | 1.84 | 0.42 |
| 41:EM:122:LYS:HA | 41:EM:122:LYS:HD3 | 1.63 | 0.42 |
| 41:EP:259:PRO:HG2 | 41:EP:263:LEU:HD12 | 2.02 | 0.42 |
| 40:FE:39:ASP:N | 40:FE:39:ASP:OD1 | 2.52 | 0.42 |
| 40:FG:318:LEU:O | 40:FG:374:VAL:HA | 2.19 | 0.42 |
| 41:GB:91:VAL:HG11 | 41:GB:116:VAL:HG22 | 2.01 | 0.42 |
| 40:GE:204:VAL:HG22 | 40:GE:302:MET:HE3 | 1.84 | 0.42 |
| 40:GE:289:ALA:O | 40:GE:290:GLU:C | 2.57 | 0.42 |
| 40:GF:177:VAL:HG12 | 41:GM:331:LEU:HD12 | 2.02 | 0.42 |
| 40:GF:408:VAL:HG23 | 40:GF:413:GLU:HA | 2.02 | 0.42 |
| 40:GI:106:GLY:O | 40:GI:148:GLY:C | 2.58 | 0.42 |
| 41:GM:214:THR:HG22 | 41:GM:297:LYS:HE2 | 2.02 | 0.42 |
| 41:GM:375:GLN:HB3 | 41:GM:422:VAL:HG13 | 2.02 | 0.42 |
| 41:GN:139:LEU:HD12 | 41:GN:139:LEU:HA | 1.75 | 0.42 |
| 41:GO:178:THR:O | 41:GO:180:VAL:N | 2.53 | 0.42 |
| 41:GP:183:TYR:OH | 41:GP:388:MET:O | 2.38 | 0.42 |
| 40:HA:133:GLN:HB3 | 40:HA:252:LEU:HD12 | 2.01 | 0.42 |
| 41:HB:68:LEU:HD23 | 41:HB:143:THR:HG23 | 2.02 | 0.42 |
| 40:HE:139:HIS:ND1 | 40:HE:140:SER:O | 2.53 | 0.42 |
| 40:HE:273:ALA:HB3 | 40:HE:274:PRO:HD3 | 2.01 | 0.42 |
| 40:HE:337:THR:O | 40:HE:338:LYS:C | 2.58 | 0.42 |
| 40:HG:68:VAL:HG11 | 40:HG:149:PHE:CE2 | 2.55 | 0.42 |
| 40:HG:315:CYS:HB2 | 40:HG:351:PHE:HD1 | 1.84 | 0.42 |
| 40:HH:288:VAL:HA | 40:HH:291:ILE:HG12 | 2.01 | 0.42 |
| 40:HI:132:LEU:HD23 | 40:HI:164:LYS:HE3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HO:138:SER:HA | 41:HO:169:VAL:HG22 | 2.02 | 0.42 |
| 41:HO:148:GLY:O | 41:HO:152:ILE:HG12 | 2.19 | 0.42 |
| 41:HO:305:PRO:HB3 | 41:HO:310:TYR:HE1 | 1.84 | 0.42 |
| 41:HP:304:ASP:OD1 | 41:HP:304:ASP:N | 2.49 | 0.42 |
| 40:IA:147:SER:OG | 40:IA:148:GLY:N | 2.53 | 0.42 |
| 41:IB:42:LEU:HD23 | 41:IB:356:ILE:HD11 | 2.00 | 0.42 |
| 40:IE:247:ALA:HB3 | 40:IE:355:ILE:HB | 2.01 | 0.42 |
| 40:IF:415:GLY:O | 40:IF:419:GLU:HG3 | 2.19 | 0.42 |
| 40:II:238:ILE:HD12 | 40:II:377:LEU:HD11 | 2.01 | 0.42 |
| 41:IM:247:ASN:O | 41:IM:252:LYS:NZ | 2.49 | 0.42 |
| 41:IN:22:GLU:HA | 41:IN:81:PHE:CD1 | 2.55 | 0.42 |
| 41:IO:49:VAL:HG21 | 41:IO:241:ARG:HG2 | 2.01 | 0.42 |
| 41:IP:133:PHE:HB2 | 41:IP:164:MET:SD | 2.60 | 0.42 |
| 41:IP:305:PRO:HB3 | 41:IP:310:TYR:CE2 | 2.55 | 0.42 |
| 40:JA:116:ASP:N | 40:JA:116:ASP:OD1 | 2.52 | 0.42 |
| 40:JA:366:ASP:OD1 | 40:JA:367:LEU:N | 2.52 | 0.42 |
| 41:JB:151:LEU:O | 41:JB:155:ILE:HG12 | 2.20 | 0.42 |
| 40:JD:167:LEU:HA | 40:JD:200:CYS:O | 2.20 | 0.42 |
| 40:JE:136:LEU:HD23 | 40:JE:167:LEU:HB2 | 2.02 | 0.42 |
| 40:JH:251:ASP:OD1 | 40:JH:252:LEU:N | 2.50 | 0.42 |
| 40:JH:255:PHE:O | 40:JH:259:LEU:HB2 | 2.19 | 0.42 |
| 41:JM:193:VAL:HG12 | 41:JM:265:PHE:CE1 | 2.55 | 0.42 |
| 41:JM:242:PHE:HB3 | 41:JM:356:ILE:HD13 | 2.01 | 0.42 |
| 40:KG:88:HIS:CE1 | 40:KG:90:GLU:HG2 | 2.55 | 0.42 |
| 41:KM:150:LEU:O | 41:KM:154:LYS:HG2 | 2.20 | 0.42 |
| 41:KO:318:ARG:HG2 | 41:KO:357:PRO:HA | 2.00 | 0.42 |
| 41:LB:8:GLN:NE2 | 41:LB:65:LEU:HD22 | 2.32 | 0.42 |
| 40:LE:421:ARG:HD2 | 40:LE:421:ARG:HA | 1.79 | 0.42 |
| 40:LG:217:LEU:O | 40:LG:219:ILE:HG13 | 2.19 | 0.42 |
| 40:LH:254:GLU:HG3 | 41:LP:98:GLY:HA2 | 2.00 | 0.42 |
| 40:LH:295:CYS:HB3 | 40:LH:376:MET:HE2 | 2.02 | 0.42 |
| 41:LM:101:TRP:HE3 | 41:LM:403:MET:HE1 | 1.84 | 0.42 |
| 41:LO:114:ASP:N | 41:LO:114:ASP:OD1 | 2.52 | 0.42 |
| 41:LO:282:ARG:HA | 41:LO:282:ARG:HD3 | 1.87 | 0.42 |
| 41:LP:46:ARG:HA | 41:LP:46:ARG:HD3 | 1.93 | 0.42 |
| 40:ME:225:THR:O | 40:ME:229:ARG:HB2 | 2.19 | 0.42 |
| 40:ME:274:PRO:HD2 | 40:ME:373:ALA:HA | 2.01 | 0.42 |
| 40:MF:407:TYR:O | 40:MF:410:GLU:HG3 | 2.19 | 0.42 |
| 40:MG:103:TYR:OH | 40:MG:193:THR:HG21 | 2.20 | 0.42 |
| 40:MG:136:LEU:HD22 | 40:MG:169:PHE:HE1 | 1.85 | 0.42 |
| 40:MG:242:LEU:HD21 | 40:MG:251:ASP:HA | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:MM:20:PHE:HA | 41:MM:230:SER:HB3 | 2.01 | 0.42 |
| 41:MN:139:LEU:HD22 | 41:MN:170:VAL:HG12 | 2.01 | 0.42 |
| 41:MO:111:GLU:H | 41:MO:111:GLU:HG3 | 1.36 | 0.42 |
| 41:MO:396:HIS:C | 41:MO:398:TYR:H | 2.24 | 0.42 |
| 40:NG:217:LEU:HD21 | 40:NG:275:VAL:HG22 | 2.01 | 0.42 |
| 40:NG:231:ILE:O | 40:NG:234:ILE:HG22 | 2.20 | 0.42 |
| 41:OB:212:PHE:O | 41:OB:216:LYS:HD2 | 2.20 | 0.42 |
| 41:OB:275:SER:OG | 41:OB:276:ARG:N | 2.52 | 0.42 |
| 41:OB:293:MET:HB2 | 41:OB:293:MET:HE3 | 1.97 | 0.42 |
| 40:OF:121:ARG:HH21 | 40:OF:124:LYS:HE2 | 1.84 | 0.42 |
| 40:OH:225:THR:HA | 40:OH:228:ASN:HD21 | 1.84 | 0.42 |
| 40:OH:298:PRO:HB3 | 40:OH:307:PRO:HD2 | 2.00 | 0.42 |
| 40:OH:355:ILE:H | 40:OH:355:ILE:HG13 | 1.60 | 0.42 |
| 40:OH:405:HIS:HE1 | 41:OO:258:VAL:O | 2.03 | 0.42 |
| 41:OM:10:GLY:O | 41:OM:14:ASN:ND2 | 2.53 | 0.42 |
| 41:ON:237:THR:HA | 41:ON:240:LEU:HD13 | 2.02 | 0.42 |
| 41:OP:121:ARG:O | 41:OP:124:ALA:N | 2.51 | 0.42 |
| 41:OP:269:GLY:HA3 | 41:OP:367:PHE:HB3 | 2.01 | 0.42 |
| 40:PE:71:GLU:HA | 40:PE:72:PRO:HD3 | 1.88 | 0.42 |
| 40:PE:213:CYS:HA | 40:PE:217:LEU:HB2 | 2.01 | 0.42 |
| 41:PN:20:PHE:HA | 41:PN:230:SER:HB3 | 2.01 | 0.42 |
| 41:PO:105:HIS:CD2 | 41:PO:150:LEU:HB2 | 2.54 | 0.42 |
| 40:QA:76:ASP:HA | 40:QA:79:ARG:HH21 | 1.84 | 0.42 |
| 40:QA:107:HIS:ND1 | 40:QA:151:SER:OG | 2.41 | 0.42 |
| 41:QB:139:LEU:O | 41:QB:141:GLY:N | 2.53 | 0.42 |
| 40:QE:89:PRO:HG2 | 40:RE:280:LYS:HZ2 | 1.83 | 0.42 |
| 40:QF:181:VAL:HG12 | 41:QM:348:ASN:HA | 2.01 | 0.42 |
| 41:QN:131:GLN:HE22 | 41:QN:250:LEU:H | 1.67 | 0.42 |
| 41:QP:250:LEU:H | 41:QP:250:LEU:HD22 | 1.85 | 0.42 |
| 41:QP:263:LEU:HB2 | 41:QP:425:ARG:HH21 | 1.85 | 0.42 |
| 40:RE:153:LEU:HG | 40:RE:157:LEU:HD23 | 2.01 | 0.42 |
| 40:RF:101:ASN:HA | 40:RF:143:GLY:HA2 | 2.01 | 0.42 |
| 40:RH:2:ARG:NH2 | 41:RP:69:GLU:OE2 | 2.42 | 0.42 |
| 40:RH:150:THR:O | 40:RH:154:MET:HG2 | 2.19 | 0.42 |
| 40:RH:320:ARG:HG2 | 40:RH:356:ASN:HD21 | 1.85 | 0.42 |
| 40:RI:31:GLN:NE2 | 40:RI:33:ASP:OD1 | 2.52 | 0.42 |
| 41:RM:314:ALA:HA | 41:RM:350:LYS:O | 2.19 | 0.42 |
| 41:RO:130:LEU:O | 41:RO:162:ARG:NH1 | 2.48 | 0.42 |
| 40:SA:311:LYS:N | 40:SA:381:THR:OG1 | 2.46 | 0.42 |
| 40:SA:389:ARG:O | 40:SA:393:LYS:HG2 | 2.20 | 0.42 |
| 40:SE:315:CYS:HA | 40:SE:377:LEU:O | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SF:276:ILE:HD12 | 40:SF:276:ILE:H | 1.84 | 0.42 |
| 41:SN:25:SER:OG | 41:SN:51:TYR:OH | 2.36 | 0.42 |
| 41:SN:105:HIS:CD2 | 41:SN:150:LEU:HB2 | 2.55 | 0.42 |
| 40:TA:20:CYS:HA | 40:TA:232:SER:HB2 | 2.02 | 0.42 |
| 40:TH:332:ILE:HA | 40:TH:335:ILE:HG22 | 2.01 | 0.42 |
| 40:TI:20:CYS:HA | 40:TI:232:SER:HB2 | 2.01 | 0.42 |
| 40:TI:230:LEU:O | 40:TI:234:ILE:HG12 | 2.20 | 0.42 |
| 41:TN:198:GLU:HG2 | 41:TN:266:PHE:HE2 | 1.84 | 0.42 |
| 41:TO:180:VAL:O | 41:TO:184:ASN:ND2 | 2.52 | 0.42 |
| 41:TP:58:LYS:HZ3 | 41:UP:280:GLN:CB | 2.21 | 0.42 |
| 40:UE:332:ILE:HG21 | 41:UM:175:VAL:HG23 | 2.02 | 0.42 |
| 40:UE:387:TRP:CD1 | 40:UE:431:TYR:HE2 | 2.38 | 0.42 |
| 40:UF:301:GLN:HG3 | 40:UF:303:VAL:HG23 | 2.01 | 0.42 |
| 40:UF:326:LYS:HD2 | 40:UF:326:LYS:HA | 1.65 | 0.42 |
| 40:UG:157:LEU:HD23 | 40:UG:157:LEU:HA | 1.88 | 0.42 |
| 40:UH:60:LYS:NZ | 40:VI:282:TYR:O | 2.42 | 0.42 |
| 40:UH:174:ALA:HB3 | 40:UH:178:SER:H | 1.85 | 0.42 |
| 40:UH:350:GLY:HA2 | 41:UP:179:VAL:HG13 | 2.01 | 0.42 |
| 40:UI:139:HIS:CG | 40:UI:140:SER:N | 2.86 | 0.42 |
| 40:UI:398:TYR:O | 40:UI:401:ARG:NH1 | 2.52 | 0.42 |
| 41:UO:163:ILE:HG21 | 41:UO:250:LEU:HB3 | 2.01 | 0.42 |
| 41:UP:271:ALA:HB3 | 41:UP:272:PRO:CD | 2.49 | 0.42 |
| 40:VA:217:LEU:HA | 40:VA:277:SER:HB2 | 2.01 | 0.42 |
| 40:VA:332:ILE:HG23 | 40:VA:351:PHE:CD2 | 2.55 | 0.42 |
| 40:VG:269:LEU:HD21 | 40:VG:302:MET:H | 1.84 | 0.42 |
| 40:VI:255:PHE:HA | 40:VI:259:LEU:HD23 | 2.02 | 0.42 |
| 41:VO:118:ASP:O | 41:VO:122:LYS:HG2 | 2.20 | 0.42 |
| 40:WA:103:TYR:CE1 | 40:WA:148:GLY:HA2 | 2.54 | 0.42 |
| 40:WA:242:LEU:H | 40:WA:242:LEU:HD23 | 1.85 | 0.42 |
| 40:WE:168:GLU:OE1 | 40:WE:194:THR:OG1 | 2.29 | 0.42 |
| 40:WE:242:LEU:HD23 | 40:WE:242:LEU:H | 1.84 | 0.42 |
| 40:WE:288:VAL:HA | 40:WE:291:ILE:HG12 | 2.00 | 0.42 |
| 40:WG:64:ARG:NE | 40:WG:129:CYS:SG | 2.92 | 0.42 |
| 40:WH:406:TRP:CE2 | 41:WO:255:VAL:HA | 2.54 | 0.42 |
| 41:WM:61:PRO:HG2 | 41:WM:84:ILE:HG23 | 2.02 | 0.42 |
| 41:WM:170:VAL:HG11 | 41:WM:377:LEU:HD21 | 2.01 | 0.42 |
| 41:WM:226:ASN:N | 41:WM:226:ASN:OD1 | 2.50 | 0.42 |
| 41:WO:21:TRP:CE3 | 41:WO:24:ILE:HD11 | 2.55 | 0.42 |
| 41:WO:142:GLY:O | 41:WO:144:GLY:N | 2.53 | 0.42 |
| 41:WP:105:HIS:CD2 | 41:WP:150:LEU:HB2 | 2.54 | 0.42 |
| 7:1S:528:TYR:CD2 | 7:1S:538:ARG:HB3 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:1Z:472:HIS:HE2 | 40:UG:369:LYS:HB2 | 1.84 | 0.42 |
| 9:2B:49:ILE:H | 9:2B:49:ILE:HG12 | 1.36 | 0.42 |
| 10:2F:47:LEU:HD11 | 40:MA:434:VAL:CG1 | 2.50 | 0.42 |
| 11:2I:249:ILE:H | 11:2I:249:ILE:HG12 | 1.49 | 0.42 |
| 12:2M:113:PHE:HB3 | 12:2M:152:PRO:HB2 | 2.02 | 0.42 |
| 12:2Q:183:GLY:HA3 | 12:2Q:235:TYR:O | 2.20 | 0.42 |
| 13:2T:46:VAL:HG11 | 13:2T:129:TRP:CH2 | 2.55 | 0.42 |
| 13:2U:183:LEU:HA | 13:2U:183:LEU:HD12 | 1.82 | 0.42 |
| 13:2V:115:LYS:HE3 | 13:2V:116:PRO:HG2 | 2.02 | 0.42 |
| 13:2W:45:LEU:HD22 | 41:WN:125:GLU:HB2 | 2.01 | 0.42 |
| 14:3A:42:ILE:HG22 | 41:MN:390:ARG:O | 2.20 | 0.42 |
| 15:3F:116:LEU:HD23 | 15:3F:116:LEU:HA | 1.93 | 0.42 |
| 15:3H:4:LEU:HB3 | 15:3H:5:LEU:H | 1.55 | 0.42 |
| 15:3H:253:LEU:HD23 | 15:3H:253:LEU:HA | 1.89 | 0.42 |
| 16:3K:370:LEU:O | 16:3K:374:GLN:HG2 | 2.20 | 0.42 |
| 16:3L:120:ARG:HH12 | 16:3L:133:VAL:HG13 | 1.84 | 0.42 |
| 17:3O:400:LEU:HB3 | 17:3R:287:VAL:HB | 2.02 | 0.42 |
| 17:3P:227:LEU:HD23 | 17:3P:227:LEU:HA | 1.85 | 0.42 |
| 17:3Q:367:LYS:HB2 | 17:3Q:367:LYS:HE2 | 1.74 | 0.42 |
| 17:3Q:421:VAL:HG13 | 17:3Q:425:TYR:CE2 | 2.55 | 0.42 |
| 17:3R:264:ALA:O | 17:3R:266:ARG:N | 2.52 | 0.42 |
| 18:3T:120:HIS:CE1 | 18:3T:265:LEU:HB3 | 2.55 | 0.42 |
| 19:3Y:176:LYS:HE3 | 19:3Y:176:LYS:HB3 | 1.63 | 0.42 |
| 20:4B:229:GLN:HB3 | 20:4B:230:ARG:H | 1.72 | 0.42 |
| 20:4B:331:LEU:H | 20:4B:331:LEU:HG | 1.68 | 0.42 |
| 21:4E:434:LYS:HE2 | 21:4E:434:LYS:HB2 | 1.95 | 0.42 |
| 21:4F:50:ASP:N | 21:4F:50:ASP:OD1 | 2.53 | 0.42 |
| 22:4K:633:GLU:O | 22:4K:634:ASN:C | 2.57 | 0.42 |
| 23:4M:113:TRP:O | 23:4M:114:ALA:C | 2.57 | 0.42 |
| 23:4M:208:GLN:H | 23:4M:208:GLN:HG2 | 1.65 | 0.42 |
| 23:4M:217:LYS:HD2 | 23:4M:217:LYS:HA | 1.42 | 0.42 |
| 24:4O:202:PHE:O | 24:4O:203:PRO:C | 2.58 | 0.42 |
| 26:4W:68:VAL:HG12 | 26:4W:73:LEU:HD13 | 2.01 | 0.42 |
| 27:4Y:235:PHE:HB3 | 27:4Y:242:LYS:HD3 | 2.02 | 0.42 |
| 31:5I:380:LYS:HG2 | 41:IB:224:ASP:HA | 2.02 | 0.42 |
| 31:5I:498:THR:HB | 41:IP:219:THR:HG21 | 2.02 | 0.42 |
| 31:5I:503:ASP:OD1 | 31:5I:503:ASP:N | 2.53 | 0.42 |
| 33:5N:176:THR:O | 33:5N:179:LYS:HG3 | 2.20 | 0.42 |
| 33:5N:238:MET:O | 33:5N:241:THR:OG1 | 2.26 | 0.42 |
| 33:5O:109:LYS:HZ2 | 41:HM:80:PRO:HA | 1.84 | 0.42 |
| 34:5Q:131:LYS:HD3 | 34:5Q:131:LYS:HA | 1.76 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:5Q:288:LEU:HD12 | 40:GE:282:TYR:CE2 | 2.54 | 0.42 |
| 36:5X:97:ALA:HB3 | 36:5X:98:ILE:HD12 | 2.02 | 0.42 |
| 40:AA:191:THR:O | 40:AA:195:LEU:HB2 | 2.20 | 0.42 |
| 41:AB:156:ARG:NE | 41:AB:195:ASN:O | 2.53 | 0.42 |
| 40:AE:180:ALA:N | 40:AE:183:GLU:OE1 | 2.34 | 0.42 |
| 40:AF:133:GLN:HB3 | 40:AF:252:LEU:HD12 | 2.02 | 0.42 |
| 40:AH:287:SER:HA | 40:AH:372:ARG:HH11 | 1.84 | 0.42 |
| 41:AL:163:ILE:HD11 | 41:AL:251:ARG:HG3 | 2.02 | 0.42 |
| 41:AM:253:LEU:O | 41:AM:257:MET:HB3 | 2.19 | 0.42 |
| 41:AO:374:ILE:O | 41:AO:375:GLN:C | 2.57 | 0.42 |
| 41:AP:128:ASP:OD1 | 41:AP:128:ASP:N | 2.53 | 0.42 |
| 41:AP:189:VAL:O | 41:AP:193:VAL:HG23 | 2.19 | 0.42 |
| 40:BH:214:ARG:NH2 | 40:BH:220:GLU:O | 2.52 | 0.42 |
| 41:BM:174:LYS:HB2 | 41:BM:174:LYS:HE3 | 1.69 | 0.42 |
| 41:BN:22:GLU:HG3 | 41:BN:81:PHE:HB2 | 2.01 | 0.42 |
| 41:BN:275:SER:C | 41:BN:278:SER:H | 2.23 | 0.42 |
| 40:CA:146:GLY:O | 40:CA:147:SER:C | 2.58 | 0.42 |
| 41:CB:203:ASP:N | 41:CB:300:MET:O | 2.46 | 0.42 |
| 41:CB:263:LEU:HD23 | 41:CB:263:LEU:HA | 1.94 | 0.42 |
| 40:CG:150:THR:O | 40:CG:154:MET:HG2 | 2.20 | 0.42 |
| 41:CN:254:ALA:O | 41:CN:258:VAL:HG12 | 2.19 | 0.42 |
| 41:CO:169:VAL:HA | 41:CO:202:ILE:O | 2.20 | 0.42 |
| 40:DA:62:VAL:CG1 | 40:EA:283:HIS:HB3 | 2.48 | 0.42 |
| 40:DA:139:HIS:CG | 40:DA:150:THR:HG21 | 2.55 | 0.42 |
| 41:DB:58:LYS:HE3 | 41:DB:58:LYS:HB3 | 1.61 | 0.42 |
| 41:DB:82:GLY:O | 41:DB:84:ILE:N | 2.53 | 0.42 |
| 41:DB:329:GLN:O | 41:DB:330:MET:C | 2.58 | 0.42 |
| 41:DB:331:LEU:HG | 40:DG:177:VAL:HA | 2.02 | 0.42 |
| 40:DE:199:ASP:O | 40:DE:266:HIS:ND1 | 2.53 | 0.42 |
| 40:DE:346:TRP:CG | 41:DM:391:ARG:HD2 | 2.54 | 0.42 |
| 40:DF:4:CYS:O | 40:DF:4:CYS:SG | 2.77 | 0.42 |
| 40:DF:194:THR:C | 40:DF:196:GLU:H | 2.22 | 0.42 |
| 40:DF:230:LEU:HG | 40:DF:367:LEU:HD11 | 2.01 | 0.42 |
| 40:DF:271:THR:HG1 | 40:DF:301:GLN:HA | 1.85 | 0.42 |
| 40:DF:298:PRO:HB3 | 40:DF:307:PRO:HD2 | 2.02 | 0.42 |
| 40:DF:326:LYS:NZ | 41:DN:211:CYS:HB2 | 2.34 | 0.42 |
| 40:DF:336:LYS:HB2 | 40:DF:336:LYS:HE3 | 1.68 | 0.42 |
| 40:DF:363:VAL:O | 40:DF:364:PRO:C | 2.57 | 0.42 |
| 40:DH:1:GLN:HB3 | 40:DH:2:ARG:H | 1.65 | 0.42 |
| 40:DH:217:LEU:C | 40:DH:219:ILE:H | 2.19 | 0.42 |
| 40:DH:223:THR:HG22 | 40:DH:226:ASN:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DH:286:LEU:HD23 | 40:DH:286:LEU:HA | 1.93 | 0.42 |
| 41:DL:388:MET:O | 41:DL:392:LYS:N | 2.53 | 0.42 |
| 41:DM:386:THR:O | 41:DM:390:ARG:HB2 | 2.20 | 0.42 |
| 41:DN:292:GLN:O | 41:DN:294:PHE:N | 2.53 | 0.42 |
| 41:DN:359:ARG:CZ | 41:DN:359:ARG:HB2 | 2.49 | 0.42 |
| 41:DP:324:LYS:HE2 | 41:DP:324:LYS:HA | 2.02 | 0.42 |
| 40:EA:123:ARG:HH11 | 40:FA:338:LYS:HE3 | 1.85 | 0.42 |
| 41:EB:258:VAL:HG23 | 40:EG:406:TRP:HE1 | 1.84 | 0.42 |
| 40:EE:205:ASP:O | 40:EE:209:ILE:HG13 | 2.20 | 0.42 |
| 40:EF:2:ARG:HG3 | 40:EF:51:THR:HG22 | 2.02 | 0.42 |
| 40:EG:264:ARG:HG2 | 40:EG:427:LEU:HD13 | 2.02 | 0.42 |
| 40:EH:172:TYR:O | 40:EH:173:PRO:C | 2.58 | 0.42 |
| 40:EI:102:ASN:O | 40:EI:103:TYR:C | 2.57 | 0.42 |
| 40:EI:123:ARG:HA | 40:EI:161:TYR:CE2 | 2.53 | 0.42 |
| 40:EI:250:VAL:HG11 | 40:EI:318:LEU:HD11 | 2.02 | 0.42 |
| 41:EM:263:LEU:HD13 | 41:EM:263:LEU:HA | 1.77 | 0.42 |
| 41:EO:69:GLU:HA | 41:EO:70:PRO:HD3 | 1.82 | 0.42 |
| 40:FA:63:PRO:HG2 | 40:FA:91:GLN:HE22 | 1.85 | 0.42 |
| 40:FA:273:ALA:HB3 | 40:FA:374:VAL:H | 1.84 | 0.42 |
| 41:FB:282:ARG:HD3 | 41:FB:283:ALA:H | 1.85 | 0.42 |
| 40:FH:263:PRO:HG3 | 41:FP:396:HIS:CD2 | 2.55 | 0.42 |
| 40:FI:57:GLY:O | 40:FI:58:ALA:HB3 | 2.20 | 0.42 |
| 41:FM:139:LEU:HB2 | 41:FM:170:VAL:HA | 2.00 | 0.42 |
| 41:FP:148:GLY:O | 41:FP:152:ILE:HG12 | 2.20 | 0.42 |
| 41:FP:346:PRO:O | 41:FP:347:ASN:ND2 | 2.53 | 0.42 |
| 40:GA:393:LYS:HD2 | 41:GN:346:PRO:HB2 | 2.01 | 0.42 |
| 40:GE:234:ILE:O | 40:GE:238:ILE:HG23 | 2.20 | 0.42 |
| 40:GF:224:TYR:HD1 | 40:GF:227:LEU:HD12 | 1.85 | 0.42 |
| 40:GF:319:TYR:HB3 | 40:GF:323:VAL:HG21 | 2.01 | 0.42 |
| 40:GF:331:ALA:O | 40:GF:335:ILE:HG12 | 2.20 | 0.42 |
| 40:GG:273:ALA:HB1 | 40:GG:274:PRO:CD | 2.49 | 0.42 |
| 40:GH:88:HIS:C | 40:GH:90:GLU:H | 2.23 | 0.42 |
| 40:GI:86:LEU:HB3 | 40:GI:87:PHE:H | 1.73 | 0.42 |
| 40:GI:189:LEU:HD21 | 40:GI:417:PHE:HA | 2.01 | 0.42 |
| 40:GI:319:TYR:HB2 | 40:GI:355:ILE:HD13 | 2.02 | 0.42 |
| 41:GN:233:MET:HE2 | 41:GN:233:MET:HB2 | 1.83 | 0.42 |
| 41:GO:238:THR:HG1 | 41:GO:354:CYS:HG | 1.67 | 0.42 |
| 41:GP:276:ARG:HD2 | 41:GP:276:ARG:HA | 1.86 | 0.42 |
| 40:HE:329:ASN:O | 40:HE:332:ILE:HG12 | 2.20 | 0.42 |
| 40:HH:27:GLU:OE2 | 40:HH:236:SER:OG | 2.38 | 0.42 |
| 40:HH:208:ALA:HA | 40:HH:211:ASP:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HI:181:VAL:HG23 | 40:HI:182:VAL:HG13 | 2.02 | 0.42 |
| 40:HI:315:CYS:HA | 40:HI:377:LEU:O | 2.20 | 0.42 |
| 41:HM:87:PRO:HD3 | 41:IM:281:TYR:HD2 | 1.85 | 0.42 |
| 41:HN:103:LYS:HB2 | 41:HN:103:LYS:HE2 | 1.48 | 0.42 |
| 41:HN:198:GLU:HG3 | 41:HN:266:PHE:CE2 | 2.54 | 0.42 |
| 41:HQ:198:GLU:OE1 | 41:HQ:200:TYR:OH | 2.31 | 0.42 |
| 40:IA:326:LYS:HE3 | 41:IB:208:TYR:HB2 | 2.01 | 0.42 |
| 40:IE:258:ASN:N | 40:IE:258:ASN:ND2 | 2.68 | 0.42 |
| 41:IP:387:ALA:HA | 41:IP:390:ARG:NH1 | 2.35 | 0.42 |
| 41:IQ:139:LEU:HG | 41:IQ:168:SER:HB2 | 2.01 | 0.42 |
| 41:JB:13:GLY:HA2 | 41:JB:16:ILE:HG22 | 2.02 | 0.42 |
| 40:JF:177:VAL:HB | 41:JM:331:LEU:HD22 | 2.00 | 0.42 |
| 40:JF:191:THR:O | 40:JF:195:LEU:HB2 | 2.19 | 0.42 |
| 40:JF:318:LEU:O | 40:JF:374:VAL:HA | 2.19 | 0.42 |
| 40:JH:405:HIS:HA | 40:JH:408:VAL:HG12 | 2.01 | 0.42 |
| 41:JM:70:PRO:HB3 | 41:JM:92:PHE:CD2 | 2.55 | 0.42 |
| 41:JM:103:LYS:HE2 | 41:JM:103:LYS:HB3 | 1.44 | 0.42 |
| 41:JM:137:HIS:CD2 | 41:JM:137:HIS:N | 2.88 | 0.42 |
| 41:JO:21:TRP:HA | 41:JO:24:ILE:HG22 | 2.02 | 0.42 |
| 40:KH:366:ASP:OD1 | 40:KH:366:ASP:N | 2.50 | 0.42 |
| 41:KM:121:ARG:HD2 | 41:KM:158:GLU:OE2 | 2.20 | 0.42 |
| 41:KN:161:ASP:N | 41:KN:161:ASP:OD2 | 2.52 | 0.42 |
| 41:KO:210:ILE:O | 41:KO:214:THR:OG1 | 2.27 | 0.42 |
| 40:LD:164:LYS:HA | 40:LD:164:LYS:HD3 | 1.79 | 0.42 |
| 40:LD:260:VAL:HG23 | 40:LD:265:ILE:O | 2.19 | 0.42 |
| 40:LE:167:LEU:HD11 | 40:LE:252:LEU:HD22 | 2.00 | 0.42 |
| 40:LG:35:GLN:HA | 40:LG:59:GLY:O | 2.19 | 0.42 |
| 40:LG:124:LYS:H | 40:LG:124:LYS:HG2 | 1.59 | 0.42 |
| 41:LM:6:HIS:O | 41:LM:63:ALA:HA | 2.20 | 0.42 |
| 40:MA:256:GLN:O | 40:MA:257:THR:C | 2.58 | 0.42 |
| 40:MH:12:ALA:CB | 40:MH:140:SER:HB3 | 2.49 | 0.42 |
| 41:ML:31:ASP:OD1 | 41:ML:34:GLY:N | 2.52 | 0.42 |
| 41:MN:317:PHE:HA | 41:MN:365:ALA:HA | 2.02 | 0.42 |
| 40:NA:199:ASP:HB3 | 40:NA:256:GLN:NE2 | 2.23 | 0.42 |
| 40:ND:423:ASP:O | 40:ND:426:ALA:HB3 | 2.20 | 0.42 |
| 40:NE:419:GLU:HA | 40:NE:422:GLU:HG3 | 2.01 | 0.42 |
| 40:NH:438:SER:HB2 | 41:NP:391:ARG:NH1 | 2.35 | 0.42 |
| 41:NL:137:HIS:NE2 | 41:NL:166:THR:OG1 | 2.53 | 0.42 |
| 41:NO:189:VAL:HA | 41:NO:192:LEU:HB2 | 2.02 | 0.42 |
| 41:OB:187:LEU:HD23 | 41:OB:187:LEU:HA | 1.92 | 0.42 |
| 41:OB:350:LYS:HZ3 | 40:OG:181:VAL:N | 2.15 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:OB:350:LYS:NZ | 40:OG:181:VAL:H | 2.17 | 0.42 |
| 40:OD:28:HIS:HB2 | 40:OD:30:ILE:HG12 | 2.02 | 0.42 |
| 40:OD:120:ASP:OD2 | 40:OD:124:LYS:NZ | 2.39 | 0.42 |
| 40:OE:389:ARG:O | 40:OE:393:LYS:HG3 | 2.20 | 0.42 |
| 40:OF:264:ARG:O | 40:OF:266:HIS:ND1 | 2.42 | 0.42 |
| 40:OH:142:GLY:O | 40:OH:143:GLY:C | 2.57 | 0.42 |
| 40:OH:157:LEU:HD23 | 40:OH:157:LEU:HA | 1.89 | 0.42 |
| 40:OH:408:VAL:O | 40:OH:409:GLY:C | 2.57 | 0.42 |
| 41:OL:87:PRO:HA | 41:OL:90:PHE:HD2 | 1.85 | 0.42 |
| 41:OL:107:THR:O | 41:OL:109:GLY:N | 2.52 | 0.42 |
| 41:OL:282:ARG:NH2 | 41:OL:284:LEU:HD21 | 2.34 | 0.42 |
| 41:ON:140:GLY:HA3 | 41:ON:181:GLU:OE1 | 2.20 | 0.42 |
| 40:PA:199:ASP:HB3 | 40:PA:256:GLN:HG2 | 2.02 | 0.42 |
| 41:PB:5:VAL:HB | 41:PB:133:PHE:CD1 | 2.54 | 0.42 |
| 40:PE:187:SER:O | 40:PE:191:THR:OG1 | 2.31 | 0.42 |
| 40:PG:277:SER:OG | 40:PG:277:SER:O | 2.34 | 0.42 |
| 41:PN:306:ARG:HG3 | 41:PN:340:TYR:CE1 | 2.54 | 0.42 |
| 41:QB:21:TRP:CH2 | 41:QB:50:TYR:HB3 | 2.55 | 0.42 |
| 41:QB:192:LEU:O | 41:QB:195:ASN:N | 2.53 | 0.42 |
| 40:QF:14:VAL:HG21 | 40:QF:75:ILE:HD13 | 2.01 | 0.42 |
| 40:QF:200:CYS:HA | 40:QF:266:HIS:HB2 | 2.01 | 0.42 |
| 41:QL:63:ALA:O | 41:QL:89:ASN:ND2 | 2.52 | 0.42 |
| 41:QM:21:TRP:HZ2 | 41:QM:63:ALA:HB2 | 1.85 | 0.42 |
| 41:QM:207:LEU:HD21 | 41:QM:229:VAL:HG13 | 2.01 | 0.42 |
| 41:QN:2:ARG:H | 41:QN:2:ARG:HG2 | 1.68 | 0.42 |
| 41:QN:12:CYS:SG | 41:QN:169:VAL:HG21 | 2.60 | 0.42 |
| 41:QN:117:LEU:HD13 | 41:QN:155:ILE:HG12 | 2.01 | 0.42 |
| 41:QN:134:GLN:HA | 41:QN:165:ASN:HB2 | 2.02 | 0.42 |
| 41:QP:236:VAL:HG23 | 41:QP:368:ILE:HG21 | 2.01 | 0.42 |
| 41:QP:426:GLY:O | 41:QP:428:CYS:SG | 2.76 | 0.42 |
| 40:RE:224:TYR:H | 41:RL:323:MET:HE1 | 1.84 | 0.42 |
| 40:RH:205:ASP:O | 40:RH:209:ILE:HG13 | 2.20 | 0.42 |
| 40:RH:297:GLU:HA | 40:RH:298:PRO:HD3 | 1.86 | 0.42 |
| 41:RL:189:VAL:O | 41:RL:193:VAL:HG23 | 2.20 | 0.42 |
| 41:RN:46:ARG:HA | 41:RN:46:ARG:HD3 | 1.68 | 0.42 |
| 41:RP:16:ILE:HG12 | 43:RP:502:GDP:N2 | 2.35 | 0.42 |
| 40:SA:290:GLU:OE2 | 40:SA:290:GLU:N | 2.42 | 0.42 |
| 40:SE:260:VAL:HG21 | 40:SE:266:HIS:HB3 | 2.02 | 0.42 |
| 40:SI:234:ILE:O | 40:SI:238:ILE:HD12 | 2.19 | 0.42 |
| 40:SI:311:LYS:N | 40:SI:381:THR:OG1 | 2.46 | 0.42 |
| 41:SM:229:VAL:O | 41:SM:232:THR:HG22 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SN:128:ASP:OD2 | 41:SN:129:CYS:N | 2.53 | 0.42 |
| 41:SN:207:LEU:HB3 | 41:SN:225:LEU:HD22 | 2.00 | 0.42 |
| 41:SO:240:LEU:HD23 | 41:SO:249:ASP:HA | 2.02 | 0.42 |
| 41:SO:397:TRP:O | 41:SO:400:GLY:N | 2.53 | 0.42 |
| 41:SO:415:MET:HA | 41:SO:418:LEU:HD12 | 2.01 | 0.42 |
| 41:TB:187:LEU:HD21 | 41:TB:408:PHE:CD1 | 2.54 | 0.42 |
| 41:TB:324:LYS:NZ | 40:TG:222:PRO:HG2 | 2.35 | 0.42 |
| 40:TE:28:HIS:CE1 | 40:TE:243:ARG:HH21 | 2.38 | 0.42 |
| 40:TG:27:GLU:OE1 | 40:TG:243:ARG:NH2 | 2.50 | 0.42 |
| 40:TH:178:SER:OG | 40:TH:179:THR:N | 2.53 | 0.42 |
| 40:TH:291:ILE:HG22 | 40:TH:374:VAL:HG12 | 2.01 | 0.42 |
| 41:TL:318:ARG:HG2 | 41:TL:358:PRO:HD3 | 2.02 | 0.42 |
| 41:TN:154:LYS:HA | 41:TN:157:GLU:HG3 | 2.02 | 0.42 |
| 41:TO:163:ILE:HD11 | 41:TO:251:ARG:HB2 | 2.02 | 0.42 |
| 41:TO:193:VAL:HG21 | 41:TO:418:LEU:HD21 | 2.02 | 0.42 |
| 41:TP:100:ASN:HB2 | 41:TP:103:LYS:HB2 | 2.01 | 0.42 |
| 40:UA:2:ARG:HB2 | 40:UA:133:GLN:HE22 | 1.85 | 0.42 |
| 40:UA:222:PRO:O | 41:UN:322:SER:OG | 2.37 | 0.42 |
| 42:UB:502:GTP:HN1 | 40:UG:228:ASN:ND2 | 2.18 | 0.42 |
| 40:UE:383:ILE:HG23 | 40:UE:383:ILE:HD12 | 1.85 | 0.42 |
| 40:UF:265:ILE:HD11 | 40:UF:379:ASN:HD21 | 1.84 | 0.42 |
| 40:UF:273:ALA:HB1 | 40:UF:291:ILE:HB | 2.01 | 0.42 |
| 40:UI:224:TYR:O | 40:UI:225:THR:C | 2.58 | 0.42 |
| 41:UM:215:LEU:HG | 41:UM:217:LEU:HD23 | 2.02 | 0.42 |
| 41:UM:237:THR:O | 41:UM:241:ARG:NE | 2.52 | 0.42 |
| 41:UN:226:ASN:ND2 | 43:UN:501:GDP:O6 | 2.53 | 0.42 |
| 41:UN:263:LEU:HD22 | 41:UN:422:VAL:HB | 2.01 | 0.42 |
| 41:UP:131:GLN:HE22 | 41:UP:240:LEU:HD13 | 1.85 | 0.42 |
| 41:UP:204:ASN:O | 41:UP:205:GLU:C | 2.57 | 0.42 |
| 41:UP:250:LEU:HA | 41:UP:250:LEU:HD23 | 1.93 | 0.42 |
| 41:VB:1:MET:HB3 | 41:VB:48:ASN:HD21 | 1.84 | 0.42 |
| 40:WF:263:PRO:HG3 | 41:WN:396:HIS:CG | 2.54 | 0.42 |
| 40:WF:326:LYS:HE3 | 41:WN:208:TYR:CD1 | 2.55 | 0.42 |
| 40:WG:7:VAL:O | 40:WG:137:ILE:HA | 2.19 | 0.42 |
| 40:WG:332:ILE:O | 40:WG:336:LYS:HG3 | 2.18 | 0.42 |
| 40:WI:240:ALA:HA | 40:WI:243:ARG:HH11 | 1.85 | 0.42 |
| 40:WI:273:ALA:HB2 | 40:WI:295:CYS:SG | 2.60 | 0.42 |
| 41:WM:51:TYR:HB3 | 41:WM:59:TYR:HB3 | 2.02 | 0.42 |
| 41:WM:260:PHE:HB3 | 41:WM:261:PRO:HD2 | 2.02 | 0.42 |
| 41:WN:245:GLN:O | 41:WN:247:ASN:N | 2.53 | 0.42 |
| 41:WN:395:LEU:C | 41:WN:397:TRP:H | 2.23 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WO:306:ARG:HA | 41:WO:340:TYR:HE2 | 1.84 | 0.42 |
| 41:WP:316:VAL:HA | 41:WP:352:ALA:HB3 | 2.02 | 0.42 |
| 7:1T:89:PHE:CZ | 41:VN:33:THR:HG22 | 2.54 | 0.42 |
| 7:1U:299:ARG:HD2 | 7:1U:304:GLN:HB2 | 2.02 | 0.42 |
| 8:1X:104:PRO:O | 8:1X:105:GLU:C | 2.59 | 0.42 |
| 10:2E:150:PRO:CD | 40:WF:221:ARG:HH12 | 2.32 | 0.42 |
| 11:2K:95:PRO:HG2 | 41:LP:405:GLU:HB3 | 2.02 | 0.42 |
| 12:2N:158:ASN:O | 12:2N:160:ARG:NH1 | 2.50 | 0.42 |
| 12:2Q:216:GLN:HE22 | 41:WP:119:VAL:HG23 | 1.85 | 0.42 |
| 13:2U:40:ASN:HA | 13:2U:43:GLN:HE21 | 1.85 | 0.42 |
| 13:2V:88:THR:O | 13:2V:157:HIS:HB2 | 2.20 | 0.42 |
| 13:2V:170:ARG:HB2 | 13:2V:171:LEU:H | 1.61 | 0.42 |
| 16:3J:139:LYS:HA | 16:3J:142:GLU:HG2 | 2.01 | 0.42 |
| 17:3P:185:LEU:HD12 | 17:3P:237:LEU:HD13 | 2.01 | 0.42 |
| 17:3P:342:LYS:HB2 | 17:3P:342:LYS:HE3 | 1.63 | 0.42 |
| 17:3Q:406:ARG:HD2 | 17:3Q:410:GLU:HG3 | 2.01 | 0.42 |
| 18:3T:332:GLN:HB3 | 18:3T:402:LEU:HD13 | 2.02 | 0.42 |
| 20:4A:160:PHE:O | 20:4A:164:LEU:HG | 2.20 | 0.42 |
| 22:4I:340:ILE:HD13 | 22:4I:353:LEU:HD23 | 2.02 | 0.42 |
| 22:4J:626:GLN:C | 22:4J:628:LYS:H | 2.23 | 0.42 |
| 23:4M:51:LEU:HB2 | 23:4M:52:ALA:H | 1.71 | 0.42 |
| 23:4M:216:MET:HE2 | 23:4M:216:MET:HB2 | 1.88 | 0.42 |
| 23:4M:240:LEU:HB2 | 23:4M:241:GLY:H | 1.74 | 0.42 |
| 23:4Q:267:ASP:O | 23:4Q:268:ALA:C | 2.59 | 0.42 |
| 23:4R:172:TYR:O | 23:4R:174:MET:N | 2.48 | 0.42 |
| 23:4R:202:PHE:N | 23:4R:203:PRO:HD2 | 2.35 | 0.42 |
| 26:4W:237:THR:O | 26:4W:239:CYS:N | 2.53 | 0.42 |
| 27:4Z:42:LYS:HE3 | 27:4Z:102:TYR:O | 2.20 | 0.42 |
| 27:4Z:61:ASP:OD1 | 27:4Z:62:GLY:N | 2.53 | 0.42 |
| 29:5E:108:VAL:CG1 | 40:GE:114:LEU:HD21 | 2.49 | 0.42 |
| 33:5N:444:ILE:HD13 | 33:5O:114:VAL:HG13 | 2.01 | 0.42 |
| 35:5T:81:HIS:O | 35:5T:85:HIS:CB | 2.68 | 0.42 |
| 36:5W:101:TRP:HD1 | 36:5W:103:VAL:HG22 | 1.85 | 0.42 |
| 36:5Y:74:SER:HB3 | 40:NG:84:ARG:HD2 | 2.01 | 0.42 |
| 41:AB:192:LEU:HA | 41:AB:196:THR:HG22 | 2.02 | 0.42 |
| 40:AG:21:TRP:HA | 40:AG:24:TYR:HD1 | 1.85 | 0.42 |
| 40:AG:204:VAL:HG11 | 40:AG:231:ILE:HG12 | 2.01 | 0.42 |
| 41:AN:152:ILE:HG22 | 41:AN:195:ASN:HB3 | 2.02 | 0.42 |
| 41:AO:260:PHE:HB2 | 41:AO:263:LEU:HD13 | 2.00 | 0.42 |
| 40:BA:241:SER:HA | 40:BA:356:ASN:HD22 | 1.85 | 0.42 |
| 40:BA:253:THR:HG23 | 41:BB:98:GLY:HA2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BA:271:THR:HG22 | 40:BA:301:GLN:HA | 2.02 | 0.42 |
| 40:BE:300:ASN:OD1 | 40:BE:300:ASN:N | 2.53 | 0.42 |
| 40:BF:293:ASN:O | 40:BF:297:GLU:HG3 | 2.20 | 0.42 |
| 40:BH:363:VAL:O | 40:BH:364:PRO:C | 2.58 | 0.42 |
| 40:BI:313:MET:HB3 | 40:BI:379:ASN:O | 2.20 | 0.42 |
| 41:BL:311:LEU:HD23 | 41:BL:342:VAL:HG11 | 2.02 | 0.42 |
| 41:BM:19:LYS:HA | 41:BM:19:LYS:HD3 | 1.74 | 0.42 |
| 41:BN:1:MET:SD | 41:BN:48:ASN:ND2 | 2.92 | 0.42 |
| 41:BN:424:THR:HG23 | 41:BN:425:ARG:HD2 | 2.02 | 0.42 |
| 40:CA:31:GLN:O | 40:CA:33:ASP:N | 2.43 | 0.42 |
| 40:CA:112:LYS:O | 40:CA:113:GLU:C | 2.57 | 0.42 |
| 40:CE:156:ARG:H | 40:CE:156:ARG:HG2 | 1.69 | 0.42 |
| 40:CG:171:ILE:HG21 | 42:CG:501:GTP:H1' | 2.02 | 0.42 |
| 40:CH:107:HIS:ND1 | 40:CH:152:LEU:HG | 2.35 | 0.42 |
| 41:CM:44:LEU:HA | 41:CM:44:LEU:HD12 | 1.92 | 0.42 |
| 41:CM:68:LEU:HD12 | 41:CM:68:LEU:HA | 1.81 | 0.42 |
| 41:CM:183:TYR:O | 41:CM:184:ASN:C | 2.58 | 0.42 |
| 41:CP:174:LYS:HD3 | 41:CP:205:GLU:HB2 | 2.01 | 0.42 |
| 41:CP:204:ASN:HD22 | 41:CP:204:ASN:HA | 1.43 | 0.42 |
| 41:CP:245:GLN:O | 41:CP:246:LEU:C | 2.59 | 0.42 |
| 41:CP:401:GLU:HB3 | 41:CP:402:GLY:H | 1.72 | 0.42 |
| 40:DA:269:LEU:HD23 | 40:DA:380:THR:OG1 | 2.19 | 0.42 |
| 40:DA:326:LYS:HG3 | 41:DB:212:PHE:CE1 | 2.55 | 0.42 |
| 41:DB:69:GLU:HA | 41:DB:93:GLY:O | 2.20 | 0.42 |
| 41:DB:324:LYS:O | 41:DB:328:GLU:N | 2.42 | 0.42 |
| 40:DF:73:THR:O | 40:DF:76:ASP:HB2 | 2.20 | 0.42 |
| 40:DF:131:GLY:C | 40:DF:133:GLN:H | 2.23 | 0.42 |
| 40:DF:176:GLN:HB3 | 40:DF:177:VAL:H | 1.55 | 0.42 |
| 40:DF:359:PRO:O | 40:DF:360:PRO:C | 2.58 | 0.42 |
| 40:DH:396:LEU:HD12 | 40:DH:396:LEU:HA | 1.84 | 0.42 |
| 41:DL:252:LYS:HB2 | 41:DL:252:LYS:HE2 | 1.61 | 0.42 |
| 41:DN:143:THR:O | 41:DN:144:GLY:C | 2.58 | 0.42 |
| 41:DN:204:ASN:ND2 | 41:DN:222:TYR:HE1 | 2.17 | 0.42 |
| 41:DN:239:CYS:C | 41:DN:241:ARG:N | 2.72 | 0.42 |
| 41:DP:89:ASN:O | 41:DP:91:VAL:HG22 | 2.20 | 0.42 |
| 41:DP:155:ILE:C | 41:DP:157:GLU:H | 2.23 | 0.42 |
| 41:DP:165:ASN:OD1 | 41:DP:165:ASN:N | 2.50 | 0.42 |
| 41:DP:226:ASN:HD22 | 41:DP:226:ASN:HA | 1.58 | 0.42 |
| 41:EB:255:VAL:HG11 | 40:EG:100:ALA:O | 2.19 | 0.42 |
| 40:EE:7:VAL:HG11 | 40:EE:153:LEU:HD21 | 2.01 | 0.42 |
| 40:EH:123:ARG:HE | 40:EH:123:ARG:HB3 | 1.40 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EH:319:TYR:HA | 40:EH:374:VAL:HA | 2.02 | 0.42 |
| 40:EI:50:ASN:C | 40:EI:52:PHE:H | 2.24 | 0.42 |
| 40:EI:183:GLU:O | 40:EI:184:PRO:C | 2.58 | 0.42 |
| 40:EI:261:PRO:HD2 | 40:EI:265:ILE:HD11 | 2.01 | 0.42 |
| 41:EM:257:MET:HE2 | 41:EM:257:MET:HB3 | 1.72 | 0.42 |
| 41:EM:416:ASN:C | 41:EM:418:LEU:H | 2.23 | 0.42 |
| 41:EN:313:VAL:O | 41:EN:349:VAL:HA | 2.20 | 0.42 |
| 41:EP:45:GLU:HG3 | 41:EP:46:ARG:N | 2.33 | 0.42 |
| 41:EP:67:ASP:O | 41:EP:92:PHE:HA | 2.20 | 0.42 |
| 41:EP:226:ASN:ND2 | 43:EP:501:GDP:HN1 | 2.18 | 0.42 |
| 40:FA:101:ASN:H | 41:FN:252:LYS:CE | 2.32 | 0.42 |
| 40:FA:269:LEU:HD22 | 40:FA:303:VAL:HG21 | 2.02 | 0.42 |
| 40:FE:297:GLU:HA | 40:FE:298:PRO:HD3 | 1.86 | 0.42 |
| 40:FF:325:PRO:HB2 | 41:FN:222:TYR:HE2 | 1.84 | 0.42 |
| 40:FG:229:ARG:HH11 | 40:FG:363:VAL:HG11 | 1.83 | 0.42 |
| 40:FH:147:SER:HB2 | 40:FH:190:THR:HG21 | 2.02 | 0.42 |
| 40:FI:216:ASN:ND2 | 40:FI:216:ASN:O | 2.53 | 0.42 |
| 40:GE:1:GLN:HB3 | 40:GE:2:ARG:H | 1.55 | 0.42 |
| 40:GE:254:GLU:OE1 | 41:GM:99:ASN:ND2 | 2.53 | 0.42 |
| 40:GH:121:ARG:HD2 | 40:GH:124:LYS:HD3 | 2.00 | 0.42 |
| 40:GH:144:GLY:O | 40:GH:145:THR:C | 2.58 | 0.42 |
| 40:GH:171:ILE:H | 40:GH:171:ILE:HG12 | 1.48 | 0.42 |
| 40:GH:326:LYS:HD2 | 40:GH:326:LYS:HA | 1.90 | 0.42 |
| 40:GI:139:HIS:CE1 | 40:GI:141:PHE:HE1 | 2.38 | 0.42 |
| 40:GI:217:LEU:HA | 40:GI:217:LEU:HD12 | 1.82 | 0.42 |
| 40:GI:222:PRO:HG2 | 41:GP:324:LYS:HZ2 | 1.85 | 0.42 |
| 40:GI:333:ALA:O | 40:GI:334:ALA:C | 2.57 | 0.42 |
| 40:GI:356:ASN:HD22 | 40:GI:356:ASN:HA | 1.64 | 0.42 |
| 41:GN:103:LYS:HB2 | 41:GN:103:LYS:HE3 | 1.89 | 0.42 |
| 41:GN:328:GLU:O | 41:GN:329:GLN:C | 2.58 | 0.42 |
| 41:GN:385:PHE:CZ | 41:GN:408:PHE:HB3 | 2.49 | 0.42 |
| 41:GP:326:VAL:O | 41:GP:330:MET:HG2 | 2.20 | 0.42 |
| 41:HB:22:GLU:HG3 | 41:HB:81:PHE:CD2 | 2.55 | 0.42 |
| 40:HI:62:VAL:HG11 | 40:II:283:HIS:HA | 2.02 | 0.42 |
| 41:HN:138:SER:O | 41:HN:139:LEU:C | 2.58 | 0.42 |
| 41:HN:218:THR:O | 41:HN:220:PRO:HD3 | 2.20 | 0.42 |
| 41:HN:398:TYR:HB3 | 41:HN:408:PHE:CZ | 2.54 | 0.42 |
| 41:HQ:16:ILE:HD11 | 41:HQ:229:VAL:HB | 2.02 | 0.42 |
| 41:HQ:105:HIS:ND1 | 41:HQ:150:LEU:HB2 | 2.34 | 0.42 |
| 41:HQ:318:ARG:NE | 41:HQ:358:PRO:HD3 | 2.35 | 0.42 |
| 40:II:223:THR:HG23 | 40:II:225:THR:HG22 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IO:138:SER:HA | 41:IO:169:VAL:HG22 | 2.02 | 0.42 |
| 40:JA:70:LEU:HD12 | 40:JA:145:THR:HA | 2.01 | 0.42 |
| 41:JB:273:LEU:HD23 | 41:JB:273:LEU:HA | 1.94 | 0.42 |
| 40:JD:7:VAL:HG11 | 40:JD:153:LEU:HD21 | 2.02 | 0.42 |
| 40:JD:102:ASN:H | 40:JD:144:GLY:HA3 | 1.85 | 0.42 |
| 40:JE:36:MET:O | 40:JE:38:SER:N | 2.53 | 0.42 |
| 40:JG:26:LEU:HD11 | 40:JG:363:VAL:HG12 | 2.02 | 0.42 |
| 41:JM:47:ILE:H | 41:JM:47:ILE:HG13 | 1.69 | 0.42 |
| 41:JM:380:ARG:HA | 41:JM:383:GLU:CD | 2.40 | 0.42 |
| 41:JN:121:ARG:O | 41:JN:124:ALA:N | 2.53 | 0.42 |
| 41:JO:8:GLN:HE21 | 41:JO:65:LEU:HD13 | 1.85 | 0.42 |
| 40:KA:11:GLN:O | 40:KA:15:GLN:HG3 | 2.20 | 0.42 |
| 40:KA:210:TYR:CZ | 40:KA:227:LEU:HD11 | 2.55 | 0.42 |
| 40:KD:231:ILE:HA | 40:KD:234:ILE:HD12 | 2.02 | 0.42 |
| 41:KL:289:LEU:H | 41:KL:289:LEU:HG | 1.65 | 0.42 |
| 41:KN:142:GLY:O | 41:KN:144:GLY:N | 2.53 | 0.42 |
| 41:KP:211:CYS:HA | 41:KP:215:LEU:HD12 | 2.02 | 0.42 |
| 41:KP:272:PRO:HD3 | 41:KP:365:ALA:H | 1.85 | 0.42 |
| 40:LF:187:SER:HB2 | 40:LF:390:LEU:HD21 | 2.02 | 0.42 |
| 40:LF:224:TYR:HA | 40:LF:227:LEU:HD12 | 2.02 | 0.42 |
| 40:MA:173:PRO:HG2 | 40:MA:187:SER:CB | 2.50 | 0.42 |
| 40:MA:223:THR:OG1 | 40:MA:224:TYR:N | 2.52 | 0.42 |
| 40:MF:163:LYS:H | 40:MF:163:LYS:HG3 | 1.70 | 0.42 |
| 40:MF:236:SER:O | 40:MF:240:ALA:HB2 | 2.19 | 0.42 |
| 40:MG:172:TYR:HE1 | 40:MG:386:ALA:HB1 | 1.85 | 0.42 |
| 40:MG:266:HIS:O | 40:MG:266:HIS:ND1 | 2.50 | 0.42 |
| 40:MH:429:LYS:HE2 | 40:MH:429:LYS:HB2 | 1.65 | 0.42 |
| 41:MN:181:GLU:HG2 | 41:MN:182:PRO:HD3 | 2.02 | 0.42 |
| 41:MO:278:SER:C | 41:MO:280:GLN:H | 2.23 | 0.42 |
| 41:NB:87:PRO:HD3 | 41:OB:281:TYR:CD2 | 2.55 | 0.42 |
| 41:NM:143:THR:OG1 | 41:NM:144:GLY:N | 2.53 | 0.42 |
| 41:NO:197:ASP:OD1 | 41:NO:197:ASP:N | 2.45 | 0.42 |
| 40:OA:140:SER:OG | 40:OA:141:PHE:N | 2.52 | 0.42 |
| 41:OB:318:ARG:HE | 41:OB:318:ARG:HB3 | 1.62 | 0.42 |
| 40:OF:113:GLU:N | 40:OF:113:GLU:OE2 | 2.53 | 0.42 |
| 40:OG:211:ASP:HB3 | 40:OG:215:ARG:HH12 | 1.85 | 0.42 |
| 40:OH:16:ILE:HA | 40:OH:228:ASN:HB2 | 2.02 | 0.42 |
| 41:OL:113:VAL:HG21 | 41:OL:150:LEU:HD23 | 2.02 | 0.42 |
| 41:OO:225:LEU:HA | 41:OO:225:LEU:HD12 | 1.79 | 0.42 |
| 41:OO:241:ARG:HG3 | 41:OO:242:PHE:CD2 | 2.55 | 0.42 |
| 41:OP:167:PHE:HZ | 41:OP:236:VAL:HG11 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:PE:23:LEU:HD12 | 40:PE:26:LEU:HD11 | 2.00 | 0.42 |
| 40:PG:288:VAL:HG21 | 40:PG:327:ASP:HB3 | 2.02 | 0.42 |
| 41:PL:16:ILE:HG13 | 41:PL:226:ASN:HB3 | 2.02 | 0.42 |
| 41:PM:24:ILE:HG12 | 41:PM:28:HIS:HD2 | 1.85 | 0.42 |
| 41:PM:197:ASP:OD1 | 41:PM:197:ASP:N | 2.51 | 0.42 |
| 41:PM:332:ASN:O | 41:PM:336:LYS:HB2 | 2.19 | 0.42 |
| 41:PP:195:ASN:HB3 | 41:PP:196:THR:H | 1.71 | 0.42 |
| 41:PP:309:ARG:H | 41:PP:372:THR:HG1 | 1.66 | 0.42 |
| 41:QB:121:ARG:O | 41:QB:123:GLU:N | 2.53 | 0.42 |
| 41:QB:420:ASN:O | 41:QB:421:PRO:C | 2.57 | 0.42 |
| 40:QG:276:ILE:HG23 | 40:QG:280:LYS:NZ | 2.35 | 0.42 |
| 40:QH:211:ASP:OD1 | 40:QH:212:ILE:N | 2.52 | 0.42 |
| 41:QL:6:HIS:HD2 | 41:QL:21:TRP:HE1 | 1.68 | 0.42 |
| 41:QL:24:ILE:HD12 | 41:QL:241:ARG:NH1 | 2.35 | 0.42 |
| 41:QL:299:MET:HG3 | 41:QL:301:ALA:H | 1.84 | 0.42 |
| 41:QL:379:LYS:O | 41:QL:382:SER:OG | 2.23 | 0.42 |
| 41:QM:199:THR:OG1 | 41:QM:265:PHE:HA | 2.20 | 0.42 |
| 41:QP:278:SER:HA | 41:QP:281:TYR:HD2 | 1.85 | 0.42 |
| 40:RF:183:GLU:OE2 | 42:RF:501:GTP:O3' | 2.38 | 0.42 |
| 40:RG:238:ILE:HG23 | 40:RG:255:PHE:CE2 | 2.55 | 0.42 |
| 40:RG:316:CYS:O | 40:RG:376:MET:HA | 2.20 | 0.42 |
| 40:RH:156:ARG:HD2 | 40:RH:156:ARG:HA | 1.85 | 0.42 |
| 40:RI:366:ASP:OD1 | 40:RI:366:ASP:N | 2.52 | 0.42 |
| 41:RP:172:SER:HB2 | 41:RP:205:GLU:HB3 | 2.02 | 0.42 |
| 41:RP:362:LYS:HE2 | 41:RP:362:LYS:HB2 | 1.98 | 0.42 |
| 40:SA:139:HIS:HE1 | 40:SA:141:PHE:CE1 | 2.38 | 0.42 |
| 41:SB:148:GLY:O | 41:SB:152:ILE:HG12 | 2.20 | 0.42 |
| 40:SF:7:VAL:O | 40:SF:137:ILE:HA | 2.19 | 0.42 |
| 40:SF:386:ALA:HA | 40:SF:389:ARG:HE | 1.85 | 0.42 |
| 40:SH:167:LEU:HD11 | 40:SH:202:PHE:HE2 | 1.84 | 0.42 |
| 40:SH:221:ARG:HA | 41:SO:324:LYS:HZ3 | 1.84 | 0.42 |
| 40:SH:421:ARG:NH1 | 40:SH:421:ARG:O | 2.53 | 0.42 |
| 41:SL:238:THR:HA | 41:SL:241:ARG:HG2 | 2.02 | 0.42 |
| 41:SM:204:ASN:H | 41:SM:204:ASN:HD22 | 1.67 | 0.42 |
| 41:SO:305:PRO:O | 41:SO:306:ARG:C | 2.59 | 0.42 |
| 41:SP:296:ALA:HB1 | 41:SP:305:PRO:HD2 | 2.02 | 0.42 |
| 41:TB:46:ARG:HD3 | 41:TB:46:ARG:HA | 1.87 | 0.42 |
| 40:TE:62:VAL:HG21 | 40:UE:283:HIS:HB3 | 2.02 | 0.42 |
| 40:TG:316:CYS:HA | 40:TG:352:LYS:HB2 | 2.02 | 0.42 |
| 40:TI:54:SER:O | 40:TI:61:HIS:HA | 2.20 | 0.42 |
| 41:TL:202:ILE:HG21 | 41:TL:229:VAL:HG22 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TO:22:GLU:HG3 | 41:TO:81:PHE:CG | 2.55 | 0.42 |
| 40:UF:298:PRO:HA | 40:UF:307:PRO:HG2 | 2.01 | 0.42 |
| 41:UM:181:GLU:HG2 | 41:UM:182:PRO:HD3 | 2.01 | 0.42 |
| 41:UP:44:LEU:O | 41:UP:47:ILE:HG13 | 2.20 | 0.42 |
| 41:UP:324:LYS:NZ | 41:UP:324:LYS:HB2 | 2.34 | 0.42 |
| 41:VB:336:LYS:HB3 | 41:VB:336:LYS:HE2 | 1.87 | 0.42 |
| 40:VG:210:TYR:CE1 | 40:VG:227:LEU:HD21 | 2.55 | 0.42 |
| 40:VG:356:ASN:OD1 | 40:VG:357:TYR:N | 2.53 | 0.42 |
| 40:VG:438:SER:HB2 | 41:VO:391:ARG:HD2 | 2.02 | 0.42 |
| 40:VH:141:PHE:HB2 | 40:VH:173:PRO:HD3 | 2.02 | 0.42 |
| 40:VI:49:PHE:HE2 | 40:VI:55:GLU:HB2 | 1.84 | 0.42 |
| 40:VI:89:PRO:HD3 | 40:WH:283:HIS:HD2 | 1.85 | 0.42 |
| 40:VI:118:VAL:HG11 | 40:VI:149:PHE:CZ | 2.55 | 0.42 |
| 41:VQ:278:SER:O | 41:VQ:278:SER:OG | 2.36 | 0.42 |
| 40:WA:150:THR:O | 40:WA:154:MET:HG2 | 2.19 | 0.42 |
| 40:WG:416:GLU:HA | 40:WG:419:GLU:HB2 | 2.02 | 0.42 |
| 40:WH:51:THR:HG21 | 40:WH:243:ARG:HG2 | 2.02 | 0.42 |
| 40:WH:69:ASP:OD2 | 40:WH:70:LEU:N | 2.52 | 0.42 |
| 41:WM:44:LEU:HD12 | 41:WM:44:LEU:HA | 1.89 | 0.42 |
| 41:WM:215:LEU:O | 41:WM:216:LYS:C | 2.59 | 0.42 |
| 41:WN:271:ALA:HB3 | 41:WN:272:PRO:CD | 2.49 | 0.42 |
| 6:1P:217:ARG:NH1 | 41:ML:417:ASP:OD1 | 2.52 | 0.41 |
| 7:1T:45:CYS:HB3 | 7:1T:65:ASN:O | 2.19 | 0.41 |
| 7:1T:236:THR:HG21 | 40:WE:39:ASP:OD2 | 2.20 | 0.41 |
| 7:1T:340:PHE:CE1 | 7:1T:348:PHE:HB3 | 2.55 | 0.41 |
| 7:1T:372:VAL:HB | 7:1T:393:TRP:CH2 | 2.55 | 0.41 |
| 8:1Y:201:CYS:SG | 8:1Y:205:ARG:HD2 | 2.60 | 0.41 |
| 8:1Z:434:ALA:HA | 8:1Z:437:VAL:HG12 | 2.02 | 0.41 |
| 11:2J:110:ALA:O | 11:2J:114:ILE:HD12 | 2.19 | 0.41 |
| 11:2J:250:ILE:O | 11:2J:251:TYR:C | 2.58 | 0.41 |
| 11:2K:252:ILE:HD12 | 11:2K:252:ILE:HA | 1.69 | 0.41 |
| 13:2T:91:VAL:HG13 | 13:2T:151:THR:HG23 | 2.02 | 0.41 |
| 13:2T:185:LEU:HD13 | 13:2T:185:LEU:HA | 1.80 | 0.41 |
| 13:2V:90:GLU:HA | 13:2V:103:PHE:O | 2.20 | 0.41 |
| 14:3B:76:PRO:HG3 | 40:LD:196:GLU:HB3 | 2.02 | 0.41 |
| 14:3C:61:TRP:HD1 | 40:MG:310:GLY:HA2 | 1.85 | 0.41 |
| 15:3F:187:ILE:H | 15:3F:187:ILE:HG13 | 1.75 | 0.41 |
| 15:3H:262:THR:HG21 | 16:3K:80:LYS:HE3 | 2.02 | 0.41 |
| 17:3O:351:ILE:CG1 | 17:3O:469:ASP:HB3 | 2.50 | 0.41 |
| 17:3Q:399:ARG:HB3 | 17:3Q:420:LEU:HD21 | 2.01 | 0.41 |
| 17:3R:181:LEU:O | 17:3R:185:LEU:HD12 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:3R:256:LYS:HE2 | 17:3R:256:LYS:HB2 | 1.84 | 0.41 |
| 20:4A:181:ALA:O | 20:4A:184:LEU:N | 2.53 | 0.41 |
| 20:4A:182:ASP:O | 20:4A:186:ASN:HB2 | 2.19 | 0.41 |
| 22:4J:282:ARG:HH12 | 41:CN:80:PRO:HB3 | 1.85 | 0.41 |
| 22:4J:495:LYS:HA | 22:4J:495:LYS:HD2 | 1.75 | 0.41 |
| 24:4O:210:LEU:HD12 | 24:4O:210:LEU:HA | 1.90 | 0.41 |
| 23:4P:198:PHE:HD2 | 41:DN:322:SER:HB3 | 1.84 | 0.41 |
| 23:4P:259:ARG:HB2 | 23:4P:264:LEU:HG | 2.02 | 0.41 |
| 23:4R:235:THR:O | 23:4R:236:TYR:C | 2.58 | 0.41 |
| 26:4W:269:ILE:HD11 | 26:4W:272:MET:HG2 | 2.02 | 0.41 |
| 26:4W:343:ARG:HE | 26:4W:353:ASN:HD21 | 1.68 | 0.41 |
| 27:4Z:75:PRO:HG3 | 27:4Z:265:MET:HE2 | 2.00 | 0.41 |
| 27:4Z:93:CYS:HB3 | 27:4Z:95:THR:HG23 | 2.01 | 0.41 |
| 31:5I:728:LYS:HD2 | 31:5I:728:LYS:HA | 1.97 | 0.41 |
| 34:5Q:164:LEU:HD21 | 34:5R:490:ILE:HG21 | 2.01 | 0.41 |
| 38:6C:203:PHE:CZ | 41:VQ:328:GLU:HG3 | 2.55 | 0.41 |
| 40:AA:68:VAL:HG22 | 40:AA:93:ILE:HB | 2.01 | 0.41 |
| 40:AA:188:ILE:HA | 40:AA:191:THR:HG22 | 2.01 | 0.41 |
| 41:AB:261:PRO:HG3 | 40:AG:405:HIS:CD2 | 2.55 | 0.41 |
| 40:AG:352:LYS:NZ | 41:AO:178:THR:C | 2.73 | 0.41 |
| 40:BE:38:SER:O | 40:BE:40:LYS:N | 2.53 | 0.41 |
| 40:BF:32:PRO:HB3 | 40:BF:83:TYR:HE1 | 1.84 | 0.41 |
| 40:BH:413:GLU:N | 40:BH:416:GLU:OE1 | 2.52 | 0.41 |
| 40:BI:73:THR:O | 40:BI:74:VAL:C | 2.58 | 0.41 |
| 40:BI:148:GLY:O | 40:BI:149:PHE:C | 2.58 | 0.41 |
| 41:BO:147:MET:HE3 | 41:BO:147:MET:HB3 | 1.88 | 0.41 |
| 41:BP:358:PRO:HG2 | 41:BP:361:LEU:HB2 | 2.01 | 0.41 |
| 40:CA:119:LEU:CD1 | 40:CA:156:ARG:HG2 | 2.50 | 0.41 |
| 40:CA:157:LEU:HD23 | 40:CA:157:LEU:HA | 1.81 | 0.41 |
| 40:CE:228:ASN:HA | 40:CE:231:ILE:HD12 | 2.02 | 0.41 |
| 40:CE:254:GLU:HG2 | 41:CM:98:GLY:HA2 | 2.02 | 0.41 |
| 41:CL:4:ILE:HD11 | 41:CL:49:VAL:HG12 | 2.02 | 0.41 |
| 41:CL:189:VAL:O | 41:CL:193:VAL:HG23 | 2.20 | 0.41 |
| 41:CL:309:ARG:O | 41:CL:372:THR:HB | 2.19 | 0.41 |
| 41:CL:420:ASN:H | 41:CL:421:PRO:HD2 | 1.85 | 0.41 |
| 41:CN:28:HIS:HA | 41:CN:43:GLN:HB3 | 2.02 | 0.41 |
| 41:CN:155:ILE:C | 41:CN:157:GLU:N | 2.73 | 0.41 |
| 41:CN:239:CYS:O | 41:CN:241:ARG:N | 2.42 | 0.41 |
| 41:CO:174:LYS:HE2 | 41:CO:175:VAL:N | 2.34 | 0.41 |
| 40:DA:2:ARG:H | 40:DA:2:ARG:HG3 | 1.53 | 0.41 |
| 40:DA:169:PHE:HA | 40:DA:202:PHE:O | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DA:249:ASN:HD22 | 40:DA:249:ASN:HA | 1.52 | 0.41 |
| 41:DB:121:ARG:O | 41:DB:122:LYS:C | 2.59 | 0.41 |
| 40:DF:177:VAL:HG21 | 40:DF:207:GLU:HB2 | 2.00 | 0.41 |
| 40:DF:188:ILE:HG12 | 40:DF:390:LEU:HD13 | 2.02 | 0.41 |
| 40:DH:70:LEU:HG | 40:DH:145:THR:HG23 | 2.02 | 0.41 |
| 40:DI:273:ALA:O | 40:DI:275:VAL:N | 2.53 | 0.41 |
| 41:DL:401:GLU:HG2 | 41:DL:401:GLU:H | 1.58 | 0.41 |
| 41:DM:8:GLN:OE1 | 41:DM:14:ASN:HA | 2.20 | 0.41 |
| 41:DN:129:CYS:O | 41:DN:131:GLN:N | 2.53 | 0.41 |
| 41:DN:178:THR:HG22 | 41:DN:180:VAL:H | 1.84 | 0.41 |
| 41:DN:318:ARG:HD3 | 41:DN:358:PRO:HD3 | 2.01 | 0.41 |
| 41:DO:237:THR:O | 41:DO:241:ARG:NH1 | 2.53 | 0.41 |
| 41:DP:67:ASP:O | 41:DP:92:PHE:HA | 2.20 | 0.41 |
| 41:DP:104:GLY:C | 41:DP:109:GLY:HA3 | 2.39 | 0.41 |
| 40:EA:406:TRP:HE1 | 41:EN:258:VAL:HB | 1.84 | 0.41 |
| 41:EB:316:VAL:HA | 41:EB:352:ALA:HB3 | 2.02 | 0.41 |
| 40:EE:297:GLU:HA | 40:EE:298:PRO:HD3 | 1.81 | 0.41 |
| 40:EG:141:PHE:HB2 | 40:EG:173:PRO:HD3 | 2.02 | 0.41 |
| 40:EI:60:LYS:HG2 | 40:FI:282:TYR:O | 2.20 | 0.41 |
| 40:EI:205:ASP:O | 40:EI:208:ALA:N | 2.52 | 0.41 |
| 40:EI:276:ILE:H | 40:EI:276:ILE:HG13 | 1.57 | 0.41 |
| 40:EI:286:LEU:H | 40:EI:286:LEU:HG | 1.64 | 0.41 |
| 41:EM:25:SER:HA | 41:EM:51:TYR:OH | 2.20 | 0.41 |
| 41:EM:50:TYR:CE1 | 41:EM:237:THR:HG21 | 2.54 | 0.41 |
| 41:EM:311:LEU:HD12 | 41:EM:311:LEU:HA | 1.74 | 0.41 |
| 41:EP:260:PHE:O | 41:EP:261:PRO:C | 2.58 | 0.41 |
| 40:FA:208:ALA:O | 40:FA:209:ILE:C | 2.58 | 0.41 |
| 41:FB:252:LYS:HG2 | 41:FB:350:LYS:HZ1 | 1.85 | 0.41 |
| 40:FH:171:ILE:HD13 | 40:FH:204:VAL:HG23 | 2.02 | 0.41 |
| 40:FH:301:GLN:OE1 | 40:FH:301:GLN:N | 2.47 | 0.41 |
| 41:FO:226:ASN:ND2 | 43:FO:502:GDP:O6 | 2.44 | 0.41 |
| 40:GA:139:HIS:O | 40:GA:170:SER:HA | 2.19 | 0.41 |
| 40:GE:76:ASP:O | 40:GE:77:GLU:C | 2.59 | 0.41 |
| 40:GE:256:GLN:HG3 | 41:GM:397:TRP:CZ2 | 2.54 | 0.41 |
| 40:GH:205:ASP:O | 40:GH:209:ILE:HG13 | 2.20 | 0.41 |
| 40:GH:213:CYS:HB3 | 40:GH:219:ILE:HD12 | 2.02 | 0.41 |
| 41:GM:102:ALA:HB2 | 41:GM:403:MET:HG2 | 2.01 | 0.41 |
| 41:GM:404:ASP:OD2 | 41:GM:405:GLU:N | 2.53 | 0.41 |
| 41:GN:63:ALA:O | 41:GN:89:ASN:HB3 | 2.20 | 0.41 |
| 41:GP:12:CYS:HB2 | 43:GP:502:GDP:O4' | 2.20 | 0.41 |
| 40:HA:230:LEU:O | 40:HA:234:ILE:HG12 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HE:269:LEU:HD21 | 40:HE:305:CYS:SG | 2.60 | 0.41 |
| 40:HG:287:SER:HA | 40:HG:372:ARG:HH12 | 1.85 | 0.41 |
| 40:HH:328:VAL:O | 40:HH:332:ILE:HG12 | 2.19 | 0.41 |
| 40:HI:313:MET:SD | 40:HI:379:ASN:ND2 | 2.93 | 0.41 |
| 41:HO:337:ASN:HB2 | 41:HO:340:TYR:HB2 | 2.01 | 0.41 |
| 41:HP:25:SER:OG | 41:HP:30:ILE:O | 2.38 | 0.41 |
| 41:HQ:134:GLN:HG2 | 41:HQ:165:ASN:HB2 | 2.02 | 0.41 |
| 41:HQ:252:LYS:HB2 | 41:HQ:252:LYS:HE2 | 1.93 | 0.41 |
| 40:IE:116:ASP:OD1 | 40:IE:116:ASP:N | 2.51 | 0.41 |
| 40:IF:60:LYS:HD3 | 41:JL:281:TYR:CE2 | 2.54 | 0.41 |
| 40:IG:2:ARG:NH1 | 41:IO:69:GLU:OE2 | 2.53 | 0.41 |
| 41:IN:139:LEU:HD22 | 41:IN:170:VAL:HG12 | 2.03 | 0.41 |
| 41:IO:150:LEU:O | 41:IO:154:LYS:HG2 | 2.20 | 0.41 |
| 41:IP:172:SER:HB2 | 41:IP:205:GLU:HG2 | 2.02 | 0.41 |
| 41:IQ:42:LEU:HD11 | 41:IQ:243:PRO:HG3 | 2.02 | 0.41 |
| 40:JF:21:TRP:CZ3 | 40:JF:52:PHE:HB3 | 2.55 | 0.41 |
| 40:JF:73:THR:O | 40:JF:77:GLU:HB2 | 2.20 | 0.41 |
| 41:JM:152:ILE:HD13 | 41:JM:196:THR:HG22 | 2.02 | 0.41 |
| 41:JM:226:ASN:HD22 | 41:JM:226:ASN:HA | 1.49 | 0.41 |
| 41:JM:233:MET:HE2 | 41:JM:233:MET:HB2 | 1.78 | 0.41 |
| 41:JO:3:GLU:O | 41:JO:131:GLN:N | 2.48 | 0.41 |
| 40:KA:238:ILE:HD12 | 40:KA:377:LEU:HD11 | 2.01 | 0.41 |
| 41:KB:186:THR:HG21 | 41:KB:385:PHE:CD1 | 2.55 | 0.41 |
| 40:KD:412:MET:HG2 | 40:KD:413:GLU:O | 2.20 | 0.41 |
| 41:KM:275:SER:O | 41:KM:279:GLN:HB2 | 2.20 | 0.41 |
| 41:LL:262:ARG:NH2 | 41:LL:414:ASN:OD1 | 2.53 | 0.41 |
| 40:MA:72:PRO:O | 40:MA:74:VAL:N | 2.52 | 0.41 |
| 40:MA:224:TYR:HD1 | 40:MA:224:TYR:HA | 1.76 | 0.41 |
| 40:MD:186:ASN:OD1 | 40:MD:407:TYR:OH | 2.28 | 0.41 |
| 40:ME:167:LEU:HD11 | 40:ME:252:LEU:HD22 | 2.02 | 0.41 |
| 40:MF:172:TYR:CE2 | 40:MF:386:ALA:HB1 | 2.50 | 0.41 |
| 40:MG:319:TYR:CD2 | 40:MG:323:VAL:HG11 | 2.56 | 0.41 |
| 41:ML:193:VAL:HG12 | 41:ML:194:GLU:HG2 | 2.02 | 0.41 |
| 41:MN:61:PRO:HD3 | 41:MN:84:ILE:HG12 | 2.02 | 0.41 |
| 41:MO:417:ASP:O | 41:MO:418:LEU:C | 2.59 | 0.41 |
| 41:MP:328:GLU:O | 41:MP:332:ASN:HB2 | 2.20 | 0.41 |
| 40:ND:68:VAL:HG11 | 40:ND:118:VAL:HG21 | 2.02 | 0.41 |
| 40:ND:323:VAL:HG23 | 40:ND:355:ILE:HG23 | 2.02 | 0.41 |
| 40:ND:433:GLU:O | 40:ND:434:VAL:C | 2.58 | 0.41 |
| 40:NG:304:LYS:HE2 | 40:NG:304:LYS:HB2 | 1.65 | 0.41 |
| 40:NH:70:LEU:HD23 | 40:NH:145:THR:HG22 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NH:404:VAL:HG13 | 40:NH:417:PHE:HE2 | 1.85 | 0.41 |
| 41:NN:268:PRO:HG2 | 41:NN:300:MET:HB2 | 2.02 | 0.41 |
| 41:NO:154:LYS:HD3 | 41:NO:154:LYS:HA | 1.86 | 0.41 |
| 41:NP:152:ILE:HA | 41:NP:155:ILE:HG22 | 2.01 | 0.41 |
| 41:NP:236:VAL:HG12 | 41:NP:368:ILE:HD11 | 2.01 | 0.41 |
| 40:OA:5:ILE:HD12 | 40:OA:135:PHE:HE2 | 1.83 | 0.41 |
| 40:OA:328:VAL:O | 40:OA:332:ILE:HG12 | 2.20 | 0.41 |
| 41:OB:128:ASP:OD2 | 41:OB:129:CYS:N | 2.50 | 0.41 |
| 41:OB:141:GLY:H | 41:OB:184:ASN:HB2 | 1.85 | 0.41 |
| 40:OD:105:ARG:NH1 | 40:OD:410:GLU:OE2 | 2.53 | 0.41 |
| 40:OE:3:GLU:OE2 | 40:OE:130:THR:N | 2.52 | 0.41 |
| 40:OF:137:ILE:HG22 | 40:OF:139:HIS:HD2 | 1.84 | 0.41 |
| 40:OH:116:ASP:O | 40:OH:117:LEU:C | 2.57 | 0.41 |
| 41:OP:7:LEU:O | 41:OP:135:LEU:HA | 2.19 | 0.41 |
| 40:PA:103:TYR:HD2 | 40:PA:189:LEU:HD13 | 1.85 | 0.41 |
| 41:PB:2:ARG:NH2 | 41:PB:131:GLN:OE1 | 2.46 | 0.41 |
| 40:PH:24:TYR:HE1 | 40:PH:236:SER:HB2 | 1.85 | 0.41 |
| 41:QB:85:PHE:HB2 | 41:QB:90:PHE:HE2 | 1.85 | 0.41 |
| 41:QB:228:LEU:O | 41:QB:231:ALA:HB3 | 2.20 | 0.41 |
| 41:QB:359:ARG:H | 41:QB:359:ARG:HG3 | 1.54 | 0.41 |
| 41:QB:371:SER:C | 41:QB:373:ALA:H | 2.23 | 0.41 |
| 40:QG:262:TYR:HE1 | 41:QO:393:ALA:HA | 1.85 | 0.41 |
| 41:QL:242:PHE:CG | 41:QL:356:ILE:HD11 | 2.55 | 0.41 |
| 41:QM:83:GLN:O | 41:RM:281:TYR:OH | 2.21 | 0.41 |
| 41:QM:412:GLU:HA | 41:QM:415:MET:SD | 2.60 | 0.41 |
| 41:QN:46:ARG:HA | 41:QN:46:ARG:HD3 | 1.88 | 0.41 |
| 41:QN:137:HIS:CE1 | 41:QN:139:LEU:CD2 | 3.03 | 0.41 |
| 41:QO:19:LYS:O | 41:QO:22:GLU:HG3 | 2.20 | 0.41 |
| 41:QO:237:THR:O | 41:QO:241:ARG:NH1 | 2.53 | 0.41 |
| 40:RA:11:GLN:OE1 | 41:RN:246:LEU:N | 2.52 | 0.41 |
| 40:RA:264:ARG:HE | 40:RA:427:LEU:HD21 | 1.85 | 0.41 |
| 40:RA:405:HIS:CD2 | 41:RN:261:PRO:HG3 | 2.55 | 0.41 |
| 41:RB:100:ASN:HB2 | 41:RB:398:TYR:HE1 | 1.85 | 0.41 |
| 41:RB:294:PHE:HD2 | 41:RB:333:VAL:HG21 | 1.85 | 0.41 |
| 40:RE:88:HIS:ND1 | 40:RE:91:GLN:HG2 | 2.35 | 0.41 |
| 40:RE:277:SER:O | 40:RE:279:GLU:N | 2.52 | 0.41 |
| 40:RG:280:LYS:HD2 | 40:RG:280:LYS:HA | 1.91 | 0.41 |
| 40:RI:211:ASP:OD1 | 40:RI:212:ILE:HD12 | 2.20 | 0.41 |
| 40:SA:278:ALA:H | 40:SA:368:ALA:HB2 | 1.85 | 0.41 |
| 40:SE:328:VAL:O | 40:SE:332:ILE:HG12 | 2.18 | 0.41 |
| 40:SF:398:TYR:O | 40:SF:401:ARG:NH1 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:SI:102:ASN:ND2 | 40:SI:105:ARG:HG3 | 2.35 | 0.41 |
| 40:SI:115:ILE:HA | 40:SI:118:VAL:HG12 | 2.02 | 0.41 |
| 40:SI:269:LEU:HD11 | 40:SI:302:MET:H | 1.84 | 0.41 |
| 41:SL:257:MET:HG3 | 41:SL:266:PHE:CE2 | 2.50 | 0.41 |
| 41:SO:70:PRO:HD3 | 41:SO:93:GLY:O | 2.20 | 0.41 |
| 41:SO:139:LEU:HB2 | 41:SO:170:VAL:HA | 2.01 | 0.41 |
| 41:SO:318:ARG:HD3 | 41:SO:354:CYS:SG | 2.59 | 0.41 |
| 41:SP:86:ARG:NH2 | 41:TP:281:TYR:HB2 | 2.35 | 0.41 |
| 41:TB:324:LYS:HE3 | 40:TG:222:PRO:HD2 | 2.01 | 0.41 |
| 40:TE:224:TYR:HD1 | 40:TE:227:LEU:HD12 | 1.85 | 0.41 |
| 40:TH:167:LEU:HA | 40:TH:200:CYS:O | 2.20 | 0.41 |
| 40:TH:228:ASN:HA | 40:TH:231:ILE:HD12 | 2.02 | 0.41 |
| 41:TL:27:GLU:OE1 | 41:TL:241:ARG:NH1 | 2.50 | 0.41 |
| 41:TM:183:TYR:OH | 41:TM:393:ALA:O | 2.33 | 0.41 |
| 40:UA:12:ALA:O | 40:UA:16:ILE:HG12 | 2.20 | 0.41 |
| 40:UE:3:GLU:OE2 | 40:UE:130:THR:N | 2.53 | 0.41 |
| 40:UF:105:ARG:HB3 | 40:UF:110:ILE:HG23 | 2.02 | 0.41 |
| 40:UG:88:HIS:HB3 | 40:UG:91:GLN:NE2 | 2.35 | 0.41 |
| 40:UI:172:TYR:CD2 | 40:UI:173:PRO:HD2 | 2.55 | 0.41 |
| 40:UI:323:VAL:HB | 40:UI:355:ILE:HD13 | 2.01 | 0.41 |
| 41:UP:30:ILE:H | 41:UP:30:ILE:HG12 | 1.44 | 0.41 |
| 41:UP:107:THR:O | 41:UP:109:GLY:N | 2.52 | 0.41 |
| 41:UP:236:VAL:HG13 | 41:UP:237:THR:HG23 | 2.02 | 0.41 |
| 40:VA:91:GLN:HG3 | 40:VA:121:ARG:HH21 | 1.85 | 0.41 |
| 41:VB:117:LEU:HA | 41:VB:117:LEU:HD23 | 1.93 | 0.41 |
| 40:VF:155:GLU:HA | 40:VF:197:HIS:CE1 | 2.55 | 0.41 |
| 40:VH:28:HIS:NE2 | 40:VH:243:ARG:HD2 | 2.35 | 0.41 |
| 40:VI:67:PHE:HB3 | 40:VI:75:ILE:HD12 | 2.02 | 0.41 |
| 40:VI:212:ILE:HD13 | 40:VI:212:ILE:HA | 1.85 | 0.41 |
| 40:VJ:8:HIS:HB2 | 40:VJ:67:PHE:HA | 2.02 | 0.41 |
| 41:WB:22:GLU:HA | 41:WB:81:PHE:CD2 | 2.55 | 0.41 |
| 40:WH:319:TYR:CD1 | 40:WH:374:VAL:HB | 2.54 | 0.41 |
| 41:WM:7:LEU:O | 41:WM:135:LEU:HA | 2.20 | 0.41 |
| 41:WN:9:ALA:HB1 | 41:WN:143:THR:HG22 | 2.01 | 0.41 |
| 7:1T:93:ILE:HG23 | 7:1T:117:LEU:HD11 | 2.00 | 0.41 |
| 7:1T:511:HIS:HA | 7:1T:553:ILE:HD12 | 2.02 | 0.41 |
| 7:1U:33:HIS:CD2 | 7:1U:34:PRO:HD2 | 2.55 | 0.41 |
| 7:1U:109:LEU:HD11 | 40:VI:42:ILE:HA | 2.02 | 0.41 |
| 7:1U:201:THR:HG22 | 7:1U:239:LEU:HB2 | 2.01 | 0.41 |
| 7:1U:559:HIS:CE1 | 7:1U:573:ASP:CG | 2.94 | 0.41 |
| 10:2E:159:TYR:HD1 | 10:2E:159:TYR:HA | 1.76 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:2F:39:GLN:HE21 | 41:MB:392:LYS:HD3 | 1.86 | 0.41 |
| 10:2G:158:GLY:N | 41:VQ:53:GLU:OE2 | 2.53 | 0.41 |
| 12:2O:143:LEU:HB3 | 12:2O:144:PRO:HD3 | 2.02 | 0.41 |
| 13:2T:182:LYS:HB2 | 13:2T:182:LYS:HE3 | 1.89 | 0.41 |
| 13:2U:156:ILE:H | 13:2U:156:ILE:HG13 | 1.60 | 0.41 |
| 13:2W:15:TYR:HD1 | 13:2W:164:ARG:HB2 | 1.85 | 0.41 |
| 13:2X:29:VAL:HG12 | 13:2X:57:THR:HG22 | 2.01 | 0.41 |
| 15:3G:323:ARG:NE | 15:3G:327:GLU:O | 2.49 | 0.41 |
| 16:3J:286:THR:HG23 | 16:3J:366:LEU:HD12 | 2.03 | 0.41 |
| 16:3L:6:VAL:HG23 | 16:3L:7:LYS:H | 1.83 | 0.41 |
| 16:3L:149:LYS:HA | 16:3L:149:LYS:HD2 | 1.89 | 0.41 |
| 16:3L:305:ARG:HH22 | 18:3U:362:HIS:CD2 | 2.38 | 0.41 |
| 17:3O:184:ALA:HA | 17:3O:187:GLU:HG3 | 2.01 | 0.41 |
| 17:3O:199:LEU:HD22 | 17:3O:219:LEU:HD13 | 2.02 | 0.41 |
| 20:4A:149:ARG:HA | 20:4A:152:HIS:HD2 | 1.85 | 0.41 |
| 20:4A:210:MET:H | 20:4A:210:MET:HG3 | 1.67 | 0.41 |
| 21:4D:407:LYS:O | 21:4D:408:ASP:C | 2.58 | 0.41 |
| 21:4E:54:VAL:HG13 | 41:LO:33:THR:HG22 | 2.03 | 0.41 |
| 21:4F:491:PHE:CD2 | 21:4F:494:ALA:HB2 | 2.53 | 0.41 |
| 22:4H:324:LYS:HB3 | 22:4H:324:LYS:HE2 | 1.73 | 0.41 |
| 22:4I:633:GLU:HB3 | 22:4I:634:ASN:H | 1.73 | 0.41 |
| 22:4J:33:ARG:NH1 | 41:MN:92:PHE:O | 2.49 | 0.41 |
| 22:4J:357:ASP:O | 22:4J:361:LYS:HG3 | 2.20 | 0.41 |
| 22:4K:583:ARG:HA | 22:4K:599:LEU:HD21 | 2.01 | 0.41 |
| 23:4M:20:PRO:HG2 | 40:BG:89:PRO:CB | 2.50 | 0.41 |
| 23:4N:255:PHE:O | 23:4N:256:GLN:NE2 | 2.54 | 0.41 |
| 23:4N:259:ARG:HB2 | 23:4N:264:LEU:HG | 2.02 | 0.41 |
| 23:4Q:20:PRO:HG2 | 40:CH:280:LYS:HG2 | 2.02 | 0.41 |
| 23:4Q:201:SER:HA | 40:DH:219:ILE:HG22 | 2.02 | 0.41 |
| 23:4Q:240:LEU:CA | 23:4Q:266:HIS:HA | 2.46 | 0.41 |
| 26:4V:65:LYS:HE3 | 26:4V:72:GLN:NE2 | 2.35 | 0.41 |
| 27:4Z:23:GLU:O | 27:4Z:27:ARG:HB2 | 2.20 | 0.41 |
| 28:5B:29:ARG:NH2 | 28:5B:33:LEU:O | 2.48 | 0.41 |
| 34:5R:405:LEU:HD13 | 34:5R:405:LEU:HA | 1.78 | 0.41 |
| 36:5Y:28:PRO:HA | 36:5Y:29:PRO:HD3 | 1.87 | 0.41 |
| 38:6D:231:LYS:HA | 38:6D:231:LYS:HD2 | 1.89 | 0.41 |
| 39:6J:113:SER:O | 39:6J:116:ARG:NH1 | 2.50 | 0.41 |
| 39:6K:52:GLN:HB2 | 39:6K:72:LEU:HD11 | 2.02 | 0.41 |
| 39:6L:135:HIS:HB2 | 39:6L:136:TYR:H | 1.69 | 0.41 |
| 40:AA:24:TYR:HE2 | 40:AA:236:SER:HB2 | 1.85 | 0.41 |
| 41:AB:46:ARG:HD3 | 41:AB:46:ARG:HA | 1.90 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AO:103:LYS:HA | 41:AO:107:THR:OG1 | 2.20 | 0.41 |
| 40:BE:8:HIS:CD2 | 40:BE:8:HIS:N | 2.88 | 0.41 |
| 40:BE:293:ASN:HA | 40:BE:335:ILE:HD11 | 2.01 | 0.41 |
| 40:BG:205:ASP:HB3 | 40:BG:303:VAL:HA | 2.02 | 0.41 |
| 40:BI:5:ILE:HG13 | 40:BI:132:LEU:CD1 | 2.51 | 0.41 |
| 40:BI:240:ALA:HA | 40:BI:243:ARG:HB2 | 2.03 | 0.41 |
| 41:BM:113:VAL:O | 41:BM:117:LEU:HG | 2.19 | 0.41 |
| 41:BO:21:TRP:HA | 41:BO:24:ILE:HG12 | 2.01 | 0.41 |
| 41:BP:377:LEU:HD13 | 41:BP:377:LEU:HA | 1.89 | 0.41 |
| 40:CA:350:GLY:CA | 41:CB:179:VAL:HG22 | 2.48 | 0.41 |
| 41:CB:237:THR:HG23 | 41:CB:241:ARG:HE | 1.84 | 0.41 |
| 40:CE:26:LEU:HD21 | 40:CE:363:VAL:HG22 | 2.01 | 0.41 |
| 40:CE:345:ASP:N | 40:CE:345:ASP:OD1 | 2.52 | 0.41 |
| 40:CF:154:MET:HG3 | 40:CF:194:THR:HG23 | 2.02 | 0.41 |
| 41:CL:48:ASN:HD22 | 41:CL:48:ASN:HA | 1.50 | 0.41 |
| 41:CL:193:VAL:HG13 | 41:CL:265:PHE:HE1 | 1.86 | 0.41 |
| 41:CM:14:ASN:HB3 | 41:CM:76:VAL:HG21 | 2.02 | 0.41 |
| 41:CM:239:CYS:CB | 41:CM:248:ALA:H | 2.33 | 0.41 |
| 41:CO:121:ARG:O | 41:CO:125:GLU:HG2 | 2.20 | 0.41 |
| 41:CO:266:PHE:CD1 | 41:CO:370:ASN:HB2 | 2.55 | 0.41 |
| 41:CO:366:THR:HG22 | 41:CO:368:ILE:HD13 | 2.01 | 0.41 |
| 40:DA:210:TYR:HD1 | 40:DA:210:TYR:HA | 1.67 | 0.41 |
| 40:DA:252:LEU:HA | 40:DA:255:PHE:CE2 | 2.55 | 0.41 |
| 40:DA:421:ARG:NH1 | 40:DA:421:ARG:O | 2.53 | 0.41 |
| 41:DB:189:VAL:O | 41:DB:192:LEU:HB2 | 2.20 | 0.41 |
| 41:DB:222:TYR:HD1 | 41:DB:222:TYR:HA | 1.78 | 0.41 |
| 41:DB:288:GLU:HA | 41:DB:291:GLN:HG3 | 2.02 | 0.41 |
| 40:DF:153:LEU:HD12 | 40:DF:153:LEU:HA | 1.73 | 0.41 |
| 40:DF:326:LYS:HE2 | 41:DN:208:TYR:HD1 | 1.85 | 0.41 |
| 40:DG:258:ASN:ND2 | 40:DG:352:LYS:HE3 | 2.35 | 0.41 |
| 40:DG:407:TYR:HB3 | 40:DG:412:MET:SD | 2.60 | 0.41 |
| 40:DH:140:SER:OG | 40:DH:146:GLY:HA3 | 2.21 | 0.41 |
| 40:DH:237:SER:O | 40:DH:318:LEU:HG | 2.20 | 0.41 |
| 40:DH:433:GLU:O | 40:DH:434:VAL:C | 2.58 | 0.41 |
| 40:DI:236:SER:OG | 40:DI:237:SER:N | 2.53 | 0.41 |
| 40:DI:262:TYR:HD2 | 40:DI:434:VAL:HG23 | 1.84 | 0.41 |
| 40:DI:334:ALA:O | 40:DI:335:ILE:C | 2.57 | 0.41 |
| 41:DM:382:SER:O | 41:DM:386:THR:HG23 | 2.19 | 0.41 |
| 41:DO:274:THR:HG21 | 41:DO:282:ARG:HD3 | 2.02 | 0.41 |
| 41:DP:4:ILE:HD12 | 41:DP:131:GLN:HB3 | 2.01 | 0.41 |
| 40:EA:169:PHE:CE1 | 40:EA:235:VAL:HG22 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EB:183:TYR:OH | 41:EB:388:MET:O | 2.38 | 0.41 |
| 40:EE:88:HIS:CE1 | 40:EE:90:GLU:CB | 3.04 | 0.41 |
| 40:EE:205:ASP:N | 40:EE:302:MET:O | 2.36 | 0.41 |
| 40:EF:326:LYS:NZ | 41:EN:204:ASN:O | 2.50 | 0.41 |
| 40:EH:206:ASN:O | 40:EH:207:GLU:C | 2.57 | 0.41 |
| 40:EH:270:ALA:O | 40:EH:302:MET:HB2 | 2.20 | 0.41 |
| 40:EH:280:LYS:H | 40:EH:280:LYS:HG3 | 1.74 | 0.41 |
| 40:EI:177:VAL:HA | 41:EP:331:LEU:HD13 | 2.02 | 0.41 |
| 40:EI:323:VAL:HG23 | 40:EI:355:ILE:HG23 | 2.02 | 0.41 |
| 40:EI:388:ALA:O | 40:EI:389:ARG:C | 2.59 | 0.41 |
| 40:EI:414:GLU:O | 40:EI:415:GLY:C | 2.57 | 0.41 |
| 41:EM:7:LEU:HD12 | 41:EM:135:LEU:HB2 | 2.02 | 0.41 |
| 41:EM:101:TRP:O | 41:EM:102:ALA:C | 2.58 | 0.41 |
| 41:EM:234:SER:OG | 41:EM:235:GLY:N | 2.54 | 0.41 |
| 41:EM:250:LEU:HD23 | 41:EM:250:LEU:HA | 1.74 | 0.41 |
| 41:EM:318:ARG:HD3 | 41:EM:358:PRO:HG3 | 2.02 | 0.41 |
| 41:EN:151:LEU:HD12 | 41:EN:151:LEU:HA | 1.90 | 0.41 |
| 41:EN:318:ARG:NE | 41:EN:358:PRO:HD3 | 2.35 | 0.41 |
| 41:EO:113:VAL:HG22 | 41:EO:117:LEU:HD23 | 2.02 | 0.41 |
| 41:EP:1:MET:HE2 | 41:EP:1:MET:HB2 | 1.94 | 0.41 |
| 40:FA:100:ALA:O | 40:FA:102:ASN:HB2 | 2.20 | 0.41 |
| 40:FH:370:VAL:HG12 | 40:FH:372:ARG:H | 1.85 | 0.41 |
| 41:FN:290:THR:HA | 41:FN:293:MET:HB3 | 2.02 | 0.41 |
| 41:FP:52:ASN:OD1 | 41:FP:53:GLU:N | 2.53 | 0.41 |
| 41:FP:239:CYS:HB3 | 41:FP:248:ALA:H | 1.85 | 0.41 |
| 41:FP:322:SER:OG | 41:FP:323:MET:N | 2.53 | 0.41 |
| 40:GH:24:TYR:HE2 | 40:GH:236:SER:HA | 1.85 | 0.41 |
| 40:GH:261:PRO:HA | 41:GP:394:PHE:CD2 | 2.55 | 0.41 |
| 40:GH:392:HIS:O | 40:GH:395:ASP:HB2 | 2.19 | 0.41 |
| 40:GI:311:LYS:HE3 | 40:GI:344:VAL:HG12 | 2.02 | 0.41 |
| 41:GN:189:VAL:O | 41:GN:190:HIS:C | 2.58 | 0.41 |
| 40:HA:21:TRP:CZ2 | 40:HA:65:ALA:HB2 | 2.55 | 0.41 |
| 41:HB:395:LEU:HD12 | 41:HB:398:TYR:HB2 | 2.02 | 0.41 |
| 40:HE:125:LEU:HD23 | 40:HE:125:LEU:HA | 1.86 | 0.41 |
| 40:HE:163:LYS:O | 40:HE:164:LYS:C | 2.58 | 0.41 |
| 40:HE:238:ILE:H | 40:HE:238:ILE:HG12 | 1.39 | 0.41 |
| 40:HF:277:SER:O | 40:HF:279:GLU:N | 2.53 | 0.41 |
| 40:HH:20:CYS:HA | 40:HH:232:SER:HB2 | 2.02 | 0.41 |
| 40:HH:116:ASP:OD1 | 40:HH:117:LEU:N | 2.51 | 0.41 |
| 40:HI:20:CYS:HA | 40:HI:232:SER:HB2 | 2.02 | 0.41 |
| 40:HI:67:PHE:HB2 | 40:HI:92:LEU:HD23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HO:52:ASN:OD1 | 41:HO:62:ARG:NH2 | 2.53 | 0.41 |
| 41:HO:60:VAL:HG11 | 41:HO:86:ARG:HB2 | 2.01 | 0.41 |
| 40:IH:206:ASN:OD1 | 42:IH:501:GTP:O2' | 2.38 | 0.41 |
| 40:IH:224:TYR:HA | 40:IH:227:LEU:HG | 2.02 | 0.41 |
| 41:IM:207:LEU:HD11 | 41:IM:300:MET:HE3 | 2.01 | 0.41 |
| 41:IN:135:LEU:HD21 | 41:IN:148:GLY:HA2 | 2.02 | 0.41 |
| 41:IO:16:ILE:HA | 41:IO:226:ASN:HB3 | 2.02 | 0.41 |
| 41:IP:189:VAL:O | 41:IP:193:VAL:HG23 | 2.20 | 0.41 |
| 41:JB:39:ASP:N | 41:JB:39:ASP:OD1 | 2.53 | 0.41 |
| 40:JE:254:GLU:O | 40:JE:258:ASN:HB2 | 2.20 | 0.41 |
| 40:JE:352:LYS:NZ | 41:JM:178:THR:C | 2.72 | 0.41 |
| 40:JH:277:SER:O | 40:JH:279:GLU:N | 2.53 | 0.41 |
| 41:JL:52:ASN:OD1 | 41:JL:62:ARG:NH2 | 2.54 | 0.41 |
| 41:JM:8:GLN:O | 41:JM:8:GLN:HG2 | 2.20 | 0.41 |
| 41:JM:226:ASN:CG | 43:JM:501:GDP:HN1 | 2.23 | 0.41 |
| 41:JO:256:ASN:ND2 | 41:JO:350:LYS:HE2 | 2.35 | 0.41 |
| 40:KA:16:ILE:CG1 | 40:KA:228:ASN:HD22 | 2.33 | 0.41 |
| 40:KD:371:GLN:OE1 | 40:KD:371:GLN:N | 2.52 | 0.41 |
| 40:KF:16:ILE:HG12 | 40:KF:228:ASN:HD22 | 1.85 | 0.41 |
| 40:KH:269:LEU:HD21 | 40:KH:383:ILE:HD12 | 2.01 | 0.41 |
| 41:KL:358:PRO:HB2 | 41:KL:361:LEU:HD12 | 2.02 | 0.41 |
| 41:KM:73:MET:HB3 | 41:KM:90:PHE:CE1 | 2.54 | 0.41 |
| 41:LB:2:ARG:HH12 | 40:LG:72:PRO:CD | 2.34 | 0.41 |
| 40:LD:136:LEU:HD22 | 40:LD:169:PHE:HE2 | 1.85 | 0.41 |
| 40:LE:359:PRO:HA | 40:LE:360:PRO:HD3 | 1.93 | 0.41 |
| 40:LG:23:LEU:O | 40:LG:27:GLU:HG3 | 2.19 | 0.41 |
| 40:LG:301:GLN:HG3 | 40:LG:307:PRO:CG | 2.50 | 0.41 |
| 40:LH:181:VAL:HG12 | 41:LO:348:ASN:HA | 2.02 | 0.41 |
| 41:LL:91:VAL:HG11 | 41:LL:116:VAL:HG22 | 2.02 | 0.41 |
| 41:LN:137:HIS:CE1 | 41:LN:168:SER:HB3 | 2.55 | 0.41 |
| 40:MA:71:GLU:HB2 | 40:MA:98:ASP:HA | 2.01 | 0.41 |
| 40:MF:11:GLN:HA | 40:MF:74:VAL:HG21 | 2.02 | 0.41 |
| 40:MH:60:LYS:O | 40:MH:62:VAL:N | 2.53 | 0.41 |
| 41:MP:180:VAL:O | 41:MP:184:ASN:ND2 | 2.53 | 0.41 |
| 40:ND:73:THR:O | 40:ND:74:VAL:C | 2.58 | 0.41 |
| 40:ND:155:GLU:H | 40:ND:155:GLU:HG3 | 1.68 | 0.41 |
| 40:ND:262:TYR:O | 40:ND:263:PRO:C | 2.58 | 0.41 |
| 40:ND:382:ALA:O | 40:ND:384:ALA:N | 2.52 | 0.41 |
| 40:NF:261:PRO:HA | 41:NN:394:PHE:CE1 | 2.55 | 0.41 |
| 41:NL:266:PHE:CE1 | 41:NL:370:ASN:HB2 | 2.55 | 0.41 |
| 41:NO:6:HIS:HE1 | 41:NO:8:GLN:HG2 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OE:88:HIS:HB3 | 40:OE:91:GLN:HG2 | 2.02 | 0.41 |
| 40:OF:73:THR:HA | 40:OF:76:ASP:HB2 | 2.02 | 0.41 |
| 40:OG:328:VAL:O | 40:OG:332:ILE:HG12 | 2.20 | 0.41 |
| 40:OH:326:LYS:HG3 | 41:OP:208:TYR:CD1 | 2.55 | 0.41 |
| 41:OO:3:GLU:HB2 | 41:OO:62:ARG:NH2 | 2.35 | 0.41 |
| 40:PA:70:LEU:HD12 | 40:PA:99:ALA:HB2 | 2.01 | 0.41 |
| 40:PF:135:PHE:CE2 | 40:PF:157:LEU:HD23 | 2.55 | 0.41 |
| 40:PH:55:GLU:HG3 | 40:PH:57:GLY:H | 1.84 | 0.41 |
| 41:PL:260:PHE:HE2 | 41:PL:425:ARG:HD3 | 1.85 | 0.41 |
| 41:PO:21:TRP:CZ2 | 41:PO:63:ALA:HB2 | 2.56 | 0.41 |
| 40:QA:239:THR:O | 40:QA:243:ARG:NE | 2.43 | 0.41 |
| 41:QB:138:SER:HA | 41:QB:169:VAL:HB | 2.02 | 0.41 |
| 41:QB:182:PRO:O | 41:QB:183:TYR:C | 2.58 | 0.41 |
| 40:QE:12:ALA:O | 40:QE:15:GLN:HG3 | 2.21 | 0.41 |
| 40:QE:311:LYS:H | 40:QE:381:THR:HB | 1.85 | 0.41 |
| 41:QL:375:GLN:NE2 | 41:QL:379:LYS:HB3 | 2.32 | 0.41 |
| 41:QM:8:GLN:HG3 | 41:QM:17:GLY:HA3 | 2.02 | 0.41 |
| 41:QP:24:ILE:HG23 | 41:QP:28:HIS:CE1 | 2.55 | 0.41 |
| 41:QP:146:GLY:O | 41:QP:149:THR:OG1 | 2.37 | 0.41 |
| 41:QP:164:MET:O | 41:QP:166:THR:HG23 | 2.20 | 0.41 |
| 41:QP:195:ASN:O | 41:QP:196:THR:C | 2.57 | 0.41 |
| 41:QP:343:GLU:O | 41:QP:344:TRP:C | 2.59 | 0.41 |
| 40:RE:105:ARG:NH1 | 40:RE:410:GLU:OE1 | 2.52 | 0.41 |
| 40:RE:263:PRO:HG3 | 41:RM:396:HIS:CG | 2.55 | 0.41 |
| 40:RF:36:MET:HG2 | 40:RF:61:HIS:CE1 | 2.56 | 0.41 |
| 40:RF:325:PRO:HA | 40:RF:328:VAL:HB | 2.01 | 0.41 |
| 40:RG:30:ILE:HA | 40:RG:36:MET:HE1 | 2.02 | 0.41 |
| 40:RG:189:LEU:HD11 | 40:RG:417:PHE:CE1 | 2.55 | 0.41 |
| 41:RL:324:LYS:O | 41:RL:328:GLU:HG3 | 2.20 | 0.41 |
| 41:RL:342:VAL:HB | 41:RL:344:TRP:CD1 | 2.55 | 0.41 |
| 41:RM:58:LYS:HA | 41:RM:58:LYS:HD3 | 1.87 | 0.41 |
| 41:RN:234:SER:O | 41:RN:238:THR:HB | 2.20 | 0.41 |
| 41:RO:19:LYS:HA | 41:RO:19:LYS:HD3 | 1.77 | 0.41 |
| 41:RO:285:THR:HB | 41:RO:287:PRO:HD2 | 2.02 | 0.41 |
| 41:RP:176:SER:OG | 41:RP:178:THR:O | 2.38 | 0.41 |
| 41:SB:149:THR:HB | 41:SB:191:GLN:HG2 | 2.01 | 0.41 |
| 40:SE:172:TYR:CD1 | 40:SE:173:PRO:HD2 | 2.55 | 0.41 |
| 40:SF:223:THR:OG1 | 40:SF:226:ASN:OD1 | 2.31 | 0.41 |
| 40:SG:324:VAL:HA | 40:SG:325:PRO:HD3 | 1.89 | 0.41 |
| 40:SH:139:HIS:CD2 | 40:SH:150:THR:HG21 | 2.55 | 0.41 |
| 40:SH:156:ARG:HA | 40:SH:156:ARG:HD2 | 1.97 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SN:178:THR:HG22 | 41:SN:180:VAL:H | 1.84 | 0.41 |
| 41:SN:192:LEU:HD23 | 41:SN:199:THR:HG21 | 2.01 | 0.41 |
| 41:SO:2:ARG:O | 41:SO:49:VAL:HA | 2.20 | 0.41 |
| 41:SO:33:THR:OG1 | 41:SO:34:GLY:N | 2.53 | 0.41 |
| 41:SO:250:LEU:HD12 | 41:SO:250:LEU:HA | 1.70 | 0.41 |
| 41:SP:296:ALA:HB3 | 41:SP:306:ARG:CZ | 2.50 | 0.41 |
| 40:TA:263:PRO:HG3 | 41:TB:396:HIS:CD2 | 2.55 | 0.41 |
| 40:TA:352:LYS:HD2 | 41:TB:179:VAL:HG13 | 2.03 | 0.41 |
| 40:TA:380:THR:OG1 | 40:TA:381:THR:N | 2.54 | 0.41 |
| 41:TB:261:PRO:HG3 | 40:TG:405:HIS:CD2 | 2.55 | 0.41 |
| 41:TM:208:TYR:HA | 41:TM:211:CYS:SG | 2.60 | 0.41 |
| 40:UE:343:PHE:HZ | 40:UE:350:GLY:HA3 | 1.85 | 0.41 |
| 40:UF:155:GLU:HG2 | 40:UF:156:ARG:N | 2.35 | 0.41 |
| 40:UH:177:VAL:HA | 41:UO:331:LEU:HD13 | 2.02 | 0.41 |
| 40:UI:429:LYS:HA | 40:UI:429:LYS:HD2 | 1.42 | 0.41 |
| 40:VH:318:LEU:O | 40:VH:374:VAL:HA | 2.20 | 0.41 |
| 40:VJ:221:ARG:NH2 | 41:VQ:325:GLU:HG3 | 2.35 | 0.41 |
| 41:VP:377:LEU:HD13 | 41:VP:380:ARG:HH12 | 1.85 | 0.41 |
| 40:WF:288:VAL:HA | 40:WF:291:ILE:HG12 | 2.02 | 0.41 |
| 40:WG:292:THR:HG22 | 40:WG:335:ILE:HD11 | 2.02 | 0.41 |
| 40:WH:387:TRP:CD1 | 40:WH:431:TYR:HE2 | 2.37 | 0.41 |
| 41:WN:5:VAL:HG23 | 41:WN:130:LEU:HD11 | 2.02 | 0.41 |
| 41:WN:9:ALA:HA | 41:WN:66:VAL:O | 2.20 | 0.41 |
| 41:WN:182:PRO:O | 41:WN:186:THR:HG23 | 2.20 | 0.41 |
| 41:WN:333:VAL:HG13 | 41:WN:337:ASN:HD21 | 1.85 | 0.41 |
| 41:WP:107:THR:O | 41:WP:110:ALA:N | 2.38 | 0.41 |
| 41:WQ:198:GLU:HG2 | 41:WQ:266:PHE:HE2 | 1.86 | 0.41 |
| 4:1J:182:LEU:HG | 40:HF:308:ARG:HH12 | 1.85 | 0.41 |
| 7:1T:336:GLU:HB2 | 7:1T:351:CYS:SG | 2.60 | 0.41 |
| 7:1T:407:ARG:H | 7:1T:407:ARG:HG3 | 1.60 | 0.41 |
| 7:1U:14:LEU:HG | 7:1U:617:PRO:HG3 | 2.02 | 0.41 |
| 8:1W:333:LEU:HA | 8:1W:336:GLN:HB2 | 2.02 | 0.41 |
| 9:2B:221:ILE:HD13 | 9:2B:221:ILE:HA | 1.84 | 0.41 |
| 10:2E:80:TYR:O | 40:AE:308:ARG:NH2 | 2.53 | 0.41 |
| 11:2K:184:ALA:O | 11:2K:185:MET:C | 2.59 | 0.41 |
| 12:2P:213:TYR:HD2 | 41:WM:86:ARG:HD2 | 1.86 | 0.41 |
| 12:2P:216:GLN:HE21 | 41:WM:118:ASP:HB2 | 1.85 | 0.41 |
| 12:2P:250:THR:HG22 | 40:AE:401:ARG:HG2 | 2.03 | 0.41 |
| 13:2V:37:ILE:HD12 | 13:2V:37:ILE:HA | 1.93 | 0.41 |
| 13:2X:61:CYS:HB3 | 13:2X:62:PRO:HD3 | 2.02 | 0.41 |
| 14:3A:9:GLN:H | 14:3A:9:GLN:HG2 | 1.72 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:3B:79:VAL:HG23 | 14:3B:113:ILE:HA | 2.01 | 0.41 |
| 15:3F:191:LEU:HD23 | 15:3G:316:ARG:HG3 | 2.01 | 0.41 |
| 16:3J:183:LEU:O | 16:3J:187:ARG:HB2 | 2.20 | 0.41 |
| 16:3L:365:ALA:O | 16:3L:368:LYS:HG3 | 2.21 | 0.41 |
| 17:3O:209:ASP:OD2 | 17:3O:465:SER:OG | 2.33 | 0.41 |
| 17:3R:215:VAL:HG22 | 17:3R:346:ALA:HB1 | 2.02 | 0.41 |
| 17:3R:215:VAL:HG22 | 17:3R:346:ALA:C | 2.41 | 0.41 |
| 17:3R:340:PHE:O | 17:3R:341:ASN:C | 2.59 | 0.41 |
| 21:4D:309:PRO:HB3 | 41:CB:361:LEU:HG | 2.01 | 0.41 |
| 22:4H:79:LEU:HD22 | 22:4H:174:THR:HA | 2.01 | 0.41 |
| 22:4H:112:THR:HG21 | 22:4H:133:ARG:HG3 | 2.02 | 0.41 |
| 22:4J:261:GLU:N | 22:4J:261:GLU:OE1 | 2.53 | 0.41 |
| 23:4Q:260:THR:HG23 | 23:4Q:263:HIS:CE1 | 2.55 | 0.41 |
| 25:4T:326:SER:HB2 | 40:JF:225:THR:HG21 | 2.01 | 0.41 |
| 26:4W:7:PHE:O | 26:4W:27:LEU:HA | 2.20 | 0.41 |
| 26:4W:95:LEU:HB2 | 26:4W:218:MET:SD | 2.60 | 0.41 |
| 27:4Z:113:LEU:HD12 | 27:4Z:183:LEU:HD11 | 2.02 | 0.41 |
| 29:5D:24:THR:O | 29:5D:27:TYR:C | 2.58 | 0.41 |
| 30:5G:56:MET:CE | 41:GN:39:ASP:HB2 | 2.49 | 0.41 |
| 31:5I:367:LEU:HD21 | 40:IA:282:TYR:CE1 | 2.54 | 0.41 |
| 31:5I:374:LYS:O | 31:5I:376:SER:N | 2.42 | 0.41 |
| 33:5N:194:GLN:NE2 | 40:HI:367:LEU:O | 2.53 | 0.41 |
| 33:5N:234:LYS:O | 33:5N:238:MET:HG2 | 2.20 | 0.41 |
| 33:5N:344:LEU:HD23 | 33:5N:344:LEU:HA | 1.89 | 0.41 |
| 33:5O:57:LEU:O | 33:5O:61:GLN:HG2 | 2.20 | 0.41 |
| 34:5R:442:SER:OG | 34:5R:443:LEU:N | 2.53 | 0.41 |
| 36:5W:121:MET:HB3 | 36:5W:140:HIS:CD2 | 2.55 | 0.41 |
| 36:5Y:167:THR:O | 40:OH:371:GLN:NE2 | 2.53 | 0.41 |
| 39:6I:129:CYS:SG | 39:6I:133:ARG:NH2 | 2.94 | 0.41 |
| 40:AF:21:TRP:CZ2 | 40:AF:65:ALA:HB2 | 2.56 | 0.41 |
| 40:AG:117:LEU:O | 40:AG:121:ARG:HG2 | 2.20 | 0.41 |
| 40:AG:178:SER:OG | 40:AG:179:THR:N | 2.53 | 0.41 |
| 41:AM:304:ASP:HB3 | 41:AM:307:HIS:ND1 | 2.35 | 0.41 |
| 41:AN:311:LEU:HD23 | 41:AN:311:LEU:HA | 1.92 | 0.41 |
| 41:AO:299:MET:HB3 | 41:AO:299:MET:HE2 | 1.87 | 0.41 |
| 40:BA:222:PRO:HD2 | 41:BN:324:LYS:NZ | 2.35 | 0.41 |
| 40:BA:242:LEU:H | 40:BA:242:LEU:HD23 | 1.85 | 0.41 |
| 41:BB:7:LEU:HD13 | 41:BB:135:LEU:HD12 | 2.02 | 0.41 |
| 41:BB:213:ARG:O | 41:BB:216:LYS:HG2 | 2.20 | 0.41 |
| 41:BB:267:MET:HG3 | 41:BB:369:GLY:O | 2.19 | 0.41 |
| 41:BB:306:ARG:HE | 41:BB:306:ARG:HB2 | 1.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:BE:20:CYS:HA | 40:BE:232:SER:HB2 | 2.01 | 0.41 |
| 40:BF:286:LEU:HD13 | 40:BF:370:VAL:HG13 | 2.01 | 0.41 |
| 40:BH:119:LEU:HD21 | 40:BH:156:ARG:HB2 | 2.01 | 0.41 |
| 40:BI:117:LEU:HD13 | 40:BI:117:LEU:HA | 1.82 | 0.41 |
| 40:BI:172:TYR:CE2 | 40:BI:386:ALA:HB1 | 2.55 | 0.41 |
| 40:BI:227:LEU:HD22 | 40:BI:227:LEU:HA | 1.81 | 0.41 |
| 40:BI:288:VAL:HA | 40:BI:291:ILE:HD13 | 2.02 | 0.41 |
| 41:BL:309:ARG:N | 41:BL:372:THR:OG1 | 2.53 | 0.41 |
| 41:BM:188:SER:O | 41:BM:189:VAL:C | 2.59 | 0.41 |
| 41:BO:383:GLU:O | 41:BO:386:THR:OG1 | 2.34 | 0.41 |
| 41:BO:420:ASN:HB2 | 41:BO:421:PRO:HD3 | 2.02 | 0.41 |
| 41:BP:51:TYR:HD1 | 41:BP:61:PRO:HA | 1.85 | 0.41 |
| 41:BP:149:THR:HB | 41:BP:191:GLN:HB2 | 2.01 | 0.41 |
| 41:BP:163:ILE:HD11 | 41:BP:251:ARG:HE | 1.84 | 0.41 |
| 41:BP:191:GLN:HE21 | 41:BP:191:GLN:HB3 | 1.51 | 0.41 |
| 41:BP:284:LEU:H | 41:BP:284:LEU:HG | 1.33 | 0.41 |
| 40:CA:265:ILE:HD11 | 40:CA:430:ASP:HB3 | 2.01 | 0.41 |
| 40:CE:222:PRO:HD2 | 41:CL:324:LYS:CB | 2.50 | 0.41 |
| 40:CF:336:LYS:HE2 | 40:CF:343:PHE:HE2 | 1.85 | 0.41 |
| 40:CG:166:LYS:HE2 | 40:CG:166:LYS:HB3 | 1.92 | 0.41 |
| 40:CH:48:SER:O | 40:CH:51:THR:HG22 | 2.20 | 0.41 |
| 40:CH:70:LEU:HD12 | 40:CH:70:LEU:HA | 1.83 | 0.41 |
| 40:CH:427:LEU:HD12 | 40:CH:427:LEU:HA | 1.93 | 0.41 |
| 41:CL:6:HIS:HB2 | 41:CL:134:GLN:NE2 | 2.36 | 0.41 |
| 41:CL:316:VAL:HG13 | 41:CL:366:THR:HB | 2.02 | 0.41 |
| 41:CL:412:GLU:HG3 | 41:CL:416:ASN:HD21 | 1.86 | 0.41 |
| 41:CM:237:THR:O | 41:CM:237:THR:OG1 | 2.37 | 0.41 |
| 41:CM:241:ARG:O | 41:CM:242:PHE:C | 2.59 | 0.41 |
| 41:CM:363:MET:HE3 | 41:CM:363:MET:HB3 | 1.88 | 0.41 |
| 41:CN:303:CYS:O | 41:CN:304:ASP:C | 2.58 | 0.41 |
| 41:CP:174:LYS:HB2 | 41:CP:174:LYS:HE2 | 1.47 | 0.41 |
| 41:CP:192:LEU:O | 41:CP:193:VAL:C | 2.58 | 0.41 |
| 41:CP:289:LEU:HD22 | 41:CP:289:LEU:HA | 1.83 | 0.41 |
| 40:DE:23:LEU:HD23 | 40:DE:23:LEU:HA | 1.81 | 0.41 |
| 40:DE:408:VAL:O | 40:DE:409:GLY:C | 2.58 | 0.41 |
| 40:DF:379:ASN:O | 40:DF:380:THR:C | 2.59 | 0.41 |
| 40:DH:63:PRO:HG3 | 40:DH:86:LEU:HG | 2.01 | 0.41 |
| 40:DH:204:VAL:HA | 40:DH:302:MET:O | 2.20 | 0.41 |
| 40:DI:104:ALA:O | 40:DI:106:GLY:N | 2.48 | 0.41 |
| 40:DI:435:GLY:O | 40:DI:436:MET:C | 2.58 | 0.41 |
| 41:DL:44:LEU:HD23 | 41:DL:44:LEU:HA | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DL:54:ALA:HA | 41:EL:283:ALA:HB2 | 2.01 | 0.41 |
| 41:DN:110:ALA:O | 41:DN:113:VAL:HG22 | 2.20 | 0.41 |
| 41:DN:257:MET:HE1 | 41:DN:312:THR:HB | 2.01 | 0.41 |
| 41:DN:313:VAL:HA | 41:DN:369:GLY:HA3 | 2.01 | 0.41 |
| 41:DN:389:PHE:O | 41:DN:392:LYS:N | 2.52 | 0.41 |
| 40:EA:150:THR:O | 40:EA:154:MET:HG2 | 2.20 | 0.41 |
| 41:EB:151:LEU:O | 41:EB:155:ILE:HG12 | 2.20 | 0.41 |
| 40:EH:102:ASN:O | 40:EH:103:TYR:C | 2.59 | 0.41 |
| 40:EH:238:ILE:HG22 | 40:EH:255:PHE:CE2 | 2.55 | 0.41 |
| 40:EI:3:GLU:H | 40:EI:3:GLU:HG2 | 1.62 | 0.41 |
| 40:EI:316:CYS:HB2 | 40:EI:377:LEU:O | 2.20 | 0.41 |
| 41:EM:288:GLU:HG3 | 41:EM:289:LEU:N | 2.35 | 0.41 |
| 41:EN:24:ILE:HG21 | 41:EN:50:TYR:HD1 | 1.85 | 0.41 |
| 41:EN:176:SER:OG | 41:EN:178:THR:O | 2.38 | 0.41 |
| 41:EP:30:ILE:HG21 | 41:EP:84:ILE:HD11 | 2.01 | 0.41 |
| 41:EP:207:LEU:O | 41:EP:210:ILE:HG12 | 2.20 | 0.41 |
| 40:FA:189:LEU:HD13 | 40:FA:189:LEU:HA | 1.90 | 0.41 |
| 41:FB:125:GLU:OE1 | 41:GB:291:GLN:NE2 | 2.52 | 0.41 |
| 40:FE:125:LEU:HD23 | 40:FE:125:LEU:HA | 1.96 | 0.41 |
| 40:FG:3:GLU:HG2 | 40:FG:131:GLY:O | 2.20 | 0.41 |
| 40:FG:7:VAL:HG13 | 40:FG:66:VAL:HG23 | 2.02 | 0.41 |
| 40:FI:107:HIS:ND1 | 40:FI:152:LEU:HB2 | 2.35 | 0.41 |
| 40:GE:48:SER:O | 40:GE:49:PHE:C | 2.59 | 0.41 |
| 40:GE:110:ILE:H | 40:GE:110:ILE:HG13 | 1.42 | 0.41 |
| 40:GF:431:TYR:HA | 40:GF:434:VAL:HG22 | 2.02 | 0.41 |
| 41:GN:267:MET:O | 41:GN:368:ILE:HA | 2.20 | 0.41 |
| 41:GN:275:SER:OG | 41:GN:276:ARG:N | 2.51 | 0.41 |
| 41:GP:11:GLN:HA | 41:GP:72:THR:HG21 | 2.01 | 0.41 |
| 40:HE:13:GLY:HA2 | 40:HE:16:ILE:HD12 | 2.03 | 0.41 |
| 40:HE:105:ARG:HG3 | 40:HE:105:ARG:H | 1.59 | 0.41 |
| 40:HE:112:LYS:H | 40:HE:112:LYS:HG3 | 1.54 | 0.41 |
| 40:HE:114:LEU:HB3 | 40:HE:149:PHE:CZ | 2.55 | 0.41 |
| 40:HH:232:SER:HA | 40:HH:235:VAL:HG22 | 2.02 | 0.41 |
| 40:HI:297:GLU:HA | 40:HI:298:PRO:HD3 | 1.90 | 0.41 |
| 41:HM:155:ILE:HD13 | 41:HM:155:ILE:HA | 1.93 | 0.41 |
| 41:HO:109:GLY:O | 41:HO:113:VAL:HG23 | 2.20 | 0.41 |
| 41:HO:310:TYR:N | 41:HO:340:TYR:O | 2.39 | 0.41 |
| 41:IB:137:HIS:ND1 | 41:IB:144:GLY:O | 2.53 | 0.41 |
| 40:IE:88:HIS:CD2 | 40:IE:90:GLU:H | 2.38 | 0.41 |
| 40:IF:404:VAL:HG13 | 40:IF:417:PHE:HE2 | 1.84 | 0.41 |
| 40:IG:89:PRO:HD3 | 41:JN:281:TYR:CE1 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:II:234:ILE:HD11 | 40:II:272:TYR:HB2 | 2.01 | 0.41 |
| 41:IO:165:ASN:ND2 | 41:IO:198:GLU:OE1 | 2.53 | 0.41 |
| 41:IP:217:LEU:HB3 | 41:IP:220:PRO:HG3 | 2.01 | 0.41 |
| 41:IQ:311:LEU:HD23 | 41:IQ:342:VAL:HG11 | 2.02 | 0.41 |
| 40:JA:278:ALA:HA | 40:JA:368:ALA:HB2 | 2.02 | 0.41 |
| 40:JE:241:SER:HA | 40:JE:356:ASN:HD22 | 1.86 | 0.41 |
| 41:JN:105:HIS:HB3 | 41:JN:106:TYR:HD1 | 1.85 | 0.41 |
| 41:JO:214:THR:HG21 | 41:JO:298:ASN:ND2 | 2.35 | 0.41 |
| 40:KA:185:TYR:HE1 | 40:KA:397:MET:HB3 | 1.85 | 0.41 |
| 41:KN:186:THR:HG22 | 41:KN:415:MET:SD | 2.60 | 0.41 |
| 41:KO:134:GLN:HA | 41:KO:165:ASN:O | 2.20 | 0.41 |
| 41:KO:321:MET:HB2 | 41:KO:321:MET:HE2 | 1.93 | 0.41 |
| 41:KO:345:ILE:O | 41:KO:348:ASN:HB3 | 2.20 | 0.41 |
| 40:LE:73:THR:HA | 41:LL:46:ARG:HH21 | 1.85 | 0.41 |
| 40:LF:51:THR:HG21 | 40:LF:243:ARG:HD3 | 2.01 | 0.41 |
| 40:LF:328:VAL:CG1 | 40:LF:353:VAL:HG11 | 2.50 | 0.41 |
| 40:LG:63:PRO:HD3 | 40:LG:86:LEU:HG | 2.01 | 0.41 |
| 40:LG:204:VAL:HG13 | 40:LG:270:ALA:HB3 | 2.02 | 0.41 |
| 40:LG:220:GLU:HG2 | 40:LG:221:ARG:N | 2.33 | 0.41 |
| 40:LG:277:SER:O | 40:LG:278:ALA:C | 2.59 | 0.41 |
| 40:LH:182:VAL:HG12 | 40:LH:186:ASN:ND2 | 2.36 | 0.41 |
| 41:LL:273:LEU:HD23 | 41:LL:273:LEU:HA | 1.90 | 0.41 |
| 41:LM:398:TYR:HB3 | 41:LM:403:MET:HG3 | 2.01 | 0.41 |
| 40:MA:11:GLN:O | 40:MA:12:ALA:C | 2.57 | 0.41 |
| 40:MA:72:PRO:HB2 | 40:MA:73:THR:H | 1.61 | 0.41 |
| 41:MB:19:LYS:HA | 41:MB:19:LYS:HD3 | 1.87 | 0.41 |
| 41:MB:67:ASP:HA | 41:MB:143:THR:HG21 | 2.03 | 0.41 |
| 41:MB:268:PRO:HG2 | 41:MB:300:MET:HB2 | 2.01 | 0.41 |
| 41:MB:314:ALA:HB3 | 41:MB:368:ILE:HB | 2.01 | 0.41 |
| 41:MB:317:PHE:HB2 | 41:MB:353:VAL:HG22 | 2.01 | 0.41 |
| 40:MF:2:ARG:O | 40:MF:51:THR:HA | 2.20 | 0.41 |
| 40:MF:3:GLU:H | 40:MF:3:GLU:HG2 | 1.72 | 0.41 |
| 40:MH:56:THR:O | 40:MH:57:GLY:C | 2.58 | 0.41 |
| 40:MH:277:SER:O | 40:MH:278:ALA:C | 2.59 | 0.41 |
| 40:MH:324:VAL:O | 40:MH:326:LYS:N | 2.53 | 0.41 |
| 40:MH:438:SER:HA | 41:MP:391:ARG:HH21 | 1.85 | 0.41 |
| 41:ML:47:ILE:HG12 | 41:ML:51:TYR:HB2 | 2.02 | 0.41 |
| 41:MO:271:ALA:HB3 | 41:MO:272:PRO:CD | 2.50 | 0.41 |
| 41:NB:113:VAL:HG21 | 41:NB:150:LEU:HG | 2.02 | 0.41 |
| 41:NB:267:MET:HE1 | 41:NB:371:SER:HB3 | 2.02 | 0.41 |
| 41:NB:310:TYR:HD1 | 41:NB:313:VAL:HG22 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:NE:185:TYR:HE2 | 40:NE:403:PHE:HB2 | 1.84 | 0.41 |
| 40:NG:228:ASN:ND2 | 42:NG:501:GTP:HN1 | 2.17 | 0.41 |
| 41:NM:2:ARG:HD2 | 41:NM:131:GLN:HE22 | 1.84 | 0.41 |
| 40:OA:212:ILE:HD12 | 40:OA:300:ASN:HA | 2.01 | 0.41 |
| 40:OD:84:ARG:NH2 | 40:OD:85:GLN:HB2 | 2.35 | 0.41 |
| 40:OG:115:ILE:HA | 40:OG:118:VAL:HG12 | 2.02 | 0.41 |
| 40:OH:115:ILE:HG23 | 40:OH:119:LEU:HD13 | 2.01 | 0.41 |
| 40:OH:164:LYS:HA | 40:OH:164:LYS:HD3 | 1.62 | 0.41 |
| 40:OH:429:LYS:HA | 40:OH:429:LYS:HD3 | 1.46 | 0.41 |
| 41:OL:273:LEU:O | 41:OL:292:GLN:NE2 | 2.53 | 0.41 |
| 41:OM:142:GLY:O | 41:OM:144:GLY:N | 2.53 | 0.41 |
| 41:ON:250:LEU:HD23 | 41:ON:250:LEU:HA | 1.87 | 0.41 |
| 41:OO:257:MET:SD | 41:OO:314:ALA:HB2 | 2.60 | 0.41 |
| 41:OO:280:GLN:HB3 | 41:OO:281:TYR:CD1 | 2.55 | 0.41 |
| 41:OO:314:ALA:HB3 | 41:OO:368:ILE:HB | 2.02 | 0.41 |
| 40:PA:212:ILE:HD13 | 40:PA:215:ARG:HH22 | 1.85 | 0.41 |
| 40:PA:267:PHE:HB3 | 40:PA:383:ILE:HD13 | 2.02 | 0.41 |
| 40:PD:295:CYS:HA | 40:PD:300:ASN:HD21 | 1.86 | 0.41 |
| 40:PF:50:ASN:O | 40:PF:64:ARG:NH2 | 2.53 | 0.41 |
| 40:PF:268:PRO:HB3 | 40:PF:379:ASN:HB3 | 2.02 | 0.41 |
| 40:PH:230:LEU:O | 40:PH:234:ILE:HG12 | 2.20 | 0.41 |
| 41:PM:145:SER:O | 41:PM:149:THR:CB | 2.69 | 0.41 |
| 41:PM:186:THR:HG23 | 41:PM:381:ILE:HG12 | 2.02 | 0.41 |
| 41:PP:8:GLN:HB3 | 41:PP:14:ASN:HA | 2.02 | 0.41 |
| 41:QB:143:THR:O | 41:QB:144:GLY:C | 2.59 | 0.41 |
| 41:QB:336:LYS:HD2 | 41:QB:336:LYS:HA | 1.83 | 0.41 |
| 41:QB:410:GLU:O | 41:QB:413:SER:HB3 | 2.20 | 0.41 |
| 40:QE:274:PRO:HG2 | 40:QE:291:ILE:HD12 | 2.01 | 0.41 |
| 40:QH:136:LEU:HD13 | 40:QH:167:LEU:HB2 | 2.01 | 0.41 |
| 41:QL:6:HIS:ND1 | 41:QL:134:GLN:O | 2.42 | 0.41 |
| 41:QL:7:LEU:O | 41:QL:135:LEU:HA | 2.20 | 0.41 |
| 41:QN:130:LEU:HD21 | 41:QN:133:PHE:CE2 | 2.55 | 0.41 |
| 41:QO:7:LEU:HD12 | 41:QO:135:LEU:HB2 | 2.02 | 0.41 |
| 41:QO:276:ARG:HD2 | 41:QO:276:ARG:HA | 1.85 | 0.41 |
| 41:QP:146:GLY:O | 41:QP:147:MET:C | 2.58 | 0.41 |
| 41:QP:192:LEU:O | 41:QP:194:GLU:N | 2.52 | 0.41 |
| 41:QP:238:THR:O | 41:QP:241:ARG:N | 2.45 | 0.41 |
| 41:QP:314:ALA:CB | 41:QP:350:LYS:H | 2.34 | 0.41 |
| 41:QP:376:GLU:HG3 | 41:QP:377:LEU:N | 2.35 | 0.41 |
| 40:RA:73:THR:HA | 40:RA:76:ASP:HB2 | 2.02 | 0.41 |
| 41:RB:137:HIS:CE1 | 41:RB:139:LEU:HD23 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RE:3:GLU:HA | 40:RE:51:THR:HA | 2.03 | 0.41 |
| 40:RG:308:ARG:HE | 40:RG:308:ARG:HB2 | 1.62 | 0.41 |
| 41:RM:318:ARG:HB2 | 41:RM:364:SER:OG | 2.20 | 0.41 |
| 41:RM:412:GLU:HA | 41:RM:415:MET:HB3 | 2.03 | 0.41 |
| 40:SF:387:TRP:HA | 40:SF:390:LEU:HB2 | 2.02 | 0.41 |
| 40:SH:222:PRO:HB3 | 40:SH:226:ASN:HD22 | 1.86 | 0.41 |
| 41:SO:151:LEU:O | 41:SO:152:ILE:C | 2.58 | 0.41 |
| 41:SO:311:LEU:HA | 41:SO:342:VAL:HG21 | 2.02 | 0.41 |
| 40:TE:319:TYR:HB2 | 40:TE:355:ILE:HD13 | 2.02 | 0.41 |
| 40:TF:6:SER:O | 40:TF:65:ALA:HA | 2.20 | 0.41 |
| 40:TF:277:SER:H | 40:TF:280:LYS:HB3 | 1.85 | 0.41 |
| 40:TI:188:ILE:HD11 | 40:TI:421:ARG:HA | 2.01 | 0.41 |
| 40:TI:286:LEU:N | 40:TI:290:GLU:OE2 | 2.52 | 0.41 |
| 41:TN:285:THR:HG23 | 41:TN:287:PRO:HD2 | 2.01 | 0.41 |
| 41:TO:184:ASN:O | 41:TO:188:SER:HB3 | 2.20 | 0.41 |
| 40:UE:207:GLU:HA | 40:UE:210:TYR:CD2 | 2.47 | 0.41 |
| 40:UF:70:LEU:HD12 | 40:UF:70:LEU:HA | 1.75 | 0.41 |
| 40:UG:262:TYR:HB2 | 40:UG:265:ILE:HG12 | 2.01 | 0.41 |
| 40:UI:123:ARG:HA | 40:UI:161:TYR:OH | 2.20 | 0.41 |
| 41:UP:4:ILE:HA | 41:UP:132:GLY:O | 2.20 | 0.41 |
| 41:UP:174:LYS:HB3 | 41:UP:174:LYS:HE2 | 1.62 | 0.41 |
| 41:UP:223:GLY:O | 41:UP:226:ASN:HB2 | 2.20 | 0.41 |
| 41:UP:285:THR:O | 41:UP:286:VAL:C | 2.58 | 0.41 |
| 41:UP:346:PRO:O | 41:UP:347:ASN:C | 2.58 | 0.41 |
| 41:VB:86:ARG:HA | 41:WB:281:TYR:HD2 | 1.85 | 0.41 |
| 40:VF:69:ASP:OD1 | 40:VF:70:LEU:N | 2.53 | 0.41 |
| 40:VG:100:ALA:HA | 41:VN:252:LYS:HB3 | 2.01 | 0.41 |
| 40:VG:228:ASN:ND2 | 42:VN:501:GTP:HN1 | 2.10 | 0.41 |
| 40:VI:204:VAL:HG11 | 40:VI:231:ILE:HD12 | 2.02 | 0.41 |
| 40:VI:210:TYR:CG | 41:VP:324:LYS:HD3 | 2.55 | 0.41 |
| 40:VI:240:ALA:HB1 | 40:VI:356:ASN:HD22 | 1.85 | 0.41 |
| 40:VI:326:LYS:NZ | 41:VQ:225:LEU:HD21 | 2.35 | 0.41 |
| 40:VI:326:LYS:HD3 | 41:VQ:208:TYR:CD1 | 2.56 | 0.41 |
| 40:VJ:107:HIS:CD2 | 40:VJ:152:LEU:HD13 | 2.55 | 0.41 |
| 41:VN:42:LEU:HD11 | 41:VN:243:PRO:HG3 | 2.02 | 0.41 |
| 41:VP:206:ALA:O | 41:VP:210:ILE:HD12 | 2.20 | 0.41 |
| 41:VQ:8:GLN:NE2 | 41:VQ:65:LEU:HG | 2.35 | 0.41 |
| 41:WB:165:ASN:HD21 | 41:WB:250:LEU:HD13 | 1.85 | 0.41 |
| 40:WE:167:LEU:HD22 | 40:WE:200:CYS:HB3 | 2.02 | 0.41 |
| 40:WG:143:GLY:N | 42:WG:501:GTP:O2A | 2.38 | 0.41 |
| 40:WG:296:PHE:HD1 | 40:WG:341:ILE:HD13 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:WH:185:TYR:CE1 | 40:WH:403:PHE:HB2 | 2.55 | 0.41 |
| 41:WM:2:ARG:HD2 | 41:WM:240:LEU:HD11 | 2.00 | 0.41 |
| 41:WM:117:LEU:HD11 | 41:WM:154:LYS:CB | 2.50 | 0.41 |
| 41:WM:260:PHE:HB3 | 41:WM:261:PRO:CD | 2.49 | 0.41 |
| 41:WN:279:GLN:C | 41:WN:281:TYR:H | 2.24 | 0.41 |
| 41:WN:427:ALA:O | 41:WN:428:CYS:C | 2.58 | 0.41 |
| 41:WO:74:ASP:OD1 | 41:WO:77:ARG:NH1 | 2.53 | 0.41 |
| 41:WO:318:ARG:NE | 41:WO:358:PRO:HD3 | 2.34 | 0.41 |
| 41:WO:354:CYS:SG | 41:WO:355:ASP:N | 2.93 | 0.41 |
| 4:1H:160:ASP:OD1 | 41:HO:306:ARG:HG2 | 2.20 | 0.41 |
| 7:1T:241:ASP:CG | 7:1T:279:PRO:HD3 | 2.41 | 0.41 |
| 8:1X:131:LYS:HB2 | 8:1X:131:LYS:HE2 | 1.61 | 0.41 |
| 10:2G:81:ASN:HB3 | 10:2G:84:SER:HB2 | 2.02 | 0.41 |
| 11:2I:215:SER:N | 41:VP:77:ARG:HH12 | 2.18 | 0.41 |
| 12:2Q:211:ILE:HG12 | 13:2V:36:ARG:HB2 | 2.03 | 0.41 |
| 12:2R:85:LEU:HD13 | 12:2R:125:PHE:CE2 | 2.55 | 0.41 |
| 13:2T:28:LYS:HB2 | 13:2T:28:LYS:HE2 | 1.53 | 0.41 |
| 13:2T:157:HIS:HB3 | 13:2T:158:ALA:H | 1.58 | 0.41 |
| 13:2U:77:VAL:HA | 13:2U:132:ILE:O | 2.20 | 0.41 |
| 13:2U:101:ARG:HE | 13:2U:101:ARG:HB3 | 1.57 | 0.41 |
| 13:2X:115:LYS:HG3 | 13:2X:118:ILE:HD12 | 2.02 | 0.41 |
| 14:3B:118:HIS:ND1 | 36:5Z:248:ASP:OD1 | 2.53 | 0.41 |
| 16:3J:387:ASP:O | 16:3J:391:MET:HG2 | 2.20 | 0.41 |
| 17:3P:129:GLN:HE21 | 17:3P:133:GLN:HG2 | 1.85 | 0.41 |
| 17:3P:438:LEU:HD12 | 17:3P:438:LEU:HA | 1.83 | 0.41 |
| 17:3R:108:LEU:HA | 17:3R:108:LEU:HD22 | 1.74 | 0.41 |
| 17:3R:181:LEU:HA | 17:3R:329:LEU:HD21 | 2.01 | 0.41 |
| 17:3R:193:GLN:HE21 | 17:3R:197:GLU:HB2 | 1.86 | 0.41 |
| 17:3R:199:LEU:HD21 | 17:3R:219:LEU:HB3 | 2.03 | 0.41 |
| 19:3Y:159:PHE:HZ | 25:4T:392:ARG:HH11 | 1.69 | 0.41 |
| 21:4E:439:VAL:O | 21:4E:440:LEU:C | 2.58 | 0.41 |
| 22:4J:92:LYS:HB2 | 41:BN:279:GLN:C | 2.41 | 0.41 |
| 22:4J:327:ASN:O | 22:4J:330:GLN:NE2 | 2.49 | 0.41 |
| 22:4K:696:ALA:O | 22:4K:698:ASN:N | 2.43 | 0.41 |
| 23:4N:233:SER:O | 23:4N:234:ARG:HB2 | 2.19 | 0.41 |
| 24:4O:269:LEU:H | 24:4O:269:LEU:HG | 1.49 | 0.41 |
| 23:4P:255:PHE:O | 23:4P:256:GLN:NE2 | 2.54 | 0.41 |
| 26:4W:295:GLU:O | 26:4W:298:GLU:HG3 | 2.21 | 0.41 |
| 26:4W:343:ARG:NE | 26:4W:353:ASN:HD21 | 2.19 | 0.41 |
| 26:4W:374:ILE:HG12 | 26:4W:374:ILE:H | 1.77 | 0.41 |
| 27:4Y:253:ASP:HB3 | 27:4Y:257:VAL:HG23 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:5B:210:TYR:C | 28:5B:212:ASN:H | 2.23 | 0.41 |
| 31:5I:380:LYS:HE2 | 41:IB:215:LEU:HD13 | 2.01 | 0.41 |
| 34:5Q:238:ILE:HG23 | 34:5Q:242:GLN:HE21 | 1.84 | 0.41 |
| 36:5W:62:VAL:HG11 | 36:5W:71:GLU:HB2 | 2.01 | 0.41 |
| 37:6A:119:THR:HA | 37:6A:122:LYS:HB3 | 2.02 | 0.41 |
| 38:6C:105:LYS:CD | 38:6C:115:GLY:HA3 | 2.49 | 0.41 |
| 38:6C:170:TYR:HB2 | 40:UH:161:TYR:CD1 | 2.55 | 0.41 |
| 41:AB:52:ASN:OD1 | 41:AB:62:ARG:NH2 | 2.39 | 0.41 |
| 40:AH:200:CYS:HA | 40:AH:266:HIS:HB2 | 2.00 | 0.41 |
| 41:AN:107:THR:O | 41:AN:110:ALA:N | 2.33 | 0.41 |
| 41:AN:271:ALA:HB1 | 41:AN:292:GLN:HB3 | 2.02 | 0.41 |
| 41:AO:131:GLN:HE22 | 41:AO:249:ASP:HB2 | 1.85 | 0.41 |
| 40:BA:2:ARG:HD3 | 40:BA:242:LEU:HB2 | 2.01 | 0.41 |
| 40:BE:263:PRO:HG3 | 41:BM:396:HIS:CG | 2.56 | 0.41 |
| 40:BE:402:ALA:O | 40:BE:403:PHE:C | 2.58 | 0.41 |
| 40:BF:12:ALA:O | 40:BF:16:ILE:HG12 | 2.20 | 0.41 |
| 40:BH:59:GLY:O | 40:BH:61:HIS:ND1 | 2.53 | 0.41 |
| 40:BI:36:MET:HE2 | 40:BI:36:MET:HB2 | 1.85 | 0.41 |
| 40:BI:390:LEU:HA | 40:BI:390:LEU:HD23 | 1.85 | 0.41 |
| 41:BL:182:PRO:HG3 | 41:BL:384:GLN:HG2 | 2.02 | 0.41 |
| 41:BL:248:ALA:HA | 41:BL:252:LYS:HD3 | 2.02 | 0.41 |
| 41:BM:215:LEU:HA | 41:BM:215:LEU:HD13 | 1.75 | 0.41 |
| 40:CA:54:SER:HA | 40:CA:64:ARG:HH21 | 1.85 | 0.41 |
| 40:CA:245:ASP:OD2 | 40:CA:245:ASP:N | 2.53 | 0.41 |
| 40:CH:60:LYS:HE3 | 40:CH:86:LEU:HA | 2.00 | 0.41 |
| 40:CH:105:ARG:HG2 | 40:CH:410:GLU:HG2 | 2.01 | 0.41 |
| 40:CH:183:GLU:O | 40:CH:184:PRO:C | 2.58 | 0.41 |
| 40:CH:258:ASN:HA | 41:CP:179:VAL:HG11 | 2.01 | 0.41 |
| 40:CI:25:CYS:HA | 40:CI:30:ILE:HB | 2.02 | 0.41 |
| 40:CI:278:ALA:H | 40:CI:368:ALA:HB2 | 1.85 | 0.41 |
| 41:CL:22:GLU:O | 41:CL:26:ASP:N | 2.53 | 0.41 |
| 41:CM:137:HIS:O | 41:CM:168:SER:HA | 2.21 | 0.41 |
| 41:CO:269:GLY:O | 41:CO:367:PHE:N | 2.49 | 0.41 |
| 40:DA:181:VAL:HG12 | 41:DN:348:ASN:HA | 2.02 | 0.41 |
| 40:DE:225:THR:HG23 | 40:DE:228:ASN:HD21 | 1.85 | 0.41 |
| 40:DE:390:LEU:HD23 | 40:DE:390:LEU:HA | 1.83 | 0.41 |
| 40:DF:31:GLN:C | 40:DF:33:ASP:N | 2.72 | 0.41 |
| 40:DF:93:ILE:HD11 | 40:DF:114:LEU:HG | 2.02 | 0.41 |
| 40:DF:335:ILE:O | 40:DF:338:LYS:HB2 | 2.20 | 0.41 |
| 40:DF:432:GLU:H | 40:DF:432:GLU:HG3 | 1.62 | 0.41 |
| 40:DH:102:ASN:HD21 | 40:DH:406:TRP:HB3 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DH:133:GLN:HB3 | 40:DH:252:LEU:CD1 | 2.50 | 0.41 |
| 40:DH:153:LEU:HD12 | 40:DH:153:LEU:HA | 1.84 | 0.41 |
| 40:DH:419:GLU:H | 40:DH:419:GLU:HG3 | 1.60 | 0.41 |
| 40:DI:115:ILE:HD12 | 40:DI:115:ILE:HA | 1.93 | 0.41 |
| 40:DI:253:THR:O | 40:DI:254:GLU:C | 2.59 | 0.41 |
| 41:DL:144:GLY:O | 41:DL:148:GLY:N | 2.52 | 0.41 |
| 41:DM:287:PRO:HA | 41:DM:329:GLN:HG3 | 2.03 | 0.41 |
| 41:DN:238:THR:O | 41:DN:241:ARG:N | 2.49 | 0.41 |
| 41:DO:305:PRO:HB3 | 41:DO:310:TYR:CE1 | 2.55 | 0.41 |
| 41:DO:313:VAL:HB | 41:DO:349:VAL:HG22 | 2.02 | 0.41 |
| 40:EA:56:THR:HG23 | 40:FA:284:GLU:O | 2.20 | 0.41 |
| 40:EA:376:MET:SD | 40:EA:378:SER:HB3 | 2.60 | 0.41 |
| 41:EB:192:LEU:HD13 | 41:EB:199:THR:HG21 | 2.01 | 0.41 |
| 40:EF:130:THR:OG1 | 40:EF:131:GLY:N | 2.53 | 0.41 |
| 40:EG:167:LEU:HD22 | 40:EG:200:CYS:HB2 | 2.03 | 0.41 |
| 40:EI:88:HIS:O | 40:EI:89:PRO:C | 2.59 | 0.41 |
| 40:EI:112:LYS:HA | 40:EI:112:LYS:HD3 | 1.84 | 0.41 |
| 40:EI:139:HIS:CD2 | 40:EI:170:SER:HB3 | 2.54 | 0.41 |
| 40:EI:259:LEU:HD11 | 40:EI:377:LEU:O | 2.20 | 0.41 |
| 41:EL:19:LYS:HE2 | 41:EL:223:GLY:HA2 | 2.01 | 0.41 |
| 41:EM:132:GLY:HA3 | 41:EM:163:ILE:O | 2.20 | 0.41 |
| 41:EM:181:GLU:HB3 | 41:EM:182:PRO:HD3 | 2.01 | 0.41 |
| 41:EP:151:LEU:O | 41:EP:152:ILE:C | 2.59 | 0.41 |
| 41:EP:192:LEU:O | 41:EP:193:VAL:C | 2.58 | 0.41 |
| 40:FA:73:THR:OG1 | 40:FA:74:VAL:N | 2.53 | 0.41 |
| 41:FB:32:PRO:HG3 | 41:FB:81:PHE:HE1 | 1.85 | 0.41 |
| 40:FG:18:ASN:O | 40:FG:22:GLU:HG2 | 2.20 | 0.41 |
| 40:FG:272:TYR:HE1 | 40:FG:367:LEU:HD11 | 1.85 | 0.41 |
| 41:FM:183:TYR:O | 41:FM:187:LEU:HG | 2.20 | 0.41 |
| 41:FN:240:LEU:H | 41:FN:240:LEU:HD23 | 1.85 | 0.41 |
| 40:GA:37:PRO:O | 40:GA:39:ASP:N | 2.54 | 0.41 |
| 41:GB:204:ASN:HD22 | 41:GB:207:LEU:HD12 | 1.85 | 0.41 |
| 40:GF:136:LEU:HB3 | 40:GF:138:PHE:HE1 | 1.85 | 0.41 |
| 40:GG:133:GLN:NE2 | 40:GG:251:ASP:OD2 | 2.54 | 0.41 |
| 40:GG:405:HIS:HA | 40:GG:408:VAL:HG22 | 2.01 | 0.41 |
| 40:GI:284:GLU:HG3 | 40:GI:285:GLN:N | 2.35 | 0.41 |
| 40:GI:429:LYS:HZ2 | 40:GI:432:GLU:HB2 | 1.85 | 0.41 |
| 41:GM:7:LEU:HD23 | 41:GM:133:PHE:HB3 | 2.03 | 0.41 |
| 41:GM:21:TRP:CZ3 | 41:GM:61:PRO:HB3 | 2.54 | 0.41 |
| 41:GM:257:MET:O | 41:GM:312:THR:OG1 | 2.28 | 0.41 |
| 41:GN:262:ARG:HH12 | 41:GN:414:ASN:HD21 | 1.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HA:394:PHE:HE1 | 40:HA:421:ARG:HB2 | 1.85 | 0.41 |
| 40:HE:3:GLU:HG2 | 40:HE:132:LEU:HA | 2.03 | 0.41 |
| 40:HE:51:THR:HG21 | 40:HE:243:ARG:HG2 | 2.03 | 0.41 |
| 40:HE:128:GLN:HE21 | 40:HE:128:GLN:HB2 | 1.62 | 0.41 |
| 40:HG:8:HIS:HD1 | 40:HG:17:GLY:HA3 | 1.84 | 0.41 |
| 40:HG:169:PHE:HE2 | 40:HG:235:VAL:HG13 | 1.85 | 0.41 |
| 40:HI:100:ALA:O | 41:HP:255:VAL:HG11 | 2.20 | 0.41 |
| 40:HI:274:PRO:HG3 | 40:HI:286:LEU:HD12 | 2.02 | 0.41 |
| 41:HN:228:LEU:H | 41:HN:228:LEU:HG | 1.61 | 0.41 |
| 41:HN:297:LYS:HB3 | 41:HN:297:LYS:HE2 | 1.54 | 0.41 |
| 40:IA:240:ALA:HB1 | 40:IA:356:ASN:HD22 | 1.85 | 0.41 |
| 40:IE:230:LEU:HD23 | 40:IE:230:LEU:HA | 1.91 | 0.41 |
| 40:IF:54:SER:HB3 | 40:IF:64:ARG:HE | 1.85 | 0.41 |
| 40:IG:116:ASP:OD1 | 40:IG:117:LEU:N | 2.53 | 0.41 |
| 40:IG:122:ILE:HG21 | 40:IG:157:LEU:HD21 | 2.02 | 0.41 |
| 40:II:139:HIS:HE1 | 40:II:141:PHE:HE1 | 1.69 | 0.41 |
| 40:II:223:THR:OG1 | 40:II:224:TYR:N | 2.53 | 0.41 |
| 40:II:292:THR:HG1 | 40:II:319:TYR:HH | 1.61 | 0.41 |
| 41:IM:312:THR:H | 41:IM:370:ASN:HB2 | 1.85 | 0.41 |
| 41:IN:138:SER:OG | 41:IN:140:GLY:O | 2.39 | 0.41 |
| 41:IP:21:TRP:CZ3 | 41:IP:50:TYR:HB3 | 2.56 | 0.41 |
| 41:IP:159:TYR:HB3 | 41:IP:162:ARG:HD3 | 2.02 | 0.41 |
| 41:IQ:134:GLN:HA | 41:IQ:165:ASN:O | 2.20 | 0.41 |
| 40:JA:71:GLU:HB3 | 40:JA:98:ASP:HA | 2.02 | 0.41 |
| 41:JB:91:VAL:HG11 | 41:JB:116:VAL:HG22 | 2.02 | 0.41 |
| 40:JD:306:ASP:HA | 40:JD:307:PRO:HD3 | 1.86 | 0.41 |
| 40:JH:108:TYR:CE2 | 40:JH:412:MET:HB2 | 2.55 | 0.41 |
| 41:JM:42:LEU:HD13 | 41:JM:42:LEU:HA | 1.84 | 0.41 |
| 41:JM:192:LEU:HD22 | 41:JM:192:LEU:HA | 1.93 | 0.41 |
| 41:JM:201:CYS:O | 41:JM:268:PRO:HD2 | 2.21 | 0.41 |
| 41:JN:239:CYS:HB3 | 41:JN:247:ASN:HB2 | 2.01 | 0.41 |
| 40:KF:16:ILE:HD13 | 40:KF:228:ASN:HB2 | 2.02 | 0.41 |
| 40:KG:264:ARG:NH2 | 40:KG:423:ASP:OD2 | 2.53 | 0.41 |
| 40:KH:28:HIS:HD1 | 40:KH:49:PHE:HA | 1.85 | 0.41 |
| 40:KH:122:ILE:HD13 | 40:KH:122:ILE:HA | 1.86 | 0.41 |
| 40:KH:298:PRO:HB3 | 40:KH:307:PRO:HD2 | 2.01 | 0.41 |
| 41:KP:221:THR:OG1 | 41:KP:224:ASP:OD2 | 2.26 | 0.41 |
| 40:LF:306:ASP:HB3 | 40:LF:309:HIS:CD2 | 2.54 | 0.41 |
| 40:LG:35:GLN:HE21 | 40:LG:35:GLN:HB3 | 1.67 | 0.41 |
| 40:LG:288:VAL:O | 40:LG:291:ILE:HG12 | 2.20 | 0.41 |
| 41:LL:398:TYR:HB3 | 41:LL:408:PHE:HZ | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:LP:25:SER:HG | 41:LP:51:TYR:HH | 1.63 | 0.41 |
| 40:MA:177:VAL:CG1 | 41:MN:327:ASP:HB3 | 2.49 | 0.41 |
| 40:MD:263:PRO:HG3 | 41:ML:396:HIS:CG | 2.55 | 0.41 |
| 40:MF:153:LEU:O | 40:MF:154:MET:C | 2.57 | 0.41 |
| 40:MF:242:LEU:H | 40:MF:242:LEU:HG | 1.69 | 0.41 |
| 40:MF:436:MET:O | 41:MN:391:ARG:NH2 | 2.44 | 0.41 |
| 40:MG:139:HIS:HE1 | 40:MG:141:PHE:HE1 | 1.69 | 0.41 |
| 40:MG:172:TYR:CE1 | 40:MG:386:ALA:HB1 | 2.56 | 0.41 |
| 40:MG:269:LEU:HD23 | 40:MG:303:VAL:HG11 | 2.02 | 0.41 |
| 40:MH:76:ASP:N | 40:MH:76:ASP:OD2 | 2.53 | 0.41 |
| 40:MH:187:SER:O | 40:MH:190:THR:HG22 | 2.20 | 0.41 |
| 41:ML:274:THR:HG23 | 41:ML:279:GLN:OE1 | 2.21 | 0.41 |
| 41:NB:306:ARG:HG3 | 41:NB:340:TYR:HE1 | 1.85 | 0.41 |
| 40:ND:217:LEU:O | 40:ND:219:ILE:HG12 | 2.21 | 0.41 |
| 40:NE:3:GLU:OE2 | 40:NE:130:THR:N | 2.53 | 0.41 |
| 40:NG:25:CYS:SG | 40:NG:86:LEU:HD11 | 2.61 | 0.41 |
| 40:NG:313:MET:HG2 | 40:NG:344:VAL:HG11 | 2.02 | 0.41 |
| 40:NH:139:HIS:O | 40:NH:170:SER:HA | 2.20 | 0.41 |
| 41:NN:142:GLY:O | 41:NN:144:GLY:N | 2.53 | 0.41 |
| 41:NN:198:GLU:HG2 | 41:NN:266:PHE:HE2 | 1.86 | 0.41 |
| 41:NN:285:THR:N | 41:NN:288:GLU:OE2 | 2.53 | 0.41 |
| 40:OE:101:ASN:HD21 | 40:OE:180:ALA:HB1 | 1.85 | 0.41 |
| 40:OF:356:ASN:OD1 | 40:OF:357:TYR:N | 2.53 | 0.41 |
| 40:OH:353:VAL:H | 40:OH:353:VAL:HG23 | 1.59 | 0.41 |
| 41:OL:19:LYS:HA | 41:OL:19:LYS:HD3 | 1.89 | 0.41 |
| 41:OM:7:LEU:O | 41:OM:135:LEU:HA | 2.21 | 0.41 |
| 41:OM:21:TRP:CZ2 | 41:OM:63:ALA:HB2 | 2.56 | 0.41 |
| 41:OO:100:ASN:HB3 | 41:OO:103:LYS:HB2 | 2.02 | 0.41 |
| 40:PD:265:ILE:HG22 | 40:PD:379:ASN:HD21 | 1.85 | 0.41 |
| 40:PF:73:THR:HA | 40:PF:76:ASP:OD1 | 2.20 | 0.41 |
| 41:PM:105:HIS:CG | 41:PM:150:LEU:HD12 | 2.55 | 0.41 |
| 41:PM:266:PHE:HD1 | 41:PM:370:ASN:HB3 | 1.85 | 0.41 |
| 40:QA:395:ASP:OD1 | 40:QA:421:ARG:NE | 2.51 | 0.41 |
| 41:QB:28:HIS:O | 41:QB:29:GLY:C | 2.58 | 0.41 |
| 41:QB:286:VAL:O | 41:QB:290:THR:HG23 | 2.21 | 0.41 |
| 41:QB:337:ASN:O | 41:QB:340:TYR:N | 2.53 | 0.41 |
| 40:QE:428:GLU:HA | 40:QE:431:TYR:HB2 | 2.02 | 0.41 |
| 40:QG:195:LEU:HD21 | 40:QG:427:LEU:HD11 | 2.01 | 0.41 |
| 41:QO:134:GLN:HG3 | 41:QO:165:ASN:HB2 | 2.03 | 0.41 |
| 40:RA:210:TYR:HE1 | 40:RA:227:LEU:HG | 1.86 | 0.41 |
| 40:RF:54:SER:OG | 40:RF:62:VAL:HG22 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:RH:175:PRO:HB2 | 40:RH:389:ARG:HH11 | 1.84 | 0.41 |
| 40:SE:176:GLN:O | 41:SL:347:ASN:ND2 | 2.54 | 0.41 |
| 40:SE:277:SER:H | 40:SE:280:LYS:HB3 | 1.85 | 0.41 |
| 40:SE:384:ALA:HB2 | 40:SE:431:TYR:CD1 | 2.55 | 0.41 |
| 40:SG:305:CYS:HB3 | 40:SG:386:ALA:HB2 | 2.03 | 0.41 |
| 40:SI:265:ILE:HD12 | 40:SI:431:TYR:HD1 | 1.86 | 0.41 |
| 41:SM:21:TRP:CZ3 | 41:SM:61:PRO:HB3 | 2.55 | 0.41 |
| 41:SO:235:GLY:O | 41:SO:236:VAL:C | 2.59 | 0.41 |
| 41:SP:148:GLY:O | 41:SP:152:ILE:HG12 | 2.21 | 0.41 |
| 40:TA:3:GLU:OE1 | 40:TA:130:THR:N | 2.54 | 0.41 |
| 40:TE:242:LEU:H | 40:TE:242:LEU:HD23 | 1.85 | 0.41 |
| 40:TF:205:ASP:HB3 | 40:TF:303:VAL:HA | 2.03 | 0.41 |
| 40:TF:210:TYR:HE1 | 40:TF:227:LEU:HD12 | 1.85 | 0.41 |
| 40:TF:257:THR:HA | 41:TN:397:TRP:CH2 | 2.55 | 0.41 |
| 41:TM:3:GLU:OE2 | 41:TM:127:CYS:HB3 | 2.20 | 0.41 |
| 41:TM:100:ASN:HB2 | 41:TM:103:LYS:HB2 | 2.01 | 0.41 |
| 41:TN:52:ASN:OD1 | 41:TN:62:ARG:NH2 | 2.53 | 0.41 |
| 41:TP:116:VAL:HA | 41:TP:119:VAL:HG22 | 2.01 | 0.41 |
| 41:TP:240:LEU:H | 41:TP:240:LEU:HD23 | 1.85 | 0.41 |
| 40:UA:326:LYS:HA | 40:UA:326:LYS:HD2 | 1.80 | 0.41 |
| 41:UB:21:TRP:HZ3 | 41:UB:50:TYR:HB3 | 1.86 | 0.41 |
| 41:UB:222:TYR:HA | 41:UB:225:LEU:HB2 | 2.03 | 0.41 |
| 40:UF:8:HIS:CD2 | 40:UF:8:HIS:H | 2.37 | 0.41 |
| 40:UF:383:ILE:HD12 | 40:UF:383:ILE:HA | 1.92 | 0.41 |
| 40:UF:397:MET:O | 40:UF:398:TYR:C | 2.58 | 0.41 |
| 40:UH:429:LYS:HA | 40:UH:432:GLU:HG2 | 2.01 | 0.41 |
| 40:UI:160:ASP:O | 40:UI:162:GLY:N | 2.54 | 0.41 |
| 40:UI:207:GLU:HA | 40:UI:210:TYR:HD2 | 1.85 | 0.41 |
| 41:UM:6:HIS:O | 41:UM:63:ALA:HA | 2.19 | 0.41 |
| 41:UM:7:LEU:HD23 | 41:UM:64:VAL:HB | 2.02 | 0.41 |
| 41:UM:290:THR:HG23 | 41:UM:329:GLN:HE21 | 1.84 | 0.41 |
| 41:UO:100:ASN:OD1 | 41:UO:101:TRP:N | 2.53 | 0.41 |
| 41:UO:375:GLN:NE2 | 41:UO:422:VAL:HG13 | 2.36 | 0.41 |
| 41:UP:127:CYS:O | 41:UP:128:ASP:C | 2.59 | 0.41 |
| 41:UP:279:GLN:O | 41:UP:282:ARG:HB2 | 2.20 | 0.41 |
| 40:VF:88:HIS:NE2 | 40:VF:90:GLU:HB2 | 2.36 | 0.41 |
| 40:VJ:67:PHE:HB2 | 40:VJ:92:LEU:HD23 | 2.02 | 0.41 |
| 40:VJ:390:LEU:HD23 | 40:VJ:390:LEU:HA | 1.85 | 0.41 |
| 41:VN:237:THR:HG22 | 41:VN:250:LEU:HD21 | 2.02 | 0.41 |
| 41:VO:290:THR:HB | 41:VO:329:GLN:NE2 | 2.36 | 0.41 |
| 41:VP:41:ASP:OD1 | 41:VP:41:ASP:N | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:WE:171:ILE:HG21 | 42:WE:501:GTP:H1' | 2.02 | 0.41 |
| 40:WF:3:GLU:HB3 | 40:WF:51:THR:HA | 2.02 | 0.41 |
| 41:WM:113:VAL:HG13 | 41:WM:117:LEU:HD12 | 2.02 | 0.41 |
| 5:1N:161:LYS:HD2 | 41:HQ:336:LYS:HZ3 | 1.81 | 0.41 |
| 7:1T:50:GLN:HB3 | 7:1T:51:ALA:H | 1.67 | 0.41 |
| 7:1T:211:ILE:HD11 | 7:1T:220:PHE:HD2 | 1.84 | 0.41 |
| 12:2O:69:PRO:HB3 | 12:2O:74:LYS:HZ1 | 1.85 | 0.41 |
| 12:2O:197:LEU:HD22 | 12:2O:225:ILE:HG12 | 2.03 | 0.41 |
| 16:3J:69:ASP:O | 16:3J:73:ARG:HG2 | 2.20 | 0.41 |
| 17:3Q:360:LYS:HA | 17:3Q:360:LYS:HD3 | 1.80 | 0.41 |
| 18:3U:167:LEU:HD23 | 18:3U:167:LEU:HA | 1.94 | 0.41 |
| 19:3Y:264:ALA:HB1 | 19:3Y:273:VAL:HB | 2.01 | 0.41 |
| 20:4B:228:ARG:HA | 20:4B:231:ARG:HE | 1.86 | 0.41 |
| 21:4E:277:GLU:OE1 | 21:4E:289:PRO:HA | 2.20 | 0.41 |
| 21:4E:452:PHE:HE1 | 21:4E:465:LYS:HE2 | 1.85 | 0.41 |
| 21:4F:107:VAL:HB | 21:4F:116:ARG:HD2 | 2.03 | 0.41 |
| 22:4H:138:LEU:HA | 22:4H:147:TYR:CE1 | 2.55 | 0.41 |
| 22:4I:542:ARG:O | 22:4I:542:ARG:HD3 | 2.21 | 0.41 |
| 22:4K:594:LEU:HD23 | 22:4K:594:LEU:HA | 1.93 | 0.41 |
| 23:4M:36:THR:O | 23:4M:37:TYR:C | 2.58 | 0.41 |
| 23:4M:171:PRO:C | 23:4M:173:SER:H | 2.23 | 0.41 |
| 24:4O:242:LEU:HD23 | 24:4O:242:LEU:HA | 1.73 | 0.41 |
| 23:4P:233:SER:O | 23:4P:234:ARG:HB2 | 2.19 | 0.41 |
| 23:4Q:178:ASP:O | 23:4Q:179:PRO:C | 2.58 | 0.41 |
| 23:4R:250:VAL:O | 23:4R:251:PRO:C | 2.59 | 0.41 |
| 25:4T:289:VAL:H | 25:4T:290:PRO:CD | 2.34 | 0.41 |
| 33:5N:449:LEU:HB3 | 33:5N:453:LYS:NZ | 2.36 | 0.41 |
| 36:5W:258:ARG:HH21 | 40:LG:440:GLU:HA | 1.85 | 0.41 |
| 36:5X:63:LYS:H | 36:5X:63:LYS:HG2 | 1.69 | 0.41 |
| 36:5X:162:LEU:HA | 36:5X:163:PRO:HD3 | 1.87 | 0.41 |
| 38:6C:105:LYS:HE3 | 38:6C:105:LYS:HB3 | 1.85 | 0.41 |
| 38:6C:210:PHE:CE2 | 38:6C:215:PRO:HD3 | 2.56 | 0.41 |
| 39:6K:74:ILE:HG21 | 39:6K:143:ILE:HD13 | 2.01 | 0.41 |
| 41:AB:67:ASP:OD1 | 41:AB:68:LEU:N | 2.53 | 0.41 |
| 40:AE:16:ILE:HD12 | 40:AE:231:ILE:HG21 | 2.03 | 0.41 |
| 40:AE:88:HIS:CD2 | 40:AE:89:PRO:HD2 | 2.56 | 0.41 |
| 40:AE:150:THR:O | 40:AE:154:MET:HG2 | 2.20 | 0.41 |
| 41:AM:417:ASP:O | 41:AM:421:PRO:HD2 | 2.21 | 0.41 |
| 41:AN:19:LYS:HD2 | 41:AN:19:LYS:HA | 1.85 | 0.41 |
| 41:AO:70:PRO:HD3 | 41:AO:94:GLN:HA | 2.01 | 0.41 |
| 41:AO:286:VAL:HG22 | 41:AO:321:MET:HE2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BB:1:MET:HE3 | 41:BB:1:MET:HB2 | 1.91 | 0.41 |
| 41:BB:2:ARG:HA | 41:BB:129:CYS:O | 2.21 | 0.41 |
| 40:BE:216:ASN:ND2 | 40:BE:275:VAL:O | 2.51 | 0.41 |
| 40:BE:326:LYS:HG3 | 41:BM:208:TYR:CD1 | 2.56 | 0.41 |
| 40:BF:224:TYR:CE2 | 41:BM:323:MET:HG3 | 2.55 | 0.41 |
| 40:BG:105:ARG:HA | 40:BG:109:THR:HG22 | 2.03 | 0.41 |
| 40:BI:177:VAL:HG13 | 41:BP:327:ASP:HB3 | 2.02 | 0.41 |
| 40:BI:394:PHE:O | 40:BI:395:ASP:C | 2.58 | 0.41 |
| 41:BM:142:GLY:O | 41:BM:144:GLY:N | 2.53 | 0.41 |
| 41:BM:203:ASP:HB2 | 41:BM:302:ALA:H | 1.85 | 0.41 |
| 41:BM:204:ASN:HD22 | 41:BM:207:LEU:HD12 | 1.84 | 0.41 |
| 41:BN:87:PRO:HA | 41:BN:90:PHE:HD2 | 1.84 | 0.41 |
| 41:BO:87:PRO:CD | 41:CO:281:TYR:HD2 | 2.33 | 0.41 |
| 41:BO:284:LEU:HA | 41:BO:284:LEU:HD23 | 1.78 | 0.41 |
| 41:BP:164:MET:H | 41:BP:164:MET:HG2 | 1.38 | 0.41 |
| 40:CA:16:ILE:H | 40:CA:16:ILE:HG13 | 1.76 | 0.41 |
| 40:CA:183:GLU:HA | 40:CA:186:ASN:HD22 | 1.86 | 0.41 |
| 40:CA:398:TYR:O | 40:CA:399:ALA:C | 2.59 | 0.41 |
| 41:CB:61:PRO:HD2 | 41:CB:85:PHE:HA | 2.02 | 0.41 |
| 41:CB:116:VAL:HA | 41:CB:119:VAL:HG22 | 2.01 | 0.41 |
| 40:CF:213:CYS:HA | 40:CF:217:LEU:HB2 | 2.01 | 0.41 |
| 40:CF:426:ALA:HA | 40:CF:429:LYS:HG2 | 2.02 | 0.41 |
| 40:CG:224:TYR:CD1 | 40:CG:227:LEU:HD12 | 2.55 | 0.41 |
| 40:CH:72:PRO:O | 40:CH:74:VAL:N | 2.53 | 0.41 |
| 40:CH:184:PRO:O | 40:CH:188:ILE:HG23 | 2.21 | 0.41 |
| 41:CL:279:GLN:H | 41:CL:279:GLN:HG3 | 1.59 | 0.41 |
| 41:CL:286:VAL:HG12 | 41:CL:329:GLN:HG3 | 2.03 | 0.41 |
| 41:CM:46:ARG:HG3 | 41:CM:241:ARG:HA | 2.01 | 0.41 |
| 41:CM:357:PRO:HB2 | 41:CM:358:PRO:HD2 | 2.01 | 0.41 |
| 41:CM:395:LEU:HD13 | 41:CM:395:LEU:HA | 1.80 | 0.41 |
| 41:CO:67:ASP:HB3 | 41:CO:73:MET:HE1 | 2.01 | 0.41 |
| 41:CO:158:GLU:HB3 | 41:CO:159:TYR:H | 1.61 | 0.41 |
| 41:CP:1:MET:N | 41:CP:1:MET:SD | 2.93 | 0.41 |
| 40:DA:184:PRO:HB3 | 40:DA:393:LYS:HB3 | 2.03 | 0.41 |
| 40:DA:266:HIS:O | 40:DA:266:HIS:ND1 | 2.53 | 0.41 |
| 40:DE:24:TYR:HA | 40:DE:27:GLU:HB2 | 2.02 | 0.41 |
| 40:DG:207:GLU:HA | 40:DG:210:TYR:CD2 | 2.56 | 0.41 |
| 40:DG:317:LEU:HD12 | 40:DG:374:VAL:HG21 | 2.03 | 0.41 |
| 40:DH:105:ARG:O | 40:DH:110:ILE:N | 2.53 | 0.41 |
| 40:DI:166:LYS:H | 40:DI:199:ASP:HB2 | 1.85 | 0.41 |
| 41:DL:233:MET:O | 41:DL:234:SER:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DM:23:VAL:HG23 | 41:DM:227:HIS:CE1 | 2.55 | 0.41 |
| 41:DM:82:GLY:C | 41:DM:84:ILE:N | 2.74 | 0.41 |
| 41:DM:254:ALA:C | 41:DM:256:ASN:H | 2.23 | 0.41 |
| 41:DM:362:LYS:H | 41:DM:362:LYS:HZ2 | 1.67 | 0.41 |
| 41:DM:375:GLN:NE2 | 41:DM:419:GLY:O | 2.36 | 0.41 |
| 41:DN:64:VAL:O | 41:DN:66:VAL:HG13 | 2.21 | 0.41 |
| 41:DN:161:ASP:O | 41:DN:162:ARG:C | 2.59 | 0.41 |
| 41:DN:394:PHE:O | 41:DN:395:LEU:C | 2.58 | 0.41 |
| 41:DP:268:PRO:HG2 | 41:DP:300:MET:HB2 | 2.03 | 0.41 |
| 41:EB:285:THR:H | 41:EB:288:GLU:HB3 | 1.84 | 0.41 |
| 41:EB:331:LEU:HG | 41:EB:334:GLN:HG3 | 2.03 | 0.41 |
| 41:EB:395:LEU:HD12 | 41:EB:398:TYR:HB2 | 2.03 | 0.41 |
| 40:EE:112:LYS:HA | 40:EE:115:ILE:HG22 | 2.02 | 0.41 |
| 40:EH:12:ALA:O | 40:EH:16:ILE:HG23 | 2.20 | 0.41 |
| 40:EH:157:LEU:HD13 | 40:EH:157:LEU:HA | 1.71 | 0.41 |
| 40:EH:168:GLU:CD | 40:EH:198:SER:HB2 | 2.40 | 0.41 |
| 40:EH:320:ARG:HE | 40:EH:360:PRO:HG3 | 1.85 | 0.41 |
| 40:EI:274:PRO:CB | 40:EI:370:VAL:HG21 | 2.50 | 0.41 |
| 41:EL:27:GLU:HA | 41:EL:359:ARG:HH12 | 1.86 | 0.41 |
| 41:EL:163:ILE:HD11 | 41:EL:250:LEU:HG | 2.02 | 0.41 |
| 41:EO:132:GLY:HA3 | 41:EO:163:ILE:O | 2.21 | 0.41 |
| 41:EP:154:LYS:H | 41:EP:154:LYS:HG2 | 1.64 | 0.41 |
| 40:FA:51:THR:HG21 | 40:FA:243:ARG:CB | 2.50 | 0.41 |
| 40:FA:51:THR:HG21 | 40:FA:243:ARG:HB3 | 2.03 | 0.41 |
| 40:FA:51:THR:HG23 | 40:FA:52:PHE:H | 1.86 | 0.41 |
| 40:FA:203:MET:HE2 | 40:FA:203:MET:HB2 | 1.78 | 0.41 |
| 40:FA:270:ALA:HA | 40:FA:376:MET:O | 2.21 | 0.41 |
| 40:FH:98:ASP:OD1 | 40:FH:98:ASP:N | 2.54 | 0.41 |
| 40:FH:231:ILE:O | 40:FH:235:VAL:HG23 | 2.21 | 0.41 |
| 40:GE:49:PHE:O | 40:GE:53:PHE:HB2 | 2.21 | 0.41 |
| 40:GE:291:ILE:O | 40:GE:292:THR:C | 2.59 | 0.41 |
| 40:GH:366:ASP:OD2 | 40:GH:366:ASP:N | 2.52 | 0.41 |
| 40:GI:15:GLN:O | 40:GI:16:ILE:C | 2.58 | 0.41 |
| 41:GN:284:LEU:HD13 | 41:GN:284:LEU:HA | 1.86 | 0.41 |
| 41:GP:6:HIS:O | 41:GP:63:ALA:HA | 2.21 | 0.41 |
| 40:HA:97:GLU:OE2 | 40:HA:105:ARG:NH1 | 2.54 | 0.41 |
| 41:HB:255:VAL:HG11 | 40:HG:100:ALA:O | 2.20 | 0.41 |
| 40:HG:136:LEU:HA | 40:HG:136:LEU:HD23 | 1.80 | 0.41 |
| 40:HH:143:GLY:N | 42:HH:501:GTP:O2A | 2.47 | 0.41 |
| 40:HH:156:ARG:HA | 40:HH:159:VAL:HG12 | 2.02 | 0.41 |
| 40:HI:234:ILE:HD11 | 40:HI:272:TYR:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HI:252:LEU:O | 40:HI:256:GLN:HG2 | 2.21 | 0.41 |
| 41:HM:61:PRO:HD3 | 41:HM:84:ILE:HG12 | 2.00 | 0.41 |
| 41:HN:186:THR:O | 41:HN:189:VAL:HG22 | 2.20 | 0.41 |
| 41:HQ:297:LYS:HD2 | 41:HQ:297:LYS:HA | 1.85 | 0.41 |
| 41:HQ:299:MET:HE1 | 41:HQ:367:PHE:HE2 | 1.85 | 0.41 |
| 41:HQ:372:THR:HG22 | 41:HQ:375:GLN:HE22 | 1.85 | 0.41 |
| 40:IA:202:PHE:HE1 | 40:IA:377:LEU:HD13 | 1.86 | 0.41 |
| 40:IE:337:THR:O | 40:IE:339:ARG:NH1 | 2.54 | 0.41 |
| 40:IF:406:TRP:CG | 41:IM:255:VAL:HG23 | 2.55 | 0.41 |
| 40:IG:269:LEU:HD23 | 40:IG:303:VAL:HB | 2.02 | 0.41 |
| 40:II:182:VAL:HA | 40:II:185:TYR:HD2 | 1.84 | 0.41 |
| 41:IN:163:ILE:HG13 | 41:IN:251:ARG:HB2 | 2.03 | 0.41 |
| 41:IN:222:TYR:HD1 | 41:IN:225:LEU:HD22 | 1.86 | 0.41 |
| 41:IN:267:MET:HG3 | 41:IN:374:ILE:HD11 | 2.02 | 0.41 |
| 41:IO:178:THR:HG22 | 41:IO:180:VAL:H | 1.84 | 0.41 |
| 41:JB:222:TYR:O | 41:JB:226:ASN:ND2 | 2.53 | 0.41 |
| 41:JB:270:PHE:O | 41:JB:298:ASN:ND2 | 2.51 | 0.41 |
| 40:JF:53:PHE:HB3 | 40:JF:61:HIS:HB3 | 2.02 | 0.41 |
| 40:JF:195:LEU:HD23 | 40:JF:264:ARG:HH21 | 1.86 | 0.41 |
| 40:JF:239:THR:O | 40:JF:243:ARG:NE | 2.47 | 0.41 |
| 41:JL:257:MET:HE3 | 41:JL:314:ALA:HB2 | 2.03 | 0.41 |
| 41:JM:56:GLY:C | 41:JM:58:LYS:H | 2.23 | 0.41 |
| 41:JM:112:LEU:O | 41:JM:113:VAL:C | 2.58 | 0.41 |
| 41:JM:137:HIS:NE2 | 41:JM:168:SER:HB3 | 2.34 | 0.41 |
| 41:JN:154:LYS:HE2 | 41:JN:154:LYS:HB2 | 1.82 | 0.41 |
| 41:JN:256:ASN:ND2 | 41:JN:350:LYS:HE2 | 2.36 | 0.41 |
| 41:JO:176:SER:OG | 41:JO:178:THR:O | 2.37 | 0.41 |
| 41:KB:62:ARG:NH1 | 41:KB:127:CYS:SG | 2.93 | 0.41 |
| 40:KF:181:VAL:HG23 | 40:KF:182:VAL:HG13 | 2.02 | 0.41 |
| 40:KG:296:PHE:CE2 | 40:KG:335:ILE:HG21 | 2.55 | 0.41 |
| 41:KL:208:TYR:O | 41:KL:209:ASP:C | 2.56 | 0.41 |
| 41:KM:213:ARG:HD2 | 41:KM:297:LYS:HD2 | 2.02 | 0.41 |
| 41:KO:8:GLN:NE2 | 41:KO:14:ASN:HA | 2.35 | 0.41 |
| 40:LF:255:PHE:CE1 | 40:LF:318:LEU:HD11 | 2.55 | 0.41 |
| 41:LM:39:ASP:OD2 | 41:LM:40:SER:N | 2.53 | 0.41 |
| 41:LM:122:LYS:HE3 | 41:MM:291:GLN:HG2 | 2.03 | 0.41 |
| 41:LN:19:LYS:HD2 | 41:LN:227:HIS:CD2 | 2.56 | 0.41 |
| 41:LO:254:ALA:O | 41:LO:258:VAL:HG22 | 2.20 | 0.41 |
| 40:MA:167:LEU:HD23 | 40:MA:202:PHE:HE2 | 1.83 | 0.41 |
| 40:MA:182:VAL:HG23 | 40:MA:186:ASN:HD21 | 1.86 | 0.41 |
| 40:MD:7:VAL:O | 40:MD:137:ILE:HA | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MF:99:ALA:HA | 40:MF:110:ILE:CD1 | 2.47 | 0.41 |
| 40:MF:320:ARG:HE | 40:MF:360:PRO:HA | 1.84 | 0.41 |
| 40:MG:256:GLN:O | 40:MG:257:THR:C | 2.59 | 0.41 |
| 41:MN:216:LYS:HB2 | 41:MN:275:SER:HB2 | 2.01 | 0.41 |
| 41:MP:205:GLU:HA | 41:MP:208:TYR:HB2 | 2.03 | 0.41 |
| 40:ND:273:ALA:O | 40:ND:275:VAL:N | 2.53 | 0.41 |
| 40:NH:331:ALA:O | 40:NH:335:ILE:HG12 | 2.19 | 0.41 |
| 41:NL:39:ASP:OD1 | 41:NL:39:ASP:N | 2.50 | 0.41 |
| 41:NM:226:ASN:ND2 | 43:NM:502:GDP:O6 | 2.45 | 0.41 |
| 41:NN:221:THR:HG23 | 41:NN:224:ASP:H | 1.85 | 0.41 |
| 41:NO:87:PRO:HA | 41:NO:90:PHE:CD2 | 2.56 | 0.41 |
| 41:NP:198:GLU:OE1 | 41:NP:200:TYR:OH | 2.31 | 0.41 |
| 40:OA:51:THR:HG23 | 40:OA:52:PHE:CD2 | 2.56 | 0.41 |
| 40:OA:172:TYR:HB2 | 40:OA:203:MET:SD | 2.61 | 0.41 |
| 41:OB:156:ARG:HA | 41:OB:156:ARG:HD2 | 1.88 | 0.41 |
| 41:OB:165:ASN:HA | 41:OB:198:GLU:O | 2.20 | 0.41 |
| 42:OB:502:GTP:O2' | 40:OG:206:ASN:OD1 | 2.24 | 0.41 |
| 40:OF:205:ASP:O | 40:OF:209:ILE:HG12 | 2.20 | 0.41 |
| 40:OG:112:LYS:HA | 40:OG:115:ILE:HG22 | 2.02 | 0.41 |
| 40:OG:325:PRO:HG2 | 41:OO:221:THR:HA | 2.01 | 0.41 |
| 40:OH:36:MET:HG2 | 40:OH:37:PRO:N | 2.36 | 0.41 |
| 41:ON:238:THR:HG21 | 41:ON:318:ARG:HD2 | 2.03 | 0.41 |
| 41:OO:183:TYR:OH | 41:OO:388:MET:O | 2.32 | 0.41 |
| 41:OP:44:LEU:HA | 41:OP:47:ILE:HG23 | 2.02 | 0.41 |
| 40:PA:129:CYS:SG | 40:PA:132:LEU:N | 2.91 | 0.41 |
| 40:PA:266:HIS:ND1 | 40:PA:266:HIS:O | 2.54 | 0.41 |
| 41:PB:324:LYS:NZ | 40:PG:222:PRO:HD2 | 2.32 | 0.41 |
| 40:PE:244:PHE:HD2 | 40:PE:356:ASN:HD21 | 1.68 | 0.41 |
| 40:PE:255:PHE:O | 40:PE:259:LEU:HB2 | 2.20 | 0.41 |
| 40:PF:185:TYR:OH | 40:PF:402:ALA:O | 2.31 | 0.41 |
| 40:PG:235:VAL:HA | 40:PG:238:ILE:HG22 | 2.02 | 0.41 |
| 41:PM:51:TYR:HB3 | 41:PM:59:TYR:HB3 | 2.03 | 0.41 |
| 41:PN:21:TRP:CZ3 | 41:PN:61:PRO:HB3 | 2.56 | 0.41 |
| 41:PP:210:ILE:O | 41:PP:214:THR:OG1 | 2.37 | 0.41 |
| 40:QA:101:ASN:HB2 | 41:QN:252:LYS:NZ | 2.35 | 0.41 |
| 40:QA:222:PRO:HG2 | 41:QN:324:LYS:HE2 | 2.02 | 0.41 |
| 40:QA:271:THR:HB | 40:QA:376:MET:HE3 | 2.02 | 0.41 |
| 40:QA:316:CYS:SG | 40:QA:377:LEU:HB2 | 2.61 | 0.41 |
| 41:QB:103:LYS:HA | 41:QB:107:THR:OG1 | 2.21 | 0.41 |
| 41:QB:147:MET:HE3 | 41:QB:147:MET:HB3 | 1.96 | 0.41 |
| 40:QF:105:ARG:HG2 | 40:QF:410:GLU:HG2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QG:89:PRO:HG2 | 40:RG:280:LYS:NZ | 2.35 | 0.41 |
| 41:QM:8:GLN:NE2 | 41:QM:65:LEU:HG | 2.35 | 0.41 |
| 41:QP:375:GLN:H | 41:QP:375:GLN:HG3 | 1.48 | 0.41 |
| 41:QP:382:SER:O | 41:QP:383:GLU:C | 2.59 | 0.41 |
| 41:QP:415:MET:O | 41:QP:416:ASN:C | 2.59 | 0.41 |
| 40:RA:230:LEU:O | 40:RA:234:ILE:HG12 | 2.20 | 0.41 |
| 40:RH:13:GLY:HA2 | 40:RH:16:ILE:HG22 | 2.03 | 0.41 |
| 40:RH:208:ALA:O | 40:RH:212:ILE:HG12 | 2.20 | 0.41 |
| 40:RI:91:GLN:HA | 40:RI:121:ARG:HH22 | 1.85 | 0.41 |
| 41:RL:193:VAL:HG22 | 41:RL:418:LEU:HD21 | 2.02 | 0.41 |
| 41:RN:87:PRO:HA | 41:RN:90:PHE:HD2 | 1.86 | 0.41 |
| 41:RN:314:ALA:HB3 | 41:RN:368:ILE:HB | 2.01 | 0.41 |
| 41:RO:100:ASN:HD22 | 41:RO:103:LYS:HE2 | 1.85 | 0.41 |
| 40:SH:120:ASP:O | 40:SH:124:LYS:HG2 | 2.20 | 0.41 |
| 40:SH:139:HIS:CG | 40:SH:150:THR:HG21 | 2.55 | 0.41 |
| 40:SI:107:HIS:HA | 40:SI:152:LEU:HD22 | 2.01 | 0.41 |
| 41:SL:309:ARG:NH1 | 41:SL:339:SER:O | 2.52 | 0.41 |
| 41:SM:3:GLU:HG3 | 41:SM:127:CYS:SG | 2.61 | 0.41 |
| 41:SM:240:LEU:HD23 | 41:SM:240:LEU:H | 1.85 | 0.41 |
| 40:TE:115:ILE:HG13 | 40:TE:119:LEU:HD12 | 2.03 | 0.41 |
| 40:TH:440:GLU:O | 41:TP:390:ARG:NH2 | 2.46 | 0.41 |
| 41:TM:148:GLY:O | 41:TM:152:ILE:HG12 | 2.21 | 0.41 |
| 41:TN:318:ARG:CZ | 41:TN:358:PRO:HG3 | 2.50 | 0.41 |
| 40:UE:233:GLN:OE1 | 40:UE:320:ARG:NH1 | 2.54 | 0.41 |
| 40:UF:251:ASP:H | 40:UF:254:GLU:HG3 | 1.85 | 0.41 |
| 40:UF:421:ARG:HD2 | 40:UF:421:ARG:HA | 1.50 | 0.41 |
| 40:UG:20:CYS:HA | 40:UG:232:SER:HB2 | 2.02 | 0.41 |
| 40:UI:2:ARG:HE | 40:UI:2:ARG:HB2 | 1.72 | 0.41 |
| 40:UI:198:SER:HB2 | 40:UI:266:HIS:CE1 | 2.56 | 0.41 |
| 41:UN:170:VAL:HG21 | 41:UN:377:LEU:HD21 | 2.03 | 0.41 |
| 41:UP:64:VAL:O | 41:UP:66:VAL:HG23 | 2.20 | 0.41 |
| 41:UP:317:PHE:HB3 | 41:UP:321:MET:SD | 2.60 | 0.41 |
| 41:UP:321:MET:HG3 | 41:UP:353:VAL:CG2 | 2.50 | 0.41 |
| 40:VA:164:LYS:HD3 | 40:VA:164:LYS:HA | 1.78 | 0.41 |
| 40:VA:325:PRO:O | 40:VA:329:ASN:ND2 | 2.54 | 0.41 |
| 40:VA:328:VAL:O | 40:VA:332:ILE:HG12 | 2.20 | 0.41 |
| 40:VF:40:LYS:NZ | 40:VF:46:ASP:HB3 | 2.36 | 0.41 |
| 40:VH:181:VAL:HG23 | 40:VH:182:VAL:HG13 | 2.02 | 0.41 |
| 40:VH:264:ARG:HA | 40:VH:264:ARG:HD2 | 1.88 | 0.41 |
| 40:VI:231:ILE:O | 40:VI:235:VAL:HG23 | 2.20 | 0.41 |
| 40:VJ:405:HIS:HA | 40:VJ:408:VAL:HG12 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:VO:305:PRO:HB3 | 41:VO:310:TYR:CE2 | 2.56 | 0.41 |
| 41:VP:104:GLY:HA3 | 41:VP:146:GLY:HA3 | 2.02 | 0.41 |
| 41:VQ:236:VAL:HG22 | 41:VQ:368:ILE:HD11 | 2.03 | 0.41 |
| 41:WB:332:ASN:OD1 | 41:WB:336:LYS:NZ | 2.40 | 0.41 |
| 40:WG:88:HIS:HB3 | 40:WG:91:GLN:HG3 | 2.02 | 0.41 |
| 40:WH:168:GLU:HB3 | 40:WH:201:ALA:HA | 2.02 | 0.41 |
| 40:WI:164:LYS:HD3 | 40:WI:164:LYS:HA | 1.90 | 0.41 |
| 41:WM:47:ILE:HD12 | 41:WM:47:ILE:HA | 1.84 | 0.41 |
| 41:WM:279:GLN:C | 41:WM:281:TYR:H | 2.24 | 0.41 |
| 41:WM:415:MET:HE3 | 41:WM:415:MET:HB3 | 1.83 | 0.41 |
| 41:WO:20:PHE:HE1 | 41:WO:234:SER:HB2 | 1.85 | 0.41 |
| 41:WP:42:LEU:HD22 | 41:WP:243:PRO:HG3 | 2.03 | 0.41 |
| 41:WQ:292:GLN:O | 41:WQ:298:ASN:ND2 | 2.53 | 0.41 |
| 2:1C:14:PRO:HB2 | 41:GM:262:ARG:NH1 | 2.35 | 0.41 |
| 2:1D:10:ARG:CZ | 40:GH:401:ARG:HG3 | 2.50 | 0.41 |
| 7:1T:20:ILE:O | 7:1T:610:ALA:HA | 2.20 | 0.41 |
| 7:1T:148:ILE:HG13 | 7:1T:148:ILE:H | 1.50 | 0.41 |
| 7:1T:216:ASP:O | 7:1T:217:ASP:C | 2.58 | 0.41 |
| 7:1T:343:GLY:O | 7:1T:597:PRO:HB2 | 2.20 | 0.41 |
| 7:1U:479:ALA:HB2 | 7:1U:508:VAL:HB | 2.01 | 0.41 |
| 7:1U:569:VAL:CG2 | 7:1U:586:HIS:CE1 | 3.02 | 0.41 |
| 11:2J:32:LYS:HE2 | 11:2J:32:LYS:HB2 | 1.88 | 0.41 |
| 11:2J:190:ASP:N | 11:2J:190:ASP:OD1 | 2.53 | 0.41 |
| 11:2K:48:THR:HG1 | 11:2K:49:MET:H | 1.68 | 0.41 |
| 12:2N:65:ARG:HD3 | 12:2N:65:ARG:HA | 1.81 | 0.41 |
| 12:2O:109:LEU:HD12 | 12:2O:109:LEU:HA | 1.78 | 0.41 |
| 12:2R:76:TYR:HE2 | 12:2R:83:ILE:HD11 | 1.86 | 0.41 |
| 13:2T:10:PHE:CZ | 13:2T:178:PRO:HD3 | 2.56 | 0.41 |
| 13:2T:102:ARG:HB2 | 13:2T:118:ILE:HA | 2.02 | 0.41 |
| 13:2X:28:LYS:HG2 | 13:2X:58:TYR:CZ | 2.56 | 0.41 |
| 16:3K:268:ARG:HA | 16:3K:268:ARG:HD2 | 1.91 | 0.41 |
| 16:3L:23:LEU:HD23 | 16:3L:23:LEU:HA | 1.88 | 0.41 |
| 16:3L:154:LYS:HG3 | 16:3L:246:THR:HG21 | 2.02 | 0.41 |
| 16:3L:270:ARG:NH2 | 16:3L:274:LYS:HE3 | 2.36 | 0.41 |
| 17:3O:185:LEU:HD21 | 17:3O:237:LEU:HD22 | 2.01 | 0.41 |
| 17:3Q:409:ILE:H | 17:3Q:409:ILE:HG12 | 1.41 | 0.41 |
| 20:4B:321:ALA:O | 20:4B:324:LEU:HG | 2.21 | 0.41 |
| 21:4E:466:TYR:O | 21:4E:467:LEU:C | 2.58 | 0.41 |
| 21:4F:348:ASP:N | 21:4F:348:ASP:OD1 | 2.51 | 0.41 |
| 21:4F:529:LEU:O | 21:4F:530:SER:C | 2.58 | 0.41 |
| 22:4H:85:LEU:HD12 | 22:4H:102:TYR:HE2 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 22:4H:117:GLU:OE2 | 22:4H:127:LYS:NZ | 2.47 | 0.41 |
| 22:4H:230:LEU:HB2 | 22:4H:253:TYR:HB3 | 2.02 | 0.41 |
| 22:4H:370:ILE:HB | 22:4H:372:ASN:HD21 | 1.86 | 0.41 |
| 22:4I:23:SER:OG | 40:MG:46:ASP:HB3 | 2.21 | 0.41 |
| 22:4I:33:ARG:HG3 | 41:MO:92:PHE:CZ | 2.55 | 0.41 |
| 22:4J:15:ILE:HD12 | 22:4J:17:LYS:HD3 | 2.02 | 0.41 |
| 22:4J:91:ASP:HB3 | 41:BN:281:TYR:CB | 2.50 | 0.41 |
| 22:4J:92:LYS:HB2 | 41:BN:279:GLN:CA | 2.50 | 0.41 |
| 23:4M:98:VAL:HG21 | 23:4M:113:TRP:CD1 | 2.55 | 0.41 |
| 23:4M:109:CYS:SG | 40:BG:218:ASP:OD2 | 2.79 | 0.41 |
| 23:4M:212:GLU:HG3 | 23:4M:213:PHE:N | 2.35 | 0.41 |
| 23:4N:170:SER:C | 23:4N:172:TYR:H | 2.24 | 0.41 |
| 23:4Q:205:LEU:HD22 | 23:4Q:205:LEU:HA | 1.82 | 0.41 |
| 23:4R:59:THR:O | 23:4R:61:LEU:N | 2.54 | 0.41 |
| 26:4W:59:ASP:O | 26:4W:64:ASN:ND2 | 2.51 | 0.41 |
| 28:5B:113:ALA:HB1 | 32:5L:63:ASN:HD21 | 1.86 | 0.41 |
| 28:5B:217:ARG:HA | 28:5B:217:ARG:HD3 | 1.66 | 0.41 |
| 29:5D:27:TYR:HD1 | 29:5D:70:VAL:HG21 | 1.85 | 0.41 |
| 30:5G:105:THR:O | 41:HB:332:ASN:ND2 | 2.43 | 0.41 |
| 31:5J:803:ILE:HG23 | 31:5J:804:PHE:CD1 | 2.55 | 0.41 |
| 33:5O:109:LYS:NZ | 33:5O:112:GLN:OE1 | 2.45 | 0.41 |
| 34:5R:432:GLU:HA | 34:5R:435:GLU:HB2 | 2.02 | 0.41 |
| 36:5W:52:ARG:HH22 | 41:NM:40:SER:C | 2.23 | 0.41 |
| 38:6C:197:LEU:HA | 41:UP:125:GLU:OE1 | 2.21 | 0.41 |
| 39:6I:48:ILE:HD11 | 39:6I:142:LEU:HD21 | 2.03 | 0.41 |
| 40:AE:168:GLU:N | 40:AE:168:GLU:OE2 | 2.54 | 0.41 |
| 40:AE:273:ALA:HB1 | 40:AE:291:ILE:HB | 2.03 | 0.41 |
| 40:AF:36:MET:HA | 40:AF:37:PRO:HD3 | 1.95 | 0.41 |
| 40:AG:103:TYR:HB2 | 40:AG:186:ASN:HD22 | 1.85 | 0.41 |
| 40:AH:251:ASP:OD1 | 40:AH:252:LEU:N | 2.48 | 0.41 |
| 41:AP:178:THR:HB | 41:AP:181:GLU:HG3 | 2.02 | 0.41 |
| 41:BB:24:ILE:HD13 | 41:BB:24:ILE:HA | 1.98 | 0.41 |
| 40:BH:195:LEU:HD12 | 40:BH:266:HIS:CE1 | 2.56 | 0.41 |
| 40:BH:224:TYR:HD1 | 40:BH:224:TYR:HA | 1.75 | 0.41 |
| 40:BI:201:ALA:O | 40:BI:203:MET:N | 2.54 | 0.41 |
| 41:BL:244:GLY:O | 41:BL:247:ASN:ND2 | 2.53 | 0.41 |
| 41:BL:312:THR:HA | 41:BL:348:ASN:HB2 | 2.03 | 0.41 |
| 41:BM:20:PHE:HZ | 41:BM:50:TYR:CE2 | 2.39 | 0.41 |
| 41:BN:51:TYR:HA | 41:BN:61:PRO:HA | 2.03 | 0.41 |
| 41:BO:107:THR:HB | 41:BO:108:GLU:H | 1.64 | 0.41 |
| 41:BO:252:LYS:O | 41:BO:253:LEU:C | 2.58 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CB:137:HIS:HE1 | 41:CB:139:LEU:HD23 | 1.85 | 0.41 |
| 40:CF:1:GLN:OE1 | 41:CN:94:GLN:NE2 | 2.54 | 0.41 |
| 40:CF:118:VAL:O | 40:CF:122:ILE:HG12 | 2.21 | 0.41 |
| 40:CH:153:LEU:HD12 | 40:CH:153:LEU:HA | 1.77 | 0.41 |
| 40:CH:177:VAL:O | 40:CH:178:SER:HB3 | 2.21 | 0.41 |
| 40:CH:191:THR:O | 40:CH:191:THR:OG1 | 2.39 | 0.41 |
| 41:CL:105:HIS:CE1 | 41:CL:191:GLN:HE22 | 2.39 | 0.41 |
| 41:CM:311:LEU:HA | 41:CM:342:VAL:HG22 | 2.03 | 0.41 |
| 41:CN:123:GLU:O | 41:CN:124:ALA:C | 2.58 | 0.41 |
| 41:CO:8:GLN:HG2 | 41:CO:14:ASN:HA | 2.03 | 0.41 |
| 41:CO:208:TYR:O | 41:CO:209:ASP:C | 2.59 | 0.41 |
| 41:CP:104:GLY:CA | 41:CP:109:GLY:HA3 | 2.50 | 0.41 |
| 41:CP:112:LEU:O | 41:CP:113:VAL:C | 2.58 | 0.41 |
| 41:CP:214:THR:HG21 | 41:CP:298:ASN:HD21 | 1.86 | 0.41 |
| 41:CP:325:GLU:H | 41:CP:325:GLU:HG3 | 1.54 | 0.41 |
| 41:DB:109:GLY:O | 41:DB:112:LEU:N | 2.41 | 0.41 |
| 41:DB:317:PHE:HB3 | 41:DB:321:MET:SD | 2.61 | 0.41 |
| 40:DE:117:LEU:H | 40:DE:117:LEU:HG | 1.49 | 0.41 |
| 40:DE:189:LEU:HA | 40:DE:189:LEU:HD23 | 1.86 | 0.41 |
| 40:DE:278:ALA:O | 40:DE:279:GLU:C | 2.59 | 0.41 |
| 40:DF:123:ARG:HA | 40:DF:123:ARG:HD3 | 1.53 | 0.41 |
| 40:DF:363:VAL:O | 40:DF:365:GLY:N | 2.54 | 0.41 |
| 40:DG:97:GLU:OE1 | 40:DG:105:ARG:NH2 | 2.54 | 0.41 |
| 40:DI:209:ILE:HG22 | 40:DI:227:LEU:HD22 | 2.02 | 0.41 |
| 40:DI:297:GLU:O | 40:DI:299:ALA:N | 2.50 | 0.41 |
| 41:DL:45:GLU:C | 41:DL:47:ILE:H | 2.20 | 0.41 |
| 41:DL:167:PHE:HD1 | 41:DL:200:TYR:CD2 | 2.38 | 0.41 |
| 41:DL:173:PRO:HD2 | 41:DL:205:GLU:HB2 | 2.02 | 0.41 |
| 41:DL:276:ARG:C | 41:DL:279:GLN:HG2 | 2.41 | 0.41 |
| 41:DM:51:TYR:HB3 | 41:DM:59:TYR:HB3 | 2.03 | 0.41 |
| 41:DM:100:ASN:HD22 | 41:DM:103:LYS:HB2 | 1.86 | 0.41 |
| 41:DM:222:TYR:HD1 | 41:DM:222:TYR:HA | 1.75 | 0.41 |
| 41:DN:90:PHE:O | 41:DN:91:VAL:C | 2.59 | 0.41 |
| 41:DN:315:ALA:HA | 41:DN:366:THR:O | 2.20 | 0.41 |
| 41:DO:375:GLN:HB2 | 41:DO:422:VAL:HG13 | 2.01 | 0.41 |
| 41:DP:73:MET:O | 41:DP:76:VAL:HB | 2.21 | 0.41 |
| 40:EA:71:GLU:OE1 | 40:EA:98:ASP:HB3 | 2.20 | 0.41 |
| 40:EE:306:ASP:OD2 | 40:EE:308:ARG:NH2 | 2.52 | 0.41 |
| 40:EG:175:PRO:O | 40:EG:389:ARG:NH2 | 2.53 | 0.41 |
| 40:EH:158:SER:OG | 40:EH:159:VAL:N | 2.54 | 0.41 |
| 40:EH:230:LEU:HD11 | 40:EH:275:VAL:HG11 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EI:399:ALA:O | 40:EI:401:ARG:N | 2.50 | 0.41 |
| 41:EM:193:VAL:CG1 | 41:EM:418:LEU:HD21 | 2.50 | 0.41 |
| 41:EM:419:GLY:O | 41:EM:423:VAL:HG13 | 2.21 | 0.41 |
| 41:EP:163:ILE:H | 41:EP:163:ILE:HG13 | 1.42 | 0.41 |
| 41:EP:284:LEU:HA | 41:EP:284:LEU:HD13 | 1.79 | 0.41 |
| 40:FA:366:ASP:O | 40:FA:367:LEU:C | 2.58 | 0.41 |
| 40:FF:170:SER:HB2 | 40:FF:203:MET:SD | 2.60 | 0.41 |
| 40:FF:407:TYR:O | 40:FF:412:MET:HG3 | 2.20 | 0.41 |
| 40:FG:70:LEU:HD23 | 40:FG:114:LEU:HD12 | 2.02 | 0.41 |
| 40:FG:351:PHE:C | 40:FG:352:LYS:HE2 | 2.40 | 0.41 |
| 40:FH:115:ILE:HG13 | 40:FH:119:LEU:HD23 | 2.03 | 0.41 |
| 40:FI:101:ASN:OD1 | 41:FP:252:LYS:NZ | 2.49 | 0.41 |
| 41:FM:7:LEU:HD23 | 41:FM:151:LEU:HD11 | 2.03 | 0.41 |
| 41:FM:105:HIS:HB3 | 41:FM:106:TYR:HD1 | 1.86 | 0.41 |
| 41:FO:186:THR:HG21 | 41:FO:385:PHE:CE2 | 2.56 | 0.41 |
| 41:FO:380:ARG:HG3 | 41:FO:384:GLN:HE22 | 1.85 | 0.41 |
| 40:GA:223:THR:HB | 40:GA:225:THR:HG22 | 2.02 | 0.41 |
| 40:GA:319:TYR:HB3 | 40:GA:323:VAL:HG11 | 2.01 | 0.41 |
| 41:GB:255:VAL:HG11 | 40:GG:100:ALA:O | 2.21 | 0.41 |
| 40:GE:17:GLY:O | 40:GE:18:ASN:C | 2.59 | 0.41 |
| 40:GE:172:TYR:HE1 | 40:GE:390:LEU:HD11 | 1.85 | 0.41 |
| 40:GE:266:HIS:O | 40:GE:268:PRO:HD3 | 2.20 | 0.41 |
| 40:GF:210:TYR:HE2 | 40:GF:227:LEU:HD11 | 1.85 | 0.41 |
| 40:GG:189:LEU:HD11 | 40:GG:417:PHE:HE1 | 1.84 | 0.41 |
| 40:GG:278:ALA:HA | 40:GG:368:ALA:CB | 2.51 | 0.41 |
| 40:GI:162:GLY:O | 40:GI:164:LYS:N | 2.54 | 0.41 |
| 40:GI:261:PRO:HD3 | 40:GI:379:ASN:ND2 | 2.36 | 0.41 |
| 40:GI:305:CYS:SG | 40:GI:305:CYS:O | 2.78 | 0.41 |
| 41:GO:316:VAL:HA | 41:GO:352:ALA:HB3 | 2.03 | 0.41 |
| 40:HA:107:HIS:ND1 | 40:HA:151:SER:OG | 2.52 | 0.41 |
| 40:HF:169:PHE:HZ | 40:HF:238:ILE:HG21 | 1.86 | 0.41 |
| 40:HG:319:TYR:HB3 | 40:HG:323:VAL:HG21 | 2.02 | 0.41 |
| 40:HH:181:VAL:HG13 | 40:HH:182:VAL:HG13 | 2.03 | 0.41 |
| 40:HH:256:GLN:HG2 | 40:HH:260:VAL:HG21 | 2.01 | 0.41 |
| 41:HN:71:GLY:O | 41:HN:74:ASP:N | 2.53 | 0.41 |
| 40:IA:251:ASP:H | 40:IA:254:GLU:HB2 | 1.85 | 0.41 |
| 41:IB:131:GLN:HE21 | 41:IB:251:ARG:HG2 | 1.86 | 0.41 |
| 40:IH:12:ALA:HB1 | 40:IH:171:ILE:HD13 | 2.03 | 0.41 |
| 41:IM:121:ARG:NH1 | 41:IM:158:GLU:OE2 | 2.54 | 0.41 |
| 41:IQ:282:ARG:NH2 | 41:IQ:288:GLU:OE2 | 2.53 | 0.41 |
| 41:JB:270:PHE:CE2 | 41:JB:272:PRO:HD2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JE:319:TYR:CD1 | 40:JE:374:VAL:HB | 2.55 | 0.41 |
| 40:JH:178:SER:OG | 40:JH:179:THR:N | 2.53 | 0.41 |
| 41:JM:363:MET:HE3 | 41:JM:363:MET:HB3 | 1.94 | 0.41 |
| 40:KG:88:HIS:ND1 | 40:KG:90:GLU:HG2 | 2.36 | 0.41 |
| 40:KH:62:VAL:HA | 40:KH:63:PRO:HD3 | 1.93 | 0.41 |
| 40:KH:71:GLU:HA | 40:KH:72:PRO:HD3 | 1.90 | 0.41 |
| 41:KM:303:CYS:SG | 41:KM:377:LEU:HB2 | 2.60 | 0.41 |
| 40:LF:157:LEU:HD12 | 40:LF:157:LEU:HA | 1.72 | 0.41 |
| 41:LO:222:TYR:CD1 | 41:LO:225:LEU:HD12 | 2.56 | 0.41 |
| 41:LP:209:ASP:CG | 41:LP:213:ARG:HH12 | 2.23 | 0.41 |
| 40:MA:91:GLN:HG2 | 40:MA:125:LEU:HD11 | 2.02 | 0.41 |
| 40:MA:111:GLY:C | 40:MA:113:GLU:H | 2.22 | 0.41 |
| 40:MG:29:GLY:O | 40:MG:30:ILE:C | 2.58 | 0.41 |
| 40:MG:75:ILE:HB | 40:MG:94:THR:HG23 | 2.02 | 0.41 |
| 40:MH:231:ILE:O | 40:MH:235:VAL:HG23 | 2.20 | 0.41 |
| 41:MO:357:PRO:HB2 | 41:MO:361:LEU:O | 2.20 | 0.41 |
| 40:NA:8:HIS:CE1 | 40:NA:21:TRP:HE1 | 2.38 | 0.41 |
| 40:NA:132:LEU:C | 40:NA:164:LYS:HZ1 | 2.24 | 0.41 |
| 41:NB:44:LEU:HA | 41:NB:47:ILE:HB | 2.01 | 0.41 |
| 41:NB:107:THR:HB | 41:NB:108:GLU:H | 1.74 | 0.41 |
| 40:NE:195:LEU:HD21 | 40:NE:264:ARG:HE | 1.85 | 0.41 |
| 40:NF:247:ALA:HB3 | 40:NF:355:ILE:HB | 2.02 | 0.41 |
| 41:NL:309:ARG:H | 41:NL:372:THR:HG1 | 1.64 | 0.41 |
| 41:NM:42:LEU:HD21 | 41:NM:243:PRO:HD2 | 2.02 | 0.41 |
| 41:NM:68:LEU:HD21 | 41:NM:109:GLY:HA2 | 2.02 | 0.41 |
| 41:NP:305:PRO:HB3 | 41:NP:310:TYR:CE1 | 2.56 | 0.41 |
| 40:OA:238:ILE:HA | 40:OA:318:LEU:HD22 | 2.01 | 0.41 |
| 40:OA:393:LYS:HE3 | 40:OA:393:LYS:HB2 | 1.76 | 0.41 |
| 40:OD:329:ASN:HD21 | 41:OL:175:VAL:HG21 | 1.85 | 0.41 |
| 40:OF:248:LEU:HB2 | 40:OF:354:GLY:HA2 | 2.02 | 0.41 |
| 40:OH:413:GLU:H | 40:OH:413:GLU:CD | 2.24 | 0.41 |
| 41:ON:3:GLU:OE2 | 41:ON:129:CYS:N | 2.54 | 0.41 |
| 41:ON:23:VAL:HG11 | 41:ON:230:SER:HB3 | 2.03 | 0.41 |
| 41:OO:105:HIS:CD2 | 41:OO:150:LEU:HB2 | 2.55 | 0.41 |
| 41:PB:44:LEU:HD12 | 41:PB:47:ILE:HG21 | 2.01 | 0.41 |
| 41:PB:139:LEU:HD12 | 41:PB:170:VAL:HG12 | 2.02 | 0.41 |
| 40:PH:240:ALA:HB1 | 40:PH:356:ASN:HD22 | 1.84 | 0.41 |
| 41:PL:167:PHE:HZ | 41:PL:236:VAL:HG11 | 1.86 | 0.41 |
| 41:PL:326:VAL:HG11 | 41:PL:351:THR:HG21 | 2.02 | 0.41 |
| 41:PM:105:HIS:CD2 | 41:PM:150:LEU:HD12 | 2.55 | 0.41 |
| 41:PM:152:ILE:HG13 | 41:PM:195:ASN:ND2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QA:226:ASN:ND2 | 40:QA:366:ASP:OD2 | 2.53 | 0.41 |
| 40:QA:248:LEU:HD11 | 43:QB:501:GDP:H5" | 2.03 | 0.41 |
| 40:QA:405:HIS:CG | 41:QN:261:PRO:HG3 | 2.56 | 0.41 |
| 41:QB:221:THR:O | 41:QB:224:ASP:N | 2.52 | 0.41 |
| 41:QB:359:ARG:HB2 | 41:QB:359:ARG:HH11 | 1.85 | 0.41 |
| 40:QE:138:PHE:HE2 | 40:QE:235:VAL:HG21 | 1.84 | 0.41 |
| 40:QF:103:TYR:CD2 | 40:QF:189:LEU:HB3 | 2.56 | 0.41 |
| 40:QH:75:ILE:HG23 | 40:QH:92:LEU:HD12 | 2.01 | 0.41 |
| 40:QH:133:GLN:HB3 | 40:QH:252:LEU:HD13 | 2.03 | 0.41 |
| 41:QP:269:GLY:O | 41:QP:366:THR:HG23 | 2.20 | 0.41 |
| 41:QP:325:GLU:O | 41:QP:326:VAL:C | 2.59 | 0.41 |
| 40:RA:236:SER:O | 40:RA:240:ALA:HB2 | 2.20 | 0.41 |
| 40:RE:135:PHE:HE2 | 40:RE:164:LYS:HD2 | 1.86 | 0.41 |
| 40:RF:107:HIS:CD2 | 40:RF:152:LEU:HB2 | 2.55 | 0.41 |
| 40:RG:24:TYR:HA | 40:RG:27:GLU:HG2 | 2.02 | 0.41 |
| 41:RN:288:GLU:HA | 41:RN:291:GLN:HG3 | 2.02 | 0.41 |
| 40:SA:167:LEU:HD21 | 40:SA:256:GLN:HE22 | 1.85 | 0.41 |
| 40:SA:247:ALA:O | 40:SA:249:ASN:N | 2.54 | 0.41 |
| 40:SA:376:MET:SD | 40:SA:378:SER:HB3 | 2.60 | 0.41 |
| 41:SB:324:LYS:HG2 | 40:SG:222:PRO:HD2 | 2.02 | 0.41 |
| 40:SE:326:LYS:HG3 | 40:SE:329:ASN:HB2 | 2.02 | 0.41 |
| 40:SF:25:CYS:HA | 40:SF:30:ILE:HB | 2.03 | 0.41 |
| 40:SF:67:PHE:HB2 | 40:SF:92:LEU:HD13 | 2.02 | 0.41 |
| 40:SF:172:TYR:HE2 | 40:SF:389:ARG:HH22 | 1.69 | 0.41 |
| 40:SH:230:LEU:O | 40:SH:234:ILE:HD12 | 2.20 | 0.41 |
| 41:SO:19:LYS:HA | 41:SO:19:LYS:HD2 | 1.29 | 0.41 |
| 41:SO:72:THR:O | 41:SO:73:MET:C | 2.59 | 0.41 |
| 40:TA:255:PHE:CE1 | 40:TA:318:LEU:HD11 | 2.55 | 0.41 |
| 40:TE:260:VAL:HG23 | 40:TE:265:ILE:O | 2.21 | 0.41 |
| 40:TG:256:GLN:O | 40:TG:260:VAL:HB | 2.21 | 0.41 |
| 40:TH:70:LEU:HD11 | 40:TH:149:PHE:HB2 | 2.03 | 0.41 |
| 40:TI:405:HIS:CD2 | 41:TP:261:PRO:HG3 | 2.56 | 0.41 |
| 41:TL:164:MET:HB2 | 41:TL:196:THR:HG1 | 1.86 | 0.41 |
| 41:TP:282:ARG:HD3 | 41:TP:283:ALA:N | 2.36 | 0.41 |
| 41:UB:142:GLY:O | 41:UB:144:GLY:N | 2.54 | 0.41 |
| 40:UE:186:ASN:ND2 | 40:UE:407:TYR:OH | 2.54 | 0.41 |
| 40:UF:1:GLN:HE21 | 41:UN:70:PRO:HG2 | 1.85 | 0.41 |
| 40:UF:156:ARG:C | 40:UF:158:SER:N | 2.72 | 0.41 |
| 40:UF:177:VAL:HG13 | 40:UF:178:SER:H | 1.85 | 0.41 |
| 40:UF:177:VAL:HG22 | 40:UF:178:SER:N | 2.36 | 0.41 |
| 40:UF:415:GLY:O | 40:UF:416:GLU:C | 2.58 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UG:150:THR:O | 40:UG:154:MET:HG2 | 2.20 | 0.41 |
| 40:UH:1:GLN:HE22 | 41:UP:94:GLN:HE22 | 1.67 | 0.41 |
| 40:UH:25:CYS:SG | 40:UH:86:LEU:HD11 | 2.61 | 0.41 |
| 40:UH:280:LYS:HE2 | 40:UH:280:LYS:HB3 | 1.75 | 0.41 |
| 41:UM:385:PHE:O | 41:UM:389:PHE:CB | 2.69 | 0.41 |
| 41:UP:173:PRO:HG2 | 41:UP:302:ALA:HB1 | 2.02 | 0.41 |
| 41:VB:226:ASN:ND2 | 43:VB:501:GDP:O6 | 2.52 | 0.41 |
| 40:VI:277:SER:O | 40:VI:279:GLU:N | 2.53 | 0.41 |
| 40:VJ:332:ILE:HG22 | 40:VJ:336:LYS:HD2 | 2.01 | 0.41 |
| 41:VO:7:LEU:O | 41:VO:135:LEU:HA | 2.21 | 0.41 |
| 41:VO:263:LEU:HD23 | 41:VO:263:LEU:HA | 1.85 | 0.41 |
| 41:VP:149:THR:HB | 41:VP:191:GLN:HG3 | 2.02 | 0.41 |
| 41:VP:262:ARG:NH2 | 41:VP:414:ASN:OD1 | 2.50 | 0.41 |
| 40:WE:140:SER:OG | 42:WE:501:GTP:O2A | 2.28 | 0.41 |
| 40:WE:153:LEU:O | 40:WE:157:LEU:HB2 | 2.20 | 0.41 |
| 40:WE:261:PRO:HG3 | 41:WM:394:PHE:CZ | 2.56 | 0.41 |
| 40:WG:28:HIS:CE1 | 40:WG:243:ARG:HD2 | 2.55 | 0.41 |
| 40:WG:167:LEU:HD22 | 40:WG:200:CYS:HB3 | 2.03 | 0.41 |
| 41:WM:151:LEU:HD13 | 41:WM:151:LEU:HA | 1.70 | 0.41 |
| 41:WM:420:ASN:HD22 | 41:WM:420:ASN:HA | 1.63 | 0.41 |
| 7:1T:205:LYS:H | 7:1T:205:LYS:HG2 | 1.61 | 0.41 |
| 7:1T:272:LEU:HD12 | 7:1T:272:LEU:HA | 1.82 | 0.41 |
| 7:1T:558:VAL:HG21 | 7:1T:620:SER:HB2 | 2.02 | 0.41 |
| 7:1U:503:THR:HB | 7:1U:523:ASP:HB3 | 2.03 | 0.41 |
| 7:1U:553:ILE:HD12 | 7:1U:560:PHE:HB3 | 2.03 | 0.41 |
| 8:1W:401:ARG:HA | 8:1W:404:GLU:HG3 | 2.03 | 0.41 |
| 8:1X:150:LYS:HB2 | 8:1X:150:LYS:HE2 | 1.75 | 0.41 |
| 10:2F:75:ARG:NH1 | 40:AA:296:PHE:HB3 | 2.36 | 0.41 |
| 10:2F:161:ARG:NH1 | 10:2F:166:GLY:H | 2.18 | 0.41 |
| 12:2O:230:GLU:OE2 | 12:2O:234:ARG:NH2 | 2.54 | 0.41 |
| 13:2V:163:ARG:HE | 13:2V:163:ARG:HB2 | 1.53 | 0.41 |
| 13:2V:183:LEU:HD12 | 13:2V:183:LEU:HA | 1.90 | 0.41 |
| 13:2W:39:ASP:HB2 | 13:2W:46:VAL:HG11 | 2.02 | 0.41 |
| 16:3J:205:PRO:HG3 | 16:3K:315:HIS:CE1 | 2.56 | 0.41 |
| 17:3P:95:THR:HB | 17:3P:96:PRO:HD2 | 2.01 | 0.41 |
| 17:3R:205:ARG:HB3 | 17:3R:209:ASP:OD2 | 2.21 | 0.41 |
| 18:3T:332:GLN:HE21 | 18:3T:401:SER:HB3 | 1.86 | 0.41 |
| 18:3T:376:ARG:HH22 | 18:3U:95:THR:HG23 | 1.85 | 0.41 |
| 18:3W:142:LEU:HA | 18:3W:145:THR:HG22 | 2.02 | 0.41 |
| 19:3Y:144:GLN:OE1 | 41:LB:279:GLN:NE2 | 2.32 | 0.41 |
| 21:4D:437:ARG:HD3 | 21:4D:437:ARG:HA | 1.43 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4D:502:ARG:HD3 | 22:4I:644:TYR:CE1 | 2.56 | 0.41 |
| 21:4F:519:ASN:HB3 | 21:4F:522:GLN:HB2 | 2.02 | 0.41 |
| 22:4I:280:GLN:HE21 | 22:4I:282:ARG:HH11 | 1.69 | 0.41 |
| 22:4J:92:LYS:CE | 41:BN:280:GLN:HB2 | 2.49 | 0.41 |
| 23:4M:198:PHE:CD1 | 40:DG:221:ARG:HD2 | 2.55 | 0.41 |
| 24:4O:178:ASP:OD1 | 24:4O:180:ARG:HB2 | 2.21 | 0.41 |
| 23:4P:235:THR:CG2 | 23:4P:240:LEU:HA | 2.51 | 0.41 |
| 23:4Q:197:LEU:HD12 | 23:4Q:197:LEU:HA | 1.86 | 0.41 |
| 23:4R:260:THR:O | 23:4R:262:GLY:N | 2.48 | 0.41 |
| 23:4R:269:LEU:H | 23:4R:269:LEU:HG | 1.62 | 0.41 |
| 25:4T:323:GLN:O | 25:4T:327:TYR:HB2 | 2.20 | 0.41 |
| 26:4V:193:ARG:NE | 26:4V:203:ASN:HD22 | 2.18 | 0.41 |
| 26:4W:258:ILE:O | 26:4W:262:ILE:HG12 | 2.21 | 0.41 |
| 34:5R:340:LYS:HB3 | 34:5R:340:LYS:HE3 | 1.63 | 0.41 |
| 34:5R:445:GLN:O | 34:5R:449:LYS:HG2 | 2.21 | 0.41 |
| 36:5W:47:ARG:NH1 | 41:NM:59:TYR:OH | 2.41 | 0.41 |
| 39:6F:152:GLU:HG3 | 39:6F:156:HIS:HE1 | 1.86 | 0.41 |
| 39:6L:8:GLU:HG3 | 39:6L:11:ARG:HH21 | 1.85 | 0.41 |
| 41:AB:226:ASN:ND2 | 43:AB:501:GDP:O6 | 2.42 | 0.41 |
| 41:AB:313:VAL:HG13 | 41:AB:367:PHE:HE1 | 1.85 | 0.41 |
| 40:AE:306:ASP:HB3 | 40:AE:309:HIS:ND1 | 2.36 | 0.41 |
| 40:AG:156:ARG:HD3 | 40:AG:156:ARG:HA | 1.85 | 0.41 |
| 40:AH:28:HIS:HD1 | 40:AH:49:PHE:HA | 1.86 | 0.41 |
| 41:AL:172:SER:HB3 | 41:AL:203:ASP:OD1 | 2.21 | 0.41 |
| 41:AL:173:PRO:HD3 | 41:AL:380:ARG:HH11 | 1.85 | 0.41 |
| 41:AO:44:LEU:HD23 | 41:AO:44:LEU:HA | 1.83 | 0.41 |
| 41:AP:404:ASP:HB3 | 41:AP:407:GLU:HG3 | 2.03 | 0.41 |
| 41:BB:165:ASN:OD1 | 41:BB:165:ASN:N | 2.54 | 0.41 |
| 40:BE:204:VAL:HG12 | 40:BE:302:MET:HB2 | 2.01 | 0.41 |
| 40:BE:273:ALA:HB1 | 40:BE:291:ILE:HB | 2.03 | 0.41 |
| 40:BG:265:ILE:HD11 | 40:BG:430:ASP:HB3 | 2.02 | 0.41 |
| 40:BG:386:ALA:HA | 40:BG:389:ARG:HG2 | 2.02 | 0.41 |
| 40:BH:10:GLY:O | 40:BH:14:VAL:HG23 | 2.21 | 0.41 |
| 40:BH:141:PHE:O | 40:BH:142:GLY:C | 2.59 | 0.41 |
| 40:BI:50:ASN:O | 40:BI:51:THR:C | 2.57 | 0.41 |
| 40:BI:84:ARG:O | 40:BI:86:LEU:N | 2.53 | 0.41 |
| 41:BO:271:ALA:HB3 | 41:BO:272:PRO:HD3 | 2.02 | 0.41 |
| 40:CA:303:VAL:O | 40:CA:304:LYS:C | 2.59 | 0.41 |
| 40:CH:6:SER:HA | 40:CH:136:LEU:O | 2.21 | 0.41 |
| 40:CH:174:ALA:HB3 | 40:CH:177:VAL:HG23 | 2.02 | 0.41 |
| 40:CI:178:SER:OG | 40:CI:179:THR:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CL:114:ASP:C | 41:CL:116:VAL:H | 2.23 | 0.41 |
| 41:CL:166:THR:HG23 | 41:CL:199:THR:HA | 2.03 | 0.41 |
| 41:CL:237:THR:O | 41:CL:237:THR:OG1 | 2.37 | 0.41 |
| 41:CL:289:LEU:HD11 | 41:CL:363:MET:HG3 | 2.02 | 0.41 |
| 41:CL:420:ASN:HD22 | 41:CL:420:ASN:HA | 1.73 | 0.41 |
| 41:CN:277:GLY:C | 41:CN:279:GLN:H | 2.24 | 0.41 |
| 40:DA:35:GLN:O | 40:DA:36:MET:C | 2.58 | 0.41 |
| 40:DA:72:PRO:O | 40:DA:73:THR:C | 2.59 | 0.41 |
| 40:DA:91:GLN:O | 40:DA:93:ILE:HG12 | 2.20 | 0.41 |
| 40:DA:191:THR:OG1 | 40:DA:192:HIS:N | 2.53 | 0.41 |
| 40:DE:20:CYS:HA | 40:DE:232:SER:HB2 | 2.03 | 0.41 |
| 40:DE:195:LEU:HA | 40:DE:266:HIS:NE2 | 2.36 | 0.41 |
| 40:DE:396:LEU:HG | 41:DL:344:TRP:O | 2.20 | 0.41 |
| 40:DE:409:GLY:O | 40:DE:411:GLY:N | 2.53 | 0.41 |
| 40:DF:207:GLU:O | 40:DF:210:TYR:HB2 | 2.21 | 0.41 |
| 40:DF:221:ARG:HB3 | 41:DM:322:SER:CB | 2.51 | 0.41 |
| 40:DG:143:GLY:N | 42:DG:501:GTP:O2A | 2.39 | 0.41 |
| 40:DH:90:GLU:O | 40:DH:91:GLN:C | 2.59 | 0.41 |
| 40:DH:129:CYS:SG | 40:DH:132:LEU:HG | 2.60 | 0.41 |
| 40:DH:397:MET:O | 40:DH:400:LYS:N | 2.53 | 0.41 |
| 40:DI:9:VAL:O | 40:DI:13:GLY:HA3 | 2.21 | 0.41 |
| 40:DI:248:LEU:O | 40:DI:355:ILE:N | 2.54 | 0.41 |
| 41:DL:156:ARG:HH11 | 41:DL:164:MET:HB2 | 1.85 | 0.41 |
| 41:DM:151:LEU:HD13 | 41:DM:151:LEU:HA | 1.77 | 0.41 |
| 41:DM:199:THR:HG23 | 41:DM:264:HIS:HD2 | 1.86 | 0.41 |
| 41:DN:7:LEU:HA | 41:DN:64:VAL:HG23 | 2.02 | 0.41 |
| 41:DO:190:HIS:CG | 41:DO:414:ASN:HD22 | 2.38 | 0.41 |
| 40:EF:241:SER:HB2 | 40:EF:250:VAL:H | 1.85 | 0.41 |
| 40:EF:255:PHE:HE1 | 40:EF:318:LEU:HD11 | 1.85 | 0.41 |
| 40:EG:217:LEU:HD23 | 40:EG:277:SER:HB3 | 2.02 | 0.41 |
| 41:EL:135:LEU:HD23 | 41:EL:152:ILE:HD11 | 2.03 | 0.41 |
| 41:EM:171:PRO:HB3 | 41:EM:181:GLU:HG3 | 2.01 | 0.41 |
| 41:EM:271:ALA:O | 41:EM:273:LEU:N | 2.44 | 0.41 |
| 41:EN:122:LYS:HD3 | 41:FN:291:GLN:HE22 | 1.85 | 0.41 |
| 41:EP:98:GLY:O | 41:EP:100:ASN:N | 2.53 | 0.41 |
| 40:FA:131:GLY:O | 40:FA:132:LEU:C | 2.59 | 0.41 |
| 40:FA:142:GLY:O | 40:FA:143:GLY:C | 2.58 | 0.41 |
| 40:FA:273:ALA:CB | 40:FA:274:PRO:CD | 2.93 | 0.41 |
| 40:FA:319:TYR:HA | 40:FA:374:VAL:HA | 2.03 | 0.41 |
| 40:FA:427:LEU:HD12 | 40:FA:427:LEU:HA | 1.87 | 0.41 |
| 41:FM:12:CYS:SG | 41:FM:138:SER:OG | 2.58 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FN:119:VAL:O | 41:FN:123:GLU:HG2 | 2.21 | 0.41 |
| 41:FN:183:TYR:OH | 41:FN:388:MET:O | 2.39 | 0.41 |
| 40:GA:121:ARG:HD3 | 40:GA:121:ARG:HA | 1.88 | 0.41 |
| 40:GA:257:THR:HG21 | 41:GB:98:GLY:O | 2.20 | 0.41 |
| 41:GB:261:PRO:HG3 | 40:GG:405:HIS:CD2 | 2.56 | 0.41 |
| 40:GG:72:PRO:HD3 | 40:GG:96:LYS:HA | 2.01 | 0.41 |
| 40:GH:311:LYS:HE3 | 40:GH:344:VAL:HG12 | 2.02 | 0.41 |
| 40:GH:346:TRP:HB3 | 41:GP:391:ARG:HG3 | 2.02 | 0.41 |
| 41:GN:153:SER:OG | 41:GN:154:LYS:N | 2.54 | 0.41 |
| 41:GN:234:SER:O | 41:GN:235:GLY:C | 2.58 | 0.41 |
| 41:GN:395:LEU:O | 41:GN:396:HIS:C | 2.58 | 0.41 |
| 41:GP:282:ARG:NH1 | 41:GP:288:GLU:OE2 | 2.54 | 0.41 |
| 40:HE:258:ASN:ND2 | 41:HM:99:ASN:HD21 | 2.17 | 0.41 |
| 40:HE:376:MET:HE3 | 40:HE:376:MET:HB3 | 1.95 | 0.41 |
| 40:HF:376:MET:SD | 40:HF:378:SER:HB3 | 2.61 | 0.41 |
| 41:HN:16:ILE:HG13 | 41:HN:226:ASN:OD1 | 2.21 | 0.41 |
| 41:HN:107:THR:OG1 | 41:HN:108:GLU:N | 2.51 | 0.41 |
| 41:HN:147:MET:O | 41:HN:148:GLY:C | 2.59 | 0.41 |
| 41:HO:318:ARG:HB3 | 41:HO:357:PRO:HA | 2.03 | 0.41 |
| 40:IA:234:ILE:O | 40:IA:238:ILE:HG12 | 2.21 | 0.41 |
| 40:IA:257:THR:HG23 | 40:IA:258:ASN:OD1 | 2.21 | 0.41 |
| 40:IF:263:PRO:HG3 | 41:IN:396:HIS:CG | 2.56 | 0.41 |
| 40:IH:274:PRO:HB3 | 40:IH:370:VAL:HG11 | 2.01 | 0.41 |
| 40:II:105:ARG:NH1 | 41:IP:251:ARG:HH12 | 2.19 | 0.41 |
| 40:II:292:THR:OG1 | 40:II:319:TYR:OH | 2.33 | 0.41 |
| 40:II:294:ALA:O | 40:II:300:ASN:ND2 | 2.39 | 0.41 |
| 41:IM:421:PRO:O | 41:IM:425:ARG:HG2 | 2.21 | 0.41 |
| 41:IN:200:TYR:HE2 | 41:IN:368:ILE:HD12 | 1.85 | 0.41 |
| 41:IN:215:LEU:HD21 | 41:IN:273:LEU:HD22 | 2.03 | 0.41 |
| 41:IN:262:ARG:NH2 | 41:IN:414:ASN:OD1 | 2.54 | 0.41 |
| 41:IP:421:PRO:O | 41:IP:425:ARG:HG3 | 2.20 | 0.41 |
| 40:JA:204:VAL:HG21 | 40:JA:231:ILE:HD11 | 2.01 | 0.41 |
| 40:JE:294:ALA:O | 40:JE:300:ASN:ND2 | 2.41 | 0.41 |
| 40:JF:329:ASN:OD1 | 41:JN:175:VAL:HG21 | 2.21 | 0.41 |
| 41:JM:389:PHE:O | 41:JM:392:LYS:HD3 | 2.20 | 0.41 |
| 41:JM:418:LEU:C | 41:JM:420:ASN:H | 2.24 | 0.41 |
| 41:JO:226:ASN:ND2 | 43:JO:502:GDP:O6 | 2.53 | 0.41 |
| 41:KB:248:ALA:HA | 41:KB:252:LYS:HD3 | 2.02 | 0.41 |
| 40:KD:366:ASP:OD1 | 40:KD:367:LEU:N | 2.54 | 0.41 |
| 40:KF:119:LEU:HA | 40:KF:122:ILE:HB | 2.03 | 0.41 |
| 41:KL:217:LEU:HD12 | 41:KL:217:LEU:HA | 1.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KM:181:GLU:HG2 | 41:KM:182:PRO:HD3 | 2.02 | 0.41 |
| 41:KN:99:ASN:HA | 41:KN:142:GLY:N | 2.36 | 0.41 |
| 41:KO:254:ALA:O | 41:KO:258:VAL:HG22 | 2.21 | 0.41 |
| 40:LA:221:ARG:NH1 | 41:LN:325:GLU:OE1 | 2.53 | 0.41 |
| 41:LB:290:THR:HG21 | 41:LB:329:GLN:HB3 | 2.03 | 0.41 |
| 40:LG:157:LEU:HD22 | 40:LG:161:TYR:CD1 | 2.56 | 0.41 |
| 40:LH:71:GLU:HB3 | 40:LH:98:ASP:HA | 2.02 | 0.41 |
| 41:LO:170:VAL:HG21 | 41:LO:377:LEU:HD11 | 2.03 | 0.41 |
| 40:MA:228:ASN:HB3 | 42:MN:501:GTP:N2 | 2.36 | 0.41 |
| 40:MA:288:VAL:O | 40:MA:291:ILE:HG12 | 2.21 | 0.41 |
| 40:ME:101:ASN:ND2 | 40:ME:143:GLY:HA2 | 2.36 | 0.41 |
| 40:MF:174:ALA:HB1 | 40:MF:175:PRO:HD2 | 2.01 | 0.41 |
| 40:MG:324:VAL:HG11 | 41:MO:220:PRO:HD2 | 2.02 | 0.41 |
| 40:MH:279:GLU:H | 40:MH:279:GLU:HG2 | 1.50 | 0.41 |
| 42:MN:501:GTP:HO2' | 42:MN:501:GTP:HO3' | 1.62 | 0.41 |
| 41:MO:139:LEU:HA | 41:MO:139:LEU:HD12 | 1.72 | 0.41 |
| 41:MP:139:LEU:HD23 | 41:MP:170:VAL:HG13 | 2.02 | 0.41 |
| 40:NA:143:GLY:H | 42:NN:501:GTP:PA | 2.44 | 0.41 |
| 41:NB:167:PHE:CE2 | 41:NB:200:TYR:HD2 | 2.38 | 0.41 |
| 40:ND:133:GLN:H | 40:ND:133:GLN:HG2 | 1.36 | 0.41 |
| 40:ND:137:ILE:HG13 | 40:ND:168:GLU:HG2 | 2.03 | 0.41 |
| 40:ND:210:TYR:HD1 | 40:ND:222:PRO:HG2 | 1.85 | 0.41 |
| 40:ND:276:ILE:HG22 | 40:ND:280:LYS:HD2 | 2.03 | 0.41 |
| 40:ND:435:GLY:O | 40:ND:437:ASP:N | 2.54 | 0.41 |
| 40:NE:167:LEU:HG | 40:NE:252:LEU:HD12 | 2.03 | 0.41 |
| 40:NF:255:PHE:CZ | 40:NF:318:LEU:HD21 | 2.55 | 0.41 |
| 40:NG:390:LEU:HD23 | 40:NG:390:LEU:HA | 1.93 | 0.41 |
| 41:NL:183:TYR:HD2 | 41:NL:398:TYR:HE2 | 1.68 | 0.41 |
| 41:NL:385:PHE:O | 41:NL:389:PHE:HB3 | 2.21 | 0.41 |
| 41:NM:21:TRP:CZ3 | 41:NM:24:ILE:HD11 | 2.55 | 0.41 |
| 40:OA:217:LEU:HA | 40:OA:277:SER:HB3 | 2.03 | 0.41 |
| 40:OD:136:LEU:HD11 | 40:OD:239:THR:HG21 | 2.02 | 0.41 |
| 40:OD:298:PRO:HB3 | 40:OD:307:PRO:HD2 | 2.03 | 0.41 |
| 40:OF:139:HIS:ND1 | 40:OF:140:SER:O | 2.43 | 0.41 |
| 40:OH:34:GLY:O | 40:OH:35:GLN:C | 2.59 | 0.41 |
| 40:OH:125:LEU:O | 40:OH:126:ALA:C | 2.59 | 0.41 |
| 41:OL:341:PHE:HB3 | 41:OL:348:ASN:HD21 | 1.85 | 0.41 |
| 41:OM:42:LEU:HG | 41:OM:356:ILE:HD11 | 2.02 | 0.41 |
| 41:PB:328:GLU:O | 41:PB:332:ASN:HB2 | 2.20 | 0.41 |
| 40:PH:20:CYS:HA | 40:PH:232:SER:HB2 | 2.02 | 0.41 |
| 40:PH:316:CYS:O | 40:PH:376:MET:HA | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:PM:112:LEU:O | 41:PM:116:VAL:HG23 | 2.21 | 0.41 |
| 41:PP:7:LEU:HB2 | 41:PP:135:LEU:HA | 2.01 | 0.41 |
| 40:QG:205:ASP:N | 40:QG:302:MET:O | 2.48 | 0.41 |
| 40:QH:229:ARG:HD3 | 40:QH:363:VAL:HG21 | 2.02 | 0.41 |
| 41:QO:103:LYS:HA | 41:QO:107:THR:OG1 | 2.20 | 0.41 |
| 41:QP:116:VAL:O | 41:QP:119:VAL:HG13 | 2.20 | 0.41 |
| 41:QP:268:PRO:HG2 | 41:QP:300:MET:HB3 | 2.02 | 0.41 |
| 40:RA:336:LYS:O | 40:RA:339:ARG:NH2 | 2.52 | 0.41 |
| 41:RB:100:ASN:HD21 | 41:RB:103:LYS:HG3 | 1.86 | 0.41 |
| 40:RE:141:PHE:HB2 | 40:RE:173:PRO:HD3 | 2.03 | 0.41 |
| 40:RE:262:TYR:OH | 41:RM:391:ARG:O | 2.29 | 0.41 |
| 40:RI:5:ILE:O | 40:RI:135:PHE:HA | 2.21 | 0.41 |
| 41:RM:7:LEU:O | 41:RM:135:LEU:HA | 2.20 | 0.41 |
| 41:RP:4:ILE:HG13 | 41:RP:131:GLN:NE2 | 2.36 | 0.41 |
| 41:RP:51:TYR:HA | 41:RP:60:VAL:O | 2.20 | 0.41 |
| 40:SA:261:PRO:O | 40:SA:262:TYR:C | 2.59 | 0.41 |
| 40:SA:326:LYS:HD2 | 41:SB:225:LEU:HD11 | 2.03 | 0.41 |
| 40:SF:293:ASN:O | 40:SF:297:GLU:HG3 | 2.21 | 0.41 |
| 40:SG:6:SER:OG | 40:SG:8:HIS:NE2 | 2.38 | 0.41 |
| 41:SL:11:GLN:HG3 | 41:SL:72:THR:HG21 | 2.02 | 0.41 |
| 41:SL:342:VAL:HG22 | 41:SL:348:ASN:HD22 | 1.86 | 0.41 |
| 40:TA:273:ALA:HB1 | 40:TA:291:ILE:HB | 2.01 | 0.41 |
| 41:TB:130:LEU:O | 41:TB:162:ARG:NE | 2.54 | 0.41 |
| 41:TB:245:GLN:HG2 | 42:TG:501:GTP:C5 | 2.56 | 0.41 |
| 40:TE:97:GLU:HG2 | 41:TL:251:ARG:HH22 | 1.85 | 0.41 |
| 40:TF:54:SER:OG | 40:TF:64:ARG:NE | 2.52 | 0.41 |
| 40:TF:231:ILE:O | 40:TF:234:ILE:HG22 | 2.21 | 0.41 |
| 40:TI:271:THR:HG22 | 40:TI:376:MET:HB3 | 2.02 | 0.41 |
| 41:TN:19:LYS:HZ1 | 41:TN:227:HIS:HB2 | 1.84 | 0.41 |
| 41:TN:300:MET:N | 41:TN:300:MET:SD | 2.94 | 0.41 |
| 40:UA:73:THR:HG22 | 41:UN:46:ARG:HH11 | 1.85 | 0.41 |
| 40:UE:325:PRO:HG2 | 41:UM:221:THR:HA | 2.03 | 0.41 |
| 40:UF:100:ALA:O | 41:UM:255:VAL:HG11 | 2.21 | 0.41 |
| 40:UF:186:ASN:O | 40:UF:187:SER:C | 2.59 | 0.41 |
| 40:UI:35:GLN:O | 40:UI:36:MET:C | 2.59 | 0.41 |
| 40:UI:376:MET:HE3 | 40:UI:376:MET:HB3 | 1.92 | 0.41 |
| 40:UI:398:TYR:O | 40:UI:399:ALA:C | 2.59 | 0.41 |
| 40:UI:402:ALA:O | 40:UI:404:VAL:HG13 | 2.20 | 0.41 |
| 41:UM:331:LEU:HD12 | 41:UM:331:LEU:HA | 1.88 | 0.41 |
| 41:UO:55:THR:H | 41:VP:283:ALA:HA | 1.85 | 0.41 |
| 41:UP:379:LYS:HB2 | 41:UP:379:LYS:HE2 | 1.75 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UP:399:THR:O | 41:UP:402:GLY:N | 2.51 | 0.41 |
| 40:VA:3:GLU:HG3 | 40:VA:64:ARG:HH22 | 1.86 | 0.41 |
| 40:VF:301:GLN:OE1 | 40:VF:307:PRO:HG3 | 2.21 | 0.41 |
| 40:VF:324:VAL:O | 40:VF:328:VAL:HG23 | 2.21 | 0.41 |
| 40:VJ:262:TYR:HB2 | 40:VJ:265:ILE:HG12 | 2.03 | 0.41 |
| 41:VO:297:LYS:HE3 | 41:VO:297:LYS:HB2 | 1.90 | 0.41 |
| 41:VP:324:LYS:NZ | 41:VP:325:GLU:OE2 | 2.54 | 0.41 |
| 41:VQ:217:LEU:HD23 | 41:VQ:217:LEU:HA | 1.93 | 0.41 |
| 40:WA:139:HIS:O | 40:WA:170:SER:HA | 2.21 | 0.41 |
| 40:WA:256:GLN:HB2 | 41:WB:397:TRP:CH2 | 2.56 | 0.41 |
| 40:WA:431:TYR:HA | 40:WA:434:VAL:HG12 | 2.02 | 0.41 |
| 40:WE:5:ILE:HD13 | 40:WE:64:ARG:HB3 | 2.03 | 0.41 |
| 40:WE:366:ASP:OD1 | 40:WE:366:ASP:N | 2.42 | 0.41 |
| 40:WF:359:PRO:HA | 40:WF:360:PRO:HD3 | 1.93 | 0.41 |
| 40:WG:394:PHE:CD1 | 40:WG:421:ARG:HD3 | 2.55 | 0.41 |
| 41:WN:213:ARG:O | 41:WN:214:THR:C | 2.59 | 0.41 |
| 7:1T:74:LYS:H | 7:1T:74:LYS:HG2 | 1.64 | 0.41 |
| 7:1T:235:ARG:HG3 | 7:1T:236:THR:HG23 | 2.01 | 0.41 |
| 7:1T:373:PRO:CB | 10:2E:137:LYS:HG3 | 2.49 | 0.41 |
| 7:1T:485:CYS:HB3 | 7:1T:499:ILE:HB | 2.03 | 0.41 |
| 7:1U:77:VAL:HG23 | 7:1U:78:TYR:CD1 | 2.56 | 0.41 |
| 7:1U:248:LYS:HB3 | 7:1U:248:LYS:HE3 | 1.64 | 0.41 |
| 8:1X:121:GLU:O | 8:1X:122:LEU:C | 2.57 | 0.41 |
| 8:1X:147:MET:O | 8:1X:148:LYS:C | 2.59 | 0.41 |
| 8:1X:163:LEU:O | 8:1X:164:GLU:C | 2.58 | 0.41 |
| 9:2B:214:ALA:HB2 | 40:SG:58:ALA:HB2 | 2.02 | 0.41 |
| 9:2B:405:ILE:O | 9:2B:409:ASP:HB2 | 2.21 | 0.41 |
| 12:2Q:158:ASN:O | 12:2Q:160:ARG:NH1 | 2.49 | 0.41 |
| 12:2R:89:SER:OG | 41:WQ:108:GLU:OE2 | 2.34 | 0.41 |
| 13:2U:136:LEU:O | 13:2U:140:THR:HG22 | 2.20 | 0.41 |
| 13:2W:77:VAL:HA | 13:2W:132:ILE:O | 2.21 | 0.41 |
| 15:3F:30:GLN:HE21 | 15:3F:30:GLN:HA | 1.86 | 0.41 |
| 15:3G:273:ASP:OD1 | 15:3G:277:LYS:NZ | 2.53 | 0.41 |
| 15:3G:359:GLN:O | 15:3G:363:LYS:HG2 | 2.21 | 0.41 |
| 17:3P:254:LEU:HD13 | 17:3P:307:ASN:HB3 | 2.02 | 0.41 |
| 17:3R:232:ARG:HE | 17:3R:328:LEU:HD12 | 1.85 | 0.41 |
| 17:3R:326:GLN:HA | 17:3R:329:LEU:HD12 | 2.02 | 0.41 |
| 20:4A:204:GLU:HA | 20:4A:207:ARG:HE | 1.85 | 0.41 |
| 20:4A:233:HIS:O | 20:4A:234:GLN:C | 2.59 | 0.41 |
| 21:4D:307:ASN:O | 41:CB:279:GLN:NE2 | 2.54 | 0.41 |
| 21:4F:222:LYS:HD2 | 40:BE:41:THR:CG2 | 2.42 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4F:480:GLU:O | 21:4F:481:ASN:C | 2.59 | 0.41 |
| 21:4F:531:ILE:O | 21:4F:535:ILE:HB | 2.20 | 0.41 |
| 22:4J:686:LYS:HB2 | 22:4J:686:LYS:HE2 | 1.71 | 0.41 |
| 22:4K:565:VAL:HA | 22:4K:568:ALA:HB3 | 2.01 | 0.41 |
| 23:4N:235:THR:CG2 | 23:4N:240:LEU:HA | 2.51 | 0.41 |
| 23:4P:172:TYR:C | 23:4P:174:MET:H | 2.23 | 0.41 |
| 23:4Q:190:TYR:O | 23:4Q:192:PRO:N | 2.54 | 0.41 |
| 23:4R:240:LEU:CB | 23:4R:266:HIS:HA | 2.50 | 0.41 |
| 23:4R:243:LEU:HD13 | 40:DI:79:ARG:HG3 | 2.02 | 0.41 |
| 25:4T:326:SER:O | 40:JF:229:ARG:NH2 | 2.53 | 0.41 |
| 28:5B:219:LEU:O | 28:5B:223:THR:HG23 | 2.21 | 0.41 |
| 34:5Q:176:VAL:O | 34:5Q:180:ARG:HG3 | 2.21 | 0.41 |
| 36:5W:184:HIS:HA | 41:OB:279:GLN:NE2 | 2.36 | 0.41 |
| 37:6A:39:VAL:HG11 | 41:TO:36:TYR:HB3 | 2.02 | 0.41 |
| 37:6A:122:LYS:HD3 | 41:TP:94:GLN:HE21 | 1.86 | 0.41 |
| 39:6H:16:LYS:NZ | 39:6H:73:ASP:OD1 | 2.43 | 0.41 |
| 39:6I:103:LYS:HA | 39:6I:106:VAL:HG12 | 2.02 | 0.41 |
| 39:6L:80:LYS:HA | 39:6L:80:LYS:HD3 | 1.94 | 0.41 |
| 40:AE:167:LEU:HA | 40:AE:200:CYS:O | 2.20 | 0.41 |
| 41:BB:128:ASP:OD1 | 41:BB:128:ASP:N | 2.54 | 0.41 |
| 41:BB:174:LYS:HG2 | 41:BB:205:GLU:HG3 | 2.02 | 0.41 |
| 40:BE:301:GLN:H | 40:BE:301:GLN:HG2 | 1.63 | 0.41 |
| 40:BE:413:GLU:O | 40:BE:414:GLU:C | 2.58 | 0.41 |
| 40:BH:72:PRO:HA | 40:BH:94:THR:CG2 | 2.51 | 0.41 |
| 40:BH:348:PRO:HB2 | 41:BP:384:GLN:OE1 | 2.20 | 0.41 |
| 40:BI:87:PHE:O | 40:BI:88:HIS:C | 2.58 | 0.41 |
| 40:BI:185:TYR:CD2 | 40:BI:417:PHE:HE1 | 2.38 | 0.41 |
| 40:BI:199:ASP:OD2 | 40:BI:199:ASP:N | 2.53 | 0.41 |
| 41:BM:167:PHE:CE2 | 41:BM:233:MET:HG2 | 2.56 | 0.41 |
| 41:BO:16:ILE:HG13 | 41:BO:226:ASN:OD1 | 2.21 | 0.41 |
| 41:BO:21:TRP:CZ3 | 41:BO:61:PRO:HB3 | 2.55 | 0.41 |
| 41:BP:385:PHE:HZ | 41:BP:408:PHE:HD2 | 1.68 | 0.41 |
| 40:CA:23:LEU:O | 40:CA:27:GLU:HG3 | 2.21 | 0.41 |
| 40:CA:215:ARG:HE | 40:CA:215:ARG:HB2 | 1.61 | 0.41 |
| 40:CA:382:ALA:C | 40:CA:384:ALA:H | 2.24 | 0.41 |
| 41:CB:26:ASP:OD1 | 41:CB:359:ARG:NH1 | 2.54 | 0.41 |
| 41:CN:180:VAL:HG13 | 41:CN:184:ASN:HB2 | 2.03 | 0.41 |
| 41:CO:218:THR:C | 41:CO:220:PRO:HD3 | 2.40 | 0.41 |
| 41:CO:258:VAL:HG12 | 41:CO:264:HIS:HA | 2.03 | 0.41 |
| 41:CP:84:ILE:O | 41:CP:85:PHE:C | 2.59 | 0.41 |
| 40:DA:124:LYS:HE3 | 40:DA:124:LYS:HB2 | 1.38 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DA:220:GLU:HB3 | 40:DA:221:ARG:H | 1.74 | 0.41 |
| 40:DA:235:VAL:O | 40:DA:239:THR:HG22 | 2.20 | 0.41 |
| 40:DA:273:ALA:HB3 | 40:DA:274:PRO:CD | 2.51 | 0.41 |
| 41:DB:42:LEU:HG | 41:DB:42:LEU:H | 1.53 | 0.41 |
| 40:DE:120:ASP:O | 40:DE:123:ARG:HB2 | 2.21 | 0.41 |
| 40:DF:110:ILE:HG23 | 40:DF:110:ILE:O | 2.21 | 0.41 |
| 40:DF:326:LYS:HE2 | 41:DN:208:TYR:CD1 | 2.55 | 0.41 |
| 40:DF:332:ILE:O | 40:DF:335:ILE:HB | 2.21 | 0.41 |
| 40:DH:68:VAL:HG21 | 40:DH:149:PHE:CE2 | 2.56 | 0.41 |
| 40:DH:250:VAL:HG23 | 40:DH:254:GLU:CB | 2.47 | 0.41 |
| 40:DH:258:ASN:HB3 | 41:DP:179:VAL:CG1 | 2.51 | 0.41 |
| 40:DH:259:LEU:HD21 | 40:DH:377:LEU:O | 2.21 | 0.41 |
| 40:DH:332:ILE:O | 40:DH:335:ILE:HB | 2.20 | 0.41 |
| 40:DI:160:ASP:O | 40:DI:162:GLY:N | 2.54 | 0.41 |
| 41:DM:388:MET:HE2 | 41:DM:388:MET:HB2 | 1.82 | 0.41 |
| 41:DP:257:MET:HE1 | 41:DP:314:ALA:HB2 | 2.02 | 0.41 |
| 41:DP:425:ARG:H | 41:DP:425:ARG:HG2 | 1.63 | 0.41 |
| 40:EA:326:LYS:HE3 | 41:EB:208:TYR:HB2 | 2.03 | 0.41 |
| 41:EB:138:SER:HA | 41:EB:169:VAL:HB | 2.02 | 0.41 |
| 40:EF:217:LEU:HA | 40:EF:277:SER:HB2 | 2.02 | 0.41 |
| 40:EF:238:ILE:HD11 | 40:EF:377:LEU:HD11 | 2.03 | 0.41 |
| 40:EI:291:ILE:HD11 | 40:EI:319:TYR:HD1 | 1.86 | 0.41 |
| 41:EL:260:PHE:HE2 | 41:EL:425:ARG:HD3 | 1.86 | 0.41 |
| 41:EM:183:TYR:CZ | 41:EM:388:MET:HB3 | 2.55 | 0.41 |
| 40:FA:105:ARG:HA | 40:FA:109:THR:HG23 | 2.02 | 0.41 |
| 40:FA:304:LYS:O | 40:FA:305:CYS:C | 2.59 | 0.41 |
| 41:FB:246:LEU:HD11 | 40:FG:179:THR:HG21 | 2.03 | 0.41 |
| 40:FF:222:PRO:O | 41:FM:322:SER:HB2 | 2.20 | 0.41 |
| 40:FG:405:HIS:HA | 40:FG:408:VAL:HG12 | 2.02 | 0.41 |
| 41:FM:246:LEU:HD21 | 42:FM:501:GTP:H8 | 1.85 | 0.41 |
| 41:FO:61:PRO:HD3 | 41:FO:84:ILE:HG12 | 2.01 | 0.41 |
| 40:GE:171:ILE:HG12 | 40:GE:171:ILE:H | 1.75 | 0.41 |
| 40:GE:393:LYS:O | 40:GE:396:LEU:HB2 | 2.21 | 0.41 |
| 40:GE:432:GLU:O | 40:GE:433:GLU:C | 2.59 | 0.41 |
| 40:GF:316:CYS:SG | 40:GF:377:LEU:HB2 | 2.61 | 0.41 |
| 40:GH:70:LEU:HD13 | 40:GH:110:ILE:HD12 | 2.01 | 0.41 |
| 40:GH:126:ALA:O | 40:GH:127:ASP:C | 2.58 | 0.41 |
| 40:GI:56:THR:HG22 | 40:GI:60:LYS:H | 1.84 | 0.41 |
| 40:GI:85:GLN:H | 40:GI:85:GLN:HG2 | 1.65 | 0.41 |
| 40:GI:172:TYR:CE2 | 40:GI:386:ALA:HB1 | 2.56 | 0.41 |
| 41:GM:87:PRO:HD3 | 41:HM:281:TYR:HD2 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:GM:396:HIS:HA | 41:GM:399:THR:HG22 | 2.02 | 0.41 |
| 41:GN:12:CYS:O | 41:GN:16:ILE:HG13 | 2.21 | 0.41 |
| 41:GN:217:LEU:HA | 41:GN:217:LEU:HD22 | 1.63 | 0.41 |
| 41:GP:324:LYS:HE2 | 41:GP:324:LYS:HB2 | 1.51 | 0.41 |
| 40:HE:57:GLY:O | 40:HE:59:GLY:N | 2.53 | 0.41 |
| 40:HE:400:LYS:H | 40:HE:400:LYS:HG2 | 1.68 | 0.41 |
| 40:HF:107:HIS:ND1 | 40:HF:151:SER:OG | 2.39 | 0.41 |
| 40:HF:312:TYR:CE2 | 40:HF:341:ILE:HG23 | 2.56 | 0.41 |
| 40:HG:97:GLU:HG2 | 40:HG:105:ARG:HH22 | 1.86 | 0.41 |
| 40:HG:157:LEU:HD23 | 40:HG:157:LEU:HA | 1.94 | 0.41 |
| 41:HN:273:LEU:HD12 | 41:HN:273:LEU:HA | 1.71 | 0.41 |
| 41:HO:20:PHE:HA | 41:HO:230:SER:OG | 2.21 | 0.41 |
| 41:HO:294:PHE:CG | 41:HO:333:VAL:HG21 | 2.56 | 0.41 |
| 41:HP:211:CYS:HA | 41:HP:215:LEU:HD12 | 2.03 | 0.41 |
| 40:IA:209:ILE:HA | 40:IA:212:ILE:HG22 | 2.02 | 0.41 |
| 40:IE:7:VAL:HG13 | 40:IE:66:VAL:HG13 | 2.02 | 0.41 |
| 40:IE:286:LEU:HD23 | 40:IE:370:VAL:HG13 | 2.02 | 0.41 |
| 40:IF:407:TYR:CD1 | 40:IF:412:MET:HG3 | 2.54 | 0.41 |
| 40:IG:7:VAL:HG13 | 40:IG:66:VAL:HG23 | 2.02 | 0.41 |
| 40:IG:109:THR:HG21 | 40:IG:410:GLU:OE2 | 2.20 | 0.41 |
| 40:IH:297:GLU:HA | 40:IH:298:PRO:HD3 | 1.86 | 0.41 |
| 40:JA:274:PRO:HD2 | 40:JA:291:ILE:HG23 | 2.03 | 0.41 |
| 41:JB:318:ARG:HB2 | 41:JB:364:SER:OG | 2.21 | 0.41 |
| 40:JD:151:SER:HB2 | 40:JD:193:THR:HG21 | 2.03 | 0.41 |
| 40:JD:202:PHE:CE1 | 40:JD:377:LEU:HD13 | 2.56 | 0.41 |
| 40:JD:376:MET:SD | 40:JD:378:SER:HB3 | 2.61 | 0.41 |
| 40:JF:224:TYR:HE2 | 41:JM:323:MET:HB2 | 1.86 | 0.41 |
| 40:JF:261:PRO:HG3 | 41:JN:394:PHE:HE1 | 1.86 | 0.41 |
| 40:JH:366:ASP:OD1 | 40:JH:367:LEU:N | 2.54 | 0.41 |
| 41:JM:174:LYS:HB2 | 41:JM:174:LYS:HE3 | 1.77 | 0.41 |
| 41:JM:388:MET:O | 41:JM:391:ARG:N | 2.54 | 0.41 |
| 41:JM:393:ALA:O | 41:JM:395:LEU:N | 2.54 | 0.41 |
| 41:JN:21:TRP:CD1 | 41:JN:85:PHE:HE1 | 2.39 | 0.41 |
| 41:KB:42:LEU:HD22 | 41:KB:243:PRO:HG3 | 2.03 | 0.41 |
| 40:KH:185:TYR:HE2 | 40:KH:404:VAL:HG22 | 1.86 | 0.41 |
| 40:KH:326:LYS:HD3 | 41:KP:208:TYR:CD1 | 2.56 | 0.41 |
| 41:KL:31:ASP:HB2 | 41:KL:32:PRO:CD | 2.42 | 0.41 |
| 41:KL:317:PHE:HB3 | 41:KL:321:MET:SD | 2.60 | 0.41 |
| 41:KN:254:ALA:O | 41:KN:258:VAL:HG12 | 2.20 | 0.41 |
| 40:LA:100:ALA:O | 41:LN:255:VAL:HG11 | 2.21 | 0.41 |
| 40:LE:167:LEU:HD22 | 40:LE:200:CYS:HB3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:LE:345:ASP:OD1 | 40:LE:345:ASP:N | 2.54 | 0.41 |
| 40:LF:114:LEU:HD23 | 40:LF:114:LEU:HA | 1.86 | 0.41 |
| 41:LO:198:GLU:OE1 | 41:LO:200:TYR:OH | 2.32 | 0.41 |
| 41:LP:413:SER:O | 41:LP:417:ASP:HB2 | 2.20 | 0.41 |
| 41:MB:105:HIS:CD2 | 41:MB:150:LEU:HB2 | 2.55 | 0.41 |
| 40:MF:324:VAL:HG12 | 40:MF:326:LYS:H | 1.86 | 0.41 |
| 40:MG:185:TYR:O | 40:MG:186:ASN:C | 2.59 | 0.41 |
| 40:MH:36:MET:O | 40:MH:37:PRO:C | 2.59 | 0.41 |
| 40:MH:37:PRO:O | 40:MH:38:SER:C | 2.59 | 0.41 |
| 40:MH:249:ASN:HD22 | 40:MH:249:ASN:HA | 1.59 | 0.41 |
| 41:ML:183:TYR:HE2 | 41:ML:394:PHE:HB2 | 1.85 | 0.41 |
| 40:ND:269:LEU:CD2 | 40:ND:380:THR:HG22 | 2.50 | 0.41 |
| 40:ND:363:VAL:O | 40:ND:365:GLY:N | 2.54 | 0.41 |
| 40:NG:107:HIS:ND1 | 40:NG:152:LEU:HB2 | 2.36 | 0.41 |
| 40:NG:141:PHE:O | 40:NG:187:SER:OG | 2.39 | 0.41 |
| 40:NH:115:ILE:HA | 40:NH:118:VAL:HG22 | 2.01 | 0.41 |
| 41:NL:270:PHE:CE2 | 41:NL:272:PRO:HD2 | 2.56 | 0.41 |
| 41:NM:7:LEU:O | 41:NM:135:LEU:HA | 2.20 | 0.41 |
| 41:NN:392:LYS:HD3 | 41:NN:395:LEU:HD23 | 2.03 | 0.41 |
| 41:NO:39:ASP:N | 41:NO:39:ASP:OD1 | 2.53 | 0.41 |
| 41:NP:139:LEU:HG | 41:NP:168:SER:HB2 | 2.01 | 0.41 |
| 41:NP:172:SER:OG | 41:NP:175:VAL:O | 2.39 | 0.41 |
| 41:NP:318:ARG:HB2 | 41:NP:354:CYS:HB3 | 2.03 | 0.41 |
| 40:OA:336:LYS:HD3 | 40:OA:343:PHE:HE2 | 1.85 | 0.41 |
| 40:OD:260:VAL:HG12 | 40:OD:266:HIS:HA | 2.03 | 0.41 |
| 40:OD:384:ALA:HA | 40:OD:387:TRP:CD1 | 2.55 | 0.41 |
| 40:OF:286:LEU:N | 40:OF:290:GLU:OE2 | 2.54 | 0.41 |
| 40:OG:137:ILE:HB | 40:OG:168:GLU:HG2 | 2.03 | 0.41 |
| 40:OH:385:GLU:O | 40:OH:388:ALA:HB3 | 2.21 | 0.41 |
| 40:OH:401:ARG:O | 40:OH:404:VAL:HB | 2.21 | 0.41 |
| 41:OO:309:ARG:H | 41:OO:372:THR:HG1 | 1.61 | 0.41 |
| 41:PB:287:PRO:O | 41:PB:291:GLN:HG2 | 2.20 | 0.41 |
| 40:PG:234:ILE:HD11 | 40:PG:272:TYR:HB2 | 2.03 | 0.41 |
| 40:PH:260:VAL:HG13 | 41:PP:397:TRP:NE1 | 2.35 | 0.41 |
| 41:PL:5:VAL:HG22 | 41:PL:62:ARG:HD2 | 2.02 | 0.41 |
| 41:PM:163:ILE:HG13 | 41:PM:251:ARG:HG3 | 2.02 | 0.41 |
| 41:PM:398:TYR:HB3 | 41:PM:403:MET:HG3 | 2.01 | 0.41 |
| 41:QB:46:ARG:HD3 | 41:QB:46:ARG:HA | 1.82 | 0.41 |
| 40:QE:11:GLN:OE1 | 41:QL:246:LEU:N | 2.54 | 0.41 |
| 40:QE:114:LEU:O | 40:QE:118:VAL:HG23 | 2.20 | 0.41 |
| 40:QH:2:ARG:NH2 | 41:QP:69:GLU:OE2 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QM:331:LEU:HD13 | 41:QM:334:GLN:HG3 | 2.02 | 0.41 |
| 41:QN:108:GLU:O | 41:QN:111:GLU:HG3 | 2.20 | 0.41 |
| 41:QP:67:ASP:HB3 | 41:QP:73:MET:CE | 2.51 | 0.41 |
| 41:QP:363:MET:HE3 | 41:QP:363:MET:HB3 | 1.91 | 0.41 |
| 40:RA:324:VAL:HA | 40:RA:325:PRO:HD3 | 1.97 | 0.41 |
| 40:RE:85:GLN:O | 40:SE:283:HIS:CE1 | 2.73 | 0.41 |
| 40:RG:21:TRP:CH2 | 40:RG:63:PRO:HB3 | 2.56 | 0.41 |
| 40:RG:172:TYR:OH | 40:RG:386:ALA:O | 2.39 | 0.41 |
| 40:RG:215:ARG:NH2 | 40:RG:300:ASN:OD1 | 2.46 | 0.41 |
| 41:RP:19:LYS:O | 41:RP:22:GLU:HG3 | 2.21 | 0.41 |
| 40:SA:100:ALA:O | 41:SN:255:VAL:HG21 | 2.20 | 0.41 |
| 40:SA:265:ILE:HG13 | 40:SA:379:ASN:HD21 | 1.85 | 0.41 |
| 40:SE:88:HIS:HA | 40:SE:89:PRO:HD3 | 1.93 | 0.41 |
| 40:SE:418:SER:O | 40:SE:421:ARG:N | 2.54 | 0.41 |
| 40:SI:70:LEU:HG | 40:SI:145:THR:HG23 | 2.02 | 0.41 |
| 40:SI:231:ILE:HA | 40:SI:234:ILE:HD12 | 2.03 | 0.41 |
| 41:SN:153:SER:HB3 | 41:SN:191:GLN:HE21 | 1.85 | 0.41 |
| 41:SN:316:VAL:HB | 41:SN:366:THR:HB | 2.02 | 0.41 |
| 41:SO:97:ALA:HB1 | 41:SO:143:THR:H | 1.86 | 0.41 |
| 40:TA:224:TYR:HB3 | 42:TN:501:GTP:N1 | 2.36 | 0.41 |
| 40:TA:412:MET:HE3 | 40:TA:412:MET:HB3 | 1.98 | 0.41 |
| 41:TB:313:VAL:HG13 | 41:TB:367:PHE:HE1 | 1.86 | 0.41 |
| 40:TE:140:SER:OG | 42:TL:501:GTP:O2A | 2.33 | 0.41 |
| 40:TI:273:ALA:HB1 | 40:TI:291:ILE:HG23 | 2.03 | 0.41 |
| 41:TP:21:TRP:O | 41:TP:25:SER:OG | 2.31 | 0.41 |
| 40:UF:212:ILE:H | 40:UF:212:ILE:HG12 | 1.42 | 0.41 |
| 40:UF:436:MET:H | 40:UF:436:MET:HG2 | 1.58 | 0.41 |
| 40:UI:96:LYS:HG3 | 41:UP:1:MET:H3 | 1.86 | 0.41 |
| 40:UI:149:PHE:HD1 | 40:UI:149:PHE:HA | 1.72 | 0.41 |
| 40:UI:359:PRO:O | 40:UI:360:PRO:C | 2.58 | 0.41 |
| 41:UM:16:ILE:HD11 | 41:UM:136:THR:HB | 2.01 | 0.41 |
| 41:UO:270:PHE:CE2 | 41:UO:272:PRO:HD2 | 2.56 | 0.41 |
| 41:UP:47:ILE:C | 41:UP:49:VAL:H | 2.24 | 0.41 |
| 41:UP:51:TYR:HB3 | 41:UP:59:TYR:HB3 | 2.02 | 0.41 |
| 40:VA:172:TYR:CD1 | 40:VA:173:PRO:HD2 | 2.56 | 0.41 |
| 40:VA:387:TRP:HB3 | 40:VA:424:MET:HE2 | 2.02 | 0.41 |
| 40:WF:11:GLN:NE2 | 41:WM:246:LEU:H | 2.18 | 0.41 |
| 40:WF:235:VAL:HA | 40:WF:238:ILE:HG12 | 2.01 | 0.41 |
| 40:WF:258:ASN:HB3 | 40:WF:352:LYS:HD2 | 2.03 | 0.41 |
| 40:WG:10:GLY:HA2 | 40:WG:145:THR:HG23 | 2.02 | 0.41 |
| 40:WG:188:ILE:HG21 | 40:WG:394:PHE:CD2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:WH:96:LYS:HD2 | 40:WH:96:LYS:HA | 1.77 | 0.41 |
| 40:WH:401:ARG:HA | 40:WH:401:ARG:HD3 | 1.74 | 0.41 |
| 40:WI:132:LEU:HD23 | 40:WI:164:LYS:HE2 | 2.02 | 0.41 |
| 40:WI:245:ASP:OD1 | 40:WI:245:ASP:N | 2.53 | 0.41 |
| 41:WM:112:LEU:HD12 | 41:WM:112:LEU:HA | 1.91 | 0.41 |
| 41:WM:422:VAL:O | 41:WM:426:GLY:N | 2.53 | 0.41 |
| 41:WN:89:ASN:HD22 | 41:WN:89:ASN:N | 2.19 | 0.41 |
| 41:WN:100:ASN:HB3 | 41:WN:103:LYS:HG3 | 2.03 | 0.41 |
| 41:WO:326:VAL:O | 41:WO:330:MET:HG2 | 2.20 | 0.41 |
| 41:WP:132:GLY:HA2 | 41:WP:162:ARG:HB3 | 2.02 | 0.41 |
| 41:WQ:7:LEU:O | 41:WQ:135:LEU:HA | 2.21 | 0.41 |
| 4:1H:33:ARG:HG2 | 41:GN:404:ASP:CG | 2.41 | 0.41 |
| 6:1P:263:ASP:HB3 | 7:1T:303:HIS:CE1 | 2.56 | 0.41 |
| 7:1T:13:LYS:HZ1 | 7:1T:614:TRP:HZ3 | 1.69 | 0.41 |
| 7:1T:413:SER:O | 7:1T:414:ASN:C | 2.59 | 0.41 |
| 7:1T:552:ASP:HB3 | 7:1T:595:ILE:HD12 | 2.03 | 0.41 |
| 7:1U:167:SER:OG | 7:1U:168:GLN:N | 2.54 | 0.41 |
| 7:1U:442:ARG:HH11 | 7:1U:453:LEU:HD11 | 1.85 | 0.41 |
| 8:1W:420:LYS:O | 8:1W:424:GLU:HG2 | 2.21 | 0.41 |
| 8:1Z:451:GLN:O | 8:1Z:455:ILE:HG12 | 2.20 | 0.41 |
| 9:2B:66:ARG:HA | 9:2B:66:ARG:NH1 | 2.35 | 0.41 |
| 9:2B:154:PHE:CG | 9:2C:475:ARG:HD3 | 2.55 | 0.41 |
| 9:2B:184:TRP:CZ2 | 41:TO:362:LYS:HG2 | 2.55 | 0.41 |
| 9:2B:303:LYS:HG2 | 41:TN:359:ARG:NH2 | 2.36 | 0.41 |
| 9:2B:394:ARG:NH2 | 41:TL:362:LYS:HG2 | 2.36 | 0.41 |
| 10:2G:162:LYS:HE3 | 10:2G:168:PHE:CE1 | 2.56 | 0.41 |
| 11:2K:209:LYS:HA | 11:2K:209:LYS:HD2 | 1.42 | 0.41 |
| 12:2O:108:TYR:O | 12:2O:109:LEU:C | 2.59 | 0.41 |
| 12:2R:197:LEU:HD12 | 12:2R:225:ILE:HG12 | 2.02 | 0.41 |
| 13:2U:54:VAL:HA | 13:2U:158:ALA:HB3 | 2.03 | 0.41 |
| 13:2U:178:PRO:O | 13:2U:181:PHE:N | 2.44 | 0.41 |
| 13:2V:83:LEU:O | 13:2V:84:LYS:C | 2.59 | 0.41 |
| 13:2V:169:ASP:OD1 | 13:2V:169:ASP:N | 2.54 | 0.41 |
| 13:2W:95:ASP:HB3 | 13:2W:146:THR:HB | 2.02 | 0.41 |
| 13:2X:134:PHE:HE1 | 13:2X:139:PHE:CG | 2.37 | 0.41 |
| 13:2X:169:ASP:OD1 | 13:2X:169:ASP:N | 2.54 | 0.41 |
| 14:3C:24:LEU:O | 40:MG:339:ARG:NE | 2.54 | 0.41 |
| 15:3F:138:LYS:HA | 15:3F:138:LYS:HD3 | 1.81 | 0.41 |
| 15:3H:180:THR:HA | 15:3H:183:THR:HG22 | 2.03 | 0.41 |
| 17:3Q:351:ILE:HD13 | 17:3Q:474:MET:HE2 | 2.03 | 0.41 |
| 17:3R:150:VAL:HG13 | 17:3R:269:ASP:OD2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:3R:253:GLU:O | 17:3R:254:LEU:C | 2.59 | 0.41 |
| 18:3T:51:TYR:N | 18:3W:167:LEU:O | 2.49 | 0.41 |
| 18:3T:411:ASN:HA | 18:3T:414:LYS:HB2 | 2.02 | 0.41 |
| 18:3W:135:LYS:HZ1 | 18:3W:198:VAL:N | 2.19 | 0.41 |
| 21:4D:244:ARG:HB2 | 40:CA:41:THR:HG21 | 2.02 | 0.41 |
| 21:4D:439:VAL:O | 21:4D:440:LEU:C | 2.60 | 0.41 |
| 21:4D:477:SER:O | 21:4D:478:SER:C | 2.59 | 0.41 |
| 21:4E:255:MET:H | 21:4E:255:MET:CE | 2.34 | 0.41 |
| 22:4H:126:PRO:HD3 | 41:BL:277:GLY:HA3 | 2.02 | 0.41 |
| 22:4H:236:TRP:CE3 | 22:4H:247:ARG:HD2 | 2.56 | 0.41 |
| 22:4I:95:GLU:HB2 | 22:4I:195:PRO:HG2 | 2.02 | 0.41 |
| 22:4I:122:ASN:HB2 | 22:4I:200:ARG:HD3 | 2.02 | 0.41 |
| 22:4I:638:LEU:HA | 22:4I:638:LEU:HD13 | 1.77 | 0.41 |
| 22:4I:686:LYS:HA | 22:4I:686:LYS:HD3 | 1.78 | 0.41 |
| 22:4I:698:ASN:HD22 | 22:4I:698:ASN:HA | 1.58 | 0.41 |
| 22:4J:663:LYS:O | 22:4J:664:SER:C | 2.59 | 0.41 |
| 22:4K:548:ALA:HA | 22:4K:598:GLU:OE2 | 2.20 | 0.41 |
| 22:4K:615:ASP:O | 22:4K:617:CYS:N | 2.54 | 0.41 |
| 22:4K:649:LYS:HD3 | 22:4K:649:LYS:HA | 1.46 | 0.41 |
| 23:4M:38:GLY:O | 23:4M:39:GLN:C | 2.59 | 0.41 |
| 23:4M:109:CYS:O | 23:4M:110:ASN:C | 2.60 | 0.41 |
| 23:4M:187:PHE:CZ | 23:4M:189:GLY:HA3 | 2.56 | 0.41 |
| 23:4N:15:ASN:O | 23:4N:16:PRO:C | 2.59 | 0.41 |
| 23:4N:257:PHE:HB3 | 41:EM:322:SER:HB2 | 2.01 | 0.41 |
| 24:4O:236:TYR:HA | 24:4O:267:ASP:HA | 2.03 | 0.41 |
| 24:4O:259:ARG:HB3 | 24:4O:260:THR:H | 1.75 | 0.41 |
| 23:4P:197:LEU:HA | 23:4P:197:LEU:HD12 | 1.76 | 0.41 |
| 23:4Q:237:PRO:O | 23:4Q:239:ASN:N | 2.54 | 0.41 |
| 25:4T:299:PHE:O | 25:4T:302:ARG:NH1 | 2.52 | 0.41 |
| 26:4V:299:MET:HA | 26:4V:351:ILE:HG23 | 2.03 | 0.41 |
| 26:4W:140:HIS:HE1 | 26:4W:146:LEU:HA | 1.86 | 0.41 |
| 26:4W:337:LEU:HD21 | 26:4W:338:ARG:HH21 | 1.86 | 0.41 |
| 28:5B:198:PHE:CE2 | 40:KH:44:GLY:HA3 | 2.56 | 0.41 |
| 31:5I:496:VAL:O | 40:IH:372:ARG:NH2 | 2.42 | 0.41 |
| 33:5N:244:TYR:HB3 | 40:HH:369:LYS:NZ | 2.36 | 0.41 |
| 36:5W:72:ARG:HD3 | 40:OF:279:GLU:HG2 | 2.02 | 0.41 |
| 37:6A:92:ILE:HG13 | 40:TH:22:GLU:HG3 | 2.02 | 0.41 |
| 38:6C:44:ARG:HD3 | 38:6C:45:GLN:H | 1.86 | 0.41 |
| 38:6D:258:TYR:HB2 | 40:UE:161:TYR:CE1 | 2.56 | 0.41 |
| 40:AA:261:PRO:HG3 | 40:AA:313:MET:SD | 2.61 | 0.41 |
| 41:AB:292:GLN:NE2 | 41:AB:298:ASN:HD21 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:AF:26:LEU:HD21 | 40:AF:363:VAL:HG12 | 2.03 | 0.41 |
| 40:AF:298:PRO:HB2 | 40:AF:308:ARG:HH21 | 1.86 | 0.41 |
| 40:AG:88:HIS:HB2 | 40:BG:283:HIS:HB3 | 2.02 | 0.41 |
| 40:AG:138:PHE:HZ | 40:AG:235:VAL:HG11 | 1.86 | 0.41 |
| 40:AH:42:ILE:HG23 | 40:AH:43:GLY:H | 1.86 | 0.41 |
| 40:AH:72:PRO:O | 40:AH:73:THR:OG1 | 2.35 | 0.41 |
| 40:AH:239:THR:O | 40:AH:243:ARG:NE | 2.50 | 0.41 |
| 41:AM:20:PHE:HA | 41:AM:230:SER:HB2 | 2.02 | 0.41 |
| 41:AN:6:HIS:HD2 | 41:AN:134:GLN:NE2 | 2.19 | 0.41 |
| 41:AO:3:GLU:HB3 | 41:AO:62:ARG:NH1 | 2.36 | 0.41 |
| 41:AO:33:THR:OG1 | 41:AO:34:GLY:N | 2.54 | 0.41 |
| 41:AO:252:LYS:HE3 | 41:AO:350:LYS:NZ | 2.35 | 0.41 |
| 41:AO:321:MET:HE3 | 41:AO:321:MET:HB3 | 1.95 | 0.41 |
| 40:BA:294:ALA:O | 40:BA:300:ASN:ND2 | 2.54 | 0.41 |
| 41:BB:6:HIS:HB3 | 41:BB:21:TRP:HZ2 | 1.86 | 0.41 |
| 41:BB:19:LYS:HD2 | 41:BB:19:LYS:HA | 1.34 | 0.41 |
| 41:BB:117:LEU:O | 41:BB:120:VAL:HG12 | 2.20 | 0.41 |
| 41:BB:150:LEU:O | 41:BB:151:LEU:C | 2.58 | 0.41 |
| 41:BB:174:LYS:HB2 | 41:BB:175:VAL:H | 1.65 | 0.41 |
| 41:BB:362:LYS:O | 41:BB:363:MET:HB2 | 2.20 | 0.41 |
| 40:BE:9:VAL:HG13 | 40:BE:68:VAL:HG13 | 2.03 | 0.41 |
| 40:BE:109:THR:HG23 | 40:BE:110:ILE:H | 1.84 | 0.41 |
| 40:BE:129:CYS:SG | 40:BE:132:LEU:HB2 | 2.60 | 0.41 |
| 40:BE:252:LEU:HD23 | 40:BE:252:LEU:HA | 1.85 | 0.41 |
| 40:BE:333:ALA:O | 40:BE:337:THR:HG23 | 2.20 | 0.41 |
| 40:BF:115:ILE:HG13 | 40:BF:119:LEU:HD23 | 2.01 | 0.41 |
| 40:BF:370:VAL:HG12 | 40:BF:372:ARG:H | 1.85 | 0.41 |
| 40:BG:51:THR:HG21 | 40:BG:243:ARG:HG2 | 2.03 | 0.41 |
| 40:BG:79:ARG:HG2 | 40:BG:92:LEU:HD13 | 2.02 | 0.41 |
| 40:BG:208:ALA:HA | 40:BG:304:LYS:HZ3 | 1.83 | 0.41 |
| 40:BG:255:PHE:CZ | 40:BG:318:LEU:HD21 | 2.55 | 0.41 |
| 40:BH:72:PRO:O | 40:BH:74:VAL:N | 2.54 | 0.41 |
| 40:BH:221:ARG:HB2 | 41:BO:322:SER:CB | 2.51 | 0.41 |
| 40:BH:329:ASN:ND2 | 41:BP:175:VAL:HG22 | 2.36 | 0.41 |
| 40:BI:36:MET:HG2 | 40:BI:61:HIS:CE1 | 2.56 | 0.41 |
| 40:BI:195:LEU:HD12 | 40:BI:266:HIS:HE1 | 1.86 | 0.41 |
| 41:BL:257:MET:HE3 | 41:BL:312:THR:HG23 | 2.03 | 0.41 |
| 41:BM:173:PRO:HD3 | 41:BM:380:ARG:NH1 | 2.35 | 0.41 |
| 41:BO:132:GLY:HA3 | 41:BO:163:ILE:O | 2.20 | 0.41 |
| 41:BO:211:CYS:HA | 41:BO:215:LEU:HB2 | 2.02 | 0.41 |
| 41:BO:258:VAL:HG22 | 41:BO:266:PHE:CZ | 2.42 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BO:293:MET:HG2 | 41:BO:294:PHE:CD1 | 2.56 | 0.41 |
| 41:BO:320:ARG:HD2 | 41:BO:320:ARG:HA | 1.31 | 0.41 |
| 40:CA:144:GLY:O | 40:CA:145:THR:C | 2.58 | 0.41 |
| 40:CA:226:ASN:N | 40:CA:226:ASN:OD1 | 2.54 | 0.41 |
| 41:CB:21:TRP:CE3 | 41:CB:24:ILE:HD11 | 2.56 | 0.41 |
| 41:CB:258:VAL:HG23 | 40:CG:406:TRP:HE1 | 1.85 | 0.41 |
| 40:CE:102:ASN:HB3 | 40:CE:105:ARG:HB2 | 2.03 | 0.41 |
| 40:CE:195:LEU:HD21 | 40:CE:264:ARG:HE | 1.84 | 0.41 |
| 40:CF:132:LEU:HD22 | 40:CF:164:LYS:HE3 | 2.02 | 0.41 |
| 40:CF:228:ASN:ND2 | 42:CF:501:GTP:HN1 | 2.08 | 0.41 |
| 40:CH:222:PRO:HD2 | 41:CO:324:LYS:CG | 2.50 | 0.41 |
| 40:CH:400:LYS:O | 40:CH:402:ALA:N | 2.54 | 0.41 |
| 41:CL:40:SER:HB2 | 41:CL:43:GLN:HG3 | 2.01 | 0.41 |
| 41:CL:165:ASN:CA | 41:CL:198:GLU:HB3 | 2.50 | 0.41 |
| 41:CM:54:ALA:O | 41:CM:55:THR:C | 2.59 | 0.41 |
| 41:CM:257:MET:CE | 41:CM:314:ALA:HB2 | 2.50 | 0.41 |
| 41:CN:19:LYS:C | 41:CN:21:TRP:H | 2.23 | 0.41 |
| 41:CO:373:ALA:C | 41:CO:375:GLN:N | 2.73 | 0.41 |
| 41:CP:36:TYR:CE2 | 41:CP:44:LEU:HD11 | 2.56 | 0.41 |
| 41:CP:322:SER:O | 41:CP:325:GLU:HG3 | 2.21 | 0.41 |
| 40:DA:5:ILE:HD11 | 40:DA:129:CYS:SG | 2.61 | 0.41 |
| 40:DA:49:PHE:O | 40:DA:50:ASN:C | 2.59 | 0.41 |
| 40:DA:274:PRO:HG3 | 40:DA:373:ALA:HB2 | 2.02 | 0.41 |
| 40:DA:416:GLU:O | 40:DA:417:PHE:C | 2.59 | 0.41 |
| 41:DB:21:TRP:HZ2 | 41:DB:63:ALA:HB2 | 1.86 | 0.41 |
| 41:DB:87:PRO:HB2 | 41:DB:88:ASP:H | 1.63 | 0.41 |
| 40:DE:12:ALA:HB2 | 42:DE:501:GTP:N9 | 2.36 | 0.41 |
| 40:DE:129:CYS:O | 40:DE:131:GLY:N | 2.53 | 0.41 |
| 40:DE:139:HIS:CE1 | 40:DE:168:GLU:HB3 | 2.56 | 0.41 |
| 40:DE:164:LYS:O | 40:DE:165:SER:C | 2.58 | 0.41 |
| 40:DE:213:CYS:C | 40:DE:215:ARG:N | 2.75 | 0.41 |
| 40:DE:307:PRO:O | 40:DE:310:GLY:N | 2.48 | 0.41 |
| 40:DE:421:ARG:HA | 40:DE:421:ARG:HD2 | 1.45 | 0.41 |
| 40:DF:26:LEU:HD12 | 40:DF:26:LEU:HA | 1.90 | 0.41 |
| 40:DF:195:LEU:HD11 | 40:DF:427:LEU:HD22 | 2.02 | 0.41 |
| 40:DF:255:PHE:HE1 | 40:DF:318:LEU:HD21 | 1.86 | 0.41 |
| 40:DF:395:ASP:C | 40:DF:397:MET:N | 2.75 | 0.41 |
| 40:DG:352:LYS:HE2 | 41:DO:178:THR:HA | 2.02 | 0.41 |
| 40:DH:254:GLU:O | 40:DH:255:PHE:C | 2.59 | 0.41 |
| 40:DI:140:SER:OG | 40:DI:146:GLY:HA3 | 2.21 | 0.41 |
| 40:DI:152:LEU:HG | 40:DI:156:ARG:HH22 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DI:187:SER:O | 40:DI:191:THR:HG23 | 2.21 | 0.41 |
| 40:DI:352:LYS:H | 40:DI:352:LYS:HG2 | 1.67 | 0.41 |
| 41:DL:192:LEU:HD22 | 41:DL:192:LEU:HA | 1.83 | 0.41 |
| 41:DL:252:LYS:HD3 | 41:DL:350:LYS:HE2 | 2.03 | 0.41 |
| 41:DL:263:LEU:HD22 | 41:DL:422:VAL:HG23 | 2.03 | 0.41 |
| 41:DL:323:MET:O | 41:DL:326:VAL:HB | 2.21 | 0.41 |
| 41:DM:31:ASP:C | 41:DM:33:THR:H | 2.24 | 0.41 |
| 41:DN:42:LEU:H | 41:DN:42:LEU:HG | 1.51 | 0.41 |
| 41:DN:165:ASN:HD21 | 41:DN:250:LEU:HB3 | 1.85 | 0.41 |
| 41:DP:68:LEU:HD12 | 41:DP:143:THR:HA | 2.03 | 0.41 |
| 41:DP:83:GLN:H | 41:DP:83:GLN:HG2 | 1.55 | 0.41 |
| 41:DP:174:LYS:HB2 | 41:DP:174:LYS:HE2 | 1.54 | 0.41 |
| 41:DP:278:SER:O | 41:DP:280:GLN:N | 2.54 | 0.41 |
| 41:DP:313:VAL:HB | 41:DP:367:PHE:CE2 | 2.55 | 0.41 |
| 40:EA:235:VAL:O | 40:EA:239:THR:HG22 | 2.21 | 0.41 |
| 41:EB:156:ARG:HD2 | 41:EB:156:ARG:HA | 1.77 | 0.41 |
| 41:EB:248:ALA:HB1 | 41:EB:350:LYS:HZ2 | 1.84 | 0.41 |
| 40:EH:27:GLU:C | 40:EH:29:GLY:N | 2.74 | 0.41 |
| 40:EH:195:LEU:HD21 | 40:EH:427:LEU:HD13 | 2.03 | 0.41 |
| 40:EH:258:ASN:ND2 | 41:EP:179:VAL:HG13 | 2.35 | 0.41 |
| 40:EH:259:LEU:HD12 | 40:EH:259:LEU:HA | 1.90 | 0.41 |
| 40:EH:332:ILE:HG12 | 40:EH:351:PHE:CD2 | 2.56 | 0.41 |
| 40:EI:51:THR:HG21 | 40:EI:243:ARG:HB3 | 2.03 | 0.41 |
| 40:EI:209:ILE:H | 40:EI:209:ILE:HG13 | 1.69 | 0.41 |
| 41:EL:262:ARG:O | 41:EL:264:HIS:ND1 | 2.53 | 0.41 |
| 41:EM:274:THR:HG23 | 41:EM:279:GLN:HG3 | 2.03 | 0.41 |
| 41:EM:335:ASN:O | 41:EM:336:LYS:C | 2.59 | 0.41 |
| 41:EN:242:PHE:HD2 | 41:EN:356:ILE:HB | 1.86 | 0.41 |
| 41:EO:28:HIS:ND1 | 41:EO:47:ILE:HG13 | 2.36 | 0.41 |
| 41:EO:42:LEU:HD13 | 41:EO:356:ILE:HD11 | 2.01 | 0.41 |
| 41:EO:58:LYS:NZ | 41:FO:280:GLN:HG3 | 2.36 | 0.41 |
| 41:EP:5:VAL:HA | 41:EP:62:ARG:HG2 | 2.03 | 0.41 |
| 41:EP:7:LEU:HD21 | 41:EP:151:LEU:HG | 2.03 | 0.41 |
| 41:EP:8:GLN:H | 41:EP:8:GLN:HG2 | 1.64 | 0.41 |
| 41:EP:193:VAL:HA | 41:EP:264:HIS:NE2 | 2.36 | 0.41 |
| 41:EP:200:TYR:N | 41:EP:200:TYR:HD2 | 2.19 | 0.41 |
| 40:FA:106:GLY:C | 40:FA:108:TYR:N | 2.74 | 0.41 |
| 40:FA:175:PRO:HD3 | 40:FA:205:ASP:OD2 | 2.21 | 0.41 |
| 40:FA:222:PRO:O | 41:FN:324:LYS:HE3 | 2.21 | 0.41 |
| 40:FA:325:PRO:HB2 | 41:FB:222:TYR:OH | 2.20 | 0.41 |
| 40:FA:328:VAL:HG11 | 40:FA:353:VAL:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FB:295:ASP:OD2 | 41:FB:297:LYS:HG2 | 2.20 | 0.41 |
| 40:FE:174:ALA:HB3 | 40:FE:178:SER:H | 1.85 | 0.41 |
| 40:FE:336:LYS:HA | 40:FE:336:LYS:HD2 | 1.91 | 0.41 |
| 40:FF:188:ILE:HG23 | 40:FF:424:MET:HG3 | 2.01 | 0.41 |
| 40:FH:206:ASN:HD22 | 40:FH:206:ASN:HA | 1.69 | 0.41 |
| 40:FH:224:TYR:HE2 | 41:FO:245:GLN:HG3 | 1.85 | 0.41 |
| 40:FI:21:TRP:CZ2 | 40:FI:65:ALA:HB2 | 2.56 | 0.41 |
| 40:FI:252:LEU:O | 40:FI:256:GLN:NE2 | 2.49 | 0.41 |
| 40:FI:320:ARG:HG3 | 40:FI:360:PRO:HD3 | 2.03 | 0.41 |
| 41:FM:354:CYS:SG | 41:FM:355:ASP:N | 2.94 | 0.41 |
| 41:FO:27:GLU:OE2 | 41:FO:318:ARG:NH2 | 2.52 | 0.41 |
| 41:FO:134:GLN:HA | 41:FO:165:ASN:O | 2.21 | 0.41 |
| 40:GA:104:ALA:HB1 | 40:GA:108:TYR:HD2 | 1.85 | 0.41 |
| 40:GA:215:ARG:HA | 40:GA:215:ARG:HD3 | 1.86 | 0.41 |
| 40:GA:224:TYR:HD1 | 42:GA:501:GTP:C2 | 2.39 | 0.41 |
| 40:GA:265:ILE:HG22 | 40:GA:379:ASN:HD21 | 1.85 | 0.41 |
| 40:GA:297:GLU:HA | 40:GA:298:PRO:HD3 | 1.89 | 0.41 |
| 40:GA:317:LEU:HD23 | 40:GA:376:MET:HB2 | 2.02 | 0.41 |
| 41:GB:252:LYS:O | 41:GB:256:ASN:HB2 | 2.20 | 0.41 |
| 41:GB:258:VAL:HG13 | 40:GG:406:TRP:HE1 | 1.86 | 0.41 |
| 40:GE:104:ALA:HB1 | 40:GE:412:MET:H | 1.86 | 0.41 |
| 40:GE:185:TYR:O | 40:GE:186:ASN:C | 2.59 | 0.41 |
| 40:GE:311:LYS:HE2 | 40:GE:311:LYS:HB2 | 1.92 | 0.41 |
| 40:GE:428:GLU:O | 40:GE:429:LYS:C | 2.59 | 0.41 |
| 40:GF:194:THR:OG1 | 40:GF:198:SER:HB2 | 2.20 | 0.41 |
| 40:GG:6:SER:O | 40:GG:65:ALA:HA | 2.20 | 0.41 |
| 40:GG:346:TRP:CE3 | 40:GG:347:CYS:HB2 | 2.56 | 0.41 |
| 40:GG:363:VAL:O | 40:GG:364:PRO:C | 2.60 | 0.41 |
| 40:GI:288:VAL:HA | 40:GI:291:ILE:CD1 | 2.51 | 0.41 |
| 40:GI:394:PHE:HZ | 40:GI:417:PHE:HB3 | 1.84 | 0.41 |
| 40:GI:418:SER:O | 40:GI:419:GLU:C | 2.59 | 0.41 |
| 41:GN:101:TRP:HD1 | 41:GN:145:SER:HB2 | 1.84 | 0.41 |
| 41:GN:213:ARG:HD3 | 41:GN:213:ARG:HA | 1.49 | 0.41 |
| 41:GN:297:LYS:HE2 | 41:GN:297:LYS:HB3 | 1.51 | 0.41 |
| 41:GO:39:ASP:OD1 | 41:GO:40:SER:N | 2.54 | 0.41 |
| 41:GP:186:THR:HG21 | 41:GP:385:PHE:CD1 | 2.56 | 0.41 |
| 41:GP:324:LYS:O | 41:GP:328:GLU:HG3 | 2.21 | 0.41 |
| 40:HA:21:TRP:CH2 | 40:HA:63:PRO:HB3 | 2.56 | 0.41 |
| 40:HA:362:VAL:HG12 | 40:HA:369:LYS:HE2 | 2.02 | 0.41 |
| 41:HB:148:GLY:O | 41:HB:152:ILE:HG12 | 2.20 | 0.41 |
| 40:HE:6:SER:HB2 | 40:HE:8:HIS:CE1 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HE:96:LYS:HA | 40:HE:96:LYS:HD3 | 1.71 | 0.41 |
| 40:HE:252:LEU:HA | 40:HE:255:PHE:HD2 | 1.86 | 0.41 |
| 40:HF:210:TYR:CD1 | 41:HM:324:LYS:HE3 | 2.56 | 0.41 |
| 40:HF:235:VAL:HA | 40:HF:238:ILE:HG22 | 2.02 | 0.41 |
| 40:HF:262:TYR:HB2 | 40:HF:265:ILE:HG12 | 2.01 | 0.41 |
| 40:HH:172:TYR:CD1 | 40:HH:173:PRO:HD2 | 2.55 | 0.41 |
| 40:HH:319:TYR:HB3 | 40:HH:323:VAL:HG21 | 2.03 | 0.41 |
| 40:HI:88:HIS:CE1 | 40:HI:90:GLU:HB2 | 2.55 | 0.41 |
| 41:HM:12:CYS:SG | 41:HM:138:SER:HB2 | 2.61 | 0.41 |
| 41:HN:87:PRO:HD3 | 41:IN:281:TYR:HE2 | 1.76 | 0.41 |
| 41:HN:260:PHE:HE2 | 41:HN:344:TRP:HZ3 | 1.69 | 0.41 |
| 41:HN:339:SER:O | 41:HN:341:PHE:N | 2.50 | 0.41 |
| 41:HN:391:ARG:O | 41:HN:393:ALA:N | 2.54 | 0.41 |
| 41:HP:105:HIS:CD2 | 41:HP:150:LEU:HD13 | 2.56 | 0.41 |
| 40:IA:14:VAL:HG22 | 40:IA:67:PHE:HD2 | 1.86 | 0.41 |
| 40:IA:54:SER:HB3 | 40:IA:64:ARG:NE | 2.35 | 0.41 |
| 40:IA:56:THR:HG21 | 41:JM:281:TYR:HA | 2.02 | 0.41 |
| 40:IA:139:HIS:CE1 | 40:IA:150:THR:HG21 | 2.56 | 0.41 |
| 40:IF:232:SER:HA | 40:IF:235:VAL:HG22 | 2.02 | 0.41 |
| 40:IG:219:ILE:HG22 | 40:IG:221:ARG:H | 1.86 | 0.41 |
| 40:IH:217:LEU:HA | 40:IH:277:SER:HB3 | 2.03 | 0.41 |
| 40:IH:264:ARG:NH2 | 40:IH:423:ASP:OD1 | 2.53 | 0.41 |
| 40:IH:406:TRP:CG | 41:IO:255:VAL:HG23 | 2.55 | 0.41 |
| 40:II:231:ILE:O | 40:II:235:VAL:HG23 | 2.21 | 0.41 |
| 41:IM:109:GLY:O | 41:IM:113:VAL:HG23 | 2.21 | 0.41 |
| 41:IO:137:HIS:O | 41:IO:168:SER:HA | 2.21 | 0.41 |
| 40:JA:123:ARG:NH1 | 40:JA:123:ARG:HA | 2.35 | 0.41 |
| 40:JA:228:ASN:ND2 | 42:JA:501:GTP:HN1 | 2.16 | 0.41 |
| 40:JA:288:VAL:HB | 40:JA:327:ASP:HB3 | 2.01 | 0.41 |
| 40:JA:352:LYS:HD2 | 40:JA:353:VAL:H | 1.86 | 0.41 |
| 41:JB:114:ASP:N | 41:JB:114:ASP:OD1 | 2.54 | 0.41 |
| 41:JB:142:GLY:O | 41:JB:144:GLY:N | 2.54 | 0.41 |
| 41:JB:186:THR:HG22 | 41:JB:415:MET:SD | 2.60 | 0.41 |
| 41:JB:284:LEU:HD21 | 41:JB:363:MET:HB2 | 2.02 | 0.41 |
| 40:JD:271:THR:OG1 | 40:JD:301:GLN:OE1 | 2.38 | 0.41 |
| 40:JD:433:GLU:HA | 40:JD:436:MET:SD | 2.61 | 0.41 |
| 40:JE:31:GLN:HG3 | 40:JE:34:GLY:H | 1.86 | 0.41 |
| 40:JE:102:ASN:HB3 | 40:JE:105:ARG:HB2 | 2.01 | 0.41 |
| 40:JE:245:ASP:OD2 | 40:JE:246:GLY:N | 2.53 | 0.41 |
| 40:JF:263:PRO:HD3 | 41:JN:396:HIS:CE1 | 2.56 | 0.41 |
| 40:JG:205:ASP:HB2 | 40:JG:303:VAL:HA | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:JH:288:VAL:HB | 40:JH:327:ASP:HB3 | 2.03 | 0.41 |
| 41:JL:117:LEU:HA | 41:JL:120:VAL:HG12 | 2.03 | 0.41 |
| 41:JM:182:PRO:O | 41:JM:186:THR:HG23 | 2.21 | 0.41 |
| 41:JM:427:ALA:O | 41:JM:428:CYS:C | 2.59 | 0.41 |
| 41:JO:313:VAL:O | 41:JO:349:VAL:HA | 2.21 | 0.41 |
| 40:KA:185:TYR:HE2 | 40:KA:404:VAL:HG22 | 1.86 | 0.41 |
| 40:KA:256:GLN:HB3 | 41:KB:397:TRP:CZ3 | 2.56 | 0.41 |
| 41:KB:207:LEU:HB3 | 41:KB:225:LEU:HG | 2.03 | 0.41 |
| 40:KD:274:PRO:HG3 | 40:KD:286:LEU:HD11 | 2.03 | 0.41 |
| 40:KD:394:PHE:CD1 | 40:KD:421:ARG:HD3 | 2.56 | 0.41 |
| 40:KE:230:LEU:HD12 | 40:KE:230:LEU:HA | 1.90 | 0.41 |
| 40:KF:132:LEU:HD22 | 40:KF:164:LYS:HG3 | 2.02 | 0.41 |
| 40:KG:7:VAL:HG23 | 40:KG:137:ILE:HA | 2.03 | 0.41 |
| 40:KG:308:ARG:HB3 | 40:NG:282:TYR:HE2 | 1.86 | 0.41 |
| 40:KG:311:LYS:H | 40:KG:381:THR:HG22 | 1.86 | 0.41 |
| 40:KH:182:VAL:HG23 | 40:KH:186:ASN:HD21 | 1.86 | 0.41 |
| 41:KL:4:ILE:HG13 | 41:KL:49:VAL:HG13 | 2.03 | 0.41 |
| 41:KL:233:MET:HE2 | 41:KL:233:MET:HB2 | 1.86 | 0.41 |
| 41:KN:133:PHE:HB2 | 41:KN:164:MET:SD | 2.61 | 0.41 |
| 41:KO:133:PHE:O | 41:KO:164:MET:HA | 2.21 | 0.41 |
| 41:KO:216:LYS:HA | 41:KO:216:LYS:HE3 | 2.03 | 0.41 |
| 40:LA:98:ASP:OD1 | 40:LA:99:ALA:N | 2.54 | 0.41 |
| 40:LA:228:ASN:ND2 | 42:LA:501:GTP:HN1 | 2.17 | 0.41 |
| 40:LA:396:LEU:HD23 | 41:LN:346:PRO:HD3 | 2.03 | 0.41 |
| 41:LB:2:ARG:HH12 | 40:LG:72:PRO:CG | 2.34 | 0.41 |
| 40:LD:152:LEU:O | 40:LD:155:GLU:HB3 | 2.21 | 0.41 |
| 40:LD:335:ILE:HD13 | 40:LD:335:ILE:HA | 1.94 | 0.41 |
| 40:LD:376:MET:SD | 40:LD:378:SER:HB3 | 2.61 | 0.41 |
| 40:LF:115:ILE:HG12 | 40:LF:156:ARG:HG3 | 2.02 | 0.41 |
| 40:LF:139:HIS:CG | 40:LF:150:THR:HG21 | 2.55 | 0.41 |
| 40:LF:238:ILE:HG22 | 40:LF:239:THR:HG23 | 2.03 | 0.41 |
| 40:LF:363:VAL:O | 40:LF:364:PRO:C | 2.59 | 0.41 |
| 40:LG:99:ALA:HA | 40:LG:105:ARG:HE | 1.86 | 0.41 |
| 40:LG:102:ASN:HB3 | 40:LG:105:ARG:CG | 2.51 | 0.41 |
| 40:LG:174:ALA:HA | 40:LG:205:ASP:OD2 | 2.21 | 0.41 |
| 40:LG:191:THR:HG23 | 40:LG:267:PHE:CZ | 2.56 | 0.41 |
| 40:LH:14:VAL:HG22 | 40:LH:67:PHE:HD2 | 1.86 | 0.41 |
| 40:LH:287:SER:O | 40:LH:291:ILE:HG23 | 2.21 | 0.41 |
| 41:LN:240:LEU:HD12 | 41:LN:241:ARG:HG3 | 2.03 | 0.41 |
| 40:MA:36:MET:HE3 | 40:MA:36:MET:HB3 | 1.81 | 0.41 |
| 40:MA:56:THR:O | 40:MA:57:GLY:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MA:291:ILE:HD13 | 40:MA:372:ARG:HG3 | 2.02 | 0.41 |
| 40:MA:346:TRP:O | 41:MB:388:MET:HG2 | 2.21 | 0.41 |
| 41:MB:11:GLN:HA | 41:MB:72:THR:HG21 | 2.03 | 0.41 |
| 40:MD:51:THR:HG21 | 40:MD:243:ARG:HD3 | 2.03 | 0.41 |
| 40:MG:110:ILE:H | 40:MG:110:ILE:HG12 | 1.35 | 0.41 |
| 40:MG:168:GLU:CD | 40:MG:198:SER:HB2 | 2.41 | 0.41 |
| 40:MG:188:ILE:HD11 | 40:MG:391:ASP:HA | 2.02 | 0.41 |
| 40:MG:305:CYS:O | 40:MG:305:CYS:SG | 2.79 | 0.41 |
| 40:MG:319:TYR:HB3 | 40:MG:323:VAL:HG11 | 2.02 | 0.41 |
| 40:MG:335:ILE:C | 40:MG:337:THR:H | 2.24 | 0.41 |
| 41:ML:134:GLN:NE2 | 41:ML:233:MET:SD | 2.94 | 0.41 |
| 41:ML:139:LEU:HA | 41:ML:139:LEU:HD12 | 1.86 | 0.41 |
| 41:MM:173:PRO:HG3 | 41:MM:380:ARG:HD3 | 2.02 | 0.41 |
| 41:MN:358:PRO:HG2 | 41:MN:361:LEU:HB2 | 2.03 | 0.41 |
| 41:MO:263:LEU:HD11 | 41:MO:425:ARG:HD3 | 2.02 | 0.41 |
| 41:MO:420:ASN:HB2 | 41:MO:421:PRO:CD | 2.50 | 0.41 |
| 41:MP:137:HIS:NE2 | 41:MP:168:SER:OG | 2.41 | 0.41 |
| 41:MP:173:PRO:HD2 | 41:MP:205:GLU:OE1 | 2.21 | 0.41 |
| 40:NA:50:ASN:HB3 | 40:NA:51:THR:H | 1.75 | 0.41 |
| 40:NA:238:ILE:HD12 | 40:NA:377:LEU:HD11 | 2.03 | 0.41 |
| 40:NA:349:THR:HB | 41:NB:176:SER:HB3 | 2.02 | 0.41 |
| 41:NB:6:HIS:HD2 | 41:NB:134:GLN:O | 2.04 | 0.41 |
| 41:NB:239:CYS:SG | 41:NB:248:ALA:N | 2.93 | 0.41 |
| 40:ND:102:ASN:O | 40:ND:105:ARG:N | 2.50 | 0.41 |
| 40:ND:106:GLY:O | 40:ND:149:PHE:N | 2.54 | 0.41 |
| 40:ND:277:SER:O | 40:ND:278:ALA:C | 2.59 | 0.41 |
| 40:NE:8:HIS:ND1 | 40:NE:17:GLY:HA3 | 2.35 | 0.41 |
| 40:NF:33:ASP:HB2 | 40:NF:85:GLN:HG2 | 2.03 | 0.41 |
| 40:NF:134:GLY:HA2 | 40:NF:165:SER:O | 2.21 | 0.41 |
| 40:NG:261:PRO:HD3 | 40:NG:379:ASN:ND2 | 2.35 | 0.41 |
| 40:NH:166:LYS:H | 40:NH:199:ASP:HB2 | 1.86 | 0.41 |
| 40:NH:238:ILE:HD12 | 40:NH:377:LEU:HD21 | 2.01 | 0.41 |
| 40:NH:352:LYS:HZ2 | 41:NP:178:THR:C | 2.24 | 0.41 |
| 41:NL:165:ASN:ND2 | 41:NL:250:LEU:HD13 | 2.35 | 0.41 |
| 41:NL:271:ALA:HB1 | 41:NL:292:GLN:HG2 | 2.02 | 0.41 |
| 41:NM:45:GLU:OE1 | 41:NM:46:ARG:HG2 | 2.21 | 0.41 |
| 41:NN:12:CYS:O | 41:NN:16:ILE:HG12 | 2.21 | 0.41 |
| 41:NN:64:VAL:HA | 41:NN:89:ASN:HB3 | 2.03 | 0.41 |
| 41:NN:262:ARG:O | 41:NN:264:HIS:ND1 | 2.53 | 0.41 |
| 41:NO:137:HIS:O | 41:NO:168:SER:HA | 2.21 | 0.41 |
| 41:NP:101:TRP:O | 41:NP:104:GLY:N | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:NP:152:ILE:HG23 | 41:NP:164:MET:HG2 | 2.03 | 0.41 |
| 40:OA:296:PHE:CD2 | 40:OA:335:ILE:HG12 | 2.56 | 0.41 |
| 40:OA:319:TYR:HB3 | 40:OA:323:VAL:HG21 | 2.02 | 0.41 |
| 41:OB:107:THR:O | 41:OB:110:ALA:N | 2.33 | 0.41 |
| 41:OB:309:ARG:HD3 | 41:OB:342:VAL:HA | 2.02 | 0.41 |
| 40:OE:273:ALA:HB1 | 40:OE:291:ILE:HG23 | 2.03 | 0.41 |
| 40:OF:174:ALA:HB3 | 40:OF:178:SER:H | 1.85 | 0.41 |
| 40:OH:195:LEU:HD11 | 40:OH:427:LEU:HD13 | 2.02 | 0.41 |
| 40:OH:369:LYS:HB2 | 40:OH:369:LYS:HE3 | 1.62 | 0.41 |
| 41:OM:398:TYR:HB3 | 41:OM:403:MET:HB2 | 2.02 | 0.41 |
| 41:ON:276:ARG:NH1 | 41:ON:276:ARG:O | 2.54 | 0.41 |
| 41:OO:232:THR:HG21 | 41:OO:268:PRO:HB2 | 2.03 | 0.41 |
| 41:OP:318:ARG:HH22 | 41:OP:358:PRO:HB3 | 1.86 | 0.41 |
| 40:PA:7:VAL:HB | 40:PA:66:VAL:HG22 | 2.03 | 0.41 |
| 40:PA:68:VAL:HG12 | 40:PA:93:ILE:HB | 2.02 | 0.41 |
| 40:PA:352:LYS:HD2 | 41:PB:178:THR:HA | 2.02 | 0.41 |
| 40:PD:436:MET:O | 41:PL:391:ARG:NH2 | 2.48 | 0.41 |
| 40:PF:105:ARG:HH12 | 41:PM:251:ARG:HH11 | 1.69 | 0.41 |
| 40:PF:251:ASP:H | 40:PF:254:GLU:HB2 | 1.86 | 0.41 |
| 40:PG:172:TYR:HB2 | 40:PG:203:MET:SD | 2.60 | 0.41 |
| 41:PL:210:ILE:O | 41:PL:214:THR:OG1 | 2.31 | 0.41 |
| 41:PM:6:HIS:O | 41:PM:63:ALA:HA | 2.21 | 0.41 |
| 41:PO:21:TRP:CZ3 | 41:PO:24:ILE:HD11 | 2.56 | 0.41 |
| 41:PO:189:VAL:O | 41:PO:193:VAL:HG23 | 2.20 | 0.41 |
| 41:PP:13:GLY:HA2 | 41:PP:136:THR:HG22 | 2.02 | 0.41 |
| 40:QA:121:ARG:HA | 40:QA:121:ARG:HD3 | 1.85 | 0.41 |
| 40:QA:346:TRP:HA | 41:QB:390:ARG:NH1 | 2.35 | 0.41 |
| 41:QB:1:MET:O | 41:QB:3:GLU:N | 2.54 | 0.41 |
| 41:QB:15:GLN:HB3 | 43:QB:501:GDP:O6 | 2.20 | 0.41 |
| 41:QB:256:ASN:HB3 | 40:QG:181:VAL:HG22 | 2.02 | 0.41 |
| 41:QB:394:PHE:O | 41:QB:395:LEU:C | 2.59 | 0.41 |
| 40:QE:51:THR:HG23 | 40:QE:52:PHE:CD1 | 2.56 | 0.41 |
| 40:QE:195:LEU:HD23 | 40:QE:195:LEU:HA | 1.95 | 0.41 |
| 40:QE:274:PRO:HD2 | 40:QE:291:ILE:HG13 | 2.03 | 0.41 |
| 41:QL:263:LEU:HD21 | 41:QL:422:VAL:HB | 2.03 | 0.41 |
| 41:QM:139:LEU:HD22 | 41:QM:188:SER:OG | 2.21 | 0.41 |
| 41:QN:202:ILE:HD13 | 41:QN:229:VAL:HG21 | 2.02 | 0.41 |
| 41:QN:375:GLN:NE2 | 41:QN:379:LYS:HB2 | 2.36 | 0.41 |
| 41:QO:3:GLU:HB2 | 41:QO:130:LEU:HD23 | 2.03 | 0.41 |
| 41:QP:103:LYS:HB3 | 41:QP:104:GLY:H | 1.69 | 0.41 |
| 41:QP:161:ASP:HB3 | 41:QP:162:ARG:HH12 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:QP:203:ASP:HB3 | 41:QP:206:ALA:HB3 | 2.02 | 0.41 |
| 41:QP:285:THR:HB | 41:QP:287:PRO:HD2 | 2.03 | 0.41 |
| 41:QP:336:LYS:HA | 41:QP:336:LYS:HD2 | 1.81 | 0.41 |
| 40:RA:97:GLU:OE2 | 41:RN:251:ARG:NE | 2.54 | 0.41 |
| 40:RA:100:ALA:HA | 41:RN:252:LYS:HG3 | 2.01 | 0.41 |
| 41:RB:199:THR:OG1 | 41:RB:265:PHE:HA | 2.20 | 0.41 |
| 40:RE:5:ILE:HD11 | 40:RE:129:CYS:SG | 2.60 | 0.41 |
| 40:RE:11:GLN:HG2 | 40:RE:15:GLN:NE2 | 2.36 | 0.41 |
| 42:RF:501:GTP:C8 | 41:RM:246:LEU:HD12 | 2.55 | 0.41 |
| 40:RG:207:GLU:HA | 40:RG:210:TYR:HD1 | 1.86 | 0.41 |
| 40:RG:277:SER:O | 40:RG:279:GLU:N | 2.54 | 0.41 |
| 40:RI:360:PRO:HG2 | 40:RI:370:VAL:HG23 | 2.03 | 0.41 |
| 41:RL:86:ARG:HB2 | 41:RL:89:ASN:HB2 | 2.02 | 0.41 |
| 41:RM:19:LYS:O | 41:RM:22:GLU:HG3 | 2.21 | 0.41 |
| 41:RM:122:LYS:NZ | 41:SM:291:GLN:HG3 | 2.35 | 0.41 |
| 41:RM:141:GLY:O | 41:RM:145:SER:OG | 2.30 | 0.41 |
| 41:RP:58:LYS:HD3 | 41:RP:58:LYS:HA | 1.89 | 0.41 |
| 40:SA:109:THR:HG23 | 40:SA:110:ILE:HD12 | 2.02 | 0.41 |
| 40:SA:236:SER:O | 40:SA:240:ALA:HB2 | 2.20 | 0.41 |
| 40:SA:259:LEU:HD12 | 40:SA:259:LEU:HA | 1.79 | 0.41 |
| 40:SA:328:VAL:O | 40:SA:332:ILE:HG12 | 2.20 | 0.41 |
| 40:SA:329:ASN:HB2 | 41:SB:175:VAL:HG11 | 2.03 | 0.41 |
| 40:SE:174:ALA:HB3 | 40:SE:178:SER:HA | 2.03 | 0.41 |
| 40:SE:207:GLU:HB2 | 40:SE:304:LYS:HE2 | 2.01 | 0.41 |
| 40:SE:405:HIS:NE2 | 41:SL:259:PRO:O | 2.54 | 0.41 |
| 40:SF:88:HIS:HB3 | 40:SF:91:GLN:HG2 | 2.01 | 0.41 |
| 40:SF:166:LYS:H | 40:SF:199:ASP:HB2 | 1.85 | 0.41 |
| 40:SF:386:ALA:HA | 40:SF:389:ARG:NE | 2.36 | 0.41 |
| 40:SG:56:THR:OG1 | 40:SG:57:GLY:N | 2.51 | 0.41 |
| 40:SH:145:THR:HG1 | 42:SH:501:GTP:PB | 2.44 | 0.41 |
| 40:SH:387:TRP:HZ3 | 40:SH:431:TYR:CE2 | 2.39 | 0.41 |
| 40:SI:140:SER:HA | 40:SI:171:ILE:H | 1.86 | 0.41 |
| 41:SM:359:ARG:H | 41:SM:359:ARG:HG2 | 1.73 | 0.41 |
| 41:SO:3:GLU:H | 41:SO:131:GLN:H | 1.69 | 0.41 |
| 41:SO:151:LEU:HD12 | 41:SO:151:LEU:HA | 1.89 | 0.41 |
| 41:SO:306:ARG:O | 41:SO:308:GLY:N | 2.46 | 0.41 |
| 41:SO:325:GLU:O | 41:SO:326:VAL:C | 2.59 | 0.41 |
| 41:SO:369:GLY:O | 41:SO:370:ASN:C | 2.59 | 0.41 |
| 41:SP:89:ASN:ND2 | 41:SP:123:GLU:OE2 | 2.53 | 0.41 |
| 41:SP:152:ILE:HA | 41:SP:155:ILE:HG12 | 2.02 | 0.41 |
| 41:SP:323:MET:HE2 | 41:SP:353:VAL:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SP:377:LEU:HA | 41:SP:380:ARG:HE | 1.86 | 0.41 |
| 41:SP:407:GLU:HA | 41:SP:410:GLU:HG3 | 2.03 | 0.41 |
| 40:TA:1:GLN:N | 40:TA:3:GLU:OE2 | 2.44 | 0.41 |
| 41:TB:42:LEU:HD23 | 41:TB:356:ILE:HD11 | 2.03 | 0.41 |
| 41:TB:167:PHE:CE2 | 41:TB:233:MET:HG3 | 2.56 | 0.41 |
| 41:TB:274:THR:HG22 | 41:TB:282:ARG:NH1 | 2.35 | 0.41 |
| 40:TE:72:PRO:HD2 | 41:TL:2:ARG:CZ | 2.51 | 0.41 |
| 40:TE:75:ILE:HG23 | 40:TE:92:LEU:HD22 | 2.02 | 0.41 |
| 40:TF:73:THR:HG22 | 41:TM:46:ARG:NE | 2.36 | 0.41 |
| 40:TG:6:SER:O | 40:TG:65:ALA:HA | 2.21 | 0.41 |
| 40:TG:120:ASP:OD1 | 40:TG:123:ARG:NH2 | 2.52 | 0.41 |
| 40:TG:229:ARG:HH11 | 40:TG:363:VAL:HG11 | 1.85 | 0.41 |
| 40:TH:270:ALA:HA | 40:TH:376:MET:O | 2.21 | 0.41 |
| 40:TI:240:ALA:HB1 | 40:TI:356:ASN:HD22 | 1.85 | 0.41 |
| 41:TL:41:ASP:N | 41:TL:41:ASP:OD1 | 2.46 | 0.41 |
| 41:TL:117:LEU:HA | 41:TL:120:VAL:HG22 | 2.02 | 0.41 |
| 41:TM:21:TRP:HZ2 | 41:TM:63:ALA:HB2 | 1.85 | 0.41 |
| 41:TN:150:LEU:O | 41:TN:154:LYS:HG2 | 2.21 | 0.41 |
| 41:TN:271:ALA:HB2 | 41:TN:298:ASN:ND2 | 2.35 | 0.41 |
| 41:TO:267:MET:N | 41:TO:369:GLY:O | 2.54 | 0.41 |
| 41:TP:27:GLU:OE1 | 41:TP:241:ARG:NH1 | 2.35 | 0.41 |
| 41:TP:417:ASP:O | 41:TP:421:PRO:HD3 | 2.21 | 0.41 |
| 40:UA:328:VAL:O | 40:UA:332:ILE:HG12 | 2.20 | 0.41 |
| 40:UF:88:HIS:O | 40:UF:89:PRO:C | 2.59 | 0.41 |
| 40:UF:99:ALA:HB3 | 40:UF:145:THR:CA | 2.50 | 0.41 |
| 40:UF:188:ILE:HG22 | 40:UF:420:ALA:HB1 | 2.03 | 0.41 |
| 40:UF:207:GLU:H | 40:UF:207:GLU:HG3 | 1.54 | 0.41 |
| 40:UF:346:TRP:HE3 | 41:UN:393:ALA:HB2 | 1.85 | 0.41 |
| 40:UG:274:PRO:HG2 | 40:UG:372:ARG:O | 2.21 | 0.41 |
| 40:UH:35:GLN:NE2 | 40:UH:36:MET:O | 2.54 | 0.41 |
| 40:UH:326:LYS:HD2 | 40:UH:329:ASN:HD21 | 1.86 | 0.41 |
| 40:UH:384:ALA:HB2 | 40:UH:431:TYR:HD2 | 1.85 | 0.41 |
| 40:UI:136:LEU:HB3 | 40:UI:169:PHE:HE1 | 1.86 | 0.41 |
| 40:UI:201:ALA:HB3 | 40:UI:267:PHE:CD1 | 2.56 | 0.41 |
| 40:UI:295:CYS:HB3 | 40:UI:376:MET:HE2 | 2.02 | 0.41 |
| 40:UI:328:VAL:HG11 | 40:UI:353:VAL:CG1 | 2.43 | 0.41 |
| 41:UN:5:VAL:HG22 | 41:UN:62:ARG:HD2 | 2.03 | 0.41 |
| 41:UN:64:VAL:HA | 41:UN:89:ASN:HB3 | 2.03 | 0.41 |
| 41:UN:230:SER:HA | 41:UN:233:MET:HB2 | 2.03 | 0.41 |
| 41:UO:30:ILE:HD12 | 41:UO:51:TYR:CE2 | 2.55 | 0.41 |
| 41:UP:44:LEU:O | 41:UP:46:ARG:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:UP:90:PHE:O | 41:UP:91:VAL:C | 2.59 | 0.41 |
| 41:UP:129:CYS:SG | 41:UP:129:CYS:O | 2.79 | 0.41 |
| 41:UP:362:LYS:H | 41:UP:362:LYS:HG3 | 1.71 | 0.41 |
| 41:UP:364:SER:OG | 41:UP:365:ALA:N | 2.54 | 0.41 |
| 40:VA:66:VAL:HG12 | 40:VA:68:VAL:HG23 | 2.02 | 0.41 |
| 40:VA:229:ARG:NH1 | 40:VA:364:PRO:O | 2.54 | 0.41 |
| 40:VA:262:TYR:OH | 41:VB:391:ARG:O | 2.32 | 0.41 |
| 41:VB:41:ASP:N | 41:VB:41:ASP:OD1 | 2.54 | 0.41 |
| 41:VB:103:LYS:HA | 41:VB:107:THR:HB | 2.03 | 0.41 |
| 40:VG:189:LEU:HD11 | 40:VG:417:PHE:HE1 | 1.85 | 0.41 |
| 40:VI:221:ARG:HH21 | 41:VP:325:GLU:HG3 | 1.85 | 0.41 |
| 41:VN:25:SER:HB3 | 41:VN:81:PHE:CE2 | 2.56 | 0.41 |
| 41:VN:122:LYS:HE2 | 41:WM:291:GLN:HG3 | 2.03 | 0.41 |
| 41:VN:149:THR:HG21 | 41:VN:188:SER:HA | 2.02 | 0.41 |
| 41:VN:215:LEU:HD21 | 41:VN:273:LEU:HD22 | 2.03 | 0.41 |
| 41:VO:375:GLN:OE1 | 41:VO:419:GLY:HA2 | 2.21 | 0.41 |
| 41:VP:152:ILE:HD12 | 41:VP:164:MET:SD | 2.61 | 0.41 |
| 41:VP:210:ILE:HG13 | 41:VP:298:ASN:HA | 2.03 | 0.41 |
| 41:VQ:122:LYS:HG2 | 41:WP:291:GLN:NE2 | 2.35 | 0.41 |
| 41:VQ:305:PRO:HB3 | 41:VQ:310:TYR:CE1 | 2.56 | 0.41 |
| 40:WA:70:LEU:HD12 | 40:WA:145:THR:HG22 | 2.02 | 0.41 |
| 40:WA:397:MET:SD | 41:WN:345:ILE:HD12 | 2.61 | 0.41 |
| 41:WB:30:ILE:HD13 | 41:WB:36:TYR:HA | 2.03 | 0.41 |
| 40:WE:245:ASP:OD1 | 40:WE:245:ASP:N | 2.54 | 0.41 |
| 40:WF:49:PHE:HE2 | 40:WF:55:GLU:HB2 | 1.86 | 0.41 |
| 40:WG:209:ILE:HA | 40:WG:212:ILE:HG22 | 2.02 | 0.41 |
| 40:WG:224:TYR:HA | 40:WG:227:LEU:HB3 | 2.03 | 0.41 |
| 40:WG:346:TRP:CD1 | 41:WO:391:ARG:HD3 | 2.56 | 0.41 |
| 40:WI:97:GLU:HB3 | 40:WI:110:ILE:HD13 | 2.02 | 0.41 |
| 41:WM:66:VAL:HG13 | 41:WM:147:MET:CE | 2.50 | 0.41 |
| 41:WM:101:TRP:O | 41:WM:102:ALA:C | 2.59 | 0.41 |
| 41:WM:224:ASP:OD1 | 41:WM:224:ASP:N | 2.54 | 0.41 |
| 41:WM:317:PHE:O | 41:WM:353:VAL:HA | 2.20 | 0.41 |
| 41:WN:103:LYS:HE2 | 41:WN:103:LYS:HB3 | 1.55 | 0.41 |
| 41:WN:116:VAL:O | 41:WN:120:VAL:HG23 | 2.21 | 0.41 |
| 41:WN:240:LEU:HD13 | 41:WN:249:ASP:HB2 | 2.02 | 0.41 |
| 41:WP:47:ILE:HD12 | 41:WP:47:ILE:HA | 1.97 | 0.41 |
| 41:WP:273:LEU:HD23 | 41:WP:273:LEU:HA | 1.88 | 0.41 |
| 7:1T:579:VAL:HG23 | 8:1Y:160:LEU:HD22 | 2.03 | 0.41 |
| 7:1U:538:ARG:HD2 | 7:1U:540:LEU:HD23 | 2.03 | 0.41 |
| 8:1W:232:VAL:O | 8:1W:236:LYS:HG2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:1W:517:LYS:HA | 8:1W:520:ILE:HG22 | 2.02 | 0.41 |
| 8:1X:103:SER:HB2 | 8:1X:107:PHE:CB | 2.47 | 0.41 |
| 8:1X:274:ALA:O | 8:1X:277:ARG:HG3 | 2.21 | 0.41 |
| 10:2F:47:LEU:HA | 10:2F:47:LEU:HD23 | 1.87 | 0.41 |
| 13:2V:102:ARG:HB3 | 13:2V:118:ILE:HG13 | 2.03 | 0.41 |
| 15:3F:275:ARG:NH2 | 15:3F:276:ASP:OD1 | 2.46 | 0.41 |
| 16:3K:144:ILE:HG12 | 16:3K:254:LEU:HD11 | 2.03 | 0.41 |
| 16:3K:293:LEU:HD22 | 16:3K:363:LEU:HD13 | 2.03 | 0.41 |
| 17:3P:215:VAL:HG21 | 17:3P:350:ARG:HB2 | 2.04 | 0.41 |
| 17:3P:320:LYS:HB2 | 17:3P:320:LYS:HE2 | 1.75 | 0.41 |
| 17:3P:406:ARG:CZ | 17:3P:412:CYS:H | 2.34 | 0.41 |
| 17:3P:410:GLU:O | 17:3P:412:CYS:N | 2.54 | 0.41 |
| 17:3Q:471:GLU:O | 17:3Q:472:LYS:HB2 | 2.21 | 0.41 |
| 17:3R:191:PRO:O | 17:3R:194:VAL:HG12 | 2.21 | 0.41 |
| 17:3R:230:GLN:O | 17:3R:234:LYS:HG3 | 2.21 | 0.41 |
| 17:3R:320:LYS:HZ3 | 17:3R:321:LEU:H | 1.69 | 0.41 |
| 18:3U:184:ARG:O | 18:3U:188:GLU:HG2 | 2.21 | 0.41 |
| 20:4A:38:MET:H | 20:4A:38:MET:HG2 | 1.69 | 0.41 |
| 20:4A:175:ARG:O | 20:4A:176:ILE:C | 2.59 | 0.41 |
| 20:4B:347:ALA:HB2 | 40:MG:278:ALA:O | 2.21 | 0.41 |
| 21:4D:427:GLU:HB2 | 21:4D:502:ARG:HB2 | 2.04 | 0.41 |
| 21:4D:430:ILE:H | 21:4D:430:ILE:HG12 | 1.61 | 0.41 |
| 21:4E:34:ARG:HB3 | 21:4E:35:ASN:H | 1.75 | 0.41 |
| 22:4J:78:VAL:HG12 | 22:4J:107:TYR:HA | 2.02 | 0.41 |
| 22:4K:619:VAL:O | 22:4K:620:MET:C | 2.58 | 0.41 |
| 23:4M:253:TYR:O | 23:4M:255:PHE:N | 2.54 | 0.41 |
| 23:4P:250:VAL:O | 23:4P:253:TYR:HB2 | 2.21 | 0.41 |
| 23:4Q:253:TYR:OH | 40:EH:220:GLU:HB2 | 2.21 | 0.41 |
| 23:4R:203:PRO:HB3 | 40:DI:279:GLU:CD | 2.41 | 0.41 |
| 26:4V:166:ASP:OD1 | 26:4V:166:ASP:N | 2.54 | 0.41 |
| 31:5I:588:ASP:N | 31:5I:588:ASP:OD1 | 2.54 | 0.41 |
| 33:5N:424:GLN:O | 33:5N:427:LEU:HG | 2.21 | 0.41 |
| 34:5Q:158:ARG:CZ | 34:5R:490:ILE:HD11 | 2.51 | 0.41 |
| 36:5Y:205:LYS:HE2 | 36:5Y:205:LYS:HB2 | 1.91 | 0.41 |
| 38:6C:170:TYR:HB2 | 40:UH:161:TYR:CE1 | 2.56 | 0.41 |
| 40:AA:202:PHE:CE1 | 40:AA:377:LEU:HD13 | 2.56 | 0.41 |
| 40:AA:335:ILE:HG23 | 40:AA:341:ILE:HD13 | 2.03 | 0.41 |
| 40:AE:259:LEU:HD23 | 40:AE:259:LEU:HA | 1.94 | 0.41 |
| 40:AG:68:VAL:HG11 | 40:AG:149:PHE:CE2 | 2.56 | 0.41 |
| 40:AG:224:TYR:CD1 | 40:AG:227:LEU:HD12 | 2.56 | 0.41 |
| 40:AG:231:ILE:O | 40:AG:235:VAL:HG23 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:AN:385:PHE:HZ | 41:AN:408:PHE:HB3 | 1.84 | 0.41 |
| 40:BA:255:PHE:O | 40:BA:259:LEU:HB2 | 2.21 | 0.41 |
| 40:BE:35:GLN:HA | 40:BE:60:LYS:HA | 2.03 | 0.41 |
| 40:BE:209:ILE:H | 40:BE:209:ILE:HG13 | 1.74 | 0.41 |
| 40:BI:86:LEU:O | 40:BI:87:PHE:C | 2.59 | 0.41 |
| 40:BI:171:ILE:HD13 | 40:BI:171:ILE:HA | 1.84 | 0.41 |
| 40:BI:224:TYR:HE2 | 41:BP:246:LEU:HD23 | 1.86 | 0.41 |
| 40:BI:398:TYR:O | 40:BI:401:ARG:N | 2.54 | 0.41 |
| 41:BL:137:HIS:O | 41:BL:168:SER:HA | 2.21 | 0.41 |
| 41:BL:293:MET:HE3 | 41:BL:293:MET:HB2 | 1.84 | 0.41 |
| 41:BL:375:GLN:HB3 | 41:BL:422:VAL:HG13 | 2.03 | 0.41 |
| 41:BM:16:ILE:HG12 | 41:BM:226:ASN:OD1 | 2.21 | 0.41 |
| 41:BM:44:LEU:O | 41:BM:46:ARG:N | 2.54 | 0.41 |
| 41:BM:250:LEU:HA | 41:BM:250:LEU:HD12 | 1.79 | 0.41 |
| 41:BP:142:GLY:O | 41:BP:144:GLY:N | 2.54 | 0.41 |
| 41:BP:233:MET:C | 41:BP:235:GLY:H | 2.24 | 0.41 |
| 40:CA:103:TYR:O | 40:CA:106:GLY:N | 2.53 | 0.41 |
| 40:CA:222:PRO:HD2 | 41:CN:324:LYS:CG | 2.51 | 0.41 |
| 40:CF:6:SER:HA | 40:CF:136:LEU:O | 2.21 | 0.41 |
| 40:CG:143:GLY:N | 42:CG:501:GTP:O2A | 2.50 | 0.41 |
| 40:CH:335:ILE:HD13 | 40:CH:335:ILE:HA | 1.88 | 0.41 |
| 40:CI:384:ALA:HA | 40:CI:387:TRP:HD1 | 1.86 | 0.41 |
| 41:CL:293:MET:HE2 | 41:CL:293:MET:HB2 | 1.81 | 0.41 |
| 41:CM:75:SER:O | 41:CM:79:GLY:N | 2.53 | 0.41 |
| 41:CM:373:ALA:C | 41:CM:375:GLN:N | 2.74 | 0.41 |
| 41:CN:2:ARG:HD2 | 41:CN:240:LEU:HD23 | 2.03 | 0.41 |
| 41:CO:292:GLN:HG3 | 41:CO:298:ASN:CG | 2.41 | 0.41 |
| 40:DA:186:ASN:O | 40:DA:187:SER:C | 2.60 | 0.41 |
| 40:DA:407:TYR:O | 40:DA:410:GLU:HB2 | 2.21 | 0.41 |
| 40:DE:183:GLU:O | 40:DE:184:PRO:C | 2.58 | 0.41 |
| 40:DE:224:TYR:HB3 | 42:DE:501:GTP:N1 | 2.36 | 0.41 |
| 40:DE:259:LEU:O | 40:DE:261:PRO:HD3 | 2.20 | 0.41 |
| 40:DF:190:THR:O | 40:DF:191:THR:C | 2.59 | 0.41 |
| 40:DH:199:ASP:O | 40:DH:200:CYS:C | 2.59 | 0.41 |
| 40:DH:258:ASN:HB3 | 41:DP:179:VAL:HG13 | 2.02 | 0.41 |
| 40:DI:320:ARG:HG2 | 40:DI:356:ASN:HB2 | 2.03 | 0.41 |
| 41:DL:34:GLY:O | 41:DL:36:TYR:N | 2.54 | 0.41 |
| 41:DL:56:GLY:O | 41:DL:58:LYS:N | 2.54 | 0.41 |
| 41:DL:62:ARG:HB2 | 41:DL:62:ARG:NH1 | 2.36 | 0.41 |
| 41:DL:135:LEU:HG | 41:DL:137:HIS:CD2 | 2.56 | 0.41 |
| 41:DM:8:GLN:NE2 | 41:DM:65:LEU:HD23 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:DM:8:GLN:NE2 | 41:DM:14:ASN:HA | 2.36 | 0.41 |
| 41:DM:107:THR:O | 41:DM:108:GLU:C | 2.60 | 0.41 |
| 41:DN:202:ILE:H | 41:DN:202:ILE:HG12 | 1.78 | 0.41 |
| 41:DN:391:ARG:HE | 41:DN:391:ARG:HB3 | 1.49 | 0.41 |
| 41:DP:389:PHE:O | 41:DP:390:ARG:C | 2.59 | 0.41 |
| 41:EB:140:GLY:HA3 | 41:EB:171:PRO:HG3 | 2.03 | 0.41 |
| 40:EE:401:ARG:HD3 | 40:EE:401:ARG:HA | 1.83 | 0.41 |
| 40:EG:328:VAL:O | 40:EG:332:ILE:HG12 | 2.21 | 0.41 |
| 40:EH:224:TYR:HD2 | 40:EH:224:TYR:HA | 1.66 | 0.41 |
| 40:EH:276:ILE:H | 40:EH:276:ILE:HG12 | 1.42 | 0.41 |
| 40:EI:139:HIS:ND1 | 40:EI:170:SER:HB3 | 2.36 | 0.41 |
| 41:EM:186:THR:HG23 | 41:EM:415:MET:HE3 | 2.03 | 0.41 |
| 41:EM:318:ARG:HG2 | 41:EM:358:PRO:HD3 | 2.02 | 0.41 |
| 41:EP:139:LEU:HB2 | 41:EP:170:VAL:HA | 2.03 | 0.41 |
| 40:FA:228:ASN:OD1 | 40:FA:228:ASN:N | 2.52 | 0.41 |
| 40:FA:304:LYS:HD2 | 40:FA:304:LYS:HA | 1.85 | 0.41 |
| 40:FA:403:PHE:CZ | 41:FN:345:ILE:HD13 | 2.55 | 0.41 |
| 41:FB:178:THR:O | 41:FB:180:VAL:N | 2.53 | 0.41 |
| 40:FE:53:PHE:HA | 40:FE:62:VAL:O | 2.21 | 0.41 |
| 40:FE:277:SER:O | 40:FE:279:GLU:N | 2.54 | 0.41 |
| 40:FE:324:VAL:HB | 40:FE:327:ASP:HB2 | 2.02 | 0.41 |
| 40:FH:324:VAL:HB | 40:FH:327:ASP:HB2 | 2.03 | 0.41 |
| 40:FI:97:GLU:OE2 | 41:FP:251:ARG:NH1 | 2.54 | 0.41 |
| 41:FM:246:LEU:HD23 | 41:FM:246:LEU:HA | 1.87 | 0.41 |
| 41:FN:177:ASP:OD1 | 41:FN:178:THR:N | 2.54 | 0.41 |
| 41:FN:310:TYR:CD1 | 41:FN:371:SER:HB3 | 2.55 | 0.41 |
| 40:GA:352:LYS:HE3 | 40:GA:352:LYS:HB3 | 1.59 | 0.41 |
| 40:GE:326:LYS:H | 40:GE:326:LYS:HG2 | 1.74 | 0.41 |
| 40:GE:435:GLY:O | 40:GE:436:MET:C | 2.58 | 0.41 |
| 40:GF:255:PHE:CZ | 40:GF:318:LEU:HD21 | 2.56 | 0.41 |
| 41:GM:183:TYR:OH | 41:GM:393:ALA:O | 2.32 | 0.41 |
| 41:GN:107:THR:O | 41:GN:109:GLY:N | 2.54 | 0.41 |
| 41:GN:128:ASP:O | 41:GN:129:CYS:HB2 | 2.20 | 0.41 |
| 41:GP:21:TRP:HA | 41:GP:24:ILE:HG22 | 2.02 | 0.41 |
| 40:HE:86:LEU:O | 40:HE:87:PHE:C | 2.59 | 0.41 |
| 40:HE:163:LYS:H | 40:HE:163:LYS:HG3 | 1.58 | 0.41 |
| 40:HE:421:ARG:HA | 40:HE:421:ARG:HD2 | 1.19 | 0.41 |
| 40:HG:205:ASP:HB3 | 40:HG:303:VAL:HA | 2.01 | 0.41 |
| 40:HH:369:LYS:HE3 | 40:HH:369:LYS:HB3 | 1.91 | 0.41 |
| 41:HM:24:ILE:HD12 | 41:HM:24:ILE:HA | 1.91 | 0.41 |
| 41:HN:28:HIS:NE2 | 41:HN:241:ARG:HD2 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:HN:39:ASP:N | 41:HN:39:ASP:OD2 | 2.54 | 0.41 |
| 41:HN:178:THR:HG23 | 41:HN:181:GLU:HG3 | 2.01 | 0.41 |
| 41:HN:200:TYR:CD1 | 41:HN:266:PHE:HB2 | 2.56 | 0.41 |
| 41:HO:112:LEU:O | 41:HO:116:VAL:HG23 | 2.21 | 0.41 |
| 40:IF:319:TYR:HB2 | 40:IF:355:ILE:HG22 | 2.03 | 0.41 |
| 40:IH:130:THR:HG22 | 41:IP:94:GLN:HG2 | 2.03 | 0.41 |
| 40:II:314:ALA:N | 40:II:379:ASN:OD1 | 2.53 | 0.41 |
| 41:IO:68:LEU:HG | 41:IO:97:ALA:HB2 | 2.02 | 0.41 |
| 40:JD:137:ILE:HD11 | 40:JD:168:GLU:HG3 | 2.03 | 0.41 |
| 40:JF:192:HIS:ND1 | 40:JF:423:ASP:OD1 | 2.36 | 0.41 |
| 40:JF:217:LEU:HD11 | 40:JF:366:ASP:HB3 | 2.03 | 0.41 |
| 40:JF:253:THR:HA | 40:JF:256:GLN:HG2 | 2.02 | 0.41 |
| 40:JF:359:PRO:HA | 40:JF:360:PRO:HD3 | 1.94 | 0.41 |
| 41:JM:85:PHE:HB2 | 41:JM:90:PHE:CE2 | 2.56 | 0.41 |
| 41:JM:421:PRO:C | 41:JM:423:VAL:H | 2.24 | 0.41 |
| 41:JN:1:MET:SD | 41:JN:128:ASP:HB2 | 2.61 | 0.41 |
| 40:KH:311:LYS:HG2 | 40:KH:342:GLN:HG2 | 2.02 | 0.41 |
| 41:KL:67:ASP:O | 41:KL:92:PHE:HA | 2.21 | 0.41 |
| 41:KO:136:THR:HG22 | 41:KO:167:PHE:HB2 | 2.03 | 0.41 |
| 41:KO:170:VAL:HG11 | 41:KO:377:LEU:HD11 | 2.02 | 0.41 |
| 41:LB:114:ASP:N | 41:LB:114:ASP:OD1 | 2.54 | 0.41 |
| 40:LD:285:GLN:HB2 | 40:LD:287:SER:HB2 | 2.03 | 0.41 |
| 40:LE:273:ALA:HB1 | 40:LE:274:PRO:HD2 | 2.03 | 0.41 |
| 40:LG:401:ARG:HA | 40:LG:401:ARG:HD3 | 1.85 | 0.41 |
| 41:LO:132:GLY:HA2 | 41:LO:162:ARG:HB3 | 2.03 | 0.41 |
| 40:MA:421:ARG:HH12 | 40:MA:425:ALA:HB2 | 1.85 | 0.41 |
| 40:MD:55:GLU:OE1 | 40:MD:61:HIS:NE2 | 2.54 | 0.41 |
| 40:MF:140:SER:O | 40:MF:142:GLY:N | 2.54 | 0.41 |
| 40:MF:316:CYS:SG | 40:MF:352:LYS:HB3 | 2.61 | 0.41 |
| 40:MF:407:TYR:HB3 | 40:MF:412:MET:SD | 2.61 | 0.41 |
| 40:MG:206:ASN:O | 40:MG:207:GLU:C | 2.58 | 0.41 |
| 40:MH:181:VAL:HG11 | 41:MO:312:THR:HG22 | 2.02 | 0.41 |
| 40:MH:324:VAL:O | 40:MH:325:PRO:C | 2.58 | 0.41 |
| 40:MH:326:LYS:HG3 | 40:MH:327:ASP:N | 2.36 | 0.41 |
| 40:MH:422:GLU:O | 40:MH:425:ALA:HB3 | 2.21 | 0.41 |
| 41:MM:328:GLU:OE2 | 41:MM:329:GLN:NE2 | 2.47 | 0.41 |
| 41:MP:131:GLN:HE21 | 41:MP:250:LEU:HB2 | 1.86 | 0.41 |
| 40:NA:177:VAL:O | 41:NN:347:ASN:ND2 | 2.51 | 0.41 |
| 40:NA:219:ILE:HD11 | 40:NA:222:PRO:HB3 | 2.02 | 0.41 |
| 40:NA:346:TRP:CD1 | 41:NB:391:ARG:HG2 | 2.56 | 0.41 |
| 41:NB:207:LEU:HB3 | 41:NB:225:LEU:HD12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:ND:104:ALA:CB | 40:ND:410:GLU:HB3 | 2.51 | 0.41 |
| 40:ND:217:LEU:HD12 | 40:ND:217:LEU:HA | 1.91 | 0.41 |
| 40:ND:265:ILE:HG23 | 40:ND:431:TYR:CZ | 2.56 | 0.41 |
| 40:NE:38:SER:OG | 40:NE:39:ASP:N | 2.54 | 0.41 |
| 40:NE:115:ILE:HA | 40:NE:118:VAL:HG22 | 2.01 | 0.41 |
| 40:NF:257:THR:HG21 | 41:NN:98:GLY:O | 2.21 | 0.41 |
| 40:NH:6:SER:O | 40:NH:65:ALA:HA | 2.20 | 0.41 |
| 40:OF:245:ASP:OD1 | 40:OF:245:ASP:N | 2.44 | 0.41 |
| 40:OH:74:VAL:HG13 | 40:OH:75:ILE:H | 1.86 | 0.41 |
| 40:OH:177:VAL:O | 40:OH:178:SER:HB3 | 2.20 | 0.41 |
| 40:OH:324:VAL:HG21 | 41:OP:219:THR:HB | 2.03 | 0.41 |
| 40:OH:391:ASP:OD1 | 40:OH:421:ARG:NE | 2.54 | 0.41 |
| 40:PA:210:TYR:CE1 | 40:PA:227:LEU:HD11 | 2.55 | 0.41 |
| 40:PD:21:TRP:HA | 40:PD:24:TYR:HD2 | 1.86 | 0.41 |
| 40:PG:121:ARG:HA | 40:PG:124:LYS:HG2 | 2.02 | 0.41 |
| 40:PH:6:SER:HA | 40:PH:136:LEU:O | 2.21 | 0.41 |
| 40:PH:51:THR:O | 40:PH:64:ARG:NH1 | 2.54 | 0.41 |
| 40:PH:88:HIS:HE1 | 40:PH:90:GLU:HB2 | 1.86 | 0.41 |
| 41:PL:16:ILE:HD11 | 43:PL:501:GDP:C2 | 2.56 | 0.41 |
| 41:PP:189:VAL:O | 41:PP:193:VAL:HG23 | 2.21 | 0.41 |
| 41:QB:137:HIS:HD2 | 41:QB:168:SER:HA | 1.86 | 0.41 |
| 41:QB:213:ARG:HE | 41:QB:213:ARG:HB2 | 1.57 | 0.41 |
| 41:QB:248:ALA:HB2 | 41:QB:352:ALA:HB2 | 2.03 | 0.41 |
| 41:QB:290:THR:HG22 | 41:QB:317:PHE:HZ | 1.84 | 0.41 |
| 40:QE:60:LYS:HZ1 | 40:RE:283:HIS:HA | 1.83 | 0.41 |
| 40:QE:213:CYS:HA | 40:QE:217:LEU:HB2 | 2.03 | 0.41 |
| 40:QE:304:LYS:HD3 | 40:QE:304:LYS:HA | 1.59 | 0.41 |
| 40:QF:56:THR:OG1 | 40:QF:60:LYS:O | 2.30 | 0.41 |
| 40:QG:200:CYS:HA | 40:QG:266:HIS:HB2 | 2.02 | 0.41 |
| 41:QM:253:LEU:HD21 | 41:QM:368:ILE:HG21 | 2.03 | 0.41 |
| 41:QN:39:ASP:N | 41:QN:39:ASP:OD1 | 2.54 | 0.41 |
| 41:QN:226:ASN:ND2 | 43:QN:502:GDP:O6 | 2.44 | 0.41 |
| 41:QP:267:MET:HE1 | 41:QP:367:PHE:CE2 | 2.52 | 0.41 |
| 40:RA:311:LYS:HE3 | 40:RA:344:VAL:HA | 2.02 | 0.41 |
| 40:RG:54:SER:OG | 40:RG:62:VAL:HG12 | 2.21 | 0.41 |
| 40:RG:176:GLN:NE2 | 40:RG:207:GLU:OE1 | 2.54 | 0.41 |
| 40:RH:31:GLN:HG2 | 40:RH:34:GLY:O | 2.21 | 0.41 |
| 40:RI:221:ARG:HG2 | 41:RP:322:SER:HB3 | 2.02 | 0.41 |
| 41:RM:39:ASP:N | 41:RM:39:ASP:OD1 | 2.54 | 0.41 |
| 41:SB:346:PRO:HG2 | 40:SG:393:LYS:NZ | 2.36 | 0.41 |
| 41:SL:226:ASN:N | 43:SL:502:GDP:HN21 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SP:12:CYS:O | 41:SP:16:ILE:HD12 | 2.20 | 0.41 |
| 40:TE:179:THR:HG21 | 41:TL:246:LEU:HD11 | 2.02 | 0.41 |
| 40:TG:167:LEU:HD11 | 40:TG:252:LEU:HD22 | 2.03 | 0.41 |
| 40:TG:236:SER:O | 40:TG:240:ALA:HB2 | 2.21 | 0.41 |
| 41:TN:226:ASN:ND2 | 43:TN:502:GDP:O6 | 2.53 | 0.41 |
| 41:TN:271:ALA:HB1 | 41:TN:292:GLN:HG2 | 2.03 | 0.41 |
| 41:TO:8:GLN:HG2 | 41:TO:14:ASN:HA | 2.03 | 0.41 |
| 41:TP:406:MET:O | 41:TP:409:THR:OG1 | 2.24 | 0.41 |
| 40:UA:316:CYS:O | 40:UA:376:MET:HA | 2.21 | 0.41 |
| 41:UB:293:MET:HE3 | 41:UB:367:PHE:HD1 | 1.85 | 0.41 |
| 40:UE:277:SER:O | 40:UE:279:GLU:N | 2.52 | 0.41 |
| 40:UF:125:LEU:HD23 | 40:UF:125:LEU:HA | 1.82 | 0.41 |
| 40:UF:136:LEU:HD13 | 40:UF:138:PHE:HZ | 1.87 | 0.41 |
| 40:UF:146:GLY:O | 40:UF:150:THR:HG23 | 2.21 | 0.41 |
| 40:UF:430:ASP:O | 40:UF:431:TYR:C | 2.59 | 0.41 |
| 40:UH:245:ASP:OD2 | 40:UH:245:ASP:N | 2.50 | 0.41 |
| 40:UI:49:PHE:O | 40:UI:51:THR:N | 2.53 | 0.41 |
| 40:UI:152:LEU:O | 40:UI:153:LEU:C | 2.58 | 0.41 |
| 40:UI:153:LEU:HD12 | 40:UI:153:LEU:HA | 1.91 | 0.41 |
| 40:UI:228:ASN:O | 40:UI:231:ILE:N | 2.54 | 0.41 |
| 40:UI:272:TYR:HD1 | 40:UI:272:TYR:HA | 1.81 | 0.41 |
| 41:UM:99:ASN:HA | 41:UM:142:GLY:HA3 | 2.02 | 0.41 |
| 41:UO:286:VAL:HB | 41:UO:325:GLU:HB3 | 2.01 | 0.41 |
| 41:UP:392:LYS:HB3 | 41:UP:392:LYS:HE3 | 1.50 | 0.41 |
| 40:VA:235:VAL:HA | 40:VA:238:ILE:HG22 | 2.02 | 0.41 |
| 41:VB:58:LYS:HA | 41:VB:58:LYS:HD3 | 1.80 | 0.41 |
| 41:VB:133:PHE:HB2 | 41:VB:164:MET:SD | 2.61 | 0.41 |
| 41:VB:245:GLN:HE22 | 41:VB:320:ARG:HH12 | 1.69 | 0.41 |
| 40:VG:79:ARG:NH2 | 40:VG:92:LEU:O | 2.54 | 0.41 |
| 40:VG:88:HIS:HA | 40:VG:89:PRO:HD3 | 1.88 | 0.41 |
| 40:VH:224:TYR:O | 40:VH:228:ASN:ND2 | 2.54 | 0.41 |
| 40:VI:118:VAL:HG11 | 40:VI:149:PHE:HZ | 1.85 | 0.41 |
| 40:VJ:112:LYS:HA | 40:VJ:115:ILE:HG22 | 2.03 | 0.41 |
| 41:VO:22:GLU:HG3 | 41:VO:81:PHE:HB2 | 2.03 | 0.41 |
| 41:WB:36:TYR:CZ | 41:WB:44:LEU:HB2 | 2.56 | 0.41 |
| 41:WB:155:ILE:HD13 | 41:WB:155:ILE:HA | 1.90 | 0.41 |
| 41:WB:324:LYS:HG2 | 40:WG:222:PRO:HD2 | 2.02 | 0.41 |
| 40:WG:31:GLN:HE21 | 40:WG:37:PRO:HG3 | 1.85 | 0.41 |
| 40:WG:271:THR:OG1 | 40:WG:376:MET:HB3 | 2.21 | 0.41 |
| 40:WG:328:VAL:O | 40:WG:332:ILE:HG12 | 2.22 | 0.41 |
| 41:WM:9:ALA:HA | 41:WM:66:VAL:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:WM:245:GLN:O | 41:WM:246:LEU:HB2 | 2.22 | 0.41 |
| 41:WN:146:GLY:O | 41:WN:147:MET:C | 2.60 | 0.41 |
| 41:WN:197:ASP:OD1 | 41:WN:197:ASP:N | 2.54 | 0.41 |
| 41:WN:239:CYS:C | 41:WN:241:ARG:H | 2.25 | 0.41 |
| 41:WP:240:LEU:HD12 | 41:WP:240:LEU:HA | 1.93 | 0.41 |
| 7:1T:264:LEU:HD12 | 7:1T:264:LEU:HA | 1.75 | 0.40 |
| 7:1U:187:LEU:HD23 | 7:1U:194:ILE:HG12 | 2.03 | 0.40 |
| 7:1U:254:SER:OG | 7:1U:293:ILE:O | 2.39 | 0.40 |
| 7:1U:282:LYS:HE2 | 7:1U:282:LYS:HB2 | 1.93 | 0.40 |
| 8:1W:228:GLN:HA | 8:1W:231:GLU:HG3 | 2.03 | 0.40 |
| 10:2F:47:LEU:HD22 | 40:MA:265:ILE:HD11 | 2.03 | 0.40 |
| 11:2I:151:TYR:OH | 40:MG:384:ALA:HB1 | 2.22 | 0.40 |
| 11:2I:186:LYS:HG3 | 11:2I:251:TYR:HD2 | 1.85 | 0.40 |
| 11:2J:123:PRO:HB2 | 11:2J:136:LEU:HB3 | 2.03 | 0.40 |
| 12:2R:41:GLY:HA3 | 41:AP:306:ARG:HH11 | 1.86 | 0.40 |
| 13:2U:70:GLY:O | 13:2U:71:ILE:C | 2.59 | 0.40 |
| 13:2V:39:ASP:HB2 | 13:2V:46:VAL:HG21 | 2.03 | 0.40 |
| 14:3B:74:VAL:HG22 | 40:LD:155:GLU:OE2 | 2.21 | 0.40 |
| 15:3E:392:HIS:HA | 15:3E:395:ARG:CZ | 2.51 | 0.40 |
| 16:3K:110:LEU:HB2 | 16:3K:144:ILE:HG21 | 2.02 | 0.40 |
| 16:3L:138:HIS:HD2 | 16:3M:4:LEU:HD13 | 1.84 | 0.40 |
| 16:3L:290:ILE:O | 16:3L:294:GLN:HG2 | 2.22 | 0.40 |
| 17:3P:274:LEU:HD12 | 17:3P:274:LEU:HA | 1.89 | 0.40 |
| 17:3Q:347:PHE:O | 17:3Q:348:THR:C | 2.59 | 0.40 |
| 18:3T:360:ARG:HH21 | 18:3T:374:GLN:HG3 | 1.86 | 0.40 |
| 20:4B:230:ARG:HB2 | 20:4B:234:GLN:HE22 | 1.87 | 0.40 |
| 21:4E:125:TYR:CE1 | 21:4E:151:ARG:HG3 | 2.56 | 0.40 |
| 21:4E:232:LEU:HD12 | 21:4E:232:LEU:HA | 1.96 | 0.40 |
| 22:4H:273:ASP:HB2 | 22:4H:275:MET:SD | 2.62 | 0.40 |
| 22:4J:263:LYS:NZ | 40:CF:46:ASP:OD2 | 2.41 | 0.40 |
| 22:4J:285:PRO:HA | 22:4J:332:PHE:HD1 | 1.85 | 0.40 |
| 22:4K:677:LEU:CA | 22:4K:680:LYS:HB2 | 2.47 | 0.40 |
| 23:4M:91:ILE:HD11 | 40:AG:79:ARG:CG | 2.51 | 0.40 |
| 23:4M:178:ASP:HB2 | 23:4M:179:PRO:HD2 | 2.03 | 0.40 |
| 23:4M:193:ARG:HE | 23:4M:196:PHE:HD2 | 1.68 | 0.40 |
| 23:4N:33:MET:HG2 | 41:CM:320:ARG:HH22 | 1.83 | 0.40 |
| 23:4N:250:VAL:O | 23:4N:253:TYR:HB2 | 2.21 | 0.40 |
| 23:4Q:19:ILE:O | 23:4Q:20:PRO:C | 2.59 | 0.40 |
| 23:4Q:269:LEU:H | 23:4Q:269:LEU:HG | 1.62 | 0.40 |
| 25:4T:422:ASP:OD1 | 25:4T:423:THR:N | 2.49 | 0.40 |
| 26:4V:140:HIS:HD2 | 26:4V:146:LEU:HD22 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:4Y:229:VAL:O | 27:4Y:246:VAL:HA | 2.21 | 0.40 |
| 30:5G:55:LYS:HB3 | 30:5G:60:LYS:HD3 | 2.02 | 0.40 |
| 31:5I:577:ARG:HA | 31:5I:577:ARG:HD3 | 1.82 | 0.40 |
| 33:5N:267:ASN:OD1 | 41:HO:362:LYS:NZ | 2.38 | 0.40 |
| 33:5O:135:LYS:HA | 33:5O:135:LYS:HE3 | 2.02 | 0.40 |
| 34:5R:375:LYS:H | 34:5R:375:LYS:HG3 | 1.49 | 0.40 |
| 36:5X:35:THR:O | 36:5X:37:ALA:N | 2.53 | 0.40 |
| 36:5X:248:ASP:OD1 | 36:5X:256:ARG:NH2 | 2.54 | 0.40 |
| 39:6H:30:ALA:HB2 | 39:6H:67:ILE:HD11 | 2.03 | 0.40 |
| 40:AA:115:ILE:HA | 40:AA:118:VAL:HG12 | 2.03 | 0.40 |
| 41:AB:100:ASN:HB3 | 41:AB:103:LYS:HB2 | 2.03 | 0.40 |
| 40:AH:215:ARG:NH2 | 40:AH:299:ALA:O | 2.54 | 0.40 |
| 41:AM:139:LEU:HD12 | 41:AM:139:LEU:HA | 1.90 | 0.40 |
| 41:BB:7:LEU:HA | 41:BB:64:VAL:HG13 | 2.03 | 0.40 |
| 41:BB:26:ASP:HB2 | 41:BB:359:ARG:HH21 | 1.86 | 0.40 |
| 41:BB:130:LEU:HD12 | 41:BB:130:LEU:HA | 1.95 | 0.40 |
| 41:BB:259:PRO:O | 40:BG:405:HIS:HE1 | 2.04 | 0.40 |
| 40:BI:72:PRO:HD2 | 41:BP:2:ARG:HH11 | 1.86 | 0.40 |
| 41:BM:216:LYS:HE2 | 41:BM:216:LYS:HB2 | 1.78 | 0.40 |
| 41:BM:393:ALA:O | 41:BM:395:LEU:N | 2.54 | 0.40 |
| 41:BN:139:LEU:HD12 | 41:BN:139:LEU:HA | 1.90 | 0.40 |
| 41:BP:211:CYS:HA | 41:BP:215:LEU:HD12 | 2.03 | 0.40 |
| 41:BP:271:ALA:HB3 | 41:BP:272:PRO:CD | 2.51 | 0.40 |
| 41:BP:271:ALA:O | 41:BP:273:LEU:N | 2.52 | 0.40 |
| 41:BP:331:LEU:HD12 | 41:BP:331:LEU:HA | 1.89 | 0.40 |
| 40:CA:280:LYS:H | 40:CA:280:LYS:HG2 | 1.50 | 0.40 |
| 41:CB:7:LEU:HB3 | 41:CB:135:LEU:HD13 | 2.04 | 0.40 |
| 41:CB:87:PRO:HA | 41:CB:90:PHE:HD1 | 1.86 | 0.40 |
| 40:CE:7:VAL:HG12 | 40:CE:9:VAL:HG23 | 2.04 | 0.40 |
| 40:CF:138:PHE:CE1 | 40:CF:235:VAL:HG11 | 2.56 | 0.40 |
| 40:CF:176:GLN:HG2 | 41:CM:331:LEU:HD11 | 2.03 | 0.40 |
| 40:CI:88:HIS:HA | 40:CI:89:PRO:HD3 | 1.90 | 0.40 |
| 41:CL:323:MET:SD | 41:CL:353:VAL:HG21 | 2.61 | 0.40 |
| 41:CM:24:ILE:HG23 | 41:CM:234:SER:HB2 | 2.03 | 0.40 |
| 41:CM:86:ARG:HH12 | 41:DM:282:ARG:HA | 1.86 | 0.40 |
| 41:CN:49:VAL:HG21 | 41:CN:240:LEU:O | 2.21 | 0.40 |
| 41:CO:284:LEU:HD12 | 41:CO:284:LEU:HA | 1.99 | 0.40 |
| 41:CO:285:THR:O | 41:CO:286:VAL:C | 2.60 | 0.40 |
| 41:CP:313:VAL:HB | 41:CP:367:PHE:CE1 | 2.50 | 0.40 |
| 40:DA:51:THR:O | 40:DA:64:ARG:HD2 | 2.20 | 0.40 |
| 40:DA:163:LYS:O | 40:DA:165:SER:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:DA:216:ASN:ND2 | 40:DA:275:VAL:HG13 | 2.36 | 0.40 |
| 40:DA:313:MET:O | 40:DA:314:ALA:HB2 | 2.21 | 0.40 |
| 40:DA:406:TRP:CE3 | 40:DA:406:TRP:HA | 2.55 | 0.40 |
| 40:DA:412:MET:O | 40:DA:413:GLU:C | 2.58 | 0.40 |
| 40:DA:435:GLY:O | 40:DA:436:MET:C | 2.59 | 0.40 |
| 41:DB:61:PRO:HG2 | 41:DB:84:ILE:CG2 | 2.44 | 0.40 |
| 41:DB:174:LYS:HD2 | 41:DB:175:VAL:HG12 | 2.02 | 0.40 |
| 41:DB:182:PRO:HG3 | 41:DB:384:GLN:HB3 | 2.02 | 0.40 |
| 40:DE:168:GLU:O | 40:DE:201:ALA:HA | 2.21 | 0.40 |
| 40:DE:216:ASN:CB | 40:DE:275:VAL:HB | 2.45 | 0.40 |
| 40:DF:98:ASP:O | 40:DF:110:ILE:HG12 | 2.21 | 0.40 |
| 40:DG:35:GLN:OE1 | 40:DG:35:GLN:N | 2.40 | 0.40 |
| 40:DG:315:CYS:HA | 40:DG:377:LEU:O | 2.21 | 0.40 |
| 40:DH:209:ILE:HB | 40:DH:227:LEU:HD12 | 2.03 | 0.40 |
| 40:DI:65:ALA:O | 40:DI:91:GLN:HG2 | 2.21 | 0.40 |
| 40:DI:288:VAL:HG22 | 40:DI:372:ARG:HD2 | 2.03 | 0.40 |
| 41:DM:27:GLU:HB3 | 41:DM:28:HIS:H | 1.73 | 0.40 |
| 41:DM:170:VAL:HB | 41:DM:171:PRO:HD2 | 2.02 | 0.40 |
| 41:DN:21:TRP:HZ2 | 41:DN:63:ALA:HB2 | 1.86 | 0.40 |
| 41:DN:290:THR:OG1 | 41:DN:291:GLN:N | 2.54 | 0.40 |
| 41:DN:334:GLN:HE22 | 41:DN:348:ASN:H | 1.69 | 0.40 |
| 41:DP:136:THR:HG23 | 41:DP:167:PHE:O | 2.20 | 0.40 |
| 40:EA:255:PHE:CZ | 40:EA:318:LEU:HD21 | 2.55 | 0.40 |
| 40:EA:311:LYS:N | 40:EA:381:THR:OG1 | 2.46 | 0.40 |
| 41:EB:260:PHE:HE2 | 41:EB:344:TRP:HH2 | 1.69 | 0.40 |
| 40:EF:10:GLY:HA2 | 40:EF:145:THR:HG23 | 2.02 | 0.40 |
| 40:EH:131:GLY:O | 40:EH:133:GLN:N | 2.54 | 0.40 |
| 40:EI:219:ILE:HD12 | 40:EI:221:ARG:H | 1.86 | 0.40 |
| 41:EL:309:ARG:N | 41:EL:372:THR:OG1 | 2.54 | 0.40 |
| 41:EM:103:LYS:O | 41:EM:105:HIS:N | 2.54 | 0.40 |
| 41:EM:342:VAL:HB | 41:EM:344:TRP:HD1 | 1.86 | 0.40 |
| 41:EM:397:TRP:O | 41:EM:400:GLY:N | 2.54 | 0.40 |
| 41:EN:3:GLU:HA | 41:EN:49:VAL:HA | 2.03 | 0.40 |
| 41:EN:28:HIS:ND1 | 41:EN:47:ILE:HG13 | 2.36 | 0.40 |
| 41:EN:167:PHE:CZ | 41:EN:233:MET:HG2 | 2.56 | 0.40 |
| 41:EO:101:TRP:HD1 | 41:EO:146:GLY:HA2 | 1.86 | 0.40 |
| 40:FA:115:ILE:HG13 | 40:FA:119:LEU:HD23 | 2.04 | 0.40 |
| 41:FB:100:ASN:HB2 | 41:FB:103:LYS:HB2 | 2.03 | 0.40 |
| 41:FB:257:MET:CE | 41:FB:314:ALA:HB2 | 2.51 | 0.40 |
| 41:FB:286:VAL:HG22 | 41:FB:321:MET:HE2 | 2.02 | 0.40 |
| 40:FE:115:ILE:HA | 40:FE:118:VAL:HG12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:FE:210:TYR:HE1 | 40:FE:227:LEU:HD11 | 1.86 | 0.40 |
| 40:FI:164:LYS:HE2 | 40:FI:164:LYS:HB2 | 1.88 | 0.40 |
| 41:FO:12:CYS:SG | 41:FO:138:SER:HB3 | 2.62 | 0.40 |
| 41:FP:149:THR:HG21 | 41:FP:188:SER:HA | 2.02 | 0.40 |
| 40:GA:171:ILE:HD12 | 42:GA:501:GTP:H1' | 2.03 | 0.40 |
| 41:GB:145:SER:HB2 | 41:GB:188:SER:HB3 | 2.02 | 0.40 |
| 40:GE:174:ALA:CB | 40:GE:178:SER:H | 2.34 | 0.40 |
| 40:GE:338:LYS:HE3 | 40:GE:338:LYS:HB3 | 1.77 | 0.40 |
| 40:GG:326:LYS:HA | 40:GG:329:ASN:HB2 | 2.02 | 0.40 |
| 40:GI:259:LEU:HD23 | 40:GI:259:LEU:HA | 1.90 | 0.40 |
| 41:GM:345:ILE:HG22 | 41:GM:348:ASN:HB3 | 2.03 | 0.40 |
| 41:GN:262:ARG:O | 41:GN:264:HIS:N | 2.54 | 0.40 |
| 40:HE:116:ASP:O | 40:HE:117:LEU:C | 2.59 | 0.40 |
| 40:HE:248:LEU:HD22 | 40:HE:248:LEU:HA | 1.76 | 0.40 |
| 40:HF:11:GLN:HG3 | 40:HF:74:VAL:HG11 | 2.03 | 0.40 |
| 40:HI:71:GLU:HB3 | 40:HI:98:ASP:HA | 2.03 | 0.40 |
| 40:HI:421:ARG:HD2 | 40:HI:421:ARG:HA | 1.63 | 0.40 |
| 41:HN:239:CYS:HB2 | 41:HN:248:ALA:H | 1.86 | 0.40 |
| 40:IF:224:TYR:CZ | 41:IM:323:MET:HG2 | 2.56 | 0.40 |
| 40:II:71:GLU:HB3 | 40:II:98:ASP:HA | 2.03 | 0.40 |
| 41:IN:159:TYR:HB3 | 41:IN:162:ARG:HD3 | 2.02 | 0.40 |
| 41:IP:87:PRO:HA | 41:IP:90:PHE:CD2 | 2.56 | 0.40 |
| 40:JA:254:GLU:O | 40:JA:258:ASN:HB2 | 2.21 | 0.40 |
| 41:JB:294:PHE:HZ | 41:JB:313:VAL:HG11 | 1.86 | 0.40 |
| 40:JD:391:ASP:HB3 | 40:JD:421:ARG:CZ | 2.51 | 0.40 |
| 40:JE:137:ILE:HG21 | 40:JE:137:ILE:HD13 | 1.89 | 0.40 |
| 40:JE:297:GLU:HA | 40:JE:298:PRO:HD3 | 1.95 | 0.40 |
| 40:JF:70:LEU:HD12 | 40:JF:99:ALA:HB2 | 2.02 | 0.40 |
| 40:JH:234:ILE:HG23 | 40:JH:375:CYS:SG | 2.61 | 0.40 |
| 41:JL:202:ILE:HD13 | 41:JL:229:VAL:HG13 | 2.03 | 0.40 |
| 41:JL:320:ARG:HE | 41:JL:320:ARG:HB3 | 1.77 | 0.40 |
| 41:JM:2:ARG:HA | 41:JM:129:CYS:O | 2.20 | 0.40 |
| 41:JM:24:ILE:O | 41:JM:27:GLU:HG3 | 2.21 | 0.40 |
| 41:JM:103:LYS:HA | 41:JM:107:THR:OG1 | 2.21 | 0.40 |
| 41:JM:167:PHE:HB3 | 41:JM:202:ILE:HD11 | 2.03 | 0.40 |
| 41:JO:274:THR:OG1 | 41:JO:282:ARG:NH1 | 2.54 | 0.40 |
| 40:KA:217:LEU:HA | 40:KA:277:SER:HB2 | 2.01 | 0.40 |
| 40:KE:349:THR:HG23 | 41:KM:176:SER:HB3 | 2.02 | 0.40 |
| 40:KF:210:TYR:CE1 | 40:KF:227:LEU:HD11 | 2.56 | 0.40 |
| 40:KG:60:LYS:HG2 | 40:LG:282:TYR:O | 2.21 | 0.40 |
| 40:KG:326:LYS:NZ | 41:KO:208:TYR:HB2 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:KH:370:VAL:HG22 | 40:KH:372:ARG:H | 1.86 | 0.40 |
| 40:KH:424:MET:O | 40:KH:428:GLU:HG2 | 2.22 | 0.40 |
| 41:KL:111:GLU:H | 41:KL:111:GLU:HG2 | 1.30 | 0.40 |
| 41:KL:294:PHE:CZ | 41:KL:313:VAL:HG11 | 2.56 | 0.40 |
| 41:LB:273:LEU:O | 41:LB:292:GLN:NE2 | 2.39 | 0.40 |
| 40:LD:28:HIS:NE2 | 40:LD:243:ARG:HD2 | 2.36 | 0.40 |
| 40:LE:70:LEU:HB2 | 40:LE:145:THR:HG22 | 2.03 | 0.40 |
| 40:LF:11:GLN:HG3 | 40:LF:15:GLN:HE21 | 1.86 | 0.40 |
| 40:LF:22:GLU:HG2 | 40:LF:26:LEU:HD23 | 2.03 | 0.40 |
| 40:LF:323:VAL:CG1 | 40:LF:355:ILE:HG23 | 2.51 | 0.40 |
| 40:LG:72:PRO:HB2 | 40:LG:73:THR:H | 1.76 | 0.40 |
| 40:LH:335:ILE:HD13 | 40:LH:335:ILE:HA | 1.90 | 0.40 |
| 41:LM:372:THR:O | 41:LM:375:GLN:HG3 | 2.21 | 0.40 |
| 41:LO:318:ARG:HG2 | 41:LO:358:PRO:HD3 | 2.02 | 0.40 |
| 40:MA:99:ALA:HB2 | 40:MA:110:ILE:HD11 | 2.02 | 0.40 |
| 40:MA:99:ALA:CB | 40:MA:144:GLY:HA3 | 2.51 | 0.40 |
| 40:MG:96:LYS:HB3 | 40:MG:96:LYS:HE3 | 1.67 | 0.40 |
| 40:MH:190:THR:O | 40:MH:194:THR:HG23 | 2.22 | 0.40 |
| 41:ML:202:ILE:HD13 | 41:ML:229:VAL:HG13 | 2.03 | 0.40 |
| 41:ML:344:TRP:HD1 | 41:ML:428:CYS:HG | 1.68 | 0.40 |
| 41:MO:147:MET:HE2 | 41:MO:147:MET:HB2 | 1.90 | 0.40 |
| 41:MO:245:GLN:H | 41:MO:245:GLN:HG2 | 1.63 | 0.40 |
| 40:NA:67:PHE:HB3 | 40:NA:75:ILE:HD12 | 2.03 | 0.40 |
| 40:NA:179:THR:HG23 | 41:NN:351:THR:HB | 2.03 | 0.40 |
| 40:NA:401:ARG:HA | 40:NA:401:ARG:HD3 | 1.95 | 0.40 |
| 40:ND:130:THR:O | 40:ND:130:THR:OG1 | 2.35 | 0.40 |
| 40:ND:290:GLU:O | 40:ND:294:ALA:N | 2.47 | 0.40 |
| 40:ND:431:TYR:O | 40:ND:434:VAL:HB | 2.21 | 0.40 |
| 40:NE:276:ILE:HD12 | 40:NE:281:ALA:HA | 2.03 | 0.40 |
| 40:NE:390:LEU:HD23 | 40:NE:390:LEU:HA | 1.94 | 0.40 |
| 40:NH:123:ARG:NH2 | 40:OH:293:ASN:OD1 | 2.51 | 0.40 |
| 41:OB:180:VAL:HG23 | 41:OB:184:ASN:HD21 | 1.86 | 0.40 |
| 40:OD:121:ARG:HD2 | 40:OD:124:LYS:NZ | 2.35 | 0.40 |
| 40:OD:145:THR:OG1 | 42:OD:501:GTP:O3B | 2.39 | 0.40 |
| 40:OE:270:ALA:HA | 40:OE:377:LEU:HD13 | 2.03 | 0.40 |
| 40:OG:9:VAL:HG23 | 40:OG:139:HIS:HB3 | 2.04 | 0.40 |
| 40:OH:69:ASP:O | 40:OH:70:LEU:C | 2.58 | 0.40 |
| 41:OM:122:LYS:NZ | 41:PM:291:GLN:HB3 | 2.36 | 0.40 |
| 41:ON:273:LEU:HD23 | 41:ON:273:LEU:HA | 1.96 | 0.40 |
| 41:OP:40:SER:HB3 | 41:OP:43:GLN:HB2 | 2.02 | 0.40 |
| 41:OP:392:LYS:HD2 | 41:OP:395:LEU:HD22 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:PA:319:TYR:HB3 | 40:PA:323:VAL:HG11 | 2.02 | 0.40 |
| 41:PB:19:LYS:HZ1 | 41:PB:227:HIS:CA | 2.29 | 0.40 |
| 41:PB:255:VAL:HG22 | 40:PG:406:TRP:CE3 | 2.56 | 0.40 |
| 40:PD:205:ASP:HB2 | 40:PD:303:VAL:HG22 | 2.02 | 0.40 |
| 40:PD:320:ARG:NH1 | 40:PD:358:GLN:O | 2.54 | 0.40 |
| 40:PF:28:HIS:HB2 | 40:PF:30:ILE:HD12 | 2.03 | 0.40 |
| 40:PF:239:THR:OG1 | 40:PF:243:ARG:NH2 | 2.53 | 0.40 |
| 41:PM:199:THR:OG1 | 41:PM:265:PHE:HA | 2.21 | 0.40 |
| 41:QB:9:ALA:HA | 41:QB:66:VAL:H | 1.85 | 0.40 |
| 41:QB:337:ASN:O | 41:QB:338:SER:C | 2.60 | 0.40 |
| 41:QB:347:ASN:HB3 | 40:QG:178:SER:OG | 2.20 | 0.40 |
| 41:QB:406:MET:O | 41:QB:407:GLU:C | 2.60 | 0.40 |
| 40:QF:191:THR:O | 40:QF:195:LEU:HG | 2.21 | 0.40 |
| 40:QF:278:ALA:HA | 40:QF:368:ALA:HB2 | 2.02 | 0.40 |
| 40:QH:345:ASP:N | 40:QH:345:ASP:OD1 | 2.55 | 0.40 |
| 41:QL:240:LEU:H | 41:QL:240:LEU:HD23 | 1.87 | 0.40 |
| 41:QM:2:ARG:HE | 41:QM:240:LEU:HD12 | 1.86 | 0.40 |
| 41:QP:70:PRO:HD3 | 41:QP:95:SER:O | 2.21 | 0.40 |
| 41:QP:79:GLY:O | 41:QP:80:PRO:C | 2.59 | 0.40 |
| 41:QP:139:LEU:HD12 | 41:QP:170:VAL:HA | 2.02 | 0.40 |
| 40:RA:205:ASP:HB3 | 40:RA:303:VAL:HA | 2.04 | 0.40 |
| 41:RB:330:MET:O | 41:RB:334:GLN:HG2 | 2.21 | 0.40 |
| 40:RG:261:PRO:HB2 | 40:RG:346:TRP:HH2 | 1.86 | 0.40 |
| 40:RH:88:HIS:HA | 40:RH:89:PRO:HD3 | 1.95 | 0.40 |
| 40:RH:181:VAL:HG23 | 40:RH:182:VAL:HG13 | 2.02 | 0.40 |
| 41:RM:41:ASP:N | 41:RM:41:ASP:OD1 | 2.48 | 0.40 |
| 41:RM:215:LEU:HD11 | 41:RM:228:LEU:HD11 | 2.04 | 0.40 |
| 41:RN:407:GLU:HA | 41:RN:410:GLU:OE2 | 2.22 | 0.40 |
| 41:RP:31:ASP:OD1 | 41:RP:34:GLY:N | 2.52 | 0.40 |
| 41:RP:217:LEU:HD22 | 41:RP:224:ASP:OD2 | 2.21 | 0.40 |
| 40:SA:91:GLN:HE22 | 40:SA:125:LEU:HD11 | 1.85 | 0.40 |
| 41:SB:229:VAL:O | 41:SB:233:MET:HG2 | 2.21 | 0.40 |
| 41:SB:256:ASN:HD21 | 40:SG:182:VAL:HG12 | 1.85 | 0.40 |
| 41:SB:413:SER:OG | 41:SB:414:ASN:N | 2.52 | 0.40 |
| 41:SM:26:ASP:N | 41:SM:26:ASP:OD1 | 2.44 | 0.40 |
| 41:SM:139:LEU:HD23 | 41:SM:139:LEU:HA | 1.91 | 0.40 |
| 41:SM:322:SER:OG | 41:SM:323:MET:N | 2.54 | 0.40 |
| 41:SO:1:MET:HB2 | 41:SO:2:ARG:H | 1.46 | 0.40 |
| 41:SO:68:LEU:HA | 41:SO:68:LEU:HD13 | 1.68 | 0.40 |
| 41:SO:152:ILE:H | 41:SO:152:ILE:HG13 | 1.71 | 0.40 |
| 41:SO:192:LEU:HD13 | 41:SO:196:THR:HG21 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:SO:303:CYS:SG | 41:SO:303:CYS:O | 2.79 | 0.40 |
| 41:TB:51:TYR:HB3 | 41:TB:59:TYR:HB3 | 2.02 | 0.40 |
| 40:TF:244:PHE:HD2 | 40:TF:356:ASN:HD21 | 1.67 | 0.40 |
| 40:TF:320:ARG:HG2 | 40:TF:373:ALA:HB3 | 2.02 | 0.40 |
| 41:TL:116:VAL:HA | 41:TL:119:VAL:HG12 | 2.03 | 0.40 |
| 41:TM:332:ASN:HA | 41:TM:335:ASN:HD22 | 1.85 | 0.40 |
| 41:UB:255:VAL:HA | 40:UG:406:TRP:CZ3 | 2.56 | 0.40 |
| 40:UG:207:GLU:HA | 40:UG:210:TYR:CD2 | 2.56 | 0.40 |
| 40:UH:115:ILE:HA | 40:UH:118:VAL:HG12 | 2.03 | 0.40 |
| 40:UI:162:GLY:C | 40:UI:164:LYS:N | 2.75 | 0.40 |
| 40:UI:208:ALA:HB3 | 40:UI:302:MET:O | 2.21 | 0.40 |
| 41:UN:121:ARG:NH2 | 41:UN:158:GLU:OE1 | 2.54 | 0.40 |
| 41:UN:134:GLN:HA | 41:UN:165:ASN:HB2 | 2.02 | 0.40 |
| 41:UN:318:ARG:O | 41:UN:363:MET:HA | 2.20 | 0.40 |
| 41:UO:70:PRO:HA | 41:UO:73:MET:HE1 | 2.03 | 0.40 |
| 41:UP:242:PHE:HB3 | 41:UP:356:ILE:HB | 2.01 | 0.40 |
| 40:VH:169:PHE:CE2 | 40:VH:235:VAL:HG22 | 2.56 | 0.40 |
| 40:VI:231:ILE:HA | 40:VI:234:ILE:HG22 | 2.03 | 0.40 |
| 40:VI:332:ILE:HG23 | 40:VI:351:PHE:HD2 | 1.86 | 0.40 |
| 41:VN:250:LEU:HD23 | 41:VN:250:LEU:HA | 1.91 | 0.40 |
| 40:WA:28:HIS:CE1 | 40:WA:243:ARG:HD2 | 2.56 | 0.40 |
| 40:WA:55:GLU:CD | 40:WA:57:GLY:H | 2.24 | 0.40 |
| 40:WE:21:TRP:CZ2 | 40:WE:65:ALA:HB2 | 2.56 | 0.40 |
| 40:WF:226:ASN:ND2 | 40:WF:366:ASP:OD2 | 2.54 | 0.40 |
| 40:WH:141:PHE:HB2 | 40:WH:173:PRO:HG3 | 2.02 | 0.40 |
| 40:WH:319:TYR:HD1 | 40:WH:374:VAL:HB | 1.86 | 0.40 |
| 41:WM:247:ASN:OD1 | 41:WM:247:ASN:N | 2.54 | 0.40 |
| 41:WN:310:TYR:CE1 | 41:WN:371:SER:HB3 | 2.57 | 0.40 |
| 41:WO:261:PRO:O | 41:WO:264:HIS:ND1 | 2.54 | 0.40 |
| 41:WP:132:GLY:HA3 | 41:WP:163:ILE:O | 2.21 | 0.40 |
| 41:WQ:267:MET:SD | 41:WQ:303:CYS:HB2 | 2.61 | 0.40 |
| 7:1T:83:GLN:HE21 | 7:1T:91:ALA:HA | 1.86 | 0.40 |
| 7:1T:398:ILE:H | 7:1T:398:ILE:HG12 | 1.64 | 0.40 |
| 7:1U:115:GLU:OE2 | 7:1U:162:THR:HA | 2.21 | 0.40 |
| 8:1X:142:THR:O | 8:1X:146:ILE:HG13 | 2.21 | 0.40 |
| 8:1Y:191:ASP:O | 8:1Y:195:ILE:HG12 | 2.21 | 0.40 |
| 9:2B:213:LEU:HD21 | 40:TG:371:GLN:NE2 | 2.36 | 0.40 |
| 11:2I:182:LYS:HD2 | 11:2I:182:LYS:HA | 1.49 | 0.40 |
| 11:2K:50:GLY:HA3 | 41:LO:121:ARG:NH1 | 2.36 | 0.40 |
| 11:2K:224:LYS:HZ3 | 11:2K:224:LYS:HG3 | 1.69 | 0.40 |
| 12:2P:254:CYS:SG | 12:2P:255:LEU:N | 2.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:2Q:174:HIS:HA | 12:2Q:177:VAL:HG12 | 2.03 | 0.40 |
| 13:2T:71:ILE:HG22 | 13:2T:151:THR:HB | 2.02 | 0.40 |
| 13:2X:24:ILE:HG13 | 13:2X:25:TRP:CD1 | 2.57 | 0.40 |
| 17:3P:453:ALA:O | 17:3P:454:THR:C | 2.60 | 0.40 |
| 17:3R:205:ARG:HB2 | 17:3R:210:LEU:CD1 | 2.50 | 0.40 |
| 18:3T:192:ARG:O | 18:3T:196:GLN:HG3 | 2.21 | 0.40 |
| 18:3V:67:ALA:O | 18:3V:71:ARG:HG2 | 2.21 | 0.40 |
| 20:4A:94:LYS:HD2 | 20:4A:94:LYS:HA | 1.32 | 0.40 |
| 20:4A:169:GLN:O | 20:4A:171:GLN:N | 2.55 | 0.40 |
| 21:4D:514:LYS:O | 21:4D:517:GLU:HG2 | 2.21 | 0.40 |
| 21:4E:478:SER:O | 21:4E:481:ASN:N | 2.54 | 0.40 |
| 21:4F:222:LYS:HA | 21:4F:222:LYS:HD3 | 1.90 | 0.40 |
| 22:4H:37:SER:HB3 | 22:4H:40:LYS:HZ2 | 1.86 | 0.40 |
| 22:4I:650:LYS:HB2 | 22:4I:652:VAL:CG2 | 2.52 | 0.40 |
| 22:4I:676:ALA:O | 22:4I:680:LYS:N | 2.55 | 0.40 |
| 22:4J:529:THR:O | 22:4J:533:MET:HG2 | 2.21 | 0.40 |
| 23:4R:19:ILE:HD13 | 23:4R:19:ILE:H | 1.84 | 0.40 |
| 26:4V:102:ALA:HB1 | 26:4V:105:LYS:HB2 | 2.03 | 0.40 |
| 28:5B:87:THR:O | 28:5B:89:TRP:N | 2.53 | 0.40 |
| 31:5J:798:LEU:HD13 | 41:IM:215:LEU:HD12 | 2.03 | 0.40 |
| 37:6A:33:LEU:HA | 41:UO:280:GLN:HE22 | 1.85 | 0.40 |
| 39:6G:78:LEU:HD23 | 39:6G:78:LEU:HA | 1.97 | 0.40 |
| 39:6G:124:VAL:HA | 39:6G:127:LEU:HD12 | 2.02 | 0.40 |
| 40:AA:6:SER:O | 40:AA:65:ALA:HA | 2.21 | 0.40 |
| 41:AL:107:THR:OG1 | 41:AL:108:GLU:N | 2.54 | 0.40 |
| 40:BA:24:TYR:HE1 | 40:BA:236:SER:HB2 | 1.86 | 0.40 |
| 41:BB:12:CYS:HB2 | 43:BB:501:GDP:O4' | 2.21 | 0.40 |
| 40:BE:221:ARG:HA | 41:BL:324:LYS:HE2 | 2.03 | 0.40 |
| 40:BG:217:LEU:HA | 40:BG:277:SER:HB3 | 2.02 | 0.40 |
| 40:BH:21:TRP:CZ2 | 40:BH:65:ALA:HB2 | 2.57 | 0.40 |
| 40:BH:252:LEU:HA | 40:BH:255:PHE:CD2 | 2.50 | 0.40 |
| 40:BH:363:VAL:O | 40:BH:365:GLY:N | 2.54 | 0.40 |
| 40:BI:279:GLU:HG2 | 40:BI:280:LYS:HG3 | 2.03 | 0.40 |
| 40:BI:400:LYS:HB3 | 40:BI:400:LYS:HE2 | 1.55 | 0.40 |
| 41:BL:152:ILE:HG23 | 41:BL:164:MET:SD | 2.60 | 0.40 |
| 41:BM:183:TYR:O | 41:BM:184:ASN:C | 2.59 | 0.40 |
| 41:BM:331:LEU:HD11 | 41:BM:335:ASN:HD21 | 1.86 | 0.40 |
| 41:BN:270:PHE:HD1 | 41:BN:273:LEU:HG | 1.86 | 0.40 |
| 41:BO:97:ALA:O | 41:BO:98:GLY:C | 2.60 | 0.40 |
| 41:BO:216:LYS:HD3 | 41:BO:216:LYS:HA | 1.77 | 0.40 |
| 41:BO:221:THR:HG23 | 41:BO:224:ASP:H | 1.87 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:BP:102:ALA:HB2 | 41:BP:403:MET:HG3 | 2.02 | 0.40 |
| 41:BP:183:TYR:CE2 | 41:BP:395:LEU:HD12 | 2.56 | 0.40 |
| 40:CA:265:ILE:H | 40:CA:265:ILE:HG12 | 1.68 | 0.40 |
| 40:CA:312:TYR:CG | 40:CA:341:ILE:HD11 | 2.55 | 0.40 |
| 40:CG:195:LEU:HG | 40:CG:266:HIS:NE2 | 2.37 | 0.40 |
| 40:CH:57:GLY:O | 40:CH:58:ALA:HB3 | 2.21 | 0.40 |
| 40:CH:109:THR:CG2 | 40:CH:410:GLU:HG3 | 2.50 | 0.40 |
| 40:CI:217:LEU:HA | 40:CI:277:SER:HB3 | 2.03 | 0.40 |
| 41:CL:58:LYS:HA | 41:CL:58:LYS:HD3 | 1.35 | 0.40 |
| 41:CM:202:ILE:HD13 | 41:CM:229:VAL:HG11 | 2.03 | 0.40 |
| 41:CP:332:ASN:HA | 41:CP:335:ASN:ND2 | 2.36 | 0.40 |
| 41:CP:425:ARG:O | 41:CP:428:CYS:N | 2.54 | 0.40 |
| 40:DA:195:LEU:HD13 | 40:DA:195:LEU:HA | 1.84 | 0.40 |
| 40:DA:418:SER:O | 40:DA:419:GLU:C | 2.59 | 0.40 |
| 41:DB:215:LEU:O | 41:DB:216:LYS:C | 2.59 | 0.40 |
| 40:DE:15:GLN:H | 40:DE:15:GLN:HG2 | 1.56 | 0.40 |
| 40:DE:159:VAL:HB | 40:DE:160:ASP:H | 1.74 | 0.40 |
| 40:DE:255:PHE:O | 40:DE:256:GLN:C | 2.58 | 0.40 |
| 40:DF:416:GLU:O | 40:DF:417:PHE:C | 2.60 | 0.40 |
| 40:DG:232:SER:HA | 40:DG:235:VAL:HG12 | 2.03 | 0.40 |
| 40:DH:86:LEU:HD12 | 40:DH:86:LEU:HA | 1.92 | 0.40 |
| 40:DH:305:CYS:O | 40:DH:305:CYS:SG | 2.79 | 0.40 |
| 40:DI:119:LEU:HG | 40:DI:120:ASP:N | 2.35 | 0.40 |
| 41:DL:86:ARG:HH12 | 41:EL:282:ARG:HA | 1.86 | 0.40 |
| 41:DL:119:VAL:O | 41:DL:120:VAL:C | 2.59 | 0.40 |
| 41:DL:273:LEU:H | 41:DL:292:GLN:HE22 | 1.69 | 0.40 |
| 41:DM:101:TRP:CD1 | 41:DM:187:LEU:HD13 | 2.56 | 0.40 |
| 41:DN:193:VAL:HG12 | 41:DN:194:GLU:H | 1.85 | 0.40 |
| 41:DN:292:GLN:O | 41:DN:295:ASP:HB2 | 2.20 | 0.40 |
| 40:EA:48:SER:O | 40:EA:51:THR:HG22 | 2.20 | 0.40 |
| 41:EB:190:HIS:CE1 | 41:EB:414:ASN:HD22 | 2.39 | 0.40 |
| 40:EF:121:ARG:HD3 | 40:EF:121:ARG:HA | 1.82 | 0.40 |
| 40:EF:238:ILE:HD12 | 40:EF:238:ILE:HA | 1.89 | 0.40 |
| 40:EG:23:LEU:HD11 | 40:EG:233:GLN:HE21 | 1.86 | 0.40 |
| 40:EG:310:GLY:HA3 | 40:EG:382:ALA:HB2 | 2.03 | 0.40 |
| 40:EH:124:LYS:HE2 | 40:EH:124:LYS:HB2 | 1.33 | 0.40 |
| 40:EH:359:PRO:O | 40:EH:360:PRO:C | 2.59 | 0.40 |
| 40:EI:278:ALA:O | 40:EI:280:LYS:N | 2.54 | 0.40 |
| 41:EM:46:ARG:HE | 41:EM:46:ARG:HB2 | 1.74 | 0.40 |
| 41:EM:104:GLY:O | 41:EM:147:MET:N | 2.54 | 0.40 |
| 41:EM:337:ASN:OD1 | 41:EM:337:ASN:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EO:117:LEU:HB3 | 41:EO:121:ARG:NH1 | 2.36 | 0.40 |
| 41:EO:255:VAL:HG13 | 41:EO:256:ASN:OD1 | 2.21 | 0.40 |
| 41:EP:201:CYS:O | 41:EP:268:PRO:HD3 | 2.21 | 0.40 |
| 40:FA:218:ASP:O | 40:FA:219:ILE:C | 2.59 | 0.40 |
| 40:FA:255:PHE:CE1 | 40:FA:318:LEU:HD21 | 2.56 | 0.40 |
| 40:FA:418:SER:OG | 40:FA:419:GLU:N | 2.54 | 0.40 |
| 41:FB:67:ASP:OD1 | 41:FB:68:LEU:N | 2.53 | 0.40 |
| 41:FB:247:ASN:OD1 | 41:FB:247:ASN:N | 2.54 | 0.40 |
| 40:FE:242:LEU:H | 40:FE:242:LEU:HD23 | 1.86 | 0.40 |
| 40:FF:255:PHE:HZ | 40:FF:318:LEU:HD21 | 1.86 | 0.40 |
| 40:FF:264:ARG:NH2 | 40:FF:423:ASP:OD1 | 2.54 | 0.40 |
| 40:FG:336:LYS:NZ | 41:FO:174:LYS:O | 2.50 | 0.40 |
| 40:FI:238:ILE:HG23 | 40:FI:239:THR:HG23 | 2.03 | 0.40 |
| 40:GA:273:ALA:HB2 | 40:GA:295:CYS:SG | 2.61 | 0.40 |
| 40:GA:393:LYS:HD3 | 41:GN:346:PRO:HG2 | 2.04 | 0.40 |
| 40:GE:288:VAL:O | 40:GE:289:ALA:C | 2.59 | 0.40 |
| 40:GF:212:ILE:HD13 | 40:GF:300:ASN:HA | 2.02 | 0.40 |
| 40:GH:13:GLY:O | 40:GH:14:VAL:C | 2.59 | 0.40 |
| 40:GI:188:ILE:HG13 | 40:GI:394:PHE:CB | 2.50 | 0.40 |
| 40:GI:326:LYS:HA | 40:GI:329:ASN:ND2 | 2.36 | 0.40 |
| 41:GN:100:ASN:O | 41:GN:103:LYS:N | 2.54 | 0.40 |
| 41:GN:221:THR:C | 41:GN:223:GLY:H | 2.24 | 0.40 |
| 41:GN:285:THR:HB | 41:GN:287:PRO:HD2 | 2.02 | 0.40 |
| 40:HA:265:ILE:HG23 | 40:HA:431:TYR:HE1 | 1.86 | 0.40 |
| 40:HE:261:PRO:HA | 41:HM:394:PHE:HE2 | 1.84 | 0.40 |
| 40:HE:316:CYS:SG | 40:HE:377:LEU:HB2 | 2.61 | 0.40 |
| 40:HF:51:THR:HG23 | 40:HF:52:PHE:CD2 | 2.56 | 0.40 |
| 40:HG:97:GLU:HG3 | 40:HG:98:ASP:H | 1.86 | 0.40 |
| 40:HG:227:LEU:O | 40:HG:231:ILE:HG12 | 2.21 | 0.40 |
| 40:HI:60:LYS:HE2 | 40:II:283:HIS:HD2 | 1.86 | 0.40 |
| 41:HN:2:ARG:H | 41:HN:2:ARG:HG2 | 1.65 | 0.40 |
| 41:HQ:271:ALA:HB1 | 41:HQ:292:GLN:HB3 | 2.03 | 0.40 |
| 40:IA:405:HIS:CG | 41:IN:261:PRO:HG3 | 2.56 | 0.40 |
| 41:IB:41:ASP:OD1 | 41:IB:41:ASP:N | 2.51 | 0.40 |
| 41:IB:273:LEU:HD23 | 41:IB:273:LEU:HA | 1.90 | 0.40 |
| 41:IB:323:MET:SD | 41:IB:353:VAL:HG21 | 2.61 | 0.40 |
| 40:IE:75:ILE:HG12 | 40:IE:92:LEU:HB3 | 2.03 | 0.40 |
| 40:IF:390:LEU:HD23 | 40:IF:390:LEU:HA | 1.88 | 0.40 |
| 40:IH:210:TYR:HE1 | 40:IH:227:LEU:HD11 | 1.86 | 0.40 |
| 41:IN:44:LEU:HD12 | 41:IN:47:ILE:HG21 | 2.03 | 0.40 |
| 41:IN:317:PHE:HB2 | 41:IN:353:VAL:HG12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IP:26:ASP:O | 41:IP:359:ARG:NE | 2.54 | 0.40 |
| 41:IQ:142:GLY:O | 41:IQ:144:GLY:N | 2.53 | 0.40 |
| 40:JD:112:LYS:HA | 40:JD:115:ILE:HG22 | 2.02 | 0.40 |
| 40:JD:217:LEU:HB3 | 40:JD:219:ILE:HG13 | 2.03 | 0.40 |
| 40:JE:254:GLU:OE2 | 41:JM:98:GLY:HA2 | 2.21 | 0.40 |
| 40:JF:224:TYR:HD2 | 41:JM:323:MET:HG3 | 1.82 | 0.40 |
| 40:JG:219:ILE:HG13 | 40:JG:222:PRO:HG3 | 2.03 | 0.40 |
| 41:JL:146:GLY:O | 41:JL:149:THR:OG1 | 2.28 | 0.40 |
| 41:JL:296:ALA:HB1 | 41:JL:305:PRO:HD2 | 2.04 | 0.40 |
| 41:JM:375:GLN:O | 41:JM:376:GLU:C | 2.59 | 0.40 |
| 41:JN:116:VAL:HG11 | 41:JN:151:LEU:HD11 | 2.03 | 0.40 |
| 41:JO:102:ALA:HB1 | 41:JO:401:GLU:HB2 | 2.02 | 0.40 |
| 41:KB:383:GLU:HA | 41:KB:386:THR:HG22 | 2.03 | 0.40 |
| 40:KD:153:LEU:HD23 | 40:KD:153:LEU:HA | 1.90 | 0.40 |
| 40:KD:202:PHE:CE1 | 40:KD:377:LEU:HD13 | 2.56 | 0.40 |
| 40:KD:206:ASN:OD1 | 42:KD:501:GTP:O2' | 2.26 | 0.40 |
| 40:KD:254:GLU:HA | 40:KD:257:THR:HG22 | 2.03 | 0.40 |
| 40:KF:13:GLY:O | 40:KF:16:ILE:HB | 2.21 | 0.40 |
| 40:KH:207:GLU:O | 40:KH:210:TYR:HB2 | 2.20 | 0.40 |
| 41:KL:39:ASP:HB2 | 41:KL:40:SER:H | 1.65 | 0.40 |
| 40:LA:217:LEU:HD21 | 40:LA:367:LEU:HD12 | 2.03 | 0.40 |
| 40:LF:397:MET:HB3 | 40:LF:402:ALA:HB3 | 2.04 | 0.40 |
| 40:LG:50:ASN:O | 40:LG:64:ARG:NH1 | 2.55 | 0.40 |
| 40:LG:71:GLU:HG2 | 40:LG:72:PRO:HD2 | 2.02 | 0.40 |
| 40:LG:352:LYS:HG2 | 41:LO:179:VAL:CG2 | 2.52 | 0.40 |
| 41:LL:32:PRO:HG3 | 41:LL:81:PHE:CE1 | 2.56 | 0.40 |
| 41:LO:138:SER:OG | 43:LO:502:GDP:O1A | 2.39 | 0.40 |
| 40:MA:88:HIS:ND1 | 40:MA:89:PRO:HD2 | 2.37 | 0.40 |
| 40:MA:107:HIS:HB2 | 40:MA:148:GLY:HA2 | 2.02 | 0.40 |
| 40:MA:228:ASN:ND2 | 42:MN:501:GTP:HN21 | 2.19 | 0.40 |
| 40:MD:371:GLN:HG3 | 40:MD:372:ARG:HH11 | 1.86 | 0.40 |
| 40:MF:349:THR:HB | 41:MN:176:SER:CB | 2.51 | 0.40 |
| 40:MG:273:ALA:HB3 | 40:MG:374:VAL:H | 1.87 | 0.40 |
| 40:NA:209:ILE:HA | 40:NA:212:ILE:HG12 | 2.04 | 0.40 |
| 41:NB:2:ARG:HG2 | 41:NB:131:GLN:HE21 | 1.87 | 0.40 |
| 40:NE:204:VAL:HG11 | 40:NE:231:ILE:HG12 | 2.04 | 0.40 |
| 40:NF:7:VAL:HG13 | 40:NF:66:VAL:HB | 2.02 | 0.40 |
| 40:NF:251:ASP:OD1 | 40:NF:252:LEU:N | 2.53 | 0.40 |
| 41:NP:107:THR:OG1 | 41:NP:108:GLU:N | 2.54 | 0.40 |
| 41:OB:46:ARG:NE | 40:OG:73:THR:OG1 | 2.45 | 0.40 |
| 40:OF:7:VAL:HG23 | 40:OF:66:VAL:HG13 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OF:209:ILE:HA | 40:OF:212:ILE:HG22 | 2.03 | 0.40 |
| 40:OH:121:ARG:HD2 | 40:OH:121:ARG:HA | 1.76 | 0.40 |
| 40:OH:412:MET:H | 40:OH:412:MET:HG2 | 1.72 | 0.40 |
| 41:OM:21:TRP:HZ3 | 41:OM:50:TYR:HB3 | 1.85 | 0.40 |
| 41:OM:267:MET:SD | 41:OM:299:MET:HE2 | 2.61 | 0.40 |
| 41:OM:291:GLN:O | 41:OM:295:ASP:HB2 | 2.22 | 0.40 |
| 41:OO:39:ASP:OD1 | 41:OO:39:ASP:N | 2.54 | 0.40 |
| 41:OP:92:PHE:HE2 | 41:OP:94:GLN:HE22 | 1.69 | 0.40 |
| 40:PE:169:PHE:HE1 | 40:PE:202:PHE:HD2 | 1.69 | 0.40 |
| 40:PF:326:LYS:HD3 | 40:PF:326:LYS:HA | 1.80 | 0.40 |
| 40:PG:413:GLU:HG2 | 40:PG:416:GLU:HG3 | 2.04 | 0.40 |
| 40:PH:191:THR:HA | 40:PH:194:THR:HG1 | 1.87 | 0.40 |
| 41:PL:19:LYS:HA | 41:PL:19:LYS:HD3 | 1.91 | 0.40 |
| 40:QA:103:TYR:N | 40:QA:186:ASN:OD1 | 2.54 | 0.40 |
| 41:QB:194:GLU:H | 41:QB:194:GLU:HG2 | 1.47 | 0.40 |
| 40:QE:56:THR:HB | 40:RE:285:GLN:HA | 2.03 | 0.40 |
| 40:QE:394:PHE:HD2 | 40:QE:421:ARG:HD3 | 1.85 | 0.40 |
| 40:QF:117:LEU:HD23 | 40:QF:117:LEU:HA | 1.90 | 0.40 |
| 40:QF:177:VAL:HG12 | 41:QM:331:LEU:HG | 2.03 | 0.40 |
| 40:QG:54:SER:OG | 40:QG:64:ARG:NE | 2.44 | 0.40 |
| 41:QL:167:PHE:HD2 | 41:QL:202:ILE:HD11 | 1.86 | 0.40 |
| 41:QP:183:TYR:O | 41:QP:186:THR:OG1 | 2.37 | 0.40 |
| 41:QP:375:GLN:O | 41:QP:376:GLU:C | 2.59 | 0.40 |
| 40:RA:88:HIS:HD2 | 40:RA:89:PRO:HD2 | 1.86 | 0.40 |
| 40:RF:169:PHE:HZ | 40:RF:238:ILE:HG13 | 1.87 | 0.40 |
| 40:RH:118:VAL:O | 40:RH:122:ILE:HG12 | 2.22 | 0.40 |
| 40:RH:278:ALA:H | 40:RH:368:ALA:HB2 | 1.86 | 0.40 |
| 40:RI:367:LEU:HD23 | 40:RI:367:LEU:HA | 1.91 | 0.40 |
| 41:RM:148:GLY:O | 41:RM:152:ILE:HG12 | 2.21 | 0.40 |
| 41:RO:211:CYS:HA | 41:RO:215:LEU:HB2 | 2.03 | 0.40 |
| 40:SA:247:ALA:O | 40:SA:248:LEU:C | 2.58 | 0.40 |
| 41:SB:31:ASP:OD1 | 41:SB:35:THR:N | 2.55 | 0.40 |
| 41:SB:102:ALA:HB2 | 41:SB:398:TYR:HA | 2.03 | 0.40 |
| 40:SF:30:ILE:HG13 | 40:SF:53:PHE:CE2 | 2.56 | 0.40 |
| 40:SF:53:PHE:HE1 | 40:SF:63:PRO:HG3 | 1.86 | 0.40 |
| 40:SG:258:ASN:HA | 41:SO:179:VAL:HG22 | 2.03 | 0.40 |
| 40:SI:405:HIS:CG | 41:SP:261:PRO:HG3 | 2.56 | 0.40 |
| 41:SM:178:THR:OG1 | 41:SM:181:GLU:HG3 | 2.21 | 0.40 |
| 41:SN:45:GLU:OE1 | 41:SN:46:ARG:HG2 | 2.22 | 0.40 |
| 41:SO:8:GLN:NE2 | 41:SO:14:ASN:HA | 2.36 | 0.40 |
| 41:SO:102:ALA:O | 41:SO:104:GLY:N | 2.49 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:TB:101:TRP:CE2 | 41:TB:187:LEU:HB3 | 2.56 | 0.40 |
| 40:TE:212:ILE:HD11 | 40:TE:216:ASN:HD21 | 1.86 | 0.40 |
| 40:TF:6:SER:HB3 | 40:TF:8:HIS:NE2 | 2.37 | 0.40 |
| 40:TF:30:ILE:HD13 | 40:TF:61:HIS:HD2 | 1.84 | 0.40 |
| 41:TO:221:THR:OG1 | 41:TO:222:TYR:N | 2.54 | 0.40 |
| 40:UA:71:GLU:HG2 | 40:UA:98:ASP:HB2 | 2.03 | 0.40 |
| 40:UA:265:ILE:HG22 | 40:UA:379:ASN:HD21 | 1.86 | 0.40 |
| 40:UA:273:ALA:HB3 | 40:UA:374:VAL:HG12 | 2.03 | 0.40 |
| 40:UE:62:VAL:HA | 40:UE:63:PRO:HD3 | 1.94 | 0.40 |
| 40:UF:48:SER:O | 40:UF:49:PHE:C | 2.59 | 0.40 |
| 40:UF:307:PRO:O | 40:UF:308:ARG:C | 2.60 | 0.40 |
| 40:UF:400:LYS:HB3 | 40:UF:400:LYS:HE3 | 1.60 | 0.40 |
| 40:UH:413:GLU:CD | 40:UH:415:GLY:H | 2.25 | 0.40 |
| 40:UI:7:VAL:HA | 40:UI:66:VAL:HG13 | 2.03 | 0.40 |
| 40:UI:177:VAL:HG13 | 41:UP:327:ASP:HB3 | 2.04 | 0.40 |
| 41:UM:23:VAL:HG23 | 41:UM:359:ARG:HH22 | 1.86 | 0.40 |
| 41:UN:206:ALA:O | 41:UN:210:ILE:HD12 | 2.20 | 0.40 |
| 41:UN:341:PHE:HD2 | 41:UN:348:ASN:HD21 | 1.69 | 0.40 |
| 41:UP:12:CYS:HB2 | 43:UP:501:GDP:O4' | 2.21 | 0.40 |
| 41:UP:206:ALA:O | 41:UP:207:LEU:C | 2.59 | 0.40 |
| 41:UP:228:LEU:HD12 | 41:UP:228:LEU:HA | 1.89 | 0.40 |
| 41:UP:294:PHE:HE1 | 41:UP:313:VAL:HG11 | 1.86 | 0.40 |
| 40:VA:111:GLY:O | 40:VA:115:ILE:HB | 2.21 | 0.40 |
| 40:VF:116:ASP:N | 40:VF:116:ASP:OD1 | 2.54 | 0.40 |
| 40:VF:349:THR:HG23 | 41:VN:179:VAL:HA | 2.03 | 0.40 |
| 40:VG:406:TRP:CG | 41:VN:255:VAL:HG23 | 2.56 | 0.40 |
| 40:VI:69:ASP:OD1 | 40:VI:70:LEU:N | 2.53 | 0.40 |
| 41:VN:77:ARG:HD2 | 41:VN:77:ARG:HA | 1.80 | 0.40 |
| 40:WA:3:GLU:HG2 | 40:WA:64:ARG:CZ | 2.52 | 0.40 |
| 40:WE:138:PHE:HE1 | 40:WE:235:VAL:HG21 | 1.86 | 0.40 |
| 40:WF:298:PRO:HG2 | 40:WF:308:ARG:HH21 | 1.86 | 0.40 |
| 40:WG:136:LEU:HD23 | 40:WG:169:PHE:HE1 | 1.86 | 0.40 |
| 41:WM:1:MET:HE2 | 41:WM:48:ASN:HB2 | 2.02 | 0.40 |
| 41:WM:19:LYS:HA | 41:WM:22:GLU:HB2 | 2.02 | 0.40 |
| 41:WM:36:TYR:CD1 | 41:WM:44:LEU:HD22 | 2.56 | 0.40 |
| 41:WM:101:TRP:O | 41:WM:103:LYS:N | 2.54 | 0.40 |
| 41:WM:303:CYS:O | 41:WM:304:ASP:C | 2.60 | 0.40 |
| 41:WN:188:SER:O | 41:WN:189:VAL:C | 2.59 | 0.40 |
| 41:WO:165:ASN:HA | 41:WO:198:GLU:O | 2.21 | 0.40 |
| 41:WO:186:THR:HG22 | 41:WO:415:MET:SD | 2.62 | 0.40 |
| 41:WO:226:ASN:ND2 | 43:WO:502:GDP:O6 | 2.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:1S:523:ASP:OD2 | 7:1S:525:LYS:N | 2.53 | 0.40 |
| 7:1T:111:LYS:H | 7:1T:111:LYS:NZ | 2.19 | 0.40 |
| 7:1T:166:PHE:HD2 | 7:1T:167:SER:H | 1.69 | 0.40 |
| 7:1T:341:PRO:HB2 | 7:1T:344:THR:CG2 | 2.51 | 0.40 |
| 7:1T:564:GLY:C | 7:1T:566:ASP:H | 2.25 | 0.40 |
| 7:1U:54:THR:OG1 | 7:1U:56:GLU:OE1 | 2.27 | 0.40 |
| 8:1W:367:ILE:HD13 | 40:VH:371:GLN:NE2 | 2.36 | 0.40 |
| 8:1X:77:ILE:O | 8:1X:87:GLU:HA | 2.21 | 0.40 |
| 11:2J:193:ARG:HD3 | 11:2J:250:ILE:HG13 | 2.02 | 0.40 |
| 12:2N:75:PHE:CD2 | 12:2N:111:LEU:HD11 | 2.56 | 0.40 |
| 12:2N:85:LEU:HD22 | 12:2N:87:HIS:CD2 | 2.56 | 0.40 |
| 13:2U:119:CYS:O | 13:2U:120:THR:C | 2.59 | 0.40 |
| 13:2V:125:LEU:HD12 | 13:2V:125:LEU:HA | 1.77 | 0.40 |
| 14:3C:9:GLN:HE21 | 41:MO:304:ASP:N | 2.19 | 0.40 |
| 15:3F:151:THR:O | 15:3F:155:GLU:HG2 | 2.21 | 0.40 |
| 15:3F:208:GLU:HB2 | 15:3F:211:SER:HB3 | 2.02 | 0.40 |
| 15:3F:348:VAL:O | 15:3F:352:LYS:HG2 | 2.21 | 0.40 |
| 17:3P:278:SER:HB3 | 17:3P:281:ILE:HD11 | 2.04 | 0.40 |
| 17:3R:190:ALA:HB3 | 17:3R:191:PRO:CD | 2.48 | 0.40 |
| 20:4A:28:SER:OG | 20:4A:29:ARG:N | 2.54 | 0.40 |
| 21:4D:81:PRO:HG2 | 40:MA:32:PRO:HG3 | 2.03 | 0.40 |
| 21:4D:425:ALA:HB2 | 21:4D:506:LEU:HD11 | 2.03 | 0.40 |
| 21:4E:414:MET:HB2 | 21:4E:415:ASN:H | 1.63 | 0.40 |
| 21:4E:487:PRO:C | 21:4E:489:ASP:H | 2.24 | 0.40 |
| 21:4F:283:ASP:OD1 | 21:4F:283:ASP:N | 2.54 | 0.40 |
| 21:4F:355:TYR:HB3 | 21:4F:361:ILE:HD11 | 2.03 | 0.40 |
| 22:4H:91:ASP:CG | 41:BL:279:GLN:HE22 | 2.21 | 0.40 |
| 22:4H:155:ASN:HA | 22:4H:167:ILE:O | 2.20 | 0.40 |
| 22:4J:637:ARG:HD2 | 41:EM:56:GLY:HA3 | 2.03 | 0.40 |
| 22:4K:636:GLU:HA | 22:4K:639:ILE:HD12 | 2.03 | 0.40 |
| 22:4K:676:ALA:HB1 | 22:4K:680:LYS:HG2 | 2.04 | 0.40 |
| 23:4N:178:ASP:O | 23:4N:179:PRO:C | 2.60 | 0.40 |
| 23:4N:250:VAL:O | 23:4N:250:VAL:HG22 | 2.21 | 0.40 |
| 23:4N:261:TYR:CE1 | 23:4N:265:THR:HG21 | 2.56 | 0.40 |
| 23:4P:250:VAL:O | 23:4P:250:VAL:HG22 | 2.21 | 0.40 |
| 27:4Y:50:LEU:HD23 | 27:4Y:50:LEU:HA | 1.92 | 0.40 |
| 27:4Z:75:PRO:HD2 | 27:4Z:77:HIS:HE1 | 1.86 | 0.40 |
| 29:5D:44:PHE:HD2 | 40:GI:31:GLN:HG2 | 1.86 | 0.40 |
| 31:5I:466:TYR:O | 31:5I:469:SER:C | 2.60 | 0.40 |
| 33:5O:106:LYS:HZ2 | 41:HM:31:ASP:HB2 | 1.87 | 0.40 |
| 34:5Q:289:GLN:HA | 40:GE:282:TYR:OH | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:5R:361:ASP:O | 34:5R:363:ILE:N | 2.54 | 0.40 |
| 34:5R:387:LYS:HB3 | 34:5R:387:LYS:HE3 | 1.35 | 0.40 |
| 37:6A:46:HIS:NE2 | 40:UH:221:ARG:HG2 | 2.35 | 0.40 |
| 41:AB:347:ASN:ND2 | 40:AG:178:SER:HB3 | 2.35 | 0.40 |
| 41:AP:7:LEU:O | 41:AP:135:LEU:HA | 2.21 | 0.40 |
| 40:BA:60:LYS:HE3 | 40:CA:283:HIS:CD2 | 2.55 | 0.40 |
| 41:BB:196:THR:HG21 | 41:BB:199:THR:HG23 | 2.03 | 0.40 |
| 40:BH:333:ALA:O | 40:BH:337:THR:HG23 | 2.20 | 0.40 |
| 40:BH:344:VAL:HG21 | 40:BH:346:TRP:CE2 | 2.56 | 0.40 |
| 40:BH:414:GLU:O | 40:BH:415:GLY:C | 2.59 | 0.40 |
| 40:BI:259:LEU:HD11 | 40:BI:377:LEU:HB3 | 2.03 | 0.40 |
| 41:BN:19:LYS:HE2 | 41:BN:227:HIS:HB2 | 2.03 | 0.40 |
| 41:BN:304:ASP:HB3 | 41:BN:307:HIS:ND1 | 2.36 | 0.40 |
| 41:BO:33:THR:OG1 | 41:BO:34:GLY:N | 2.54 | 0.40 |
| 41:BO:103:LYS:O | 41:BO:108:GLU:HG3 | 2.21 | 0.40 |
| 41:BO:134:GLN:HB3 | 41:BO:167:PHE:HE2 | 1.87 | 0.40 |
| 41:BO:217:LEU:HA | 41:BO:217:LEU:HD22 | 1.68 | 0.40 |
| 41:BO:271:ALA:HB1 | 41:BO:289:LEU:HD22 | 2.04 | 0.40 |
| 41:BP:320:ARG:HA | 41:BP:320:ARG:HD2 | 1.57 | 0.40 |
| 40:CA:114:LEU:HB3 | 40:CA:149:PHE:HZ | 1.83 | 0.40 |
| 40:CA:126:ALA:O | 40:CA:127:ASP:C | 2.59 | 0.40 |
| 40:CE:238:ILE:HA | 40:CE:318:LEU:HD22 | 2.03 | 0.40 |
| 40:CF:9:VAL:HG12 | 40:CF:146:GLY:HA2 | 2.03 | 0.40 |
| 40:CF:235:VAL:O | 40:CF:239:THR:HG22 | 2.21 | 0.40 |
| 40:CF:254:GLU:HB3 | 41:CN:98:GLY:HA3 | 1.97 | 0.40 |
| 40:CF:254:GLU:O | 40:CF:258:ASN:ND2 | 2.32 | 0.40 |
| 40:CG:274:PRO:HB3 | 40:CG:370:VAL:HG11 | 2.03 | 0.40 |
| 40:CH:207:GLU:OE1 | 40:CH:304:LYS:HG3 | 2.22 | 0.40 |
| 40:CH:401:ARG:HD3 | 40:CH:404:VAL:HG11 | 2.02 | 0.40 |
| 40:CI:3:GLU:HG2 | 40:CI:64:ARG:CZ | 2.50 | 0.40 |
| 40:CI:21:TRP:CZ2 | 40:CI:65:ALA:HB2 | 2.56 | 0.40 |
| 41:CL:97:ALA:HA | 41:CL:103:LYS:HD2 | 2.03 | 0.40 |
| 41:CL:379:LYS:HZ3 | 41:CL:379:LYS:HG2 | 1.78 | 0.40 |
| 41:CM:233:MET:HE2 | 41:CM:233:MET:HB3 | 1.48 | 0.40 |
| 41:CM:394:PHE:HD1 | 41:CM:397:TRP:CH2 | 2.39 | 0.40 |
| 41:CN:13:GLY:HA3 | 41:CN:136:THR:O | 2.21 | 0.40 |
| 41:CN:270:PHE:CD2 | 41:CN:272:PRO:HD2 | 2.56 | 0.40 |
| 41:CO:115:SER:O | 41:CO:118:ASP:HB2 | 2.21 | 0.40 |
| 41:CO:252:LYS:HB2 | 41:CO:252:LYS:HE3 | 1.18 | 0.40 |
| 41:CO:256:ASN:ND2 | 41:CO:350:LYS:HB2 | 2.36 | 0.40 |
| 41:CO:368:ILE:HD12 | 41:CO:368:ILE:HA | 1.88 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:CP:116:VAL:O | 41:CP:120:VAL:HG23 | 2.22 | 0.40 |
| 40:DA:126:ALA:O | 40:DA:127:ASP:C | 2.60 | 0.40 |
| 40:DA:153:LEU:HD12 | 40:DA:153:LEU:HA | 1.80 | 0.40 |
| 40:DA:245:ASP:O | 40:DA:357:TYR:HB2 | 2.21 | 0.40 |
| 40:DE:7:VAL:HG11 | 40:DE:153:LEU:HD11 | 2.02 | 0.40 |
| 40:DE:269:LEU:HG | 40:DE:378:SER:O | 2.21 | 0.40 |
| 40:DF:8:HIS:CD2 | 40:DF:8:HIS:H | 2.37 | 0.40 |
| 40:DF:9:VAL:HA | 40:DF:68:VAL:HG13 | 2.03 | 0.40 |
| 40:DF:69:ASP:O | 40:DF:94:THR:HA | 2.22 | 0.40 |
| 40:DF:287:SER:O | 40:DF:290:GLU:N | 2.54 | 0.40 |
| 40:DG:21:TRP:CZ3 | 40:DG:52:PHE:HB3 | 2.57 | 0.40 |
| 40:DI:14:VAL:C | 40:DI:16:ILE:N | 2.75 | 0.40 |
| 40:DI:31:GLN:C | 40:DI:33:ASP:N | 2.74 | 0.40 |
| 41:DM:254:ALA:C | 41:DM:256:ASN:N | 2.75 | 0.40 |
| 41:DM:263:LEU:HD11 | 41:DM:422:VAL:HG23 | 2.03 | 0.40 |
| 41:DM:296:ALA:HB2 | 41:DM:306:ARG:HH12 | 1.86 | 0.40 |
| 41:DM:322:SER:O | 41:DM:323:MET:C | 2.59 | 0.40 |
| 41:DN:54:ALA:O | 41:DN:55:THR:C | 2.59 | 0.40 |
| 40:EA:51:THR:HG23 | 40:EA:52:PHE:HD1 | 1.86 | 0.40 |
| 41:EB:7:LEU:HG | 41:EB:135:LEU:HD12 | 2.03 | 0.40 |
| 41:EB:122:LYS:HE3 | 41:FB:291:GLN:HE22 | 1.86 | 0.40 |
| 41:EB:313:VAL:HG13 | 41:EB:367:PHE:HE1 | 1.87 | 0.40 |
| 40:EE:105:ARG:NE | 40:EE:410:GLU:OE1 | 2.33 | 0.40 |
| 40:EE:371:GLN:HG2 | 40:EE:372:ARG:HE | 1.85 | 0.40 |
| 40:EF:393:LYS:HD2 | 41:EM:346:PRO:CG | 2.51 | 0.40 |
| 40:EG:190:THR:HA | 40:EG:193:THR:HG22 | 2.03 | 0.40 |
| 40:EG:297:GLU:HA | 40:EG:298:PRO:HD3 | 1.88 | 0.40 |
| 40:EH:100:ALA:C | 40:EH:102:ASN:H | 2.25 | 0.40 |
| 40:EI:23:LEU:O | 40:EI:27:GLU:HG3 | 2.21 | 0.40 |
| 41:EN:7:LEU:O | 41:EN:135:LEU:HA | 2.22 | 0.40 |
| 41:EN:113:VAL:HG22 | 41:EN:117:LEU:HD23 | 2.04 | 0.40 |
| 41:EO:330:MET:SD | 41:EO:349:VAL:HG11 | 2.62 | 0.40 |
| 41:EP:21:TRP:CE3 | 41:EP:24:ILE:HD11 | 2.57 | 0.40 |
| 41:EP:253:LEU:HD13 | 41:EP:253:LEU:HA | 1.83 | 0.40 |
| 40:FA:88:HIS:O | 40:FA:91:GLN:N | 2.47 | 0.40 |
| 40:FA:254:GLU:O | 40:FA:258:ASN:HB2 | 2.22 | 0.40 |
| 40:FE:247:ALA:O | 41:FM:11:GLN:NE2 | 2.53 | 0.40 |
| 40:FF:139:HIS:CE1 | 40:FF:150:THR:HG21 | 2.57 | 0.40 |
| 40:FG:273:ALA:HB1 | 40:FG:274:PRO:HD2 | 2.02 | 0.40 |
| 40:FI:93:ILE:HD13 | 40:FI:118:VAL:HG12 | 2.04 | 0.40 |
| 41:FM:253:LEU:O | 41:FM:257:MET:HG3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:FN:6:HIS:O | 41:FN:63:ALA:HA | 2.20 | 0.40 |
| 40:GA:177:VAL:HG23 | 41:GN:331:LEU:HB2 | 2.04 | 0.40 |
| 41:GB:70:PRO:HG2 | 41:GB:94:GLN:HG3 | 2.02 | 0.40 |
| 40:GH:278:ALA:HA | 40:GH:368:ALA:CB | 2.45 | 0.40 |
| 40:GI:20:CYS:HA | 40:GI:232:SER:HB2 | 2.03 | 0.40 |
| 40:GI:203:MET:HE2 | 40:GI:203:MET:HB2 | 1.73 | 0.40 |
| 41:GN:425:ARG:CZ | 41:GN:425:ARG:HB2 | 2.52 | 0.40 |
| 41:GP:272:PRO:HG3 | 41:GP:364:SER:HA | 2.03 | 0.40 |
| 40:HE:88:HIS:NE2 | 40:IE:283:HIS:HB2 | 2.36 | 0.40 |
| 40:HE:280:LYS:HB3 | 40:HE:280:LYS:HE3 | 1.66 | 0.40 |
| 40:HE:284:GLU:H | 40:HE:284:GLU:HG2 | 1.66 | 0.40 |
| 40:HE:297:GLU:C | 40:HE:299:ALA:H | 2.25 | 0.40 |
| 40:HF:21:TRP:CZ3 | 40:HF:52:PHE:HB3 | 2.56 | 0.40 |
| 40:HG:69:ASP:OD2 | 40:HG:71:GLU:HG2 | 2.22 | 0.40 |
| 40:HG:294:ALA:O | 40:HG:300:ASN:ND2 | 2.46 | 0.40 |
| 41:HO:134:GLN:HA | 41:HO:165:ASN:O | 2.21 | 0.40 |
| 41:HQ:102:ALA:HB2 | 41:HQ:403:MET:HE2 | 2.04 | 0.40 |
| 41:HQ:289:LEU:HD13 | 41:HQ:365:ALA:HB2 | 2.03 | 0.40 |
| 40:IA:261:PRO:HG2 | 40:IA:265:ILE:HD11 | 2.03 | 0.40 |
| 40:IH:391:ASP:OD2 | 40:IH:421:ARG:NE | 2.54 | 0.40 |
| 40:II:291:ILE:HD13 | 40:II:291:ILE:HG21 | 1.92 | 0.40 |
| 41:IM:170:VAL:HG21 | 41:IM:377:LEU:HD21 | 2.03 | 0.40 |
| 41:IN:395:LEU:HD12 | 41:IN:398:TYR:HD1 | 1.87 | 0.40 |
| 41:IP:211:CYS:HA | 41:IP:215:LEU:HB2 | 2.04 | 0.40 |
| 40:JA:376:MET:SD | 40:JA:378:SER:HB3 | 2.61 | 0.40 |
| 40:JD:88:HIS:CE1 | 40:JD:90:GLU:HB2 | 2.56 | 0.40 |
| 40:JF:174:ALA:HB3 | 40:JF:178:SER:H | 1.86 | 0.40 |
| 40:JG:181:VAL:O | 40:JG:184:PRO:HD2 | 2.21 | 0.40 |
| 40:JH:119:LEU:HD23 | 40:JH:119:LEU:HA | 1.89 | 0.40 |
| 40:JH:205:ASP:HB3 | 40:JH:303:VAL:HA | 2.03 | 0.40 |
| 40:JH:212:ILE:HD13 | 40:JH:212:ILE:HA | 1.87 | 0.40 |
| 41:JM:239:CYS:C | 41:JM:241:ARG:N | 2.74 | 0.40 |
| 40:KA:171:ILE:HD13 | 40:KA:204:VAL:HG13 | 2.03 | 0.40 |
| 40:KA:224:TYR:CE2 | 42:KN:501:GTP:H2' | 2.57 | 0.40 |
| 41:KB:322:SER:O | 41:KB:326:VAL:HG23 | 2.21 | 0.40 |
| 40:KD:401:ARG:HB3 | 40:KD:404:VAL:HG11 | 2.03 | 0.40 |
| 40:KE:405:HIS:CG | 41:KL:261:PRO:HG3 | 2.56 | 0.40 |
| 40:KH:239:THR:O | 40:KH:243:ARG:NH1 | 2.54 | 0.40 |
| 41:KO:313:VAL:HG13 | 41:KO:367:PHE:CE1 | 2.57 | 0.40 |
| 41:KO:420:ASN:HA | 41:KO:423:VAL:HG12 | 2.02 | 0.40 |
| 41:KP:42:LEU:HD23 | 41:KP:356:ILE:HD11 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:KP:51:TYR:HB3 | 41:KP:59:TYR:HB3 | 2.03 | 0.40 |
| 40:LF:372:ARG:HE | 40:LF:372:ARG:HB2 | 1.51 | 0.40 |
| 40:LG:261:PRO:HG2 | 40:LG:262:TYR:H | 1.86 | 0.40 |
| 40:LG:286:LEU:HD13 | 40:LG:370:VAL:HG12 | 2.02 | 0.40 |
| 40:LG:287:SER:O | 40:LG:288:VAL:C | 2.59 | 0.40 |
| 41:LM:322:SER:OG | 41:LM:325:GLU:HB2 | 2.22 | 0.40 |
| 40:MA:136:LEU:HB3 | 40:MA:169:PHE:HE1 | 1.86 | 0.40 |
| 41:MB:21:TRP:CZ3 | 41:MB:50:TYR:HB3 | 2.57 | 0.40 |
| 41:MB:176:SER:OG | 41:MB:181:GLU:OE1 | 2.32 | 0.40 |
| 40:MD:169:PHE:HE1 | 40:MD:202:PHE:CD1 | 2.39 | 0.40 |
| 40:MF:139:HIS:CD2 | 40:MF:139:HIS:N | 2.87 | 0.40 |
| 40:MF:324:VAL:HG21 | 41:MN:219:THR:HB | 2.03 | 0.40 |
| 40:MH:259:LEU:O | 40:MH:261:PRO:N | 2.55 | 0.40 |
| 41:MO:16:ILE:HA | 41:MO:226:ASN:OD1 | 2.20 | 0.40 |
| 41:MO:29:GLY:O | 41:MO:30:ILE:C | 2.60 | 0.40 |
| 41:MO:222:TYR:HD1 | 41:MO:222:TYR:HA | 1.77 | 0.40 |
| 40:NA:88:HIS:NE2 | 40:NA:90:GLU:HB2 | 2.36 | 0.40 |
| 40:NA:234:ILE:O | 40:NA:238:ILE:HG12 | 2.22 | 0.40 |
| 41:NB:266:PHE:CD1 | 41:NB:370:ASN:HB2 | 2.57 | 0.40 |
| 40:NE:7:VAL:HG22 | 40:NE:66:VAL:HB | 2.02 | 0.40 |
| 40:NF:231:ILE:HD13 | 40:NF:231:ILE:HA | 1.86 | 0.40 |
| 41:NL:16:ILE:HG22 | 41:NL:20:PHE:CZ | 2.56 | 0.40 |
| 41:NL:322:SER:OG | 41:NL:323:MET:N | 2.54 | 0.40 |
| 41:NO:318:ARG:HE | 41:NO:358:PRO:HD3 | 1.87 | 0.40 |
| 40:OD:81:GLY:O | 40:OD:83:TYR:N | 2.55 | 0.40 |
| 40:OG:66:VAL:HG23 | 40:OG:91:GLN:HB2 | 2.04 | 0.40 |
| 40:OG:199:ASP:OD1 | 40:OG:200:CYS:N | 2.54 | 0.40 |
| 40:OG:360:PRO:HG3 | 40:OG:373:ALA:HB2 | 2.02 | 0.40 |
| 40:OH:84:ARG:C | 40:OH:86:LEU:H | 2.25 | 0.40 |
| 41:ON:133:PHE:CE1 | 41:ON:155:ILE:HG12 | 2.56 | 0.40 |
| 40:PA:188:ILE:HD11 | 40:PA:390:LEU:HB3 | 2.03 | 0.40 |
| 40:PA:298:PRO:HB3 | 40:PA:307:PRO:HD2 | 2.03 | 0.40 |
| 41:PB:305:PRO:HB3 | 41:PB:310:TYR:CE1 | 2.55 | 0.40 |
| 40:PE:101:ASN:O | 40:PE:407:TYR:OH | 2.39 | 0.40 |
| 40:PE:139:HIS:HE1 | 40:PE:141:PHE:HE1 | 1.70 | 0.40 |
| 40:PG:21:TRP:CZ2 | 40:PG:65:ALA:HB2 | 2.57 | 0.40 |
| 41:PL:171:PRO:HB3 | 41:PL:181:GLU:HG2 | 2.03 | 0.40 |
| 41:PP:134:GLN:HA | 41:PP:165:ASN:O | 2.21 | 0.40 |
| 40:QA:221:ARG:HB3 | 41:QN:322:SER:HB2 | 2.02 | 0.40 |
| 41:QB:31:ASP:H | 41:QB:36:TYR:HA | 1.87 | 0.40 |
| 41:QB:290:THR:C | 41:QB:292:GLN:N | 2.75 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:QE:211:ASP:OD1 | 40:QE:212:ILE:N | 2.55 | 0.40 |
| 40:QG:6:SER:O | 40:QG:65:ALA:HA | 2.21 | 0.40 |
| 40:QG:224:TYR:HA | 40:QG:227:LEU:HD12 | 2.03 | 0.40 |
| 41:QN:145:SER:OG | 41:QN:188:SER:OG | 2.32 | 0.40 |
| 41:QN:178:THR:HB | 41:QN:181:GLU:HG3 | 2.04 | 0.40 |
| 41:QP:7:LEU:N | 41:QP:134:GLN:O | 2.54 | 0.40 |
| 41:QP:55:THR:O | 41:QP:58:LYS:HB3 | 2.21 | 0.40 |
| 41:QP:420:ASN:HB2 | 41:QP:421:PRO:CD | 2.52 | 0.40 |
| 40:RA:396:LEU:HD21 | 41:RN:343:GLU:O | 2.22 | 0.40 |
| 40:RF:172:TYR:N | 40:RF:204:VAL:O | 2.54 | 0.40 |
| 40:RF:229:ARG:HH22 | 40:RF:365:GLY:HA3 | 1.86 | 0.40 |
| 40:RG:428:GLU:HA | 40:RG:431:TYR:HB3 | 2.03 | 0.40 |
| 40:RH:75:ILE:HG21 | 40:RH:94:THR:HB | 2.03 | 0.40 |
| 41:RL:31:ASP:OD1 | 41:RL:35:THR:N | 2.54 | 0.40 |
| 41:RL:306:ARG:HA | 41:RL:340:TYR:HE2 | 1.85 | 0.40 |
| 41:RL:314:ALA:HA | 41:RL:350:LYS:HB3 | 2.04 | 0.40 |
| 40:SA:169:PHE:CZ | 40:SA:238:ILE:HD13 | 2.57 | 0.40 |
| 40:SA:206:ASN:HD22 | 40:SA:206:ASN:HA | 1.68 | 0.40 |
| 40:SE:180:ALA:HB3 | 40:SE:183:GLU:HG3 | 2.02 | 0.40 |
| 40:SF:322:ASP:O | 40:SF:372:ARG:NH1 | 2.54 | 0.40 |
| 40:SH:248:LEU:HB2 | 40:SH:354:GLY:HA2 | 2.03 | 0.40 |
| 40:SH:396:LEU:HD22 | 41:SO:346:PRO:HD3 | 2.03 | 0.40 |
| 40:SI:12:ALA:O | 40:SI:16:ILE:HD12 | 2.22 | 0.40 |
| 40:SI:391:ASP:HB3 | 40:SI:421:ARG:NH1 | 2.37 | 0.40 |
| 41:SM:135:LEU:O | 41:SM:166:THR:HA | 2.21 | 0.40 |
| 41:SO:142:GLY:O | 41:SO:145:SER:N | 2.53 | 0.40 |
| 41:SO:216:LYS:HE2 | 41:SO:216:LYS:HB2 | 1.83 | 0.40 |
| 41:SO:419:GLY:O | 41:SO:422:VAL:HG12 | 2.21 | 0.40 |
| 41:SP:12:CYS:SG | 41:SP:138:SER:HB3 | 2.62 | 0.40 |
| 40:TA:168:GLU:OE1 | 40:TA:198:SER:OG | 2.34 | 0.40 |
| 40:TE:326:LYS:HD3 | 41:TM:208:TYR:CD1 | 2.56 | 0.40 |
| 40:TF:288:VAL:HG23 | 40:TF:319:TYR:CE2 | 2.56 | 0.40 |
| 40:TF:316:CYS:HA | 40:TF:352:LYS:HB2 | 2.04 | 0.40 |
| 40:TH:53:PHE:HB3 | 40:TH:61:HIS:HB3 | 2.03 | 0.40 |
| 40:TH:104:ALA:O | 40:TH:108:TYR:HB2 | 2.21 | 0.40 |
| 40:TI:31:GLN:HE21 | 40:TI:37:PRO:HD3 | 1.85 | 0.40 |
| 41:TL:21:TRP:CZ3 | 41:TL:50:TYR:HB3 | 2.56 | 0.40 |
| 41:TL:202:ILE:HG23 | 41:TL:300:MET:HB3 | 2.02 | 0.40 |
| 41:TM:193:VAL:HG22 | 41:TM:418:LEU:HD21 | 2.03 | 0.40 |
| 41:TO:5:VAL:HB | 41:TO:133:PHE:CD2 | 2.57 | 0.40 |
| 41:TP:309:ARG:N | 41:TP:372:THR:HG1 | 2.20 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:UE:171:ILE:HG21 | 42:UE:501:GTP:H1' | 2.03 | 0.40 |
| 40:UE:262:TYR:HE1 | 41:UM:393:ALA:HA | 1.87 | 0.40 |
| 40:UG:136:LEU:HD22 | 40:UG:169:PHE:HE2 | 1.85 | 0.40 |
| 40:UG:274:PRO:HG3 | 40:UG:286:LEU:HD12 | 2.03 | 0.40 |
| 40:UI:2:ARG:CZ | 40:UI:242:LEU:HA | 2.51 | 0.40 |
| 40:UI:20:CYS:HA | 40:UI:232:SER:HB2 | 2.02 | 0.40 |
| 40:UI:273:ALA:HB3 | 40:UI:274:PRO:HD3 | 2.04 | 0.40 |
| 40:UI:427:LEU:HG | 40:UI:431:TYR:CE2 | 2.56 | 0.40 |
| 41:UN:257:MET:HG3 | 41:UN:312:THR:HG23 | 2.02 | 0.40 |
| 41:UO:323:MET:HG2 | 41:UO:323:MET:O | 2.21 | 0.40 |
| 41:UP:137:HIS:HD2 | 41:UP:168:SER:HB3 | 1.86 | 0.40 |
| 40:VF:115:ILE:HA | 40:VF:118:VAL:HG12 | 2.02 | 0.40 |
| 40:VF:167:LEU:HD23 | 40:VF:200:CYS:HB3 | 2.03 | 0.40 |
| 40:VG:236:SER:HG | 40:VG:243:ARG:HH22 | 1.69 | 0.40 |
| 40:VJ:231:ILE:O | 40:VJ:235:VAL:HG23 | 2.21 | 0.40 |
| 41:VN:280:GLN:H | 41:VN:280:GLN:HG2 | 1.74 | 0.40 |
| 41:VO:156:ARG:HD3 | 41:VO:160:PRO:HA | 2.03 | 0.40 |
| 41:VP:163:ILE:HG12 | 41:VP:250:LEU:HB3 | 2.02 | 0.40 |
| 41:VQ:286:VAL:HG13 | 41:VQ:329:GLN:NE2 | 2.36 | 0.40 |
| 40:WE:319:TYR:CE2 | 40:WE:328:VAL:HG13 | 2.53 | 0.40 |
| 40:WE:346:TRP:CD1 | 41:WM:391:ARG:HD3 | 2.56 | 0.40 |
| 40:WF:319:TYR:HE2 | 40:WF:328:VAL:HG22 | 1.86 | 0.40 |
| 40:WG:96:LYS:HA | 40:WG:96:LYS:HD2 | 1.78 | 0.40 |
| 40:WH:71:GLU:N | 40:WH:71:GLU:OE1 | 2.54 | 0.40 |
| 40:WI:189:LEU:HD21 | 40:WI:417:PHE:HD1 | 1.86 | 0.40 |
| 41:WM:292:GLN:O | 41:WM:298:ASN:HB2 | 2.21 | 0.40 |
| 41:WN:12:CYS:CB | 41:WN:138:SER:HB3 | 2.51 | 0.40 |
| 6:1P:263:ASP:HB3 | 7:1T:303:HIS:HE1 | 1.87 | 0.40 |
| 7:1T:99:LYS:HE3 | 7:1T:100:LYS:HZ2 | 1.87 | 0.40 |
| 7:1U:433:ILE:HG22 | 7:1U:467:ILE:HD13 | 2.04 | 0.40 |
| 7:1U:504:LEU:HD12 | 7:1U:522:THR:HG21 | 2.02 | 0.40 |
| 8:1W:399:GLU:O | 8:1W:403:LYS:HG2 | 2.21 | 0.40 |
| 8:1Z:477:ARG:HH22 | 40:TG:60:LYS:CE | 2.34 | 0.40 |
| 9:2B:210:ARG:NH2 | 40:SG:59:GLY:H | 2.20 | 0.40 |
| 10:2E:157:ARG:O | 41:VN:48:ASN:ND2 | 2.52 | 0.40 |
| 11:2J:229:LYS:HE3 | 11:2J:229:LYS:HB3 | 1.94 | 0.40 |
| 11:2K:185:MET:HB3 | 11:2K:186:LYS:H | 1.47 | 0.40 |
| 12:2Q:89:SER:OG | 41:WP:108:GLU:OE2 | 2.27 | 0.40 |
| 13:2T:71:ILE:HG21 | 13:2T:167:PHE:CD2 | 2.56 | 0.40 |
| 13:2U:35:LYS:HB3 | 13:2U:35:LYS:HE3 | 1.48 | 0.40 |
| 13:2V:82:ASN:HB2 | 13:2V:130:ASN:HD21 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:2W:134:PHE:HE1 | 13:2W:139:PHE:CG | 2.39 | 0.40 |
| 14:3A:8:ASN:HB2 | 14:3A:9:GLN:H | 1.76 | 0.40 |
| 15:3E:296:MET:O | 15:3E:299:LEU:N | 2.55 | 0.40 |
| 15:3F:16:TRP:NE1 | 15:3G:126:ASP:OD1 | 2.33 | 0.40 |
| 16:3J:350:ALA:C | 16:3J:352:LEU:N | 2.75 | 0.40 |
| 16:3L:75:LYS:HD3 | 16:3L:183:LEU:HD12 | 2.03 | 0.40 |
| 16:3L:166:GLN:HE21 | 16:3L:166:GLN:HB3 | 1.72 | 0.40 |
| 17:3O:393:LEU:HD13 | 17:3O:427:VAL:HB | 2.03 | 0.40 |
| 21:4D:474:LYS:HB2 | 21:4D:485:TYR:CE1 | 2.56 | 0.40 |
| 21:4D:528:LEU:O | 21:4D:532:GLN:HB3 | 2.21 | 0.40 |
| 21:4E:357:GLU:HG3 | 21:4E:358:LYS:HE3 | 2.04 | 0.40 |
| 21:4E:508:SER:OG | 21:4E:509:ASP:N | 2.54 | 0.40 |
| 21:4F:169:ASN:H | 21:4F:172:ILE:HD13 | 1.86 | 0.40 |
| 21:4F:453:GLU:HB3 | 21:4F:464:GLY:H | 1.86 | 0.40 |
| 22:4I:680:LYS:HB3 | 22:4I:681:PHE:CD1 | 2.57 | 0.40 |
| 22:4J:82:ASP:HA | 22:4J:102:TYR:O | 2.22 | 0.40 |
| 23:4N:109:CYS:C | 23:4N:111:GLN:H | 2.25 | 0.40 |
| 23:4P:261:TYR:CE1 | 23:4P:265:THR:HG21 | 2.56 | 0.40 |
| 26:4V:207:GLY:HA2 | 26:4V:208:PRO:HD3 | 1.93 | 0.40 |
| 26:4V:244:ILE:HD11 | 26:4V:371:PHE:HD2 | 1.85 | 0.40 |
| 26:4V:318:PRO:O | 26:4V:320:MET:N | 2.54 | 0.40 |
| 27:4Y:136:VAL:HG22 | 27:4Y:139:GLN:HG3 | 2.03 | 0.40 |
| 29:5D:36:ALA:O | 29:5D:38:PHE:N | 2.55 | 0.40 |
| 29:5D:50:LYS:HB2 | 29:5D:50:LYS:HE2 | 1.84 | 0.40 |
| 34:5R:438:ALA:O | 34:5R:442:SER:N | 2.47 | 0.40 |
| 38:6C:114:TYR:CD1 | 40:UG:96:LYS:HE2 | 2.55 | 0.40 |
| 39:6J:44:PRO:HB3 | 39:6J:135:HIS:HA | 2.04 | 0.40 |
| 41:AB:246:LEU:HD21 | 42:AG:501:GTP:H3' | 2.03 | 0.40 |
| 40:AF:88:HIS:HA | 40:AF:89:PRO:HD3 | 1.97 | 0.40 |
| 41:AM:207:LEU:HB3 | 41:AM:225:LEU:HG | 2.04 | 0.40 |
| 41:AM:271:ALA:HB1 | 41:AM:292:GLN:HB3 | 2.03 | 0.40 |
| 41:AN:207:LEU:HB3 | 41:AN:225:LEU:HG | 2.02 | 0.40 |
| 41:BB:289:LEU:HD11 | 41:BB:363:MET:O | 2.21 | 0.40 |
| 40:BG:164:LYS:HD3 | 40:BG:164:LYS:HA | 1.73 | 0.40 |
| 40:BH:75:ILE:HG22 | 40:BH:94:THR:HG23 | 2.04 | 0.40 |
| 40:BH:173:PRO:HG2 | 40:BH:390:LEU:HD11 | 2.04 | 0.40 |
| 41:BO:68:LEU:HB2 | 41:BO:143:THR:HG23 | 2.03 | 0.40 |
| 41:BP:343:GLU:C | 41:BP:345:ILE:H | 2.25 | 0.40 |
| 40:CA:222:PRO:HD2 | 41:CN:324:LYS:HB2 | 2.04 | 0.40 |
| 40:CE:400:LYS:HB3 | 40:CE:400:LYS:HE3 | 1.77 | 0.40 |
| 40:CG:376:MET:SD | 40:CG:378:SER:HB3 | 2.61 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CH:174:ALA:CB | 40:CH:177:VAL:HG23 | 2.52 | 0.40 |
| 40:CH:179:THR:HG21 | 41:CO:246:LEU:HD21 | 2.02 | 0.40 |
| 40:CH:333:ALA:O | 40:CH:337:THR:HG23 | 2.22 | 0.40 |
| 41:CL:3:GLU:O | 41:CL:131:GLN:HG3 | 2.22 | 0.40 |
| 41:CM:117:LEU:HD23 | 41:CM:117:LEU:HA | 1.81 | 0.40 |
| 41:CM:233:MET:C | 41:CM:235:GLY:H | 2.25 | 0.40 |
| 41:CN:226:ASN:O | 41:CN:227:HIS:C | 2.60 | 0.40 |
| 41:CO:178:THR:O | 41:CO:181:GLU:HB2 | 2.21 | 0.40 |
| 41:CO:257:MET:HE3 | 41:CO:314:ALA:HB2 | 2.02 | 0.40 |
| 41:CO:297:LYS:HB3 | 41:CO:297:LYS:HE3 | 1.27 | 0.40 |
| 41:CO:308:GLY:O | 41:CO:309:ARG:C | 2.60 | 0.40 |
| 41:CO:389:PHE:O | 41:CO:392:LYS:N | 2.55 | 0.40 |
| 41:CP:149:THR:HG21 | 41:CP:188:SER:HB3 | 2.03 | 0.40 |
| 40:DA:12:ALA:O | 40:DA:15:GLN:NE2 | 2.54 | 0.40 |
| 40:DA:121:ARG:HD2 | 40:DA:121:ARG:HA | 1.46 | 0.40 |
| 40:DA:138:PHE:CD1 | 40:DA:138:PHE:N | 2.90 | 0.40 |
| 40:DA:175:PRO:O | 40:DA:177:VAL:HG12 | 2.22 | 0.40 |
| 40:DA:307:PRO:O | 40:DA:308:ARG:C | 2.60 | 0.40 |
| 40:DE:9:VAL:HG13 | 40:DE:68:VAL:HG13 | 2.03 | 0.40 |
| 40:DE:129:CYS:HB3 | 40:DE:132:LEU:HB2 | 2.03 | 0.40 |
| 40:DF:96:LYS:HA | 40:DF:96:LYS:HD3 | 1.80 | 0.40 |
| 40:DG:17:GLY:HA2 | 40:DG:20:CYS:HB2 | 2.04 | 0.40 |
| 40:DH:217:LEU:HB2 | 40:DH:219:ILE:CG1 | 2.51 | 0.40 |
| 40:DH:291:ILE:H | 40:DH:291:ILE:HG12 | 1.71 | 0.40 |
| 40:DI:88:HIS:O | 40:DI:91:GLN:N | 2.52 | 0.40 |
| 40:DI:150:THR:O | 40:DI:154:MET:N | 2.49 | 0.40 |
| 40:DI:216:ASN:CG | 40:DI:275:VAL:HB | 2.42 | 0.40 |
| 40:DI:271:THR:OG1 | 40:DI:272:TYR:N | 2.53 | 0.40 |
| 41:DL:19:LYS:HD3 | 41:DL:227:HIS:HB2 | 2.03 | 0.40 |
| 41:DL:276:ARG:HD3 | 41:DL:276:ARG:HA | 1.49 | 0.40 |
| 41:DM:30:ILE:HG12 | 41:DM:84:ILE:HD11 | 2.03 | 0.40 |
| 41:DM:80:PRO:HB2 | 41:DM:81:PHE:H | 1.64 | 0.40 |
| 41:DM:188:SER:O | 41:DM:192:LEU:HB2 | 2.22 | 0.40 |
| 41:DM:338:SER:O | 41:DM:339:SER:C | 2.59 | 0.40 |
| 41:DM:371:SER:C | 41:DM:373:ALA:H | 2.23 | 0.40 |
| 41:DO:64:VAL:HG21 | 41:DO:120:VAL:HG22 | 2.03 | 0.40 |
| 40:EG:136:LEU:HD23 | 40:EG:167:LEU:HB2 | 2.04 | 0.40 |
| 40:EH:209:ILE:O | 40:EH:212:ILE:HG12 | 2.21 | 0.40 |
| 40:EI:124:LYS:H | 40:EI:124:LYS:HG3 | 1.66 | 0.40 |
| 40:EI:198:SER:O | 40:EI:199:ASP:C | 2.60 | 0.40 |
| 41:EM:321:MET:HE3 | 41:EM:321:MET:HB3 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:EM:355:ASP:O | 41:EM:356:ILE:C | 2.58 | 0.40 |
| 41:EM:415:MET:HA | 41:EM:418:LEU:HD12 | 2.03 | 0.40 |
| 40:FA:49:PHE:O | 40:FA:51:THR:N | 2.54 | 0.40 |
| 40:FE:7:VAL:O | 40:FE:137:ILE:HA | 2.22 | 0.40 |
| 40:FF:56:THR:OG1 | 40:FF:57:GLY:N | 2.53 | 0.40 |
| 40:FG:155:GLU:HG2 | 40:FG:197:HIS:CD2 | 2.56 | 0.40 |
| 40:FI:28:HIS:HD1 | 40:FI:53:PHE:HD1 | 1.69 | 0.40 |
| 41:FM:87:PRO:HG2 | 41:GM:278:SER:HB3 | 2.04 | 0.40 |
| 41:FM:95:SER:OG | 41:FM:96:GLY:N | 2.54 | 0.40 |
| 41:FM:404:ASP:N | 41:FM:404:ASP:OD1 | 2.54 | 0.40 |
| 41:GB:323:MET:HA | 41:GB:326:VAL:HG12 | 2.02 | 0.40 |
| 40:GE:243:ARG:HB2 | 40:GE:244:PHE:H | 1.55 | 0.40 |
| 40:GE:324:VAL:O | 40:GE:325:PRO:C | 2.60 | 0.40 |
| 40:GE:326:LYS:O | 40:GE:327:ASP:C | 2.59 | 0.40 |
| 40:GG:79:ARG:HG3 | 40:GG:92:LEU:HD12 | 2.04 | 0.40 |
| 40:GG:188:ILE:HD12 | 40:GG:424:MET:HG3 | 2.03 | 0.40 |
| 40:GH:119:LEU:HD13 | 40:GH:119:LEU:HA | 1.74 | 0.40 |
| 40:GI:315:CYS:SG | 40:GI:376:MET:SD | 3.20 | 0.40 |
| 40:GI:406:TRP:CD1 | 41:GP:255:VAL:HA | 2.56 | 0.40 |
| 41:GN:263:LEU:HD13 | 41:GN:263:LEU:HA | 1.73 | 0.40 |
| 41:GO:273:LEU:HD23 | 41:GO:273:LEU:HA | 1.86 | 0.40 |
| 41:GP:316:VAL:HG23 | 41:GP:366:THR:HB | 2.02 | 0.40 |
| 41:HB:189:VAL:O | 41:HB:193:VAL:HG23 | 2.22 | 0.40 |
| 40:HE:173:PRO:HD2 | 40:HE:390:LEU:HD11 | 2.04 | 0.40 |
| 40:HE:177:VAL:HG12 | 40:HE:178:SER:N | 2.37 | 0.40 |
| 40:HE:239:THR:OG1 | 40:HE:243:ARG:NH2 | 2.54 | 0.40 |
| 40:HE:274:PRO:HD3 | 40:HE:373:ALA:HA | 2.02 | 0.40 |
| 40:HE:339:ARG:O | 40:HE:340:SER:C | 2.60 | 0.40 |
| 40:HH:73:THR:HA | 40:HH:76:ASP:HB2 | 2.03 | 0.40 |
| 40:HH:219:ILE:HD12 | 40:HH:222:PRO:HB3 | 2.03 | 0.40 |
| 40:HI:6:SER:O | 40:HI:65:ALA:HA | 2.21 | 0.40 |
| 41:HN:380:ARG:HG3 | 41:HN:380:ARG:H | 1.69 | 0.40 |
| 41:HO:7:LEU:HD12 | 41:HO:151:LEU:HD21 | 2.02 | 0.40 |
| 41:HP:237:THR:HG22 | 41:HP:250:LEU:HD21 | 2.02 | 0.40 |
| 41:HP:270:PHE:CE2 | 41:HP:272:PRO:HD2 | 2.57 | 0.40 |
| 40:IG:188:ILE:HG21 | 40:IG:394:PHE:CE1 | 2.57 | 0.40 |
| 40:IG:228:ASN:ND2 | 42:IG:501:GTP:HN1 | 2.08 | 0.40 |
| 40:IH:119:LEU:O | 40:IH:123:ARG:HG2 | 2.21 | 0.40 |
| 40:II:236:SER:OG | 40:II:243:ARG:NH2 | 2.54 | 0.40 |
| 40:II:274:PRO:HG3 | 40:II:286:LEU:HD22 | 2.03 | 0.40 |
| 40:II:401:ARG:HD3 | 40:II:401:ARG:HA | 1.91 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:IO:289:LEU:HD11 | 41:IO:363:MET:HB3 | 2.04 | 0.40 |
| 41:IP:289:LEU:HD11 | 41:IP:363:MET:HG3 | 2.03 | 0.40 |
| 40:JF:20:CYS:HA | 40:JF:232:SER:HB2 | 2.04 | 0.40 |
| 40:JH:21:TRP:CZ2 | 40:JH:65:ALA:HB2 | 2.56 | 0.40 |
| 40:JH:27:GLU:OE2 | 40:JH:243:ARG:NH2 | 2.43 | 0.40 |
| 41:JL:13:GLY:HA2 | 41:JL:16:ILE:HG22 | 2.03 | 0.40 |
| 40:KA:226:ASN:HD22 | 40:KA:366:ASP:HB3 | 1.87 | 0.40 |
| 41:KB:257:MET:HE3 | 41:KB:370:ASN:HB2 | 2.03 | 0.40 |
| 40:KD:124:LYS:HE2 | 40:KD:124:LYS:HB2 | 1.95 | 0.40 |
| 40:KD:254:GLU:HG2 | 41:KL:98:GLY:HA2 | 2.03 | 0.40 |
| 40:KF:26:LEU:HD23 | 40:KF:26:LEU:HA | 1.93 | 0.40 |
| 40:KG:215:ARG:HH21 | 40:KG:299:ALA:HB1 | 1.86 | 0.40 |
| 40:KH:175:PRO:HB3 | 40:KH:389:ARG:HE | 1.86 | 0.40 |
| 41:KO:375:GLN:HG3 | 41:KO:379:LYS:HG3 | 2.01 | 0.40 |
| 41:KP:122:LYS:HD2 | 41:LP:291:GLN:HE22 | 1.87 | 0.40 |
| 40:LA:384:ALA:HA | 40:LA:387:TRP:HD1 | 1.87 | 0.40 |
| 40:LD:53:PHE:HB3 | 40:LD:61:HIS:HB3 | 2.04 | 0.40 |
| 40:LF:204:VAL:HG12 | 40:LF:302:MET:HG2 | 2.04 | 0.40 |
| 40:LG:279:GLU:H | 40:LG:279:GLU:HG2 | 1.60 | 0.40 |
| 40:MA:247:ALA:O | 40:MA:249:ASN:N | 2.54 | 0.40 |
| 40:MD:393:LYS:HD2 | 40:MD:393:LYS:HA | 1.79 | 0.40 |
| 40:MF:75:ILE:HG21 | 40:MF:92:LEU:HB3 | 2.04 | 0.40 |
| 40:MF:123:ARG:HE | 40:MF:123:ARG:HB3 | 1.63 | 0.40 |
| 40:MF:288:VAL:HB | 40:MF:327:ASP:HB3 | 2.04 | 0.40 |
| 40:MH:262:TYR:OH | 41:MP:391:ARG:HB3 | 2.21 | 0.40 |
| 41:MN:52:ASN:OD1 | 41:MN:62:ARG:NH1 | 2.53 | 0.40 |
| 41:MN:176:SER:OG | 41:MN:178:THR:O | 2.39 | 0.40 |
| 41:NB:139:LEU:HB2 | 41:NB:168:SER:HB2 | 2.03 | 0.40 |
| 41:NB:203:ASP:HB2 | 41:NB:302:ALA:H | 1.86 | 0.40 |
| 40:ND:17:GLY:HA2 | 40:ND:20:CYS:HB2 | 2.03 | 0.40 |
| 40:ND:96:LYS:HA | 40:ND:96:LYS:HD3 | 1.78 | 0.40 |
| 40:ND:374:VAL:HG22 | 40:ND:375:CYS:N | 2.37 | 0.40 |
| 40:NF:393:LYS:HE2 | 41:NM:346:PRO:HB2 | 2.04 | 0.40 |
| 41:NL:142:GLY:O | 41:NL:144:GLY:N | 2.54 | 0.40 |
| 41:NN:113:VAL:HG22 | 41:NN:117:LEU:HD23 | 2.04 | 0.40 |
| 41:NO:47:ILE:HG12 | 41:NO:59:TYR:CD2 | 2.56 | 0.40 |
| 41:NP:10:GLY:O | 41:NP:14:ASN:HB2 | 2.21 | 0.40 |
| 41:NP:54:ALA:HB3 | 41:NP:58:LYS:HB3 | 2.03 | 0.40 |
| 40:OA:88:HIS:CE1 | 40:PA:280:LYS:HB2 | 2.57 | 0.40 |
| 40:OD:190:THR:O | 40:OD:194:THR:HG23 | 2.21 | 0.40 |
| 40:OD:320:ARG:HH21 | 40:OD:360:PRO:HA | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:OG:150:THR:O | 40:OG:154:MET:HB2 | 2.21 | 0.40 |
| 40:OG:395:ASP:OD2 | 40:OG:421:ARG:NH2 | 2.50 | 0.40 |
| 40:OH:22:GLU:O | 40:OH:25:CYS:N | 2.51 | 0.40 |
| 40:OH:155:GLU:HG2 | 40:OH:197:HIS:HD1 | 1.85 | 0.40 |
| 41:OM:103:LYS:HB2 | 41:OM:103:LYS:HE2 | 1.83 | 0.40 |
| 41:ON:19:LYS:HZ1 | 41:ON:227:HIS:CA | 2.35 | 0.40 |
| 41:ON:222:TYR:O | 41:ON:226:ASN:ND2 | 2.54 | 0.40 |
| 41:OO:209:ASP:O | 41:OO:213:ARG:HB2 | 2.21 | 0.40 |
| 41:OP:313:VAL:O | 41:OP:349:VAL:HA | 2.21 | 0.40 |
| 40:PA:313:MET:HE3 | 40:PA:379:ASN:HB3 | 2.04 | 0.40 |
| 40:PD:88:HIS:CE1 | 40:PD:90:GLU:HB2 | 2.56 | 0.40 |
| 40:PF:319:TYR:HE2 | 40:PF:328:VAL:HG13 | 1.86 | 0.40 |
| 40:PG:326:LYS:HE3 | 41:PO:208:TYR:HB2 | 2.03 | 0.40 |
| 40:PG:352:LYS:HD2 | 41:PO:179:VAL:HG13 | 2.03 | 0.40 |
| 40:PH:28:HIS:NE2 | 40:PH:243:ARG:HD2 | 2.36 | 0.40 |
| 41:PL:421:PRO:O | 41:PL:425:ARG:HG2 | 2.21 | 0.40 |
| 41:PM:18:ALA:HB2 | 41:PM:76:VAL:HG23 | 2.04 | 0.40 |
| 41:PO:21:TRP:CZ3 | 41:PO:61:PRO:HB3 | 2.57 | 0.40 |
| 41:PP:260:PHE:HA | 41:PP:261:PRO:HD3 | 1.98 | 0.40 |
| 40:QA:62:VAL:HA | 40:QA:63:PRO:HD3 | 1.94 | 0.40 |
| 40:QA:228:ASN:ND2 | 42:QN:501:GTP:HN1 | 2.19 | 0.40 |
| 41:QB:137:HIS:O | 41:QB:169:VAL:HG23 | 2.22 | 0.40 |
| 41:QB:290:THR:HG22 | 41:QB:317:PHE:CZ | 2.57 | 0.40 |
| 40:QF:230:LEU:HD23 | 40:QF:230:LEU:HA | 1.93 | 0.40 |
| 40:QG:191:THR:O | 40:QG:195:LEU:HG | 2.21 | 0.40 |
| 40:QH:405:HIS:CD2 | 41:QO:261:PRO:HG3 | 2.56 | 0.40 |
| 41:QL:189:VAL:O | 41:QL:193:VAL:HG23 | 2.22 | 0.40 |
| 41:QM:226:ASN:ND2 | 43:QM:501:GDP:O6 | 2.44 | 0.40 |
| 40:RA:103:TYR:CD1 | 40:RA:189:LEU:HB3 | 2.57 | 0.40 |
| 40:RA:405:HIS:CG | 41:RN:261:PRO:HG3 | 2.57 | 0.40 |
| 41:RB:107:THR:O | 41:RB:109:GLY:N | 2.54 | 0.40 |
| 41:RB:299:MET:HE3 | 41:RB:305:PRO:HG2 | 2.04 | 0.40 |
| 40:RE:67:PHE:HB2 | 40:RE:92:LEU:HA | 2.03 | 0.40 |
| 40:RE:177:VAL:HA | 41:RL:331:LEU:HD11 | 2.03 | 0.40 |
| 40:RF:68:VAL:HG22 | 40:RF:93:ILE:HB | 2.04 | 0.40 |
| 40:RF:118:VAL:O | 40:RF:122:ILE:HG12 | 2.21 | 0.40 |
| 40:RF:332:ILE:HD12 | 40:RF:351:PHE:CD2 | 2.56 | 0.40 |
| 40:RG:99:ALA:HA | 40:RG:110:ILE:HD11 | 2.03 | 0.40 |
| 40:RI:100:ALA:HA | 41:RP:252:LYS:HE2 | 2.03 | 0.40 |
| 40:RI:123:ARG:HH22 | 40:RI:124:LYS:NZ | 2.19 | 0.40 |
| 40:RI:188:ILE:HD12 | 40:RI:424:MET:HG3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RM:174:LYS:HB3 | 41:RM:174:LYS:HE3 | 1.82 | 0.40 |
| 41:RM:309:ARG:NH1 | 41:RM:339:SER:O | 2.55 | 0.40 |
| 41:RN:315:ALA:HB1 | 41:RN:317:PHE:CE2 | 2.56 | 0.40 |
| 41:RO:241:ARG:HG3 | 41:RO:242:PHE:CD1 | 2.55 | 0.40 |
| 41:RP:63:ALA:O | 41:RP:89:ASN:ND2 | 2.54 | 0.40 |
| 40:SA:139:HIS:HE1 | 40:SA:141:PHE:HE1 | 1.69 | 0.40 |
| 40:SA:255:PHE:CZ | 40:SA:318:LEU:HD21 | 2.56 | 0.40 |
| 41:SB:103:LYS:HA | 41:SB:107:THR:HG21 | 2.04 | 0.40 |
| 41:SB:330:MET:HE1 | 41:SB:349:VAL:HG11 | 2.04 | 0.40 |
| 40:SH:132:LEU:HB3 | 40:SH:164:LYS:HZ1 | 1.85 | 0.40 |
| 40:SH:188:ILE:HD12 | 40:SH:424:MET:HG3 | 2.04 | 0.40 |
| 40:SI:26:LEU:HD21 | 40:SI:363:VAL:HG23 | 2.03 | 0.40 |
| 41:SL:15:GLN:HB2 | 41:SL:19:LYS:HZ3 | 1.85 | 0.40 |
| 41:SM:204:ASN:HD22 | 41:SM:204:ASN:N | 2.20 | 0.40 |
| 41:SO:271:ALA:HB3 | 41:SO:272:PRO:CD | 2.45 | 0.40 |
| 41:SO:362:LYS:HA | 41:SO:362:LYS:HD3 | 1.44 | 0.40 |
| 41:TB:131:GLN:NE2 | 41:TB:240:LEU:HD22 | 2.35 | 0.40 |
| 40:TF:229:ARG:NH1 | 40:TF:363:VAL:HG11 | 2.37 | 0.40 |
| 40:TH:271:THR:HG22 | 40:TH:376:MET:HB3 | 2.02 | 0.40 |
| 40:TI:112:LYS:HA | 40:TI:115:ILE:HG22 | 2.03 | 0.40 |
| 40:TI:115:ILE:HA | 40:TI:118:VAL:HG22 | 2.03 | 0.40 |
| 41:TL:288:GLU:O | 41:TL:292:GLN:HB3 | 2.22 | 0.40 |
| 41:TP:32:PRO:HG3 | 41:TP:81:PHE:CE1 | 2.57 | 0.40 |
| 41:TP:196:THR:HG23 | 41:TP:264:HIS:CE1 | 2.56 | 0.40 |
| 40:UA:2:ARG:HH22 | 41:UB:71:GLY:HA2 | 1.86 | 0.40 |
| 40:UE:102:ASN:HD22 | 40:UE:105:ARG:HG3 | 1.85 | 0.40 |
| 40:UF:248:LEU:HD13 | 40:UF:248:LEU:HA | 1.91 | 0.40 |
| 40:UF:361:THR:OG1 | 40:UF:362:VAL:N | 2.55 | 0.40 |
| 40:UF:440:GLU:H | 40:UF:440:GLU:HG2 | 1.69 | 0.40 |
| 40:UG:139:HIS:NE2 | 40:UG:168:GLU:OE1 | 2.47 | 0.40 |
| 40:UG:191:THR:HA | 40:UG:194:THR:HG22 | 2.03 | 0.40 |
| 40:UI:106:GLY:C | 40:UI:148:GLY:HA3 | 2.41 | 0.40 |
| 40:UI:217:LEU:O | 40:UI:218:ASP:C | 2.59 | 0.40 |
| 40:UI:418:SER:OG | 40:UI:419:GLU:N | 2.55 | 0.40 |
| 41:UM:142:GLY:O | 41:UM:144:GLY:N | 2.54 | 0.40 |
| 41:UM:319:GLY:HA2 | 41:UM:357:PRO:HD3 | 2.04 | 0.40 |
| 41:UN:138:SER:HB2 | 41:UN:169:VAL:HB | 2.02 | 0.40 |
| 41:UN:260:PHE:HE2 | 41:UN:425:ARG:HD2 | 1.87 | 0.40 |
| 41:UP:207:LEU:HD12 | 41:UP:207:LEU:HA | 1.88 | 0.40 |
| 40:VA:261:PRO:HG2 | 40:VA:265:ILE:HD11 | 2.02 | 0.40 |
| 40:VA:326:LYS:HD3 | 41:VB:208:TYR:CD1 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:VF:210:TYR:HE1 | 40:VF:227:LEU:HD21 | 1.87 | 0.40 |
| 40:VH:3:GLU:HG3 | 40:VH:64:ARG:NH2 | 2.37 | 0.40 |
| 40:VJ:70:LEU:HD12 | 40:VJ:110:ILE:HG22 | 2.03 | 0.40 |
| 40:VJ:169:PHE:CZ | 40:VJ:238:ILE:HG21 | 2.57 | 0.40 |
| 41:VO:314:ALA:HB3 | 41:VO:368:ILE:HB | 2.03 | 0.40 |
| 41:WB:30:ILE:HG13 | 41:WB:51:TYR:CE2 | 2.57 | 0.40 |
| 41:WB:95:SER:OG | 41:WB:96:GLY:N | 2.54 | 0.40 |
| 41:WB:165:ASN:ND2 | 41:WB:250:LEU:HD13 | 2.37 | 0.40 |
| 41:WB:226:ASN:ND2 | 43:WB:501:GDP:O6 | 2.47 | 0.40 |
| 41:WB:344:TRP:HZ3 | 40:WG:402:ALA:HB2 | 1.87 | 0.40 |
| 40:WE:228:ASN:ND2 | 42:WE:501:GTP:HN1 | 2.13 | 0.40 |
| 40:WF:265:ILE:HG21 | 40:WF:313:MET:HE1 | 2.04 | 0.40 |
| 40:WF:394:PHE:CD2 | 40:WF:421:ARG:HD3 | 2.56 | 0.40 |
| 40:WH:112:LYS:HB3 | 40:WH:112:LYS:HE3 | 1.83 | 0.40 |
| 40:WI:112:LYS:HA | 40:WI:115:ILE:HG22 | 2.03 | 0.40 |
| 41:WN:245:GLN:H | 41:WN:245:GLN:HG2 | 1.65 | 0.40 |
| 41:WP:20:PHE:HZ | 41:WP:50:TYR:CZ | 2.39 | 0.40 |
| 41:WQ:4:ILE:HG22 | 41:WQ:49:VAL:HG12 | 2.03 | 0.40 |
| 41:WQ:273:LEU:HB2 | 41:WQ:292:GLN:NE2 | 2.37 | 0.40 |
| 41:WQ:289:LEU:HD11 | 41:WQ:363:MET:HG3 | 2.03 | 0.40 |
| 7:1T:362:LEU:HD13 | 7:1T:362:LEU:HA | 1.81 | 0.40 |
| 7:1T:507:CYS:HB2 | 7:1T:551:MET:HB2 | 2.04 | 0.40 |
| 8:1W:260:VAL:HA | 40:VJ:282:TYR:OH | 2.20 | 0.40 |
| 9:2B:389:GLU:CG | 9:2B:392:ARG:HE | 2.33 | 0.40 |
| 11:2I:195:ALA:O | 11:2I:196:VAL:C | 2.59 | 0.40 |
| 12:2P:215:GLN:HE21 | 12:2P:215:GLN:HB3 | 1.67 | 0.40 |
| 14:3A:73:LYS:HB3 | 14:3A:73:LYS:HE2 | 1.78 | 0.40 |
| 15:3E:66:ARG:O | 15:3E:70:VAL:HG23 | 2.22 | 0.40 |
| 16:3J:321:ARG:HD2 | 16:3L:64:LEU:HD21 | 2.03 | 0.40 |
| 16:3L:297:ILE:HD13 | 16:3L:360:GLN:HG2 | 2.04 | 0.40 |
| 17:3P:97:ASP:O | 17:3P:98:ASP:C | 2.60 | 0.40 |
| 17:3R:199:LEU:O | 17:3R:200:PHE:C | 2.60 | 0.40 |
| 17:3R:205:ARG:HB2 | 17:3R:205:ARG:HE | 1.60 | 0.40 |
| 18:3U:414:LYS:HA | 18:3U:414:LYS:HD3 | 1.73 | 0.40 |
| 18:3W:429:LYS:HE2 | 18:3W:429:LYS:HB2 | 1.80 | 0.40 |
| 19:3Y:207:GLU:HA | 19:3Y:210:THR:HG22 | 2.02 | 0.40 |
| 20:4B:292:GLN:O | 20:4B:296:LYS:HG2 | 2.22 | 0.40 |
| 21:4D:81:PRO:HA | 21:4D:82:PRO:HD3 | 1.90 | 0.40 |
| 21:4D:258:GLU:OE2 | 21:4D:285:ARG:NH2 | 2.51 | 0.40 |
| 21:4D:299:LYS:HG2 | 21:4D:300:VAL:H | 1.86 | 0.40 |
| 21:4E:280:GLU:HG2 | 21:4E:283:ASP:HB3 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:4F:171:GLY:HA2 | 21:4F:183:ILE:O | 2.22 | 0.40 |
| 22:4I:292:VAL:HB | 41:CO:227:HIS:HE1 | 1.87 | 0.40 |
| 22:4I:594:LEU:HD23 | 22:4I:594:LEU:HA | 1.82 | 0.40 |
| 22:4J:90:PRO:C | 41:BN:282:ARG:HB2 | 2.41 | 0.40 |
| 22:4J:659:LYS:HD3 | 22:4J:678:LEU:HG | 2.02 | 0.40 |
| 22:4K:580:ASN:OD1 | 22:4K:581:THR:N | 2.55 | 0.40 |
| 23:4M:19:ILE:O | 23:4M:20:PRO:C | 2.60 | 0.40 |
| 24:4O:213:PHE:O | 24:4O:214:ASP:C | 2.59 | 0.40 |
| 27:4Y:198:PRO:HB3 | 27:4Y:263:HIS:CD2 | 2.57 | 0.40 |
| 27:4Z:73:VAL:HG21 | 27:4Z:119:LYS:NZ | 2.37 | 0.40 |
| 30:5G:43:ARG:O | 30:5G:46:HIS:ND1 | 2.54 | 0.40 |
| 31:5I:489:HIS:CE1 | 31:5I:491:PHE:H | 2.39 | 0.40 |
| 34:5R:309:LEU:HD12 | 34:5R:310:ASN:ND2 | 2.37 | 0.40 |
| 36:5W:60:LEU:HD11 | 41:NM:45:GLU:HG2 | 2.04 | 0.40 |
| 36:5Y:48:LEU:HD23 | 41:NB:56:GLY:O | 2.21 | 0.40 |
| 38:6C:15:LEU:HD22 | 40:VG:211:ASP:HB2 | 2.03 | 0.40 |
| 38:6C:54:MET:HE1 | 40:VA:218:ASP:HA | 2.03 | 0.40 |
| 38:6D:238:LYS:HA | 38:6D:238:LYS:HD2 | 1.86 | 0.40 |
| 39:6G:115:LEU:HD12 | 39:6G:115:LEU:HA | 1.92 | 0.40 |
| 39:6L:13:VAL:HG21 | 39:6L:81:LEU:HD11 | 2.03 | 0.40 |
| 40:AE:402:ALA:HB2 | 41:AL:344:TRP:HZ3 | 1.87 | 0.40 |
| 40:AG:228:ASN:OD1 | 42:AG:501:GTP:N1 | 2.50 | 0.40 |
| 40:AG:293:ASN:O | 40:AG:297:GLU:HG3 | 2.22 | 0.40 |
| 41:AM:309:ARG:H | 41:AM:309:ARG:HG2 | 1.73 | 0.40 |
| 40:BA:325:PRO:O | 40:BA:328:VAL:HB | 2.21 | 0.40 |
| 41:BB:101:TRP:NE1 | 41:BB:145:SER:O | 2.54 | 0.40 |
| 40:BE:109:THR:OG1 | 40:BE:110:ILE:N | 2.53 | 0.40 |
| 40:BE:401:ARG:H | 40:BE:401:ARG:HG2 | 1.81 | 0.40 |
| 40:BH:152:LEU:HD12 | 40:BH:152:LEU:HA | 1.90 | 0.40 |
| 40:BH:180:ALA:O | 41:BO:347:ASN:ND2 | 2.54 | 0.40 |
| 41:BL:101:TRP:HB3 | 41:BL:398:TYR:HE1 | 1.87 | 0.40 |
| 41:BM:130:LEU:HB3 | 41:BM:162:ARG:HD2 | 2.04 | 0.40 |
| 41:BM:202:ILE:CD1 | 41:BM:268:PRO:HG3 | 2.51 | 0.40 |
| 41:BO:170:VAL:HB | 41:BO:377:LEU:HD11 | 2.02 | 0.40 |
| 41:BO:221:THR:OG1 | 41:BO:222:TYR:N | 2.54 | 0.40 |
| 41:BO:293:MET:HE3 | 41:BO:293:MET:HB3 | 1.95 | 0.40 |
| 41:BP:151:LEU:HG | 41:BP:155:ILE:HD12 | 2.04 | 0.40 |
| 41:BP:183:TYR:HA | 41:BP:385:PHE:CE2 | 2.57 | 0.40 |
| 41:BP:303:CYS:O | 41:BP:304:ASP:C | 2.59 | 0.40 |
| 40:CA:177:VAL:O | 40:CA:178:SER:HB2 | 2.21 | 0.40 |
| 40:CA:244:PHE:HB2 | 40:CA:356:ASN:OD1 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CA:262:TYR:CZ | 41:CB:393:ALA:HB2 | 2.57 | 0.40 |
| 40:CA:385:GLU:H | 40:CA:385:GLU:HG3 | 1.55 | 0.40 |
| 40:CA:404:VAL:O | 40:CA:408:VAL:HG12 | 2.22 | 0.40 |
| 40:CE:62:VAL:HG21 | 40:DE:283:HIS:HB3 | 2.02 | 0.40 |
| 40:CF:254:GLU:HA | 40:CF:257:THR:HB | 2.03 | 0.40 |
| 40:CG:167:LEU:HD13 | 40:CG:200:CYS:HB3 | 2.02 | 0.40 |
| 40:CI:73:THR:O | 40:CI:77:GLU:HG3 | 2.21 | 0.40 |
| 40:CI:258:ASN:HD22 | 40:CI:352:LYS:HG2 | 1.85 | 0.40 |
| 40:CI:390:LEU:HD23 | 40:CI:390:LEU:HA | 1.90 | 0.40 |
| 41:CM:7:LEU:HB2 | 41:CM:135:LEU:HD13 | 2.02 | 0.40 |
| 41:CM:12:CYS:HB3 | 41:CM:138:SER:HB3 | 2.03 | 0.40 |
| 41:CM:263:LEU:H | 41:CM:263:LEU:HG | 1.65 | 0.40 |
| 41:CM:303:CYS:SG | 41:CM:374:ILE:HA | 2.61 | 0.40 |
| 41:CN:32:PRO:HG3 | 41:CN:81:PHE:CZ | 2.57 | 0.40 |
| 41:CN:47:ILE:H | 41:CN:47:ILE:HG13 | 1.27 | 0.40 |
| 41:CN:263:LEU:HD23 | 41:CN:263:LEU:HA | 1.85 | 0.40 |
| 41:CO:9:ALA:HB2 | 41:CO:66:VAL:HG13 | 2.02 | 0.40 |
| 41:CO:253:LEU:HD22 | 41:CO:253:LEU:HA | 1.90 | 0.40 |
| 41:CP:102:ALA:C | 41:CP:104:GLY:H | 2.25 | 0.40 |
| 41:CP:170:VAL:HG21 | 41:CP:377:LEU:HD21 | 2.04 | 0.40 |
| 40:DA:171:ILE:HA | 40:DA:204:VAL:HG12 | 2.03 | 0.40 |
| 40:DA:416:GLU:H | 40:DA:416:GLU:HG2 | 1.39 | 0.40 |
| 41:DB:84:ILE:HD12 | 41:DB:84:ILE:HA | 1.65 | 0.40 |
| 40:DF:62:VAL:HG21 | 40:EF:283:HIS:O | 2.22 | 0.40 |
| 40:DF:84:ARG:C | 40:DF:86:LEU:H | 2.25 | 0.40 |
| 40:DG:142:GLY:HA2 | 40:DG:183:GLU:HG2 | 2.04 | 0.40 |
| 40:DG:196:GLU:N | 40:DG:196:GLU:OE2 | 2.54 | 0.40 |
| 40:DH:5:ILE:HD13 | 40:DH:64:ARG:HD2 | 2.04 | 0.40 |
| 40:DH:157:LEU:O | 40:DH:158:SER:C | 2.60 | 0.40 |
| 41:DL:77:ARG:NH2 | 41:DL:85:PHE:O | 2.54 | 0.40 |
| 41:DL:80:PRO:HB2 | 41:DL:81:PHE:H | 1.75 | 0.40 |
| 41:DL:121:ARG:HG2 | 41:DL:121:ARG:H | 1.76 | 0.40 |
| 41:DL:135:LEU:HB3 | 41:DL:166:THR:HG22 | 2.02 | 0.40 |
| 41:DL:165:ASN:ND2 | 41:DL:198:GLU:HG2 | 2.37 | 0.40 |
| 41:DL:233:MET:HE2 | 41:DL:233:MET:HB2 | 1.85 | 0.40 |
| 41:DL:387:ALA:HA | 41:DL:390:ARG:HH21 | 1.87 | 0.40 |
| 41:DM:137:HIS:HD2 | 41:DM:168:SER:HB3 | 1.86 | 0.40 |
| 41:DM:257:MET:HA | 41:DM:312:THR:CB | 2.51 | 0.40 |
| 41:DP:2:ARG:H | 41:DP:2:ARG:HG3 | 1.36 | 0.40 |
| 41:DP:171:PRO:HB3 | 41:DP:181:GLU:HG2 | 2.03 | 0.40 |
| 41:DP:417:ASP:O | 41:DP:421:PRO:HD2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:EA:9:VAL:HG12 | 40:EA:68:VAL:HG13 | 2.03 | 0.40 |
| 40:EA:242:LEU:H | 40:EA:242:LEU:HD23 | 1.87 | 0.40 |
| 40:EA:262:TYR:HB2 | 40:EA:265:ILE:HG12 | 2.03 | 0.40 |
| 40:EE:223:THR:HG23 | 40:EE:225:THR:HG22 | 2.02 | 0.40 |
| 40:EF:195:LEU:HD21 | 40:EF:264:ARG:HG3 | 2.03 | 0.40 |
| 40:EF:406:TRP:HE1 | 41:EM:258:VAL:HB | 1.86 | 0.40 |
| 40:EH:90:GLU:O | 40:EH:92:LEU:N | 2.55 | 0.40 |
| 40:EH:403:PHE:HA | 40:EH:405:HIS:CE1 | 2.56 | 0.40 |
| 40:EI:103:TYR:OH | 40:EI:193:THR:HG21 | 2.21 | 0.40 |
| 40:EI:415:GLY:O | 40:EI:417:PHE:N | 2.53 | 0.40 |
| 40:EI:429:LYS:HD2 | 40:EI:429:LYS:HA | 1.54 | 0.40 |
| 41:EM:160:PRO:O | 41:EM:161:ASP:HB2 | 2.22 | 0.40 |
| 41:EM:386:THR:C | 41:EM:388:MET:H | 2.25 | 0.40 |
| 41:EN:63:ALA:O | 41:EN:89:ASN:ND2 | 2.55 | 0.40 |
| 41:EN:386:THR:O | 41:EN:390:ARG:NH2 | 2.54 | 0.40 |
| 41:EP:285:THR:HB | 41:EP:287:PRO:HD2 | 2.03 | 0.40 |
| 40:FA:88:HIS:O | 40:FA:90:GLU:N | 2.55 | 0.40 |
| 40:FA:124:LYS:H | 40:FA:124:LYS:HG2 | 1.56 | 0.40 |
| 40:FA:390:LEU:HD23 | 40:FA:390:LEU:HA | 1.82 | 0.40 |
| 40:FG:124:LYS:HA | 40:FG:124:LYS:HD3 | 1.85 | 0.40 |
| 40:FH:7:VAL:O | 40:FH:137:ILE:HA | 2.21 | 0.40 |
| 40:FH:224:TYR:O | 40:FH:228:ASN:HB2 | 2.22 | 0.40 |
| 41:FO:105:HIS:CD2 | 41:FO:150:LEU:HD13 | 2.57 | 0.40 |
| 40:GA:26:LEU:O | 40:GA:27:GLU:C | 2.60 | 0.40 |
| 40:GA:235:VAL:O | 40:GA:239:THR:HG22 | 2.21 | 0.40 |
| 41:GB:68:LEU:HB2 | 41:GB:97:ALA:HB2 | 2.03 | 0.40 |
| 40:GE:299:ALA:C | 40:GE:301:GLN:H | 2.25 | 0.40 |
| 40:GE:359:PRO:HB2 | 40:GE:360:PRO:CD | 2.52 | 0.40 |
| 40:GF:294:ALA:O | 40:GF:300:ASN:ND2 | 2.47 | 0.40 |
| 40:GI:288:VAL:O | 40:GI:289:ALA:C | 2.58 | 0.40 |
| 41:GN:141:GLY:HA3 | 43:GN:501:GDP:O1A | 2.22 | 0.40 |
| 41:GN:216:LYS:HA | 41:GN:216:LYS:HD3 | 1.87 | 0.40 |
| 41:GO:105:HIS:HB3 | 41:GO:106:TYR:HD1 | 1.86 | 0.40 |
| 41:GO:269:GLY:O | 41:GO:367:PHE:N | 2.46 | 0.40 |
| 40:HA:107:HIS:CE1 | 40:HA:151:SER:HG | 2.39 | 0.40 |
| 40:HA:255:PHE:O | 40:HA:259:LEU:HB2 | 2.21 | 0.40 |
| 40:HE:128:GLN:O | 40:HE:129:CYS:C | 2.60 | 0.40 |
| 40:HE:281:ALA:HA | 40:HE:284:GLU:HG2 | 2.03 | 0.40 |
| 40:HG:14:VAL:HG22 | 40:HG:67:PHE:HD1 | 1.87 | 0.40 |
| 40:HG:276:ILE:HD12 | 40:HG:276:ILE:HG23 | 1.93 | 0.40 |
| 40:HI:8:HIS:HD1 | 40:HI:17:GLY:HA3 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:HI:287:SER:N | 40:HI:290:GLU:OE2 | 2.54 | 0.40 |
| 41:HN:46:ARG:C | 41:HN:48:ASN:N | 2.72 | 0.40 |
| 41:HN:93:GLY:O | 41:HN:94:GLN:C | 2.60 | 0.40 |
| 41:HN:94:GLN:O | 41:HN:95:SER:HB2 | 2.21 | 0.40 |
| 40:IA:79:ARG:HG2 | 40:IA:92:LEU:HD13 | 2.02 | 0.40 |
| 40:IA:181:VAL:HG23 | 40:IA:182:VAL:HG13 | 2.03 | 0.40 |
| 40:IE:117:LEU:O | 40:IE:121:ARG:HG2 | 2.22 | 0.40 |
| 40:IE:278:ALA:H | 40:IE:368:ALA:HB2 | 1.87 | 0.40 |
| 40:IF:28:HIS:CE1 | 40:IF:243:ARG:HD2 | 2.55 | 0.40 |
| 40:IG:254:GLU:HB3 | 40:IG:352:LYS:NZ | 2.37 | 0.40 |
| 40:IG:260:VAL:HG23 | 40:IG:265:ILE:O | 2.22 | 0.40 |
| 40:IH:297:GLU:OE2 | 40:IH:300:ASN:ND2 | 2.54 | 0.40 |
| 40:II:242:LEU:HD23 | 40:II:242:LEU:H | 1.87 | 0.40 |
| 41:IN:361:LEU:HD23 | 41:IN:361:LEU:HA | 1.92 | 0.40 |
| 40:JA:88:HIS:HB3 | 40:JA:91:GLN:HG2 | 2.03 | 0.40 |
| 41:JB:226:ASN:ND2 | 43:JB:501:GDP:O6 | 2.54 | 0.40 |
| 40:JE:48:SER:O | 40:JE:51:THR:HG22 | 2.21 | 0.40 |
| 40:JE:352:LYS:HZ3 | 41:JM:178:THR:CA | 2.34 | 0.40 |
| 40:JG:343:PHE:HE2 | 40:JG:350:GLY:HA3 | 1.87 | 0.40 |
| 41:JL:189:VAL:HG21 | 41:JL:378:PHE:HE2 | 1.87 | 0.40 |
| 41:JM:3:GLU:O | 41:JM:131:GLN:N | 2.55 | 0.40 |
| 41:JM:72:THR:O | 41:JM:73:MET:C | 2.60 | 0.40 |
| 41:JN:7:LEU:HD13 | 41:JN:151:LEU:HD13 | 2.03 | 0.40 |
| 41:JN:306:ARG:HG3 | 41:JN:340:TYR:CZ | 2.56 | 0.40 |
| 41:JN:309:ARG:NH1 | 41:JN:339:SER:O | 2.53 | 0.40 |
| 41:KB:156:ARG:HD3 | 41:KB:164:MET:HG3 | 2.03 | 0.40 |
| 40:KD:88:HIS:HB3 | 40:KD:91:GLN:HG3 | 2.03 | 0.40 |
| 40:KD:234:ILE:HD11 | 40:KD:302:MET:SD | 2.62 | 0.40 |
| 40:KE:207:GLU:HA | 40:KE:210:TYR:CD2 | 2.57 | 0.40 |
| 40:KE:400:LYS:HZ3 | 41:KL:344:TRP:HB2 | 1.86 | 0.40 |
| 41:KL:183:TYR:O | 41:KL:184:ASN:C | 2.60 | 0.40 |
| 41:KP:134:GLN:HE21 | 41:KP:167:PHE:HE1 | 1.69 | 0.40 |
| 41:KP:192:LEU:O | 41:KP:196:THR:OG1 | 2.28 | 0.40 |
| 40:LF:144:GLY:O | 40:LF:148:GLY:N | 2.51 | 0.40 |
| 40:LF:212:ILE:HD13 | 40:LF:212:ILE:HA | 1.82 | 0.40 |
| 40:LG:21:TRP:CE3 | 40:LG:24:TYR:HD1 | 2.38 | 0.40 |
| 40:LG:256:GLN:HG3 | 41:LO:397:TRP:CZ2 | 2.57 | 0.40 |
| 41:LL:53:GLU:HG3 | 41:LL:59:TYR:HE1 | 1.87 | 0.40 |
| 41:LN:31:ASP:OD1 | 41:LN:31:ASP:N | 2.55 | 0.40 |
| 41:LO:274:THR:HG21 | 41:LO:279:GLN:HG3 | 2.03 | 0.40 |
| 41:LP:7:LEU:HD23 | 41:LP:151:LEU:HD21 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:MA:143:GLY:HA3 | 42:MN:501:GTP:O1A | 2.22 | 0.40 |
| 40:MG:274:PRO:HD2 | 40:MG:291:ILE:HB | 2.04 | 0.40 |
| 40:MH:49:PHE:HE1 | 40:MH:55:GLU:HB2 | 1.86 | 0.40 |
| 40:MH:413:GLU:O | 40:MH:414:GLU:C | 2.60 | 0.40 |
| 41:MO:363:MET:HE2 | 41:MO:363:MET:HB2 | 1.63 | 0.40 |
| 41:MP:163:ILE:HG21 | 41:MP:250:LEU:HB3 | 2.03 | 0.40 |
| 40:NF:311:LYS:N | 40:NF:381:THR:OG1 | 2.44 | 0.40 |
| 41:NM:143:THR:OG1 | 43:NM:502:GDP:O1B | 2.39 | 0.40 |
| 41:NP:7:LEU:HD22 | 41:NP:64:VAL:HB | 2.03 | 0.40 |
| 40:OA:234:ILE:HD13 | 40:OA:272:TYR:HB2 | 2.04 | 0.40 |
| 40:OD:66:VAL:HG12 | 40:OD:68:VAL:HG13 | 2.02 | 0.40 |
| 40:OG:317:LEU:HD12 | 40:OG:353:VAL:HG12 | 2.04 | 0.40 |
| 41:OL:323:MET:HE3 | 41:OL:323:MET:HB3 | 1.84 | 0.40 |
| 41:OM:210:ILE:HG22 | 41:OM:215:LEU:HD23 | 2.04 | 0.40 |
| 41:ON:32:PRO:HD3 | 41:ON:81:PHE:CZ | 2.57 | 0.40 |
| 41:OP:21:TRP:CZ3 | 41:OP:24:ILE:HD11 | 2.57 | 0.40 |
| 40:PE:180:ALA:HA | 41:PL:256:ASN:HD21 | 1.85 | 0.40 |
| 40:PF:139:HIS:ND1 | 40:PF:140:SER:O | 2.55 | 0.40 |
| 40:PF:212:ILE:HG23 | 40:PF:216:ASN:ND2 | 2.36 | 0.40 |
| 40:PG:68:VAL:HG11 | 40:PG:149:PHE:CE2 | 2.57 | 0.40 |
| 40:PG:88:HIS:CE1 | 40:QG:280:LYS:HE2 | 2.56 | 0.40 |
| 40:PG:317:LEU:HD23 | 40:PG:376:MET:HB2 | 2.04 | 0.40 |
| 40:PH:18:ASN:OD1 | 40:PH:19:ALA:N | 2.55 | 0.40 |
| 40:PH:75:ILE:O | 40:PH:79:ARG:HG3 | 2.20 | 0.40 |
| 40:PH:320:ARG:HG2 | 40:PH:358:GLN:O | 2.22 | 0.40 |
| 41:PL:137:HIS:ND1 | 41:PL:144:GLY:O | 2.54 | 0.40 |
| 40:QA:268:PRO:HA | 40:QA:379:ASN:HA | 2.03 | 0.40 |
| 41:QB:16:ILE:HA | 41:QB:226:ASN:HB3 | 2.03 | 0.40 |
| 41:QB:31:ASP:HB3 | 41:QB:35:THR:O | 2.22 | 0.40 |
| 41:QB:393:ALA:C | 41:QB:395:LEU:N | 2.74 | 0.40 |
| 40:QE:15:GLN:NE2 | 40:QE:228:ASN:HD21 | 2.19 | 0.40 |
| 40:QF:33:ASP:OD1 | 40:QF:34:GLY:N | 2.55 | 0.40 |
| 40:QG:135:PHE:HD1 | 40:QG:157:LEU:HD21 | 1.86 | 0.40 |
| 40:QG:216:ASN:OD1 | 40:QG:275:VAL:HG13 | 2.20 | 0.40 |
| 40:QG:416:GLU:OE2 | 40:QG:416:GLU:N | 2.54 | 0.40 |
| 41:QP:225:LEU:HB3 | 43:QP:501:GDP:N2 | 2.36 | 0.40 |
| 40:RA:53:PHE:HB3 | 40:RA:61:HIS:HB3 | 2.04 | 0.40 |
| 40:RA:100:ALA:O | 41:RN:255:VAL:HG11 | 2.22 | 0.40 |
| 40:RA:223:THR:HA | 41:RN:323:MET:SD | 2.60 | 0.40 |
| 40:RG:178:SER:OG | 40:RG:179:THR:N | 2.53 | 0.40 |
| 41:RL:12:CYS:O | 41:RL:16:ILE:HD12 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:RN:232:THR:HG22 | 41:RN:270:PHE:HB2 | 2.02 | 0.40 |
| 41:RP:87:PRO:HD3 | 41:SP:281:TYR:HD1 | 1.86 | 0.40 |
| 41:RP:211:CYS:HA | 41:RP:215:LEU:HD12 | 2.03 | 0.40 |
| 40:SE:242:LEU:HD23 | 40:SE:242:LEU:H | 1.87 | 0.40 |
| 40:SF:121:ARG:HH21 | 40:SF:124:LYS:HG2 | 1.86 | 0.40 |
| 40:SG:16:ILE:O | 40:SG:20:CYS:HB2 | 2.21 | 0.40 |
| 41:SN:385:PHE:HA | 41:SN:388:MET:HG3 | 2.03 | 0.40 |
| 40:TA:73:THR:HG22 | 41:TN:46:ARG:HE | 1.86 | 0.40 |
| 40:TA:347:CYS:HA | 41:TB:388:MET:HE2 | 2.04 | 0.40 |
| 40:TE:80:THR:HA | 40:TE:84:ARG:HD3 | 2.03 | 0.40 |
| 40:TG:33:ASP:OD1 | 40:TG:34:GLY:N | 2.55 | 0.40 |
| 40:TH:273:ALA:HB2 | 40:TH:295:CYS:SG | 2.61 | 0.40 |
| 40:TH:351:PHE:C | 40:TH:352:LYS:HE2 | 2.42 | 0.40 |
| 40:TI:33:ASP:O | 40:TI:60:LYS:NZ | 2.48 | 0.40 |
| 41:TM:253:LEU:O | 41:TM:257:MET:HG2 | 2.21 | 0.40 |
| 40:UA:298:PRO:HB3 | 40:UA:307:PRO:HD2 | 2.03 | 0.40 |
| 40:UF:88:HIS:CD2 | 40:VG:283:HIS:HB2 | 2.57 | 0.40 |
| 40:UF:183:GLU:HB3 | 40:UF:184:PRO:CD | 2.48 | 0.40 |
| 40:VA:295:CYS:O | 40:VA:301:GLN:NE2 | 2.40 | 0.40 |
| 41:VB:156:ARG:HD2 | 41:VB:156:ARG:HA | 1.92 | 0.40 |
| 41:VB:178:THR:OG1 | 41:VB:181:GLU:HG3 | 2.22 | 0.40 |
| 40:VF:75:ILE:HD12 | 40:VF:94:THR:HG22 | 2.04 | 0.40 |
| 40:VF:189:LEU:HD11 | 40:VF:417:PHE:CE1 | 2.56 | 0.40 |
| 40:VG:7:VAL:HG11 | 40:VG:153:LEU:HD21 | 2.04 | 0.40 |
| 40:WA:180:ALA:HA | 41:WN:256:ASN:ND2 | 2.36 | 0.40 |
| 40:WA:291:ILE:HD13 | 40:WA:372:ARG:HB3 | 2.03 | 0.40 |
| 40:WG:431:TYR:HA | 40:WG:434:VAL:HG12 | 2.04 | 0.40 |
| 41:WM:158:GLU:O | 41:WM:160:PRO:HD3 | 2.21 | 0.40 |
| 41:WO:149:THR:HA | 41:WO:152:ILE:HD12 | 2.04 | 0.40 |
| 41:WP:36:TYR:CZ | 41:WP:44:LEU:HB2 | 2.57 | 0.40 |
| 41:WQ:133:PHE:HB2 | 41:WQ:164:MET:SD | 2.62 | 0.40 |
| 41:WQ:240:LEU:HA | 41:WQ:240:LEU:HD23 | 1.81 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 583/1048 (56%) | 561 (96%) | 20 (3%) | 2 (0%) | 37 | 67 |
| 1 | 1B | 147/1048 (14%) | 145 (99%) | 2 (1%) | 0 | 100 | 100 |
| 2 | 1C | 207/685 (30%) | 189 (91%) | 16 (8%) | 2 (1%) | 13 | 44 |
| 2 | 1D | 207/685 (30%) | 193 (93%) | 12 (6%) | 2 (1%) | 13 | 44 |
| 3 | 1F | 163/262 (62%) | 145 (89%) | 16 (10%) | 2 (1%) | 11 | 40 |
| 3 | 1G | 163/262 (62%) | 76 (47%) | 61 (37%) | 26 (16%) | 0 | 2 |
| 4 | 1H | 191/711 (27%) | 187 (98%) | 3 (2%) | 1 (0%) | 25 | 57 |
| 4 | 1I | 86/711 (12%) | 82 (95%) | 3 (4%) | 1 (1%) | 11 | 40 |
| 4 | 1J | 111/711 (16%) | 108 (97%) | 3 (3%) | 0 | 100 | 100 |
| 5 | 1L | 153/620 (25%) | 143 (94%) | 6 (4%) | 4 (3%) | 4 | 27 |
| 5 | 1M | 246/620 (40%) | 235 (96%) | 7 (3%) | 4 (2%) | 8 | 35 |
| 5 | 1N | 101/620 (16%) | 98 (97%) | 3 (3%) | 0 | 100 | 100 |
| 6 | 1P | 82/1456 (6%) | 77 (94%) | 5 (6%) | 0 | 100 | 100 |
| 6 | 1Q | 79/1456 (5%) | 69 (87%) | 10 (13%) | 0 | 100 | 100 |
| 7 | 1S | 609/620 (98%) | 537 (88%) | 64 (10%) | 8 (1%) | 10 | 39 |
| 7 | 1T | 609/620 (98%) | 427 (70%) | 148 (24%) | 34 (6%) | 1 | 15 |
| 7 | 1U | 609/620 (98%) | 533 (88%) | 75 (12%) | 1 (0%) | 44 | 72 |
| 8 | 1W | 314/549 (57%) | 307 (98%) | 7 (2%) | 0 | 100 | 100 |
| 8 | 1X | 273/549 (50%) | 234 (86%) | 33 (12%) | 6 (2%) | 5 | 30 |
| 8 | 1Y | 160/549 (29%) | 149 (93%) | 11 (7%) | 0 | 100 | 100 |
| 8 | 1Z | 194/549 (35%) | 189 (97%) | 4 (2%) | 1 (0%) | 25 | 57 |
| 9 | 2B | 371/552 (67%) | 353 (95%) | 16 (4%) | 2 (0%) | 25 | 57 |
| 9 | 2C | 78/552 (14%) | 73 (94%) | 4 (5%) | 1 (1%) | 10 | 39 |
| 10 | 2E | 111/170 (65%) | 93 (84%) | 17 (15%) | 1 (1%) | 14 | 46 |
| 10 | 2F | 111/170 (65%) | 95 (86%) | 15 (14%) | 1 (1%) | 14 | 46 |
| 10 | 2G | 111/170 (65%) | 97 (87%) | 13 (12%) | 1 (1%) | 14 | 46 |
| 11 | 2I | 243/256 (95%) | 191 (79%) | 51 (21%) | 1 (0%) | 30 | 62 |
| 11 | 2J | 243/256 (95%) | 217 (89%) | 21 (9%) | 5 (2%) | 5 | 31 |
| 11 | 2K | 225/256 (88%) | 189 (84%) | 31 (14%) | 5 (2%) | 5 | 30 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 12 | 2M | 217/257 (84%) | 194 (89%) | 23 (11%) | 0 | 100 | 100 |
| 12 | 2N | 217/257 (84%) | 196 (90%) | 21 (10%) | 0 | 100 | 100 |
| 12 | 2O | 217/257 (84%) | 184 (85%) | 29 (13%) | 4 (2%) | 7 | 33 |
| 12 | 2P | 217/257 (84%) | 195 (90%) | 22 (10%) | 0 | 100 | 100 |
| 12 | 2Q | 217/257 (84%) | 197 (91%) | 20 (9%) | 0 | 100 | 100 |
| 12 | 2R | 217/257 (84%) | 189 (87%) | 28 (13%) | 0 | 100 | 100 |
| 13 | 2T | 183/193 (95%) | 146 (80%) | 28 (15%) | 9 (5%) | 2 | 17 |
| 13 | 2U | 183/193 (95%) | 137 (75%) | 38 (21%) | 8 (4%) | 2 | 19 |
| 13 | 2V | 183/193 (95%) | 140 (76%) | 37 (20%) | 6 (3%) | 3 | 24 |
| 13 | 2W | 183/193 (95%) | 132 (72%) | 39 (21%) | 12 (7%) | 1 | 13 |
| 13 | 2X | 183/193 (95%) | 130 (71%) | 42 (23%) | 11 (6%) | 1 | 14 |
| 14 | 3A | 116/177 (66%) | 107 (92%) | 9 (8%) | 0 | 100 | 100 |
| 14 | 3B | 116/177 (66%) | 102 (88%) | 14 (12%) | 0 | 100 | 100 |
| 14 | 3C | 116/177 (66%) | 100 (86%) | 16 (14%) | 0 | 100 | 100 |
| 15 | 3E | 392/418 (94%) | 381 (97%) | 10 (3%) | 1 (0%) | 37 | 67 |
| 15 | 3F | 395/418 (94%) | 375 (95%) | 19 (5%) | 1 (0%) | 37 | 67 |
| 15 | 3G | 132/418 (32%) | 127 (96%) | 5 (4%) | 0 | 100 | 100 |
| 15 | 3H | 294/418 (70%) | 280 (95%) | 13 (4%) | 1 (0%) | 37 | 67 |
| 16 | 3J | 395/430 (92%) | 377 (95%) | 15 (4%) | 3 (1%) | 16 | 48 |
| 16 | 3K | 312/430 (73%) | 304 (97%) | 7 (2%) | 1 (0%) | 37 | 67 |
| 16 | 3L | 395/430 (92%) | 377 (95%) | 16 (4%) | 2 (0%) | 25 | 57 |
| 16 | 3M | 110/430 (26%) | 106 (96%) | 4 (4%) | 0 | 100 | 100 |
| 17 | 3O | 389/490 (79%) | 366 (94%) | 22 (6%) | 1 (0%) | 37 | 67 |
| 17 | 3P | 389/490 (79%) | 334 (86%) | 50 (13%) | 5 (1%) | 10 | 39 |
| 17 | 3Q | 129/490 (26%) | 107 (83%) | 15 (12%) | 7 (5%) | 1 | 16 |
| 17 | 3R | 262/490 (54%) | 164 (63%) | 80 (30%) | 18 (7%) | 1 | 12 |
| 18 | 3T | 396/447 (89%) | 381 (96%) | 15 (4%) | 0 | 100 | 100 |
| 18 | 3U | 397/447 (89%) | 381 (96%) | 16 (4%) | 0 | 100 | 100 |
| 18 | 3V | 166/447 (37%) | 162 (98%) | 4 (2%) | 0 | 100 | 100 |
| 18 | 3W | 255/447 (57%) | 241 (94%) | 14 (6%) | 0 | 100 | 100 |
| 19 | 3Y | 354/377 (94%) | 344 (97%) | 10 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
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| 19 | 3Z | 20/377 (5%) | 19 (95%) | 1 (5%) | 0 | 100 | 100 |
| 20 | 4A | 177/379 (47%) | 145 (82%) | 26 (15%) | 6 (3%) | 3 | 24 |
| 20 | 4B | 111/379 (29%) | 87 (78%) | 19 (17%) | 5 (4%) | 2 | 18 |
| 21 | 4D | 462/640 (72%) | 373 (81%) | 67 (14%) | 22 (5%) | 2 | 17 |
| 21 | 4E | 462/640 (72%) | 373 (81%) | 73 (16%) | 16 (4%) | 3 | 23 |
| 21 | 4F | 462/640 (72%) | 379 (82%) | 67 (14%) | 16 (4%) | 3 | 23 |
| 22 | 4H | 348/748 (46%) | 296 (85%) | 50 (14%) | 2 (1%) | 22 | 54 |
| 22 | 4I | 600/748 (80%) | 500 (83%) | 90 (15%) | 10 (2%) | 7 | 34 |
| 22 | 4J | 605/748 (81%) | 471 (78%) | 115 (19%) | 19 (3%) | 3 | 25 |
| 22 | 4K | 234/748 (31%) | 160 (68%) | 65 (28%) | 9 (4%) | 2 | 21 |
| 23 | 4M | 162/272 (60%) | 84 (52%) | 58 (36%) | 20 (12%) | 0 | 3 |
| 23 | 4N | 162/272 (60%) | 84 (52%) | 51 (32%) | 27 (17%) | 0 | 2 |
| 23 | 4P | 83/272 (30%) | 44 (53%) | 24 (29%) | 15 (18%) | 0 | 1 |
| 23 | 4Q | 128/272 (47%) | 71 (56%) | 41 (32%) | 16 (12%) | 0 | 3 |
| 23 | 4R | 157/272 (58%) | 83 (53%) | 55 (35%) | 19 (12%) | 0 | 4 |
| 24 | 4O | 83/252 (33%) | 37 (45%) | 42 (51%) | 4 (5%) | 2 | 17 |
| 25 | 4T | 158/469 (34%) | 122 (77%) | 31 (20%) | 5 (3%) | 3 | 24 |
| 26 | 4V | 371/377 (98%) | 312 (84%) | 57 (15%) | 2 (0%) | 25 | 57 |
| 26 | 4W | 371/377 (98%) | 317 (85%) | 47 (13%) | 7 (2%) | 6 | 33 |
| 27 | 4Y | 263/314 (84%) | 236 (90%) | 25 (10%) | 2 (1%) | 16 | 48 |
| 27 | 4Z | 268/314 (85%) | 230 (86%) | 35 (13%) | 3 (1%) | 12 | 42 |
| 28 | 5B | 196/230 (85%) | 165 (84%) | 30 (15%) | 1 (0%) | 25 | 57 |
| 29 | 5D | 82/136 (60%) | 68 (83%) | 13 (16%) | 1 (1%) | 11 | 40 |
| 29 | 5E | 31/136 (23%) | 24 (77%) | 6 (19%) | 1 (3%) | 3 | 24 |
| 30 | 5G | 91/121 (75%) | 71 (78%) | 19 (21%) | 1 (1%) | 12 | 42 |
| 31 | 5I | 437/879 (50%) | 366 (84%) | 65 (15%) | 6 (1%) | 9 | 37 |
| 31 | 5J | 108/879 (12%) | 101 (94%) | 6 (6%) | 1 (1%) | 14 | 46 |
| 32 | 5L | 90/101 (89%) | 90 (100%) | 0 | 0 | 100 | 100 |
| 33 | 5N | 332/495 (67%) | 324 (98%) | 8 (2%) | 0 | 100 | 100 |
| 33 | 5O | 149/495 (30%) | 147 (99%) | 2 (1%) | 0 | 100 | 100 |
| 34 | 5Q | 260/514 (51%) | 250 (96%) | 9 (4%) | 1 (0%) | 30 | 62 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
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| 34 | 5R | 194/514 (38%) | 155 (80%) | 36 (19%) | 3 (2%) | 8 | 36 |
| 35 | 5T | 125/196 (64%) | 109 (87%) | 15 (12%) | 1 (1%) | 16 | 48 |
| 35 | 5U | 26/196 (13%) | 19 (73%) | 7 (27%) | 0 | 100 | 100 |
| 36 | 5W | 225/282 (80%) | 190 (84%) | 27 (12%) | 8 (4%) | 3 | 22 |
| 36 | 5X | 225/282 (80%) | 189 (84%) | 29 (13%) | 7 (3%) | 3 | 25 |
| 36 | 5Y | 179/282 (64%) | 151 (84%) | 22 (12%) | 6 (3%) | 3 | 24 |
| 36 | 5Z | 57/282 (20%) | 52 (91%) | 5 (9%) | 0 | 100 | 100 |
| 37 | 6A | 114/135 (84%) | 96 (84%) | 17 (15%) | 1 (1%) | 14 | 46 |
| 38 | 6C | 210/310 (68%) | 168 (80%) | 34 (16%) | 8 (4%) | 2 | 21 |
| 38 | 6D | 61/310 (20%) | 51 (84%) | 9 (15%) | 1 (2%) | 8 | 35 |
| 39 | 6F | 155/223 (70%) | 148 (96%) | 6 (4%) | 1 (1%) | 22 | 54 |
| 39 | 6G | 155/223 (70%) | 147 (95%) | 7 (4%) | 1 (1%) | 22 | 54 |
| 39 | 6H | 133/223 (60%) | 120 (90%) | 13 (10%) | 0 | 100 | 100 |
| 39 | 6I | 155/223 (70%) | 149 (96%) | 6 (4%) | 0 | 100 | 100 |
| 39 | 6J | 155/223 (70%) | 150 (97%) | 5 (3%) | 0 | 100 | 100 |
| 39 | 6K | 155/223 (70%) | 150 (97%) | 5 (3%) | 0 | 100 | 100 |
| 39 | 6L | 131/223 (59%) | 117 (89%) | 12 (9%) | 2 (2%) | 8 | 36 |
| 40 | AA | 438/447 (98%) | 402 (92%) | 36 (8%) | 0 | 100 | 100 |
| 40 | AE | 438/447 (98%) | 402 (92%) | 33 (8%) | 3 (1%) | 19 | 51 |
| 40 | AF | 438/447 (98%) | 408 (93%) | 29 (7%) | 1 (0%) | 44 | 72 |
| 40 | AG | 438/447 (98%) | 412 (94%) | 24 (6%) | 2 (0%) | 25 | 57 |
| 40 | AH | 438/447 (98%) | 401 (92%) | 35 (8%) | 2 (0%) | 25 | 57 |
| 40 | BA | 438/447 (98%) | 410 (94%) | 27 (6%) | 1 (0%) | 44 | 72 |
| 40 | BE | 438/447 (98%) | 324 (74%) | 82 (19%) | 32 (7%) | 1 | 11 |
| 40 | BF | 429/447 (96%) | 400 (93%) | 26 (6%) | 3 (1%) | 19 | 51 |
| 40 | BG | 428/447 (96%) | 393 (92%) | 34 (8%) | 1 (0%) | 44 | 72 |
| 40 | BH | 438/447 (98%) | 323 (74%) | 82 (19%) | 33 (8%) | 1 | 10 |
| 40 | BI | 365/447 (82%) | 249 (68%) | 84 (23%) | 32 (9%) | 0 | 7 |
| 40 | CA | 438/447 (98%) | 301 (69%) | 101 (23%) | 36 (8%) | 1 | 8 |
| 40 | CE | 438/447 (98%) | 402 (92%) | 34 (8%) | 2 (0%) | 25 | 57 |
| 40 | CF | 438/447 (98%) | 404 (92%) | 31 (7%) | 3 (1%) | 19 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
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| 40 | CG | 438/447 (98%) | 404 (92%) | 32 (7%) | 2 (0%) | 25 | 57 |
| 40 | CH | 438/447 (98%) | 313 (72%) | 87 (20%) | 38 (9%) | 0 | 7 |
| 40 | CI | 438/447 (98%) | 409 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 40 | DA | 428/447 (96%) | 245 (57%) | 130 (30%) | 53 (12%) | 0 | 3 |
| 40 | DE | 431/447 (96%) | 276 (64%) | 112 (26%) | 43 (10%) | 0 | 6 |
| 40 | DF | 428/447 (96%) | 271 (63%) | 126 (29%) | 31 (7%) | 1 | 11 |
| 40 | DG | 429/447 (96%) | 391 (91%) | 37 (9%) | 1 (0%) | 44 | 72 |
| 40 | DH | 429/447 (96%) | 273 (64%) | 123 (29%) | 33 (8%) | 1 | 9 |
| 40 | DI | 428/447 (96%) | 252 (59%) | 131 (31%) | 45 (10%) | 0 | 5 |
| 40 | EA | 430/447 (96%) | 399 (93%) | 29 (7%) | 2 (0%) | 25 | 57 |
| 40 | EE | 431/447 (96%) | 398 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 40 | EF | 431/447 (96%) | 397 (92%) | 33 (8%) | 1 (0%) | 44 | 72 |
| 40 | EG | 430/447 (96%) | 393 (91%) | 35 (8%) | 2 (0%) | 25 | 57 |
| 40 | EH | 429/447 (96%) | 279 (65%) | 108 (25%) | 42 (10%) | 0 | 6 |
| 40 | EI | 430/447 (96%) | 257 (60%) | 137 (32%) | 36 (8%) | 0 | 8 |
| 40 | FA | 430/447 (96%) | 280 (65%) | 114 (26%) | 36 (8%) | 0 | 8 |
| 40 | FE | 430/447 (96%) | 394 (92%) | 36 (8%) | 0 | 100 | 100 |
| 40 | FF | 430/447 (96%) | 389 (90%) | 39 (9%) | 2 (0%) | 25 | 57 |
| 40 | FG | 429/447 (96%) | 392 (91%) | 36 (8%) | 1 (0%) | 44 | 72 |
| 40 | FH | 430/447 (96%) | 393 (91%) | 37 (9%) | 0 | 100 | 100 |
| 40 | FI | 430/447 (96%) | 384 (89%) | 45 (10%) | 1 (0%) | 44 | 72 |
| 40 | GA | 430/447 (96%) | 399 (93%) | 28 (6%) | 3 (1%) | 19 | 51 |
| 40 | GE | 430/447 (96%) | 261 (61%) | 135 (31%) | 34 (8%) | 1 | 9 |
| 40 | GF | 429/447 (96%) | 390 (91%) | 36 (8%) | 3 (1%) | 19 | 51 |
| 40 | GG | 429/447 (96%) | 390 (91%) | 34 (8%) | 5 (1%) | 11 | 40 |
| 40 | GH | 429/447 (96%) | 289 (67%) | 107 (25%) | 33 (8%) | 1 | 9 |
| 40 | GI | 430/447 (96%) | 278 (65%) | 117 (27%) | 35 (8%) | 1 | 8 |
| 40 | HA | 431/447 (96%) | 386 (90%) | 42 (10%) | 3 (1%) | 19 | 51 |
| 40 | HE | 429/447 (96%) | 261 (61%) | 127 (30%) | 41 (10%) | 0 | 6 |
| 40 | HF | 428/447 (96%) | 391 (91%) | 36 (8%) | 1 (0%) | 44 | 72 |
| 40 | HG | 430/447 (96%) | 383 (89%) | 44 (10%) | 3 (1%) | 19 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
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| 40 | HH | 430/447 (96%) | 401 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 40 | HI | 431/447 (96%) | 397 (92%) | 33 (8%) | 1 (0%) | 44 | 72 |
| 40 | IA | 430/447 (96%) | 388 (90%) | 41 (10%) | 1 (0%) | 44 | 72 |
| 40 | IE | 414/447 (93%) | 387 (94%) | 25 (6%) | 2 (0%) | 25 | 57 |
| 40 | IF | 430/447 (96%) | 390 (91%) | 38 (9%) | 2 (0%) | 25 | 57 |
| 40 | IG | 429/447 (96%) | 391 (91%) | 37 (9%) | 1 (0%) | 44 | 72 |
| 40 | IH | 430/447 (96%) | 401 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 40 | II | 430/447 (96%) | 394 (92%) | 34 (8%) | 2 (0%) | 25 | 57 |
| 40 | JA | 430/447 (96%) | 391 (91%) | 38 (9%) | 1 (0%) | 44 | 72 |
| 40 | JD | 430/447 (96%) | 397 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 40 | JE | 430/447 (96%) | 399 (93%) | 29 (7%) | 2 (0%) | 25 | 57 |
| 40 | JF | 429/447 (96%) | 395 (92%) | 33 (8%) | 1 (0%) | 44 | 72 |
| 40 | JG | 438/447 (98%) | 407 (93%) | 30 (7%) | 1 (0%) | 44 | 72 |
| 40 | JH | 429/447 (96%) | 392 (91%) | 36 (8%) | 1 (0%) | 44 | 72 |
| 40 | KA | 430/447 (96%) | 397 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 40 | KD | 429/447 (96%) | 394 (92%) | 32 (8%) | 3 (1%) | 19 | 51 |
| 40 | KE | 430/447 (96%) | 392 (91%) | 36 (8%) | 2 (0%) | 25 | 57 |
| 40 | KF | 430/447 (96%) | 397 (92%) | 32 (7%) | 1 (0%) | 44 | 72 |
| 40 | KG | 438/447 (98%) | 409 (93%) | 28 (6%) | 1 (0%) | 44 | 72 |
| 40 | KH | 438/447 (98%) | 395 (90%) | 42 (10%) | 1 (0%) | 44 | 72 |
| 40 | LA | 438/447 (98%) | 408 (93%) | 29 (7%) | 1 (0%) | 44 | 72 |
| 40 | LD | 429/447 (96%) | 400 (93%) | 28 (6%) | 1 (0%) | 44 | 72 |
| 40 | LE | 438/447 (98%) | 400 (91%) | 36 (8%) | 2 (0%) | 25 | 57 |
| 40 | LF | 429/447 (96%) | 333 (78%) | 72 (17%) | 24 (6%) | 1 | 15 |
| 40 | LG | 430/447 (96%) | 335 (78%) | 67 (16%) | 28 (6%) | 1 | 13 |
| 40 | LH | 430/447 (96%) | 400 (93%) | 29 (7%) | 1 (0%) | 44 | 72 |
| 40 | MA | 428/447 (96%) | 329 (77%) | 74 (17%) | 25 (6%) | 1 | 14 |
| 40 | MD | 430/447 (96%) | 393 (91%) | 33 (8%) | 4 (1%) | 14 | 46 |
| 40 | ME | 430/447 (96%) | 396 (92%) | 32 (7%) | 2 (0%) | 25 | 57 |
| 40 | MF | 429/447 (96%) | 325 (76%) | 77 (18%) | 27 (6%) | 1 | 13 |
| 40 | MG | 429/447 (96%) | 316 (74%) | 94 (22%) | 19 (4%) | 2 | 19 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
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| 40 | MH | 429/447 (96%) | 323 (75%) | 82 (19%) | 24 (6%) | 1 | 15 |
| 40 | NA | 428/447 (96%) | 396 (92%) | 31 (7%) | 1 (0%) | 44 | 72 |
| 40 | ND | 429/447 (96%) | 289 (67%) | 103 (24%) | 37 (9%) | 0 | 8 |
| 40 | NE | 430/447 (96%) | 392 (91%) | 35 (8%) | 3 (1%) | 19 | 51 |
| 40 | NF | 429/447 (96%) | 397 (92%) | 32 (8%) | 0 | 100 | 100 |
| 40 | NG | 428/447 (96%) | 391 (91%) | 36 (8%) | 1 (0%) | 44 | 72 |
| 40 | NH | 429/447 (96%) | 398 (93%) | 29 (7%) | 2 (0%) | 25 | 57 |
| 40 | OA | 432/447 (97%) | 387 (90%) | 45 (10%) | 0 | 100 | 100 |
| 40 | OD | 430/447 (96%) | 390 (91%) | 34 (8%) | 6 (1%) | 9 | 37 |
| 40 | OE | 430/447 (96%) | 393 (91%) | 35 (8%) | 2 (0%) | 25 | 57 |
| 40 | OF | 432/447 (97%) | 397 (92%) | 34 (8%) | 1 (0%) | 44 | 72 |
| 40 | OG | 432/447 (97%) | 398 (92%) | 33 (8%) | 1 (0%) | 44 | 72 |
| 40 | OH | 432/447 (97%) | 275 (64%) | 120 (28%) | 37 (9%) | 0 | 8 |
| 40 | PA | 428/447 (96%) | 384 (90%) | 41 (10%) | 3 (1%) | 19 | 51 |
| 40 | PD | 400/447 (90%) | 364 (91%) | 35 (9%) | 1 (0%) | 37 | 67 |
| 40 | PE | 429/447 (96%) | 388 (90%) | 41 (10%) | 0 | 100 | 100 |
| 40 | PF | 429/447 (96%) | 393 (92%) | 36 (8%) | 0 | 100 | 100 |
| 40 | PG | 427/447 (96%) | 386 (90%) | 39 (9%) | 2 (0%) | 25 | 57 |
| 40 | PH | 427/447 (96%) | 401 (94%) | 26 (6%) | 0 | 100 | 100 |
| 40 | QA | 428/447 (96%) | 393 (92%) | 34 (8%) | 1 (0%) | 44 | 72 |
| 40 | QE | 427/447 (96%) | 391 (92%) | 35 (8%) | 1 (0%) | 44 | 72 |
| 40 | QF | 427/447 (96%) | 395 (92%) | 31 (7%) | 1 (0%) | 44 | 72 |
| 40 | QG | 428/447 (96%) | 396 (92%) | 31 (7%) | 1 (0%) | 44 | 72 |
| 40 | QH | 429/447 (96%) | 399 (93%) | 28 (6%) | 2 (0%) | 25 | 57 |
| 40 | RA | 428/447 (96%) | 391 (91%) | 36 (8%) | 1 (0%) | 44 | 72 |
| 40 | RE | 427/447 (96%) | 388 (91%) | 37 (9%) | 2 (0%) | 25 | 57 |
| 40 | RF | 427/447 (96%) | 384 (90%) | 42 (10%) | 1 (0%) | 44 | 72 |
| 40 | RG | 428/447 (96%) | 384 (90%) | 44 (10%) | 0 | 100 | 100 |
| 40 | RH | 427/447 (96%) | 387 (91%) | 37 (9%) | 3 (1%) | 19 | 51 |
| 40 | RI | 368/447 (82%) | 343 (93%) | 24 (6%) | 1 (0%) | 37 | 67 |
| 40 | SA | 428/447 (96%) | 381 (89%) | 40 (9%) | 7 (2%) | 8 | 35 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
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| 40 | SE | 430/447 (96%) | 392 (91%) | 36 (8%) | 2 (0%) | 25 | 57 |
| 40 | SF | 428/447 (96%) | 392 (92%) | 35 (8%) | 1 (0%) | 44 | 72 |
| 40 | SG | 430/447 (96%) | 380 (88%) | 48 (11%) | 2 (0%) | 25 | 57 |
| 40 | SH | 429/447 (96%) | 392 (91%) | 36 (8%) | 1 (0%) | 44 | 72 |
| 40 | SI | 429/447 (96%) | 394 (92%) | 34 (8%) | 1 (0%) | 44 | 72 |
| 40 | TA | 428/447 (96%) | 397 (93%) | 31 (7%) | 0 | 100 | 100 |
| 40 | TE | 428/447 (96%) | 394 (92%) | 33 (8%) | 1 (0%) | 44 | 72 |
| 40 | TF | 428/447 (96%) | 392 (92%) | 34 (8%) | 2 (0%) | 25 | 57 |
| 40 | TG | 430/447 (96%) | 383 (89%) | 46 (11%) | 1 (0%) | 44 | 72 |
| 40 | TH | 429/447 (96%) | 394 (92%) | 33 (8%) | 2 (0%) | 25 | 57 |
| 40 | TI | 429/447 (96%) | 398 (93%) | 29 (7%) | 2 (0%) | 25 | 57 |
| 40 | UA | 429/447 (96%) | 384 (90%) | 43 (10%) | 2 (0%) | 25 | 57 |
| 40 | UE | 430/447 (96%) | 397 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 40 | UF | 430/447 (96%) | 276 (64%) | 119 (28%) | 35 (8%) | 1 | 8 |
| 40 | UG | 430/447 (96%) | 389 (90%) | 39 (9%) | 2 (0%) | 25 | 57 |
| 40 | UH | 429/447 (96%) | 389 (91%) | 38 (9%) | 2 (0%) | 25 | 57 |
| 40 | UI | 429/447 (96%) | 274 (64%) | 119 (28%) | 36 (8%) | 0 | 8 |
| 40 | VA | 438/447 (98%) | 393 (90%) | 41 (9%) | 4 (1%) | 14 | 46 |
| 40 | VF | 438/447 (98%) | 403 (92%) | 31 (7%) | 4 (1%) | 14 | 46 |
| 40 | VG | 429/447 (96%) | 393 (92%) | 33 (8%) | 3 (1%) | 19 | 51 |
| 40 | VH | 430/447 (96%) | 387 (90%) | 41 (10%) | 2 (0%) | 25 | 57 |
| 40 | VI | 438/447 (98%) | 401 (92%) | 36 (8%) | 1 (0%) | 44 | 72 |
| 40 | VJ | 429/447 (96%) | 388 (90%) | 40 (9%) | 1 (0%) | 44 | 72 |
| 40 | WA | 438/447 (98%) | 410 (94%) | 26 (6%) | 2 (0%) | 25 | 57 |
| 40 | WE | 438/447 (98%) | 404 (92%) | 33 (8%) | 1 (0%) | 44 | 72 |
| 40 | WF | 429/447 (96%) | 385 (90%) | 43 (10%) | 1 (0%) | 44 | 72 |
| 40 | WG | 428/447 (96%) | 393 (92%) | 33 (8%) | 2 (0%) | 25 | 57 |
| 40 | WH | 438/447 (98%) | 403 (92%) | 34 (8%) | 1 (0%) | 44 | 72 |
| 40 | WI | 429/447 (96%) | 398 (93%) | 31 (7%) | 0 | 100 | 100 |
| 41 | AB | 426/449 (95%) | 400 (94%) | 25 (6%) | 1 (0%) | 44 | 72 |
| 41 | AL | 426/449 (95%) | 393 (92%) | 30 (7%) | 3 (1%) | 19 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
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| 41 | AM | 426/449 (95%) | 398 (93%) | 25 (6%) | 3 (1%) | 19 | 51 |
| 41 | AN | 426/449 (95%) | 398 (93%) | 25 (6%) | 3 (1%) | 19 | 51 |
| 41 | AO | 426/449 (95%) | 335 (79%) | 70 (16%) | 21 (5%) | 2 | 17 |
| 41 | AP | 426/449 (95%) | 396 (93%) | 28 (7%) | 2 (0%) | 25 | 57 |
| 41 | BB | 426/449 (95%) | 326 (76%) | 75 (18%) | 25 (6%) | 1 | 14 |
| 41 | BL | 426/449 (95%) | 397 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 41 | BM | 426/449 (95%) | 312 (73%) | 84 (20%) | 30 (7%) | 1 | 11 |
| 41 | BN | 426/449 (95%) | 388 (91%) | 35 (8%) | 3 (1%) | 19 | 51 |
| 41 | BO | 426/449 (95%) | 322 (76%) | 81 (19%) | 23 (5%) | 1 | 16 |
| 41 | BP | 426/449 (95%) | 322 (76%) | 75 (18%) | 29 (7%) | 1 | 12 |
| 41 | CB | 426/449 (95%) | 398 (93%) | 27 (6%) | 1 (0%) | 44 | 72 |
| 41 | CL | 426/449 (95%) | 306 (72%) | 84 (20%) | 36 (8%) | 0 | 8 |
| 41 | CM | 426/449 (95%) | 305 (72%) | 93 (22%) | 28 (7%) | 1 | 13 |
| 41 | CN | 426/449 (95%) | 298 (70%) | 98 (23%) | 30 (7%) | 1 | 11 |
| 41 | CO | 426/449 (95%) | 279 (66%) | 110 (26%) | 37 (9%) | 0 | 7 |
| 41 | CP | 426/449 (95%) | 276 (65%) | 112 (26%) | 38 (9%) | 0 | 7 |
| 41 | DB | 426/449 (95%) | 260 (61%) | 125 (29%) | 41 (10%) | 0 | 6 |
| 41 | DL | 426/449 (95%) | 252 (59%) | 126 (30%) | 48 (11%) | 0 | 4 |
| 41 | DM | 426/449 (95%) | 268 (63%) | 121 (28%) | 37 (9%) | 0 | 7 |
| 41 | DN | 426/449 (95%) | 257 (60%) | 120 (28%) | 49 (12%) | 0 | 4 |
| 41 | DO | 426/449 (95%) | 396 (93%) | 28 (7%) | 2 (0%) | 25 | 57 |
| 41 | DP | 426/449 (95%) | 272 (64%) | 121 (28%) | 33 (8%) | 1 | 9 |
| 41 | EB | 426/449 (95%) | 400 (94%) | 23 (5%) | 3 (1%) | 19 | 51 |
| 41 | EL | 356/449 (79%) | 329 (92%) | 26 (7%) | 1 (0%) | 37 | 67 |
| 41 | EM | 426/449 (95%) | 270 (63%) | 116 (27%) | 40 (9%) | 0 | 7 |
| 41 | EN | 426/449 (95%) | 399 (94%) | 26 (6%) | 1 (0%) | 44 | 72 |
| 41 | EO | 426/449 (95%) | 396 (93%) | 28 (7%) | 2 (0%) | 25 | 57 |
| 41 | EP | 426/449 (95%) | 276 (65%) | 123 (29%) | 27 (6%) | 1 | 13 |
| 41 | FB | 426/449 (95%) | 393 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 41 | FM | 426/449 (95%) | 393 (92%) | 30 (7%) | 3 (1%) | 19 | 51 |
| 41 | FN | 426/449 (95%) | 391 (92%) | 34 (8%) | 1 (0%) | 44 | 72 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
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| 41 | FO | 426/449 (95%) | 393 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 41 | FP | 426/449 (95%) | 393 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 41 | GB | 426/449 (95%) | 398 (93%) | 26 (6%) | 2 (0%) | 25 | 57 |
| 41 | GM | 426/449 (95%) | 399 (94%) | 25 (6%) | 2 (0%) | 25 | 57 |
| 41 | GN | 426/449 (95%) | 277 (65%) | 118 (28%) | 31 (7%) | 1 | 11 |
| 41 | GO | 426/449 (95%) | 401 (94%) | 23 (5%) | 2 (0%) | 25 | 57 |
| 41 | GP | 426/449 (95%) | 393 (92%) | 32 (8%) | 1 (0%) | 44 | 72 |
| 41 | HB | 426/449 (95%) | 397 (93%) | 26 (6%) | 3 (1%) | 19 | 51 |
| 41 | HM | 426/449 (95%) | 399 (94%) | 25 (6%) | 2 (0%) | 25 | 57 |
| 41 | HN | 426/449 (95%) | 289 (68%) | 110 (26%) | 27 (6%) | 1 | 13 |
| 41 | HO | 426/449 (95%) | 401 (94%) | 24 (6%) | 1 (0%) | 44 | 72 |
| 41 | HP | 426/449 (95%) | 392 (92%) | 32 (8%) | 2 (0%) | 25 | 57 |
| 41 | HQ | 426/449 (95%) | 397 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 41 | IB | 426/449 (95%) | 401 (94%) | 23 (5%) | 2 (0%) | 25 | 57 |
| 41 | IM | 426/449 (95%) | 398 (93%) | 26 (6%) | 2 (0%) | 25 | 57 |
| 41 | IN | 426/449 (95%) | 398 (93%) | 26 (6%) | 2 (0%) | 25 | 57 |
| 41 | IO | 426/449 (95%) | 399 (94%) | 25 (6%) | 2 (0%) | 25 | 57 |
| 41 | IP | 426/449 (95%) | 397 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 41 | IQ | 426/449 (95%) | 389 (91%) | 35 (8%) | 2 (0%) | 25 | 57 |
| 41 | JB | 426/449 (95%) | 395 (93%) | 29 (7%) | 2 (0%) | 25 | 57 |
| 41 | JL | 426/449 (95%) | 394 (92%) | 30 (7%) | 2 (0%) | 25 | 57 |
| 41 | JM | 426/449 (95%) | 286 (67%) | 110 (26%) | 30 (7%) | 1 | 11 |
| 41 | JN | 426/449 (95%) | 393 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 41 | JO | 426/449 (95%) | 396 (93%) | 28 (7%) | 2 (0%) | 25 | 57 |
| 41 | KB | 426/449 (95%) | 397 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 41 | KL | 426/449 (95%) | 305 (72%) | 100 (24%) | 21 (5%) | 2 | 17 |
| 41 | KM | 426/449 (95%) | 399 (94%) | 26 (6%) | 1 (0%) | 44 | 72 |
| 41 | KN | 426/449 (95%) | 403 (95%) | 21 (5%) | 2 (0%) | 25 | 57 |
| 41 | KO | 426/449 (95%) | 389 (91%) | 35 (8%) | 2 (0%) | 25 | 57 |
| 41 | KP | 380/449 (85%) | 356 (94%) | 22 (6%) | 2 (0%) | 25 | 57 |
| 41 | LB | 426/449 (95%) | 393 (92%) | 32 (8%) | 1 (0%) | 44 | 72 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 41 | LL | 426/449 (95%) | 392 (92%) | 32 (8%) | 2 (0%) | 25 | 57 |
| 41 | LM | 426/449 (95%) | 393 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 41 | LN | 426/449 (95%) | 403 (95%) | 22 (5%) | 1 (0%) | 44 | 72 |
| 41 | LO | 426/449 (95%) | 399 (94%) | 24 (6%) | 3 (1%) | 19 | 51 |
| 41 | LP | 426/449 (95%) | 403 (95%) | 22 (5%) | 1 (0%) | 44 | 72 |
| 41 | MB | 426/449 (95%) | 402 (94%) | 23 (5%) | 1 (0%) | 44 | 72 |
| 41 | ML | 426/449 (95%) | 392 (92%) | 32 (8%) | 2 (0%) | 25 | 57 |
| 41 | MM | 426/449 (95%) | 396 (93%) | 27 (6%) | 3 (1%) | 19 | 51 |
| 41 | MN | 426/449 (95%) | 400 (94%) | 25 (6%) | 1 (0%) | 44 | 72 |
| 41 | MO | 426/449 (95%) | 334 (78%) | 71 (17%) | 21 (5%) | 2 | 17 |
| 41 | MP | 426/449 (95%) | 401 (94%) | 23 (5%) | 2 (0%) | 25 | 57 |
| 41 | NB | 426/449 (95%) | 392 (92%) | 32 (8%) | 2 (0%) | 25 | 57 |
| 41 | NL | 426/449 (95%) | 398 (93%) | 25 (6%) | 3 (1%) | 19 | 51 |
| 41 | NM | 426/449 (95%) | 390 (92%) | 35 (8%) | 1 (0%) | 44 | 72 |
| 41 | NN | 426/449 (95%) | 397 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 41 | NO | 426/449 (95%) | 394 (92%) | 30 (7%) | 2 (0%) | 25 | 57 |
| 41 | NP | 412/449 (92%) | 382 (93%) | 27 (7%) | 3 (1%) | 19 | 51 |
| 41 | OB | 426/449 (95%) | 404 (95%) | 20 (5%) | 2 (0%) | 25 | 57 |
| 41 | OL | 426/449 (95%) | 396 (93%) | 27 (6%) | 3 (1%) | 19 | 51 |
| 41 | OM | 426/449 (95%) | 383 (90%) | 42 (10%) | 1 (0%) | 44 | 72 |
| 41 | ON | 426/449 (95%) | 389 (91%) | 35 (8%) | 2 (0%) | 25 | 57 |
| 41 | OO | 426/449 (95%) | 390 (92%) | 33 (8%) | 3 (1%) | 19 | 51 |
| 41 | OP | 426/449 (95%) | 391 (92%) | 33 (8%) | 2 (0%) | 25 | 57 |
| 41 | PB | 426/449 (95%) | 392 (92%) | 32 (8%) | 2 (0%) | 25 | 57 |
| 41 | PL | 426/449 (95%) | 399 (94%) | 25 (6%) | 2 (0%) | 25 | 57 |
| 41 | PM | 426/449 (95%) | 395 (93%) | 29 (7%) | 2 (0%) | 25 | 57 |
| 41 | PN | 426/449 (95%) | 394 (92%) | 30 (7%) | 2 (0%) | 25 | 57 |
| 41 | PO | 426/449 (95%) | 397 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 41 | PP | 426/449 (95%) | 392 (92%) | 32 (8%) | 2 (0%) | 25 | 57 |
| 41 | QB | 426/449 (95%) | 244 (57%) | 127 (30%) | 55 (13%) | 0 | 3 |
| 41 | QL | 426/449 (95%) | 389 (91%) | 34 (8%) | 3 (1%) | 19 | 51 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 41 | QM | 426/449 (95%) | 391 (92%) | 32 (8%) | 3 (1%) | 19 | 51 |
| 41 | QN | 426/449 (95%) | 393 (92%) | 30 (7%) | 3 (1%) | 19 | 51 |
| 41 | QO | 426/449 (95%) | 391 (92%) | 32 (8%) | 3 (1%) | 19 | 51 |
| 41 | QP | 426/449 (95%) | 233 (55%) | 133 (31%) | 60 (14%) | 0 | 3 |
| 41 | RB | 426/449 (95%) | 396 (93%) | 28 (7%) | 2 (0%) | 25 | 57 |
| 41 | RL | 426/449 (95%) | 397 (93%) | 28 (7%) | 1 (0%) | 44 | 72 |
| 41 | RM | 426/449 (95%) | 398 (93%) | 27 (6%) | 1 (0%) | 44 | 72 |
| 41 | RN | 426/449 (95%) | 389 (91%) | 35 (8%) | 2 (0%) | 25 | 57 |
| 41 | RO | 426/449 (95%) | 392 (92%) | 31 (7%) | 3 (1%) | 19 | 51 |
| 41 | RP | 426/449 (95%) | 385 (90%) | 39 (9%) | 2 (0%) | 25 | 57 |
| 41 | SB | 426/449 (95%) | 376 (88%) | 45 (11%) | 5 (1%) | 11 | 40 |
| 41 | SL | 373/449 (83%) | 347 (93%) | 24 (6%) | 2 (0%) | 25 | 57 |
| 41 | SM | 426/449 (95%) | 391 (92%) | 32 (8%) | 3 (1%) | 19 | 51 |
| 41 | SN | 426/449 (95%) | 393 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 41 | SO | 426/449 (95%) | 243 (57%) | 146 (34%) | 37 (9%) | 0 | 7 |
| 41 | SP | 426/449 (95%) | 388 (91%) | 36 (8%) | 2 (0%) | 25 | 57 |
| 41 | TB | 426/449 (95%) | 391 (92%) | 32 (8%) | 3 (1%) | 19 | 51 |
| 41 | TL | 381/449 (85%) | 350 (92%) | 29 (8%) | 2 (0%) | 25 | 57 |
| 41 | TM | 426/449 (95%) | 398 (93%) | 27 (6%) | 1 (0%) | 44 | 72 |
| 41 | TN | 426/449 (95%) | 396 (93%) | 28 (7%) | 2 (0%) | 25 | 57 |
| 41 | TO | 426/449 (95%) | 394 (92%) | 31 (7%) | 1 (0%) | 44 | 72 |
| 41 | TP | 426/449 (95%) | 399 (94%) | 26 (6%) | 1 (0%) | 44 | 72 |
| 41 | UB | 426/449 (95%) | 400 (94%) | 25 (6%) | 1 (0%) | 44 | 72 |
| 41 | UM | 426/449 (95%) | 397 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 41 | UN | 426/449 (95%) | 391 (92%) | 34 (8%) | 1 (0%) | 44 | 72 |
| 41 | UO | 426/449 (95%) | 396 (93%) | 28 (7%) | 2 (0%) | 25 | 57 |
| 41 | UP | 426/449 (95%) | 277 (65%) | 116 (27%) | 33 (8%) | 1 | 9 |
| 41 | VB | 426/449 (95%) | 393 (92%) | 31 (7%) | 2 (0%) | 25 | 57 |
| 41 | VN | 426/449 (95%) | 392 (92%) | 32 (8%) | 2 (0%) | 25 | 57 |
| 41 | VO | 426/449 (95%) | 398 (93%) | 27 (6%) | 1 (0%) | 44 | 72 |
| 41 | VP | 426/449 (95%) | 390 (92%) | 34 (8%) | 2 (0%) | 25 | 57 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 41 | VQ | 426/449 (95%) | 390 (92%) | 35 (8%) | 1 (0%) | 44 | 72 |
| 41 | WB | 426/449 (95%) | 400 (94%) | 25 (6%) | 1 (0%) | 44 | 72 |
| 41 | WM | 426/449 (95%) | 316 (74%) | 91 (21%) | 19 (4%) | 2 | 18 |
| 41 | WN | 426/449 (95%) | 298 (70%) | 102 (24%) | 26 (6%) | 1 | 14 |
| 41 | WO | 426/449 (95%) | 392 (92%) | 33 (8%) | 1 (0%) | 44 | 72 |
| 41 | WP | 426/449 (95%) | 397 (93%) | 27 (6%) | 2 (0%) | 25 | 57 |
| 41 | WQ | 417/449 (93%) | 385 (92%) | 31 (7%) | 1 (0%) | 44 | 72 |
| All | All | 139272/166243 (84%) | 121168 (87%) | 15381 (11%) | 2723 (2%) | 8 | 32 |

All (2723) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1C | 133 | SER |
| 2 | 1C | 256 | GLN |
| 2 | 1D | 256 | GLN |
| 3 | 1F | 240 | PRO |
| 3 | 1G | 65 | ILE |
| 3 | 1G | 103 | ALA |
| 3 | 1G | 135 | VAL |
| 3 | 1G | 158 | TYR |
| 3 | 1G | 239 | LEU |
| 3 | 1G | 240 | PRO |
| 3 | 1G | 242 | PRO |
| 4 | 1H | 32 | GLN |
| 4 | 1I | 32 | GLN |
| 5 | 1M | 122 | ASP |
| 7 | 1S | 279 | PRO |
| 7 | 1T | 15 | GLU |
| 7 | 1T | 22 | PHE |
| 7 | 1T | 163 | SER |
| 7 | 1T | 279 | PRO |
| 7 | 1T | 280 | SER |
| 7 | 1T | 354 | LYS |
| 7 | 1T | 384 | ARG |
| 7 | 1T | 404 | GLU |
| 7 | 1T | 415 | ALA |
| 9 | 2B | 328 | ILE |
| 10 | 2E | 42 | GLU |
| 10 | 2F | 42 | GLU |
| 10 | 2G | 42 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | 2I | 252 | ILE |
| 11 | 2J | 216 | VAL |
| 11 | 2K | 185 | MET |
| 11 | 2K | 218 | ILE |
| 13 | 2W | 70 | GLY |
| 13 | 2W | 174 | GLU |
| 13 | 2X | 55 | SER |
| 13 | 2X | 174 | GLU |
| 15 | 3E | 204 | ALA |
| 15 | 3F | 204 | ALA |
| 15 | 3H | 204 | ALA |
| 16 | 3J | 195 | LYS |
| 17 | 3Q | 410 | GLU |
| 17 | 3Q | 411 | LEU |
| 20 | 4A | 37 | VAL |
| 21 | 4D | 292 | MET |
| 21 | 4D | 474 | LYS |
| 21 | 4D | 477 | SER |
| 21 | 4D | 520 | PRO |
| 21 | 4D | 521 | ALA |
| 21 | 4E | 475 | PRO |
| 21 | 4F | 462 | ILE |
| 21 | 4F | 477 | SER |
| 21 | 4F | 485 | TYR |
| 21 | 4F | 520 | PRO |
| 21 | 4F | 533 | ASN |
| 22 | 4H | 36 | VAL |
| 22 | 4I | 36 | VAL |
| 22 | 4J | 36 | VAL |
| 22 | 4J | 90 | PRO |
| 22 | 4J | 650 | LYS |
| 22 | 4J | 651 | LYS |
| 22 | 4K | 557 | SER |
| 22 | 4K | 617 | CYS |
| 23 | 4M | 92 | PRO |
| 23 | 4M | 116 | ALA |
| 23 | 4M | 235 | THR |
| 23 | 4M | 266 | HIS |
| 23 | 4N | 35 | GLN |
| 23 | 4N | 185 | SER |
| 23 | 4N | 235 | THR |
| 23 | 4N | 266 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 4O | 181 | LYS |
| 23 | 4P | 187 | PHE |
| 23 | 4P | 235 | THR |
| 23 | 4P | 266 | HIS |
| 23 | 4R | 20 | PRO |
| 23 | 4R | 235 | THR |
| 25 | 4T | 289 | VAL |
| 25 | 4T | 383 | VAL |
| 27 | 4Y | 102 | TYR |
| 27 | 4Z | 42 | LYS |
| 27 | 4Z | 44 | ARG |
| 29 | 5D | 50 | LYS |
| 31 | 5I | 725 | SER |
| 31 | 5J | 851 | HIS |
| 34 | 5R | 493 | THR |
| 36 | 5W | 39 | ILE |
| 36 | 5W | 50 | VAL |
| 36 | 5X | 131 | VAL |
| 36 | 5X | 269 | VAL |
| 36 | 5Y | 26 | ILE |
| 36 | 5Y | 50 | VAL |
| 36 | 5Y | 166 | MET |
| 36 | 5Y | 178 | PHE |
| 38 | 6C | 157 | ILE |
| 38 | 6C | 172 | ALA |
| 40 | AF | 274 | PRO |
| 40 | AG | 274 | PRO |
| 40 | AH | 42 | ILE |
| 40 | AH | 274 | PRO |
| 41 | AL | 143 | THR |
| 41 | AO | 160 | PRO |
| 41 | AO | 216 | LYS |
| 41 | AP | 143 | THR |
| 40 | BA | 274 | PRO |
| 41 | BB | 259 | PRO |
| 40 | BE | 73 | THR |
| 40 | BE | 177 | VAL |
| 40 | BE | 401 | ARG |
| 40 | BF | 274 | PRO |
| 40 | BG | 274 | PRO |
| 40 | BH | 30 | ILE |
| 40 | BH | 51 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BH | 110 | ILE |
| 40 | BH | 403 | PHE |
| 40 | BI | 72 | PRO |
| 40 | BI | 73 | THR |
| 40 | BI | 161 | TYR |
| 40 | BI | 261 | PRO |
| 40 | BI | 265 | ILE |
| 40 | BI | 274 | PRO |
| 40 | BI | 303 | VAL |
| 41 | BL | 143 | THR |
| 41 | BM | 108 | GLU |
| 41 | BM | 161 | ASP |
| 41 | BM | 246 | LEU |
| 41 | BN | 143 | THR |
| 41 | BO | 80 | PRO |
| 41 | BP | 55 | THR |
| 41 | BP | 57 | GLY |
| 41 | BP | 91 | VAL |
| 41 | BP | 139 | LEU |
| 41 | BP | 143 | THR |
| 41 | BP | 174 | LYS |
| 41 | BP | 355 | ASP |
| 41 | BP | 361 | LEU |
| 40 | CA | 72 | PRO |
| 40 | CA | 101 | ASN |
| 40 | CA | 141 | PHE |
| 40 | CA | 220 | GLU |
| 40 | CA | 279 | GLU |
| 40 | CA | 364 | PRO |
| 40 | CA | 403 | PHE |
| 41 | CB | 143 | THR |
| 40 | CF | 274 | PRO |
| 40 | CG | 274 | PRO |
| 40 | CH | 40 | LYS |
| 40 | CH | 46 | ASP |
| 40 | CH | 60 | LYS |
| 40 | CH | 101 | ASN |
| 40 | CH | 110 | ILE |
| 40 | CH | 177 | VAL |
| 40 | CH | 199 | ASP |
| 40 | CI | 274 | PRO |
| 41 | CL | 57 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CL | 59 | TYR |
| 41 | CL | 95 | SER |
| 41 | CL | 174 | LYS |
| 41 | CL | 195 | ASN |
| 41 | CL | 278 | SER |
| 41 | CM | 94 | GLN |
| 41 | CM | 198 | GLU |
| 41 | CM | 213 | ARG |
| 41 | CM | 214 | THR |
| 41 | CN | 2 | ARG |
| 41 | CN | 129 | CYS |
| 41 | CN | 173 | PRO |
| 41 | CO | 143 | THR |
| 41 | CO | 423 | VAL |
| 41 | CP | 58 | LYS |
| 41 | CP | 95 | SER |
| 41 | CP | 127 | CYS |
| 41 | CP | 173 | PRO |
| 41 | CP | 238 | THR |
| 41 | CP | 284 | LEU |
| 40 | DA | 2 | ARG |
| 40 | DA | 37 | PRO |
| 40 | DA | 74 | VAL |
| 40 | DA | 91 | GLN |
| 40 | DA | 165 | SER |
| 40 | DA | 177 | VAL |
| 40 | DA | 220 | GLU |
| 40 | DA | 280 | LYS |
| 40 | DA | 344 | VAL |
| 41 | DB | 87 | PRO |
| 41 | DB | 89 | ASN |
| 41 | DB | 90 | PHE |
| 41 | DB | 110 | ALA |
| 41 | DB | 129 | CYS |
| 41 | DB | 246 | LEU |
| 41 | DB | 338 | SER |
| 41 | DB | 392 | LYS |
| 40 | DE | 84 | ARG |
| 40 | DE | 142 | GLY |
| 40 | DE | 160 | ASP |
| 40 | DE | 202 | PHE |
| 40 | DE | 241 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DE | 282 | TYR |
| 40 | DF | 37 | PRO |
| 40 | DF | 73 | THR |
| 40 | DF | 74 | VAL |
| 40 | DF | 133 | GLN |
| 40 | DF | 177 | VAL |
| 40 | DF | 263 | PRO |
| 40 | DF | 299 | ALA |
| 40 | DG | 274 | PRO |
| 40 | DH | 74 | VAL |
| 40 | DH | 91 | GLN |
| 40 | DH | 103 | TYR |
| 40 | DH | 303 | VAL |
| 40 | DI | 74 | VAL |
| 40 | DI | 84 | ARG |
| 40 | DI | 110 | ILE |
| 40 | DI | 112 | LYS |
| 40 | DI | 177 | VAL |
| 40 | DI | 261 | PRO |
| 40 | DI | 304 | LYS |
| 41 | DL | 161 | ASP |
| 41 | DL | 284 | LEU |
| 41 | DL | 322 | SER |
| 41 | DM | 143 | THR |
| 41 | DM | 174 | LYS |
| 41 | DM | 259 | PRO |
| 41 | DN | 42 | LEU |
| 41 | DN | 69 | GLU |
| 41 | DN | 80 | PRO |
| 41 | DN | 101 | TRP |
| 41 | DN | 124 | ALA |
| 41 | DN | 194 | GLU |
| 41 | DN | 195 | ASN |
| 41 | DN | 216 | LYS |
| 41 | DN | 259 | PRO |
| 41 | DN | 271 | ALA |
| 41 | DN | 293 | MET |
| 41 | DO | 108 | GLU |
| 41 | DO | 143 | THR |
| 41 | DP | 80 | PRO |
| 40 | EA | 274 | PRO |
| 40 | EE | 274 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | EF | 274 | PRO |
| 40 | EG | 274 | PRO |
| 40 | EH | 37 | PRO |
| 40 | EH | 38 | SER |
| 40 | EH | 58 | ALA |
| 40 | EH | 100 | ALA |
| 40 | EH | 165 | SER |
| 40 | EH | 175 | PRO |
| 40 | EH | 177 | VAL |
| 40 | EH | 191 | THR |
| 40 | EH | 248 | LEU |
| 40 | EH | 274 | PRO |
| 40 | EH | 401 | ARG |
| 40 | EI | 91 | GLN |
| 40 | EI | 175 | PRO |
| 40 | EI | 177 | VAL |
| 40 | EI | 218 | ASP |
| 40 | EI | 364 | PRO |
| 40 | EI | 414 | GLU |
| 41 | EL | 143 | THR |
| 41 | EM | 39 | ASP |
| 41 | EM | 80 | PRO |
| 41 | EM | 87 | PRO |
| 41 | EM | 113 | VAL |
| 41 | EM | 161 | ASP |
| 41 | EM | 173 | PRO |
| 41 | EM | 174 | LYS |
| 41 | EM | 236 | VAL |
| 41 | EN | 143 | THR |
| 41 | EO | 143 | THR |
| 41 | EO | 195 | ASN |
| 41 | EP | 103 | LYS |
| 41 | EP | 129 | CYS |
| 41 | EP | 161 | ASP |
| 41 | EP | 173 | PRO |
| 40 | FA | 73 | THR |
| 40 | FA | 82 | THR |
| 40 | FA | 89 | PRO |
| 40 | FA | 110 | ILE |
| 40 | FA | 144 | GLY |
| 40 | FA | 261 | PRO |
| 40 | FA | 274 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | FA | 278 | ALA |
| 40 | FA | 280 | LYS |
| 40 | FA | 401 | ARG |
| 41 | FB | 143 | THR |
| 40 | FF | 274 | PRO |
| 40 | FG | 274 | PRO |
| 40 | FI | 274 | PRO |
| 41 | FM | 143 | THR |
| 41 | FO | 195 | ASN |
| 41 | FP | 143 | THR |
| 40 | GA | 274 | PRO |
| 40 | GE | 73 | THR |
| 40 | GE | 219 | ILE |
| 40 | GE | 288 | VAL |
| 40 | GF | 274 | PRO |
| 40 | GG | 274 | PRO |
| 40 | GH | 30 | ILE |
| 40 | GH | 32 | PRO |
| 40 | GH | 33 | ASP |
| 40 | GH | 58 | ALA |
| 40 | GH | 67 | PHE |
| 40 | GH | 72 | PRO |
| 40 | GH | 85 | GLN |
| 40 | GH | 341 | ILE |
| 40 | GH | 358 | GLN |
| 40 | GH | 403 | PHE |
| 40 | GI | 38 | SER |
| 40 | GI | 110 | ILE |
| 40 | GI | 161 | TYR |
| 40 | GI | 177 | VAL |
| 40 | GI | 264 | ARG |
| 40 | GI | 274 | PRO |
| 40 | GI | 279 | GLU |
| 40 | GI | 283 | HIS |
| 41 | GN | 129 | CYS |
| 41 | GO | 143 | THR |
| 41 | GP | 143 | THR |
| 40 | HA | 30 | ILE |
| 40 | HA | 274 | PRO |
| 40 | HE | 48 | SER |
| 40 | HE | 72 | PRO |
| 40 | HE | 86 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | HE | 261 | PRO |
| 40 | HF | 274 | PRO |
| 40 | HG | 51 | THR |
| 40 | HG | 82 | THR |
| 40 | HG | 274 | PRO |
| 40 | HH | 274 | PRO |
| 40 | HI | 274 | PRO |
| 41 | HN | 158 | GLU |
| 41 | HN | 161 | ASP |
| 41 | HN | 162 | ARG |
| 41 | HN | 302 | ALA |
| 41 | HO | 143 | THR |
| 41 | HP | 143 | THR |
| 40 | IA | 274 | PRO |
| 41 | IB | 143 | THR |
| 40 | IE | 274 | PRO |
| 40 | IF | 30 | ILE |
| 40 | IF | 274 | PRO |
| 40 | IG | 274 | PRO |
| 40 | IH | 178 | SER |
| 40 | IH | 274 | PRO |
| 40 | II | 178 | SER |
| 40 | II | 274 | PRO |
| 41 | IM | 143 | THR |
| 41 | IN | 143 | THR |
| 41 | IO | 143 | THR |
| 41 | IP | 143 | THR |
| 41 | IQ | 143 | THR |
| 40 | JA | 274 | PRO |
| 41 | JB | 143 | THR |
| 40 | JD | 30 | ILE |
| 40 | JD | 274 | PRO |
| 40 | JE | 274 | PRO |
| 40 | JF | 274 | PRO |
| 40 | JG | 274 | PRO |
| 40 | JH | 274 | PRO |
| 41 | JL | 143 | THR |
| 41 | JL | 195 | ASN |
| 41 | JM | 80 | PRO |
| 41 | JM | 95 | SER |
| 41 | JM | 173 | PRO |
| 41 | JM | 174 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | JN | 143 | THR |
| 41 | JO | 195 | ASN |
| 40 | KA | 48 | SER |
| 40 | KA | 274 | PRO |
| 40 | KD | 274 | PRO |
| 40 | KE | 274 | PRO |
| 40 | KF | 274 | PRO |
| 40 | KG | 274 | PRO |
| 40 | KH | 274 | PRO |
| 41 | KL | 80 | PRO |
| 41 | KL | 173 | PRO |
| 41 | KL | 392 | LYS |
| 41 | KM | 143 | THR |
| 41 | KN | 143 | THR |
| 41 | KO | 195 | ASN |
| 41 | KP | 143 | THR |
| 40 | LA | 274 | PRO |
| 41 | LB | 143 | THR |
| 40 | LD | 274 | PRO |
| 40 | LE | 274 | PRO |
| 40 | LF | 263 | PRO |
| 40 | LG | 72 | PRO |
| 40 | LG | 263 | PRO |
| 40 | LG | 274 | PRO |
| 40 | LH | 274 | PRO |
| 41 | LL | 143 | THR |
| 41 | LM | 143 | THR |
| 41 | LN | 143 | THR |
| 41 | LO | 143 | THR |
| 41 | LP | 143 | THR |
| 40 | MA | 72 | PRO |
| 40 | MA | 200 | CYS |
| 40 | MA | 278 | ALA |
| 40 | MA | 304 | LYS |
| 41 | MB | 143 | THR |
| 40 | MD | 274 | PRO |
| 40 | ME | 274 | PRO |
| 40 | MF | 73 | THR |
| 40 | MF | 163 | LYS |
| 40 | MF | 261 | PRO |
| 40 | MG | 110 | ILE |
| 40 | MG | 274 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MG | 412 | MET |
| 40 | MH | 59 | GLY |
| 40 | MH | 61 | HIS |
| 40 | MH | 273 | ALA |
| 41 | ML | 143 | THR |
| 41 | MM | 143 | THR |
| 41 | MN | 143 | THR |
| 41 | MO | 261 | PRO |
| 41 | MP | 143 | THR |
| 40 | NA | 274 | PRO |
| 41 | NB | 143 | THR |
| 40 | ND | 107 | HIS |
| 40 | ND | 110 | ILE |
| 40 | ND | 264 | ARG |
| 40 | ND | 265 | ILE |
| 40 | ND | 274 | PRO |
| 40 | NE | 274 | PRO |
| 40 | NH | 274 | PRO |
| 41 | NL | 143 | THR |
| 41 | NN | 143 | THR |
| 41 | NO | 143 | THR |
| 41 | NP | 143 | THR |
| 41 | OB | 143 | THR |
| 40 | OD | 85 | GLN |
| 40 | OD | 274 | PRO |
| 40 | OH | 313 | MET |
| 40 | OH | 355 | ILE |
| 41 | OL | 195 | ASN |
| 41 | OM | 143 | THR |
| 41 | OO | 143 | THR |
| 41 | OO | 195 | ASN |
| 41 | OP | 143 | THR |
| 41 | PB | 143 | THR |
| 40 | PG | 274 | PRO |
| 41 | PL | 143 | THR |
| 41 | PM | 143 | THR |
| 41 | PO | 143 | THR |
| 41 | QB | 80 | PRO |
| 41 | QB | 94 | GLN |
| 41 | QB | 100 | ASN |
| 41 | QB | 114 | ASP |
| 41 | QB | 174 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QB | 216 | LYS |
| 41 | QB | 297 | LYS |
| 41 | QB | 298 | ASN |
| 41 | QB | 396 | HIS |
| 40 | QE | 274 | PRO |
| 40 | QH | 274 | PRO |
| 41 | QL | 108 | GLU |
| 41 | QL | 143 | THR |
| 41 | QM | 143 | THR |
| 41 | QM | 195 | ASN |
| 41 | QN | 143 | THR |
| 41 | QO | 143 | THR |
| 41 | QO | 195 | ASN |
| 41 | QP | 2 | ARG |
| 41 | QP | 41 | ASP |
| 41 | QP | 80 | PRO |
| 41 | QP | 125 | GLU |
| 41 | QP | 174 | LYS |
| 41 | QP | 270 | PHE |
| 41 | QP | 323 | MET |
| 41 | QP | 336 | LYS |
| 41 | QP | 342 | VAL |
| 41 | QP | 346 | PRO |
| 40 | RA | 274 | PRO |
| 41 | RB | 195 | ASN |
| 40 | RE | 48 | SER |
| 40 | RE | 274 | PRO |
| 40 | RF | 274 | PRO |
| 40 | RH | 48 | SER |
| 40 | RH | 274 | PRO |
| 41 | RM | 143 | THR |
| 41 | RN | 143 | THR |
| 41 | RO | 195 | ASN |
| 41 | SB | 143 | THR |
| 40 | SE | 274 | PRO |
| 40 | SF | 274 | PRO |
| 40 | SG | 274 | PRO |
| 40 | SI | 274 | PRO |
| 41 | SL | 143 | THR |
| 41 | SM | 143 | THR |
| 41 | SM | 195 | ASN |
| 41 | SN | 143 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | SO | 90 | PHE |
| 41 | SO | 143 | THR |
| 41 | SO | 173 | PRO |
| 41 | SO | 259 | PRO |
| 41 | SO | 271 | ALA |
| 41 | SO | 303 | CYS |
| 41 | SO | 323 | MET |
| 41 | SO | 342 | VAL |
| 41 | SP | 143 | THR |
| 40 | TE | 274 | PRO |
| 40 | TF | 274 | PRO |
| 40 | TH | 274 | PRO |
| 40 | TI | 274 | PRO |
| 41 | TL | 143 | THR |
| 41 | TM | 143 | THR |
| 41 | TN | 195 | ASN |
| 41 | TO | 143 | THR |
| 41 | TP | 143 | THR |
| 40 | UA | 274 | PRO |
| 41 | UB | 143 | THR |
| 40 | UE | 48 | SER |
| 40 | UE | 274 | PRO |
| 40 | UF | 261 | PRO |
| 40 | UF | 275 | VAL |
| 40 | UG | 274 | PRO |
| 40 | UH | 48 | SER |
| 40 | UH | 58 | ALA |
| 40 | UI | 29 | GLY |
| 40 | UI | 50 | ASN |
| 40 | UI | 51 | THR |
| 40 | UI | 278 | ALA |
| 40 | UI | 355 | ILE |
| 41 | UM | 143 | THR |
| 41 | UN | 143 | THR |
| 41 | UP | 59 | TYR |
| 41 | UP | 91 | VAL |
| 41 | UP | 101 | TRP |
| 41 | UP | 108 | GLU |
| 40 | VA | 274 | PRO |
| 41 | VB | 143 | THR |
| 40 | VF | 38 | SER |
| 40 | VF | 274 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | VG | 274 | PRO |
| 40 | VI | 274 | PRO |
| 40 | VJ | 274 | PRO |
| 41 | VN | 143 | THR |
| 41 | VO | 143 | THR |
| 41 | VP | 143 | THR |
| 41 | VQ | 143 | THR |
| 40 | WA | 51 | THR |
| 40 | WA | 274 | PRO |
| 41 | WB | 143 | THR |
| 40 | WE | 274 | PRO |
| 40 | WF | 274 | PRO |
| 40 | WG | 274 | PRO |
| 40 | WH | 178 | SER |
| 41 | WM | 101 | TRP |
| 41 | WM | 271 | ALA |
| 41 | WM | 303 | CYS |
| 41 | WM | 311 | LEU |
| 41 | WO | 143 | THR |
| 41 | WQ | 143 | THR |
| 1 | 1A | 854 | PRO |
| 3 | 1G | 108 | LEU |
| 3 | 1G | 110 | VAL |
| 3 | 1G | 114 | MET |
| 3 | 1G | 164 | ASP |
| 3 | 1G | 177 | VAL |
| 5 | 1L | 284 | ASP |
| 5 | 1L | 286 | GLU |
| 7 | 1T | 14 | LEU |
| 7 | 1T | 109 | LEU |
| 7 | 1T | 123 | ASP |
| 7 | 1T | 179 | ASN |
| 7 | 1T | 322 | PHE |
| 7 | 1T | 362 | LEU |
| 7 | 1T | 374 | ASN |
| 7 | 1T | 484 | THR |
| 7 | 1T | 493 | LEU |
| 7 | 1T | 526 | ILE |
| 8 | 1X | 115 | HIS |
| 9 | 2B | 46 | VAL |
| 11 | 2K | 253 | ALA |
| 12 | 2O | 149 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2T | 55 | SER |
| 13 | 2T | 63 | ALA |
| 13 | 2T | 120 | THR |
| 13 | 2T | 132 | ILE |
| 13 | 2U | 63 | ALA |
| 13 | 2W | 74 | PRO |
| 13 | 2W | 143 | ALA |
| 13 | 2W | 145 | GLY |
| 13 | 2W | 172 | TYR |
| 13 | 2X | 70 | GLY |
| 13 | 2X | 145 | GLY |
| 17 | 3P | 472 | LYS |
| 17 | 3Q | 409 | ILE |
| 17 | 3Q | 472 | LYS |
| 17 | 3R | 94 | TYR |
| 17 | 3R | 208 | ILE |
| 17 | 3R | 331 | VAL |
| 20 | 4A | 150 | SER |
| 20 | 4B | 254 | THR |
| 20 | 4B | 258 | GLN |
| 21 | 4D | 338 | LEU |
| 21 | 4D | 409 | VAL |
| 21 | 4D | 431 | PRO |
| 21 | 4D | 436 | ARG |
| 21 | 4D | 462 | ILE |
| 21 | 4D | 478 | SER |
| 21 | 4D | 485 | TYR |
| 21 | 4D | 492 | ILE |
| 21 | 4E | 463 | GLY |
| 21 | 4E | 477 | SER |
| 21 | 4E | 478 | SER |
| 21 | 4E | 499 | PHE |
| 21 | 4E | 501 | HIS |
| 21 | 4F | 408 | ASP |
| 21 | 4F | 436 | ARG |
| 22 | 4I | 458 | LEU |
| 22 | 4I | 649 | LYS |
| 22 | 4I | 681 | PHE |
| 22 | 4J | 631 | ALA |
| 22 | 4J | 648 | GLU |
| 22 | 4K | 559 | SER |
| 22 | 4K | 616 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 4K | 618 | ILE |
| 23 | 4M | 103 | PHE |
| 23 | 4M | 262 | GLY |
| 23 | 4N | 94 | TYR |
| 23 | 4N | 177 | ARG |
| 23 | 4N | 184 | MET |
| 23 | 4N | 261 | TYR |
| 24 | 4O | 187 | PHE |
| 23 | 4P | 180 | ARG |
| 23 | 4P | 184 | MET |
| 23 | 4P | 185 | SER |
| 23 | 4P | 261 | TYR |
| 23 | 4Q | 238 | HIS |
| 23 | 4Q | 239 | ASN |
| 23 | 4R | 60 | LEU |
| 23 | 4R | 181 | LYS |
| 23 | 4R | 185 | SER |
| 23 | 4R | 187 | PHE |
| 25 | 4T | 291 | SER |
| 26 | 4V | 319 | THR |
| 26 | 4W | 228 | CYS |
| 26 | 4W | 363 | ASP |
| 26 | 4W | 373 | LYS |
| 27 | 4Y | 132 | ALA |
| 28 | 5B | 209 | ILE |
| 29 | 5E | 108 | VAL |
| 31 | 5I | 461 | ALA |
| 36 | 5W | 26 | ILE |
| 38 | 6C | 26 | ASP |
| 38 | 6C | 41 | SER |
| 41 | AB | 143 | THR |
| 40 | AE | 46 | ASP |
| 41 | AL | 108 | GLU |
| 41 | AL | 195 | ASN |
| 41 | AM | 108 | GLU |
| 41 | AM | 143 | THR |
| 41 | AM | 195 | ASN |
| 41 | AN | 108 | GLU |
| 41 | AN | 143 | THR |
| 41 | AN | 195 | ASN |
| 41 | AO | 80 | PRO |
| 41 | AO | 142 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | AO | 195 | ASN |
| 41 | AO | 271 | ALA |
| 41 | AO | 347 | ASN |
| 41 | AO | 359 | ARG |
| 41 | AP | 195 | ASN |
| 41 | BB | 45 | GLU |
| 41 | BB | 83 | GLN |
| 41 | BB | 94 | GLN |
| 41 | BB | 99 | ASN |
| 41 | BB | 143 | THR |
| 41 | BB | 195 | ASN |
| 41 | BB | 355 | ASP |
| 41 | BB | 363 | MET |
| 41 | BB | 394 | PHE |
| 40 | BE | 12 | ALA |
| 40 | BE | 39 | ASP |
| 40 | BE | 45 | GLY |
| 40 | BE | 46 | ASP |
| 40 | BE | 74 | VAL |
| 40 | BE | 160 | ASP |
| 40 | BE | 265 | ILE |
| 40 | BE | 280 | LYS |
| 40 | BE | 299 | ALA |
| 40 | BE | 305 | CYS |
| 40 | BH | 96 | LYS |
| 40 | BH | 142 | GLY |
| 40 | BH | 162 | GLY |
| 40 | BH | 177 | VAL |
| 40 | BH | 243 | ARG |
| 40 | BH | 261 | PRO |
| 40 | BH | 364 | PRO |
| 40 | BI | 37 | PRO |
| 40 | BI | 53 | PHE |
| 40 | BI | 64 | ARG |
| 40 | BI | 66 | VAL |
| 40 | BI | 86 | LEU |
| 40 | BI | 101 | ASN |
| 40 | BI | 110 | ILE |
| 40 | BI | 141 | PHE |
| 40 | BI | 160 | ASP |
| 40 | BI | 163 | LYS |
| 40 | BI | 177 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BI | 202 | PHE |
| 40 | BI | 219 | ILE |
| 40 | BI | 412 | MET |
| 41 | BM | 45 | GLU |
| 41 | BM | 91 | VAL |
| 41 | BM | 99 | ASN |
| 41 | BM | 144 | GLY |
| 41 | BM | 195 | ASN |
| 41 | BM | 259 | PRO |
| 41 | BM | 336 | LYS |
| 41 | BM | 392 | LYS |
| 41 | BM | 394 | PHE |
| 41 | BN | 108 | GLU |
| 41 | BO | 59 | TYR |
| 41 | BO | 94 | GLN |
| 41 | BO | 143 | THR |
| 41 | BO | 144 | GLY |
| 41 | BO | 145 | SER |
| 41 | BO | 195 | ASN |
| 41 | BO | 315 | ALA |
| 41 | BP | 59 | TYR |
| 41 | BP | 95 | SER |
| 41 | BP | 99 | ASN |
| 41 | BP | 112 | LEU |
| 41 | BP | 144 | GLY |
| 41 | BP | 263 | LEU |
| 40 | CA | 46 | ASP |
| 40 | CA | 110 | ILE |
| 40 | CA | 132 | LEU |
| 40 | CA | 177 | VAL |
| 40 | CA | 258 | ASN |
| 40 | CA | 261 | PRO |
| 40 | CA | 340 | SER |
| 40 | CF | 72 | PRO |
| 40 | CG | 178 | SER |
| 40 | CH | 34 | GLY |
| 40 | CH | 47 | ASP |
| 40 | CH | 72 | PRO |
| 40 | CH | 73 | THR |
| 40 | CH | 212 | ILE |
| 40 | CH | 261 | PRO |
| 40 | CH | 304 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CH | 319 | TYR |
| 40 | CH | 322 | ASP |
| 40 | CH | 364 | PRO |
| 40 | CH | 401 | ARG |
| 40 | CH | 406 | TRP |
| 41 | CL | 2 | ARG |
| 41 | CL | 80 | PRO |
| 41 | CL | 98 | GLY |
| 41 | CL | 99 | ASN |
| 41 | CL | 130 | LEU |
| 41 | CL | 143 | THR |
| 41 | CL | 144 | GLY |
| 41 | CL | 198 | GLU |
| 41 | CL | 246 | LEU |
| 41 | CL | 272 | PRO |
| 41 | CL | 320 | ARG |
| 41 | CM | 127 | CYS |
| 41 | CM | 143 | THR |
| 41 | CM | 259 | PRO |
| 41 | CM | 303 | CYS |
| 41 | CM | 392 | LYS |
| 41 | CM | 422 | VAL |
| 41 | CN | 47 | ILE |
| 41 | CN | 80 | PRO |
| 41 | CN | 95 | SER |
| 41 | CN | 98 | GLY |
| 41 | CN | 99 | ASN |
| 41 | CN | 101 | TRP |
| 41 | CN | 139 | LEU |
| 41 | CN | 140 | GLY |
| 41 | CN | 195 | ASN |
| 41 | CN | 259 | PRO |
| 41 | CN | 263 | LEU |
| 41 | CN | 307 | HIS |
| 41 | CN | 362 | LYS |
| 41 | CO | 98 | GLY |
| 41 | CO | 99 | ASN |
| 41 | CO | 112 | LEU |
| 41 | CO | 146 | GLY |
| 41 | CO | 246 | LEU |
| 41 | CO | 255 | VAL |
| 41 | CO | 256 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CO | 293 | MET |
| 41 | CO | 315 | ALA |
| 41 | CO | 392 | LYS |
| 41 | CP | 29 | GLY |
| 41 | CP | 55 | THR |
| 41 | CP | 80 | PRO |
| 41 | CP | 146 | GLY |
| 41 | CP | 158 | GLU |
| 41 | CP | 241 | ARG |
| 41 | CP | 255 | VAL |
| 41 | CP | 300 | MET |
| 41 | CP | 426 | GLY |
| 40 | DA | 60 | LYS |
| 40 | DA | 72 | PRO |
| 40 | DA | 90 | GLU |
| 40 | DA | 101 | ASN |
| 40 | DA | 142 | GLY |
| 40 | DA | 159 | VAL |
| 40 | DA | 164 | LYS |
| 40 | DA | 217 | LEU |
| 40 | DA | 218 | ASP |
| 40 | DA | 263 | PRO |
| 40 | DA | 299 | ALA |
| 40 | DA | 364 | PRO |
| 40 | DA | 414 | GLU |
| 40 | DA | 415 | GLY |
| 41 | DB | 80 | PRO |
| 41 | DB | 109 | GLY |
| 41 | DB | 128 | ASP |
| 41 | DB | 140 | GLY |
| 41 | DB | 163 | ILE |
| 41 | DB | 183 | TYR |
| 41 | DB | 193 | VAL |
| 41 | DB | 315 | ALA |
| 40 | DE | 2 | ARG |
| 40 | DE | 60 | LYS |
| 40 | DE | 107 | HIS |
| 40 | DE | 109 | THR |
| 40 | DE | 130 | THR |
| 40 | DE | 147 | SER |
| 40 | DE | 163 | LYS |
| 40 | DE | 164 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DE | 175 | PRO |
| 40 | DE | 184 | PRO |
| 40 | DE | 261 | PRO |
| 40 | DE | 264 | ARG |
| 40 | DE | 265 | ILE |
| 40 | DE | 299 | ALA |
| 40 | DE | 408 | VAL |
| 40 | DF | 99 | ALA |
| 40 | DF | 160 | ASP |
| 40 | DF | 261 | PRO |
| 40 | DF | 338 | LYS |
| 40 | DH | 52 | PHE |
| 40 | DH | 72 | PRO |
| 40 | DH | 83 | TYR |
| 40 | DH | 90 | GLU |
| 40 | DH | 176 | GLN |
| 40 | DH | 219 | ILE |
| 40 | DH | 304 | LYS |
| 40 | DI | 66 | VAL |
| 40 | DI | 98 | ASP |
| 40 | DI | 99 | ALA |
| 40 | DI | 113 | GLU |
| 40 | DI | 141 | PHE |
| 40 | DI | 179 | THR |
| 40 | DI | 217 | LEU |
| 40 | DI | 273 | ALA |
| 40 | DI | 296 | PHE |
| 40 | DI | 299 | ALA |
| 40 | DI | 323 | VAL |
| 40 | DI | 338 | LYS |
| 40 | DI | 356 | ASN |
| 40 | DI | 357 | TYR |
| 40 | DI | 364 | PRO |
| 40 | DI | 438 | SER |
| 41 | DL | 35 | THR |
| 41 | DL | 80 | PRO |
| 41 | DL | 90 | PHE |
| 41 | DL | 94 | GLN |
| 41 | DL | 138 | SER |
| 41 | DL | 173 | PRO |
| 41 | DL | 193 | VAL |
| 41 | DL | 320 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DL | 323 | MET |
| 41 | DL | 363 | MET |
| 41 | DL | 402 | GLY |
| 41 | DM | 48 | ASN |
| 41 | DM | 49 | VAL |
| 41 | DM | 76 | VAL |
| 41 | DM | 80 | PRO |
| 41 | DM | 129 | CYS |
| 41 | DM | 130 | LEU |
| 41 | DM | 140 | GLY |
| 41 | DM | 161 | ASP |
| 41 | DM | 193 | VAL |
| 41 | DM | 194 | GLU |
| 41 | DM | 201 | CYS |
| 41 | DM | 246 | LEU |
| 41 | DM | 326 | VAL |
| 41 | DN | 83 | GLN |
| 41 | DN | 90 | PHE |
| 41 | DN | 94 | GLN |
| 41 | DN | 97 | ALA |
| 41 | DN | 98 | GLY |
| 41 | DN | 130 | LEU |
| 41 | DN | 146 | GLY |
| 41 | DN | 246 | LEU |
| 41 | DN | 263 | LEU |
| 41 | DN | 336 | LYS |
| 41 | DN | 392 | LYS |
| 41 | DN | 396 | HIS |
| 41 | DP | 44 | LEU |
| 41 | DP | 45 | GLU |
| 41 | DP | 129 | CYS |
| 41 | DP | 140 | GLY |
| 41 | DP | 173 | PRO |
| 41 | DP | 174 | LYS |
| 41 | DP | 214 | THR |
| 41 | DP | 246 | LEU |
| 41 | EB | 143 | THR |
| 41 | EB | 195 | ASN |
| 40 | EH | 89 | PRO |
| 40 | EH | 91 | GLN |
| 40 | EH | 110 | ILE |
| 40 | EH | 132 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | EH | 136 | LEU |
| 40 | EH | 176 | GLN |
| 40 | EH | 244 | PHE |
| 40 | EH | 364 | PRO |
| 40 | EH | 434 | VAL |
| 40 | EI | 92 | LEU |
| 40 | EI | 101 | ASN |
| 40 | EI | 109 | THR |
| 40 | EI | 141 | PHE |
| 40 | EI | 184 | PRO |
| 40 | EI | 247 | ALA |
| 40 | EI | 415 | GLY |
| 40 | EI | 416 | GLU |
| 40 | EI | 438 | SER |
| 41 | EM | 65 | LEU |
| 41 | EM | 202 | ILE |
| 41 | EM | 245 | GLN |
| 41 | EM | 255 | VAL |
| 41 | EM | 257 | MET |
| 41 | EM | 259 | PRO |
| 41 | EM | 262 | ARG |
| 41 | EP | 99 | ASN |
| 41 | EP | 130 | LEU |
| 41 | EP | 163 | ILE |
| 41 | EP | 216 | LYS |
| 41 | EP | 339 | SER |
| 41 | EP | 377 | LEU |
| 40 | FA | 49 | PHE |
| 40 | FA | 100 | ALA |
| 40 | FA | 101 | ASN |
| 40 | FA | 107 | HIS |
| 40 | FA | 145 | THR |
| 40 | FA | 177 | VAL |
| 40 | FA | 273 | ALA |
| 40 | FA | 364 | PRO |
| 40 | FA | 412 | MET |
| 41 | FB | 195 | ASN |
| 41 | FM | 108 | GLU |
| 41 | FM | 195 | ASN |
| 41 | FN | 195 | ASN |
| 41 | FO | 143 | THR |
| 41 | FP | 195 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GA | 38 | SER |
| 41 | GB | 143 | THR |
| 40 | GE | 38 | SER |
| 40 | GE | 50 | ASN |
| 40 | GE | 51 | THR |
| 40 | GE | 160 | ASP |
| 40 | GE | 161 | TYR |
| 40 | GE | 202 | PHE |
| 40 | GE | 261 | PRO |
| 40 | GE | 264 | ARG |
| 40 | GE | 348 | PRO |
| 40 | GG | 362 | VAL |
| 40 | GH | 57 | GLY |
| 40 | GH | 86 | LEU |
| 40 | GH | 110 | ILE |
| 40 | GH | 175 | PRO |
| 40 | GH | 177 | VAL |
| 40 | GH | 261 | PRO |
| 40 | GH | 286 | LEU |
| 40 | GH | 340 | SER |
| 40 | GH | 364 | PRO |
| 40 | GI | 51 | THR |
| 40 | GI | 61 | HIS |
| 40 | GI | 72 | PRO |
| 40 | GI | 86 | LEU |
| 40 | GI | 163 | LYS |
| 40 | GI | 248 | LEU |
| 40 | GI | 261 | PRO |
| 40 | GI | 282 | TYR |
| 40 | GI | 304 | LYS |
| 40 | GI | 401 | ARG |
| 41 | GM | 143 | THR |
| 41 | GN | 55 | THR |
| 41 | GN | 59 | TYR |
| 41 | GN | 95 | SER |
| 41 | GN | 195 | ASN |
| 41 | GN | 246 | LEU |
| 41 | GN | 262 | ARG |
| 41 | GN | 299 | MET |
| 41 | GN | 302 | ALA |
| 40 | HA | 38 | SER |
| 41 | HB | 143 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | HB | 195 | ASN |
| 40 | HE | 29 | GLY |
| 40 | HE | 49 | PHE |
| 40 | HE | 54 | SER |
| 40 | HE | 56 | THR |
| 40 | HE | 58 | ALA |
| 40 | HE | 73 | THR |
| 40 | HE | 85 | GLN |
| 40 | HE | 110 | ILE |
| 40 | HE | 160 | ASP |
| 40 | HE | 364 | PRO |
| 40 | HE | 436 | MET |
| 41 | HM | 143 | THR |
| 41 | HN | 93 | GLY |
| 41 | HN | 95 | SER |
| 41 | HN | 143 | THR |
| 41 | HP | 108 | GLU |
| 41 | HQ | 143 | THR |
| 41 | IO | 195 | ASN |
| 41 | IP | 195 | ASN |
| 40 | JE | 38 | SER |
| 41 | JM | 49 | VAL |
| 41 | JM | 195 | ASN |
| 41 | JM | 259 | PRO |
| 41 | JM | 263 | LEU |
| 41 | JM | 392 | LYS |
| 41 | JO | 143 | THR |
| 41 | KB | 143 | THR |
| 41 | KL | 103 | LYS |
| 41 | KL | 143 | THR |
| 41 | KL | 336 | LYS |
| 41 | KN | 108 | GLU |
| 41 | KO | 143 | THR |
| 41 | KP | 195 | ASN |
| 40 | LE | 58 | ALA |
| 40 | LF | 30 | ILE |
| 40 | LF | 58 | ALA |
| 40 | LF | 162 | GLY |
| 40 | LF | 177 | VAL |
| 40 | LF | 261 | PRO |
| 40 | LF | 304 | LYS |
| 40 | LF | 348 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | LF | 364 | PRO |
| 40 | LG | 142 | GLY |
| 40 | LG | 160 | ASP |
| 40 | LG | 176 | GLN |
| 40 | LG | 261 | PRO |
| 40 | LG | 278 | ALA |
| 40 | LG | 286 | LEU |
| 41 | LL | 195 | ASN |
| 41 | LO | 108 | GLU |
| 41 | LO | 195 | ASN |
| 40 | MA | 29 | GLY |
| 40 | MA | 58 | ALA |
| 40 | MA | 73 | THR |
| 40 | MA | 161 | TYR |
| 40 | MA | 176 | GLN |
| 40 | MA | 177 | VAL |
| 40 | MA | 248 | LEU |
| 40 | MA | 279 | GLU |
| 40 | MA | 348 | PRO |
| 40 | MA | 364 | PRO |
| 40 | ME | 38 | SER |
| 40 | MF | 74 | VAL |
| 40 | MF | 101 | ASN |
| 40 | MF | 159 | VAL |
| 40 | MF | 164 | LYS |
| 40 | MF | 199 | ASP |
| 40 | MF | 273 | ALA |
| 40 | MF | 327 | ASP |
| 40 | MF | 364 | PRO |
| 40 | MF | 401 | ARG |
| 40 | MG | 47 | ASP |
| 40 | MG | 72 | PRO |
| 40 | MG | 160 | ASP |
| 40 | MG | 261 | PRO |
| 40 | MG | 265 | ILE |
| 40 | MG | 364 | PRO |
| 40 | MH | 49 | PHE |
| 40 | MH | 72 | PRO |
| 40 | MH | 74 | VAL |
| 40 | MH | 110 | ILE |
| 40 | MH | 160 | ASP |
| 40 | MH | 177 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MH | 434 | VAL |
| 41 | ML | 195 | ASN |
| 41 | MM | 195 | ASN |
| 41 | MO | 95 | SER |
| 41 | MO | 112 | LEU |
| 41 | MO | 173 | PRO |
| 41 | MO | 195 | ASN |
| 41 | MO | 262 | ARG |
| 41 | MO | 263 | LEU |
| 41 | MO | 271 | ALA |
| 41 | MO | 392 | LYS |
| 41 | MP | 195 | ASN |
| 41 | NB | 195 | ASN |
| 40 | ND | 73 | THR |
| 40 | ND | 160 | ASP |
| 40 | ND | 176 | GLN |
| 40 | ND | 177 | VAL |
| 40 | ND | 247 | ALA |
| 40 | ND | 261 | PRO |
| 40 | ND | 280 | LYS |
| 40 | ND | 304 | LYS |
| 40 | ND | 341 | ILE |
| 40 | ND | 436 | MET |
| 40 | NE | 38 | SER |
| 40 | NG | 178 | SER |
| 40 | NH | 178 | SER |
| 41 | NL | 108 | GLU |
| 41 | NL | 195 | ASN |
| 41 | NM | 143 | THR |
| 41 | NN | 195 | ASN |
| 41 | NP | 108 | GLU |
| 41 | NP | 284 | LEU |
| 40 | OD | 86 | LEU |
| 40 | OE | 38 | SER |
| 40 | OF | 46 | ASP |
| 40 | OH | 73 | THR |
| 40 | OH | 100 | ALA |
| 40 | OH | 101 | ASN |
| 40 | OH | 261 | PRO |
| 40 | OH | 263 | PRO |
| 40 | OH | 276 | ILE |
| 40 | OH | 299 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OH | 309 | HIS |
| 40 | OH | 412 | MET |
| 41 | OL | 143 | THR |
| 41 | ON | 143 | THR |
| 41 | ON | 195 | ASN |
| 41 | OP | 195 | ASN |
| 41 | PL | 195 | ASN |
| 41 | PM | 195 | ASN |
| 41 | PN | 143 | THR |
| 41 | PN | 195 | ASN |
| 41 | PO | 195 | ASN |
| 41 | PP | 143 | THR |
| 41 | QB | 54 | ALA |
| 41 | QB | 56 | GLY |
| 41 | QB | 57 | GLY |
| 41 | QB | 68 | LEU |
| 41 | QB | 109 | GLY |
| 41 | QB | 123 | GLU |
| 41 | QB | 126 | SER |
| 41 | QB | 128 | ASP |
| 41 | QB | 130 | LEU |
| 41 | QB | 140 | GLY |
| 41 | QB | 146 | GLY |
| 41 | QB | 173 | PRO |
| 41 | QB | 190 | HIS |
| 41 | QB | 236 | VAL |
| 41 | QB | 259 | PRO |
| 41 | QB | 317 | PHE |
| 41 | QB | 323 | MET |
| 41 | QB | 392 | LYS |
| 41 | QB | 417 | ASP |
| 41 | QN | 195 | ASN |
| 41 | QP | 18 | ALA |
| 41 | QP | 35 | THR |
| 41 | QP | 36 | TYR |
| 41 | QP | 42 | LEU |
| 41 | QP | 49 | VAL |
| 41 | QP | 98 | GLY |
| 41 | QP | 101 | TRP |
| 41 | QP | 127 | CYS |
| 41 | QP | 139 | LEU |
| 41 | QP | 140 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QP | 143 | THR |
| 41 | QP | 173 | PRO |
| 41 | QP | 193 | VAL |
| 41 | QP | 222 | TYR |
| 41 | QP | 259 | PRO |
| 41 | QP | 299 | MET |
| 41 | QP | 321 | MET |
| 41 | QP | 322 | SER |
| 41 | QP | 387 | ALA |
| 41 | QP | 402 | GLY |
| 41 | QP | 417 | ASP |
| 41 | RO | 108 | GLU |
| 41 | RO | 143 | THR |
| 40 | SA | 247 | ALA |
| 40 | SA | 261 | PRO |
| 41 | SB | 377 | LEU |
| 41 | SB | 396 | HIS |
| 41 | SL | 195 | ASN |
| 41 | SN | 108 | GLU |
| 41 | SO | 80 | PRO |
| 41 | SO | 83 | GLN |
| 41 | SO | 162 | ARG |
| 41 | SO | 210 | ILE |
| 41 | SO | 320 | ARG |
| 41 | SP | 195 | ASN |
| 41 | TB | 143 | THR |
| 41 | TB | 195 | ASN |
| 41 | TN | 143 | THR |
| 40 | UF | 38 | SER |
| 40 | UF | 164 | LYS |
| 40 | UF | 177 | VAL |
| 40 | UF | 202 | PHE |
| 40 | UF | 364 | PRO |
| 40 | UF | 367 | LEU |
| 40 | UG | 48 | SER |
| 40 | UI | 26 | LEU |
| 40 | UI | 27 | GLU |
| 40 | UI | 66 | VAL |
| 40 | UI | 72 | PRO |
| 40 | UI | 110 | ILE |
| 40 | UI | 177 | VAL |
| 40 | UI | 202 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | UI | 247 | ALA |
| 40 | UI | 263 | PRO |
| 40 | UI | 265 | ILE |
| 40 | UI | 357 | TYR |
| 40 | UI | 438 | SER |
| 41 | UM | 108 | GLU |
| 41 | UO | 143 | THR |
| 41 | UO | 195 | ASN |
| 41 | UP | 83 | GLN |
| 41 | UP | 98 | GLY |
| 41 | UP | 99 | ASN |
| 41 | UP | 143 | THR |
| 41 | UP | 161 | ASP |
| 41 | UP | 173 | PRO |
| 41 | UP | 182 | PRO |
| 41 | UP | 261 | PRO |
| 41 | UP | 265 | PHE |
| 41 | UP | 271 | ALA |
| 41 | VN | 195 | ASN |
| 41 | VP | 195 | ASN |
| 40 | WG | 178 | SER |
| 41 | WM | 129 | CYS |
| 41 | WM | 161 | ASP |
| 41 | WM | 173 | PRO |
| 41 | WM | 195 | ASN |
| 41 | WM | 300 | MET |
| 41 | WM | 427 | ALA |
| 41 | WN | 30 | ILE |
| 41 | WN | 95 | SER |
| 41 | WN | 143 | THR |
| 41 | WN | 197 | ASP |
| 41 | WN | 216 | LYS |
| 41 | WN | 246 | LEU |
| 41 | WN | 271 | ALA |
| 41 | WN | 311 | LEU |
| 41 | WN | 392 | LYS |
| 41 | WP | 143 | THR |
| 41 | WP | 195 | ASN |
| 1 | 1A | 853 | ASN |
| 2 | 1D | 133 | SER |
| 3 | 1F | 239 | LEU |
| 3 | 1G | 76 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1G | 109 | HIS |
| 3 | 1G | 138 | SER |
| 3 | 1G | 208 | MET |
| 3 | 1G | 227 | GLU |
| 5 | 1L | 285 | LEU |
| 5 | 1M | 93 | ASN |
| 7 | 1S | 586 | HIS |
| 7 | 1T | 101 | ARG |
| 7 | 1T | 133 | ASP |
| 7 | 1T | 217 | ASP |
| 7 | 1T | 245 | ALA |
| 7 | 1T | 364 | ASN |
| 7 | 1T | 414 | ASN |
| 7 | 1T | 524 | ARG |
| 7 | 1T | 575 | ASN |
| 8 | 1X | 84 | MET |
| 8 | 1X | 100 | LEU |
| 8 | 1X | 113 | ALA |
| 9 | 2C | 490 | HIS |
| 11 | 2J | 251 | TYR |
| 11 | 2K | 215 | SER |
| 12 | 2O | 141 | LYS |
| 13 | 2T | 98 | ASN |
| 13 | 2U | 127 | ASP |
| 13 | 2U | 171 | LEU |
| 13 | 2V | 63 | ALA |
| 13 | 2V | 98 | ASN |
| 13 | 2V | 143 | ALA |
| 13 | 2V | 172 | TYR |
| 13 | 2W | 63 | ALA |
| 13 | 2W | 127 | ASP |
| 13 | 2W | 175 | ASP |
| 13 | 2X | 74 | PRO |
| 13 | 2X | 109 | GLN |
| 13 | 2X | 143 | ALA |
| 16 | 3J | 325 | PRO |
| 17 | 3P | 411 | LEU |
| 17 | 3Q | 408 | ASN |
| 17 | 3Q | 471 | GLU |
| 17 | 3R | 96 | PRO |
| 17 | 3R | 217 | THR |
| 17 | 3R | 218 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | 4A | 233 | HIS |
| 20 | 4B | 229 | GLN |
| 20 | 4B | 251 | ASP |
| 20 | 4B | 358 | ASN |
| 21 | 4D | 499 | PHE |
| 21 | 4E | 436 | ARG |
| 21 | 4E | 474 | LYS |
| 21 | 4F | 474 | LYS |
| 22 | 4I | 633 | GLU |
| 22 | 4I | 676 | ALA |
| 22 | 4I | 701 | ALA |
| 22 | 4J | 54 | LYS |
| 22 | 4J | 677 | LEU |
| 23 | 4M | 55 | PRO |
| 23 | 4M | 109 | CYS |
| 23 | 4M | 181 | LYS |
| 23 | 4M | 187 | PHE |
| 23 | 4M | 242 | LEU |
| 23 | 4N | 50 | GLY |
| 23 | 4N | 180 | ARG |
| 23 | 4N | 196 | PHE |
| 23 | 4N | 245 | LYS |
| 23 | 4N | 256 | GLN |
| 24 | 4O | 192 | PRO |
| 23 | 4P | 245 | LYS |
| 23 | 4P | 256 | GLN |
| 23 | 4Q | 187 | PHE |
| 23 | 4R | 35 | GLN |
| 23 | 4R | 101 | ALA |
| 23 | 4R | 107 | LYS |
| 23 | 4R | 237 | PRO |
| 23 | 4R | 262 | GLY |
| 25 | 4T | 308 | LEU |
| 26 | 4W | 203 | ASN |
| 26 | 4W | 361 | PRO |
| 26 | 4W | 364 | GLY |
| 30 | 5G | 97 | TYR |
| 31 | 5I | 387 | PRO |
| 36 | 5W | 108 | PRO |
| 36 | 5W | 234 | LEU |
| 36 | 5X | 167 | THR |
| 38 | 6C | 205 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | 6L | 120 | PRO |
| 40 | AE | 299 | ALA |
| 41 | AO | 71 | GLY |
| 41 | AO | 95 | SER |
| 41 | AO | 173 | PRO |
| 41 | AO | 261 | PRO |
| 41 | AO | 262 | ARG |
| 41 | BB | 29 | GLY |
| 41 | BB | 59 | TYR |
| 41 | BB | 80 | PRO |
| 41 | BB | 93 | GLY |
| 41 | BB | 271 | ALA |
| 40 | BE | 38 | SER |
| 40 | BE | 72 | PRO |
| 40 | BE | 101 | ASN |
| 40 | BE | 131 | GLY |
| 40 | BE | 155 | GLU |
| 40 | BE | 161 | TYR |
| 40 | BE | 261 | PRO |
| 40 | BE | 273 | ALA |
| 40 | BE | 322 | ASP |
| 40 | BE | 348 | PRO |
| 40 | BE | 364 | PRO |
| 40 | BE | 438 | SER |
| 40 | BH | 38 | SER |
| 40 | BH | 39 | ASP |
| 40 | BH | 41 | THR |
| 40 | BH | 52 | PHE |
| 40 | BH | 72 | PRO |
| 40 | BH | 73 | THR |
| 40 | BH | 101 | ASN |
| 40 | BH | 163 | LYS |
| 40 | BH | 265 | ILE |
| 40 | BH | 309 | HIS |
| 40 | BH | 349 | THR |
| 40 | BH | 412 | MET |
| 40 | BI | 74 | VAL |
| 40 | BI | 85 | GLN |
| 40 | BI | 96 | LYS |
| 40 | BI | 114 | LEU |
| 40 | BI | 264 | ARG |
| 41 | BM | 98 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BM | 104 | GLY |
| 41 | BM | 111 | GLU |
| 41 | BM | 143 | THR |
| 41 | BM | 216 | LYS |
| 41 | BM | 271 | ALA |
| 41 | BO | 139 | LEU |
| 41 | BO | 271 | ALA |
| 41 | BO | 361 | LEU |
| 41 | BP | 67 | ASP |
| 41 | BP | 80 | PRO |
| 41 | BP | 92 | PHE |
| 41 | BP | 140 | GLY |
| 41 | BP | 158 | GLU |
| 41 | BP | 173 | PRO |
| 41 | BP | 259 | PRO |
| 41 | BP | 261 | PRO |
| 41 | BP | 262 | ARG |
| 41 | BP | 271 | ALA |
| 41 | BP | 394 | PHE |
| 40 | CA | 40 | LYS |
| 40 | CA | 61 | HIS |
| 40 | CA | 73 | THR |
| 40 | CA | 109 | THR |
| 40 | CA | 148 | GLY |
| 40 | CA | 160 | ASP |
| 40 | CA | 263 | PRO |
| 40 | CA | 265 | ILE |
| 40 | CA | 273 | ALA |
| 40 | CA | 438 | SER |
| 40 | CE | 51 | THR |
| 40 | CF | 73 | THR |
| 40 | CH | 51 | THR |
| 40 | CH | 59 | GLY |
| 40 | CH | 148 | GLY |
| 40 | CH | 242 | LEU |
| 40 | CH | 243 | ARG |
| 40 | CH | 265 | ILE |
| 40 | CH | 367 | LEU |
| 41 | CL | 146 | GLY |
| 41 | CL | 173 | PRO |
| 41 | CL | 197 | ASP |
| 41 | CL | 271 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CM | 107 | THR |
| 41 | CM | 162 | ARG |
| 41 | CM | 173 | PRO |
| 41 | CM | 271 | ALA |
| 41 | CN | 240 | LEU |
| 41 | CN | 241 | ARG |
| 41 | CN | 261 | PRO |
| 41 | CN | 271 | ALA |
| 41 | CO | 58 | LYS |
| 41 | CO | 82 | GLY |
| 41 | CO | 107 | THR |
| 41 | CO | 158 | GLU |
| 41 | CO | 173 | PRO |
| 41 | CO | 402 | GLY |
| 41 | CP | 97 | ALA |
| 41 | CP | 271 | ALA |
| 41 | CP | 293 | MET |
| 41 | CP | 302 | ALA |
| 41 | CP | 310 | TYR |
| 41 | CP | 323 | MET |
| 40 | DA | 83 | TYR |
| 40 | DA | 130 | THR |
| 40 | DA | 178 | SER |
| 40 | DA | 213 | CYS |
| 40 | DA | 216 | ASN |
| 40 | DA | 261 | PRO |
| 40 | DA | 265 | ILE |
| 40 | DA | 273 | ALA |
| 40 | DA | 357 | TYR |
| 40 | DA | 401 | ARG |
| 41 | DB | 97 | ALA |
| 41 | DB | 108 | GLU |
| 41 | DB | 130 | LEU |
| 41 | DB | 167 | PHE |
| 41 | DB | 174 | LYS |
| 41 | DB | 240 | LEU |
| 41 | DB | 339 | SER |
| 41 | DB | 347 | ASN |
| 40 | DE | 219 | ILE |
| 40 | DE | 240 | ALA |
| 40 | DE | 255 | PHE |
| 40 | DE | 281 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DE | 364 | PRO |
| 40 | DE | 406 | TRP |
| 40 | DE | 410 | GLU |
| 40 | DE | 411 | GLY |
| 40 | DF | 265 | ILE |
| 40 | DF | 364 | PRO |
| 40 | DH | 33 | ASP |
| 40 | DH | 38 | SER |
| 40 | DH | 87 | PHE |
| 40 | DH | 132 | LEU |
| 40 | DH | 160 | ASP |
| 40 | DH | 261 | PRO |
| 40 | DH | 365 | GLY |
| 40 | DI | 61 | HIS |
| 40 | DI | 72 | PRO |
| 40 | DI | 125 | LEU |
| 40 | DI | 161 | TYR |
| 40 | DI | 164 | LYS |
| 40 | DI | 248 | LEU |
| 40 | DI | 303 | VAL |
| 41 | DL | 95 | SER |
| 41 | DL | 144 | GLY |
| 41 | DL | 158 | GLU |
| 41 | DL | 182 | PRO |
| 41 | DL | 211 | CYS |
| 41 | DL | 213 | ARG |
| 41 | DL | 246 | LEU |
| 41 | DL | 311 | LEU |
| 41 | DL | 362 | LYS |
| 41 | DM | 173 | PRO |
| 41 | DM | 336 | LYS |
| 41 | DM | 347 | ASN |
| 41 | DM | 417 | ASP |
| 41 | DN | 29 | GLY |
| 41 | DN | 71 | GLY |
| 41 | DN | 99 | ASN |
| 41 | DN | 107 | THR |
| 41 | DN | 126 | SER |
| 41 | DN | 193 | VAL |
| 41 | DN | 294 | PHE |
| 41 | DP | 83 | GLN |
| 41 | DP | 99 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DP | 124 | ALA |
| 41 | DP | 139 | LEU |
| 41 | DP | 143 | THR |
| 41 | DP | 241 | ARG |
| 41 | DP | 259 | PRO |
| 41 | DP | 279 | GLN |
| 41 | DP | 283 | ALA |
| 41 | DP | 326 | VAL |
| 41 | DP | 347 | ASN |
| 41 | DP | 400 | GLY |
| 40 | EG | 73 | THR |
| 40 | EH | 105 | ARG |
| 40 | EH | 160 | ASP |
| 40 | EH | 162 | GLY |
| 40 | EH | 163 | LYS |
| 40 | EH | 258 | ASN |
| 40 | EH | 299 | ALA |
| 40 | EH | 348 | PRO |
| 40 | EH | 399 | ALA |
| 40 | EH | 411 | GLY |
| 40 | EI | 32 | PRO |
| 40 | EI | 37 | PRO |
| 40 | EI | 51 | THR |
| 40 | EI | 84 | ARG |
| 40 | EI | 90 | GLU |
| 40 | EI | 244 | PHE |
| 40 | EI | 248 | LEU |
| 40 | EI | 279 | GLU |
| 41 | EM | 88 | ASP |
| 41 | EM | 95 | SER |
| 41 | EM | 97 | ALA |
| 41 | EM | 99 | ASN |
| 41 | EM | 143 | THR |
| 41 | EM | 182 | PRO |
| 41 | EM | 184 | ASN |
| 41 | EM | 203 | ASP |
| 41 | EM | 271 | ALA |
| 41 | EM | 359 | ARG |
| 41 | EM | 377 | LEU |
| 41 | EM | 392 | LYS |
| 41 | EP | 160 | PRO |
| 41 | EP | 246 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | EP | 271 | ALA |
| 41 | EP | 284 | LEU |
| 41 | EP | 299 | MET |
| 41 | EP | 320 | ARG |
| 41 | EP | 359 | ARG |
| 41 | EP | 419 | GLY |
| 40 | FA | 50 | ASN |
| 40 | FA | 143 | GLY |
| 40 | FA | 175 | PRO |
| 40 | FA | 322 | ASP |
| 40 | FA | 348 | PRO |
| 40 | GE | 128 | GLN |
| 40 | GE | 178 | SER |
| 40 | GE | 273 | ALA |
| 40 | GE | 278 | ALA |
| 40 | GE | 286 | LEU |
| 40 | GE | 304 | LYS |
| 40 | GE | 305 | CYS |
| 40 | GE | 323 | VAL |
| 40 | GE | 360 | PRO |
| 40 | GE | 364 | PRO |
| 40 | GE | 411 | GLY |
| 40 | GH | 73 | THR |
| 40 | GH | 197 | HIS |
| 40 | GH | 264 | ARG |
| 40 | GH | 265 | ILE |
| 40 | GH | 289 | ALA |
| 40 | GH | 304 | LYS |
| 40 | GH | 339 | ARG |
| 40 | GH | 371 | GLN |
| 40 | GI | 73 | THR |
| 40 | GI | 259 | LEU |
| 40 | GI | 263 | PRO |
| 40 | GI | 286 | LEU |
| 41 | GM | 108 | GLU |
| 41 | GN | 50 | TYR |
| 41 | GN | 70 | PRO |
| 41 | GN | 94 | GLN |
| 41 | GN | 107 | THR |
| 41 | GN | 112 | LEU |
| 41 | GN | 158 | GLU |
| 41 | GN | 201 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | GN | 271 | ALA |
| 41 | GN | 394 | PHE |
| 40 | HE | 50 | ASN |
| 40 | HE | 201 | ALA |
| 40 | HE | 247 | ALA |
| 40 | HE | 278 | ALA |
| 40 | HE | 327 | ASP |
| 40 | HE | 381 | THR |
| 40 | HE | 382 | ALA |
| 41 | HN | 59 | TYR |
| 41 | HN | 94 | GLN |
| 41 | HN | 108 | GLU |
| 41 | HN | 173 | PRO |
| 41 | HN | 263 | LEU |
| 41 | HN | 271 | ALA |
| 41 | HN | 362 | LYS |
| 41 | HN | 392 | LYS |
| 41 | HN | 417 | ASP |
| 41 | IM | 108 | GLU |
| 41 | IN | 108 | GLU |
| 41 | JB | 195 | ASN |
| 41 | JM | 2 | ARG |
| 41 | JM | 130 | LEU |
| 41 | JM | 182 | PRO |
| 41 | JM | 271 | ALA |
| 41 | JM | 294 | PHE |
| 41 | JM | 303 | CYS |
| 41 | JM | 355 | ASP |
| 41 | JM | 427 | ALA |
| 41 | KB | 195 | ASN |
| 41 | KL | 174 | LYS |
| 41 | KL | 259 | PRO |
| 41 | KL | 271 | ALA |
| 41 | KL | 293 | MET |
| 41 | KL | 417 | ASP |
| 40 | LF | 111 | GLY |
| 40 | LF | 160 | ASP |
| 40 | LF | 161 | TYR |
| 40 | LF | 280 | LYS |
| 40 | LG | 100 | ALA |
| 40 | LG | 101 | ASN |
| 40 | LG | 110 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | LG | 161 | TYR |
| 40 | LG | 177 | VAL |
| 40 | LG | 302 | MET |
| 40 | LG | 304 | LYS |
| 40 | LG | 364 | PRO |
| 40 | MA | 49 | PHE |
| 40 | MA | 259 | LEU |
| 40 | MD | 279 | GLU |
| 40 | MD | 280 | LYS |
| 40 | MF | 72 | PRO |
| 40 | MF | 141 | PHE |
| 40 | MF | 403 | PHE |
| 40 | MG | 59 | GLY |
| 40 | MG | 161 | TYR |
| 40 | MG | 259 | LEU |
| 40 | MG | 304 | LYS |
| 40 | MG | 348 | PRO |
| 40 | MH | 109 | THR |
| 40 | MH | 161 | TYR |
| 40 | MH | 348 | PRO |
| 40 | MH | 364 | PRO |
| 41 | MO | 70 | PRO |
| 41 | MO | 80 | PRO |
| 41 | MO | 143 | THR |
| 41 | MO | 174 | LYS |
| 41 | MO | 259 | PRO |
| 41 | MO | 302 | ALA |
| 40 | ND | 12 | ALA |
| 40 | ND | 61 | HIS |
| 40 | ND | 64 | ARG |
| 40 | ND | 96 | LYS |
| 40 | ND | 132 | LEU |
| 40 | ND | 141 | PHE |
| 40 | ND | 194 | THR |
| 40 | ND | 364 | PRO |
| 40 | ND | 411 | GLY |
| 40 | OD | 82 | THR |
| 40 | OD | 84 | ARG |
| 40 | OH | 61 | HIS |
| 40 | OH | 63 | PRO |
| 40 | OH | 97 | GLU |
| 40 | OH | 148 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OH | 364 | PRO |
| 40 | OH | 407 | TYR |
| 40 | PA | 103 | TYR |
| 40 | PG | 178 | SER |
| 41 | PP | 195 | ASN |
| 41 | QB | 2 | ARG |
| 41 | QB | 88 | ASP |
| 41 | QB | 121 | ARG |
| 41 | QB | 129 | CYS |
| 41 | QB | 271 | ALA |
| 41 | QB | 277 | GLY |
| 41 | QB | 326 | VAL |
| 41 | QB | 400 | GLY |
| 41 | QB | 402 | GLY |
| 41 | QL | 195 | ASN |
| 41 | QP | 11 | GLN |
| 41 | QP | 37 | HIS |
| 41 | QP | 50 | TYR |
| 41 | QP | 124 | ALA |
| 41 | QP | 126 | SER |
| 41 | QP | 151 | LEU |
| 41 | QP | 183 | TYR |
| 41 | QP | 303 | CYS |
| 41 | QP | 335 | ASN |
| 41 | QP | 384 | GLN |
| 41 | QP | 385 | PHE |
| 41 | RB | 108 | GLU |
| 40 | RI | 178 | SER |
| 41 | RL | 143 | THR |
| 41 | RP | 143 | THR |
| 41 | RP | 195 | ASN |
| 40 | SA | 248 | LEU |
| 40 | SA | 256 | GLN |
| 40 | SG | 278 | ALA |
| 41 | SO | 49 | VAL |
| 41 | SO | 87 | PRO |
| 41 | SO | 99 | ASN |
| 41 | SO | 104 | GLY |
| 41 | SO | 174 | LYS |
| 41 | SO | 198 | GLU |
| 41 | SO | 252 | LYS |
| 41 | SO | 255 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | SO | 299 | MET |
| 41 | SO | 359 | ARG |
| 40 | TI | 58 | ALA |
| 40 | UA | 27 | GLU |
| 40 | UF | 106 | GLY |
| 40 | UF | 109 | THR |
| 40 | UF | 130 | THR |
| 40 | UF | 192 | HIS |
| 40 | UF | 214 | ARG |
| 40 | UF | 220 | GLU |
| 40 | UF | 256 | GLN |
| 40 | UF | 263 | PRO |
| 40 | UF | 273 | ALA |
| 40 | UF | 338 | LYS |
| 40 | UF | 403 | PHE |
| 40 | UI | 49 | PHE |
| 40 | UI | 160 | ASP |
| 40 | UI | 161 | TYR |
| 40 | UI | 168 | GLU |
| 40 | UI | 273 | ALA |
| 40 | UI | 350 | GLY |
| 41 | UP | 80 | PRO |
| 41 | UP | 126 | SER |
| 41 | UP | 144 | GLY |
| 41 | UP | 184 | ASN |
| 41 | UP | 259 | PRO |
| 41 | UP | 323 | MET |
| 41 | UP | 417 | ASP |
| 40 | VA | 41 | THR |
| 40 | VF | 40 | LYS |
| 40 | VH | 38 | SER |
| 41 | WM | 80 | PRO |
| 41 | WM | 102 | ALA |
| 41 | WM | 301 | ALA |
| 41 | WN | 80 | PRO |
| 41 | WN | 94 | GLN |
| 41 | WN | 129 | CYS |
| 41 | WN | 297 | LYS |
| 41 | WN | 347 | ASN |
| 3 | 1G | 219 | PRO |
| 3 | 1G | 244 | SER |
| 3 | 1G | 252 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 1S | 577 | GLY |
| 7 | 1T | 62 | GLY |
| 7 | 1T | 227 | GLY |
| 7 | 1T | 448 | HIS |
| 7 | 1T | 501 | ALA |
| 7 | 1T | 574 | TYR |
| 11 | 2J | 248 | LYS |
| 11 | 2K | 216 | VAL |
| 13 | 2T | 74 | PRO |
| 13 | 2T | 103 | PHE |
| 13 | 2T | 169 | ASP |
| 13 | 2U | 75 | PHE |
| 13 | 2U | 116 | PRO |
| 13 | 2U | 120 | THR |
| 13 | 2U | 126 | ASP |
| 13 | 2V | 52 | THR |
| 13 | 2W | 41 | ASP |
| 13 | 2X | 54 | VAL |
| 16 | 3J | 351 | ALA |
| 17 | 3O | 408 | ASN |
| 17 | 3P | 212 | HIS |
| 17 | 3Q | 470 | GLN |
| 17 | 3R | 253 | GLU |
| 17 | 3R | 279 | ASP |
| 17 | 3R | 320 | LYS |
| 17 | 3R | 350 | ARG |
| 21 | 4D | 414 | MET |
| 21 | 4D | 427 | GLU |
| 21 | 4D | 428 | SER |
| 21 | 4D | 458 | ASN |
| 21 | 4D | 475 | PRO |
| 21 | 4E | 338 | LEU |
| 21 | 4E | 414 | MET |
| 21 | 4F | 428 | SER |
| 21 | 4F | 429 | PRO |
| 22 | 4I | 616 | THR |
| 22 | 4I | 648 | GLU |
| 22 | 4J | 56 | LYS |
| 22 | 4J | 571 | CYS |
| 22 | 4J | 643 | VAL |
| 22 | 4J | 672 | ASP |
| 22 | 4J | 676 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 4K | 555 | GLU |
| 22 | 4K | 633 | GLU |
| 22 | 4K | 634 | ASN |
| 23 | 4M | 35 | GLN |
| 23 | 4M | 261 | TYR |
| 23 | 4N | 20 | PRO |
| 23 | 4N | 216 | MET |
| 23 | 4N | 242 | LEU |
| 24 | 4O | 243 | LEU |
| 23 | 4P | 242 | LEU |
| 23 | 4Q | 176 | ASP |
| 23 | 4Q | 184 | MET |
| 23 | 4Q | 235 | THR |
| 23 | 4Q | 242 | LEU |
| 23 | 4R | 103 | PHE |
| 23 | 4R | 105 | PHE |
| 23 | 4R | 243 | LEU |
| 26 | 4W | 238 | ASN |
| 31 | 5I | 683 | TYR |
| 34 | 5R | 361 | ASP |
| 36 | 5W | 166 | MET |
| 36 | 5X | 26 | ILE |
| 36 | 5X | 36 | VAL |
| 36 | 5Y | 39 | ILE |
| 38 | 6D | 288 | VAL |
| 39 | 6F | 118 | LYS |
| 39 | 6L | 136 | TYR |
| 41 | AO | 83 | GLN |
| 41 | AO | 161 | ASP |
| 41 | AO | 241 | ARG |
| 41 | AO | 254 | ALA |
| 41 | BB | 174 | LYS |
| 41 | BB | 402 | GLY |
| 40 | BE | 341 | ILE |
| 40 | BH | 114 | LEU |
| 40 | BH | 273 | ALA |
| 40 | BH | 325 | PRO |
| 40 | BI | 84 | ARG |
| 40 | BI | 364 | PRO |
| 41 | BL | 195 | ASN |
| 41 | BM | 92 | PHE |
| 41 | BM | 356 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BO | 95 | SER |
| 41 | BO | 108 | GLU |
| 41 | BO | 214 | THR |
| 41 | BO | 259 | PRO |
| 41 | BP | 292 | GLN |
| 40 | CA | 60 | LYS |
| 40 | CA | 140 | SER |
| 40 | CA | 202 | PHE |
| 40 | CA | 281 | ALA |
| 40 | CH | 58 | ALA |
| 40 | CH | 278 | ALA |
| 40 | CH | 300 | ASN |
| 40 | CH | 438 | SER |
| 41 | CL | 106 | TYR |
| 41 | CL | 160 | PRO |
| 41 | CL | 183 | TYR |
| 41 | CL | 240 | LEU |
| 41 | CL | 259 | PRO |
| 41 | CL | 385 | PHE |
| 41 | CM | 34 | GLY |
| 41 | CM | 39 | ASP |
| 41 | CM | 80 | PRO |
| 41 | CM | 174 | LYS |
| 41 | CN | 268 | PRO |
| 41 | CN | 392 | LYS |
| 41 | CN | 394 | PHE |
| 41 | CO | 89 | ASN |
| 41 | CO | 97 | ALA |
| 41 | CO | 181 | GLU |
| 41 | CO | 241 | ARG |
| 41 | CO | 243 | PRO |
| 41 | CO | 363 | MET |
| 41 | CP | 239 | CYS |
| 41 | CP | 256 | ASN |
| 41 | CP | 259 | PRO |
| 41 | CP | 294 | PHE |
| 41 | CP | 301 | ALA |
| 41 | CP | 303 | CYS |
| 41 | CP | 392 | LYS |
| 41 | CP | 420 | ASN |
| 40 | DA | 82 | THR |
| 40 | DA | 100 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DA | 109 | THR |
| 40 | DA | 279 | GLU |
| 40 | DA | 305 | CYS |
| 40 | DA | 438 | SER |
| 41 | DB | 46 | ARG |
| 41 | DB | 88 | ASP |
| 41 | DB | 104 | GLY |
| 41 | DB | 162 | ARG |
| 41 | DB | 173 | PRO |
| 41 | DB | 211 | CYS |
| 40 | DE | 64 | ARG |
| 40 | DE | 100 | ALA |
| 40 | DE | 159 | VAL |
| 40 | DE | 242 | LEU |
| 40 | DF | 91 | GLN |
| 40 | DF | 116 | ASP |
| 40 | DH | 100 | ALA |
| 40 | DH | 335 | ILE |
| 40 | DH | 339 | ARG |
| 40 | DH | 438 | SER |
| 40 | DI | 15 | GLN |
| 40 | DI | 155 | GLU |
| 40 | DI | 270 | ALA |
| 40 | DI | 350 | GLY |
| 41 | DL | 59 | TYR |
| 41 | DL | 121 | ARG |
| 41 | DL | 131 | GLN |
| 41 | DL | 195 | ASN |
| 41 | DL | 262 | ARG |
| 41 | DL | 293 | MET |
| 41 | DL | 307 | HIS |
| 41 | DL | 347 | ASN |
| 41 | DM | 311 | LEU |
| 41 | DM | 335 | ASN |
| 41 | DM | 339 | SER |
| 41 | DM | 422 | VAL |
| 41 | DN | 123 | GLU |
| 41 | DN | 127 | CYS |
| 41 | DN | 128 | ASP |
| 41 | DN | 162 | ARG |
| 41 | DN | 182 | PRO |
| 41 | DN | 212 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DN | 240 | LEU |
| 41 | DN | 292 | GLN |
| 41 | DP | 87 | PRO |
| 41 | DP | 238 | THR |
| 40 | EH | 90 | GLU |
| 40 | EH | 99 | ALA |
| 40 | EH | 178 | SER |
| 40 | EH | 195 | LEU |
| 40 | EH | 326 | LYS |
| 40 | EH | 438 | SER |
| 40 | EI | 38 | SER |
| 40 | EI | 130 | THR |
| 40 | EI | 187 | SER |
| 40 | EI | 278 | ALA |
| 40 | EI | 301 | GLN |
| 40 | EI | 400 | LYS |
| 41 | EM | 27 | GLU |
| 41 | EM | 126 | SER |
| 41 | EM | 134 | GLN |
| 41 | EM | 248 | ALA |
| 41 | EM | 299 | MET |
| 41 | EP | 96 | GLY |
| 41 | EP | 402 | GLY |
| 40 | FA | 109 | THR |
| 40 | FA | 169 | PHE |
| 40 | FA | 403 | PHE |
| 40 | GE | 27 | GLU |
| 40 | GE | 72 | PRO |
| 40 | GE | 176 | GLN |
| 40 | GE | 215 | ARG |
| 40 | GH | 37 | PRO |
| 40 | GH | 259 | LEU |
| 40 | GI | 32 | PRO |
| 40 | GI | 106 | GLY |
| 40 | GI | 175 | PRO |
| 40 | GI | 367 | LEU |
| 40 | GI | 412 | MET |
| 41 | GN | 71 | GLY |
| 41 | GN | 108 | GLU |
| 41 | GN | 160 | PRO |
| 41 | GN | 249 | ASP |
| 41 | GN | 259 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | GN | 277 | GLY |
| 41 | GN | 355 | ASP |
| 41 | HB | 108 | GLU |
| 40 | HE | 27 | GLU |
| 40 | HE | 47 | ASP |
| 40 | HE | 100 | ALA |
| 40 | HE | 142 | GLY |
| 40 | HE | 248 | LEU |
| 40 | HE | 304 | LYS |
| 40 | HE | 367 | LEU |
| 41 | HN | 70 | PRO |
| 41 | HN | 90 | PHE |
| 41 | HN | 160 | PRO |
| 41 | HN | 261 | PRO |
| 41 | HN | 284 | LEU |
| 41 | IB | 195 | ASN |
| 40 | IE | 178 | SER |
| 41 | IQ | 195 | ASN |
| 41 | JM | 29 | GLY |
| 41 | JM | 102 | ALA |
| 41 | JM | 124 | ALA |
| 41 | JM | 128 | ASP |
| 41 | JM | 143 | THR |
| 41 | JM | 158 | GLU |
| 41 | JN | 195 | ASN |
| 41 | KL | 71 | GLY |
| 41 | KL | 195 | ASN |
| 41 | KL | 306 | ARG |
| 41 | KL | 394 | PHE |
| 40 | LF | 73 | THR |
| 40 | LF | 105 | ARG |
| 40 | LF | 131 | GLY |
| 40 | LF | 349 | THR |
| 40 | LG | 73 | THR |
| 40 | LG | 265 | ILE |
| 40 | LG | 306 | ASP |
| 40 | LG | 414 | GLU |
| 41 | LM | 195 | ASN |
| 40 | MA | 247 | ALA |
| 40 | MA | 412 | MET |
| 40 | MD | 278 | ALA |
| 40 | MF | 257 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MF | 278 | ALA |
| 40 | MG | 73 | THR |
| 40 | MG | 273 | ALA |
| 40 | MG | 434 | VAL |
| 40 | MH | 261 | PRO |
| 40 | MH | 322 | ASP |
| 41 | MO | 34 | GLY |
| 41 | MO | 40 | SER |
| 41 | MO | 71 | GLY |
| 41 | MO | 347 | ASN |
| 40 | ND | 72 | PRO |
| 40 | ND | 133 | GLN |
| 40 | ND | 282 | TYR |
| 40 | ND | 283 | HIS |
| 40 | ND | 357 | TYR |
| 40 | ND | 367 | LEU |
| 41 | NO | 108 | GLU |
| 40 | OH | 60 | LYS |
| 40 | OH | 83 | TYR |
| 40 | OH | 144 | GLY |
| 40 | OH | 195 | LEU |
| 40 | OH | 317 | LEU |
| 40 | OH | 437 | ASP |
| 41 | OL | 108 | GLU |
| 41 | PB | 196 | THR |
| 41 | QB | 49 | VAL |
| 41 | QB | 108 | GLU |
| 41 | QB | 193 | VAL |
| 41 | QB | 195 | ASN |
| 41 | QB | 291 | GLN |
| 41 | QB | 296 | ALA |
| 41 | QB | 359 | ARG |
| 41 | QP | 129 | CYS |
| 41 | QP | 152 | ILE |
| 41 | QP | 189 | VAL |
| 41 | QP | 291 | GLN |
| 41 | QP | 313 | VAL |
| 41 | QP | 424 | THR |
| 41 | SO | 92 | PHE |
| 41 | SO | 107 | THR |
| 41 | SO | 226 | ASN |
| 41 | SO | 340 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | SO | 377 | LEU |
| 41 | SO | 417 | ASP |
| 40 | TG | 38 | SER |
| 40 | UF | 50 | ASN |
| 40 | UF | 72 | PRO |
| 40 | UF | 73 | THR |
| 40 | UF | 160 | ASP |
| 40 | UF | 176 | GLN |
| 40 | UF | 184 | PRO |
| 40 | UF | 243 | ARG |
| 40 | UF | 433 | GLU |
| 40 | UF | 437 | ASP |
| 40 | UI | 56 | THR |
| 40 | UI | 74 | VAL |
| 40 | UI | 364 | PRO |
| 41 | UP | 41 | ASP |
| 41 | UP | 146 | GLY |
| 41 | UP | 275 | SER |
| 41 | VB | 195 | ASN |
| 40 | VF | 46 | ASP |
| 41 | WM | 174 | LYS |
| 41 | WM | 212 | PHE |
| 41 | WM | 246 | LEU |
| 41 | WN | 90 | PHE |
| 41 | WN | 104 | GLY |
| 41 | WN | 130 | LEU |
| 41 | WN | 160 | PRO |
| 41 | WN | 174 | LYS |
| 41 | WN | 259 | PRO |
| 41 | WN | 420 | ASN |
| 3 | 1G | 74 | GLU |
| 3 | 1G | 107 | ILE |
| 3 | 1G | 160 | PHE |
| 3 | 1G | 174 | GLU |
| 3 | 1G | 243 | LYS |
| 5 | 1L | 280 | ASN |
| 5 | 1M | 134 | LYS |
| 7 | 1S | 240 | ALA |
| 7 | 1S | 576 | GLU |
| 7 | 1S | 579 | VAL |
| 8 | 1X | 83 | ASP |
| 8 | 1Z | 528 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | 2O | 98 | VAL |
| 13 | 2U | 41 | ASP |
| 13 | 2V | 126 | ASP |
| 13 | 2W | 52 | THR |
| 13 | 2X | 172 | TYR |
| 16 | 3K | 325 | PRO |
| 17 | 3P | 297 | PRO |
| 17 | 3R | 165 | ASP |
| 17 | 3R | 265 | TYR |
| 20 | 4A | 177 | ASP |
| 21 | 4D | 466 | TYR |
| 21 | 4E | 429 | PRO |
| 21 | 4E | 445 | ALA |
| 21 | 4E | 481 | ASN |
| 21 | 4E | 496 | ILE |
| 21 | 4F | 414 | MET |
| 21 | 4F | 415 | ASN |
| 21 | 4F | 458 | ASN |
| 21 | 4F | 478 | SER |
| 21 | 4F | 531 | ILE |
| 22 | 4H | 17 | LYS |
| 22 | 4I | 677 | LEU |
| 22 | 4J | 668 | PRO |
| 22 | 4J | 684 | SER |
| 22 | 4K | 556 | GLU |
| 23 | 4M | 117 | LEU |
| 23 | 4M | 254 | LYS |
| 23 | 4N | 55 | PRO |
| 23 | 4N | 60 | LEU |
| 23 | 4N | 92 | PRO |
| 23 | 4N | 116 | ALA |
| 23 | 4N | 179 | PRO |
| 23 | 4N | 203 | PRO |
| 23 | 4N | 262 | GLY |
| 23 | 4P | 262 | GLY |
| 23 | 4Q | 175 | ASP |
| 23 | 4Q | 185 | SER |
| 23 | 4R | 16 | PRO |
| 23 | 4R | 100 | GLN |
| 23 | 4R | 112 | VAL |
| 23 | 4R | 251 | PRO |
| 27 | 4Z | 106 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 31 | 5I | 687 | ILE |
| 35 | 5T | 103 | ASN |
| 36 | 5X | 166 | MET |
| 37 | 6A | 81 | LYS |
| 39 | 6G | 118 | LYS |
| 41 | AO | 84 | ILE |
| 41 | BB | 263 | LEU |
| 41 | BB | 361 | LEU |
| 41 | BB | 420 | ASN |
| 40 | BE | 109 | THR |
| 40 | BE | 142 | GLY |
| 40 | BF | 178 | SER |
| 40 | BH | 178 | SER |
| 40 | BH | 263 | PRO |
| 40 | BH | 326 | LYS |
| 40 | BH | 436 | MET |
| 40 | BI | 100 | ALA |
| 40 | BI | 309 | HIS |
| 41 | BM | 80 | PRO |
| 41 | BM | 96 | GLY |
| 41 | BM | 304 | ASP |
| 41 | BO | 210 | ILE |
| 41 | BO | 268 | PRO |
| 41 | BO | 394 | PHE |
| 40 | CA | 178 | SER |
| 40 | CE | 52 | PHE |
| 40 | CH | 100 | ALA |
| 40 | CH | 109 | THR |
| 40 | CH | 273 | ALA |
| 40 | CH | 436 | MET |
| 41 | CL | 108 | GLU |
| 41 | CL | 145 | SER |
| 41 | CL | 353 | VAL |
| 41 | CM | 87 | PRO |
| 41 | CM | 99 | ASN |
| 41 | CM | 263 | LEU |
| 41 | CM | 304 | ASP |
| 41 | CM | 347 | ASN |
| 41 | CM | 358 | PRO |
| 41 | CN | 320 | ARG |
| 41 | CO | 29 | GLY |
| 41 | CO | 68 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CO | 75 | SER |
| 41 | CO | 124 | ALA |
| 41 | CO | 183 | TYR |
| 41 | CO | 316 | VAL |
| 41 | CO | 421 | PRO |
| 41 | CP | 225 | LEU |
| 40 | DA | 191 | THR |
| 40 | DA | 252 | LEU |
| 40 | DA | 255 | PHE |
| 40 | DA | 283 | HIS |
| 40 | DA | 328 | VAL |
| 40 | DA | 403 | PHE |
| 41 | DB | 123 | GLU |
| 41 | DB | 216 | LYS |
| 41 | DB | 259 | PRO |
| 41 | DB | 272 | PRO |
| 41 | DB | 340 | TYR |
| 40 | DE | 74 | VAL |
| 40 | DE | 89 | PRO |
| 40 | DE | 105 | ARG |
| 40 | DE | 139 | HIS |
| 40 | DE | 185 | TYR |
| 40 | DE | 248 | LEU |
| 40 | DE | 283 | HIS |
| 40 | DE | 401 | ARG |
| 40 | DE | 405 | HIS |
| 40 | DF | 4 | CYS |
| 40 | DF | 109 | THR |
| 40 | DF | 243 | ARG |
| 40 | DF | 253 | THR |
| 40 | DF | 259 | LEU |
| 40 | DF | 264 | ARG |
| 40 | DF | 358 | GLN |
| 40 | DF | 359 | PRO |
| 40 | DF | 408 | VAL |
| 40 | DH | 37 | PRO |
| 40 | DH | 66 | VAL |
| 40 | DH | 110 | ILE |
| 40 | DH | 188 | ILE |
| 40 | DH | 364 | PRO |
| 40 | DH | 436 | MET |
| 40 | DI | 175 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DI | 185 | TYR |
| 40 | DI | 274 | PRO |
| 40 | DI | 365 | GLY |
| 41 | DL | 42 | LEU |
| 41 | DL | 83 | GLN |
| 41 | DL | 123 | GLU |
| 41 | DL | 271 | ALA |
| 41 | DL | 272 | PRO |
| 41 | DL | 287 | PRO |
| 41 | DL | 294 | PHE |
| 41 | DM | 83 | GLN |
| 41 | DM | 195 | ASN |
| 41 | DM | 342 | VAL |
| 41 | DM | 392 | LYS |
| 41 | DM | 421 | PRO |
| 41 | DN | 95 | SER |
| 41 | DN | 129 | CYS |
| 41 | DN | 183 | TYR |
| 41 | DN | 197 | ASP |
| 41 | DN | 211 | CYS |
| 41 | DN | 347 | ASN |
| 41 | DP | 49 | VAL |
| 41 | DP | 88 | ASP |
| 41 | DP | 107 | THR |
| 41 | DP | 271 | ALA |
| 40 | EH | 29 | GLY |
| 40 | EH | 256 | GLN |
| 40 | EH | 386 | ALA |
| 40 | EH | 410 | GLU |
| 40 | EI | 52 | PHE |
| 40 | EI | 116 | ASP |
| 40 | EI | 216 | ASN |
| 41 | EM | 89 | ASN |
| 41 | EM | 96 | GLY |
| 41 | EM | 254 | ALA |
| 41 | EP | 80 | PRO |
| 41 | EP | 87 | PRO |
| 41 | EP | 90 | PHE |
| 41 | EP | 210 | ILE |
| 40 | FA | 178 | SER |
| 40 | FA | 279 | GLU |
| 40 | FF | 178 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GE | 265 | ILE |
| 40 | GE | 280 | LYS |
| 40 | GG | 278 | ALA |
| 40 | GH | 89 | PRO |
| 40 | GH | 273 | ALA |
| 40 | GH | 280 | LYS |
| 40 | GH | 312 | TYR |
| 40 | GI | 333 | ALA |
| 40 | GI | 364 | PRO |
| 41 | GN | 57 | GLY |
| 41 | GN | 287 | PRO |
| 40 | HE | 37 | PRO |
| 40 | HE | 263 | PRO |
| 40 | HE | 273 | ALA |
| 40 | HE | 411 | GLY |
| 40 | HH | 178 | SER |
| 41 | HM | 108 | GLU |
| 41 | HN | 92 | PHE |
| 41 | HN | 304 | ASP |
| 41 | JM | 70 | PRO |
| 41 | JM | 420 | ASN |
| 40 | KD | 33 | ASP |
| 41 | KL | 163 | ILE |
| 41 | KL | 182 | PRO |
| 41 | KL | 214 | THR |
| 41 | KL | 401 | GLU |
| 40 | LF | 37 | PRO |
| 40 | LF | 103 | TYR |
| 40 | LG | 38 | SER |
| 40 | LG | 411 | GLY |
| 40 | MF | 160 | ASP |
| 40 | MF | 178 | SER |
| 40 | MF | 439 | VAL |
| 40 | MH | 281 | ALA |
| 41 | MO | 241 | ARG |
| 40 | ND | 32 | PRO |
| 40 | ND | 287 | SER |
| 40 | ND | 398 | TYR |
| 40 | ND | 414 | GLU |
| 40 | NE | 178 | SER |
| 40 | OD | 93 | ILE |
| 40 | OE | 178 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OG | 178 | SER |
| 40 | OH | 52 | PHE |
| 40 | OH | 70 | LEU |
| 40 | OH | 218 | ASP |
| 40 | OH | 277 | SER |
| 40 | PA | 72 | PRO |
| 40 | PA | 110 | ILE |
| 41 | QB | 61 | PRO |
| 41 | QB | 158 | GLU |
| 41 | QB | 218 | THR |
| 41 | QB | 246 | LEU |
| 41 | QB | 253 | LEU |
| 41 | QB | 263 | LEU |
| 41 | QB | 362 | LYS |
| 41 | QM | 108 | GLU |
| 41 | QO | 108 | GLU |
| 41 | QP | 43 | GLN |
| 41 | QP | 51 | TYR |
| 41 | QP | 83 | GLN |
| 41 | QP | 114 | ASP |
| 41 | QP | 156 | ARG |
| 41 | QP | 377 | LEU |
| 41 | RN | 195 | ASN |
| 40 | SA | 178 | SER |
| 40 | SA | 259 | LEU |
| 40 | SA | 263 | PRO |
| 41 | SB | 394 | PHE |
| 41 | SB | 397 | TRP |
| 41 | SO | 261 | PRO |
| 41 | SO | 322 | SER |
| 41 | SO | 344 | TRP |
| 41 | TB | 108 | GLU |
| 40 | TF | 178 | SER |
| 41 | TL | 195 | ASN |
| 40 | UF | 49 | PHE |
| 40 | UF | 178 | SER |
| 40 | UI | 12 | ALA |
| 40 | UI | 190 | THR |
| 40 | UI | 268 | PRO |
| 40 | UI | 271 | THR |
| 40 | UI | 353 | VAL |
| 40 | UI | 370 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | UP | 192 | LEU |
| 41 | UP | 377 | LEU |
| 41 | UP | 379 | LYS |
| 40 | VA | 39 | ASP |
| 40 | VG | 178 | SER |
| 41 | WM | 139 | LEU |
| 41 | WM | 338 | SER |
| 41 | WN | 35 | THR |
| 7 | 1T | 76 | GLY |
| 7 | 1U | 244 | PRO |
| 12 | 2O | 49 | LYS |
| 17 | 3R | 113 | SER |
| 17 | 3R | 324 | ASP |
| 20 | 4A | 42 | VAL |
| 21 | 4D | 500 | GLY |
| 21 | 4E | 488 | SER |
| 22 | 4J | 276 | SER |
| 22 | 4J | 633 | GLU |
| 22 | 4J | 681 | PHE |
| 22 | 4J | 697 | LEU |
| 23 | 4M | 243 | LEU |
| 23 | 4N | 254 | LYS |
| 23 | 4P | 198 | PHE |
| 23 | 4P | 254 | LYS |
| 23 | 4Q | 179 | PRO |
| 23 | 4Q | 181 | LYS |
| 26 | 4V | 374 | ILE |
| 31 | 5I | 386 | GLN |
| 34 | 5Q | 119 | LYS |
| 36 | 5X | 108 | PRO |
| 36 | 5Y | 131 | VAL |
| 38 | 6C | 156 | ASN |
| 40 | AE | 178 | SER |
| 40 | AG | 178 | SER |
| 41 | AO | 259 | PRO |
| 41 | BB | 182 | PRO |
| 40 | BE | 288 | VAL |
| 40 | BE | 298 | PRO |
| 40 | BE | 306 | ASP |
| 40 | BH | 338 | LYS |
| 40 | BI | 370 | VAL |
| 41 | BM | 47 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BM | 53 | GLU |
| 41 | BM | 95 | SER |
| 41 | BM | 355 | ASP |
| 41 | BO | 99 | ASN |
| 41 | BO | 175 | VAL |
| 41 | BO | 352 | ALA |
| 41 | BO | 422 | VAL |
| 40 | CA | 304 | LYS |
| 40 | CA | 399 | ALA |
| 40 | CH | 405 | HIS |
| 41 | CL | 107 | THR |
| 41 | CL | 182 | PRO |
| 41 | CL | 347 | ASN |
| 41 | CM | 29 | GLY |
| 41 | CM | 55 | THR |
| 41 | CM | 268 | PRO |
| 41 | CM | 417 | ASP |
| 41 | CN | 29 | GLY |
| 41 | CN | 146 | GLY |
| 41 | CN | 171 | PRO |
| 41 | CN | 212 | PHE |
| 41 | CO | 271 | ALA |
| 41 | CP | 91 | VAL |
| 41 | CP | 107 | THR |
| 40 | DA | 141 | PHE |
| 40 | DA | 176 | GLN |
| 40 | DA | 179 | THR |
| 40 | DA | 298 | PRO |
| 41 | DB | 139 | LEU |
| 41 | DB | 182 | PRO |
| 40 | DF | 159 | VAL |
| 40 | DF | 328 | VAL |
| 40 | DH | 184 | PRO |
| 40 | DH | 185 | TYR |
| 40 | DH | 222 | PRO |
| 40 | DH | 273 | ALA |
| 40 | DI | 222 | PRO |
| 41 | DL | 46 | ARG |
| 41 | DL | 57 | GLY |
| 41 | DL | 184 | ASN |
| 41 | DL | 189 | VAL |
| 41 | DL | 239 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DL | 335 | ASN |
| 41 | DL | 344 | TRP |
| 41 | DM | 57 | GLY |
| 41 | DM | 271 | ALA |
| 41 | DM | 297 | LYS |
| 41 | DM | 420 | ASN |
| 41 | DN | 174 | LYS |
| 41 | DN | 311 | LEU |
| 41 | DP | 81 | PHE |
| 41 | DP | 127 | CYS |
| 41 | DP | 128 | ASP |
| 40 | EA | 178 | SER |
| 41 | EB | 108 | GLU |
| 40 | EE | 178 | SER |
| 40 | EH | 49 | PHE |
| 40 | EH | 125 | LEU |
| 40 | EH | 325 | PRO |
| 40 | EI | 142 | GLY |
| 40 | EI | 178 | SER |
| 41 | EM | 180 | VAL |
| 41 | EM | 284 | LEU |
| 40 | FA | 153 | LEU |
| 40 | GA | 32 | PRO |
| 41 | GB | 347 | ASN |
| 40 | GE | 37 | PRO |
| 40 | GE | 89 | PRO |
| 40 | GE | 197 | HIS |
| 40 | GF | 178 | SER |
| 40 | GF | 278 | ALA |
| 40 | GG | 178 | SER |
| 40 | GG | 364 | PRO |
| 40 | GI | 85 | GLN |
| 40 | GI | 438 | SER |
| 41 | GN | 173 | PRO |
| 41 | GN | 182 | PRO |
| 41 | HN | 212 | PHE |
| 41 | JM | 261 | PRO |
| 41 | JM | 295 | ASP |
| 41 | KL | 54 | ALA |
| 40 | LF | 80 | THR |
| 40 | LF | 178 | SER |
| 40 | LG | 365 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MA | 273 | ALA |
| 40 | MA | 340 | SER |
| 40 | MA | 431 | TYR |
| 40 | MH | 141 | PHE |
| 40 | MH | 259 | LEU |
| 40 | MH | 412 | MET |
| 41 | MM | 108 | GLU |
| 41 | OB | 108 | GLU |
| 40 | OH | 29 | GLY |
| 40 | OH | 308 | ARG |
| 41 | OO | 108 | GLU |
| 41 | QB | 32 | PRO |
| 41 | QB | 182 | PRO |
| 41 | QB | 420 | ASN |
| 41 | QN | 108 | GLU |
| 41 | QP | 32 | PRO |
| 40 | RH | 29 | GLY |
| 40 | SE | 178 | SER |
| 41 | SO | 248 | ALA |
| 41 | SO | 421 | PRO |
| 40 | TH | 178 | SER |
| 40 | UF | 101 | ASN |
| 40 | UF | 350 | GLY |
| 40 | UI | 82 | THR |
| 41 | UP | 29 | GLY |
| 41 | UP | 316 | VAL |
| 41 | UP | 338 | SER |
| 40 | VA | 178 | SER |
| 41 | WN | 326 | VAL |
| 13 | 2X | 21 | PRO |
| 20 | 4A | 176 | ILE |
| 23 | 4N | 243 | LEU |
| 23 | 4P | 243 | LEU |
| 23 | 4Q | 16 | PRO |
| 34 | 5R | 336 | ILE |
| 36 | 5W | 131 | VAL |
| 38 | 6C | 29 | VAL |
| 40 | BE | 144 | GLY |
| 41 | BP | 146 | GLY |
| 40 | CA | 348 | PRO |
| 40 | CA | 408 | VAL |
| 40 | CH | 146 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CH | 184 | PRO |
| 41 | CL | 189 | VAL |
| 41 | CO | 259 | PRO |
| 41 | CO | 422 | VAL |
| 41 | CP | 84 | ILE |
| 41 | CP | 104 | GLY |
| 40 | DA | 32 | PRO |
| 41 | DB | 349 | VAL |
| 40 | DF | 32 | PRO |
| 40 | DI | 358 | GLN |
| 41 | DP | 193 | VAL |
| 40 | EI | 72 | PRO |
| 40 | FA | 74 | VAL |
| 40 | GE | 74 | VAL |
| 40 | GI | 66 | VAL |
| 41 | GO | 272 | PRO |
| 40 | HE | 106 | GLY |
| 40 | HE | 177 | VAL |
| 41 | HN | 104 | GLY |
| 41 | HN | 163 | ILE |
| 40 | LF | 34 | GLY |
| 40 | LF | 74 | VAL |
| 40 | LF | 411 | GLY |
| 40 | LG | 30 | ILE |
| 40 | MA | 341 | ILE |
| 40 | MF | 250 | VAL |
| 40 | MH | 89 | PRO |
| 40 | MH | 325 | PRO |
| 40 | ND | 365 | GLY |
| 40 | OH | 106 | GLY |
| 40 | OH | 238 | ILE |
| 40 | QG | 274 | PRO |
| 41 | QP | 271 | ALA |
| 41 | SO | 98 | GLY |
| 41 | SO | 268 | PRO |
| 40 | UF | 131 | GLY |
| 41 | UP | 287 | PRO |
| 5 | 1M | 94 | ILE |
| 11 | 2J | 249 | ILE |
| 13 | 2W | 116 | PRO |
| 17 | 3R | 281 | ILE |
| 17 | 3R | 319 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 3R | 330 | VAL |
| 23 | 4N | 104 | ILE |
| 23 | 4Q | 20 | PRO |
| 23 | 4Q | 243 | LEU |
| 41 | AO | 255 | VAL |
| 41 | BB | 84 | ILE |
| 41 | BB | 104 | GLY |
| 41 | BB | 146 | GLY |
| 41 | BB | 316 | VAL |
| 40 | BF | 29 | GLY |
| 40 | BH | 106 | GLY |
| 40 | BH | 370 | VAL |
| 41 | BN | 272 | PRO |
| 40 | CA | 303 | VAL |
| 40 | CI | 42 | ILE |
| 41 | CL | 109 | GLY |
| 41 | CN | 426 | GLY |
| 41 | CO | 160 | PRO |
| 41 | CO | 268 | PRO |
| 41 | CP | 49 | VAL |
| 41 | CP | 175 | VAL |
| 41 | CP | 272 | PRO |
| 40 | DA | 358 | GLN |
| 41 | DB | 189 | VAL |
| 40 | DF | 63 | PRO |
| 40 | DF | 175 | PRO |
| 40 | DI | 106 | GLY |
| 40 | EI | 263 | PRO |
| 40 | FA | 30 | ILE |
| 40 | FA | 250 | VAL |
| 40 | GI | 212 | ILE |
| 40 | GI | 219 | ILE |
| 41 | GN | 104 | GLY |
| 40 | HE | 439 | VAL |
| 41 | KL | 160 | PRO |
| 40 | LG | 131 | GLY |
| 40 | MA | 261 | PRO |
| 40 | MF | 66 | VAL |
| 40 | MF | 177 | VAL |
| 40 | MF | 328 | VAL |
| 40 | ND | 298 | PRO |
| 40 | OH | 37 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OH | 146 | GLY |
| 41 | QP | 71 | GLY |
| 40 | SH | 274 | PRO |
| 41 | SO | 109 | GLY |
| 40 | UF | 347 | CYS |
| 40 | UI | 354 | GLY |
| 40 | UI | 411 | GLY |
| 41 | UP | 140 | GLY |
| 41 | UP | 268 | PRO |
| 41 | WN | 182 | PRO |
| 7 | 1S | 244 | PRO |
| 7 | 1T | 293 | ILE |
| 13 | 2T | 116 | PRO |
| 13 | 2X | 132 | ILE |
| 16 | 3L | 325 | PRO |
| 23 | 4M | 50 | GLY |
| 23 | 4M | 54 | PRO |
| 23 | 4Q | 171 | PRO |
| 40 | BI | 273 | ALA |
| 41 | BM | 173 | PRO |
| 41 | BP | 71 | GLY |
| 40 | CA | 306 | ASP |
| 41 | CL | 304 | ASP |
| 41 | CN | 144 | GLY |
| 40 | DA | 34 | GLY |
| 40 | DA | 148 | GLY |
| 41 | DB | 120 | VAL |
| 41 | DB | 326 | VAL |
| 40 | DH | 177 | VAL |
| 40 | DI | 162 | GLY |
| 40 | DI | 173 | PRO |
| 40 | DI | 298 | PRO |
| 41 | DM | 181 | GLU |
| 41 | DP | 181 | GLU |
| 41 | EM | 342 | VAL |
| 41 | EP | 287 | PRO |
| 41 | EP | 319 | GLY |
| 40 | FA | 36 | MET |
| 40 | FA | 66 | VAL |
| 40 | FA | 131 | GLY |
| 40 | GE | 246 | GLY |
| 41 | GN | 80 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | HE | 291 | ILE |
| 40 | HE | 348 | PRO |
| 41 | HN | 259 | PRO |
| 40 | KD | 34 | GLY |
| 40 | LG | 273 | ALA |
| 40 | MA | 303 | VAL |
| 40 | MF | 265 | ILE |
| 40 | MG | 89 | PRO |
| 40 | MH | 111 | GLY |
| 40 | OH | 143 | GLY |
| 40 | OH | 347 | CYS |
| 40 | QA | 274 | PRO |
| 41 | QP | 57 | GLY |
| 41 | QP | 400 | GLY |
| 40 | UF | 288 | VAL |
| 40 | UI | 275 | VAL |
| 40 | VG | 57 | GLY |
| 41 | WM | 236 | VAL |
| 41 | WN | 223 | GLY |
| 41 | WN | 268 | PRO |
| 7 | 1S | 585 | GLY |
| 8 | 1X | 110 | ILE |
| 16 | 3L | 126 | ILE |
| 17 | 3P | 281 | ILE |
| 17 | 3R | 215 | VAL |
| 21 | 4D | 461 | ILE |
| 21 | 4E | 492 | ILE |
| 21 | 4F | 464 | GLY |
| 23 | 4M | 251 | PRO |
| 23 | 4P | 179 | PRO |
| 23 | 4Q | 244 | PRO |
| 23 | 4R | 104 | ILE |
| 25 | 4T | 401 | PRO |
| 38 | 6C | 64 | PRO |
| 41 | AO | 140 | GLY |
| 41 | BM | 109 | GLY |
| 41 | BM | 260 | PHE |
| 41 | BP | 243 | PRO |
| 40 | CA | 37 | PRO |
| 41 | CO | 400 | GLY |
| 40 | DE | 66 | VAL |
| 40 | DF | 298 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DF | 360 | PRO |
| 41 | DL | 49 | VAL |
| 41 | DL | 64 | VAL |
| 41 | DL | 268 | PRO |
| 41 | DM | 160 | PRO |
| 41 | DM | 272 | PRO |
| 41 | DM | 423 | VAL |
| 41 | DN | 32 | PRO |
| 41 | DN | 70 | PRO |
| 41 | DN | 326 | VAL |
| 41 | DP | 422 | VAL |
| 41 | EM | 70 | PRO |
| 41 | EM | 193 | VAL |
| 41 | EP | 261 | PRO |
| 40 | HE | 159 | VAL |
| 40 | HE | 265 | ILE |
| 40 | HE | 415 | GLY |
| 41 | JM | 140 | GLY |
| 41 | JM | 402 | GLY |
| 40 | KE | 72 | PRO |
| 40 | LG | 111 | GLY |
| 40 | MA | 57 | GLY |
| 40 | MG | 142 | GLY |
| 40 | ND | 142 | GLY |
| 40 | PD | 274 | PRO |
| 40 | QH | 57 | GLY |
| 41 | QP | 223 | GLY |
| 41 | SM | 272 | PRO |
| 40 | VH | 274 | PRO |
| 3 | 1G | 237 | PRO |
| 11 | 2J | 252 | ILE |
| 23 | 4M | 20 | PRO |
| 23 | 4N | 48 | SER |
| 36 | 5W | 251 | PRO |
| 41 | BO | 61 | PRO |
| 40 | CH | 204 | VAL |
| 41 | CP | 189 | VAL |
| 40 | DI | 14 | VAL |
| 40 | GI | 273 | ALA |
| 41 | HQ | 272 | PRO |
| 41 | JM | 79 | GLY |
| 40 | MF | 131 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MF | 275 | VAL |
| 40 | MH | 275 | VAL |
| 41 | MO | 304 | ASP |
| 40 | OH | 221 | ARG |
| 40 | OH | 415 | GLY |
| 41 | QB | 29 | GLY |
| 40 | QF | 274 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 1A | 489/903 (54%) | 488 (100%) | 1 (0%) | 92 96 |
| 1 | 1B | 121/903 (13%) | 121 (100%) | 0 | 100 100 |
| 2 | 1C | 181/588 (31%) | 180 (99%) | 1 (1%) | 84 90 |
| 2 | 1D | 181/588 (31%) | 181 (100%) | 0 | 100 100 |
| 3 | 1F | 153/229 (67%) | 151 (99%) | 2 (1%) | 65 77 |
| 3 | 1G | 153/229 (67%) | 82 (54%) | 71 (46%) | 0 0 |
| 4 | 1H | 181/623 (29%) | 180 (99%) | 1 (1%) | 84 90 |
| 4 | 1I | 80/623 (13%) | 79 (99%) | 1 (1%) | 65 77 |
| 4 | 1J | 108/623 (17%) | 107 (99%) | 1 (1%) | 75 84 |
| 5 | 1L | 141/547 (26%) | 127 (90%) | 14 (10%) | 6 26 |
| 5 | 1M | 226/547 (41%) | 224 (99%) | 2 (1%) | 75 84 |
| 5 | 1N | 94/547 (17%) | 92 (98%) | 2 (2%) | 48 67 |
| 6 | 1P | 74/1287 (6%) | 74 (100%) | 0 | 100 100 |
| 6 | 1Q | 71/1287 (6%) | 71 (100%) | 0 | 100 100 |
| 7 | 1S | 517/525 (98%) | 505 (98%) | 12 (2%) | 45 64 |
| 7 | 1T | 517/525 (98%) | 357 (69%) | 160 (31%) | 0 1 |
| 7 | 1U | 517/525 (98%) | 510 (99%) | 7 (1%) | 62 77 |
| 8 | 1W | 287/498 (58%) | 284 (99%) | 3 (1%) | 73 82 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 8 | 1X | 251/498 (50%) | 199 (79%) | 52 (21%) | 1 | 6 |
| 8 | 1Y | 149/498 (30%) | 146 (98%) | 3 (2%) | 50 | 68 |
| 8 | 1Z | 173/498 (35%) | 171 (99%) | 2 (1%) | 67 | 79 |
| 9 | 2B | 338/493 (69%) | 327 (97%) | 11 (3%) | 33 | 56 |
| 9 | 2C | 71/493 (14%) | 70 (99%) | 1 (1%) | 62 | 77 |
| 10 | 2E | 104/154 (68%) | 104 (100%) | 0 | 100 | 100 |
| 10 | 2F | 104/154 (68%) | 104 (100%) | 0 | 100 | 100 |
| 10 | 2G | 104/154 (68%) | 104 (100%) | 0 | 100 | 100 |
| 11 | 2I | 227/237 (96%) | 186 (82%) | 41 (18%) | 1 | 8 |
| 11 | 2J | 228/237 (96%) | 221 (97%) | 7 (3%) | 35 | 57 |
| 11 | 2K | 219/237 (92%) | 194 (89%) | 25 (11%) | 4 | 21 |
| 12 | 2M | 192/228 (84%) | 192 (100%) | 0 | 100 | 100 |
| 12 | 2N | 192/228 (84%) | 192 (100%) | 0 | 100 | 100 |
| 12 | 2O | 192/228 (84%) | 182 (95%) | 10 (5%) | 19 | 45 |
| 12 | 2P | 192/228 (84%) | 191 (100%) | 1 (0%) | 86 | 92 |
| 12 | 2Q | 192/228 (84%) | 191 (100%) | 1 (0%) | 86 | 92 |
| 12 | 2R | 192/228 (84%) | 192 (100%) | 0 | 100 | 100 |
| 13 | 2T | 173/180 (96%) | 116 (67%) | 57 (33%) | 0 | 1 |
| 13 | 2U | 173/180 (96%) | 117 (68%) | 56 (32%) | 0 | 1 |
| 13 | 2V | 173/180 (96%) | 114 (66%) | 59 (34%) | 0 | 1 |
| 13 | 2W | 173/180 (96%) | 121 (70%) | 52 (30%) | 0 | 2 |
| 13 | 2X | 173/180 (96%) | 110 (64%) | 63 (36%) | 0 | 0 |
| 14 | 3A | 99/150 (66%) | 98 (99%) | 1 (1%) | 73 | 82 |
| 14 | 3B | 99/150 (66%) | 98 (99%) | 1 (1%) | 73 | 82 |
| 14 | 3C | 99/150 (66%) | 99 (100%) | 0 | 100 | 100 |
| 15 | 3E | 358/375 (96%) | 357 (100%) | 1 (0%) | 91 | 94 |
| 15 | 3F | 361/375 (96%) | 356 (99%) | 5 (1%) | 62 | 77 |
| 15 | 3G | 117/375 (31%) | 117 (100%) | 0 | 100 | 100 |
| 15 | 3H | 278/375 (74%) | 276 (99%) | 2 (1%) | 81 | 88 |
| 16 | 3J | 356/387 (92%) | 348 (98%) | 8 (2%) | 47 | 65 |
| 16 | 3K | 278/387 (72%) | 276 (99%) | 2 (1%) | 81 | 88 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 16 | 3L | 356/387 (92%) | 354 (99%) | 2 (1%) | 84 | 90 |
| 16 | 3M | 107/387 (28%) | 107 (100%) | 0 | 100 | 100 |
| 17 | 3O | 354/442 (80%) | 331 (94%) | 23 (6%) | 14 | 39 |
| 17 | 3P | 354/442 (80%) | 249 (70%) | 105 (30%) | 0 | 2 |
| 17 | 3Q | 117/442 (26%) | 72 (62%) | 45 (38%) | 0 | 0 |
| 17 | 3R | 238/442 (54%) | 144 (60%) | 94 (40%) | 0 | 0 |
| 18 | 3T | 358/396 (90%) | 356 (99%) | 2 (1%) | 84 | 90 |
| 18 | 3U | 358/396 (90%) | 356 (99%) | 2 (1%) | 84 | 90 |
| 18 | 3V | 149/396 (38%) | 149 (100%) | 0 | 100 | 100 |
| 18 | 3W | 235/396 (59%) | 234 (100%) | 1 (0%) | 89 | 93 |
| 19 | 3Y | 317/337 (94%) | 310 (98%) | 7 (2%) | 47 | 65 |
| 19 | 3Z | 22/337 (6%) | 20 (91%) | 2 (9%) | 7 | 29 |
| 20 | 4A | 155/331 (47%) | 96 (62%) | 59 (38%) | 0 | 0 |
| 20 | 4B | 98/331 (30%) | 60 (61%) | 38 (39%) | 0 | 0 |
| 21 | 4D | 424/580 (73%) | 375 (88%) | 49 (12%) | 4 | 21 |
| 21 | 4E | 424/580 (73%) | 379 (89%) | 45 (11%) | 5 | 24 |
| 21 | 4F | 424/580 (73%) | 378 (89%) | 46 (11%) | 5 | 23 |
| 22 | 4H | 319/683 (47%) | 311 (98%) | 8 (2%) | 42 | 61 |
| 22 | 4I | 556/683 (81%) | 515 (93%) | 41 (7%) | 11 | 35 |
| 22 | 4J | 559/683 (82%) | 519 (93%) | 40 (7%) | 12 | 36 |
| 22 | 4K | 218/683 (32%) | 173 (79%) | 45 (21%) | 1 | 6 |
| 23 | 4M | 139/230 (60%) | 80 (58%) | 59 (42%) | 0 | 0 |
| 23 | 4N | 136/230 (59%) | 78 (57%) | 58 (43%) | 0 | 0 |
| 23 | 4P | 74/230 (32%) | 38 (51%) | 36 (49%) | 0 | 0 |
| 23 | 4Q | 107/230 (46%) | 60 (56%) | 47 (44%) | 0 | 0 |
| 23 | 4R | 139/230 (60%) | 84 (60%) | 55 (40%) | 0 | 0 |
| 24 | 4O | 73/213 (34%) | 37 (51%) | 36 (49%) | 0 | 0 |
| 25 | 4T | 148/394 (38%) | 143 (97%) | 5 (3%) | 32 | 55 |
| 26 | 4V | 319/323 (99%) | 317 (99%) | 2 (1%) | 84 | 90 |
| 26 | 4W | 319/323 (99%) | 312 (98%) | 7 (2%) | 47 | 65 |
| 27 | 4Y | 231/268 (86%) | 231 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 27 | 4Z | 231/268 (86%) | 229 (99%) | 2 (1%) | 75 | 84 |
| 28 | 5B | 177/209 (85%) | 171 (97%) | 6 (3%) | 32 | 55 |
| 29 | 5D | 74/122 (61%) | 74 (100%) | 0 | 100 | 100 |
| 29 | 5E | 32/122 (26%) | 32 (100%) | 0 | 100 | 100 |
| 30 | 5G | 75/114 (66%) | 73 (97%) | 2 (3%) | 40 | 60 |
| 31 | 5I | 386/760 (51%) | 382 (99%) | 4 (1%) | 73 | 82 |
| 31 | 5J | 99/760 (13%) | 97 (98%) | 2 (2%) | 50 | 68 |
| 32 | 5L | 72/92 (78%) | 71 (99%) | 1 (1%) | 62 | 77 |
| 33 | 5N | 310/456 (68%) | 306 (99%) | 4 (1%) | 65 | 77 |
| 33 | 5O | 137/456 (30%) | 137 (100%) | 0 | 100 | 100 |
| 34 | 5Q | 239/469 (51%) | 238 (100%) | 1 (0%) | 89 | 93 |
| 34 | 5R | 177/469 (38%) | 101 (57%) | 76 (43%) | 0 | 0 |
| 35 | 5T | 118/182 (65%) | 117 (99%) | 1 (1%) | 79 | 86 |
| 35 | 5U | 22/182 (12%) | 20 (91%) | 2 (9%) | 7 | 29 |
| 36 | 5W | 201/251 (80%) | 200 (100%) | 1 (0%) | 86 | 92 |
| 36 | 5X | 201/251 (80%) | 198 (98%) | 3 (2%) | 60 | 75 |
| 36 | 5Y | 162/251 (64%) | 160 (99%) | 2 (1%) | 67 | 79 |
| 36 | 5Z | 51/251 (20%) | 51 (100%) | 0 | 100 | 100 |
| 37 | 6A | 108/124 (87%) | 107 (99%) | 1 (1%) | 75 | 84 |
| 38 | 6C | 178/260 (68%) | 171 (96%) | 7 (4%) | 27 | 52 |
| 38 | 6D | 55/260 (21%) | 55 (100%) | 0 | 100 | 100 |
| 39 | 6F | 144/196 (74%) | 139 (96%) | 5 (4%) | 31 | 55 |
| 39 | 6G | 144/196 (74%) | 141 (98%) | 3 (2%) | 48 | 67 |
| 39 | 6H | 129/196 (66%) | 127 (98%) | 2 (2%) | 58 | 74 |
| 39 | 6I | 144/196 (74%) | 144 (100%) | 0 | 100 | 100 |
| 39 | 6J | 144/196 (74%) | 144 (100%) | 0 | 100 | 100 |
| 39 | 6K | 144/196 (74%) | 144 (100%) | 0 | 100 | 100 |
| 39 | 6L | 126/196 (64%) | 120 (95%) | 6 (5%) | 21 | 47 |
| 40 | AA | 371/376 (99%) | 371 (100%) | 0 | 100 | 100 |
| 40 | AE | 371/376 (99%) | 368 (99%) | 3 (1%) | 79 | 86 |
| 40 | AF | 371/376 (99%) | 370 (100%) | 1 (0%) | 91 | 94 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 40 | AG | 371/376 (99%) | 371 (100%) | 0 | 100 | 100 |
| 40 | AH | 371/376 (99%) | 371 (100%) | 0 | 100 | 100 |
| 40 | BA | 371/376 (99%) | 371 (100%) | 0 | 100 | 100 |
| 40 | BE | 371/376 (99%) | 241 (65%) | 130 (35%) | 0 | 0 |
| 40 | BF | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | BG | 366/376 (97%) | 364 (100%) | 2 (0%) | 86 | 92 |
| 40 | BH | 371/376 (99%) | 273 (74%) | 98 (26%) | 0 | 3 |
| 40 | BI | 316/376 (84%) | 201 (64%) | 115 (36%) | 0 | 0 |
| 40 | CA | 371/376 (99%) | 244 (66%) | 127 (34%) | 0 | 1 |
| 40 | CE | 370/376 (98%) | 367 (99%) | 3 (1%) | 79 | 86 |
| 40 | CF | 371/376 (99%) | 364 (98%) | 7 (2%) | 52 | 69 |
| 40 | CG | 371/376 (99%) | 368 (99%) | 3 (1%) | 79 | 86 |
| 40 | CH | 371/376 (99%) | 236 (64%) | 135 (36%) | 0 | 0 |
| 40 | CI | 371/376 (99%) | 371 (100%) | 0 | 100 | 100 |
| 40 | DA | 366/376 (97%) | 245 (67%) | 121 (33%) | 0 | 1 |
| 40 | DE | 368/376 (98%) | 238 (65%) | 130 (35%) | 0 | 0 |
| 40 | DF | 366/376 (97%) | 231 (63%) | 135 (37%) | 0 | 0 |
| 40 | DG | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | DH | 367/376 (98%) | 241 (66%) | 126 (34%) | 0 | 1 |
| 40 | DI | 366/376 (97%) | 241 (66%) | 125 (34%) | 0 | 1 |
| 40 | EA | 368/376 (98%) | 366 (100%) | 2 (0%) | 86 | 92 |
| 40 | EE | 369/376 (98%) | 363 (98%) | 6 (2%) | 58 | 74 |
| 40 | EF | 369/376 (98%) | 368 (100%) | 1 (0%) | 91 | 94 |
| 40 | EG | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | EH | 367/376 (98%) | 245 (67%) | 122 (33%) | 0 | 1 |
| 40 | EI | 368/376 (98%) | 223 (61%) | 145 (39%) | 0 | 0 |
| 40 | FA | 368/376 (98%) | 244 (66%) | 124 (34%) | 0 | 1 |
| 40 | FE | 368/376 (98%) | 368 (100%) | 0 | 100 | 100 |
| 40 | FF | 368/376 (98%) | 368 (100%) | 0 | 100 | 100 |
| 40 | FG | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | FH | 368/376 (98%) | 368 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 40 | FI | 367/376 (98%) | 363 (99%) | 4 (1%) | 70 | 81 |
| 40 | GA | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | GE | 368/376 (98%) | 235 (64%) | 133 (36%) | 0 | 0 |
| 40 | GF | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | GG | 367/376 (98%) | 356 (97%) | 11 (3%) | 36 | 58 |
| 40 | GH | 367/376 (98%) | 254 (69%) | 113 (31%) | 0 | 1 |
| 40 | GI | 368/376 (98%) | 241 (66%) | 127 (34%) | 0 | 1 |
| 40 | HA | 368/376 (98%) | 366 (100%) | 2 (0%) | 86 | 92 |
| 40 | HE | 367/376 (98%) | 235 (64%) | 132 (36%) | 0 | 0 |
| 40 | HF | 366/376 (97%) | 365 (100%) | 1 (0%) | 91 | 94 |
| 40 | HG | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | HH | 368/376 (98%) | 368 (100%) | 0 | 100 | 100 |
| 40 | HI | 369/376 (98%) | 369 (100%) | 0 | 100 | 100 |
| 40 | IA | 368/376 (98%) | 367 (100%) | 1 (0%) | 91 | 94 |
| 40 | IE | 358/376 (95%) | 356 (99%) | 2 (1%) | 84 | 90 |
| 40 | IF | 368/376 (98%) | 367 (100%) | 1 (0%) | 91 | 94 |
| 40 | IG | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | IH | 368/376 (98%) | 366 (100%) | 2 (0%) | 86 | 92 |
| 40 | II | 368/376 (98%) | 367 (100%) | 1 (0%) | 91 | 94 |
| 40 | JA | 368/376 (98%) | 368 (100%) | 0 | 100 | 100 |
| 40 | JD | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | JE | 368/376 (98%) | 368 (100%) | 0 | 100 | 100 |
| 40 | JF | 367/376 (98%) | 365 (100%) | 2 (0%) | 86 | 92 |
| 40 | JG | 371/376 (99%) | 367 (99%) | 4 (1%) | 70 | 81 |
| 40 | JH | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | KA | 368/376 (98%) | 366 (100%) | 2 (0%) | 86 | 92 |
| 40 | KD | 367/376 (98%) | 365 (100%) | 2 (0%) | 86 | 92 |
| 40 | KE | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | KF | 368/376 (98%) | 367 (100%) | 1 (0%) | 91 | 94 |
| 40 | KG | 371/376 (99%) | 371 (100%) | 0 | 100 | 100 |
| 40 | KH | 371/376 (99%) | 370 (100%) | 1 (0%) | 91 | 94 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 40 | LA | 371/376 (99%) | 369 (100%) | 2 (0%) | 86 | 92 |
| 40 | LD | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | LE | 371/376 (99%) | 364 (98%) | 7 (2%) | 52 | 69 |
| 40 | LF | 367/376 (98%) | 276 (75%) | 91 (25%) | 0 | 4 |
| 40 | LG | 368/376 (98%) | 268 (73%) | 100 (27%) | 0 | 2 |
| 40 | LH | 368/376 (98%) | 367 (100%) | 1 (0%) | 91 | 94 |
| 40 | MA | 366/376 (97%) | 279 (76%) | 87 (24%) | 0 | 4 |
| 40 | MD | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | ME | 368/376 (98%) | 366 (100%) | 2 (0%) | 86 | 92 |
| 40 | MF | 367/376 (98%) | 277 (76%) | 90 (24%) | 0 | 4 |
| 40 | MG | 367/376 (98%) | 272 (74%) | 95 (26%) | 0 | 3 |
| 40 | MH | 367/376 (98%) | 276 (75%) | 91 (25%) | 0 | 4 |
| 40 | NA | 366/376 (97%) | 366 (100%) | 0 | 100 | 100 |
| 40 | ND | 367/376 (98%) | 239 (65%) | 128 (35%) | 0 | 0 |
| 40 | NE | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | NF | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | NG | 366/376 (97%) | 364 (100%) | 2 (0%) | 86 | 92 |
| 40 | NH | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | OA | 370/376 (98%) | 369 (100%) | 1 (0%) | 91 | 94 |
| 40 | OD | 368/376 (98%) | 360 (98%) | 8 (2%) | 47 | 65 |
| 40 | OE | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | OF | 369/376 (98%) | 367 (100%) | 2 (0%) | 86 | 92 |
| 40 | OG | 368/376 (98%) | 366 (100%) | 2 (0%) | 86 | 92 |
| 40 | OH | 369/376 (98%) | 224 (61%) | 145 (39%) | 0 | 0 |
| 40 | PA | 366/376 (97%) | 366 (100%) | 0 | 100 | 100 |
| 40 | PD | 349/376 (93%) | 348 (100%) | 1 (0%) | 91 | 94 |
| 40 | PE | 367/376 (98%) | 364 (99%) | 3 (1%) | 79 | 86 |
| 40 | PF | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | PG | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 40 | PH | 365/376 (97%) | 365 (100%) | 0 | 100 | 100 |
| 40 | QA | 366/376 (97%) | 363 (99%) | 3 (1%) | 79 | 86 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 40 | QE | 365/376 (97%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 40 | QF | 365/376 (97%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 40 | QG | 366/376 (97%) | 366 (100%) | 0 | 100 | 100 |
| 40 | QH | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | RA | 366/376 (97%) | 363 (99%) | 3 (1%) | 79 | 86 |
| 40 | RE | 365/376 (97%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 40 | RF | 365/376 (97%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 40 | RG | 366/376 (97%) | 365 (100%) | 1 (0%) | 91 | 94 |
| 40 | RH | 365/376 (97%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 40 | RI | 320/376 (85%) | 318 (99%) | 2 (1%) | 84 | 90 |
| 40 | SA | 366/376 (97%) | 355 (97%) | 11 (3%) | 36 | 58 |
| 40 | SE | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | SF | 366/376 (97%) | 363 (99%) | 3 (1%) | 79 | 86 |
| 40 | SG | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | SH | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | SI | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | TA | 366/376 (97%) | 365 (100%) | 1 (0%) | 91 | 94 |
| 40 | TE | 366/376 (97%) | 366 (100%) | 0 | 100 | 100 |
| 40 | TF | 366/376 (97%) | 363 (99%) | 3 (1%) | 79 | 86 |
| 40 | TG | 368/376 (98%) | 366 (100%) | 2 (0%) | 86 | 92 |
| 40 | TH | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | TI | 367/376 (98%) | 365 (100%) | 2 (0%) | 86 | 92 |
| 40 | UA | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | UE | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | UF | 368/376 (98%) | 250 (68%) | 118 (32%) | 0 | 1 |
| 40 | UG | 368/376 (98%) | 365 (99%) | 3 (1%) | 79 | 86 |
| 40 | UH | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |
| 40 | UI | 367/376 (98%) | 239 (65%) | 128 (35%) | 0 | 0 |
| 40 | VA | 371/376 (99%) | 370 (100%) | 1 (0%) | 91 | 94 |
| 40 | VF | 371/376 (99%) | 370 (100%) | 1 (0%) | 91 | 94 |
| 40 | VG | 367/376 (98%) | 367 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 40 | VH | 368/376 (98%) | 367 (100%) | 1 (0%) | 91 | 94 |
| 40 | VI | 371/376 (99%) | 368 (99%) | 3 (1%) | 79 | 86 |
| 40 | VJ | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | WA | 371/376 (99%) | 369 (100%) | 2 (0%) | 86 | 92 |
| 40 | WE | 371/376 (99%) | 369 (100%) | 2 (0%) | 86 | 92 |
| 40 | WF | 367/376 (98%) | 366 (100%) | 1 (0%) | 91 | 94 |
| 40 | WG | 366/376 (97%) | 366 (100%) | 0 | 100 | 100 |
| 40 | WH | 371/376 (99%) | 370 (100%) | 1 (0%) | 91 | 94 |
| 40 | WI | 367/376 (98%) | 365 (100%) | 2 (0%) | 86 | 92 |
| 41 | AB | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | AL | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | AM | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | AN | 365/381 (96%) | 361 (99%) | 4 (1%) | 70 | 81 |
| 41 | AO | 365/381 (96%) | 266 (73%) | 99 (27%) | 0 | 2 |
| 41 | AP | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | BB | 365/381 (96%) | 252 (69%) | 113 (31%) | 0 | 1 |
| 41 | BL | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | BM | 365/381 (96%) | 251 (69%) | 114 (31%) | 0 | 1 |
| 41 | BN | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | BO | 365/381 (96%) | 251 (69%) | 114 (31%) | 0 | 1 |
| 41 | BP | 365/381 (96%) | 253 (69%) | 112 (31%) | 0 | 1 |
| 41 | CB | 365/381 (96%) | 362 (99%) | 3 (1%) | 79 | 86 |
| 41 | CL | 365/381 (96%) | 217 (60%) | 148 (40%) | 0 | 0 |
| 41 | CM | 365/381 (96%) | 263 (72%) | 102 (28%) | 0 | 2 |
| 41 | CN | 365/381 (96%) | 236 (65%) | 129 (35%) | 0 | 0 |
| 41 | CO | 365/381 (96%) | 248 (68%) | 117 (32%) | 0 | 1 |
| 41 | CP | 365/381 (96%) | 225 (62%) | 140 (38%) | 0 | 0 |
| 41 | DB | 365/381 (96%) | 234 (64%) | 131 (36%) | 0 | 0 |
| 41 | DL | 365/381 (96%) | 227 (62%) | 138 (38%) | 0 | 0 |
| 41 | DM | 365/381 (96%) | 219 (60%) | 146 (40%) | 0 | 0 |
| 41 | DN | 365/381 (96%) | 222 (61%) | 143 (39%) | 0 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 41 | DO | 365/381 (96%) | 362 (99%) | 3 (1%) | 79 | 86 |
| 41 | DP | 364/381 (96%) | 241 (66%) | 123 (34%) | 0 | 1 |
| 41 | EB | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | EL | 312/381 (82%) | 311 (100%) | 1 (0%) | 91 | 94 |
| 41 | EM | 365/381 (96%) | 237 (65%) | 128 (35%) | 0 | 0 |
| 41 | EN | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | EO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | EP | 365/381 (96%) | 252 (69%) | 113 (31%) | 0 | 1 |
| 41 | FB | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | FM | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | FN | 365/381 (96%) | 361 (99%) | 4 (1%) | 70 | 81 |
| 41 | FO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | FP | 365/381 (96%) | 362 (99%) | 3 (1%) | 79 | 86 |
| 41 | GB | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | GM | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | GN | 365/381 (96%) | 249 (68%) | 116 (32%) | 0 | 1 |
| 41 | GO | 364/381 (96%) | 361 (99%) | 3 (1%) | 79 | 86 |
| 41 | GP | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | HB | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | HM | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | HN | 365/381 (96%) | 238 (65%) | 127 (35%) | 0 | 0 |
| 41 | HO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | HP | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | HQ | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | IB | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | IM | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | IN | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | IO | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | IP | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | IQ | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | JB | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 41 | JL | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | JM | 365/381 (96%) | 235 (64%) | 130 (36%) | 0 | 0 |
| 41 | JN | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | JO | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | KB | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | KL | 365/381 (96%) | 256 (70%) | 109 (30%) | 0 | 2 |
| 41 | KM | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | KN | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | KO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | KP | 326/381 (86%) | 326 (100%) | 0 | 100 | 100 |
| 41 | LB | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | LL | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | LM | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | LN | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | LO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | LP | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | MB | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | ML | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | MM | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | MN | 365/381 (96%) | 360 (99%) | 5 (1%) | 62 | 77 |
| 41 | MO | 365/381 (96%) | 270 (74%) | 95 (26%) | 0 | 3 |
| 41 | MP | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | NB | 365/381 (96%) | 362 (99%) | 3 (1%) | 79 | 86 |
| 41 | NL | 365/381 (96%) | 362 (99%) | 3 (1%) | 79 | 86 |
| 41 | NM | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | NN | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | NO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | NP | 356/381 (93%) | 352 (99%) | 4 (1%) | 70 | 81 |
| 41 | OB | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | OL | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | OM | 365/381 (96%) | 362 (99%) | 3 (1%) | 79 | 86 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 41 | ON | 365/381 (96%) | 361 (99%) | 4 (1%) | 70 | 81 |
| 41 | OO | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | OP | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | PB | 365/381 (96%) | 361 (99%) | 4 (1%) | 70 | 81 |
| 41 | PL | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | PM | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | PN | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | PO | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | PP | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | QB | 365/381 (96%) | 223 (61%) | 142 (39%) | 0 | 0 |
| 41 | QL | 365/381 (96%) | 361 (99%) | 4 (1%) | 70 | 81 |
| 41 | QM | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | QN | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | QO | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | QP | 361/381 (95%) | 223 (62%) | 138 (38%) | 0 | 0 |
| 41 | RB | 365/381 (96%) | 362 (99%) | 3 (1%) | 79 | 86 |
| 41 | RL | 365/381 (96%) | 361 (99%) | 4 (1%) | 70 | 81 |
| 41 | RM | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | RN | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | RO | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | RP | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | SB | 365/381 (96%) | 349 (96%) | 16 (4%) | 24 | 49 |
| 41 | SL | 328/381 (86%) | 326 (99%) | 2 (1%) | 84 | 90 |
| 41 | SM | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | SN | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | SO | 365/381 (96%) | 252 (69%) | 113 (31%) | 0 | 1 |
| 41 | SP | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | TB | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | TL | 335/381 (88%) | 333 (99%) | 2 (1%) | 84 | 90 |
| 41 | TM | 365/381 (96%) | 361 (99%) | 4 (1%) | 70 | 81 |
| 41 | TN | 365/381 (96%) | 361 (99%) | 4 (1%) | 70 | 81 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 41 | TO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | TP | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | UB | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | UM | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | UN | 365/381 (96%) | 365 (100%) | 0 | 100 | 100 |
| 41 | UO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | UP | 365/381 (96%) | 232 (64%) | 133 (36%) | 0 | 0 |
| 41 | VB | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | VN | 365/381 (96%) | 362 (99%) | 3 (1%) | 79 | 86 |
| 41 | VO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | VP | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | VQ | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | WB | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | WM | 365/381 (96%) | 241 (66%) | 124 (34%) | 0 | 1 |
| 41 | WN | 365/381 (96%) | 225 (62%) | 140 (38%) | 0 | 0 |
| 41 | WO | 365/381 (96%) | 364 (100%) | 1 (0%) | 91 | 94 |
| 41 | WP | 365/381 (96%) | 363 (100%) | 2 (0%) | 86 | 92 |
| 41 | WQ | 358/381 (94%) | 357 (100%) | 1 (0%) | 91 | 94 |
| All | All | 120294/142337 (84%) | 111437 (93%) | 8857 (7%) | 14 | 35 |

All (8857) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 941 | LYS |
| 2 | 1C | 117 | LYS |
| 3 | 1F | 58 | ASN |
| 3 | 1F | 173 | LYS |
| 3 | 1G | 54 | LYS |
| 3 | 1G | 57 | LEU |
| 3 | 1G | 65 | ILE |
| 3 | 1G | 66 | PHE |
| 3 | 1G | 70 | VAL |
| 3 | 1G | 71 | ASN |
| 3 | 1G | 75 | VAL |
| 3 | 1G | 76 | LYS |
| 3 | 1G | 77 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1G | 78 | LEU |
| 3 | 1G | 80 | SER |
| 3 | 1G | 81 | LEU |
| 3 | 1G | 85 | LEU |
| 3 | 1G | 86 | VAL |
| 3 | 1G | 106 | ASN |
| 3 | 1G | 109 | HIS |
| 3 | 1G | 111 | THR |
| 3 | 1G | 114 | MET |
| 3 | 1G | 115 | THR |
| 3 | 1G | 118 | MET |
| 3 | 1G | 120 | MET |
| 3 | 1G | 121 | ASP |
| 3 | 1G | 122 | ARG |
| 3 | 1G | 127 | PHE |
| 3 | 1G | 129 | LYS |
| 3 | 1G | 131 | ASN |
| 3 | 1G | 132 | ASP |
| 3 | 1G | 134 | CYS |
| 3 | 1G | 138 | SER |
| 3 | 1G | 142 | TYR |
| 3 | 1G | 144 | LEU |
| 3 | 1G | 145 | SER |
| 3 | 1G | 148 | LEU |
| 3 | 1G | 149 | ARG |
| 3 | 1G | 151 | THR |
| 3 | 1G | 152 | LEU |
| 3 | 1G | 155 | LYS |
| 3 | 1G | 156 | MET |
| 3 | 1G | 165 | LEU |
| 3 | 1G | 168 | ASP |
| 3 | 1G | 170 | PHE |
| 3 | 1G | 171 | ILE |
| 3 | 1G | 173 | LYS |
| 3 | 1G | 174 | GLU |
| 3 | 1G | 175 | GLU |
| 3 | 1G | 178 | HIS |
| 3 | 1G | 181 | LYS |
| 3 | 1G | 184 | LEU |
| 3 | 1G | 185 | LEU |
| 3 | 1G | 186 | LYS |
| 3 | 1G | 204 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | 1G | 206 | LYS |
| 3 | 1G | 207 | LYS |
| 3 | 1G | 209 | ASP |
| 3 | 1G | 216 | LEU |
| 3 | 1G | 217 | SER |
| 3 | 1G | 220 | ASP |
| 3 | 1G | 221 | TYR |
| 3 | 1G | 222 | GLU |
| 3 | 1G | 230 | LEU |
| 3 | 1G | 239 | LEU |
| 3 | 1G | 240 | PRO |
| 3 | 1G | 243 | LYS |
| 3 | 1G | 245 | GLN |
| 3 | 1G | 246 | LYS |
| 3 | 1G | 247 | GLU |
| 3 | 1G | 248 | PHE |
| 3 | 1G | 249 | GLU |
| 3 | 1G | 251 | GLN |
| 3 | 1G | 254 | LYS |
| 3 | 1G | 255 | ASP |
| 4 | 1H | 222 | ARG |
| 4 | 1I | 62 | ARG |
| 4 | 1J | 127 | ARG |
| 5 | 1L | 272 | LEU |
| 5 | 1L | 273 | ASN |
| 5 | 1L | 275 | ARG |
| 5 | 1L | 279 | LYS |
| 5 | 1L | 282 | LEU |
| 5 | 1L | 285 | LEU |
| 5 | 1L | 287 | GLU |
| 5 | 1L | 290 | LEU |
| 5 | 1L | 291 | ARG |
| 5 | 1L | 292 | GLU |
| 5 | 1L | 293 | ARG |
| 5 | 1L | 296 | ARG |
| 5 | 1L | 310 | ARG |
| 5 | 1L | 311 | LYS |
| 5 | 1M | 68 | GLN |
| 5 | 1M | 310 | ARG |
| 5 | 1N | 68 | GLN |
| 5 | 1N | 84 | LYS |
| 7 | 1S | 239 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 1S | 246 | LYS |
| 7 | 1S | 278 | SER |
| 7 | 1S | 285 | LYS |
| 7 | 1S | 458 | LYS |
| 7 | 1S | 569 | VAL |
| 7 | 1S | 570 | LYS |
| 7 | 1S | 575 | ASN |
| 7 | 1S | 579 | VAL |
| 7 | 1S | 580 | THR |
| 7 | 1S | 582 | VAL |
| 7 | 1S | 584 | VAL |
| 7 | 1T | 10 | GLU |
| 7 | 1T | 11 | VAL |
| 7 | 1T | 14 | LEU |
| 7 | 1T | 16 | LEU |
| 7 | 1T | 19 | VAL |
| 7 | 1T | 20 | ILE |
| 7 | 1T | 35 | ASP |
| 7 | 1T | 37 | GLU |
| 7 | 1T | 38 | HIS |
| 7 | 1T | 40 | ILE |
| 7 | 1T | 53 | LYS |
| 7 | 1T | 54 | THR |
| 7 | 1T | 57 | GLN |
| 7 | 1T | 60 | LEU |
| 7 | 1T | 70 | VAL |
| 7 | 1T | 72 | ILE |
| 7 | 1T | 73 | SER |
| 7 | 1T | 74 | LYS |
| 7 | 1T | 84 | VAL |
| 7 | 1T | 85 | THR |
| 7 | 1T | 95 | LEU |
| 7 | 1T | 97 | ASP |
| 7 | 1T | 99 | LYS |
| 7 | 1T | 100 | LYS |
| 7 | 1T | 101 | ARG |
| 7 | 1T | 102 | GLU |
| 7 | 1T | 103 | LEU |
| 7 | 1T | 104 | MET |
| 7 | 1T | 106 | ARG |
| 7 | 1T | 111 | LYS |
| 7 | 1T | 113 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 1T | 120 | SER |
| 7 | 1T | 124 | LEU |
| 7 | 1T | 125 | TYR |
| 7 | 1T | 126 | LEU |
| 7 | 1T | 127 | VAL |
| 7 | 1T | 139 | VAL |
| 7 | 1T | 141 | SER |
| 7 | 1T | 142 | ILE |
| 7 | 1T | 144 | LYS |
| 7 | 1T | 146 | GLU |
| 7 | 1T | 148 | ILE |
| 7 | 1T | 151 | SER |
| 7 | 1T | 156 | LEU |
| 7 | 1T | 163 | SER |
| 7 | 1T | 166 | PHE |
| 7 | 1T | 167 | SER |
| 7 | 1T | 170 | HIS |
| 7 | 1T | 174 | PHE |
| 7 | 1T | 181 | THR |
| 7 | 1T | 183 | ARG |
| 7 | 1T | 192 | ARG |
| 7 | 1T | 193 | LYS |
| 7 | 1T | 201 | THR |
| 7 | 1T | 205 | LYS |
| 7 | 1T | 208 | VAL |
| 7 | 1T | 211 | ILE |
| 7 | 1T | 215 | SER |
| 7 | 1T | 222 | LEU |
| 7 | 1T | 228 | ASP |
| 7 | 1T | 235 | ARG |
| 7 | 1T | 237 | LYS |
| 7 | 1T | 238 | LEU |
| 7 | 1T | 241 | ASP |
| 7 | 1T | 246 | LYS |
| 7 | 1T | 258 | CYS |
| 7 | 1T | 260 | LYS |
| 7 | 1T | 264 | LEU |
| 7 | 1T | 277 | ARG |
| 7 | 1T | 278 | SER |
| 7 | 1T | 279 | PRO |
| 7 | 1T | 280 | SER |
| 7 | 1T | 286 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 1T | 287 | ILE |
| 7 | 1T | 294 | THR |
| 7 | 1T | 297 | SER |
| 7 | 1T | 305 | PHE |
| 7 | 1T | 307 | VAL |
| 7 | 1T | 312 | SER |
| 7 | 1T | 316 | ARG |
| 7 | 1T | 321 | ASP |
| 7 | 1T | 323 | LYS |
| 7 | 1T | 327 | VAL |
| 7 | 1T | 328 | THR |
| 7 | 1T | 330 | CYS |
| 7 | 1T | 332 | PHE |
| 7 | 1T | 336 | GLU |
| 7 | 1T | 346 | GLU |
| 7 | 1T | 347 | LEU |
| 7 | 1T | 351 | CYS |
| 7 | 1T | 353 | LYS |
| 7 | 1T | 354 | LYS |
| 7 | 1T | 362 | LEU |
| 7 | 1T | 365 | ARG |
| 7 | 1T | 367 | LEU |
| 7 | 1T | 374 | ASN |
| 7 | 1T | 380 | ILE |
| 7 | 1T | 383 | MET |
| 7 | 1T | 384 | ARG |
| 7 | 1T | 394 | ASP |
| 7 | 1T | 397 | LYS |
| 7 | 1T | 398 | ILE |
| 7 | 1T | 407 | ARG |
| 7 | 1T | 408 | LEU |
| 7 | 1T | 411 | VAL |
| 7 | 1T | 413 | SER |
| 7 | 1T | 414 | ASN |
| 7 | 1T | 418 | ILE |
| 7 | 1T | 428 | ASP |
| 7 | 1T | 430 | THR |
| 7 | 1T | 433 | ILE |
| 7 | 1T | 441 | VAL |
| 7 | 1T | 442 | ARG |
| 7 | 1T | 443 | VAL |
| 7 | 1T | 445 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 1T | 450 | THR |
| 7 | 1T | 452 | LYS |
| 7 | 1T | 455 | GLU |
| 7 | 1T | 458 | LYS |
| 7 | 1T | 461 | LYS |
| 7 | 1T | 464 | VAL |
| 7 | 1T | 468 | ARG |
| 7 | 1T | 471 | LYS |
| 7 | 1T | 476 | CYS |
| 7 | 1T | 482 | ASP |
| 7 | 1T | 486 | ILE |
| 7 | 1T | 493 | LEU |
| 7 | 1T | 494 | ARG |
| 7 | 1T | 496 | ASN |
| 7 | 1T | 497 | GLN |
| 7 | 1T | 500 | LEU |
| 7 | 1T | 506 | GLN |
| 7 | 1T | 507 | CYS |
| 7 | 1T | 509 | CYS |
| 7 | 1T | 513 | GLU |
| 7 | 1T | 514 | GLU |
| 7 | 1T | 515 | PHE |
| 7 | 1T | 517 | ILE |
| 7 | 1T | 520 | SER |
| 7 | 1T | 523 | ASP |
| 7 | 1T | 524 | ARG |
| 7 | 1T | 525 | LYS |
| 7 | 1T | 530 | GLU |
| 7 | 1T | 537 | ILE |
| 7 | 1T | 538 | ARG |
| 7 | 1T | 541 | ASP |
| 7 | 1T | 543 | SER |
| 7 | 1T | 544 | LEU |
| 7 | 1T | 549 | ASN |
| 7 | 1T | 551 | MET |
| 7 | 1T | 553 | ILE |
| 7 | 1T | 558 | VAL |
| 7 | 1T | 560 | PHE |
| 7 | 1T | 568 | LEU |
| 7 | 1T | 569 | VAL |
| 7 | 1T | 570 | LYS |
| 7 | 1T | 575 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 1T | 576 | GLU |
| 7 | 1T | 579 | VAL |
| 7 | 1T | 584 | VAL |
| 7 | 1U | 231 | LYS |
| 7 | 1U | 232 | MET |
| 7 | 1U | 237 | LYS |
| 7 | 1U | 246 | LYS |
| 7 | 1U | 247 | ASP |
| 7 | 1U | 248 | LYS |
| 7 | 1U | 458 | LYS |
| 8 | 1W | 240 | ARG |
| 8 | 1W | 247 | LYS |
| 8 | 1W | 531 | LYS |
| 8 | 1X | 75 | GLU |
| 8 | 1X | 76 | THR |
| 8 | 1X | 77 | ILE |
| 8 | 1X | 79 | LEU |
| 8 | 1X | 80 | ILE |
| 8 | 1X | 81 | THR |
| 8 | 1X | 82 | ARG |
| 8 | 1X | 83 | ASP |
| 8 | 1X | 86 | ARG |
| 8 | 1X | 89 | ILE |
| 8 | 1X | 90 | ILE |
| 8 | 1X | 93 | LYS |
| 8 | 1X | 98 | GLU |
| 8 | 1X | 99 | SER |
| 8 | 1X | 100 | LEU |
| 8 | 1X | 101 | ILE |
| 8 | 1X | 103 | SER |
| 8 | 1X | 108 | GLU |
| 8 | 1X | 109 | ARG |
| 8 | 1X | 116 | VAL |
| 8 | 1X | 118 | THR |
| 8 | 1X | 119 | ARG |
| 8 | 1X | 120 | GLU |
| 8 | 1X | 121 | GLU |
| 8 | 1X | 125 | LYS |
| 8 | 1X | 126 | GLU |
| 8 | 1X | 127 | GLN |
| 8 | 1X | 129 | CYS |
| 8 | 1X | 130 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 1X | 131 | LYS |
| 8 | 1X | 133 | LYS |
| 8 | 1X | 134 | GLU |
| 8 | 1X | 140 | VAL |
| 8 | 1X | 148 | LYS |
| 8 | 1X | 152 | MET |
| 8 | 1X | 155 | ARG |
| 8 | 1X | 157 | ASN |
| 8 | 1X | 158 | GLN |
| 8 | 1X | 159 | LYS |
| 8 | 1X | 161 | SER |
| 8 | 1X | 164 | GLU |
| 8 | 1X | 168 | LYS |
| 8 | 1X | 175 | LEU |
| 8 | 1X | 176 | GLN |
| 8 | 1X | 180 | GLN |
| 8 | 1X | 181 | LEU |
| 8 | 1X | 182 | ARG |
| 8 | 1X | 186 | GLU |
| 8 | 1X | 187 | GLU |
| 8 | 1X | 224 | LYS |
| 8 | 1X | 252 | ARG |
| 8 | 1X | 262 | GLN |
| 8 | 1Y | 125 | LYS |
| 8 | 1Y | 224 | LYS |
| 8 | 1Y | 225 | ARG |
| 8 | 1Z | 401 | ARG |
| 8 | 1Z | 507 | LYS |
| 9 | 2B | 43 | LEU |
| 9 | 2B | 44 | ARG |
| 9 | 2B | 49 | ILE |
| 9 | 2B | 52 | ASN |
| 9 | 2B | 57 | ILE |
| 9 | 2B | 59 | ASP |
| 9 | 2B | 61 | LEU |
| 9 | 2B | 62 | ASP |
| 9 | 2B | 289 | GLN |
| 9 | 2B | 311 | LYS |
| 9 | 2B | 327 | ARG |
| 9 | 2C | 421 | ARG |
| 11 | 2I | 91 | ARG |
| 11 | 2I | 158 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | 2I | 160 | LYS |
| 11 | 2I | 164 | GLU |
| 11 | 2I | 165 | VAL |
| 11 | 2I | 166 | LYS |
| 11 | 2I | 167 | LYS |
| 11 | 2I | 175 | TYR |
| 11 | 2I | 177 | GLN |
| 11 | 2I | 178 | GLU |
| 11 | 2I | 180 | LEU |
| 11 | 2I | 181 | ARG |
| 11 | 2I | 182 | LYS |
| 11 | 2I | 186 | LYS |
| 11 | 2I | 187 | ARG |
| 11 | 2I | 188 | LEU |
| 11 | 2I | 189 | SER |
| 11 | 2I | 193 | ARG |
| 11 | 2I | 194 | GLU |
| 11 | 2I | 200 | LEU |
| 11 | 2I | 201 | LYS |
| 11 | 2I | 203 | ASN |
| 11 | 2I | 207 | VAL |
| 11 | 2I | 209 | LYS |
| 11 | 2I | 215 | SER |
| 11 | 2I | 224 | LYS |
| 11 | 2I | 226 | ARG |
| 11 | 2I | 229 | LYS |
| 11 | 2I | 230 | LEU |
| 11 | 2I | 231 | GLU |
| 11 | 2I | 234 | MET |
| 11 | 2I | 238 | GLU |
| 11 | 2I | 239 | HIS |
| 11 | 2I | 241 | ILE |
| 11 | 2I | 243 | VAL |
| 11 | 2I | 244 | LEU |
| 11 | 2I | 246 | LYS |
| 11 | 2I | 249 | ILE |
| 11 | 2I | 250 | ILE |
| 11 | 2I | 251 | TYR |
| 11 | 2I | 255 | LYS |
| 11 | 2J | 91 | ARG |
| 11 | 2J | 120 | LYS |
| 11 | 2J | 129 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | 2J | 247 | HIS |
| 11 | 2J | 248 | LYS |
| 11 | 2J | 250 | ILE |
| 11 | 2J | 252 | ILE |
| 11 | 2K | 185 | MET |
| 11 | 2K | 186 | LYS |
| 11 | 2K | 189 | SER |
| 11 | 2K | 197 | LEU |
| 11 | 2K | 200 | LEU |
| 11 | 2K | 201 | LYS |
| 11 | 2K | 202 | LYS |
| 11 | 2K | 209 | LYS |
| 11 | 2K | 212 | GLN |
| 11 | 2K | 214 | LEU |
| 11 | 2K | 216 | VAL |
| 11 | 2K | 218 | ILE |
| 11 | 2K | 221 | ILE |
| 11 | 2K | 223 | LYS |
| 11 | 2K | 229 | LYS |
| 11 | 2K | 231 | GLU |
| 11 | 2K | 234 | MET |
| 11 | 2K | 235 | LYS |
| 11 | 2K | 239 | HIS |
| 11 | 2K | 243 | VAL |
| 11 | 2K | 244 | LEU |
| 11 | 2K | 246 | LYS |
| 11 | 2K | 252 | ILE |
| 11 | 2K | 254 | ASN |
| 11 | 2K | 255 | LYS |
| 12 | 2O | 99 | GLU |
| 12 | 2O | 100 | ILE |
| 12 | 2O | 102 | LYS |
| 12 | 2O | 107 | HIS |
| 12 | 2O | 114 | ASP |
| 12 | 2O | 120 | THR |
| 12 | 2O | 140 | ASN |
| 12 | 2O | 141 | LYS |
| 12 | 2O | 143 | LEU |
| 12 | 2O | 148 | GLN |
| 12 | 2P | 215 | GLN |
| 12 | 2Q | 206 | ASN |
| 13 | 2T | 20 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2T | 23 | GLN |
| 13 | 2T | 24 | ILE |
| 13 | 2T | 26 | ASP |
| 13 | 2T | 27 | LYS |
| 13 | 2T | 28 | LYS |
| 13 | 2T | 29 | VAL |
| 13 | 2T | 35 | LYS |
| 13 | 2T | 37 | ILE |
| 13 | 2T | 46 | VAL |
| 13 | 2T | 47 | LEU |
| 13 | 2T | 48 | GLU |
| 13 | 2T | 49 | ILE |
| 13 | 2T | 57 | THR |
| 13 | 2T | 59 | ILE |
| 13 | 2T | 66 | LYS |
| 13 | 2T | 68 | THR |
| 13 | 2T | 71 | ILE |
| 13 | 2T | 72 | LYS |
| 13 | 2T | 77 | VAL |
| 13 | 2T | 78 | MET |
| 13 | 2T | 79 | ILE |
| 13 | 2T | 81 | LYS |
| 13 | 2T | 83 | LEU |
| 13 | 2T | 85 | LYS |
| 13 | 2T | 88 | THR |
| 13 | 2T | 89 | PHE |
| 13 | 2T | 93 | VAL |
| 13 | 2T | 95 | ASP |
| 13 | 2T | 97 | LYS |
| 13 | 2T | 99 | VAL |
| 13 | 2T | 100 | ARG |
| 13 | 2T | 101 | ARG |
| 13 | 2T | 102 | ARG |
| 13 | 2T | 103 | PHE |
| 13 | 2T | 104 | ARG |
| 13 | 2T | 106 | SER |
| 13 | 2T | 113 | ARG |
| 13 | 2T | 114 | VAL |
| 13 | 2T | 118 | ILE |
| 13 | 2T | 121 | MET |
| 13 | 2T | 123 | MET |
| 13 | 2T | 124 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2T | 125 | LEU |
| 13 | 2T | 130 | ASN |
| 13 | 2T | 138 | ASP |
| 13 | 2T | 141 | ARG |
| 13 | 2T | 153 | ARG |
| 13 | 2T | 154 | VAL |
| 13 | 2T | 162 | ILE |
| 13 | 2T | 171 | LEU |
| 13 | 2T | 173 | SER |
| 13 | 2T | 175 | ASP |
| 13 | 2T | 176 | GLU |
| 13 | 2T | 180 | GLU |
| 13 | 2T | 182 | LYS |
| 13 | 2T | 185 | LEU |
| 13 | 2U | 35 | LYS |
| 13 | 2U | 37 | ILE |
| 13 | 2U | 43 | GLN |
| 13 | 2U | 44 | SER |
| 13 | 2U | 47 | LEU |
| 13 | 2U | 48 | GLU |
| 13 | 2U | 50 | GLU |
| 13 | 2U | 57 | THR |
| 13 | 2U | 59 | ILE |
| 13 | 2U | 64 | ASP |
| 13 | 2U | 66 | LYS |
| 13 | 2U | 67 | LYS |
| 13 | 2U | 71 | ILE |
| 13 | 2U | 73 | LEU |
| 13 | 2U | 75 | PHE |
| 13 | 2U | 78 | MET |
| 13 | 2U | 80 | ILE |
| 13 | 2U | 83 | LEU |
| 13 | 2U | 84 | LYS |
| 13 | 2U | 88 | THR |
| 13 | 2U | 89 | PHE |
| 13 | 2U | 91 | VAL |
| 13 | 2U | 93 | VAL |
| 13 | 2U | 97 | LYS |
| 13 | 2U | 100 | ARG |
| 13 | 2U | 101 | ARG |
| 13 | 2U | 102 | ARG |
| 13 | 2U | 111 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2U | 112 | THR |
| 13 | 2U | 115 | LYS |
| 13 | 2U | 117 | PHE |
| 13 | 2U | 118 | ILE |
| 13 | 2U | 120 | THR |
| 13 | 2U | 121 | MET |
| 13 | 2U | 124 | ARG |
| 13 | 2U | 127 | ASP |
| 13 | 2U | 130 | ASN |
| 13 | 2U | 138 | ASP |
| 13 | 2U | 141 | ARG |
| 13 | 2U | 142 | ARG |
| 13 | 2U | 146 | THR |
| 13 | 2U | 152 | LEU |
| 13 | 2U | 154 | VAL |
| 13 | 2U | 160 | CYS |
| 13 | 2U | 161 | ARG |
| 13 | 2U | 162 | ILE |
| 13 | 2U | 163 | ARG |
| 13 | 2U | 169 | ASP |
| 13 | 2U | 170 | ARG |
| 13 | 2U | 171 | LEU |
| 13 | 2U | 174 | GLU |
| 13 | 2U | 176 | GLU |
| 13 | 2U | 177 | LEU |
| 13 | 2U | 180 | GLU |
| 13 | 2U | 184 | TYR |
| 13 | 2U | 185 | LEU |
| 13 | 2V | 36 | ARG |
| 13 | 2V | 37 | ILE |
| 13 | 2V | 40 | ASN |
| 13 | 2V | 46 | VAL |
| 13 | 2V | 47 | LEU |
| 13 | 2V | 52 | THR |
| 13 | 2V | 57 | THR |
| 13 | 2V | 59 | ILE |
| 13 | 2V | 64 | ASP |
| 13 | 2V | 66 | LYS |
| 13 | 2V | 67 | LYS |
| 13 | 2V | 68 | THR |
| 13 | 2V | 72 | LYS |
| 13 | 2V | 73 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2V | 78 | MET |
| 13 | 2V | 80 | ILE |
| 13 | 2V | 84 | LYS |
| 13 | 2V | 85 | LYS |
| 13 | 2V | 88 | THR |
| 13 | 2V | 94 | LEU |
| 13 | 2V | 97 | LYS |
| 13 | 2V | 99 | VAL |
| 13 | 2V | 100 | ARG |
| 13 | 2V | 101 | ARG |
| 13 | 2V | 102 | ARG |
| 13 | 2V | 112 | THR |
| 13 | 2V | 115 | LYS |
| 13 | 2V | 118 | ILE |
| 13 | 2V | 121 | MET |
| 13 | 2V | 124 | ARG |
| 13 | 2V | 125 | LEU |
| 13 | 2V | 126 | ASP |
| 13 | 2V | 127 | ASP |
| 13 | 2V | 130 | ASN |
| 13 | 2V | 131 | GLN |
| 13 | 2V | 133 | GLN |
| 13 | 2V | 134 | PHE |
| 13 | 2V | 135 | ASN |
| 13 | 2V | 137 | SER |
| 13 | 2V | 138 | ASP |
| 13 | 2V | 140 | THR |
| 13 | 2V | 141 | ARG |
| 13 | 2V | 144 | TYR |
| 13 | 2V | 146 | THR |
| 13 | 2V | 150 | GLU |
| 13 | 2V | 151 | THR |
| 13 | 2V | 153 | ARG |
| 13 | 2V | 154 | VAL |
| 13 | 2V | 156 | ILE |
| 13 | 2V | 162 | ILE |
| 13 | 2V | 163 | ARG |
| 13 | 2V | 168 | SER |
| 13 | 2V | 170 | ARG |
| 13 | 2V | 171 | LEU |
| 13 | 2V | 173 | SER |
| 13 | 2V | 175 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2V | 176 | GLU |
| 13 | 2V | 180 | GLU |
| 13 | 2V | 185 | LEU |
| 13 | 2W | 35 | LYS |
| 13 | 2W | 37 | ILE |
| 13 | 2W | 40 | ASN |
| 13 | 2W | 43 | GLN |
| 13 | 2W | 46 | VAL |
| 13 | 2W | 48 | GLU |
| 13 | 2W | 50 | GLU |
| 13 | 2W | 57 | THR |
| 13 | 2W | 64 | ASP |
| 13 | 2W | 66 | LYS |
| 13 | 2W | 67 | LYS |
| 13 | 2W | 72 | LYS |
| 13 | 2W | 73 | LEU |
| 13 | 2W | 78 | MET |
| 13 | 2W | 85 | LYS |
| 13 | 2W | 88 | THR |
| 13 | 2W | 91 | VAL |
| 13 | 2W | 93 | VAL |
| 13 | 2W | 97 | LYS |
| 13 | 2W | 99 | VAL |
| 13 | 2W | 101 | ARG |
| 13 | 2W | 104 | ARG |
| 13 | 2W | 109 | GLN |
| 13 | 2W | 111 | THR |
| 13 | 2W | 113 | ARG |
| 13 | 2W | 115 | LYS |
| 13 | 2W | 118 | ILE |
| 13 | 2W | 120 | THR |
| 13 | 2W | 121 | MET |
| 13 | 2W | 123 | MET |
| 13 | 2W | 124 | ARG |
| 13 | 2W | 126 | ASP |
| 13 | 2W | 130 | ASN |
| 13 | 2W | 131 | GLN |
| 13 | 2W | 134 | PHE |
| 13 | 2W | 140 | THR |
| 13 | 2W | 141 | ARG |
| 13 | 2W | 142 | ARG |
| 13 | 2W | 144 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2W | 150 | GLU |
| 13 | 2W | 152 | LEU |
| 13 | 2W | 153 | ARG |
| 13 | 2W | 156 | ILE |
| 13 | 2W | 157 | HIS |
| 13 | 2W | 161 | ARG |
| 13 | 2W | 168 | SER |
| 13 | 2W | 170 | ARG |
| 13 | 2W | 171 | LEU |
| 13 | 2W | 173 | SER |
| 13 | 2W | 175 | ASP |
| 13 | 2W | 180 | GLU |
| 13 | 2W | 184 | TYR |
| 13 | 2X | 1 | MET |
| 13 | 2X | 3 | LYS |
| 13 | 2X | 6 | PHE |
| 13 | 2X | 10 | PHE |
| 13 | 2X | 11 | LEU |
| 13 | 2X | 13 | ILE |
| 13 | 2X | 20 | LYS |
| 13 | 2X | 24 | ILE |
| 13 | 2X | 26 | ASP |
| 13 | 2X | 29 | VAL |
| 13 | 2X | 30 | ARG |
| 13 | 2X | 35 | LYS |
| 13 | 2X | 37 | ILE |
| 13 | 2X | 40 | ASN |
| 13 | 2X | 43 | GLN |
| 13 | 2X | 47 | LEU |
| 13 | 2X | 48 | GLU |
| 13 | 2X | 56 | THR |
| 13 | 2X | 57 | THR |
| 13 | 2X | 64 | ASP |
| 13 | 2X | 66 | LYS |
| 13 | 2X | 67 | LYS |
| 13 | 2X | 69 | LEU |
| 13 | 2X | 72 | LYS |
| 13 | 2X | 73 | LEU |
| 13 | 2X | 78 | MET |
| 13 | 2X | 80 | ILE |
| 13 | 2X | 85 | LYS |
| 13 | 2X | 89 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2X | 91 | VAL |
| 13 | 2X | 94 | LEU |
| 13 | 2X | 97 | LYS |
| 13 | 2X | 99 | VAL |
| 13 | 2X | 100 | ARG |
| 13 | 2X | 106 | SER |
| 13 | 2X | 107 | ASN |
| 13 | 2X | 111 | THR |
| 13 | 2X | 115 | LYS |
| 13 | 2X | 116 | PRO |
| 13 | 2X | 118 | ILE |
| 13 | 2X | 121 | MET |
| 13 | 2X | 124 | ARG |
| 13 | 2X | 126 | ASP |
| 13 | 2X | 127 | ASP |
| 13 | 2X | 130 | ASN |
| 13 | 2X | 131 | GLN |
| 13 | 2X | 134 | PHE |
| 13 | 2X | 140 | THR |
| 13 | 2X | 141 | ARG |
| 13 | 2X | 142 | ARG |
| 13 | 2X | 144 | TYR |
| 13 | 2X | 154 | VAL |
| 13 | 2X | 160 | CYS |
| 13 | 2X | 162 | ILE |
| 13 | 2X | 163 | ARG |
| 13 | 2X | 168 | SER |
| 13 | 2X | 170 | ARG |
| 13 | 2X | 171 | LEU |
| 13 | 2X | 175 | ASP |
| 13 | 2X | 176 | GLU |
| 13 | 2X | 180 | GLU |
| 13 | 2X | 182 | LYS |
| 13 | 2X | 183 | LEU |
| 14 | 3A | 110 | ARG |
| 14 | 3B | 104 | LYS |
| 15 | 3E | 395 | ARG |
| 15 | 3F | 30 | GLN |
| 15 | 3F | 172 | GLU |
| 15 | 3F | 173 | LYS |
| 15 | 3F | 180 | THR |
| 15 | 3F | 186 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | 3H | 54 | LYS |
| 15 | 3H | 206 | ARG |
| 16 | 3J | 63 | ARG |
| 16 | 3J | 332 | ASP |
| 16 | 3J | 333 | GLN |
| 16 | 3J | 335 | GLN |
| 16 | 3J | 340 | ASP |
| 16 | 3J | 341 | GLU |
| 16 | 3J | 344 | GLN |
| 16 | 3J | 345 | LEU |
| 16 | 3K | 73 | ARG |
| 16 | 3K | 124 | ARG |
| 16 | 3L | 166 | GLN |
| 16 | 3L | 368 | LYS |
| 17 | 3O | 350 | ARG |
| 17 | 3O | 356 | ASP |
| 17 | 3O | 361 | MET |
| 17 | 3O | 362 | GLN |
| 17 | 3O | 363 | ILE |
| 17 | 3O | 367 | LYS |
| 17 | 3O | 372 | ILE |
| 17 | 3O | 376 | GLU |
| 17 | 3O | 383 | LYS |
| 17 | 3O | 384 | LYS |
| 17 | 3O | 389 | LYS |
| 17 | 3O | 393 | LEU |
| 17 | 3O | 400 | LEU |
| 17 | 3O | 401 | ASP |
| 17 | 3O | 405 | ARG |
| 17 | 3O | 408 | ASN |
| 17 | 3O | 409 | ILE |
| 17 | 3O | 415 | MET |
| 17 | 3O | 418 | LEU |
| 17 | 3O | 426 | GLU |
| 17 | 3O | 429 | ASP |
| 17 | 3O | 431 | ILE |
| 17 | 3O | 457 | HIS |
| 17 | 3P | 93 | ARG |
| 17 | 3P | 104 | LEU |
| 17 | 3P | 107 | TYR |
| 17 | 3P | 110 | SER |
| 17 | 3P | 117 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 3P | 126 | ARG |
| 17 | 3P | 130 | ASP |
| 17 | 3P | 131 | LYS |
| 17 | 3P | 135 | THR |
| 17 | 3P | 136 | ARG |
| 17 | 3P | 137 | LYS |
| 17 | 3P | 139 | GLN |
| 17 | 3P | 141 | ASP |
| 17 | 3P | 142 | SER |
| 17 | 3P | 157 | LYS |
| 17 | 3P | 162 | HIS |
| 17 | 3P | 174 | LEU |
| 17 | 3P | 175 | THR |
| 17 | 3P | 176 | ASP |
| 17 | 3P | 178 | LYS |
| 17 | 3P | 179 | LYS |
| 17 | 3P | 182 | GLU |
| 17 | 3P | 186 | MET |
| 17 | 3P | 189 | GLU |
| 17 | 3P | 192 | LEU |
| 17 | 3P | 196 | ARG |
| 17 | 3P | 198 | CYS |
| 17 | 3P | 199 | LEU |
| 17 | 3P | 203 | GLU |
| 17 | 3P | 204 | LYS |
| 17 | 3P | 205 | ARG |
| 17 | 3P | 206 | MET |
| 17 | 3P | 211 | VAL |
| 17 | 3P | 218 | GLU |
| 17 | 3P | 220 | LEU |
| 17 | 3P | 222 | GLU |
| 17 | 3P | 226 | ILE |
| 17 | 3P | 228 | CYS |
| 17 | 3P | 231 | GLU |
| 17 | 3P | 235 | LEU |
| 17 | 3P | 237 | LEU |
| 17 | 3P | 239 | LYS |
| 17 | 3P | 243 | GLN |
| 17 | 3P | 248 | ARG |
| 17 | 3P | 251 | GLN |
| 17 | 3P | 252 | HIS |
| 17 | 3P | 254 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 3P | 256 | LYS |
| 17 | 3P | 258 | LEU |
| 17 | 3P | 269 | ASP |
| 17 | 3P | 275 | ARG |
| 17 | 3P | 276 | ASN |
| 17 | 3P | 278 | SER |
| 17 | 3P | 279 | ASP |
| 17 | 3P | 282 | SER |
| 17 | 3P | 285 | ARG |
| 17 | 3P | 288 | GLU |
| 17 | 3P | 289 | ARG |
| 17 | 3P | 293 | THR |
| 17 | 3P | 296 | VAL |
| 17 | 3P | 302 | LYS |
| 17 | 3P | 303 | PHE |
| 17 | 3P | 304 | THR |
| 17 | 3P | 305 | ASP |
| 17 | 3P | 310 | ARG |
| 17 | 3P | 311 | SER |
| 17 | 3P | 312 | GLN |
| 17 | 3P | 322 | ARG |
| 17 | 3P | 323 | ASP |
| 17 | 3P | 328 | LEU |
| 17 | 3P | 329 | LEU |
| 17 | 3P | 342 | LYS |
| 17 | 3P | 345 | LEU |
| 17 | 3P | 347 | PHE |
| 17 | 3P | 350 | ARG |
| 17 | 3P | 353 | GLU |
| 17 | 3P | 360 | LYS |
| 17 | 3P | 361 | MET |
| 17 | 3P | 369 | LEU |
| 17 | 3P | 372 | ILE |
| 17 | 3P | 384 | LYS |
| 17 | 3P | 387 | ARG |
| 17 | 3P | 388 | ASP |
| 17 | 3P | 395 | VAL |
| 17 | 3P | 405 | ARG |
| 17 | 3P | 408 | ASN |
| 17 | 3P | 409 | ILE |
| 17 | 3P | 415 | MET |
| 17 | 3P | 419 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 3P | 420 | LEU |
| 17 | 3P | 421 | VAL |
| 17 | 3P | 429 | ASP |
| 17 | 3P | 434 | LEU |
| 17 | 3P | 435 | GLN |
| 17 | 3P | 437 | ARG |
| 17 | 3P | 438 | LEU |
| 17 | 3P | 440 | ASP |
| 17 | 3P | 444 | THR |
| 17 | 3P | 452 | LYS |
| 17 | 3P | 455 | LEU |
| 17 | 3P | 465 | SER |
| 17 | 3P | 468 | ILE |
| 17 | 3P | 472 | LYS |
| 17 | 3P | 478 | LYS |
| 17 | 3P | 483 | THR |
| 17 | 3Q | 345 | LEU |
| 17 | 3Q | 347 | PHE |
| 17 | 3Q | 350 | ARG |
| 17 | 3Q | 351 | ILE |
| 17 | 3Q | 353 | GLU |
| 17 | 3Q | 356 | ASP |
| 17 | 3Q | 358 | LYS |
| 17 | 3Q | 360 | LYS |
| 17 | 3Q | 364 | HIS |
| 17 | 3Q | 371 | GLU |
| 17 | 3Q | 379 | ILE |
| 17 | 3Q | 383 | LYS |
| 17 | 3Q | 384 | LYS |
| 17 | 3Q | 387 | ARG |
| 17 | 3Q | 388 | ASP |
| 17 | 3Q | 389 | LYS |
| 17 | 3Q | 398 | THR |
| 17 | 3Q | 401 | ASP |
| 17 | 3Q | 409 | ILE |
| 17 | 3Q | 410 | GLU |
| 17 | 3Q | 412 | CYS |
| 17 | 3Q | 413 | ARG |
| 17 | 3Q | 414 | ASP |
| 17 | 3Q | 415 | MET |
| 17 | 3Q | 418 | LEU |
| 17 | 3Q | 419 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 3Q | 420 | LEU |
| 17 | 3Q | 421 | VAL |
| 17 | 3Q | 429 | ASP |
| 17 | 3Q | 431 | ILE |
| 17 | 3Q | 434 | LEU |
| 17 | 3Q | 435 | GLN |
| 17 | 3Q | 437 | ARG |
| 17 | 3Q | 438 | LEU |
| 17 | 3Q | 444 | THR |
| 17 | 3Q | 446 | GLN |
| 17 | 3Q | 452 | LYS |
| 17 | 3Q | 458 | ASP |
| 17 | 3Q | 459 | LEU |
| 17 | 3Q | 462 | LYS |
| 17 | 3Q | 465 | SER |
| 17 | 3Q | 466 | LEU |
| 17 | 3Q | 470 | GLN |
| 17 | 3Q | 471 | GLU |
| 17 | 3Q | 472 | LYS |
| 17 | 3R | 93 | ARG |
| 17 | 3R | 95 | THR |
| 17 | 3R | 97 | ASP |
| 17 | 3R | 98 | ASP |
| 17 | 3R | 101 | ARG |
| 17 | 3R | 104 | LEU |
| 17 | 3R | 106 | ASN |
| 17 | 3R | 108 | LEU |
| 17 | 3R | 109 | GLU |
| 17 | 3R | 110 | SER |
| 17 | 3R | 117 | SER |
| 17 | 3R | 119 | ARG |
| 17 | 3R | 120 | LEU |
| 17 | 3R | 126 | ARG |
| 17 | 3R | 130 | ASP |
| 17 | 3R | 133 | GLN |
| 17 | 3R | 134 | GLN |
| 17 | 3R | 135 | THR |
| 17 | 3R | 136 | ARG |
| 17 | 3R | 143 | THR |
| 17 | 3R | 144 | GLN |
| 17 | 3R | 146 | LEU |
| 17 | 3R | 151 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 3R | 156 | TRP |
| 17 | 3R | 157 | LYS |
| 17 | 3R | 159 | GLU |
| 17 | 3R | 162 | HIS |
| 17 | 3R | 165 | ASP |
| 17 | 3R | 172 | ASN |
| 17 | 3R | 176 | ASP |
| 17 | 3R | 178 | LYS |
| 17 | 3R | 179 | LYS |
| 17 | 3R | 183 | ARG |
| 17 | 3R | 185 | LEU |
| 17 | 3R | 189 | GLU |
| 17 | 3R | 193 | GLN |
| 17 | 3R | 204 | LYS |
| 17 | 3R | 206 | MET |
| 17 | 3R | 208 | ILE |
| 17 | 3R | 210 | LEU |
| 17 | 3R | 211 | VAL |
| 17 | 3R | 213 | ASP |
| 17 | 3R | 214 | GLU |
| 17 | 3R | 216 | GLU |
| 17 | 3R | 217 | THR |
| 17 | 3R | 220 | LEU |
| 17 | 3R | 223 | VAL |
| 17 | 3R | 225 | ILE |
| 17 | 3R | 228 | CYS |
| 17 | 3R | 232 | ARG |
| 17 | 3R | 234 | LYS |
| 17 | 3R | 235 | LEU |
| 17 | 3R | 236 | HIS |
| 17 | 3R | 237 | LEU |
| 17 | 3R | 238 | ASP |
| 17 | 3R | 239 | LYS |
| 17 | 3R | 253 | GLU |
| 17 | 3R | 254 | LEU |
| 17 | 3R | 258 | LEU |
| 17 | 3R | 260 | ASP |
| 17 | 3R | 261 | LYS |
| 17 | 3R | 266 | ARG |
| 17 | 3R | 269 | ASP |
| 17 | 3R | 270 | LYS |
| 17 | 3R | 275 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | 3R | 279 | ASP |
| 17 | 3R | 282 | SER |
| 17 | 3R | 283 | TYR |
| 17 | 3R | 285 | ARG |
| 17 | 3R | 289 | ARG |
| 17 | 3R | 290 | VAL |
| 17 | 3R | 291 | ASP |
| 17 | 3R | 298 | GLU |
| 17 | 3R | 302 | LYS |
| 17 | 3R | 305 | ASP |
| 17 | 3R | 307 | ASN |
| 17 | 3R | 309 | LEU |
| 17 | 3R | 310 | ARG |
| 17 | 3R | 311 | SER |
| 17 | 3R | 313 | SER |
| 17 | 3R | 320 | LYS |
| 17 | 3R | 321 | LEU |
| 17 | 3R | 323 | ASP |
| 17 | 3R | 324 | ASP |
| 17 | 3R | 328 | LEU |
| 17 | 3R | 331 | VAL |
| 17 | 3R | 334 | ASN |
| 17 | 3R | 339 | GLN |
| 17 | 3R | 342 | LYS |
| 17 | 3R | 345 | LEU |
| 17 | 3R | 347 | PHE |
| 17 | 3R | 349 | ASN |
| 17 | 3R | 350 | ARG |
| 17 | 3R | 353 | GLU |
| 18 | 3T | 421 | ASN |
| 18 | 3T | 426 | ASN |
| 18 | 3U | 136 | GLN |
| 18 | 3U | 307 | ARG |
| 18 | 3W | 306 | ARG |
| 19 | 3Y | 166 | GLU |
| 19 | 3Y | 176 | LYS |
| 19 | 3Y | 180 | GLU |
| 19 | 3Y | 182 | GLN |
| 19 | 3Y | 215 | CYS |
| 19 | 3Y | 220 | GLU |
| 19 | 3Y | 223 | LYS |
| 19 | 3Z | 380 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | 3Z | 382 | ARG |
| 20 | 4A | 11 | LYS |
| 20 | 4A | 16 | ILE |
| 20 | 4A | 20 | ARG |
| 20 | 4A | 23 | GLU |
| 20 | 4A | 25 | GLU |
| 20 | 4A | 26 | ARG |
| 20 | 4A | 27 | GLN |
| 20 | 4A | 29 | ARG |
| 20 | 4A | 31 | LEU |
| 20 | 4A | 32 | ASN |
| 20 | 4A | 34 | ARG |
| 20 | 4A | 36 | ARG |
| 20 | 4A | 38 | MET |
| 20 | 4A | 41 | ASP |
| 20 | 4A | 42 | VAL |
| 20 | 4A | 45 | LEU |
| 20 | 4A | 51 | GLU |
| 20 | 4A | 52 | ARG |
| 20 | 4A | 54 | LEU |
| 20 | 4A | 56 | GLU |
| 20 | 4A | 69 | ASN |
| 20 | 4A | 70 | GLN |
| 20 | 4A | 74 | ASP |
| 20 | 4A | 82 | LYS |
| 20 | 4A | 84 | GLN |
| 20 | 4A | 93 | LYS |
| 20 | 4A | 94 | LYS |
| 20 | 4A | 97 | GLU |
| 20 | 4A | 100 | GLU |
| 20 | 4A | 149 | ARG |
| 20 | 4A | 155 | MET |
| 20 | 4A | 158 | GLU |
| 20 | 4A | 160 | PHE |
| 20 | 4A | 167 | GLN |
| 20 | 4A | 168 | LEU |
| 20 | 4A | 170 | GLU |
| 20 | 4A | 173 | GLN |
| 20 | 4A | 178 | TYR |
| 20 | 4A | 183 | MET |
| 20 | 4A | 185 | ASN |
| 20 | 4A | 189 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | 4A | 192 | MET |
| 20 | 4A | 194 | MET |
| 20 | 4A | 195 | ARG |
| 20 | 4A | 198 | GLN |
| 20 | 4A | 199 | MET |
| 20 | 4A | 202 | LEU |
| 20 | 4A | 203 | GLU |
| 20 | 4A | 204 | GLU |
| 20 | 4A | 207 | ARG |
| 20 | 4A | 208 | MET |
| 20 | 4A | 214 | MET |
| 20 | 4A | 216 | ASN |
| 20 | 4A | 219 | LYS |
| 20 | 4A | 228 | ARG |
| 20 | 4A | 230 | ARG |
| 20 | 4A | 232 | GLU |
| 20 | 4A | 233 | HIS |
| 20 | 4A | 234 | GLN |
| 20 | 4B | 228 | ARG |
| 20 | 4B | 230 | ARG |
| 20 | 4B | 231 | ARG |
| 20 | 4B | 232 | GLU |
| 20 | 4B | 233 | HIS |
| 20 | 4B | 234 | GLN |
| 20 | 4B | 241 | LEU |
| 20 | 4B | 243 | GLU |
| 20 | 4B | 246 | ASN |
| 20 | 4B | 247 | GLN |
| 20 | 4B | 248 | ILE |
| 20 | 4B | 254 | THR |
| 20 | 4B | 258 | GLN |
| 20 | 4B | 259 | VAL |
| 20 | 4B | 277 | MET |
| 20 | 4B | 280 | GLU |
| 20 | 4B | 282 | ARG |
| 20 | 4B | 285 | ILE |
| 20 | 4B | 286 | ARG |
| 20 | 4B | 287 | LYS |
| 20 | 4B | 290 | GLU |
| 20 | 4B | 294 | HIS |
| 20 | 4B | 311 | GLU |
| 20 | 4B | 312 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | 4B | 319 | ARG |
| 20 | 4B | 323 | GLU |
| 20 | 4B | 324 | LEU |
| 20 | 4B | 325 | GLU |
| 20 | 4B | 329 | ARG |
| 20 | 4B | 331 | LEU |
| 20 | 4B | 339 | LEU |
| 20 | 4B | 344 | GLN |
| 20 | 4B | 349 | GLU |
| 20 | 4B | 351 | LYS |
| 20 | 4B | 353 | GLN |
| 20 | 4B | 356 | TYR |
| 20 | 4B | 357 | LEU |
| 20 | 4B | 358 | ASN |
| 21 | 4D | 34 | ARG |
| 21 | 4D | 407 | LYS |
| 21 | 4D | 408 | ASP |
| 21 | 4D | 410 | ILE |
| 21 | 4D | 411 | LYS |
| 21 | 4D | 412 | MET |
| 21 | 4D | 415 | ASN |
| 21 | 4D | 416 | ASP |
| 21 | 4D | 417 | ASN |
| 21 | 4D | 418 | LYS |
| 21 | 4D | 421 | ARG |
| 21 | 4D | 426 | LEU |
| 21 | 4D | 430 | ILE |
| 21 | 4D | 432 | GLU |
| 21 | 4D | 434 | LYS |
| 21 | 4D | 436 | ARG |
| 21 | 4D | 437 | ARG |
| 21 | 4D | 439 | VAL |
| 21 | 4D | 440 | LEU |
| 21 | 4D | 448 | MET |
| 21 | 4D | 449 | ILE |
| 21 | 4D | 450 | SER |
| 21 | 4D | 456 | VAL |
| 21 | 4D | 457 | ARG |
| 21 | 4D | 458 | ASN |
| 21 | 4D | 461 | ILE |
| 21 | 4D | 465 | LYS |
| 21 | 4D | 466 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | 4D | 469 | ARG |
| 21 | 4D | 471 | LYS |
| 21 | 4D | 474 | LYS |
| 21 | 4D | 479 | MET |
| 21 | 4D | 483 | ILE |
| 21 | 4D | 492 | ILE |
| 21 | 4D | 501 | HIS |
| 21 | 4D | 502 | ARG |
| 21 | 4D | 504 | VAL |
| 21 | 4D | 505 | ILE |
| 21 | 4D | 506 | LEU |
| 21 | 4D | 509 | ASP |
| 21 | 4D | 510 | ASP |
| 21 | 4D | 513 | LEU |
| 21 | 4D | 516 | MET |
| 21 | 4D | 517 | GLU |
| 21 | 4D | 528 | LEU |
| 21 | 4D | 531 | ILE |
| 21 | 4D | 532 | GLN |
| 21 | 4D | 533 | ASN |
| 21 | 4D | 535 | ILE |
| 21 | 4E | 407 | LYS |
| 21 | 4E | 408 | ASP |
| 21 | 4E | 411 | LYS |
| 21 | 4E | 412 | MET |
| 21 | 4E | 417 | ASN |
| 21 | 4E | 419 | VAL |
| 21 | 4E | 421 | ARG |
| 21 | 4E | 427 | GLU |
| 21 | 4E | 428 | SER |
| 21 | 4E | 430 | ILE |
| 21 | 4E | 434 | LYS |
| 21 | 4E | 437 | ARG |
| 21 | 4E | 439 | VAL |
| 21 | 4E | 440 | LEU |
| 21 | 4E | 442 | TYR |
| 21 | 4E | 444 | LEU |
| 21 | 4E | 446 | THR |
| 21 | 4E | 447 | ASP |
| 21 | 4E | 449 | ILE |
| 21 | 4E | 451 | ILE |
| 21 | 4E | 453 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | 4E | 456 | VAL |
| 21 | 4E | 461 | ILE |
| 21 | 4E | 462 | ILE |
| 21 | 4E | 465 | LYS |
| 21 | 4E | 466 | TYR |
| 21 | 4E | 467 | LEU |
| 21 | 4E | 469 | ARG |
| 21 | 4E | 472 | VAL |
| 21 | 4E | 474 | LYS |
| 21 | 4E | 477 | SER |
| 21 | 4E | 480 | GLU |
| 21 | 4E | 481 | ASN |
| 21 | 4E | 485 | TYR |
| 21 | 4E | 488 | SER |
| 21 | 4E | 496 | ILE |
| 21 | 4E | 497 | GLU |
| 21 | 4E | 501 | HIS |
| 21 | 4E | 506 | LEU |
| 21 | 4E | 509 | ASP |
| 21 | 4E | 517 | GLU |
| 21 | 4E | 526 | GLU |
| 21 | 4E | 530 | SER |
| 21 | 4E | 531 | ILE |
| 21 | 4E | 532 | GLN |
| 21 | 4F | 281 | ARG |
| 21 | 4F | 407 | LYS |
| 21 | 4F | 408 | ASP |
| 21 | 4F | 411 | LYS |
| 21 | 4F | 413 | LEU |
| 21 | 4F | 414 | MET |
| 21 | 4F | 415 | ASN |
| 21 | 4F | 418 | LYS |
| 21 | 4F | 419 | VAL |
| 21 | 4F | 421 | ARG |
| 21 | 4F | 422 | TYR |
| 21 | 4F | 430 | ILE |
| 21 | 4F | 433 | ASP |
| 21 | 4F | 434 | LYS |
| 21 | 4F | 436 | ARG |
| 21 | 4F | 437 | ARG |
| 21 | 4F | 439 | VAL |
| 21 | 4F | 446 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | 4F | 450 | SER |
| 21 | 4F | 453 | GLU |
| 21 | 4F | 456 | VAL |
| 21 | 4F | 461 | ILE |
| 21 | 4F | 462 | ILE |
| 21 | 4F | 465 | LYS |
| 21 | 4F | 467 | LEU |
| 21 | 4F | 471 | LYS |
| 21 | 4F | 472 | VAL |
| 21 | 4F | 474 | LYS |
| 21 | 4F | 476 | ASP |
| 21 | 4F | 483 | ILE |
| 21 | 4F | 489 | ASP |
| 21 | 4F | 498 | VAL |
| 21 | 4F | 502 | ARG |
| 21 | 4F | 504 | VAL |
| 21 | 4F | 505 | ILE |
| 21 | 4F | 506 | LEU |
| 21 | 4F | 508 | SER |
| 21 | 4F | 510 | ASP |
| 21 | 4F | 513 | LEU |
| 21 | 4F | 514 | LYS |
| 21 | 4F | 519 | ASN |
| 21 | 4F | 520 | PRO |
| 21 | 4F | 522 | GLN |
| 21 | 4F | 526 | GLU |
| 21 | 4F | 534 | HIS |
| 21 | 4F | 535 | ILE |
| 22 | 4H | 6 | LEU |
| 22 | 4H | 9 | ASN |
| 22 | 4H | 10 | SER |
| 22 | 4H | 12 | ASN |
| 22 | 4H | 14 | ASN |
| 22 | 4H | 17 | LYS |
| 22 | 4H | 19 | LYS |
| 22 | 4H | 21 | HIS |
| 22 | 4I | 272 | ARG |
| 22 | 4I | 615 | ASP |
| 22 | 4I | 617 | CYS |
| 22 | 4I | 618 | ILE |
| 22 | 4I | 619 | VAL |
| 22 | 4I | 624 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 4I | 628 | LYS |
| 22 | 4I | 629 | LYS |
| 22 | 4I | 633 | GLU |
| 22 | 4I | 635 | PHE |
| 22 | 4I | 637 | ARG |
| 22 | 4I | 638 | LEU |
| 22 | 4I | 642 | CYS |
| 22 | 4I | 643 | VAL |
| 22 | 4I | 644 | TYR |
| 22 | 4I | 646 | ASP |
| 22 | 4I | 649 | LYS |
| 22 | 4I | 650 | LYS |
| 22 | 4I | 651 | LYS |
| 22 | 4I | 652 | VAL |
| 22 | 4I | 653 | LEU |
| 22 | 4I | 655 | SER |
| 22 | 4I | 656 | LYS |
| 22 | 4I | 658 | ILE |
| 22 | 4I | 659 | LYS |
| 22 | 4I | 660 | ARG |
| 22 | 4I | 663 | LYS |
| 22 | 4I | 664 | SER |
| 22 | 4I | 665 | SER |
| 22 | 4I | 667 | LEU |
| 22 | 4I | 670 | ASN |
| 22 | 4I | 673 | LEU |
| 22 | 4I | 677 | LEU |
| 22 | 4I | 680 | LYS |
| 22 | 4I | 685 | GLU |
| 22 | 4I | 690 | TYR |
| 22 | 4I | 691 | GLU |
| 22 | 4I | 695 | CYS |
| 22 | 4I | 698 | ASN |
| 22 | 4I | 700 | ARG |
| 22 | 4I | 702 | ASN |
| 22 | 4J | 31 | ASN |
| 22 | 4J | 615 | ASP |
| 22 | 4J | 618 | ILE |
| 22 | 4J | 620 | MET |
| 22 | 4J | 626 | GLN |
| 22 | 4J | 627 | LEU |
| 22 | 4J | 628 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 4J | 629 | LYS |
| 22 | 4J | 630 | HIS |
| 22 | 4J | 633 | GLU |
| 22 | 4J | 635 | PHE |
| 22 | 4J | 637 | ARG |
| 22 | 4J | 639 | ILE |
| 22 | 4J | 646 | ASP |
| 22 | 4J | 649 | LYS |
| 22 | 4J | 650 | LYS |
| 22 | 4J | 651 | LYS |
| 22 | 4J | 652 | VAL |
| 22 | 4J | 656 | LYS |
| 22 | 4J | 659 | LYS |
| 22 | 4J | 660 | ARG |
| 22 | 4J | 663 | LYS |
| 22 | 4J | 666 | ARG |
| 22 | 4J | 667 | LEU |
| 22 | 4J | 669 | PHE |
| 22 | 4J | 670 | ASN |
| 22 | 4J | 671 | ASP |
| 22 | 4J | 672 | ASP |
| 22 | 4J | 674 | LEU |
| 22 | 4J | 677 | LEU |
| 22 | 4J | 678 | LEU |
| 22 | 4J | 680 | LYS |
| 22 | 4J | 685 | GLU |
| 22 | 4J | 686 | LYS |
| 22 | 4J | 688 | ILE |
| 22 | 4J | 690 | TYR |
| 22 | 4J | 695 | CYS |
| 22 | 4J | 699 | TRP |
| 22 | 4J | 700 | ARG |
| 22 | 4J | 702 | ASN |
| 22 | 4K | 435 | ARG |
| 22 | 4K | 551 | LYS |
| 22 | 4K | 553 | LYS |
| 22 | 4K | 555 | GLU |
| 22 | 4K | 558 | LYS |
| 22 | 4K | 560 | ARG |
| 22 | 4K | 561 | GLU |
| 22 | 4K | 562 | LEU |
| 22 | 4K | 615 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 22 | 4K | 617 | CYS |
| 22 | 4K | 618 | ILE |
| 22 | 4K | 619 | VAL |
| 22 | 4K | 620 | MET |
| 22 | 4K | 628 | LYS |
| 22 | 4K | 629 | LYS |
| 22 | 4K | 633 | GLU |
| 22 | 4K | 635 | PHE |
| 22 | 4K | 636 | GLU |
| 22 | 4K | 637 | ARG |
| 22 | 4K | 638 | LEU |
| 22 | 4K | 646 | ASP |
| 22 | 4K | 647 | ARG |
| 22 | 4K | 649 | LYS |
| 22 | 4K | 650 | LYS |
| 22 | 4K | 651 | LYS |
| 22 | 4K | 652 | VAL |
| 22 | 4K | 653 | LEU |
| 22 | 4K | 656 | LYS |
| 22 | 4K | 657 | ASP |
| 22 | 4K | 659 | LYS |
| 22 | 4K | 660 | ARG |
| 22 | 4K | 663 | LYS |
| 22 | 4K | 670 | ASN |
| 22 | 4K | 672 | ASP |
| 22 | 4K | 673 | LEU |
| 22 | 4K | 678 | LEU |
| 22 | 4K | 680 | LYS |
| 22 | 4K | 686 | LYS |
| 22 | 4K | 690 | TYR |
| 22 | 4K | 695 | CYS |
| 22 | 4K | 697 | LEU |
| 22 | 4K | 698 | ASN |
| 22 | 4K | 699 | TRP |
| 22 | 4K | 700 | ARG |
| 22 | 4K | 702 | ASN |
| 23 | 4M | 17 | HIS |
| 23 | 4M | 19 | ILE |
| 23 | 4M | 20 | PRO |
| 23 | 4M | 30 | ARG |
| 23 | 4M | 33 | MET |
| 23 | 4M | 35 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | 4M | 36 | THR |
| 23 | 4M | 40 | THR |
| 23 | 4M | 43 | GLN |
| 23 | 4M | 45 | LEU |
| 23 | 4M | 51 | LEU |
| 23 | 4M | 61 | LEU |
| 23 | 4M | 86 | LEU |
| 23 | 4M | 90 | MET |
| 23 | 4M | 100 | GLN |
| 23 | 4M | 102 | GLN |
| 23 | 4M | 103 | PHE |
| 23 | 4M | 104 | ILE |
| 23 | 4M | 110 | ASN |
| 23 | 4M | 115 | GLU |
| 23 | 4M | 118 | ASN |
| 23 | 4M | 174 | MET |
| 23 | 4M | 176 | ASP |
| 23 | 4M | 177 | ARG |
| 23 | 4M | 180 | ARG |
| 23 | 4M | 183 | PHE |
| 23 | 4M | 184 | MET |
| 23 | 4M | 190 | TYR |
| 23 | 4M | 191 | VAL |
| 23 | 4M | 195 | ARG |
| 23 | 4M | 197 | LEU |
| 23 | 4M | 198 | PHE |
| 23 | 4M | 201 | SER |
| 23 | 4M | 204 | VAL |
| 23 | 4M | 208 | GLN |
| 23 | 4M | 210 | LEU |
| 23 | 4M | 211 | GLN |
| 23 | 4M | 212 | GLU |
| 23 | 4M | 215 | GLN |
| 23 | 4M | 216 | MET |
| 23 | 4M | 217 | LYS |
| 23 | 4M | 219 | GLN |
| 23 | 4M | 233 | SER |
| 23 | 4M | 234 | ARG |
| 23 | 4M | 239 | ASN |
| 23 | 4M | 240 | LEU |
| 23 | 4M | 242 | LEU |
| 23 | 4M | 243 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | 4M | 245 | LYS |
| 23 | 4M | 249 | TYR |
| 23 | 4M | 250 | VAL |
| 23 | 4M | 254 | LYS |
| 23 | 4M | 255 | PHE |
| 23 | 4M | 256 | GLN |
| 23 | 4M | 260 | THR |
| 23 | 4M | 261 | TYR |
| 23 | 4M | 263 | HIS |
| 23 | 4M | 267 | ASP |
| 23 | 4M | 269 | LEU |
| 23 | 4N | 17 | HIS |
| 23 | 4N | 19 | ILE |
| 23 | 4N | 20 | PRO |
| 23 | 4N | 26 | CYS |
| 23 | 4N | 33 | MET |
| 23 | 4N | 40 | THR |
| 23 | 4N | 45 | LEU |
| 23 | 4N | 46 | ARG |
| 23 | 4N | 48 | SER |
| 23 | 4N | 58 | ARG |
| 23 | 4N | 61 | LEU |
| 23 | 4N | 86 | LEU |
| 23 | 4N | 87 | SER |
| 23 | 4N | 90 | MET |
| 23 | 4N | 91 | ILE |
| 23 | 4N | 102 | GLN |
| 23 | 4N | 104 | ILE |
| 23 | 4N | 107 | LYS |
| 23 | 4N | 111 | GLN |
| 23 | 4N | 118 | ASN |
| 23 | 4N | 173 | SER |
| 23 | 4N | 174 | MET |
| 23 | 4N | 175 | ASP |
| 23 | 4N | 177 | ARG |
| 23 | 4N | 180 | ARG |
| 23 | 4N | 181 | LYS |
| 23 | 4N | 182 | PHE |
| 23 | 4N | 183 | PHE |
| 23 | 4N | 195 | ARG |
| 23 | 4N | 196 | PHE |
| 23 | 4N | 197 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | 4N | 198 | PHE |
| 23 | 4N | 201 | SER |
| 23 | 4N | 204 | VAL |
| 23 | 4N | 205 | LEU |
| 23 | 4N | 206 | SER |
| 23 | 4N | 208 | GLN |
| 23 | 4N | 210 | LEU |
| 23 | 4N | 211 | GLN |
| 23 | 4N | 212 | GLU |
| 23 | 4N | 215 | GLN |
| 23 | 4N | 233 | SER |
| 23 | 4N | 236 | TYR |
| 23 | 4N | 239 | ASN |
| 23 | 4N | 240 | LEU |
| 23 | 4N | 242 | LEU |
| 23 | 4N | 245 | LYS |
| 23 | 4N | 246 | TYR |
| 23 | 4N | 250 | VAL |
| 23 | 4N | 254 | LYS |
| 23 | 4N | 255 | PHE |
| 23 | 4N | 256 | GLN |
| 23 | 4N | 257 | PHE |
| 23 | 4N | 260 | THR |
| 23 | 4N | 261 | TYR |
| 23 | 4N | 263 | HIS |
| 23 | 4N | 267 | ASP |
| 23 | 4N | 269 | LEU |
| 24 | 4O | 170 | SER |
| 24 | 4O | 172 | TYR |
| 24 | 4O | 176 | ASP |
| 24 | 4O | 177 | ARG |
| 24 | 4O | 178 | ASP |
| 24 | 4O | 180 | ARG |
| 24 | 4O | 181 | LYS |
| 24 | 4O | 182 | PHE |
| 24 | 4O | 184 | MET |
| 24 | 4O | 185 | SER |
| 24 | 4O | 191 | VAL |
| 24 | 4O | 192 | PRO |
| 24 | 4O | 196 | PHE |
| 24 | 4O | 197 | LEU |
| 24 | 4O | 202 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | 4O | 208 | GLN |
| 24 | 4O | 210 | LEU |
| 24 | 4O | 211 | GLN |
| 24 | 4O | 213 | PHE |
| 24 | 4O | 214 | ASP |
| 24 | 4O | 217 | LYS |
| 24 | 4O | 218 | SER |
| 24 | 4O | 234 | ARG |
| 24 | 4O | 235 | THR |
| 24 | 4O | 239 | ASN |
| 24 | 4O | 240 | LEU |
| 24 | 4O | 242 | LEU |
| 24 | 4O | 243 | LEU |
| 24 | 4O | 245 | LYS |
| 24 | 4O | 250 | VAL |
| 24 | 4O | 255 | PHE |
| 24 | 4O | 257 | PHE |
| 24 | 4O | 259 | ARG |
| 24 | 4O | 266 | HIS |
| 24 | 4O | 267 | ASP |
| 24 | 4O | 269 | LEU |
| 23 | 4P | 177 | ARG |
| 23 | 4P | 180 | ARG |
| 23 | 4P | 181 | LYS |
| 23 | 4P | 183 | PHE |
| 23 | 4P | 184 | MET |
| 23 | 4P | 185 | SER |
| 23 | 4P | 191 | VAL |
| 23 | 4P | 193 | ARG |
| 23 | 4P | 195 | ARG |
| 23 | 4P | 196 | PHE |
| 23 | 4P | 197 | LEU |
| 23 | 4P | 198 | PHE |
| 23 | 4P | 200 | SER |
| 23 | 4P | 206 | SER |
| 23 | 4P | 210 | LEU |
| 23 | 4P | 211 | GLN |
| 23 | 4P | 215 | GLN |
| 23 | 4P | 216 | MET |
| 23 | 4P | 217 | LYS |
| 23 | 4P | 233 | SER |
| 23 | 4P | 236 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | 4P | 239 | ASN |
| 23 | 4P | 240 | LEU |
| 23 | 4P | 242 | LEU |
| 23 | 4P | 245 | LYS |
| 23 | 4P | 246 | TYR |
| 23 | 4P | 250 | VAL |
| 23 | 4P | 254 | LYS |
| 23 | 4P | 255 | PHE |
| 23 | 4P | 256 | GLN |
| 23 | 4P | 257 | PHE |
| 23 | 4P | 260 | THR |
| 23 | 4P | 261 | TYR |
| 23 | 4P | 263 | HIS |
| 23 | 4P | 267 | ASP |
| 23 | 4P | 269 | LEU |
| 23 | 4Q | 15 | ASN |
| 23 | 4Q | 17 | HIS |
| 23 | 4Q | 19 | ILE |
| 23 | 4Q | 20 | PRO |
| 23 | 4Q | 32 | SER |
| 23 | 4Q | 100 | GLN |
| 23 | 4Q | 102 | GLN |
| 23 | 4Q | 107 | LYS |
| 23 | 4Q | 110 | ASN |
| 23 | 4Q | 115 | GLU |
| 23 | 4Q | 174 | MET |
| 23 | 4Q | 175 | ASP |
| 23 | 4Q | 177 | ARG |
| 23 | 4Q | 180 | ARG |
| 23 | 4Q | 182 | PHE |
| 23 | 4Q | 183 | PHE |
| 23 | 4Q | 184 | MET |
| 23 | 4Q | 191 | VAL |
| 23 | 4Q | 195 | ARG |
| 23 | 4Q | 196 | PHE |
| 23 | 4Q | 200 | SER |
| 23 | 4Q | 201 | SER |
| 23 | 4Q | 204 | VAL |
| 23 | 4Q | 205 | LEU |
| 23 | 4Q | 208 | GLN |
| 23 | 4Q | 210 | LEU |
| 23 | 4Q | 214 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | 4Q | 215 | GLN |
| 23 | 4Q | 217 | LYS |
| 23 | 4Q | 219 | GLN |
| 23 | 4Q | 234 | ARG |
| 23 | 4Q | 239 | ASN |
| 23 | 4Q | 240 | LEU |
| 23 | 4Q | 242 | LEU |
| 23 | 4Q | 243 | LEU |
| 23 | 4Q | 246 | TYR |
| 23 | 4Q | 250 | VAL |
| 23 | 4Q | 254 | LYS |
| 23 | 4Q | 255 | PHE |
| 23 | 4Q | 257 | PHE |
| 23 | 4Q | 259 | ARG |
| 23 | 4Q | 260 | THR |
| 23 | 4Q | 261 | TYR |
| 23 | 4Q | 263 | HIS |
| 23 | 4Q | 266 | HIS |
| 23 | 4Q | 267 | ASP |
| 23 | 4Q | 269 | LEU |
| 23 | 4R | 15 | ASN |
| 23 | 4R | 17 | HIS |
| 23 | 4R | 18 | TYR |
| 23 | 4R | 19 | ILE |
| 23 | 4R | 26 | CYS |
| 23 | 4R | 30 | ARG |
| 23 | 4R | 33 | MET |
| 23 | 4R | 40 | THR |
| 23 | 4R | 43 | GLN |
| 23 | 4R | 45 | LEU |
| 23 | 4R | 60 | LEU |
| 23 | 4R | 61 | LEU |
| 23 | 4R | 86 | LEU |
| 23 | 4R | 90 | MET |
| 23 | 4R | 102 | GLN |
| 23 | 4R | 104 | ILE |
| 23 | 4R | 105 | PHE |
| 23 | 4R | 107 | LYS |
| 23 | 4R | 108 | ASN |
| 23 | 4R | 113 | TRP |
| 23 | 4R | 117 | LEU |
| 23 | 4R | 174 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | 4R | 176 | ASP |
| 23 | 4R | 177 | ARG |
| 23 | 4R | 182 | PHE |
| 23 | 4R | 183 | PHE |
| 23 | 4R | 184 | MET |
| 23 | 4R | 185 | SER |
| 23 | 4R | 191 | VAL |
| 23 | 4R | 195 | ARG |
| 23 | 4R | 198 | PHE |
| 23 | 4R | 201 | SER |
| 23 | 4R | 204 | VAL |
| 23 | 4R | 206 | SER |
| 23 | 4R | 210 | LEU |
| 23 | 4R | 211 | GLN |
| 23 | 4R | 215 | GLN |
| 23 | 4R | 216 | MET |
| 23 | 4R | 217 | LYS |
| 23 | 4R | 219 | GLN |
| 23 | 4R | 233 | SER |
| 23 | 4R | 234 | ARG |
| 23 | 4R | 239 | ASN |
| 23 | 4R | 240 | LEU |
| 23 | 4R | 242 | LEU |
| 23 | 4R | 243 | LEU |
| 23 | 4R | 245 | LYS |
| 23 | 4R | 250 | VAL |
| 23 | 4R | 253 | TYR |
| 23 | 4R | 254 | LYS |
| 23 | 4R | 257 | PHE |
| 23 | 4R | 263 | HIS |
| 23 | 4R | 266 | HIS |
| 23 | 4R | 267 | ASP |
| 23 | 4R | 269 | LEU |
| 25 | 4T | 269 | ARG |
| 25 | 4T | 397 | ARG |
| 25 | 4T | 399 | GLU |
| 25 | 4T | 401 | PRO |
| 25 | 4T | 428 | ASN |
| 26 | 4V | 373 | LYS |
| 26 | 4V | 376 | ASP |
| 26 | 4W | 42 | ASN |
| 26 | 4W | 165 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 26 | 4W | 290 | LYS |
| 26 | 4W | 365 | LEU |
| 26 | 4W | 373 | LYS |
| 26 | 4W | 374 | ILE |
| 26 | 4W | 376 | ASP |
| 27 | 4Z | 125 | ASN |
| 27 | 4Z | 167 | ARG |
| 28 | 5B | 209 | ILE |
| 28 | 5B | 212 | ASN |
| 28 | 5B | 214 | TYR |
| 28 | 5B | 217 | ARG |
| 28 | 5B | 218 | LYS |
| 28 | 5B | 219 | LEU |
| 30 | 5G | 65 | ASN |
| 30 | 5G | 110 | ARG |
| 31 | 5I | 589 | ARG |
| 31 | 5I | 622 | LYS |
| 31 | 5I | 675 | LYS |
| 31 | 5I | 686 | ARG |
| 31 | 5J | 779 | ARG |
| 31 | 5J | 807 | LYS |
| 32 | 5L | 42 | ARG |
| 33 | 5N | 179 | LYS |
| 33 | 5N | 287 | LYS |
| 33 | 5N | 353 | ASN |
| 33 | 5N | 450 | LYS |
| 34 | 5Q | 192 | ARG |
| 34 | 5R | 309 | LEU |
| 34 | 5R | 311 | MET |
| 34 | 5R | 312 | LYS |
| 34 | 5R | 320 | ASN |
| 34 | 5R | 322 | GLN |
| 34 | 5R | 323 | GLU |
| 34 | 5R | 327 | LYS |
| 34 | 5R | 328 | LYS |
| 34 | 5R | 329 | LYS |
| 34 | 5R | 330 | GLN |
| 34 | 5R | 331 | LYS |
| 34 | 5R | 334 | ASP |
| 34 | 5R | 337 | ARG |
| 34 | 5R | 338 | GLU |
| 34 | 5R | 339 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | 5R | 340 | LYS |
| 34 | 5R | 348 | GLN |
| 34 | 5R | 349 | ARG |
| 34 | 5R | 351 | GLU |
| 34 | 5R | 352 | GLU |
| 34 | 5R | 353 | GLU |
| 34 | 5R | 356 | GLN |
| 34 | 5R | 359 | GLU |
| 34 | 5R | 360 | LEU |
| 34 | 5R | 362 | ARG |
| 34 | 5R | 363 | ILE |
| 34 | 5R | 364 | LEU |
| 34 | 5R | 365 | GLU |
| 34 | 5R | 366 | LYS |
| 34 | 5R | 368 | LYS |
| 34 | 5R | 370 | LYS |
| 34 | 5R | 371 | LYS |
| 34 | 5R | 374 | GLU |
| 34 | 5R | 375 | LYS |
| 34 | 5R | 376 | ASP |
| 34 | 5R | 380 | ARG |
| 34 | 5R | 386 | ARG |
| 34 | 5R | 387 | LYS |
| 34 | 5R | 388 | GLN |
| 34 | 5R | 389 | LEU |
| 34 | 5R | 396 | THR |
| 34 | 5R | 397 | ARG |
| 34 | 5R | 398 | LYS |
| 34 | 5R | 399 | LEU |
| 34 | 5R | 400 | GLN |
| 34 | 5R | 403 | GLU |
| 34 | 5R | 405 | LEU |
| 34 | 5R | 407 | ARG |
| 34 | 5R | 410 | LYS |
| 34 | 5R | 417 | MET |
| 34 | 5R | 418 | GLU |
| 34 | 5R | 419 | GLN |
| 34 | 5R | 422 | ILE |
| 34 | 5R | 426 | LEU |
| 34 | 5R | 427 | LYS |
| 34 | 5R | 428 | GLU |
| 34 | 5R | 430 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | 5R | 431 | ARG |
| 34 | 5R | 432 | GLU |
| 34 | 5R | 435 | GLU |
| 34 | 5R | 440 | ARG |
| 34 | 5R | 445 | GLN |
| 34 | 5R | 449 | LYS |
| 34 | 5R | 450 | GLN |
| 34 | 5R | 451 | LEU |
| 34 | 5R | 452 | GLN |
| 34 | 5R | 453 | MET |
| 34 | 5R | 459 | GLN |
| 34 | 5R | 460 | GLN |
| 34 | 5R | 462 | ARG |
| 34 | 5R | 463 | GLU |
| 34 | 5R | 466 | LYS |
| 34 | 5R | 497 | LEU |
| 34 | 5R | 499 | ARG |
| 34 | 5R | 501 | ILE |
| 34 | 5R | 502 | HIS |
| 35 | 5T | 159 | ARG |
| 35 | 5U | 26 | ARG |
| 35 | 5U | 38 | LYS |
| 36 | 5W | 105 | LYS |
| 36 | 5X | 123 | ARG |
| 36 | 5X | 134 | ARG |
| 36 | 5X | 264 | ARG |
| 36 | 5Y | 32 | ARG |
| 36 | 5Y | 171 | ARG |
| 37 | 6A | 53 | MET |
| 38 | 6C | 47 | LEU |
| 38 | 6C | 83 | ARG |
| 38 | 6C | 92 | LYS |
| 38 | 6C | 105 | LYS |
| 38 | 6C | 187 | LEU |
| 38 | 6C | 188 | LEU |
| 38 | 6C | 189 | LYS |
| 39 | 6F | 116 | ARG |
| 39 | 6F | 118 | LYS |
| 39 | 6F | 119 | TYR |
| 39 | 6F | 121 | HIS |
| 39 | 6F | 124 | VAL |
| 39 | 6G | 24 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | 6G | 116 | ARG |
| 39 | 6G | 118 | LYS |
| 39 | 6H | 11 | ARG |
| 39 | 6H | 43 | ARG |
| 39 | 6L | 115 | LEU |
| 39 | 6L | 118 | LYS |
| 39 | 6L | 119 | TYR |
| 39 | 6L | 124 | VAL |
| 39 | 6L | 127 | LEU |
| 39 | 6L | 128 | SER |
| 40 | AE | 297 | GLU |
| 40 | AE | 302 | MET |
| 40 | AE | 305 | CYS |
| 40 | AF | 2 | ARG |
| 41 | AM | 306 | ARG |
| 41 | AN | 2 | ARG |
| 41 | AN | 58 | LYS |
| 41 | AN | 162 | ARG |
| 41 | AN | 306 | ARG |
| 41 | AO | 1 | MET |
| 41 | AO | 2 | ARG |
| 41 | AO | 19 | LYS |
| 41 | AO | 39 | ASP |
| 41 | AO | 40 | SER |
| 41 | AO | 42 | LEU |
| 41 | AO | 44 | LEU |
| 41 | AO | 45 | GLU |
| 41 | AO | 47 | ILE |
| 41 | AO | 52 | ASN |
| 41 | AO | 58 | LYS |
| 41 | AO | 67 | ASP |
| 41 | AO | 77 | ARG |
| 41 | AO | 88 | ASP |
| 41 | AO | 90 | PHE |
| 41 | AO | 103 | LYS |
| 41 | AO | 107 | THR |
| 41 | AO | 114 | ASP |
| 41 | AO | 120 | VAL |
| 41 | AO | 121 | ARG |
| 41 | AO | 122 | LYS |
| 41 | AO | 126 | SER |
| 41 | AO | 128 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | AO | 131 | GLN |
| 41 | AO | 135 | LEU |
| 41 | AO | 136 | THR |
| 41 | AO | 138 | SER |
| 41 | AO | 139 | LEU |
| 41 | AO | 154 | LYS |
| 41 | AO | 162 | ARG |
| 41 | AO | 164 | MET |
| 41 | AO | 166 | THR |
| 41 | AO | 170 | VAL |
| 41 | AO | 172 | SER |
| 41 | AO | 174 | LYS |
| 41 | AO | 177 | ASP |
| 41 | AO | 179 | VAL |
| 41 | AO | 180 | VAL |
| 41 | AO | 191 | GLN |
| 41 | AO | 194 | GLU |
| 41 | AO | 197 | ASP |
| 41 | AO | 199 | THR |
| 41 | AO | 202 | ILE |
| 41 | AO | 205 | GLU |
| 41 | AO | 209 | ASP |
| 41 | AO | 213 | ARG |
| 41 | AO | 216 | LYS |
| 41 | AO | 219 | THR |
| 41 | AO | 222 | TYR |
| 41 | AO | 228 | LEU |
| 41 | AO | 234 | SER |
| 41 | AO | 239 | CYS |
| 41 | AO | 240 | LEU |
| 41 | AO | 241 | ARG |
| 41 | AO | 245 | GLN |
| 41 | AO | 246 | LEU |
| 41 | AO | 252 | LYS |
| 41 | AO | 262 | ARG |
| 41 | AO | 264 | HIS |
| 41 | AO | 267 | MET |
| 41 | AO | 274 | THR |
| 41 | AO | 275 | SER |
| 41 | AO | 276 | ARG |
| 41 | AO | 280 | GLN |
| 41 | AO | 284 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | AO | 285 | THR |
| 41 | AO | 292 | GLN |
| 41 | AO | 293 | MET |
| 41 | AO | 297 | LYS |
| 41 | AO | 298 | ASN |
| 41 | AO | 306 | ARG |
| 41 | AO | 311 | LEU |
| 41 | AO | 316 | VAL |
| 41 | AO | 320 | ARG |
| 41 | AO | 321 | MET |
| 41 | AO | 322 | SER |
| 41 | AO | 324 | LYS |
| 41 | AO | 330 | MET |
| 41 | AO | 337 | ASN |
| 41 | AO | 348 | ASN |
| 41 | AO | 350 | LYS |
| 41 | AO | 351 | THR |
| 41 | AO | 354 | CYS |
| 41 | AO | 362 | LYS |
| 41 | AO | 364 | SER |
| 41 | AO | 368 | ILE |
| 41 | AO | 372 | THR |
| 41 | AO | 379 | LYS |
| 41 | AO | 380 | ARG |
| 41 | AO | 382 | SER |
| 41 | AO | 392 | LYS |
| 41 | AO | 397 | TRP |
| 41 | AO | 404 | ASP |
| 41 | AO | 405 | GLU |
| 41 | AO | 406 | MET |
| 41 | AO | 416 | ASN |
| 41 | AO | 423 | VAL |
| 41 | AO | 425 | ARG |
| 41 | AO | 428 | CYS |
| 41 | AP | 306 | ARG |
| 41 | BB | 1 | MET |
| 41 | BB | 2 | ARG |
| 41 | BB | 3 | GLU |
| 41 | BB | 4 | ILE |
| 41 | BB | 7 | LEU |
| 41 | BB | 12 | CYS |
| 41 | BB | 19 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BB | 22 | GLU |
| 41 | BB | 25 | SER |
| 41 | BB | 26 | ASP |
| 41 | BB | 31 | ASP |
| 41 | BB | 40 | SER |
| 41 | BB | 41 | ASP |
| 41 | BB | 42 | LEU |
| 41 | BB | 46 | ARG |
| 41 | BB | 47 | ILE |
| 41 | BB | 55 | THR |
| 41 | BB | 58 | LYS |
| 41 | BB | 64 | VAL |
| 41 | BB | 66 | VAL |
| 41 | BB | 68 | LEU |
| 41 | BB | 69 | GLU |
| 41 | BB | 77 | ARG |
| 41 | BB | 88 | ASP |
| 41 | BB | 90 | PHE |
| 41 | BB | 91 | VAL |
| 41 | BB | 100 | ASN |
| 41 | BB | 103 | LYS |
| 41 | BB | 108 | GLU |
| 41 | BB | 111 | GLU |
| 41 | BB | 114 | ASP |
| 41 | BB | 117 | LEU |
| 41 | BB | 119 | VAL |
| 41 | BB | 120 | VAL |
| 41 | BB | 121 | ARG |
| 41 | BB | 125 | GLU |
| 41 | BB | 128 | ASP |
| 41 | BB | 129 | CYS |
| 41 | BB | 131 | GLN |
| 41 | BB | 135 | LEU |
| 41 | BB | 143 | THR |
| 41 | BB | 145 | SER |
| 41 | BB | 147 | MET |
| 41 | BB | 151 | LEU |
| 41 | BB | 154 | LYS |
| 41 | BB | 159 | TYR |
| 41 | BB | 161 | ASP |
| 41 | BB | 162 | ARG |
| 41 | BB | 170 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BB | 174 | LYS |
| 41 | BB | 175 | VAL |
| 41 | BB | 178 | THR |
| 41 | BB | 180 | VAL |
| 41 | BB | 189 | VAL |
| 41 | BB | 191 | GLN |
| 41 | BB | 194 | GLU |
| 41 | BB | 195 | ASN |
| 41 | BB | 199 | THR |
| 41 | BB | 201 | CYS |
| 41 | BB | 203 | ASP |
| 41 | BB | 204 | ASN |
| 41 | BB | 207 | LEU |
| 41 | BB | 215 | LEU |
| 41 | BB | 217 | LEU |
| 41 | BB | 221 | THR |
| 41 | BB | 222 | TYR |
| 41 | BB | 224 | ASP |
| 41 | BB | 232 | THR |
| 41 | BB | 233 | MET |
| 41 | BB | 245 | GLN |
| 41 | BB | 251 | ARG |
| 41 | BB | 252 | LYS |
| 41 | BB | 253 | LEU |
| 41 | BB | 264 | HIS |
| 41 | BB | 267 | MET |
| 41 | BB | 270 | PHE |
| 41 | BB | 275 | SER |
| 41 | BB | 276 | ARG |
| 41 | BB | 280 | GLN |
| 41 | BB | 282 | ARG |
| 41 | BB | 288 | GLU |
| 41 | BB | 289 | LEU |
| 41 | BB | 290 | THR |
| 41 | BB | 292 | GLN |
| 41 | BB | 293 | MET |
| 41 | BB | 297 | LYS |
| 41 | BB | 299 | MET |
| 41 | BB | 306 | ARG |
| 41 | BB | 310 | TYR |
| 41 | BB | 312 | THR |
| 41 | BB | 313 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BB | 316 | VAL |
| 41 | BB | 318 | ARG |
| 41 | BB | 322 | SER |
| 41 | BB | 327 | ASP |
| 41 | BB | 331 | LEU |
| 41 | BB | 337 | ASN |
| 41 | BB | 350 | LYS |
| 41 | BB | 351 | THR |
| 41 | BB | 359 | ARG |
| 41 | BB | 362 | LYS |
| 41 | BB | 364 | SER |
| 41 | BB | 374 | ILE |
| 41 | BB | 375 | GLN |
| 41 | BB | 376 | GLU |
| 41 | BB | 379 | LYS |
| 41 | BB | 391 | ARG |
| 41 | BB | 395 | LEU |
| 41 | BB | 396 | HIS |
| 41 | BB | 404 | ASP |
| 41 | BB | 405 | GLU |
| 41 | BB | 416 | ASN |
| 41 | BB | 423 | VAL |
| 40 | BE | 1 | GLN |
| 40 | BE | 2 | ARG |
| 40 | BE | 3 | GLU |
| 40 | BE | 6 | SER |
| 40 | BE | 9 | VAL |
| 40 | BE | 11 | GLN |
| 40 | BE | 16 | ILE |
| 40 | BE | 22 | GLU |
| 40 | BE | 25 | CYS |
| 40 | BE | 26 | LEU |
| 40 | BE | 30 | ILE |
| 40 | BE | 33 | ASP |
| 40 | BE | 39 | ASP |
| 40 | BE | 40 | LYS |
| 40 | BE | 41 | THR |
| 40 | BE | 42 | ILE |
| 40 | BE | 46 | ASP |
| 40 | BE | 47 | ASP |
| 40 | BE | 51 | THR |
| 40 | BE | 60 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BE | 68 | VAL |
| 40 | BE | 70 | LEU |
| 40 | BE | 75 | ILE |
| 40 | BE | 76 | ASP |
| 40 | BE | 77 | GLU |
| 40 | BE | 79 | ARG |
| 40 | BE | 80 | THR |
| 40 | BE | 82 | THR |
| 40 | BE | 90 | GLU |
| 40 | BE | 94 | THR |
| 40 | BE | 96 | LYS |
| 40 | BE | 101 | ASN |
| 40 | BE | 105 | ARG |
| 40 | BE | 109 | THR |
| 40 | BE | 114 | LEU |
| 40 | BE | 116 | ASP |
| 40 | BE | 119 | LEU |
| 40 | BE | 120 | ASP |
| 40 | BE | 123 | ARG |
| 40 | BE | 124 | LYS |
| 40 | BE | 128 | GLN |
| 40 | BE | 129 | CYS |
| 40 | BE | 141 | PHE |
| 40 | BE | 145 | THR |
| 40 | BE | 147 | SER |
| 40 | BE | 153 | LEU |
| 40 | BE | 156 | ARG |
| 40 | BE | 157 | LEU |
| 40 | BE | 158 | SER |
| 40 | BE | 161 | TYR |
| 40 | BE | 163 | LYS |
| 40 | BE | 164 | LYS |
| 40 | BE | 166 | LYS |
| 40 | BE | 167 | LEU |
| 40 | BE | 178 | SER |
| 40 | BE | 179 | THR |
| 40 | BE | 184 | PRO |
| 40 | BE | 186 | ASN |
| 40 | BE | 187 | SER |
| 40 | BE | 188 | ILE |
| 40 | BE | 190 | THR |
| 40 | BE | 191 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BE | 192 | HIS |
| 40 | BE | 195 | LEU |
| 40 | BE | 200 | CYS |
| 40 | BE | 203 | MET |
| 40 | BE | 204 | VAL |
| 40 | BE | 205 | ASP |
| 40 | BE | 206 | ASN |
| 40 | BE | 212 | ILE |
| 40 | BE | 214 | ARG |
| 40 | BE | 215 | ARG |
| 40 | BE | 216 | ASN |
| 40 | BE | 218 | ASP |
| 40 | BE | 221 | ARG |
| 40 | BE | 223 | THR |
| 40 | BE | 224 | TYR |
| 40 | BE | 225 | THR |
| 40 | BE | 230 | LEU |
| 40 | BE | 237 | SER |
| 40 | BE | 239 | THR |
| 40 | BE | 241 | SER |
| 40 | BE | 242 | LEU |
| 40 | BE | 243 | ARG |
| 40 | BE | 248 | LEU |
| 40 | BE | 259 | LEU |
| 40 | BE | 264 | ARG |
| 40 | BE | 265 | ILE |
| 40 | BE | 269 | LEU |
| 40 | BE | 271 | THR |
| 40 | BE | 272 | TYR |
| 40 | BE | 276 | ILE |
| 40 | BE | 277 | SER |
| 40 | BE | 279 | GLU |
| 40 | BE | 280 | LYS |
| 40 | BE | 284 | GLU |
| 40 | BE | 290 | GLU |
| 40 | BE | 291 | ILE |
| 40 | BE | 300 | ASN |
| 40 | BE | 302 | MET |
| 40 | BE | 308 | ARG |
| 40 | BE | 311 | LYS |
| 40 | BE | 315 | CYS |
| 40 | BE | 318 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BE | 326 | LYS |
| 40 | BE | 339 | ARG |
| 40 | BE | 341 | ILE |
| 40 | BE | 349 | THR |
| 40 | BE | 356 | ASN |
| 40 | BE | 361 | THR |
| 40 | BE | 362 | VAL |
| 40 | BE | 369 | LYS |
| 40 | BE | 372 | ARG |
| 40 | BE | 376 | MET |
| 40 | BE | 378 | SER |
| 40 | BE | 389 | ARG |
| 40 | BE | 393 | LYS |
| 40 | BE | 396 | LEU |
| 40 | BE | 400 | LYS |
| 40 | BE | 401 | ARG |
| 40 | BE | 412 | MET |
| 40 | BE | 414 | GLU |
| 40 | BE | 419 | GLU |
| 40 | BE | 429 | LYS |
| 40 | BE | 431 | TYR |
| 40 | BE | 434 | VAL |
| 40 | BE | 436 | MET |
| 40 | BE | 437 | ASP |
| 40 | BE | 438 | SER |
| 40 | BE | 439 | VAL |
| 40 | BG | 128 | GLN |
| 40 | BG | 256 | GLN |
| 40 | BH | 2 | ARG |
| 40 | BH | 3 | GLU |
| 40 | BH | 6 | SER |
| 40 | BH | 9 | VAL |
| 40 | BH | 22 | GLU |
| 40 | BH | 26 | LEU |
| 40 | BH | 46 | ASP |
| 40 | BH | 47 | ASP |
| 40 | BH | 52 | PHE |
| 40 | BH | 53 | PHE |
| 40 | BH | 60 | LYS |
| 40 | BH | 66 | VAL |
| 40 | BH | 70 | LEU |
| 40 | BH | 71 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BH | 75 | ILE |
| 40 | BH | 84 | ARG |
| 40 | BH | 92 | LEU |
| 40 | BH | 94 | THR |
| 40 | BH | 110 | ILE |
| 40 | BH | 112 | LYS |
| 40 | BH | 113 | GLU |
| 40 | BH | 114 | LEU |
| 40 | BH | 116 | ASP |
| 40 | BH | 117 | LEU |
| 40 | BH | 122 | ILE |
| 40 | BH | 124 | LYS |
| 40 | BH | 128 | GLN |
| 40 | BH | 129 | CYS |
| 40 | BH | 130 | THR |
| 40 | BH | 132 | LEU |
| 40 | BH | 135 | PHE |
| 40 | BH | 137 | ILE |
| 40 | BH | 139 | HIS |
| 40 | BH | 151 | SER |
| 40 | BH | 154 | MET |
| 40 | BH | 155 | GLU |
| 40 | BH | 159 | VAL |
| 40 | BH | 160 | ASP |
| 40 | BH | 163 | LYS |
| 40 | BH | 164 | LYS |
| 40 | BH | 167 | LEU |
| 40 | BH | 176 | GLN |
| 40 | BH | 181 | VAL |
| 40 | BH | 192 | HIS |
| 40 | BH | 198 | SER |
| 40 | BH | 200 | CYS |
| 40 | BH | 206 | ASN |
| 40 | BH | 214 | ARG |
| 40 | BH | 215 | ARG |
| 40 | BH | 220 | GLU |
| 40 | BH | 224 | TYR |
| 40 | BH | 234 | ILE |
| 40 | BH | 238 | ILE |
| 40 | BH | 241 | SER |
| 40 | BH | 242 | LEU |
| 40 | BH | 250 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BH | 254 | GLU |
| 40 | BH | 257 | THR |
| 40 | BH | 264 | ARG |
| 40 | BH | 266 | HIS |
| 40 | BH | 272 | TYR |
| 40 | BH | 275 | VAL |
| 40 | BH | 276 | ILE |
| 40 | BH | 279 | GLU |
| 40 | BH | 285 | GLN |
| 40 | BH | 286 | LEU |
| 40 | BH | 293 | ASN |
| 40 | BH | 297 | GLU |
| 40 | BH | 304 | LYS |
| 40 | BH | 308 | ARG |
| 40 | BH | 311 | LYS |
| 40 | BH | 315 | CYS |
| 40 | BH | 318 | LEU |
| 40 | BH | 324 | VAL |
| 40 | BH | 326 | LYS |
| 40 | BH | 339 | ARG |
| 40 | BH | 361 | THR |
| 40 | BH | 362 | VAL |
| 40 | BH | 363 | VAL |
| 40 | BH | 367 | LEU |
| 40 | BH | 369 | LYS |
| 40 | BH | 371 | GLN |
| 40 | BH | 374 | VAL |
| 40 | BH | 375 | CYS |
| 40 | BH | 379 | ASN |
| 40 | BH | 389 | ARG |
| 40 | BH | 390 | LEU |
| 40 | BH | 396 | LEU |
| 40 | BH | 397 | MET |
| 40 | BH | 400 | LYS |
| 40 | BH | 401 | ARG |
| 40 | BH | 412 | MET |
| 40 | BH | 421 | ARG |
| 40 | BH | 423 | ASP |
| 40 | BH | 428 | GLU |
| 40 | BH | 436 | MET |
| 40 | BH | 437 | ASP |
| 40 | BH | 439 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BI | 7 | VAL |
| 40 | BI | 9 | VAL |
| 40 | BI | 14 | VAL |
| 40 | BI | 16 | ILE |
| 40 | BI | 26 | LEU |
| 40 | BI | 28 | HIS |
| 40 | BI | 36 | MET |
| 40 | BI | 37 | PRO |
| 40 | BI | 50 | ASN |
| 40 | BI | 51 | THR |
| 40 | BI | 52 | PHE |
| 40 | BI | 53 | PHE |
| 40 | BI | 54 | SER |
| 40 | BI | 56 | THR |
| 40 | BI | 60 | LYS |
| 40 | BI | 66 | VAL |
| 40 | BI | 68 | VAL |
| 40 | BI | 70 | LEU |
| 40 | BI | 71 | GLU |
| 40 | BI | 73 | THR |
| 40 | BI | 74 | VAL |
| 40 | BI | 76 | ASP |
| 40 | BI | 82 | THR |
| 40 | BI | 84 | ARG |
| 40 | BI | 89 | PRO |
| 40 | BI | 93 | ILE |
| 40 | BI | 94 | THR |
| 40 | BI | 96 | LYS |
| 40 | BI | 102 | ASN |
| 40 | BI | 107 | HIS |
| 40 | BI | 112 | LYS |
| 40 | BI | 114 | LEU |
| 40 | BI | 117 | LEU |
| 40 | BI | 119 | LEU |
| 40 | BI | 123 | ARG |
| 40 | BI | 124 | LYS |
| 40 | BI | 128 | GLN |
| 40 | BI | 133 | GLN |
| 40 | BI | 145 | THR |
| 40 | BI | 153 | LEU |
| 40 | BI | 155 | GLU |
| 40 | BI | 156 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BI | 157 | LEU |
| 40 | BI | 159 | VAL |
| 40 | BI | 161 | TYR |
| 40 | BI | 163 | LYS |
| 40 | BI | 168 | GLU |
| 40 | BI | 170 | SER |
| 40 | BI | 171 | ILE |
| 40 | BI | 176 | GLN |
| 40 | BI | 179 | THR |
| 40 | BI | 186 | ASN |
| 40 | BI | 191 | THR |
| 40 | BI | 192 | HIS |
| 40 | BI | 193 | THR |
| 40 | BI | 196 | GLU |
| 40 | BI | 199 | ASP |
| 40 | BI | 200 | CYS |
| 40 | BI | 204 | VAL |
| 40 | BI | 209 | ILE |
| 40 | BI | 211 | ASP |
| 40 | BI | 212 | ILE |
| 40 | BI | 214 | ARG |
| 40 | BI | 219 | ILE |
| 40 | BI | 220 | GLU |
| 40 | BI | 224 | TYR |
| 40 | BI | 227 | LEU |
| 40 | BI | 229 | ARG |
| 40 | BI | 242 | LEU |
| 40 | BI | 264 | ARG |
| 40 | BI | 265 | ILE |
| 40 | BI | 269 | LEU |
| 40 | BI | 271 | THR |
| 40 | BI | 274 | PRO |
| 40 | BI | 275 | VAL |
| 40 | BI | 277 | SER |
| 40 | BI | 282 | TYR |
| 40 | BI | 288 | VAL |
| 40 | BI | 291 | ILE |
| 40 | BI | 295 | CYS |
| 40 | BI | 297 | GLU |
| 40 | BI | 301 | GLN |
| 40 | BI | 303 | VAL |
| 40 | BI | 304 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BI | 305 | CYS |
| 40 | BI | 308 | ARG |
| 40 | BI | 311 | LYS |
| 40 | BI | 313 | MET |
| 40 | BI | 316 | CYS |
| 40 | BI | 358 | GLN |
| 40 | BI | 361 | THR |
| 40 | BI | 362 | VAL |
| 40 | BI | 363 | VAL |
| 40 | BI | 366 | ASP |
| 40 | BI | 367 | LEU |
| 40 | BI | 369 | LYS |
| 40 | BI | 374 | VAL |
| 40 | BI | 376 | MET |
| 40 | BI | 377 | LEU |
| 40 | BI | 380 | THR |
| 40 | BI | 389 | ARG |
| 40 | BI | 391 | ASP |
| 40 | BI | 397 | MET |
| 40 | BI | 400 | LYS |
| 40 | BI | 401 | ARG |
| 40 | BI | 406 | TRP |
| 40 | BI | 412 | MET |
| 40 | BI | 413 | GLU |
| 40 | BI | 416 | GLU |
| 40 | BI | 421 | ARG |
| 40 | BI | 423 | ASP |
| 40 | BI | 427 | LEU |
| 40 | BI | 428 | GLU |
| 40 | BI | 429 | LYS |
| 40 | BI | 434 | VAL |
| 41 | BL | 174 | LYS |
| 41 | BL | 306 | ARG |
| 41 | BM | 1 | MET |
| 41 | BM | 2 | ARG |
| 41 | BM | 3 | GLU |
| 41 | BM | 7 | LEU |
| 41 | BM | 12 | CYS |
| 41 | BM | 16 | ILE |
| 41 | BM | 19 | LYS |
| 41 | BM | 24 | ILE |
| 41 | BM | 26 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BM | 31 | ASP |
| 41 | BM | 39 | ASP |
| 41 | BM | 40 | SER |
| 41 | BM | 42 | LEU |
| 41 | BM | 58 | LYS |
| 41 | BM | 60 | VAL |
| 41 | BM | 62 | ARG |
| 41 | BM | 66 | VAL |
| 41 | BM | 68 | LEU |
| 41 | BM | 72 | THR |
| 41 | BM | 73 | MET |
| 41 | BM | 74 | ASP |
| 41 | BM | 84 | ILE |
| 41 | BM | 91 | VAL |
| 41 | BM | 100 | ASN |
| 41 | BM | 103 | LYS |
| 41 | BM | 115 | SER |
| 41 | BM | 119 | VAL |
| 41 | BM | 121 | ARG |
| 41 | BM | 122 | LYS |
| 41 | BM | 128 | ASP |
| 41 | BM | 129 | CYS |
| 41 | BM | 130 | LEU |
| 41 | BM | 135 | LEU |
| 41 | BM | 138 | SER |
| 41 | BM | 139 | LEU |
| 41 | BM | 143 | THR |
| 41 | BM | 147 | MET |
| 41 | BM | 151 | LEU |
| 41 | BM | 153 | SER |
| 41 | BM | 154 | LYS |
| 41 | BM | 162 | ARG |
| 41 | BM | 163 | ILE |
| 41 | BM | 164 | MET |
| 41 | BM | 168 | SER |
| 41 | BM | 170 | VAL |
| 41 | BM | 172 | SER |
| 41 | BM | 174 | LYS |
| 41 | BM | 175 | VAL |
| 41 | BM | 180 | VAL |
| 41 | BM | 194 | GLU |
| 41 | BM | 195 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BM | 196 | THR |
| 41 | BM | 204 | ASN |
| 41 | BM | 205 | GLU |
| 41 | BM | 209 | ASP |
| 41 | BM | 212 | PHE |
| 41 | BM | 215 | LEU |
| 41 | BM | 216 | LYS |
| 41 | BM | 221 | THR |
| 41 | BM | 222 | TYR |
| 41 | BM | 225 | LEU |
| 41 | BM | 227 | HIS |
| 41 | BM | 228 | LEU |
| 41 | BM | 238 | THR |
| 41 | BM | 246 | LEU |
| 41 | BM | 252 | LYS |
| 41 | BM | 258 | VAL |
| 41 | BM | 263 | LEU |
| 41 | BM | 264 | HIS |
| 41 | BM | 270 | PHE |
| 41 | BM | 275 | SER |
| 41 | BM | 279 | GLN |
| 41 | BM | 280 | GLN |
| 41 | BM | 282 | ARG |
| 41 | BM | 289 | LEU |
| 41 | BM | 291 | GLN |
| 41 | BM | 292 | GLN |
| 41 | BM | 293 | MET |
| 41 | BM | 297 | LYS |
| 41 | BM | 298 | ASN |
| 41 | BM | 300 | MET |
| 41 | BM | 303 | CYS |
| 41 | BM | 306 | ARG |
| 41 | BM | 309 | ARG |
| 41 | BM | 313 | VAL |
| 41 | BM | 320 | ARG |
| 41 | BM | 321 | MET |
| 41 | BM | 329 | GLN |
| 41 | BM | 331 | LEU |
| 41 | BM | 337 | ASN |
| 41 | BM | 338 | SER |
| 41 | BM | 343 | GLU |
| 41 | BM | 347 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BM | 350 | LYS |
| 41 | BM | 353 | VAL |
| 41 | BM | 354 | CYS |
| 41 | BM | 359 | ARG |
| 41 | BM | 361 | LEU |
| 41 | BM | 363 | MET |
| 41 | BM | 364 | SER |
| 41 | BM | 368 | ILE |
| 41 | BM | 375 | GLN |
| 41 | BM | 380 | ARG |
| 41 | BM | 382 | SER |
| 41 | BM | 383 | GLU |
| 41 | BM | 390 | ARG |
| 41 | BM | 391 | ARG |
| 41 | BM | 392 | LYS |
| 41 | BM | 403 | MET |
| 41 | BM | 406 | MET |
| 41 | BM | 416 | ASN |
| 41 | BM | 423 | VAL |
| 41 | BM | 425 | ARG |
| 41 | BM | 428 | CYS |
| 41 | BN | 2 | ARG |
| 41 | BO | 1 | MET |
| 41 | BO | 2 | ARG |
| 41 | BO | 3 | GLU |
| 41 | BO | 7 | LEU |
| 41 | BO | 12 | CYS |
| 41 | BO | 19 | LYS |
| 41 | BO | 22 | GLU |
| 41 | BO | 27 | GLU |
| 41 | BO | 45 | GLU |
| 41 | BO | 53 | GLU |
| 41 | BO | 60 | VAL |
| 41 | BO | 61 | PRO |
| 41 | BO | 62 | ARG |
| 41 | BO | 65 | LEU |
| 41 | BO | 68 | LEU |
| 41 | BO | 72 | THR |
| 41 | BO | 75 | SER |
| 41 | BO | 86 | ARG |
| 41 | BO | 100 | ASN |
| 41 | BO | 103 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BO | 107 | THR |
| 41 | BO | 108 | GLU |
| 41 | BO | 114 | ASP |
| 41 | BO | 120 | VAL |
| 41 | BO | 125 | GLU |
| 41 | BO | 130 | LEU |
| 41 | BO | 131 | GLN |
| 41 | BO | 135 | LEU |
| 41 | BO | 143 | THR |
| 41 | BO | 147 | MET |
| 41 | BO | 151 | LEU |
| 41 | BO | 155 | ILE |
| 41 | BO | 157 | GLU |
| 41 | BO | 161 | ASP |
| 41 | BO | 162 | ARG |
| 41 | BO | 163 | ILE |
| 41 | BO | 164 | MET |
| 41 | BO | 165 | ASN |
| 41 | BO | 166 | THR |
| 41 | BO | 170 | VAL |
| 41 | BO | 172 | SER |
| 41 | BO | 174 | LYS |
| 41 | BO | 180 | VAL |
| 41 | BO | 188 | SER |
| 41 | BO | 191 | GLN |
| 41 | BO | 193 | VAL |
| 41 | BO | 194 | GLU |
| 41 | BO | 196 | THR |
| 41 | BO | 198 | GLU |
| 41 | BO | 201 | CYS |
| 41 | BO | 202 | ILE |
| 41 | BO | 205 | GLU |
| 41 | BO | 208 | TYR |
| 41 | BO | 209 | ASP |
| 41 | BO | 210 | ILE |
| 41 | BO | 213 | ARG |
| 41 | BO | 214 | THR |
| 41 | BO | 216 | LYS |
| 41 | BO | 217 | LEU |
| 41 | BO | 222 | TYR |
| 41 | BO | 238 | THR |
| 41 | BO | 240 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BO | 241 | ARG |
| 41 | BO | 245 | GLN |
| 41 | BO | 246 | LEU |
| 41 | BO | 252 | LYS |
| 41 | BO | 255 | VAL |
| 41 | BO | 257 | MET |
| 41 | BO | 264 | HIS |
| 41 | BO | 270 | PHE |
| 41 | BO | 274 | THR |
| 41 | BO | 275 | SER |
| 41 | BO | 276 | ARG |
| 41 | BO | 279 | GLN |
| 41 | BO | 284 | LEU |
| 41 | BO | 285 | THR |
| 41 | BO | 288 | GLU |
| 41 | BO | 290 | THR |
| 41 | BO | 293 | MET |
| 41 | BO | 297 | LYS |
| 41 | BO | 299 | MET |
| 41 | BO | 303 | CYS |
| 41 | BO | 306 | ARG |
| 41 | BO | 312 | THR |
| 41 | BO | 313 | VAL |
| 41 | BO | 318 | ARG |
| 41 | BO | 320 | ARG |
| 41 | BO | 321 | MET |
| 41 | BO | 322 | SER |
| 41 | BO | 324 | LYS |
| 41 | BO | 326 | VAL |
| 41 | BO | 331 | LEU |
| 41 | BO | 334 | GLN |
| 41 | BO | 336 | LYS |
| 41 | BO | 337 | ASN |
| 41 | BO | 338 | SER |
| 41 | BO | 344 | TRP |
| 41 | BO | 348 | ASN |
| 41 | BO | 350 | LYS |
| 41 | BO | 354 | CYS |
| 41 | BO | 356 | ILE |
| 41 | BO | 359 | ARG |
| 41 | BO | 372 | THR |
| 41 | BO | 374 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BO | 375 | GLN |
| 41 | BO | 379 | LYS |
| 41 | BO | 380 | ARG |
| 41 | BO | 392 | LYS |
| 41 | BO | 394 | PHE |
| 41 | BO | 395 | LEU |
| 41 | BO | 403 | MET |
| 41 | BO | 405 | GLU |
| 41 | BO | 413 | SER |
| 41 | BO | 428 | CYS |
| 41 | BP | 1 | MET |
| 41 | BP | 7 | LEU |
| 41 | BP | 16 | ILE |
| 41 | BP | 19 | LYS |
| 41 | BP | 20 | PHE |
| 41 | BP | 22 | GLU |
| 41 | BP | 24 | ILE |
| 41 | BP | 25 | SER |
| 41 | BP | 26 | ASP |
| 41 | BP | 31 | ASP |
| 41 | BP | 39 | ASP |
| 41 | BP | 41 | ASP |
| 41 | BP | 42 | LEU |
| 41 | BP | 44 | LEU |
| 41 | BP | 47 | ILE |
| 41 | BP | 48 | ASN |
| 41 | BP | 53 | GLU |
| 41 | BP | 55 | THR |
| 41 | BP | 58 | LYS |
| 41 | BP | 62 | ARG |
| 41 | BP | 64 | VAL |
| 41 | BP | 66 | VAL |
| 41 | BP | 68 | LEU |
| 41 | BP | 69 | GLU |
| 41 | BP | 72 | THR |
| 41 | BP | 86 | ARG |
| 41 | BP | 91 | VAL |
| 41 | BP | 94 | GLN |
| 41 | BP | 99 | ASN |
| 41 | BP | 103 | LYS |
| 41 | BP | 107 | THR |
| 41 | BP | 111 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BP | 112 | LEU |
| 41 | BP | 114 | ASP |
| 41 | BP | 117 | LEU |
| 41 | BP | 118 | ASP |
| 41 | BP | 119 | VAL |
| 41 | BP | 121 | ARG |
| 41 | BP | 125 | GLU |
| 41 | BP | 131 | GLN |
| 41 | BP | 137 | HIS |
| 41 | BP | 139 | LEU |
| 41 | BP | 145 | SER |
| 41 | BP | 147 | MET |
| 41 | BP | 151 | LEU |
| 41 | BP | 154 | LYS |
| 41 | BP | 155 | ILE |
| 41 | BP | 159 | TYR |
| 41 | BP | 162 | ARG |
| 41 | BP | 164 | MET |
| 41 | BP | 170 | VAL |
| 41 | BP | 172 | SER |
| 41 | BP | 174 | LYS |
| 41 | BP | 191 | GLN |
| 41 | BP | 192 | LEU |
| 41 | BP | 193 | VAL |
| 41 | BP | 194 | GLU |
| 41 | BP | 199 | THR |
| 41 | BP | 203 | ASP |
| 41 | BP | 204 | ASN |
| 41 | BP | 209 | ASP |
| 41 | BP | 211 | CYS |
| 41 | BP | 212 | PHE |
| 41 | BP | 213 | ARG |
| 41 | BP | 214 | THR |
| 41 | BP | 217 | LEU |
| 41 | BP | 222 | TYR |
| 41 | BP | 240 | LEU |
| 41 | BP | 241 | ARG |
| 41 | BP | 245 | GLN |
| 41 | BP | 246 | LEU |
| 41 | BP | 249 | ASP |
| 41 | BP | 252 | LYS |
| 41 | BP | 263 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BP | 264 | HIS |
| 41 | BP | 276 | ARG |
| 41 | BP | 278 | SER |
| 41 | BP | 284 | LEU |
| 41 | BP | 288 | GLU |
| 41 | BP | 292 | GLN |
| 41 | BP | 293 | MET |
| 41 | BP | 297 | LYS |
| 41 | BP | 306 | ARG |
| 41 | BP | 310 | TYR |
| 41 | BP | 316 | VAL |
| 41 | BP | 320 | ARG |
| 41 | BP | 321 | MET |
| 41 | BP | 322 | SER |
| 41 | BP | 337 | ASN |
| 41 | BP | 348 | ASN |
| 41 | BP | 349 | VAL |
| 41 | BP | 350 | LYS |
| 41 | BP | 351 | THR |
| 41 | BP | 359 | ARG |
| 41 | BP | 362 | LYS |
| 41 | BP | 363 | MET |
| 41 | BP | 364 | SER |
| 41 | BP | 370 | ASN |
| 41 | BP | 377 | LEU |
| 41 | BP | 380 | ARG |
| 41 | BP | 382 | SER |
| 41 | BP | 383 | GLU |
| 41 | BP | 395 | LEU |
| 41 | BP | 397 | TRP |
| 41 | BP | 404 | ASP |
| 41 | BP | 406 | MET |
| 41 | BP | 407 | GLU |
| 41 | BP | 409 | THR |
| 41 | BP | 414 | ASN |
| 41 | BP | 422 | VAL |
| 41 | BP | 423 | VAL |
| 41 | BP | 425 | ARG |
| 40 | CA | 3 | GLU |
| 40 | CA | 4 | CYS |
| 40 | CA | 9 | VAL |
| 40 | CA | 22 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CA | 23 | LEU |
| 40 | CA | 30 | ILE |
| 40 | CA | 36 | MET |
| 40 | CA | 38 | SER |
| 40 | CA | 39 | ASP |
| 40 | CA | 40 | LYS |
| 40 | CA | 41 | THR |
| 40 | CA | 42 | ILE |
| 40 | CA | 51 | THR |
| 40 | CA | 52 | PHE |
| 40 | CA | 62 | VAL |
| 40 | CA | 66 | VAL |
| 40 | CA | 67 | PHE |
| 40 | CA | 70 | LEU |
| 40 | CA | 73 | THR |
| 40 | CA | 74 | VAL |
| 40 | CA | 79 | ARG |
| 40 | CA | 82 | THR |
| 40 | CA | 90 | GLU |
| 40 | CA | 96 | LYS |
| 40 | CA | 105 | ARG |
| 40 | CA | 110 | ILE |
| 40 | CA | 112 | LYS |
| 40 | CA | 114 | LEU |
| 40 | CA | 115 | ILE |
| 40 | CA | 120 | ASP |
| 40 | CA | 122 | ILE |
| 40 | CA | 123 | ARG |
| 40 | CA | 125 | LEU |
| 40 | CA | 132 | LEU |
| 40 | CA | 133 | GLN |
| 40 | CA | 137 | ILE |
| 40 | CA | 139 | HIS |
| 40 | CA | 141 | PHE |
| 40 | CA | 149 | PHE |
| 40 | CA | 151 | SER |
| 40 | CA | 152 | LEU |
| 40 | CA | 156 | ARG |
| 40 | CA | 163 | LYS |
| 40 | CA | 164 | LYS |
| 40 | CA | 166 | LYS |
| 40 | CA | 170 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CA | 171 | ILE |
| 40 | CA | 177 | VAL |
| 40 | CA | 183 | GLU |
| 40 | CA | 187 | SER |
| 40 | CA | 190 | THR |
| 40 | CA | 191 | THR |
| 40 | CA | 193 | THR |
| 40 | CA | 195 | LEU |
| 40 | CA | 196 | GLU |
| 40 | CA | 200 | CYS |
| 40 | CA | 203 | MET |
| 40 | CA | 204 | VAL |
| 40 | CA | 209 | ILE |
| 40 | CA | 211 | ASP |
| 40 | CA | 213 | CYS |
| 40 | CA | 214 | ARG |
| 40 | CA | 215 | ARG |
| 40 | CA | 220 | GLU |
| 40 | CA | 221 | ARG |
| 40 | CA | 223 | THR |
| 40 | CA | 226 | ASN |
| 40 | CA | 227 | LEU |
| 40 | CA | 229 | ARG |
| 40 | CA | 231 | ILE |
| 40 | CA | 232 | SER |
| 40 | CA | 234 | ILE |
| 40 | CA | 235 | VAL |
| 40 | CA | 242 | LEU |
| 40 | CA | 252 | LEU |
| 40 | CA | 253 | THR |
| 40 | CA | 256 | GLN |
| 40 | CA | 258 | ASN |
| 40 | CA | 259 | LEU |
| 40 | CA | 266 | HIS |
| 40 | CA | 269 | LEU |
| 40 | CA | 272 | TYR |
| 40 | CA | 275 | VAL |
| 40 | CA | 276 | ILE |
| 40 | CA | 279 | GLU |
| 40 | CA | 280 | LYS |
| 40 | CA | 284 | GLU |
| 40 | CA | 285 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CA | 293 | ASN |
| 40 | CA | 295 | CYS |
| 40 | CA | 302 | MET |
| 40 | CA | 303 | VAL |
| 40 | CA | 304 | LYS |
| 40 | CA | 308 | ARG |
| 40 | CA | 311 | LYS |
| 40 | CA | 316 | CYS |
| 40 | CA | 317 | LEU |
| 40 | CA | 318 | LEU |
| 40 | CA | 320 | ARG |
| 40 | CA | 335 | ILE |
| 40 | CA | 339 | ARG |
| 40 | CA | 344 | VAL |
| 40 | CA | 349 | THR |
| 40 | CA | 363 | VAL |
| 40 | CA | 367 | LEU |
| 40 | CA | 369 | LYS |
| 40 | CA | 370 | VAL |
| 40 | CA | 372 | ARG |
| 40 | CA | 374 | VAL |
| 40 | CA | 376 | MET |
| 40 | CA | 378 | SER |
| 40 | CA | 385 | GLU |
| 40 | CA | 390 | LEU |
| 40 | CA | 395 | ASP |
| 40 | CA | 400 | LYS |
| 40 | CA | 401 | ARG |
| 40 | CA | 408 | VAL |
| 40 | CA | 414 | GLU |
| 40 | CA | 416 | GLU |
| 40 | CA | 421 | ARG |
| 40 | CA | 424 | MET |
| 40 | CA | 429 | LYS |
| 40 | CA | 432 | GLU |
| 40 | CA | 436 | MET |
| 40 | CA | 437 | ASP |
| 40 | CA | 438 | SER |
| 40 | CA | 439 | VAL |
| 41 | CB | 213 | ARG |
| 41 | CB | 306 | ARG |
| 41 | CB | 347 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CE | 2 | ARG |
| 40 | CE | 256 | GLN |
| 40 | CE | 379 | ASN |
| 40 | CF | 74 | VAL |
| 40 | CF | 75 | ILE |
| 40 | CF | 76 | ASP |
| 40 | CF | 84 | ARG |
| 40 | CF | 163 | LYS |
| 40 | CF | 206 | ASN |
| 40 | CF | 256 | GLN |
| 40 | CG | 2 | ARG |
| 40 | CG | 256 | GLN |
| 40 | CG | 285 | GLN |
| 40 | CH | 2 | ARG |
| 40 | CH | 3 | GLU |
| 40 | CH | 4 | CYS |
| 40 | CH | 9 | VAL |
| 40 | CH | 20 | CYS |
| 40 | CH | 22 | GLU |
| 40 | CH | 23 | LEU |
| 40 | CH | 27 | GLU |
| 40 | CH | 30 | ILE |
| 40 | CH | 35 | GLN |
| 40 | CH | 36 | MET |
| 40 | CH | 38 | SER |
| 40 | CH | 40 | LYS |
| 40 | CH | 50 | ASN |
| 40 | CH | 51 | THR |
| 40 | CH | 52 | PHE |
| 40 | CH | 53 | PHE |
| 40 | CH | 56 | THR |
| 40 | CH | 60 | LYS |
| 40 | CH | 70 | LEU |
| 40 | CH | 73 | THR |
| 40 | CH | 78 | VAL |
| 40 | CH | 90 | GLU |
| 40 | CH | 92 | LEU |
| 40 | CH | 94 | THR |
| 40 | CH | 96 | LYS |
| 40 | CH | 101 | ASN |
| 40 | CH | 109 | THR |
| 40 | CH | 110 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CH | 113 | GLU |
| 40 | CH | 114 | LEU |
| 40 | CH | 115 | ILE |
| 40 | CH | 116 | ASP |
| 40 | CH | 120 | ASP |
| 40 | CH | 121 | ARG |
| 40 | CH | 123 | ARG |
| 40 | CH | 124 | LYS |
| 40 | CH | 128 | GLN |
| 40 | CH | 129 | CYS |
| 40 | CH | 136 | LEU |
| 40 | CH | 137 | ILE |
| 40 | CH | 145 | THR |
| 40 | CH | 149 | PHE |
| 40 | CH | 153 | LEU |
| 40 | CH | 154 | MET |
| 40 | CH | 155 | GLU |
| 40 | CH | 161 | TYR |
| 40 | CH | 163 | LYS |
| 40 | CH | 164 | LYS |
| 40 | CH | 166 | LYS |
| 40 | CH | 170 | SER |
| 40 | CH | 177 | VAL |
| 40 | CH | 182 | VAL |
| 40 | CH | 184 | PRO |
| 40 | CH | 187 | SER |
| 40 | CH | 188 | ILE |
| 40 | CH | 189 | LEU |
| 40 | CH | 191 | THR |
| 40 | CH | 195 | LEU |
| 40 | CH | 196 | GLU |
| 40 | CH | 198 | SER |
| 40 | CH | 199 | ASP |
| 40 | CH | 200 | CYS |
| 40 | CH | 203 | MET |
| 40 | CH | 204 | VAL |
| 40 | CH | 205 | ASP |
| 40 | CH | 206 | ASN |
| 40 | CH | 209 | ILE |
| 40 | CH | 211 | ASP |
| 40 | CH | 212 | ILE |
| 40 | CH | 213 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CH | 214 | ARG |
| 40 | CH | 215 | ARG |
| 40 | CH | 217 | LEU |
| 40 | CH | 218 | ASP |
| 40 | CH | 221 | ARG |
| 40 | CH | 229 | ARG |
| 40 | CH | 232 | SER |
| 40 | CH | 237 | SER |
| 40 | CH | 238 | ILE |
| 40 | CH | 248 | LEU |
| 40 | CH | 250 | VAL |
| 40 | CH | 253 | THR |
| 40 | CH | 254 | GLU |
| 40 | CH | 257 | THR |
| 40 | CH | 259 | LEU |
| 40 | CH | 260 | VAL |
| 40 | CH | 269 | LEU |
| 40 | CH | 275 | VAL |
| 40 | CH | 276 | ILE |
| 40 | CH | 279 | GLU |
| 40 | CH | 280 | LYS |
| 40 | CH | 284 | GLU |
| 40 | CH | 286 | LEU |
| 40 | CH | 287 | SER |
| 40 | CH | 295 | CYS |
| 40 | CH | 300 | ASN |
| 40 | CH | 302 | MET |
| 40 | CH | 303 | VAL |
| 40 | CH | 304 | LYS |
| 40 | CH | 305 | CYS |
| 40 | CH | 311 | LYS |
| 40 | CH | 315 | CYS |
| 40 | CH | 317 | LEU |
| 40 | CH | 318 | LEU |
| 40 | CH | 320 | ARG |
| 40 | CH | 326 | LYS |
| 40 | CH | 332 | ILE |
| 40 | CH | 339 | ARG |
| 40 | CH | 340 | SER |
| 40 | CH | 342 | GLN |
| 40 | CH | 343 | PHE |
| 40 | CH | 345 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | CH | 347 | CYS |
| 40 | CH | 362 | VAL |
| 40 | CH | 363 | VAL |
| 40 | CH | 366 | ASP |
| 40 | CH | 371 | GLN |
| 40 | CH | 377 | LEU |
| 40 | CH | 381 | THR |
| 40 | CH | 385 | GLU |
| 40 | CH | 389 | ARG |
| 40 | CH | 395 | ASP |
| 40 | CH | 400 | LYS |
| 40 | CH | 403 | PHE |
| 40 | CH | 404 | VAL |
| 40 | CH | 414 | GLU |
| 40 | CH | 416 | GLU |
| 40 | CH | 419 | GLU |
| 40 | CH | 424 | MET |
| 40 | CH | 429 | LYS |
| 40 | CH | 434 | VAL |
| 40 | CH | 436 | MET |
| 40 | CH | 438 | SER |
| 40 | CH | 439 | VAL |
| 41 | CL | 1 | MET |
| 41 | CL | 2 | ARG |
| 41 | CL | 4 | ILE |
| 41 | CL | 8 | GLN |
| 41 | CL | 11 | GLN |
| 41 | CL | 16 | ILE |
| 41 | CL | 19 | LYS |
| 41 | CL | 24 | ILE |
| 41 | CL | 25 | SER |
| 41 | CL | 26 | ASP |
| 41 | CL | 31 | ASP |
| 41 | CL | 33 | THR |
| 41 | CL | 36 | TYR |
| 41 | CL | 39 | ASP |
| 41 | CL | 40 | SER |
| 41 | CL | 47 | ILE |
| 41 | CL | 48 | ASN |
| 41 | CL | 53 | GLU |
| 41 | CL | 55 | THR |
| 41 | CL | 58 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CL | 64 | VAL |
| 41 | CL | 65 | LEU |
| 41 | CL | 66 | VAL |
| 41 | CL | 67 | ASP |
| 41 | CL | 73 | MET |
| 41 | CL | 74 | ASP |
| 41 | CL | 75 | SER |
| 41 | CL | 88 | ASP |
| 41 | CL | 90 | PHE |
| 41 | CL | 91 | VAL |
| 41 | CL | 92 | PHE |
| 41 | CL | 99 | ASN |
| 41 | CL | 105 | HIS |
| 41 | CL | 107 | THR |
| 41 | CL | 108 | GLU |
| 41 | CL | 111 | GLU |
| 41 | CL | 112 | LEU |
| 41 | CL | 114 | ASP |
| 41 | CL | 115 | SER |
| 41 | CL | 117 | LEU |
| 41 | CL | 119 | VAL |
| 41 | CL | 121 | ARG |
| 41 | CL | 122 | LYS |
| 41 | CL | 128 | ASP |
| 41 | CL | 129 | CYS |
| 41 | CL | 130 | LEU |
| 41 | CL | 131 | GLN |
| 41 | CL | 134 | GLN |
| 41 | CL | 143 | THR |
| 41 | CL | 145 | SER |
| 41 | CL | 147 | MET |
| 41 | CL | 150 | LEU |
| 41 | CL | 156 | ARG |
| 41 | CL | 158 | GLU |
| 41 | CL | 159 | TYR |
| 41 | CL | 162 | ARG |
| 41 | CL | 163 | ILE |
| 41 | CL | 165 | ASN |
| 41 | CL | 166 | THR |
| 41 | CL | 168 | SER |
| 41 | CL | 169 | VAL |
| 41 | CL | 170 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CL | 174 | LYS |
| 41 | CL | 175 | VAL |
| 41 | CL | 177 | ASP |
| 41 | CL | 178 | THR |
| 41 | CL | 179 | VAL |
| 41 | CL | 180 | VAL |
| 41 | CL | 181 | GLU |
| 41 | CL | 187 | LEU |
| 41 | CL | 192 | LEU |
| 41 | CL | 193 | VAL |
| 41 | CL | 194 | GLU |
| 41 | CL | 195 | ASN |
| 41 | CL | 201 | CYS |
| 41 | CL | 202 | ILE |
| 41 | CL | 205 | GLU |
| 41 | CL | 209 | ASP |
| 41 | CL | 211 | CYS |
| 41 | CL | 217 | LEU |
| 41 | CL | 221 | THR |
| 41 | CL | 224 | ASP |
| 41 | CL | 230 | SER |
| 41 | CL | 233 | MET |
| 41 | CL | 245 | GLN |
| 41 | CL | 249 | ASP |
| 41 | CL | 250 | LEU |
| 41 | CL | 251 | ARG |
| 41 | CL | 252 | LYS |
| 41 | CL | 253 | LEU |
| 41 | CL | 256 | ASN |
| 41 | CL | 257 | MET |
| 41 | CL | 262 | ARG |
| 41 | CL | 264 | HIS |
| 41 | CL | 276 | ARG |
| 41 | CL | 279 | GLN |
| 41 | CL | 280 | GLN |
| 41 | CL | 282 | ARG |
| 41 | CL | 285 | THR |
| 41 | CL | 288 | GLU |
| 41 | CL | 289 | LEU |
| 41 | CL | 290 | THR |
| 41 | CL | 297 | LYS |
| 41 | CL | 299 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CL | 300 | MET |
| 41 | CL | 306 | ARG |
| 41 | CL | 312 | THR |
| 41 | CL | 316 | VAL |
| 41 | CL | 318 | ARG |
| 41 | CL | 320 | ARG |
| 41 | CL | 322 | SER |
| 41 | CL | 324 | LYS |
| 41 | CL | 325 | GLU |
| 41 | CL | 330 | MET |
| 41 | CL | 332 | ASN |
| 41 | CL | 336 | LYS |
| 41 | CL | 337 | ASN |
| 41 | CL | 339 | SER |
| 41 | CL | 341 | PHE |
| 41 | CL | 347 | ASN |
| 41 | CL | 350 | LYS |
| 41 | CL | 351 | THR |
| 41 | CL | 353 | VAL |
| 41 | CL | 359 | ARG |
| 41 | CL | 362 | LYS |
| 41 | CL | 363 | MET |
| 41 | CL | 371 | SER |
| 41 | CL | 372 | THR |
| 41 | CL | 374 | ILE |
| 41 | CL | 375 | GLN |
| 41 | CL | 377 | LEU |
| 41 | CL | 379 | LYS |
| 41 | CL | 380 | ARG |
| 41 | CL | 383 | GLU |
| 41 | CL | 385 | PHE |
| 41 | CL | 388 | MET |
| 41 | CL | 391 | ARG |
| 41 | CL | 392 | LYS |
| 41 | CL | 395 | LEU |
| 41 | CL | 397 | TRP |
| 41 | CL | 399 | THR |
| 41 | CL | 401 | GLU |
| 41 | CL | 403 | MET |
| 41 | CL | 406 | MET |
| 41 | CL | 413 | SER |
| 41 | CL | 415 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CL | 420 | ASN |
| 41 | CL | 425 | ARG |
| 41 | CM | 7 | LEU |
| 41 | CM | 12 | CYS |
| 41 | CM | 19 | LYS |
| 41 | CM | 20 | PHE |
| 41 | CM | 30 | ILE |
| 41 | CM | 31 | ASP |
| 41 | CM | 33 | THR |
| 41 | CM | 35 | THR |
| 41 | CM | 40 | SER |
| 41 | CM | 43 | GLN |
| 41 | CM | 47 | ILE |
| 41 | CM | 50 | TYR |
| 41 | CM | 53 | GLU |
| 41 | CM | 55 | THR |
| 41 | CM | 60 | VAL |
| 41 | CM | 64 | VAL |
| 41 | CM | 65 | LEU |
| 41 | CM | 66 | VAL |
| 41 | CM | 68 | LEU |
| 41 | CM | 73 | MET |
| 41 | CM | 83 | GLN |
| 41 | CM | 88 | ASP |
| 41 | CM | 89 | ASN |
| 41 | CM | 91 | VAL |
| 41 | CM | 94 | GLN |
| 41 | CM | 106 | TYR |
| 41 | CM | 108 | GLU |
| 41 | CM | 113 | VAL |
| 41 | CM | 115 | SER |
| 41 | CM | 121 | ARG |
| 41 | CM | 122 | LYS |
| 41 | CM | 128 | ASP |
| 41 | CM | 136 | THR |
| 41 | CM | 139 | LEU |
| 41 | CM | 151 | LEU |
| 41 | CM | 156 | ARG |
| 41 | CM | 161 | ASP |
| 41 | CM | 162 | ARG |
| 41 | CM | 165 | ASN |
| 41 | CM | 166 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CM | 168 | SER |
| 41 | CM | 174 | LYS |
| 41 | CM | 180 | VAL |
| 41 | CM | 199 | THR |
| 41 | CM | 202 | ILE |
| 41 | CM | 211 | CYS |
| 41 | CM | 215 | LEU |
| 41 | CM | 216 | LYS |
| 41 | CM | 227 | HIS |
| 41 | CM | 228 | LEU |
| 41 | CM | 232 | THR |
| 41 | CM | 241 | ARG |
| 41 | CM | 245 | GLN |
| 41 | CM | 246 | LEU |
| 41 | CM | 249 | ASP |
| 41 | CM | 253 | LEU |
| 41 | CM | 256 | ASN |
| 41 | CM | 258 | VAL |
| 41 | CM | 262 | ARG |
| 41 | CM | 263 | LEU |
| 41 | CM | 270 | PHE |
| 41 | CM | 274 | THR |
| 41 | CM | 279 | GLN |
| 41 | CM | 280 | GLN |
| 41 | CM | 282 | ARG |
| 41 | CM | 284 | LEU |
| 41 | CM | 289 | LEU |
| 41 | CM | 293 | MET |
| 41 | CM | 295 | ASP |
| 41 | CM | 297 | LYS |
| 41 | CM | 298 | ASN |
| 41 | CM | 299 | MET |
| 41 | CM | 303 | CYS |
| 41 | CM | 306 | ARG |
| 41 | CM | 309 | ARG |
| 41 | CM | 310 | TYR |
| 41 | CM | 313 | VAL |
| 41 | CM | 316 | VAL |
| 41 | CM | 318 | ARG |
| 41 | CM | 321 | MET |
| 41 | CM | 322 | SER |
| 41 | CM | 324 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CM | 326 | VAL |
| 41 | CM | 329 | GLN |
| 41 | CM | 330 | MET |
| 41 | CM | 335 | ASN |
| 41 | CM | 337 | ASN |
| 41 | CM | 348 | ASN |
| 41 | CM | 353 | VAL |
| 41 | CM | 354 | CYS |
| 41 | CM | 359 | ARG |
| 41 | CM | 363 | MET |
| 41 | CM | 374 | ILE |
| 41 | CM | 375 | GLN |
| 41 | CM | 379 | LYS |
| 41 | CM | 388 | MET |
| 41 | CM | 390 | ARG |
| 41 | CM | 392 | LYS |
| 41 | CM | 395 | LEU |
| 41 | CM | 404 | ASP |
| 41 | CM | 422 | VAL |
| 41 | CM | 423 | VAL |
| 41 | CN | 1 | MET |
| 41 | CN | 7 | LEU |
| 41 | CN | 8 | GLN |
| 41 | CN | 12 | CYS |
| 41 | CN | 19 | LYS |
| 41 | CN | 22 | GLU |
| 41 | CN | 26 | ASP |
| 41 | CN | 31 | ASP |
| 41 | CN | 33 | THR |
| 41 | CN | 35 | THR |
| 41 | CN | 40 | SER |
| 41 | CN | 41 | ASP |
| 41 | CN | 45 | GLU |
| 41 | CN | 47 | ILE |
| 41 | CN | 50 | TYR |
| 41 | CN | 53 | GLU |
| 41 | CN | 58 | LYS |
| 41 | CN | 60 | VAL |
| 41 | CN | 64 | VAL |
| 41 | CN | 65 | LEU |
| 41 | CN | 69 | GLU |
| 41 | CN | 72 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CN | 77 | ARG |
| 41 | CN | 83 | GLN |
| 41 | CN | 86 | ARG |
| 41 | CN | 88 | ASP |
| 41 | CN | 99 | ASN |
| 41 | CN | 108 | GLU |
| 41 | CN | 112 | LEU |
| 41 | CN | 114 | ASP |
| 41 | CN | 115 | SER |
| 41 | CN | 122 | LYS |
| 41 | CN | 125 | GLU |
| 41 | CN | 128 | ASP |
| 41 | CN | 130 | LEU |
| 41 | CN | 131 | GLN |
| 41 | CN | 134 | GLN |
| 41 | CN | 135 | LEU |
| 41 | CN | 137 | HIS |
| 41 | CN | 145 | SER |
| 41 | CN | 147 | MET |
| 41 | CN | 151 | LEU |
| 41 | CN | 154 | LYS |
| 41 | CN | 162 | ARG |
| 41 | CN | 165 | ASN |
| 41 | CN | 166 | THR |
| 41 | CN | 168 | SER |
| 41 | CN | 170 | VAL |
| 41 | CN | 172 | SER |
| 41 | CN | 174 | LYS |
| 41 | CN | 175 | VAL |
| 41 | CN | 177 | ASP |
| 41 | CN | 180 | VAL |
| 41 | CN | 181 | GLU |
| 41 | CN | 186 | THR |
| 41 | CN | 191 | GLN |
| 41 | CN | 194 | GLU |
| 41 | CN | 196 | THR |
| 41 | CN | 197 | ASP |
| 41 | CN | 199 | THR |
| 41 | CN | 202 | ILE |
| 41 | CN | 204 | ASN |
| 41 | CN | 211 | CYS |
| 41 | CN | 214 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CN | 215 | LEU |
| 41 | CN | 218 | THR |
| 41 | CN | 222 | TYR |
| 41 | CN | 230 | SER |
| 41 | CN | 233 | MET |
| 41 | CN | 238 | THR |
| 41 | CN | 240 | LEU |
| 41 | CN | 241 | ARG |
| 41 | CN | 245 | GLN |
| 41 | CN | 246 | LEU |
| 41 | CN | 249 | ASP |
| 41 | CN | 252 | LYS |
| 41 | CN | 263 | LEU |
| 41 | CN | 267 | MET |
| 41 | CN | 270 | PHE |
| 41 | CN | 275 | SER |
| 41 | CN | 279 | GLN |
| 41 | CN | 280 | GLN |
| 41 | CN | 284 | LEU |
| 41 | CN | 285 | THR |
| 41 | CN | 288 | GLU |
| 41 | CN | 289 | LEU |
| 41 | CN | 293 | MET |
| 41 | CN | 297 | LYS |
| 41 | CN | 299 | MET |
| 41 | CN | 303 | CYS |
| 41 | CN | 306 | ARG |
| 41 | CN | 309 | ARG |
| 41 | CN | 313 | VAL |
| 41 | CN | 316 | VAL |
| 41 | CN | 318 | ARG |
| 41 | CN | 320 | ARG |
| 41 | CN | 322 | SER |
| 41 | CN | 324 | LYS |
| 41 | CN | 325 | GLU |
| 41 | CN | 327 | ASP |
| 41 | CN | 329 | GLN |
| 41 | CN | 331 | LEU |
| 41 | CN | 342 | VAL |
| 41 | CN | 343 | GLU |
| 41 | CN | 347 | ASN |
| 41 | CN | 348 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CN | 350 | LYS |
| 41 | CN | 353 | VAL |
| 41 | CN | 354 | CYS |
| 41 | CN | 359 | ARG |
| 41 | CN | 362 | LYS |
| 41 | CN | 363 | MET |
| 41 | CN | 371 | SER |
| 41 | CN | 372 | THR |
| 41 | CN | 374 | ILE |
| 41 | CN | 376 | GLU |
| 41 | CN | 379 | LYS |
| 41 | CN | 381 | ILE |
| 41 | CN | 382 | SER |
| 41 | CN | 390 | ARG |
| 41 | CN | 395 | LEU |
| 41 | CN | 403 | MET |
| 41 | CN | 404 | ASP |
| 41 | CN | 409 | THR |
| 41 | CN | 413 | SER |
| 41 | CN | 415 | MET |
| 41 | CN | 423 | VAL |
| 41 | CN | 425 | ARG |
| 41 | CN | 428 | CYS |
| 41 | CO | 1 | MET |
| 41 | CO | 2 | ARG |
| 41 | CO | 3 | GLU |
| 41 | CO | 4 | ILE |
| 41 | CO | 6 | HIS |
| 41 | CO | 7 | LEU |
| 41 | CO | 12 | CYS |
| 41 | CO | 16 | ILE |
| 41 | CO | 19 | LYS |
| 41 | CO | 22 | GLU |
| 41 | CO | 26 | ASP |
| 41 | CO | 30 | ILE |
| 41 | CO | 31 | ASP |
| 41 | CO | 35 | THR |
| 41 | CO | 37 | HIS |
| 41 | CO | 39 | ASP |
| 41 | CO | 40 | SER |
| 41 | CO | 41 | ASP |
| 41 | CO | 47 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CO | 50 | TYR |
| 41 | CO | 55 | THR |
| 41 | CO | 62 | ARG |
| 41 | CO | 65 | LEU |
| 41 | CO | 66 | VAL |
| 41 | CO | 72 | THR |
| 41 | CO | 73 | MET |
| 41 | CO | 74 | ASP |
| 41 | CO | 75 | SER |
| 41 | CO | 77 | ARG |
| 41 | CO | 83 | GLN |
| 41 | CO | 86 | ARG |
| 41 | CO | 88 | ASP |
| 41 | CO | 99 | ASN |
| 41 | CO | 103 | LYS |
| 41 | CO | 106 | TYR |
| 41 | CO | 111 | GLU |
| 41 | CO | 112 | LEU |
| 41 | CO | 113 | VAL |
| 41 | CO | 115 | SER |
| 41 | CO | 119 | VAL |
| 41 | CO | 121 | ARG |
| 41 | CO | 128 | ASP |
| 41 | CO | 130 | LEU |
| 41 | CO | 131 | GLN |
| 41 | CO | 134 | GLN |
| 41 | CO | 136 | THR |
| 41 | CO | 139 | LEU |
| 41 | CO | 147 | MET |
| 41 | CO | 151 | LEU |
| 41 | CO | 154 | LYS |
| 41 | CO | 162 | ARG |
| 41 | CO | 163 | ILE |
| 41 | CO | 166 | THR |
| 41 | CO | 170 | VAL |
| 41 | CO | 172 | SER |
| 41 | CO | 174 | LYS |
| 41 | CO | 176 | SER |
| 41 | CO | 178 | THR |
| 41 | CO | 180 | VAL |
| 41 | CO | 188 | SER |
| 41 | CO | 190 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CO | 191 | GLN |
| 41 | CO | 192 | LEU |
| 41 | CO | 194 | GLU |
| 41 | CO | 199 | THR |
| 41 | CO | 204 | ASN |
| 41 | CO | 209 | ASP |
| 41 | CO | 213 | ARG |
| 41 | CO | 218 | THR |
| 41 | CO | 222 | TYR |
| 41 | CO | 225 | LEU |
| 41 | CO | 232 | THR |
| 41 | CO | 236 | VAL |
| 41 | CO | 240 | LEU |
| 41 | CO | 249 | ASP |
| 41 | CO | 252 | LYS |
| 41 | CO | 253 | LEU |
| 41 | CO | 267 | MET |
| 41 | CO | 275 | SER |
| 41 | CO | 280 | GLN |
| 41 | CO | 282 | ARG |
| 41 | CO | 288 | GLU |
| 41 | CO | 292 | GLN |
| 41 | CO | 297 | LYS |
| 41 | CO | 299 | MET |
| 41 | CO | 303 | CYS |
| 41 | CO | 306 | ARG |
| 41 | CO | 310 | TYR |
| 41 | CO | 313 | VAL |
| 41 | CO | 316 | VAL |
| 41 | CO | 318 | ARG |
| 41 | CO | 320 | ARG |
| 41 | CO | 322 | SER |
| 41 | CO | 324 | LYS |
| 41 | CO | 328 | GLU |
| 41 | CO | 331 | LEU |
| 41 | CO | 341 | PHE |
| 41 | CO | 343 | GLU |
| 41 | CO | 347 | ASN |
| 41 | CO | 359 | ARG |
| 41 | CO | 362 | LYS |
| 41 | CO | 364 | SER |
| 41 | CO | 368 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CO | 374 | ILE |
| 41 | CO | 375 | GLN |
| 41 | CO | 376 | GLU |
| 41 | CO | 380 | ARG |
| 41 | CO | 381 | ILE |
| 41 | CO | 388 | MET |
| 41 | CO | 391 | ARG |
| 41 | CO | 395 | LEU |
| 41 | CO | 406 | MET |
| 41 | CO | 413 | SER |
| 41 | CO | 415 | MET |
| 41 | CO | 418 | LEU |
| 41 | CO | 422 | VAL |
| 41 | CO | 425 | ARG |
| 41 | CP | 1 | MET |
| 41 | CP | 2 | ARG |
| 41 | CP | 4 | ILE |
| 41 | CP | 6 | HIS |
| 41 | CP | 7 | LEU |
| 41 | CP | 8 | GLN |
| 41 | CP | 11 | GLN |
| 41 | CP | 12 | CYS |
| 41 | CP | 19 | LYS |
| 41 | CP | 20 | PHE |
| 41 | CP | 22 | GLU |
| 41 | CP | 27 | GLU |
| 41 | CP | 30 | ILE |
| 41 | CP | 31 | ASP |
| 41 | CP | 35 | THR |
| 41 | CP | 39 | ASP |
| 41 | CP | 40 | SER |
| 41 | CP | 42 | LEU |
| 41 | CP | 44 | LEU |
| 41 | CP | 45 | GLU |
| 41 | CP | 47 | ILE |
| 41 | CP | 50 | TYR |
| 41 | CP | 53 | GLU |
| 41 | CP | 55 | THR |
| 41 | CP | 59 | TYR |
| 41 | CP | 65 | LEU |
| 41 | CP | 69 | GLU |
| 41 | CP | 73 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CP | 75 | SER |
| 41 | CP | 77 | ARG |
| 41 | CP | 86 | ARG |
| 41 | CP | 99 | ASN |
| 41 | CP | 103 | LYS |
| 41 | CP | 107 | THR |
| 41 | CP | 114 | ASP |
| 41 | CP | 122 | LYS |
| 41 | CP | 128 | ASP |
| 41 | CP | 129 | CYS |
| 41 | CP | 130 | LEU |
| 41 | CP | 135 | LEU |
| 41 | CP | 137 | HIS |
| 41 | CP | 139 | LEU |
| 41 | CP | 147 | MET |
| 41 | CP | 151 | LEU |
| 41 | CP | 158 | GLU |
| 41 | CP | 159 | TYR |
| 41 | CP | 162 | ARG |
| 41 | CP | 163 | ILE |
| 41 | CP | 164 | MET |
| 41 | CP | 165 | ASN |
| 41 | CP | 166 | THR |
| 41 | CP | 168 | SER |
| 41 | CP | 170 | VAL |
| 41 | CP | 172 | SER |
| 41 | CP | 174 | LYS |
| 41 | CP | 175 | VAL |
| 41 | CP | 176 | SER |
| 41 | CP | 178 | THR |
| 41 | CP | 179 | VAL |
| 41 | CP | 180 | VAL |
| 41 | CP | 188 | SER |
| 41 | CP | 197 | ASP |
| 41 | CP | 198 | GLU |
| 41 | CP | 199 | THR |
| 41 | CP | 201 | CYS |
| 41 | CP | 202 | ILE |
| 41 | CP | 203 | ASP |
| 41 | CP | 204 | ASN |
| 41 | CP | 208 | TYR |
| 41 | CP | 212 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CP | 213 | ARG |
| 41 | CP | 216 | LYS |
| 41 | CP | 218 | THR |
| 41 | CP | 219 | THR |
| 41 | CP | 224 | ASP |
| 41 | CP | 227 | HIS |
| 41 | CP | 232 | THR |
| 41 | CP | 233 | MET |
| 41 | CP | 238 | THR |
| 41 | CP | 240 | LEU |
| 41 | CP | 241 | ARG |
| 41 | CP | 245 | GLN |
| 41 | CP | 251 | ARG |
| 41 | CP | 252 | LYS |
| 41 | CP | 256 | ASN |
| 41 | CP | 258 | VAL |
| 41 | CP | 262 | ARG |
| 41 | CP | 267 | MET |
| 41 | CP | 273 | LEU |
| 41 | CP | 274 | THR |
| 41 | CP | 278 | SER |
| 41 | CP | 280 | GLN |
| 41 | CP | 282 | ARG |
| 41 | CP | 284 | LEU |
| 41 | CP | 288 | GLU |
| 41 | CP | 289 | LEU |
| 41 | CP | 293 | MET |
| 41 | CP | 297 | LYS |
| 41 | CP | 300 | MET |
| 41 | CP | 303 | CYS |
| 41 | CP | 306 | ARG |
| 41 | CP | 309 | ARG |
| 41 | CP | 312 | THR |
| 41 | CP | 313 | VAL |
| 41 | CP | 316 | VAL |
| 41 | CP | 318 | ARG |
| 41 | CP | 320 | ARG |
| 41 | CP | 321 | MET |
| 41 | CP | 322 | SER |
| 41 | CP | 323 | MET |
| 41 | CP | 324 | LYS |
| 41 | CP | 325 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CP | 326 | VAL |
| 41 | CP | 327 | ASP |
| 41 | CP | 330 | MET |
| 41 | CP | 335 | ASN |
| 41 | CP | 336 | LYS |
| 41 | CP | 337 | ASN |
| 41 | CP | 342 | VAL |
| 41 | CP | 347 | ASN |
| 41 | CP | 350 | LYS |
| 41 | CP | 353 | VAL |
| 41 | CP | 356 | ILE |
| 41 | CP | 359 | ARG |
| 41 | CP | 362 | LYS |
| 41 | CP | 363 | MET |
| 41 | CP | 374 | ILE |
| 41 | CP | 375 | GLN |
| 41 | CP | 377 | LEU |
| 41 | CP | 380 | ARG |
| 41 | CP | 386 | THR |
| 41 | CP | 388 | MET |
| 41 | CP | 390 | ARG |
| 41 | CP | 392 | LYS |
| 41 | CP | 395 | LEU |
| 41 | CP | 409 | THR |
| 41 | CP | 418 | LEU |
| 41 | CP | 420 | ASN |
| 41 | CP | 423 | VAL |
| 41 | CP | 428 | CYS |
| 40 | DA | 2 | ARG |
| 40 | DA | 4 | CYS |
| 40 | DA | 6 | SER |
| 40 | DA | 11 | GLN |
| 40 | DA | 16 | ILE |
| 40 | DA | 23 | LEU |
| 40 | DA | 26 | LEU |
| 40 | DA | 27 | GLU |
| 40 | DA | 33 | ASP |
| 40 | DA | 35 | GLN |
| 40 | DA | 36 | MET |
| 40 | DA | 38 | SER |
| 40 | DA | 48 | SER |
| 40 | DA | 51 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DA | 54 | SER |
| 40 | DA | 66 | VAL |
| 40 | DA | 71 | GLU |
| 40 | DA | 73 | THR |
| 40 | DA | 75 | ILE |
| 40 | DA | 80 | THR |
| 40 | DA | 84 | ARG |
| 40 | DA | 94 | THR |
| 40 | DA | 96 | LYS |
| 40 | DA | 97 | GLU |
| 40 | DA | 109 | THR |
| 40 | DA | 110 | ILE |
| 40 | DA | 112 | LYS |
| 40 | DA | 114 | LEU |
| 40 | DA | 116 | ASP |
| 40 | DA | 117 | LEU |
| 40 | DA | 119 | LEU |
| 40 | DA | 120 | ASP |
| 40 | DA | 121 | ARG |
| 40 | DA | 122 | ILE |
| 40 | DA | 123 | ARG |
| 40 | DA | 124 | LYS |
| 40 | DA | 132 | LEU |
| 40 | DA | 137 | ILE |
| 40 | DA | 138 | PHE |
| 40 | DA | 140 | SER |
| 40 | DA | 156 | ARG |
| 40 | DA | 160 | ASP |
| 40 | DA | 163 | LYS |
| 40 | DA | 164 | LYS |
| 40 | DA | 165 | SER |
| 40 | DA | 166 | LYS |
| 40 | DA | 168 | GLU |
| 40 | DA | 169 | PHE |
| 40 | DA | 170 | SER |
| 40 | DA | 172 | TYR |
| 40 | DA | 179 | THR |
| 40 | DA | 182 | VAL |
| 40 | DA | 187 | SER |
| 40 | DA | 188 | ILE |
| 40 | DA | 195 | LEU |
| 40 | DA | 198 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DA | 199 | ASP |
| 40 | DA | 202 | PHE |
| 40 | DA | 203 | MET |
| 40 | DA | 204 | VAL |
| 40 | DA | 206 | ASN |
| 40 | DA | 210 | TYR |
| 40 | DA | 211 | ASP |
| 40 | DA | 214 | ARG |
| 40 | DA | 217 | LEU |
| 40 | DA | 221 | ARG |
| 40 | DA | 224 | TYR |
| 40 | DA | 227 | LEU |
| 40 | DA | 232 | SER |
| 40 | DA | 235 | VAL |
| 40 | DA | 238 | ILE |
| 40 | DA | 242 | LEU |
| 40 | DA | 243 | ARG |
| 40 | DA | 248 | LEU |
| 40 | DA | 249 | ASN |
| 40 | DA | 250 | VAL |
| 40 | DA | 255 | PHE |
| 40 | DA | 259 | LEU |
| 40 | DA | 264 | ARG |
| 40 | DA | 265 | ILE |
| 40 | DA | 277 | SER |
| 40 | DA | 287 | SER |
| 40 | DA | 291 | ILE |
| 40 | DA | 302 | MET |
| 40 | DA | 303 | VAL |
| 40 | DA | 304 | LYS |
| 40 | DA | 311 | LYS |
| 40 | DA | 315 | CYS |
| 40 | DA | 316 | CYS |
| 40 | DA | 318 | LEU |
| 40 | DA | 323 | VAL |
| 40 | DA | 326 | LYS |
| 40 | DA | 332 | ILE |
| 40 | DA | 335 | ILE |
| 40 | DA | 339 | ARG |
| 40 | DA | 342 | GLN |
| 40 | DA | 343 | PHE |
| 40 | DA | 352 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DA | 357 | TYR |
| 40 | DA | 362 | VAL |
| 40 | DA | 369 | LYS |
| 40 | DA | 370 | VAL |
| 40 | DA | 371 | GLN |
| 40 | DA | 376 | MET |
| 40 | DA | 380 | THR |
| 40 | DA | 383 | ILE |
| 40 | DA | 385 | GLU |
| 40 | DA | 389 | ARG |
| 40 | DA | 390 | LEU |
| 40 | DA | 397 | MET |
| 40 | DA | 400 | LYS |
| 40 | DA | 412 | MET |
| 40 | DA | 416 | GLU |
| 40 | DA | 421 | ARG |
| 40 | DA | 423 | ASP |
| 40 | DA | 424 | MET |
| 40 | DA | 427 | LEU |
| 40 | DA | 429 | LYS |
| 40 | DA | 430 | ASP |
| 40 | DA | 436 | MET |
| 40 | DA | 438 | SER |
| 41 | DB | 1 | MET |
| 41 | DB | 4 | ILE |
| 41 | DB | 7 | LEU |
| 41 | DB | 12 | CYS |
| 41 | DB | 14 | ASN |
| 41 | DB | 15 | GLN |
| 41 | DB | 16 | ILE |
| 41 | DB | 19 | LYS |
| 41 | DB | 22 | GLU |
| 41 | DB | 26 | ASP |
| 41 | DB | 27 | GLU |
| 41 | DB | 31 | ASP |
| 41 | DB | 33 | THR |
| 41 | DB | 35 | THR |
| 41 | DB | 37 | HIS |
| 41 | DB | 40 | SER |
| 41 | DB | 42 | LEU |
| 41 | DB | 43 | GLN |
| 41 | DB | 55 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DB | 58 | LYS |
| 41 | DB | 62 | ARG |
| 41 | DB | 64 | VAL |
| 41 | DB | 69 | GLU |
| 41 | DB | 73 | MET |
| 41 | DB | 75 | SER |
| 41 | DB | 77 | ARG |
| 41 | DB | 81 | PHE |
| 41 | DB | 83 | GLN |
| 41 | DB | 84 | ILE |
| 41 | DB | 86 | ARG |
| 41 | DB | 88 | ASP |
| 41 | DB | 90 | PHE |
| 41 | DB | 94 | GLN |
| 41 | DB | 99 | ASN |
| 41 | DB | 101 | TRP |
| 41 | DB | 111 | GLU |
| 41 | DB | 114 | ASP |
| 41 | DB | 115 | SER |
| 41 | DB | 122 | LYS |
| 41 | DB | 123 | GLU |
| 41 | DB | 125 | GLU |
| 41 | DB | 128 | ASP |
| 41 | DB | 134 | GLN |
| 41 | DB | 135 | LEU |
| 41 | DB | 151 | LEU |
| 41 | DB | 153 | SER |
| 41 | DB | 155 | ILE |
| 41 | DB | 158 | GLU |
| 41 | DB | 161 | ASP |
| 41 | DB | 162 | ARG |
| 41 | DB | 163 | ILE |
| 41 | DB | 164 | MET |
| 41 | DB | 166 | THR |
| 41 | DB | 167 | PHE |
| 41 | DB | 168 | SER |
| 41 | DB | 172 | SER |
| 41 | DB | 174 | LYS |
| 41 | DB | 175 | VAL |
| 41 | DB | 176 | SER |
| 41 | DB | 180 | VAL |
| 41 | DB | 181 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DB | 188 | SER |
| 41 | DB | 192 | LEU |
| 41 | DB | 196 | THR |
| 41 | DB | 202 | ILE |
| 41 | DB | 204 | ASN |
| 41 | DB | 205 | GLU |
| 41 | DB | 208 | TYR |
| 41 | DB | 216 | LYS |
| 41 | DB | 222 | TYR |
| 41 | DB | 224 | ASP |
| 41 | DB | 226 | ASN |
| 41 | DB | 227 | HIS |
| 41 | DB | 228 | LEU |
| 41 | DB | 233 | MET |
| 41 | DB | 236 | VAL |
| 41 | DB | 238 | THR |
| 41 | DB | 240 | LEU |
| 41 | DB | 245 | GLN |
| 41 | DB | 246 | LEU |
| 41 | DB | 253 | LEU |
| 41 | DB | 262 | ARG |
| 41 | DB | 263 | LEU |
| 41 | DB | 266 | PHE |
| 41 | DB | 276 | ARG |
| 41 | DB | 279 | GLN |
| 41 | DB | 292 | GLN |
| 41 | DB | 293 | MET |
| 41 | DB | 300 | MET |
| 41 | DB | 306 | ARG |
| 41 | DB | 309 | ARG |
| 41 | DB | 310 | TYR |
| 41 | DB | 311 | LEU |
| 41 | DB | 318 | ARG |
| 41 | DB | 320 | ARG |
| 41 | DB | 322 | SER |
| 41 | DB | 324 | LYS |
| 41 | DB | 331 | LEU |
| 41 | DB | 332 | ASN |
| 41 | DB | 334 | GLN |
| 41 | DB | 336 | LYS |
| 41 | DB | 338 | SER |
| 41 | DB | 342 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DB | 347 | ASN |
| 41 | DB | 349 | VAL |
| 41 | DB | 350 | LYS |
| 41 | DB | 353 | VAL |
| 41 | DB | 354 | CYS |
| 41 | DB | 361 | LEU |
| 41 | DB | 362 | LYS |
| 41 | DB | 363 | MET |
| 41 | DB | 366 | THR |
| 41 | DB | 367 | PHE |
| 41 | DB | 376 | GLU |
| 41 | DB | 379 | LYS |
| 41 | DB | 381 | ILE |
| 41 | DB | 382 | SER |
| 41 | DB | 389 | PHE |
| 41 | DB | 390 | ARG |
| 41 | DB | 392 | LYS |
| 41 | DB | 395 | LEU |
| 41 | DB | 396 | HIS |
| 41 | DB | 403 | MET |
| 41 | DB | 404 | ASP |
| 41 | DB | 406 | MET |
| 41 | DB | 409 | THR |
| 41 | DB | 410 | GLU |
| 41 | DB | 415 | MET |
| 41 | DB | 416 | ASN |
| 41 | DB | 423 | VAL |
| 41 | DB | 425 | ARG |
| 40 | DE | 2 | ARG |
| 40 | DE | 5 | ILE |
| 40 | DE | 14 | VAL |
| 40 | DE | 15 | GLN |
| 40 | DE | 22 | GLU |
| 40 | DE | 23 | LEU |
| 40 | DE | 25 | CYS |
| 40 | DE | 26 | LEU |
| 40 | DE | 30 | ILE |
| 40 | DE | 31 | GLN |
| 40 | DE | 33 | ASP |
| 40 | DE | 36 | MET |
| 40 | DE | 48 | SER |
| 40 | DE | 51 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DE | 64 | ARG |
| 40 | DE | 66 | VAL |
| 40 | DE | 68 | VAL |
| 40 | DE | 74 | VAL |
| 40 | DE | 75 | ILE |
| 40 | DE | 78 | VAL |
| 40 | DE | 80 | THR |
| 40 | DE | 84 | ARG |
| 40 | DE | 88 | HIS |
| 40 | DE | 93 | ILE |
| 40 | DE | 96 | LYS |
| 40 | DE | 107 | HIS |
| 40 | DE | 108 | TYR |
| 40 | DE | 109 | THR |
| 40 | DE | 110 | ILE |
| 40 | DE | 112 | LYS |
| 40 | DE | 113 | GLU |
| 40 | DE | 115 | ILE |
| 40 | DE | 116 | ASP |
| 40 | DE | 117 | LEU |
| 40 | DE | 120 | ASP |
| 40 | DE | 123 | ARG |
| 40 | DE | 128 | GLN |
| 40 | DE | 129 | CYS |
| 40 | DE | 136 | LEU |
| 40 | DE | 138 | PHE |
| 40 | DE | 139 | HIS |
| 40 | DE | 140 | SER |
| 40 | DE | 141 | PHE |
| 40 | DE | 152 | LEU |
| 40 | DE | 153 | LEU |
| 40 | DE | 155 | GLU |
| 40 | DE | 157 | LEU |
| 40 | DE | 159 | VAL |
| 40 | DE | 163 | LYS |
| 40 | DE | 164 | LYS |
| 40 | DE | 170 | SER |
| 40 | DE | 171 | ILE |
| 40 | DE | 181 | VAL |
| 40 | DE | 182 | VAL |
| 40 | DE | 184 | PRO |
| 40 | DE | 195 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DE | 199 | ASP |
| 40 | DE | 200 | CYS |
| 40 | DE | 205 | ASP |
| 40 | DE | 206 | ASN |
| 40 | DE | 209 | ILE |
| 40 | DE | 211 | ASP |
| 40 | DE | 219 | ILE |
| 40 | DE | 220 | GLU |
| 40 | DE | 221 | ARG |
| 40 | DE | 229 | ARG |
| 40 | DE | 230 | LEU |
| 40 | DE | 235 | VAL |
| 40 | DE | 242 | LEU |
| 40 | DE | 249 | ASN |
| 40 | DE | 250 | VAL |
| 40 | DE | 254 | GLU |
| 40 | DE | 256 | GLN |
| 40 | DE | 257 | THR |
| 40 | DE | 258 | ASN |
| 40 | DE | 262 | TYR |
| 40 | DE | 264 | ARG |
| 40 | DE | 267 | PHE |
| 40 | DE | 275 | VAL |
| 40 | DE | 276 | ILE |
| 40 | DE | 280 | LYS |
| 40 | DE | 283 | HIS |
| 40 | DE | 284 | GLU |
| 40 | DE | 286 | LEU |
| 40 | DE | 291 | ILE |
| 40 | DE | 293 | ASN |
| 40 | DE | 295 | CYS |
| 40 | DE | 296 | PHE |
| 40 | DE | 302 | MET |
| 40 | DE | 303 | VAL |
| 40 | DE | 308 | ARG |
| 40 | DE | 311 | LYS |
| 40 | DE | 313 | MET |
| 40 | DE | 315 | CYS |
| 40 | DE | 320 | ARG |
| 40 | DE | 322 | ASP |
| 40 | DE | 323 | VAL |
| 40 | DE | 324 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DE | 326 | LYS |
| 40 | DE | 327 | ASP |
| 40 | DE | 335 | ILE |
| 40 | DE | 336 | LYS |
| 40 | DE | 339 | ARG |
| 40 | DE | 341 | ILE |
| 40 | DE | 343 | PHE |
| 40 | DE | 349 | THR |
| 40 | DE | 352 | LYS |
| 40 | DE | 355 | ILE |
| 40 | DE | 358 | GLN |
| 40 | DE | 363 | VAL |
| 40 | DE | 366 | ASP |
| 40 | DE | 367 | LEU |
| 40 | DE | 371 | GLN |
| 40 | DE | 378 | SER |
| 40 | DE | 380 | THR |
| 40 | DE | 381 | THR |
| 40 | DE | 383 | ILE |
| 40 | DE | 387 | TRP |
| 40 | DE | 389 | ARG |
| 40 | DE | 390 | LEU |
| 40 | DE | 400 | LYS |
| 40 | DE | 401 | ARG |
| 40 | DE | 405 | HIS |
| 40 | DE | 421 | ARG |
| 40 | DE | 423 | ASP |
| 40 | DE | 429 | LYS |
| 40 | DE | 436 | MET |
| 40 | DE | 437 | ASP |
| 40 | DE | 439 | VAL |
| 40 | DE | 440 | GLU |
| 40 | DF | 2 | ARG |
| 40 | DF | 3 | GLU |
| 40 | DF | 6 | SER |
| 40 | DF | 11 | GLN |
| 40 | DF | 15 | GLN |
| 40 | DF | 16 | ILE |
| 40 | DF | 22 | GLU |
| 40 | DF | 23 | LEU |
| 40 | DF | 26 | LEU |
| 40 | DF | 27 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DF | 33 | ASP |
| 40 | DF | 36 | MET |
| 40 | DF | 55 | GLU |
| 40 | DF | 60 | LYS |
| 40 | DF | 62 | VAL |
| 40 | DF | 66 | VAL |
| 40 | DF | 68 | VAL |
| 40 | DF | 74 | VAL |
| 40 | DF | 75 | ILE |
| 40 | DF | 79 | ARG |
| 40 | DF | 84 | ARG |
| 40 | DF | 92 | LEU |
| 40 | DF | 93 | ILE |
| 40 | DF | 94 | THR |
| 40 | DF | 97 | GLU |
| 40 | DF | 98 | ASP |
| 40 | DF | 105 | ARG |
| 40 | DF | 112 | LYS |
| 40 | DF | 116 | ASP |
| 40 | DF | 120 | ASP |
| 40 | DF | 122 | ILE |
| 40 | DF | 123 | ARG |
| 40 | DF | 128 | GLN |
| 40 | DF | 132 | LEU |
| 40 | DF | 133 | GLN |
| 40 | DF | 138 | PHE |
| 40 | DF | 141 | PHE |
| 40 | DF | 145 | THR |
| 40 | DF | 147 | SER |
| 40 | DF | 153 | LEU |
| 40 | DF | 157 | LEU |
| 40 | DF | 159 | VAL |
| 40 | DF | 160 | ASP |
| 40 | DF | 161 | TYR |
| 40 | DF | 163 | LYS |
| 40 | DF | 164 | LYS |
| 40 | DF | 169 | PHE |
| 40 | DF | 171 | ILE |
| 40 | DF | 182 | VAL |
| 40 | DF | 187 | SER |
| 40 | DF | 188 | ILE |
| 40 | DF | 195 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DF | 198 | SER |
| 40 | DF | 199 | ASP |
| 40 | DF | 203 | MET |
| 40 | DF | 204 | VAL |
| 40 | DF | 205 | ASP |
| 40 | DF | 207 | GLU |
| 40 | DF | 209 | ILE |
| 40 | DF | 212 | ILE |
| 40 | DF | 213 | CYS |
| 40 | DF | 214 | ARG |
| 40 | DF | 215 | ARG |
| 40 | DF | 217 | LEU |
| 40 | DF | 220 | GLU |
| 40 | DF | 221 | ARG |
| 40 | DF | 226 | ASN |
| 40 | DF | 227 | LEU |
| 40 | DF | 231 | ILE |
| 40 | DF | 239 | THR |
| 40 | DF | 241 | SER |
| 40 | DF | 242 | LEU |
| 40 | DF | 244 | PHE |
| 40 | DF | 245 | ASP |
| 40 | DF | 248 | LEU |
| 40 | DF | 249 | ASN |
| 40 | DF | 250 | VAL |
| 40 | DF | 251 | ASP |
| 40 | DF | 253 | THR |
| 40 | DF | 256 | GLN |
| 40 | DF | 257 | THR |
| 40 | DF | 259 | LEU |
| 40 | DF | 275 | VAL |
| 40 | DF | 276 | ILE |
| 40 | DF | 277 | SER |
| 40 | DF | 284 | GLU |
| 40 | DF | 286 | LEU |
| 40 | DF | 287 | SER |
| 40 | DF | 291 | ILE |
| 40 | DF | 300 | ASN |
| 40 | DF | 302 | MET |
| 40 | DF | 303 | VAL |
| 40 | DF | 308 | ARG |
| 40 | DF | 311 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DF | 315 | CYS |
| 40 | DF | 316 | CYS |
| 40 | DF | 318 | LEU |
| 40 | DF | 323 | VAL |
| 40 | DF | 324 | VAL |
| 40 | DF | 327 | ASP |
| 40 | DF | 329 | ASN |
| 40 | DF | 336 | LYS |
| 40 | DF | 338 | LYS |
| 40 | DF | 339 | ARG |
| 40 | DF | 340 | SER |
| 40 | DF | 349 | THR |
| 40 | DF | 359 | PRO |
| 40 | DF | 363 | VAL |
| 40 | DF | 366 | ASP |
| 40 | DF | 367 | LEU |
| 40 | DF | 370 | VAL |
| 40 | DF | 372 | ARG |
| 40 | DF | 376 | MET |
| 40 | DF | 377 | LEU |
| 40 | DF | 379 | ASN |
| 40 | DF | 383 | ILE |
| 40 | DF | 385 | GLU |
| 40 | DF | 390 | LEU |
| 40 | DF | 397 | MET |
| 40 | DF | 401 | ARG |
| 40 | DF | 404 | VAL |
| 40 | DF | 405 | HIS |
| 40 | DF | 408 | VAL |
| 40 | DF | 410 | GLU |
| 40 | DF | 413 | GLU |
| 40 | DF | 418 | SER |
| 40 | DF | 419 | GLU |
| 40 | DF | 421 | ARG |
| 40 | DF | 423 | ASP |
| 40 | DF | 432 | GLU |
| 40 | DF | 436 | MET |
| 40 | DF | 437 | ASP |
| 40 | DF | 438 | SER |
| 40 | DF | 439 | VAL |
| 40 | DF | 440 | GLU |
| 40 | DG | 308 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DH | 2 | ARG |
| 40 | DH | 5 | ILE |
| 40 | DH | 6 | SER |
| 40 | DH | 7 | VAL |
| 40 | DH | 11 | GLN |
| 40 | DH | 15 | GLN |
| 40 | DH | 20 | CYS |
| 40 | DH | 23 | LEU |
| 40 | DH | 26 | LEU |
| 40 | DH | 51 | THR |
| 40 | DH | 52 | PHE |
| 40 | DH | 54 | SER |
| 40 | DH | 62 | VAL |
| 40 | DH | 64 | ARG |
| 40 | DH | 66 | VAL |
| 40 | DH | 68 | VAL |
| 40 | DH | 71 | GLU |
| 40 | DH | 74 | VAL |
| 40 | DH | 75 | ILE |
| 40 | DH | 80 | THR |
| 40 | DH | 85 | GLN |
| 40 | DH | 92 | LEU |
| 40 | DH | 96 | LYS |
| 40 | DH | 112 | LYS |
| 40 | DH | 113 | GLU |
| 40 | DH | 114 | LEU |
| 40 | DH | 116 | ASP |
| 40 | DH | 121 | ARG |
| 40 | DH | 123 | ARG |
| 40 | DH | 128 | GLN |
| 40 | DH | 140 | SER |
| 40 | DH | 141 | PHE |
| 40 | DH | 158 | SER |
| 40 | DH | 164 | LYS |
| 40 | DH | 165 | SER |
| 40 | DH | 166 | LYS |
| 40 | DH | 168 | GLU |
| 40 | DH | 169 | PHE |
| 40 | DH | 171 | ILE |
| 40 | DH | 172 | TYR |
| 40 | DH | 177 | VAL |
| 40 | DH | 187 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DH | 188 | ILE |
| 40 | DH | 191 | THR |
| 40 | DH | 192 | HIS |
| 40 | DH | 195 | LEU |
| 40 | DH | 196 | GLU |
| 40 | DH | 198 | SER |
| 40 | DH | 199 | ASP |
| 40 | DH | 200 | CYS |
| 40 | DH | 203 | MET |
| 40 | DH | 204 | VAL |
| 40 | DH | 205 | ASP |
| 40 | DH | 206 | ASN |
| 40 | DH | 209 | ILE |
| 40 | DH | 214 | ARG |
| 40 | DH | 215 | ARG |
| 40 | DH | 220 | GLU |
| 40 | DH | 221 | ARG |
| 40 | DH | 224 | TYR |
| 40 | DH | 226 | ASN |
| 40 | DH | 229 | ARG |
| 40 | DH | 230 | LEU |
| 40 | DH | 231 | ILE |
| 40 | DH | 239 | THR |
| 40 | DH | 241 | SER |
| 40 | DH | 242 | LEU |
| 40 | DH | 243 | ARG |
| 40 | DH | 245 | ASP |
| 40 | DH | 248 | LEU |
| 40 | DH | 264 | ARG |
| 40 | DH | 269 | LEU |
| 40 | DH | 275 | VAL |
| 40 | DH | 276 | ILE |
| 40 | DH | 279 | GLU |
| 40 | DH | 282 | TYR |
| 40 | DH | 283 | HIS |
| 40 | DH | 285 | GLN |
| 40 | DH | 291 | ILE |
| 40 | DH | 295 | CYS |
| 40 | DH | 302 | MET |
| 40 | DH | 304 | LYS |
| 40 | DH | 306 | ASP |
| 40 | DH | 308 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DH | 311 | LYS |
| 40 | DH | 313 | MET |
| 40 | DH | 316 | CYS |
| 40 | DH | 317 | LEU |
| 40 | DH | 318 | LEU |
| 40 | DH | 320 | ARG |
| 40 | DH | 322 | ASP |
| 40 | DH | 324 | VAL |
| 40 | DH | 326 | LYS |
| 40 | DH | 328 | VAL |
| 40 | DH | 336 | LYS |
| 40 | DH | 337 | THR |
| 40 | DH | 339 | ARG |
| 40 | DH | 342 | GLN |
| 40 | DH | 343 | PHE |
| 40 | DH | 344 | VAL |
| 40 | DH | 356 | ASN |
| 40 | DH | 357 | TYR |
| 40 | DH | 361 | THR |
| 40 | DH | 362 | VAL |
| 40 | DH | 363 | VAL |
| 40 | DH | 367 | LEU |
| 40 | DH | 369 | LYS |
| 40 | DH | 372 | ARG |
| 40 | DH | 383 | ILE |
| 40 | DH | 385 | GLU |
| 40 | DH | 389 | ARG |
| 40 | DH | 390 | LEU |
| 40 | DH | 395 | ASP |
| 40 | DH | 398 | TYR |
| 40 | DH | 400 | LYS |
| 40 | DH | 401 | ARG |
| 40 | DH | 414 | GLU |
| 40 | DH | 418 | SER |
| 40 | DH | 419 | GLU |
| 40 | DH | 423 | ASP |
| 40 | DH | 424 | MET |
| 40 | DH | 427 | LEU |
| 40 | DH | 429 | LYS |
| 40 | DH | 436 | MET |
| 40 | DH | 439 | VAL |
| 40 | DH | 440 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DI | 2 | ARG |
| 40 | DI | 3 | GLU |
| 40 | DI | 4 | CYS |
| 40 | DI | 6 | SER |
| 40 | DI | 11 | GLN |
| 40 | DI | 22 | GLU |
| 40 | DI | 25 | CYS |
| 40 | DI | 26 | LEU |
| 40 | DI | 33 | ASP |
| 40 | DI | 38 | SER |
| 40 | DI | 60 | LYS |
| 40 | DI | 62 | VAL |
| 40 | DI | 66 | VAL |
| 40 | DI | 68 | VAL |
| 40 | DI | 71 | GLU |
| 40 | DI | 75 | ILE |
| 40 | DI | 79 | ARG |
| 40 | DI | 85 | GLN |
| 40 | DI | 91 | GLN |
| 40 | DI | 92 | LEU |
| 40 | DI | 93 | ILE |
| 40 | DI | 94 | THR |
| 40 | DI | 96 | LYS |
| 40 | DI | 101 | ASN |
| 40 | DI | 109 | THR |
| 40 | DI | 112 | LYS |
| 40 | DI | 113 | GLU |
| 40 | DI | 114 | LEU |
| 40 | DI | 116 | ASP |
| 40 | DI | 117 | LEU |
| 40 | DI | 119 | LEU |
| 40 | DI | 120 | ASP |
| 40 | DI | 123 | ARG |
| 40 | DI | 124 | LYS |
| 40 | DI | 128 | GLN |
| 40 | DI | 130 | THR |
| 40 | DI | 133 | GLN |
| 40 | DI | 138 | PHE |
| 40 | DI | 139 | HIS |
| 40 | DI | 152 | LEU |
| 40 | DI | 153 | LEU |
| 40 | DI | 156 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DI | 163 | LYS |
| 40 | DI | 164 | LYS |
| 40 | DI | 166 | LYS |
| 40 | DI | 167 | LEU |
| 40 | DI | 169 | PHE |
| 40 | DI | 171 | ILE |
| 40 | DI | 176 | GLN |
| 40 | DI | 179 | THR |
| 40 | DI | 181 | VAL |
| 40 | DI | 182 | VAL |
| 40 | DI | 190 | THR |
| 40 | DI | 192 | HIS |
| 40 | DI | 195 | LEU |
| 40 | DI | 199 | ASP |
| 40 | DI | 203 | MET |
| 40 | DI | 204 | VAL |
| 40 | DI | 206 | ASN |
| 40 | DI | 207 | GLU |
| 40 | DI | 209 | ILE |
| 40 | DI | 211 | ASP |
| 40 | DI | 212 | ILE |
| 40 | DI | 214 | ARG |
| 40 | DI | 215 | ARG |
| 40 | DI | 216 | ASN |
| 40 | DI | 218 | ASP |
| 40 | DI | 220 | GLU |
| 40 | DI | 224 | TYR |
| 40 | DI | 226 | ASN |
| 40 | DI | 234 | ILE |
| 40 | DI | 236 | SER |
| 40 | DI | 237 | SER |
| 40 | DI | 242 | LEU |
| 40 | DI | 243 | ARG |
| 40 | DI | 249 | ASN |
| 40 | DI | 250 | VAL |
| 40 | DI | 256 | GLN |
| 40 | DI | 257 | THR |
| 40 | DI | 259 | LEU |
| 40 | DI | 269 | LEU |
| 40 | DI | 275 | VAL |
| 40 | DI | 276 | ILE |
| 40 | DI | 277 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DI | 280 | LYS |
| 40 | DI | 283 | HIS |
| 40 | DI | 284 | GLU |
| 40 | DI | 287 | SER |
| 40 | DI | 301 | GLN |
| 40 | DI | 304 | LYS |
| 40 | DI | 306 | ASP |
| 40 | DI | 313 | MET |
| 40 | DI | 315 | CYS |
| 40 | DI | 316 | CYS |
| 40 | DI | 317 | LEU |
| 40 | DI | 320 | ARG |
| 40 | DI | 322 | ASP |
| 40 | DI | 324 | VAL |
| 40 | DI | 326 | LYS |
| 40 | DI | 332 | ILE |
| 40 | DI | 338 | LYS |
| 40 | DI | 340 | SER |
| 40 | DI | 341 | ILE |
| 40 | DI | 347 | CYS |
| 40 | DI | 355 | ILE |
| 40 | DI | 357 | TYR |
| 40 | DI | 363 | VAL |
| 40 | DI | 366 | ASP |
| 40 | DI | 367 | LEU |
| 40 | DI | 369 | LYS |
| 40 | DI | 376 | MET |
| 40 | DI | 377 | LEU |
| 40 | DI | 380 | THR |
| 40 | DI | 385 | GLU |
| 40 | DI | 390 | LEU |
| 40 | DI | 391 | ASP |
| 40 | DI | 397 | MET |
| 40 | DI | 400 | LYS |
| 40 | DI | 404 | VAL |
| 40 | DI | 412 | MET |
| 40 | DI | 414 | GLU |
| 40 | DI | 421 | ARG |
| 40 | DI | 423 | ASP |
| 40 | DI | 424 | MET |
| 40 | DI | 436 | MET |
| 41 | DL | 1 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DL | 2 | ARG |
| 41 | DL | 3 | GLU |
| 41 | DL | 4 | ILE |
| 41 | DL | 5 | VAL |
| 41 | DL | 7 | LEU |
| 41 | DL | 15 | GLN |
| 41 | DL | 22 | GLU |
| 41 | DL | 26 | ASP |
| 41 | DL | 30 | ILE |
| 41 | DL | 31 | ASP |
| 41 | DL | 35 | THR |
| 41 | DL | 36 | TYR |
| 41 | DL | 39 | ASP |
| 41 | DL | 40 | SER |
| 41 | DL | 45 | GLU |
| 41 | DL | 46 | ARG |
| 41 | DL | 49 | VAL |
| 41 | DL | 58 | LYS |
| 41 | DL | 60 | VAL |
| 41 | DL | 62 | ARG |
| 41 | DL | 64 | VAL |
| 41 | DL | 65 | LEU |
| 41 | DL | 66 | VAL |
| 41 | DL | 68 | LEU |
| 41 | DL | 69 | GLU |
| 41 | DL | 72 | THR |
| 41 | DL | 73 | MET |
| 41 | DL | 77 | ARG |
| 41 | DL | 78 | SER |
| 41 | DL | 81 | PHE |
| 41 | DL | 84 | ILE |
| 41 | DL | 88 | ASP |
| 41 | DL | 89 | ASN |
| 41 | DL | 92 | PHE |
| 41 | DL | 101 | TRP |
| 41 | DL | 108 | GLU |
| 41 | DL | 114 | ASP |
| 41 | DL | 115 | SER |
| 41 | DL | 122 | LYS |
| 41 | DL | 125 | GLU |
| 41 | DL | 128 | ASP |
| 41 | DL | 131 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DL | 133 | PHE |
| 41 | DL | 134 | GLN |
| 41 | DL | 135 | LEU |
| 41 | DL | 137 | HIS |
| 41 | DL | 147 | MET |
| 41 | DL | 154 | LYS |
| 41 | DL | 155 | ILE |
| 41 | DL | 156 | ARG |
| 41 | DL | 162 | ARG |
| 41 | DL | 166 | THR |
| 41 | DL | 167 | PHE |
| 41 | DL | 169 | VAL |
| 41 | DL | 172 | SER |
| 41 | DL | 177 | ASP |
| 41 | DL | 180 | VAL |
| 41 | DL | 181 | GLU |
| 41 | DL | 190 | HIS |
| 41 | DL | 192 | LEU |
| 41 | DL | 194 | GLU |
| 41 | DL | 197 | ASP |
| 41 | DL | 198 | GLU |
| 41 | DL | 199 | THR |
| 41 | DL | 202 | ILE |
| 41 | DL | 208 | TYR |
| 41 | DL | 209 | ASP |
| 41 | DL | 210 | ILE |
| 41 | DL | 211 | CYS |
| 41 | DL | 212 | PHE |
| 41 | DL | 213 | ARG |
| 41 | DL | 214 | THR |
| 41 | DL | 215 | LEU |
| 41 | DL | 216 | LYS |
| 41 | DL | 221 | THR |
| 41 | DL | 224 | ASP |
| 41 | DL | 226 | ASN |
| 41 | DL | 228 | LEU |
| 41 | DL | 233 | MET |
| 41 | DL | 234 | SER |
| 41 | DL | 237 | THR |
| 41 | DL | 238 | THR |
| 41 | DL | 240 | LEU |
| 41 | DL | 245 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DL | 246 | LEU |
| 41 | DL | 247 | ASN |
| 41 | DL | 252 | LYS |
| 41 | DL | 262 | ARG |
| 41 | DL | 267 | MET |
| 41 | DL | 270 | PHE |
| 41 | DL | 273 | LEU |
| 41 | DL | 274 | THR |
| 41 | DL | 276 | ARG |
| 41 | DL | 279 | GLN |
| 41 | DL | 282 | ARG |
| 41 | DL | 284 | LEU |
| 41 | DL | 291 | GLN |
| 41 | DL | 293 | MET |
| 41 | DL | 297 | LYS |
| 41 | DL | 298 | ASN |
| 41 | DL | 300 | MET |
| 41 | DL | 309 | ARG |
| 41 | DL | 311 | LEU |
| 41 | DL | 317 | PHE |
| 41 | DL | 318 | ARG |
| 41 | DL | 321 | MET |
| 41 | DL | 323 | MET |
| 41 | DL | 330 | MET |
| 41 | DL | 331 | LEU |
| 41 | DL | 333 | VAL |
| 41 | DL | 334 | GLN |
| 41 | DL | 341 | PHE |
| 41 | DL | 344 | TRP |
| 41 | DL | 348 | ASN |
| 41 | DL | 349 | VAL |
| 41 | DL | 350 | LYS |
| 41 | DL | 351 | THR |
| 41 | DL | 354 | CYS |
| 41 | DL | 355 | ASP |
| 41 | DL | 359 | ARG |
| 41 | DL | 362 | LYS |
| 41 | DL | 366 | THR |
| 41 | DL | 371 | SER |
| 41 | DL | 372 | THR |
| 41 | DL | 377 | LEU |
| 41 | DL | 380 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DL | 382 | SER |
| 41 | DL | 388 | MET |
| 41 | DL | 390 | ARG |
| 41 | DL | 395 | LEU |
| 41 | DL | 401 | GLU |
| 41 | DL | 406 | MET |
| 41 | DL | 415 | MET |
| 41 | DL | 417 | ASP |
| 41 | DL | 418 | LEU |
| 41 | DL | 422 | VAL |
| 41 | DL | 425 | ARG |
| 41 | DM | 1 | MET |
| 41 | DM | 2 | ARG |
| 41 | DM | 7 | LEU |
| 41 | DM | 8 | GLN |
| 41 | DM | 15 | GLN |
| 41 | DM | 19 | LYS |
| 41 | DM | 20 | PHE |
| 41 | DM | 22 | GLU |
| 41 | DM | 26 | ASP |
| 41 | DM | 30 | ILE |
| 41 | DM | 33 | THR |
| 41 | DM | 35 | THR |
| 41 | DM | 39 | ASP |
| 41 | DM | 41 | ASP |
| 41 | DM | 42 | LEU |
| 41 | DM | 43 | GLN |
| 41 | DM | 44 | LEU |
| 41 | DM | 46 | ARG |
| 41 | DM | 47 | ILE |
| 41 | DM | 48 | ASN |
| 41 | DM | 49 | VAL |
| 41 | DM | 53 | GLU |
| 41 | DM | 58 | LYS |
| 41 | DM | 62 | ARG |
| 41 | DM | 65 | LEU |
| 41 | DM | 72 | THR |
| 41 | DM | 73 | MET |
| 41 | DM | 83 | GLN |
| 41 | DM | 86 | ARG |
| 41 | DM | 88 | ASP |
| 41 | DM | 90 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DM | 91 | VAL |
| 41 | DM | 99 | ASN |
| 41 | DM | 100 | ASN |
| 41 | DM | 103 | LYS |
| 41 | DM | 108 | GLU |
| 41 | DM | 112 | LEU |
| 41 | DM | 114 | ASP |
| 41 | DM | 115 | SER |
| 41 | DM | 119 | VAL |
| 41 | DM | 121 | ARG |
| 41 | DM | 122 | LYS |
| 41 | DM | 123 | GLU |
| 41 | DM | 125 | GLU |
| 41 | DM | 128 | ASP |
| 41 | DM | 131 | GLN |
| 41 | DM | 135 | LEU |
| 41 | DM | 137 | HIS |
| 41 | DM | 151 | LEU |
| 41 | DM | 154 | LYS |
| 41 | DM | 156 | ARG |
| 41 | DM | 162 | ARG |
| 41 | DM | 163 | ILE |
| 41 | DM | 166 | THR |
| 41 | DM | 168 | SER |
| 41 | DM | 169 | VAL |
| 41 | DM | 174 | LYS |
| 41 | DM | 175 | VAL |
| 41 | DM | 176 | SER |
| 41 | DM | 177 | ASP |
| 41 | DM | 179 | VAL |
| 41 | DM | 180 | VAL |
| 41 | DM | 181 | GLU |
| 41 | DM | 183 | TYR |
| 41 | DM | 192 | LEU |
| 41 | DM | 194 | GLU |
| 41 | DM | 196 | THR |
| 41 | DM | 197 | ASP |
| 41 | DM | 203 | ASP |
| 41 | DM | 205 | GLU |
| 41 | DM | 207 | LEU |
| 41 | DM | 212 | PHE |
| 41 | DM | 213 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DM | 214 | THR |
| 41 | DM | 215 | LEU |
| 41 | DM | 216 | LYS |
| 41 | DM | 218 | THR |
| 41 | DM | 219 | THR |
| 41 | DM | 222 | TYR |
| 41 | DM | 224 | ASP |
| 41 | DM | 226 | ASN |
| 41 | DM | 227 | HIS |
| 41 | DM | 229 | VAL |
| 41 | DM | 232 | THR |
| 41 | DM | 233 | MET |
| 41 | DM | 236 | VAL |
| 41 | DM | 238 | THR |
| 41 | DM | 241 | ARG |
| 41 | DM | 245 | GLN |
| 41 | DM | 246 | LEU |
| 41 | DM | 249 | ASP |
| 41 | DM | 250 | LEU |
| 41 | DM | 252 | LYS |
| 41 | DM | 253 | LEU |
| 41 | DM | 263 | LEU |
| 41 | DM | 267 | MET |
| 41 | DM | 274 | THR |
| 41 | DM | 282 | ARG |
| 41 | DM | 284 | LEU |
| 41 | DM | 291 | GLN |
| 41 | DM | 297 | LYS |
| 41 | DM | 300 | MET |
| 41 | DM | 306 | ARG |
| 41 | DM | 307 | HIS |
| 41 | DM | 311 | LEU |
| 41 | DM | 318 | ARG |
| 41 | DM | 320 | ARG |
| 41 | DM | 321 | MET |
| 41 | DM | 323 | MET |
| 41 | DM | 324 | LYS |
| 41 | DM | 327 | ASP |
| 41 | DM | 334 | GLN |
| 41 | DM | 336 | LYS |
| 41 | DM | 338 | SER |
| 41 | DM | 341 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DM | 342 | VAL |
| 41 | DM | 345 | ILE |
| 41 | DM | 347 | ASN |
| 41 | DM | 348 | ASN |
| 41 | DM | 350 | LYS |
| 41 | DM | 354 | CYS |
| 41 | DM | 355 | ASP |
| 41 | DM | 359 | ARG |
| 41 | DM | 362 | LYS |
| 41 | DM | 366 | THR |
| 41 | DM | 367 | PHE |
| 41 | DM | 374 | ILE |
| 41 | DM | 377 | LEU |
| 41 | DM | 381 | ILE |
| 41 | DM | 382 | SER |
| 41 | DM | 383 | GLU |
| 41 | DM | 388 | MET |
| 41 | DM | 389 | PHE |
| 41 | DM | 390 | ARG |
| 41 | DM | 391 | ARG |
| 41 | DM | 392 | LYS |
| 41 | DM | 399 | THR |
| 41 | DM | 401 | GLU |
| 41 | DM | 404 | ASP |
| 41 | DM | 405 | GLU |
| 41 | DM | 406 | MET |
| 41 | DM | 418 | LEU |
| 41 | DM | 423 | VAL |
| 41 | DM | 424 | THR |
| 41 | DM | 425 | ARG |
| 41 | DM | 428 | CYS |
| 41 | DN | 1 | MET |
| 41 | DN | 6 | HIS |
| 41 | DN | 7 | LEU |
| 41 | DN | 12 | CYS |
| 41 | DN | 19 | LYS |
| 41 | DN | 22 | GLU |
| 41 | DN | 25 | SER |
| 41 | DN | 26 | ASP |
| 41 | DN | 31 | ASP |
| 41 | DN | 33 | THR |
| 41 | DN | 35 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DN | 39 | ASP |
| 41 | DN | 40 | SER |
| 41 | DN | 41 | ASP |
| 41 | DN | 42 | LEU |
| 41 | DN | 44 | LEU |
| 41 | DN | 46 | ARG |
| 41 | DN | 53 | GLU |
| 41 | DN | 55 | THR |
| 41 | DN | 58 | LYS |
| 41 | DN | 62 | ARG |
| 41 | DN | 68 | LEU |
| 41 | DN | 73 | MET |
| 41 | DN | 74 | ASP |
| 41 | DN | 75 | SER |
| 41 | DN | 83 | GLN |
| 41 | DN | 88 | ASP |
| 41 | DN | 90 | PHE |
| 41 | DN | 99 | ASN |
| 41 | DN | 101 | TRP |
| 41 | DN | 105 | HIS |
| 41 | DN | 114 | ASP |
| 41 | DN | 115 | SER |
| 41 | DN | 117 | LEU |
| 41 | DN | 118 | ASP |
| 41 | DN | 121 | ARG |
| 41 | DN | 128 | ASP |
| 41 | DN | 129 | CYS |
| 41 | DN | 131 | GLN |
| 41 | DN | 138 | SER |
| 41 | DN | 139 | LEU |
| 41 | DN | 150 | LEU |
| 41 | DN | 156 | ARG |
| 41 | DN | 157 | GLU |
| 41 | DN | 159 | TYR |
| 41 | DN | 162 | ARG |
| 41 | DN | 164 | MET |
| 41 | DN | 166 | THR |
| 41 | DN | 168 | SER |
| 41 | DN | 170 | VAL |
| 41 | DN | 172 | SER |
| 41 | DN | 174 | LYS |
| 41 | DN | 175 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DN | 179 | VAL |
| 41 | DN | 181 | GLU |
| 41 | DN | 182 | PRO |
| 41 | DN | 191 | GLN |
| 41 | DN | 192 | LEU |
| 41 | DN | 194 | GLU |
| 41 | DN | 197 | ASP |
| 41 | DN | 200 | TYR |
| 41 | DN | 202 | ILE |
| 41 | DN | 204 | ASN |
| 41 | DN | 205 | GLU |
| 41 | DN | 209 | ASP |
| 41 | DN | 212 | PHE |
| 41 | DN | 213 | ARG |
| 41 | DN | 214 | THR |
| 41 | DN | 215 | LEU |
| 41 | DN | 216 | LYS |
| 41 | DN | 218 | THR |
| 41 | DN | 219 | THR |
| 41 | DN | 222 | TYR |
| 41 | DN | 224 | ASP |
| 41 | DN | 227 | HIS |
| 41 | DN | 228 | LEU |
| 41 | DN | 229 | VAL |
| 41 | DN | 236 | VAL |
| 41 | DN | 238 | THR |
| 41 | DN | 240 | LEU |
| 41 | DN | 241 | ARG |
| 41 | DN | 245 | GLN |
| 41 | DN | 250 | LEU |
| 41 | DN | 252 | LYS |
| 41 | DN | 253 | LEU |
| 41 | DN | 256 | ASN |
| 41 | DN | 262 | ARG |
| 41 | DN | 263 | LEU |
| 41 | DN | 266 | PHE |
| 41 | DN | 267 | MET |
| 41 | DN | 273 | LEU |
| 41 | DN | 274 | THR |
| 41 | DN | 278 | SER |
| 41 | DN | 282 | ARG |
| 41 | DN | 288 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DN | 293 | MET |
| 41 | DN | 297 | LYS |
| 41 | DN | 300 | MET |
| 41 | DN | 303 | CYS |
| 41 | DN | 306 | ARG |
| 41 | DN | 309 | ARG |
| 41 | DN | 313 | VAL |
| 41 | DN | 317 | PHE |
| 41 | DN | 318 | ARG |
| 41 | DN | 321 | MET |
| 41 | DN | 323 | MET |
| 41 | DN | 333 | VAL |
| 41 | DN | 337 | ASN |
| 41 | DN | 338 | SER |
| 41 | DN | 340 | TYR |
| 41 | DN | 341 | PHE |
| 41 | DN | 345 | ILE |
| 41 | DN | 347 | ASN |
| 41 | DN | 348 | ASN |
| 41 | DN | 354 | CYS |
| 41 | DN | 359 | ARG |
| 41 | DN | 361 | LEU |
| 41 | DN | 362 | LYS |
| 41 | DN | 363 | MET |
| 41 | DN | 366 | THR |
| 41 | DN | 367 | PHE |
| 41 | DN | 368 | ILE |
| 41 | DN | 372 | THR |
| 41 | DN | 374 | ILE |
| 41 | DN | 375 | GLN |
| 41 | DN | 380 | ARG |
| 41 | DN | 381 | ILE |
| 41 | DN | 383 | GLU |
| 41 | DN | 384 | GLN |
| 41 | DN | 385 | PHE |
| 41 | DN | 388 | MET |
| 41 | DN | 390 | ARG |
| 41 | DN | 391 | ARG |
| 41 | DN | 392 | LYS |
| 41 | DN | 395 | LEU |
| 41 | DN | 401 | GLU |
| 41 | DN | 407 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DN | 410 | GLU |
| 41 | DN | 412 | GLU |
| 41 | DN | 415 | MET |
| 41 | DN | 423 | VAL |
| 41 | DN | 425 | ARG |
| 41 | DN | 428 | CYS |
| 41 | DO | 2 | ARG |
| 41 | DO | 99 | ASN |
| 41 | DO | 216 | LYS |
| 41 | DP | 2 | ARG |
| 41 | DP | 4 | ILE |
| 41 | DP | 7 | LEU |
| 41 | DP | 11 | GLN |
| 41 | DP | 12 | CYS |
| 41 | DP | 19 | LYS |
| 41 | DP | 22 | GLU |
| 41 | DP | 24 | ILE |
| 41 | DP | 26 | ASP |
| 41 | DP | 33 | THR |
| 41 | DP | 35 | THR |
| 41 | DP | 41 | ASP |
| 41 | DP | 42 | LEU |
| 41 | DP | 46 | ARG |
| 41 | DP | 55 | THR |
| 41 | DP | 62 | ARG |
| 41 | DP | 65 | LEU |
| 41 | DP | 68 | LEU |
| 41 | DP | 69 | GLU |
| 41 | DP | 73 | MET |
| 41 | DP | 75 | SER |
| 41 | DP | 77 | ARG |
| 41 | DP | 86 | ARG |
| 41 | DP | 88 | ASP |
| 41 | DP | 90 | PHE |
| 41 | DP | 91 | VAL |
| 41 | DP | 94 | GLN |
| 41 | DP | 103 | LYS |
| 41 | DP | 111 | GLU |
| 41 | DP | 118 | ASP |
| 41 | DP | 121 | ARG |
| 41 | DP | 125 | GLU |
| 41 | DP | 130 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DP | 135 | LEU |
| 41 | DP | 147 | MET |
| 41 | DP | 149 | THR |
| 41 | DP | 151 | LEU |
| 41 | DP | 154 | LYS |
| 41 | DP | 159 | TYR |
| 41 | DP | 170 | VAL |
| 41 | DP | 172 | SER |
| 41 | DP | 174 | LYS |
| 41 | DP | 177 | ASP |
| 41 | DP | 178 | THR |
| 41 | DP | 179 | VAL |
| 41 | DP | 193 | VAL |
| 41 | DP | 194 | GLU |
| 41 | DP | 196 | THR |
| 41 | DP | 197 | ASP |
| 41 | DP | 202 | ILE |
| 41 | DP | 203 | ASP |
| 41 | DP | 208 | TYR |
| 41 | DP | 213 | ARG |
| 41 | DP | 214 | THR |
| 41 | DP | 216 | LYS |
| 41 | DP | 228 | LEU |
| 41 | DP | 233 | MET |
| 41 | DP | 234 | SER |
| 41 | DP | 236 | VAL |
| 41 | DP | 240 | LEU |
| 41 | DP | 246 | LEU |
| 41 | DP | 249 | ASP |
| 41 | DP | 250 | LEU |
| 41 | DP | 251 | ARG |
| 41 | DP | 252 | LYS |
| 41 | DP | 253 | LEU |
| 41 | DP | 257 | MET |
| 41 | DP | 262 | ARG |
| 41 | DP | 266 | PHE |
| 41 | DP | 267 | MET |
| 41 | DP | 270 | PHE |
| 41 | DP | 273 | LEU |
| 41 | DP | 275 | SER |
| 41 | DP | 276 | ARG |
| 41 | DP | 279 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DP | 284 | LEU |
| 41 | DP | 292 | GLN |
| 41 | DP | 293 | MET |
| 41 | DP | 297 | LYS |
| 41 | DP | 298 | ASN |
| 41 | DP | 299 | MET |
| 41 | DP | 300 | MET |
| 41 | DP | 309 | ARG |
| 41 | DP | 311 | LEU |
| 41 | DP | 312 | THR |
| 41 | DP | 313 | VAL |
| 41 | DP | 316 | VAL |
| 41 | DP | 318 | ARG |
| 41 | DP | 320 | ARG |
| 41 | DP | 323 | MET |
| 41 | DP | 328 | GLU |
| 41 | DP | 330 | MET |
| 41 | DP | 336 | LYS |
| 41 | DP | 337 | ASN |
| 41 | DP | 347 | ASN |
| 41 | DP | 348 | ASN |
| 41 | DP | 350 | LYS |
| 41 | DP | 351 | THR |
| 41 | DP | 353 | VAL |
| 41 | DP | 354 | CYS |
| 41 | DP | 359 | ARG |
| 41 | DP | 361 | LEU |
| 41 | DP | 362 | LYS |
| 41 | DP | 372 | THR |
| 41 | DP | 376 | GLU |
| 41 | DP | 377 | LEU |
| 41 | DP | 379 | LYS |
| 41 | DP | 380 | ARG |
| 41 | DP | 383 | GLU |
| 41 | DP | 388 | MET |
| 41 | DP | 389 | PHE |
| 41 | DP | 391 | ARG |
| 41 | DP | 396 | HIS |
| 41 | DP | 399 | THR |
| 41 | DP | 401 | GLU |
| 41 | DP | 403 | MET |
| 41 | DP | 406 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DP | 407 | GLU |
| 41 | DP | 409 | THR |
| 41 | DP | 413 | SER |
| 41 | DP | 422 | VAL |
| 41 | DP | 425 | ARG |
| 41 | DP | 428 | CYS |
| 40 | EA | 84 | ARG |
| 40 | EA | 308 | ARG |
| 41 | EB | 334 | GLN |
| 40 | EE | 88 | HIS |
| 40 | EE | 221 | ARG |
| 40 | EE | 308 | ARG |
| 40 | EE | 369 | LYS |
| 40 | EE | 372 | ARG |
| 40 | EE | 379 | ASN |
| 40 | EF | 308 | ARG |
| 40 | EG | 221 | ARG |
| 40 | EG | 308 | ARG |
| 40 | EG | 329 | ASN |
| 40 | EH | 2 | ARG |
| 40 | EH | 3 | GLU |
| 40 | EH | 5 | ILE |
| 40 | EH | 7 | VAL |
| 40 | EH | 8 | HIS |
| 40 | EH | 9 | VAL |
| 40 | EH | 11 | GLN |
| 40 | EH | 26 | LEU |
| 40 | EH | 28 | HIS |
| 40 | EH | 30 | ILE |
| 40 | EH | 36 | MET |
| 40 | EH | 38 | SER |
| 40 | EH | 52 | PHE |
| 40 | EH | 55 | GLU |
| 40 | EH | 62 | VAL |
| 40 | EH | 68 | VAL |
| 40 | EH | 75 | ILE |
| 40 | EH | 84 | ARG |
| 40 | EH | 96 | LYS |
| 40 | EH | 103 | TYR |
| 40 | EH | 105 | ARG |
| 40 | EH | 109 | THR |
| 40 | EH | 110 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | EH | 112 | LYS |
| 40 | EH | 114 | LEU |
| 40 | EH | 119 | LEU |
| 40 | EH | 121 | ARG |
| 40 | EH | 122 | ILE |
| 40 | EH | 123 | ARG |
| 40 | EH | 124 | LYS |
| 40 | EH | 125 | LEU |
| 40 | EH | 129 | CYS |
| 40 | EH | 132 | LEU |
| 40 | EH | 137 | ILE |
| 40 | EH | 151 | SER |
| 40 | EH | 156 | ARG |
| 40 | EH | 157 | LEU |
| 40 | EH | 163 | LYS |
| 40 | EH | 167 | LEU |
| 40 | EH | 171 | ILE |
| 40 | EH | 176 | GLN |
| 40 | EH | 177 | VAL |
| 40 | EH | 186 | ASN |
| 40 | EH | 187 | SER |
| 40 | EH | 189 | LEU |
| 40 | EH | 195 | LEU |
| 40 | EH | 198 | SER |
| 40 | EH | 199 | ASP |
| 40 | EH | 207 | GLU |
| 40 | EH | 209 | ILE |
| 40 | EH | 211 | ASP |
| 40 | EH | 214 | ARG |
| 40 | EH | 223 | THR |
| 40 | EH | 224 | TYR |
| 40 | EH | 227 | LEU |
| 40 | EH | 229 | ARG |
| 40 | EH | 230 | LEU |
| 40 | EH | 234 | ILE |
| 40 | EH | 236 | SER |
| 40 | EH | 237 | SER |
| 40 | EH | 238 | ILE |
| 40 | EH | 242 | LEU |
| 40 | EH | 245 | ASP |
| 40 | EH | 250 | VAL |
| 40 | EH | 256 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | EH | 257 | THR |
| 40 | EH | 258 | ASN |
| 40 | EH | 265 | ILE |
| 40 | EH | 269 | LEU |
| 40 | EH | 272 | TYR |
| 40 | EH | 274 | PRO |
| 40 | EH | 276 | ILE |
| 40 | EH | 277 | SER |
| 40 | EH | 279 | GLU |
| 40 | EH | 280 | LYS |
| 40 | EH | 285 | GLN |
| 40 | EH | 286 | LEU |
| 40 | EH | 287 | SER |
| 40 | EH | 291 | ILE |
| 40 | EH | 293 | ASN |
| 40 | EH | 295 | CYS |
| 40 | EH | 300 | ASN |
| 40 | EH | 301 | GLN |
| 40 | EH | 308 | ARG |
| 40 | EH | 311 | LYS |
| 40 | EH | 315 | CYS |
| 40 | EH | 318 | LEU |
| 40 | EH | 320 | ARG |
| 40 | EH | 326 | LYS |
| 40 | EH | 328 | VAL |
| 40 | EH | 338 | LYS |
| 40 | EH | 339 | ARG |
| 40 | EH | 340 | SER |
| 40 | EH | 352 | LYS |
| 40 | EH | 353 | VAL |
| 40 | EH | 361 | THR |
| 40 | EH | 362 | VAL |
| 40 | EH | 363 | VAL |
| 40 | EH | 369 | LYS |
| 40 | EH | 371 | GLN |
| 40 | EH | 372 | ARG |
| 40 | EH | 375 | CYS |
| 40 | EH | 376 | MET |
| 40 | EH | 378 | SER |
| 40 | EH | 385 | GLU |
| 40 | EH | 390 | LEU |
| 40 | EH | 392 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | EH | 395 | ASP |
| 40 | EH | 396 | LEU |
| 40 | EH | 400 | LYS |
| 40 | EH | 401 | ARG |
| 40 | EH | 410 | GLU |
| 40 | EH | 413 | GLU |
| 40 | EH | 419 | GLU |
| 40 | EH | 421 | ARG |
| 40 | EH | 423 | ASP |
| 40 | EH | 429 | LYS |
| 40 | EH | 430 | ASP |
| 40 | EH | 432 | GLU |
| 40 | EH | 436 | MET |
| 40 | EH | 439 | VAL |
| 40 | EH | 440 | GLU |
| 40 | EI | 2 | ARG |
| 40 | EI | 3 | GLU |
| 40 | EI | 4 | CYS |
| 40 | EI | 7 | VAL |
| 40 | EI | 9 | VAL |
| 40 | EI | 11 | GLN |
| 40 | EI | 16 | ILE |
| 40 | EI | 20 | CYS |
| 40 | EI | 22 | GLU |
| 40 | EI | 23 | LEU |
| 40 | EI | 25 | CYS |
| 40 | EI | 26 | LEU |
| 40 | EI | 30 | ILE |
| 40 | EI | 39 | ASP |
| 40 | EI | 47 | ASP |
| 40 | EI | 54 | SER |
| 40 | EI | 55 | GLU |
| 40 | EI | 68 | VAL |
| 40 | EI | 70 | LEU |
| 40 | EI | 71 | GLU |
| 40 | EI | 75 | ILE |
| 40 | EI | 76 | ASP |
| 40 | EI | 77 | GLU |
| 40 | EI | 84 | ARG |
| 40 | EI | 90 | GLU |
| 40 | EI | 92 | LEU |
| 40 | EI | 94 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | EI | 97 | GLU |
| 40 | EI | 105 | ARG |
| 40 | EI | 110 | ILE |
| 40 | EI | 112 | LYS |
| 40 | EI | 114 | LEU |
| 40 | EI | 116 | ASP |
| 40 | EI | 119 | LEU |
| 40 | EI | 120 | ASP |
| 40 | EI | 122 | ILE |
| 40 | EI | 124 | LYS |
| 40 | EI | 130 | THR |
| 40 | EI | 132 | LEU |
| 40 | EI | 137 | ILE |
| 40 | EI | 139 | HIS |
| 40 | EI | 140 | SER |
| 40 | EI | 151 | SER |
| 40 | EI | 152 | LEU |
| 40 | EI | 154 | MET |
| 40 | EI | 156 | ARG |
| 40 | EI | 157 | LEU |
| 40 | EI | 158 | SER |
| 40 | EI | 161 | TYR |
| 40 | EI | 163 | LYS |
| 40 | EI | 164 | LYS |
| 40 | EI | 166 | LYS |
| 40 | EI | 171 | ILE |
| 40 | EI | 178 | SER |
| 40 | EI | 179 | THR |
| 40 | EI | 181 | VAL |
| 40 | EI | 183 | GLU |
| 40 | EI | 184 | PRO |
| 40 | EI | 187 | SER |
| 40 | EI | 189 | LEU |
| 40 | EI | 192 | HIS |
| 40 | EI | 194 | THR |
| 40 | EI | 195 | LEU |
| 40 | EI | 196 | GLU |
| 40 | EI | 199 | ASP |
| 40 | EI | 200 | CYS |
| 40 | EI | 203 | MET |
| 40 | EI | 204 | VAL |
| 40 | EI | 206 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | EI | 212 | ILE |
| 40 | EI | 214 | ARG |
| 40 | EI | 215 | ARG |
| 40 | EI | 217 | LEU |
| 40 | EI | 219 | ILE |
| 40 | EI | 220 | GLU |
| 40 | EI | 224 | TYR |
| 40 | EI | 226 | ASN |
| 40 | EI | 230 | LEU |
| 40 | EI | 237 | SER |
| 40 | EI | 238 | ILE |
| 40 | EI | 243 | ARG |
| 40 | EI | 244 | PHE |
| 40 | EI | 245 | ASP |
| 40 | EI | 248 | LEU |
| 40 | EI | 250 | VAL |
| 40 | EI | 259 | LEU |
| 40 | EI | 264 | ARG |
| 40 | EI | 269 | LEU |
| 40 | EI | 271 | THR |
| 40 | EI | 272 | TYR |
| 40 | EI | 276 | ILE |
| 40 | EI | 279 | GLU |
| 40 | EI | 280 | LYS |
| 40 | EI | 285 | GLN |
| 40 | EI | 286 | LEU |
| 40 | EI | 287 | SER |
| 40 | EI | 288 | VAL |
| 40 | EI | 291 | ILE |
| 40 | EI | 293 | ASN |
| 40 | EI | 304 | LYS |
| 40 | EI | 308 | ARG |
| 40 | EI | 312 | TYR |
| 40 | EI | 315 | CYS |
| 40 | EI | 316 | CYS |
| 40 | EI | 317 | LEU |
| 40 | EI | 318 | LEU |
| 40 | EI | 320 | ARG |
| 40 | EI | 323 | VAL |
| 40 | EI | 324 | VAL |
| 40 | EI | 326 | LYS |
| 40 | EI | 329 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | EI | 332 | ILE |
| 40 | EI | 336 | LYS |
| 40 | EI | 338 | LYS |
| 40 | EI | 341 | ILE |
| 40 | EI | 342 | GLN |
| 40 | EI | 352 | LYS |
| 40 | EI | 358 | GLN |
| 40 | EI | 363 | VAL |
| 40 | EI | 367 | LEU |
| 40 | EI | 372 | ARG |
| 40 | EI | 375 | CYS |
| 40 | EI | 380 | THR |
| 40 | EI | 383 | ILE |
| 40 | EI | 385 | GLU |
| 40 | EI | 389 | ARG |
| 40 | EI | 390 | LEU |
| 40 | EI | 391 | ASP |
| 40 | EI | 395 | ASP |
| 40 | EI | 397 | MET |
| 40 | EI | 400 | LYS |
| 40 | EI | 401 | ARG |
| 40 | EI | 404 | VAL |
| 40 | EI | 405 | HIS |
| 40 | EI | 410 | GLU |
| 40 | EI | 413 | GLU |
| 40 | EI | 421 | ARG |
| 40 | EI | 422 | GLU |
| 40 | EI | 424 | MET |
| 40 | EI | 427 | LEU |
| 40 | EI | 429 | LYS |
| 40 | EI | 430 | ASP |
| 40 | EI | 432 | GLU |
| 40 | EI | 436 | MET |
| 40 | EI | 439 | VAL |
| 41 | EL | 306 | ARG |
| 41 | EM | 2 | ARG |
| 41 | EM | 4 | ILE |
| 41 | EM | 6 | HIS |
| 41 | EM | 7 | LEU |
| 41 | EM | 12 | CYS |
| 41 | EM | 19 | LYS |
| 41 | EM | 22 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | EM | 24 | ILE |
| 41 | EM | 30 | ILE |
| 41 | EM | 39 | ASP |
| 41 | EM | 42 | LEU |
| 41 | EM | 46 | ARG |
| 41 | EM | 47 | ILE |
| 41 | EM | 49 | VAL |
| 41 | EM | 58 | LYS |
| 41 | EM | 60 | VAL |
| 41 | EM | 62 | ARG |
| 41 | EM | 65 | LEU |
| 41 | EM | 67 | ASP |
| 41 | EM | 68 | LEU |
| 41 | EM | 69 | GLU |
| 41 | EM | 73 | MET |
| 41 | EM | 77 | ARG |
| 41 | EM | 86 | ARG |
| 41 | EM | 88 | ASP |
| 41 | EM | 94 | GLN |
| 41 | EM | 100 | ASN |
| 41 | EM | 105 | HIS |
| 41 | EM | 106 | TYR |
| 41 | EM | 108 | GLU |
| 41 | EM | 114 | ASP |
| 41 | EM | 121 | ARG |
| 41 | EM | 122 | LYS |
| 41 | EM | 128 | ASP |
| 41 | EM | 129 | CYS |
| 41 | EM | 131 | GLN |
| 41 | EM | 135 | LEU |
| 41 | EM | 145 | SER |
| 41 | EM | 147 | MET |
| 41 | EM | 149 | THR |
| 41 | EM | 150 | LEU |
| 41 | EM | 151 | LEU |
| 41 | EM | 152 | ILE |
| 41 | EM | 153 | SER |
| 41 | EM | 156 | ARG |
| 41 | EM | 157 | GLU |
| 41 | EM | 162 | ARG |
| 41 | EM | 165 | ASN |
| 41 | EM | 168 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | EM | 170 | VAL |
| 41 | EM | 172 | SER |
| 41 | EM | 176 | SER |
| 41 | EM | 180 | VAL |
| 41 | EM | 187 | LEU |
| 41 | EM | 188 | SER |
| 41 | EM | 192 | LEU |
| 41 | EM | 196 | THR |
| 41 | EM | 203 | ASP |
| 41 | EM | 207 | LEU |
| 41 | EM | 210 | ILE |
| 41 | EM | 212 | PHE |
| 41 | EM | 216 | LYS |
| 41 | EM | 217 | LEU |
| 41 | EM | 218 | THR |
| 41 | EM | 221 | THR |
| 41 | EM | 222 | TYR |
| 41 | EM | 224 | ASP |
| 41 | EM | 225 | LEU |
| 41 | EM | 228 | LEU |
| 41 | EM | 230 | SER |
| 41 | EM | 236 | VAL |
| 41 | EM | 239 | CYS |
| 41 | EM | 245 | GLN |
| 41 | EM | 250 | LEU |
| 41 | EM | 252 | LYS |
| 41 | EM | 253 | LEU |
| 41 | EM | 257 | MET |
| 41 | EM | 262 | ARG |
| 41 | EM | 263 | LEU |
| 41 | EM | 273 | LEU |
| 41 | EM | 274 | THR |
| 41 | EM | 276 | ARG |
| 41 | EM | 280 | GLN |
| 41 | EM | 282 | ARG |
| 41 | EM | 284 | LEU |
| 41 | EM | 288 | GLU |
| 41 | EM | 289 | LEU |
| 41 | EM | 291 | GLN |
| 41 | EM | 292 | GLN |
| 41 | EM | 293 | MET |
| 41 | EM | 295 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | EM | 299 | MET |
| 41 | EM | 300 | MET |
| 41 | EM | 310 | TYR |
| 41 | EM | 311 | LEU |
| 41 | EM | 312 | THR |
| 41 | EM | 313 | VAL |
| 41 | EM | 321 | MET |
| 41 | EM | 323 | MET |
| 41 | EM | 330 | MET |
| 41 | EM | 331 | LEU |
| 41 | EM | 332 | ASN |
| 41 | EM | 336 | LYS |
| 41 | EM | 337 | ASN |
| 41 | EM | 347 | ASN |
| 41 | EM | 348 | ASN |
| 41 | EM | 350 | LYS |
| 41 | EM | 353 | VAL |
| 41 | EM | 359 | ARG |
| 41 | EM | 361 | LEU |
| 41 | EM | 362 | LYS |
| 41 | EM | 366 | THR |
| 41 | EM | 367 | PHE |
| 41 | EM | 374 | ILE |
| 41 | EM | 378 | PHE |
| 41 | EM | 379 | LYS |
| 41 | EM | 381 | ILE |
| 41 | EM | 382 | SER |
| 41 | EM | 383 | GLU |
| 41 | EM | 390 | ARG |
| 41 | EM | 392 | LYS |
| 41 | EM | 395 | LEU |
| 41 | EM | 399 | THR |
| 41 | EM | 403 | MET |
| 41 | EM | 412 | GLU |
| 41 | EM | 415 | MET |
| 41 | EM | 421 | PRO |
| 41 | EM | 425 | ARG |
| 41 | EO | 306 | ARG |
| 41 | EP | 1 | MET |
| 41 | EP | 2 | ARG |
| 41 | EP | 7 | LEU |
| 41 | EP | 16 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | EP | 19 | LYS |
| 41 | EP | 30 | ILE |
| 41 | EP | 31 | ASP |
| 41 | EP | 35 | THR |
| 41 | EP | 39 | ASP |
| 41 | EP | 42 | LEU |
| 41 | EP | 45 | GLU |
| 41 | EP | 47 | ILE |
| 41 | EP | 48 | ASN |
| 41 | EP | 60 | VAL |
| 41 | EP | 65 | LEU |
| 41 | EP | 66 | VAL |
| 41 | EP | 68 | LEU |
| 41 | EP | 73 | MET |
| 41 | EP | 77 | ARG |
| 41 | EP | 83 | GLN |
| 41 | EP | 86 | ARG |
| 41 | EP | 94 | GLN |
| 41 | EP | 108 | GLU |
| 41 | EP | 111 | GLU |
| 41 | EP | 113 | VAL |
| 41 | EP | 115 | SER |
| 41 | EP | 117 | LEU |
| 41 | EP | 119 | VAL |
| 41 | EP | 120 | VAL |
| 41 | EP | 129 | CYS |
| 41 | EP | 130 | LEU |
| 41 | EP | 131 | GLN |
| 41 | EP | 137 | HIS |
| 41 | EP | 147 | MET |
| 41 | EP | 151 | LEU |
| 41 | EP | 154 | LYS |
| 41 | EP | 156 | ARG |
| 41 | EP | 162 | ARG |
| 41 | EP | 163 | ILE |
| 41 | EP | 164 | MET |
| 41 | EP | 166 | THR |
| 41 | EP | 170 | VAL |
| 41 | EP | 172 | SER |
| 41 | EP | 175 | VAL |
| 41 | EP | 176 | SER |
| 41 | EP | 192 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | EP | 194 | GLU |
| 41 | EP | 196 | THR |
| 41 | EP | 197 | ASP |
| 41 | EP | 202 | ILE |
| 41 | EP | 215 | LEU |
| 41 | EP | 216 | LYS |
| 41 | EP | 217 | LEU |
| 41 | EP | 219 | THR |
| 41 | EP | 221 | THR |
| 41 | EP | 228 | LEU |
| 41 | EP | 230 | SER |
| 41 | EP | 232 | THR |
| 41 | EP | 238 | THR |
| 41 | EP | 240 | LEU |
| 41 | EP | 245 | GLN |
| 41 | EP | 246 | LEU |
| 41 | EP | 252 | LYS |
| 41 | EP | 262 | ARG |
| 41 | EP | 267 | MET |
| 41 | EP | 273 | LEU |
| 41 | EP | 275 | SER |
| 41 | EP | 279 | GLN |
| 41 | EP | 280 | GLN |
| 41 | EP | 284 | LEU |
| 41 | EP | 290 | THR |
| 41 | EP | 298 | ASN |
| 41 | EP | 303 | CYS |
| 41 | EP | 304 | ASP |
| 41 | EP | 309 | ARG |
| 41 | EP | 311 | LEU |
| 41 | EP | 312 | THR |
| 41 | EP | 322 | SER |
| 41 | EP | 323 | MET |
| 41 | EP | 326 | VAL |
| 41 | EP | 328 | GLU |
| 41 | EP | 330 | MET |
| 41 | EP | 332 | ASN |
| 41 | EP | 336 | LYS |
| 41 | EP | 337 | ASN |
| 41 | EP | 350 | LYS |
| 41 | EP | 351 | THR |
| 41 | EP | 353 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | EP | 354 | CYS |
| 41 | EP | 356 | ILE |
| 41 | EP | 359 | ARG |
| 41 | EP | 361 | LEU |
| 41 | EP | 362 | LYS |
| 41 | EP | 367 | PHE |
| 41 | EP | 372 | THR |
| 41 | EP | 375 | GLN |
| 41 | EP | 377 | LEU |
| 41 | EP | 379 | LYS |
| 41 | EP | 381 | ILE |
| 41 | EP | 383 | GLU |
| 41 | EP | 386 | THR |
| 41 | EP | 391 | ARG |
| 41 | EP | 395 | LEU |
| 41 | EP | 397 | TRP |
| 41 | EP | 398 | TYR |
| 41 | EP | 399 | THR |
| 41 | EP | 405 | GLU |
| 41 | EP | 406 | MET |
| 41 | EP | 409 | THR |
| 41 | EP | 413 | SER |
| 41 | EP | 422 | VAL |
| 41 | EP | 423 | VAL |
| 41 | EP | 425 | ARG |
| 40 | FA | 1 | GLN |
| 40 | FA | 2 | ARG |
| 40 | FA | 3 | GLU |
| 40 | FA | 5 | ILE |
| 40 | FA | 9 | VAL |
| 40 | FA | 22 | GLU |
| 40 | FA | 23 | LEU |
| 40 | FA | 26 | LEU |
| 40 | FA | 30 | ILE |
| 40 | FA | 33 | ASP |
| 40 | FA | 39 | ASP |
| 40 | FA | 46 | ASP |
| 40 | FA | 51 | THR |
| 40 | FA | 52 | PHE |
| 40 | FA | 54 | SER |
| 40 | FA | 56 | THR |
| 40 | FA | 62 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | FA | 66 | VAL |
| 40 | FA | 74 | VAL |
| 40 | FA | 75 | ILE |
| 40 | FA | 76 | ASP |
| 40 | FA | 92 | LEU |
| 40 | FA | 93 | ILE |
| 40 | FA | 102 | ASN |
| 40 | FA | 105 | ARG |
| 40 | FA | 107 | HIS |
| 40 | FA | 110 | ILE |
| 40 | FA | 112 | LYS |
| 40 | FA | 113 | GLU |
| 40 | FA | 114 | LEU |
| 40 | FA | 119 | LEU |
| 40 | FA | 122 | ILE |
| 40 | FA | 124 | LYS |
| 40 | FA | 125 | LEU |
| 40 | FA | 130 | THR |
| 40 | FA | 132 | LEU |
| 40 | FA | 136 | LEU |
| 40 | FA | 140 | SER |
| 40 | FA | 141 | PHE |
| 40 | FA | 152 | LEU |
| 40 | FA | 154 | MET |
| 40 | FA | 156 | ARG |
| 40 | FA | 163 | LYS |
| 40 | FA | 165 | SER |
| 40 | FA | 166 | LYS |
| 40 | FA | 170 | SER |
| 40 | FA | 176 | GLN |
| 40 | FA | 178 | SER |
| 40 | FA | 183 | GLU |
| 40 | FA | 188 | ILE |
| 40 | FA | 196 | GLU |
| 40 | FA | 199 | ASP |
| 40 | FA | 200 | CYS |
| 40 | FA | 203 | MET |
| 40 | FA | 204 | VAL |
| 40 | FA | 209 | ILE |
| 40 | FA | 211 | ASP |
| 40 | FA | 214 | ARG |
| 40 | FA | 216 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | FA | 217 | LEU |
| 40 | FA | 219 | ILE |
| 40 | FA | 220 | GLU |
| 40 | FA | 221 | ARG |
| 40 | FA | 228 | ASN |
| 40 | FA | 238 | ILE |
| 40 | FA | 239 | THR |
| 40 | FA | 241 | SER |
| 40 | FA | 242 | LEU |
| 40 | FA | 245 | ASP |
| 40 | FA | 251 | ASP |
| 40 | FA | 256 | GLN |
| 40 | FA | 258 | ASN |
| 40 | FA | 260 | VAL |
| 40 | FA | 262 | TYR |
| 40 | FA | 265 | ILE |
| 40 | FA | 271 | THR |
| 40 | FA | 274 | PRO |
| 40 | FA | 275 | VAL |
| 40 | FA | 276 | ILE |
| 40 | FA | 280 | LYS |
| 40 | FA | 284 | GLU |
| 40 | FA | 285 | GLN |
| 40 | FA | 287 | SER |
| 40 | FA | 288 | VAL |
| 40 | FA | 291 | ILE |
| 40 | FA | 295 | CYS |
| 40 | FA | 297 | GLU |
| 40 | FA | 300 | ASN |
| 40 | FA | 304 | LYS |
| 40 | FA | 305 | CYS |
| 40 | FA | 308 | ARG |
| 40 | FA | 311 | LYS |
| 40 | FA | 315 | CYS |
| 40 | FA | 316 | CYS |
| 40 | FA | 326 | LYS |
| 40 | FA | 328 | VAL |
| 40 | FA | 329 | ASN |
| 40 | FA | 332 | ILE |
| 40 | FA | 335 | ILE |
| 40 | FA | 339 | ARG |
| 40 | FA | 341 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | FA | 351 | PHE |
| 40 | FA | 363 | VAL |
| 40 | FA | 366 | ASP |
| 40 | FA | 367 | LEU |
| 40 | FA | 372 | ARG |
| 40 | FA | 380 | THR |
| 40 | FA | 383 | ILE |
| 40 | FA | 387 | TRP |
| 40 | FA | 398 | TYR |
| 40 | FA | 400 | LYS |
| 40 | FA | 404 | VAL |
| 40 | FA | 412 | MET |
| 40 | FA | 419 | GLU |
| 40 | FA | 421 | ARG |
| 40 | FA | 423 | ASP |
| 40 | FA | 424 | MET |
| 40 | FA | 428 | GLU |
| 40 | FA | 429 | LYS |
| 40 | FA | 432 | GLU |
| 40 | FA | 436 | MET |
| 40 | FA | 437 | ASP |
| 40 | FA | 438 | SER |
| 40 | FA | 439 | VAL |
| 41 | FB | 2 | ARG |
| 41 | FB | 174 | LYS |
| 40 | FG | 372 | ARG |
| 40 | FI | 2 | ARG |
| 40 | FI | 54 | SER |
| 40 | FI | 62 | VAL |
| 40 | FI | 379 | ASN |
| 41 | FM | 280 | GLN |
| 41 | FN | 297 | LYS |
| 41 | FN | 298 | ASN |
| 41 | FN | 307 | HIS |
| 41 | FN | 334 | GLN |
| 41 | FO | 291 | GLN |
| 41 | FP | 2 | ARG |
| 41 | FP | 291 | GLN |
| 41 | FP | 347 | ASN |
| 40 | GA | 15 | GLN |
| 40 | GA | 23 | LEU |
| 40 | GA | 36 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GE | 2 | ARG |
| 40 | GE | 3 | GLU |
| 40 | GE | 6 | SER |
| 40 | GE | 7 | VAL |
| 40 | GE | 14 | VAL |
| 40 | GE | 16 | ILE |
| 40 | GE | 23 | LEU |
| 40 | GE | 25 | CYS |
| 40 | GE | 26 | LEU |
| 40 | GE | 27 | GLU |
| 40 | GE | 30 | ILE |
| 40 | GE | 35 | GLN |
| 40 | GE | 39 | ASP |
| 40 | GE | 48 | SER |
| 40 | GE | 52 | PHE |
| 40 | GE | 54 | SER |
| 40 | GE | 55 | GLU |
| 40 | GE | 60 | LYS |
| 40 | GE | 66 | VAL |
| 40 | GE | 68 | VAL |
| 40 | GE | 69 | ASP |
| 40 | GE | 70 | LEU |
| 40 | GE | 71 | GLU |
| 40 | GE | 74 | VAL |
| 40 | GE | 78 | VAL |
| 40 | GE | 79 | ARG |
| 40 | GE | 80 | THR |
| 40 | GE | 84 | ARG |
| 40 | GE | 87 | PHE |
| 40 | GE | 94 | THR |
| 40 | GE | 96 | LYS |
| 40 | GE | 105 | ARG |
| 40 | GE | 109 | THR |
| 40 | GE | 110 | ILE |
| 40 | GE | 112 | LYS |
| 40 | GE | 114 | LEU |
| 40 | GE | 116 | ASP |
| 40 | GE | 118 | VAL |
| 40 | GE | 119 | LEU |
| 40 | GE | 121 | ARG |
| 40 | GE | 122 | ILE |
| 40 | GE | 123 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GE | 124 | LYS |
| 40 | GE | 135 | PHE |
| 40 | GE | 139 | HIS |
| 40 | GE | 141 | PHE |
| 40 | GE | 145 | THR |
| 40 | GE | 149 | PHE |
| 40 | GE | 151 | SER |
| 40 | GE | 152 | LEU |
| 40 | GE | 153 | LEU |
| 40 | GE | 154 | MET |
| 40 | GE | 157 | LEU |
| 40 | GE | 160 | ASP |
| 40 | GE | 161 | TYR |
| 40 | GE | 163 | LYS |
| 40 | GE | 165 | SER |
| 40 | GE | 171 | ILE |
| 40 | GE | 183 | GLU |
| 40 | GE | 193 | THR |
| 40 | GE | 196 | GLU |
| 40 | GE | 200 | CYS |
| 40 | GE | 203 | MET |
| 40 | GE | 211 | ASP |
| 40 | GE | 212 | ILE |
| 40 | GE | 214 | ARG |
| 40 | GE | 215 | ARG |
| 40 | GE | 218 | ASP |
| 40 | GE | 220 | GLU |
| 40 | GE | 221 | ARG |
| 40 | GE | 223 | THR |
| 40 | GE | 224 | TYR |
| 40 | GE | 225 | THR |
| 40 | GE | 228 | ASN |
| 40 | GE | 229 | ARG |
| 40 | GE | 234 | ILE |
| 40 | GE | 235 | VAL |
| 40 | GE | 238 | ILE |
| 40 | GE | 241 | SER |
| 40 | GE | 243 | ARG |
| 40 | GE | 244 | PHE |
| 40 | GE | 248 | LEU |
| 40 | GE | 250 | VAL |
| 40 | GE | 251 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GE | 255 | PHE |
| 40 | GE | 256 | GLN |
| 40 | GE | 260 | VAL |
| 40 | GE | 264 | ARG |
| 40 | GE | 265 | ILE |
| 40 | GE | 271 | THR |
| 40 | GE | 275 | VAL |
| 40 | GE | 283 | HIS |
| 40 | GE | 286 | LEU |
| 40 | GE | 291 | ILE |
| 40 | GE | 295 | CYS |
| 40 | GE | 296 | PHE |
| 40 | GE | 303 | VAL |
| 40 | GE | 304 | LYS |
| 40 | GE | 315 | CYS |
| 40 | GE | 316 | CYS |
| 40 | GE | 320 | ARG |
| 40 | GE | 322 | ASP |
| 40 | GE | 328 | VAL |
| 40 | GE | 336 | LYS |
| 40 | GE | 339 | ARG |
| 40 | GE | 341 | ILE |
| 40 | GE | 345 | ASP |
| 40 | GE | 347 | CYS |
| 40 | GE | 349 | THR |
| 40 | GE | 358 | GLN |
| 40 | GE | 362 | VAL |
| 40 | GE | 367 | LEU |
| 40 | GE | 369 | LYS |
| 40 | GE | 372 | ARG |
| 40 | GE | 377 | LEU |
| 40 | GE | 381 | THR |
| 40 | GE | 383 | ILE |
| 40 | GE | 397 | MET |
| 40 | GE | 400 | LYS |
| 40 | GE | 401 | ARG |
| 40 | GE | 403 | PHE |
| 40 | GE | 412 | MET |
| 40 | GE | 416 | GLU |
| 40 | GE | 417 | PHE |
| 40 | GE | 421 | ARG |
| 40 | GE | 423 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GE | 424 | MET |
| 40 | GE | 427 | LEU |
| 40 | GE | 429 | LYS |
| 40 | GE | 434 | VAL |
| 40 | GE | 436 | MET |
| 40 | GE | 437 | ASP |
| 40 | GE | 439 | VAL |
| 40 | GG | 18 | ASN |
| 40 | GG | 274 | PRO |
| 40 | GG | 275 | VAL |
| 40 | GG | 276 | ILE |
| 40 | GG | 286 | LEU |
| 40 | GG | 361 | THR |
| 40 | GG | 362 | VAL |
| 40 | GG | 363 | VAL |
| 40 | GG | 366 | ASP |
| 40 | GG | 369 | LYS |
| 40 | GG | 371 | GLN |
| 40 | GH | 2 | ARG |
| 40 | GH | 3 | GLU |
| 40 | GH | 6 | SER |
| 40 | GH | 11 | GLN |
| 40 | GH | 22 | GLU |
| 40 | GH | 23 | LEU |
| 40 | GH | 26 | LEU |
| 40 | GH | 30 | ILE |
| 40 | GH | 33 | ASP |
| 40 | GH | 36 | MET |
| 40 | GH | 38 | SER |
| 40 | GH | 51 | THR |
| 40 | GH | 52 | PHE |
| 40 | GH | 55 | GLU |
| 40 | GH | 60 | LYS |
| 40 | GH | 62 | VAL |
| 40 | GH | 64 | ARG |
| 40 | GH | 66 | VAL |
| 40 | GH | 90 | GLU |
| 40 | GH | 92 | LEU |
| 40 | GH | 93 | ILE |
| 40 | GH | 94 | THR |
| 40 | GH | 97 | GLU |
| 40 | GH | 105 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GH | 109 | THR |
| 40 | GH | 110 | ILE |
| 40 | GH | 114 | LEU |
| 40 | GH | 116 | ASP |
| 40 | GH | 117 | LEU |
| 40 | GH | 119 | LEU |
| 40 | GH | 120 | ASP |
| 40 | GH | 123 | ARG |
| 40 | GH | 125 | LEU |
| 40 | GH | 132 | LEU |
| 40 | GH | 137 | ILE |
| 40 | GH | 141 | PHE |
| 40 | GH | 151 | SER |
| 40 | GH | 152 | LEU |
| 40 | GH | 156 | ARG |
| 40 | GH | 157 | LEU |
| 40 | GH | 160 | ASP |
| 40 | GH | 161 | TYR |
| 40 | GH | 164 | LYS |
| 40 | GH | 166 | LYS |
| 40 | GH | 168 | GLU |
| 40 | GH | 171 | ILE |
| 40 | GH | 176 | GLN |
| 40 | GH | 179 | THR |
| 40 | GH | 189 | LEU |
| 40 | GH | 190 | THR |
| 40 | GH | 192 | HIS |
| 40 | GH | 193 | THR |
| 40 | GH | 196 | GLU |
| 40 | GH | 200 | CYS |
| 40 | GH | 203 | MET |
| 40 | GH | 205 | ASP |
| 40 | GH | 210 | TYR |
| 40 | GH | 212 | ILE |
| 40 | GH | 214 | ARG |
| 40 | GH | 215 | ARG |
| 40 | GH | 221 | ARG |
| 40 | GH | 228 | ASN |
| 40 | GH | 229 | ARG |
| 40 | GH | 241 | SER |
| 40 | GH | 242 | LEU |
| 40 | GH | 243 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GH | 248 | LEU |
| 40 | GH | 250 | VAL |
| 40 | GH | 251 | ASP |
| 40 | GH | 256 | GLN |
| 40 | GH | 271 | THR |
| 40 | GH | 272 | TYR |
| 40 | GH | 277 | SER |
| 40 | GH | 279 | GLU |
| 40 | GH | 280 | LYS |
| 40 | GH | 284 | GLU |
| 40 | GH | 286 | LEU |
| 40 | GH | 287 | SER |
| 40 | GH | 295 | CYS |
| 40 | GH | 304 | LYS |
| 40 | GH | 305 | CYS |
| 40 | GH | 318 | LEU |
| 40 | GH | 320 | ARG |
| 40 | GH | 328 | VAL |
| 40 | GH | 335 | ILE |
| 40 | GH | 337 | THR |
| 40 | GH | 341 | ILE |
| 40 | GH | 342 | GLN |
| 40 | GH | 343 | PHE |
| 40 | GH | 349 | THR |
| 40 | GH | 351 | PHE |
| 40 | GH | 352 | LYS |
| 40 | GH | 355 | ILE |
| 40 | GH | 362 | VAL |
| 40 | GH | 363 | VAL |
| 40 | GH | 369 | LYS |
| 40 | GH | 370 | VAL |
| 40 | GH | 372 | ARG |
| 40 | GH | 377 | LEU |
| 40 | GH | 381 | THR |
| 40 | GH | 396 | LEU |
| 40 | GH | 400 | LYS |
| 40 | GH | 403 | PHE |
| 40 | GH | 410 | GLU |
| 40 | GH | 412 | MET |
| 40 | GH | 417 | PHE |
| 40 | GH | 423 | ASP |
| 40 | GH | 424 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GH | 429 | LYS |
| 40 | GH | 434 | VAL |
| 40 | GH | 436 | MET |
| 40 | GH | 437 | ASP |
| 40 | GH | 439 | VAL |
| 40 | GI | 1 | GLN |
| 40 | GI | 2 | ARG |
| 40 | GI | 4 | CYS |
| 40 | GI | 7 | VAL |
| 40 | GI | 9 | VAL |
| 40 | GI | 20 | CYS |
| 40 | GI | 26 | LEU |
| 40 | GI | 33 | ASP |
| 40 | GI | 36 | MET |
| 40 | GI | 39 | ASP |
| 40 | GI | 47 | ASP |
| 40 | GI | 52 | PHE |
| 40 | GI | 55 | GLU |
| 40 | GI | 60 | LYS |
| 40 | GI | 66 | VAL |
| 40 | GI | 71 | GLU |
| 40 | GI | 75 | ILE |
| 40 | GI | 79 | ARG |
| 40 | GI | 85 | GLN |
| 40 | GI | 94 | THR |
| 40 | GI | 96 | LYS |
| 40 | GI | 110 | ILE |
| 40 | GI | 116 | ASP |
| 40 | GI | 120 | ASP |
| 40 | GI | 123 | ARG |
| 40 | GI | 124 | LYS |
| 40 | GI | 128 | GLN |
| 40 | GI | 129 | CYS |
| 40 | GI | 130 | THR |
| 40 | GI | 132 | LEU |
| 40 | GI | 133 | GLN |
| 40 | GI | 137 | ILE |
| 40 | GI | 139 | HIS |
| 40 | GI | 145 | THR |
| 40 | GI | 149 | PHE |
| 40 | GI | 152 | LEU |
| 40 | GI | 153 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GI | 154 | MET |
| 40 | GI | 160 | ASP |
| 40 | GI | 161 | TYR |
| 40 | GI | 163 | LYS |
| 40 | GI | 164 | LYS |
| 40 | GI | 166 | LYS |
| 40 | GI | 170 | SER |
| 40 | GI | 176 | GLN |
| 40 | GI | 177 | VAL |
| 40 | GI | 179 | THR |
| 40 | GI | 181 | VAL |
| 40 | GI | 188 | ILE |
| 40 | GI | 190 | THR |
| 40 | GI | 192 | HIS |
| 40 | GI | 203 | MET |
| 40 | GI | 205 | ASP |
| 40 | GI | 207 | GLU |
| 40 | GI | 209 | ILE |
| 40 | GI | 210 | TYR |
| 40 | GI | 214 | ARG |
| 40 | GI | 215 | ARG |
| 40 | GI | 216 | ASN |
| 40 | GI | 221 | ARG |
| 40 | GI | 223 | THR |
| 40 | GI | 225 | THR |
| 40 | GI | 229 | ARG |
| 40 | GI | 230 | LEU |
| 40 | GI | 233 | GLN |
| 40 | GI | 234 | ILE |
| 40 | GI | 236 | SER |
| 40 | GI | 239 | THR |
| 40 | GI | 242 | LEU |
| 40 | GI | 243 | ARG |
| 40 | GI | 248 | LEU |
| 40 | GI | 250 | VAL |
| 40 | GI | 253 | THR |
| 40 | GI | 254 | GLU |
| 40 | GI | 258 | ASN |
| 40 | GI | 259 | LEU |
| 40 | GI | 264 | ARG |
| 40 | GI | 271 | THR |
| 40 | GI | 272 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GI | 275 | VAL |
| 40 | GI | 276 | ILE |
| 40 | GI | 280 | LYS |
| 40 | GI | 282 | TYR |
| 40 | GI | 285 | GLN |
| 40 | GI | 287 | SER |
| 40 | GI | 291 | ILE |
| 40 | GI | 293 | ASN |
| 40 | GI | 304 | LYS |
| 40 | GI | 311 | LYS |
| 40 | GI | 313 | MET |
| 40 | GI | 318 | LEU |
| 40 | GI | 323 | VAL |
| 40 | GI | 326 | LYS |
| 40 | GI | 328 | VAL |
| 40 | GI | 332 | ILE |
| 40 | GI | 339 | ARG |
| 40 | GI | 341 | ILE |
| 40 | GI | 345 | ASP |
| 40 | GI | 349 | THR |
| 40 | GI | 351 | PHE |
| 40 | GI | 352 | LYS |
| 40 | GI | 353 | VAL |
| 40 | GI | 356 | ASN |
| 40 | GI | 357 | TYR |
| 40 | GI | 358 | GLN |
| 40 | GI | 362 | VAL |
| 40 | GI | 363 | VAL |
| 40 | GI | 366 | ASP |
| 40 | GI | 367 | LEU |
| 40 | GI | 369 | LYS |
| 40 | GI | 370 | VAL |
| 40 | GI | 372 | ARG |
| 40 | GI | 376 | MET |
| 40 | GI | 383 | ILE |
| 40 | GI | 389 | ARG |
| 40 | GI | 410 | GLU |
| 40 | GI | 412 | MET |
| 40 | GI | 413 | GLU |
| 40 | GI | 416 | GLU |
| 40 | GI | 419 | GLU |
| 40 | GI | 421 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | GI | 422 | GLU |
| 40 | GI | 424 | MET |
| 40 | GI | 428 | GLU |
| 40 | GI | 429 | LYS |
| 40 | GI | 433 | GLU |
| 40 | GI | 439 | VAL |
| 41 | GN | 2 | ARG |
| 41 | GN | 3 | GLU |
| 41 | GN | 5 | VAL |
| 41 | GN | 7 | LEU |
| 41 | GN | 12 | CYS |
| 41 | GN | 19 | LYS |
| 41 | GN | 24 | ILE |
| 41 | GN | 31 | ASP |
| 41 | GN | 39 | ASP |
| 41 | GN | 45 | GLU |
| 41 | GN | 46 | ARG |
| 41 | GN | 47 | ILE |
| 41 | GN | 48 | ASN |
| 41 | GN | 49 | VAL |
| 41 | GN | 55 | THR |
| 41 | GN | 58 | LYS |
| 41 | GN | 64 | VAL |
| 41 | GN | 67 | ASP |
| 41 | GN | 77 | ARG |
| 41 | GN | 83 | GLN |
| 41 | GN | 86 | ARG |
| 41 | GN | 88 | ASP |
| 41 | GN | 100 | ASN |
| 41 | GN | 103 | LYS |
| 41 | GN | 107 | THR |
| 41 | GN | 108 | GLU |
| 41 | GN | 114 | ASP |
| 41 | GN | 117 | LEU |
| 41 | GN | 122 | LYS |
| 41 | GN | 136 | THR |
| 41 | GN | 137 | HIS |
| 41 | GN | 139 | LEU |
| 41 | GN | 143 | THR |
| 41 | GN | 147 | MET |
| 41 | GN | 150 | LEU |
| 41 | GN | 152 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | GN | 155 | ILE |
| 41 | GN | 157 | GLU |
| 41 | GN | 162 | ARG |
| 41 | GN | 163 | ILE |
| 41 | GN | 164 | MET |
| 41 | GN | 166 | THR |
| 41 | GN | 168 | SER |
| 41 | GN | 170 | VAL |
| 41 | GN | 172 | SER |
| 41 | GN | 174 | LYS |
| 41 | GN | 175 | VAL |
| 41 | GN | 176 | SER |
| 41 | GN | 177 | ASP |
| 41 | GN | 180 | VAL |
| 41 | GN | 187 | LEU |
| 41 | GN | 202 | ILE |
| 41 | GN | 205 | GLU |
| 41 | GN | 209 | ASP |
| 41 | GN | 213 | ARG |
| 41 | GN | 214 | THR |
| 41 | GN | 217 | LEU |
| 41 | GN | 224 | ASP |
| 41 | GN | 227 | HIS |
| 41 | GN | 228 | LEU |
| 41 | GN | 230 | SER |
| 41 | GN | 233 | MET |
| 41 | GN | 240 | LEU |
| 41 | GN | 249 | ASP |
| 41 | GN | 251 | ARG |
| 41 | GN | 252 | LYS |
| 41 | GN | 253 | LEU |
| 41 | GN | 262 | ARG |
| 41 | GN | 263 | LEU |
| 41 | GN | 275 | SER |
| 41 | GN | 276 | ARG |
| 41 | GN | 279 | GLN |
| 41 | GN | 282 | ARG |
| 41 | GN | 284 | LEU |
| 41 | GN | 285 | THR |
| 41 | GN | 290 | THR |
| 41 | GN | 293 | MET |
| 41 | GN | 297 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | GN | 299 | MET |
| 41 | GN | 300 | MET |
| 41 | GN | 307 | HIS |
| 41 | GN | 309 | ARG |
| 41 | GN | 310 | TYR |
| 41 | GN | 313 | VAL |
| 41 | GN | 318 | ARG |
| 41 | GN | 322 | SER |
| 41 | GN | 327 | ASP |
| 41 | GN | 328 | GLU |
| 41 | GN | 330 | MET |
| 41 | GN | 334 | GLN |
| 41 | GN | 338 | SER |
| 41 | GN | 345 | ILE |
| 41 | GN | 347 | ASN |
| 41 | GN | 348 | ASN |
| 41 | GN | 350 | LYS |
| 41 | GN | 353 | VAL |
| 41 | GN | 354 | CYS |
| 41 | GN | 355 | ASP |
| 41 | GN | 362 | LYS |
| 41 | GN | 366 | THR |
| 41 | GN | 374 | ILE |
| 41 | GN | 376 | GLU |
| 41 | GN | 377 | LEU |
| 41 | GN | 379 | LYS |
| 41 | GN | 384 | GLN |
| 41 | GN | 392 | LYS |
| 41 | GN | 395 | LEU |
| 41 | GN | 396 | HIS |
| 41 | GN | 397 | TRP |
| 41 | GN | 406 | MET |
| 41 | GN | 410 | GLU |
| 41 | GN | 414 | ASN |
| 41 | GN | 415 | MET |
| 41 | GN | 422 | VAL |
| 41 | GN | 425 | ARG |
| 41 | GN | 428 | CYS |
| 41 | GO | 251 | ARG |
| 41 | GO | 274 | THR |
| 41 | GO | 279 | GLN |
| 40 | HA | 2 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | HA | 206 | ASN |
| 40 | HE | 1 | GLN |
| 40 | HE | 2 | ARG |
| 40 | HE | 3 | GLU |
| 40 | HE | 4 | CYS |
| 40 | HE | 6 | SER |
| 40 | HE | 7 | VAL |
| 40 | HE | 9 | VAL |
| 40 | HE | 20 | CYS |
| 40 | HE | 22 | GLU |
| 40 | HE | 28 | HIS |
| 40 | HE | 31 | GLN |
| 40 | HE | 38 | SER |
| 40 | HE | 46 | ASP |
| 40 | HE | 50 | ASN |
| 40 | HE | 52 | PHE |
| 40 | HE | 56 | THR |
| 40 | HE | 60 | LYS |
| 40 | HE | 66 | VAL |
| 40 | HE | 68 | VAL |
| 40 | HE | 71 | GLU |
| 40 | HE | 74 | VAL |
| 40 | HE | 75 | ILE |
| 40 | HE | 79 | ARG |
| 40 | HE | 80 | THR |
| 40 | HE | 84 | ARG |
| 40 | HE | 94 | THR |
| 40 | HE | 96 | LYS |
| 40 | HE | 98 | ASP |
| 40 | HE | 105 | ARG |
| 40 | HE | 109 | THR |
| 40 | HE | 110 | ILE |
| 40 | HE | 112 | LYS |
| 40 | HE | 113 | GLU |
| 40 | HE | 114 | LEU |
| 40 | HE | 116 | ASP |
| 40 | HE | 117 | LEU |
| 40 | HE | 120 | ASP |
| 40 | HE | 122 | ILE |
| 40 | HE | 123 | ARG |
| 40 | HE | 128 | GLN |
| 40 | HE | 129 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | HE | 137 | ILE |
| 40 | HE | 138 | PHE |
| 40 | HE | 145 | THR |
| 40 | HE | 149 | PHE |
| 40 | HE | 151 | SER |
| 40 | HE | 152 | LEU |
| 40 | HE | 153 | LEU |
| 40 | HE | 154 | MET |
| 40 | HE | 160 | ASP |
| 40 | HE | 161 | TYR |
| 40 | HE | 163 | LYS |
| 40 | HE | 164 | LYS |
| 40 | HE | 165 | SER |
| 40 | HE | 166 | LYS |
| 40 | HE | 167 | LEU |
| 40 | HE | 170 | SER |
| 40 | HE | 171 | ILE |
| 40 | HE | 182 | VAL |
| 40 | HE | 183 | GLU |
| 40 | HE | 194 | THR |
| 40 | HE | 195 | LEU |
| 40 | HE | 200 | CYS |
| 40 | HE | 204 | VAL |
| 40 | HE | 205 | ASP |
| 40 | HE | 209 | ILE |
| 40 | HE | 210 | TYR |
| 40 | HE | 212 | ILE |
| 40 | HE | 214 | ARG |
| 40 | HE | 215 | ARG |
| 40 | HE | 218 | ASP |
| 40 | HE | 219 | ILE |
| 40 | HE | 220 | GLU |
| 40 | HE | 226 | ASN |
| 40 | HE | 232 | SER |
| 40 | HE | 234 | ILE |
| 40 | HE | 238 | ILE |
| 40 | HE | 241 | SER |
| 40 | HE | 242 | LEU |
| 40 | HE | 243 | ARG |
| 40 | HE | 244 | PHE |
| 40 | HE | 248 | LEU |
| 40 | HE | 253 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | HE | 256 | GLN |
| 40 | HE | 264 | ARG |
| 40 | HE | 271 | THR |
| 40 | HE | 272 | TYR |
| 40 | HE | 275 | VAL |
| 40 | HE | 277 | SER |
| 40 | HE | 280 | LYS |
| 40 | HE | 284 | GLU |
| 40 | HE | 290 | GLU |
| 40 | HE | 291 | ILE |
| 40 | HE | 304 | LYS |
| 40 | HE | 308 | ARG |
| 40 | HE | 309 | HIS |
| 40 | HE | 311 | LYS |
| 40 | HE | 313 | MET |
| 40 | HE | 317 | LEU |
| 40 | HE | 318 | LEU |
| 40 | HE | 323 | VAL |
| 40 | HE | 324 | VAL |
| 40 | HE | 326 | LYS |
| 40 | HE | 329 | ASN |
| 40 | HE | 338 | LYS |
| 40 | HE | 340 | SER |
| 40 | HE | 342 | GLN |
| 40 | HE | 363 | VAL |
| 40 | HE | 366 | ASP |
| 40 | HE | 367 | LEU |
| 40 | HE | 369 | LYS |
| 40 | HE | 370 | VAL |
| 40 | HE | 374 | VAL |
| 40 | HE | 376 | MET |
| 40 | HE | 377 | LEU |
| 40 | HE | 378 | SER |
| 40 | HE | 380 | THR |
| 40 | HE | 381 | THR |
| 40 | HE | 383 | ILE |
| 40 | HE | 385 | GLU |
| 40 | HE | 391 | ASP |
| 40 | HE | 396 | LEU |
| 40 | HE | 400 | LYS |
| 40 | HE | 401 | ARG |
| 40 | HE | 403 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | HE | 410 | GLU |
| 40 | HE | 421 | ARG |
| 40 | HE | 427 | LEU |
| 40 | HE | 429 | LYS |
| 40 | HE | 430 | ASP |
| 40 | HE | 434 | VAL |
| 40 | HE | 439 | VAL |
| 40 | HF | 329 | ASN |
| 41 | HM | 2 | ARG |
| 41 | HM | 359 | ARG |
| 41 | HN | 1 | MET |
| 41 | HN | 2 | ARG |
| 41 | HN | 3 | GLU |
| 41 | HN | 4 | ILE |
| 41 | HN | 7 | LEU |
| 41 | HN | 8 | GLN |
| 41 | HN | 12 | CYS |
| 41 | HN | 15 | GLN |
| 41 | HN | 16 | ILE |
| 41 | HN | 19 | LYS |
| 41 | HN | 23 | VAL |
| 41 | HN | 27 | GLU |
| 41 | HN | 31 | ASP |
| 41 | HN | 35 | THR |
| 41 | HN | 40 | SER |
| 41 | HN | 41 | ASP |
| 41 | HN | 53 | GLU |
| 41 | HN | 58 | LYS |
| 41 | HN | 62 | ARG |
| 41 | HN | 65 | LEU |
| 41 | HN | 66 | VAL |
| 41 | HN | 68 | LEU |
| 41 | HN | 69 | GLU |
| 41 | HN | 72 | THR |
| 41 | HN | 74 | ASP |
| 41 | HN | 75 | SER |
| 41 | HN | 84 | ILE |
| 41 | HN | 91 | VAL |
| 41 | HN | 103 | LYS |
| 41 | HN | 108 | GLU |
| 41 | HN | 111 | GLU |
| 41 | HN | 114 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | HN | 115 | SER |
| 41 | HN | 117 | LEU |
| 41 | HN | 121 | ARG |
| 41 | HN | 123 | GLU |
| 41 | HN | 128 | ASP |
| 41 | HN | 130 | LEU |
| 41 | HN | 131 | GLN |
| 41 | HN | 135 | LEU |
| 41 | HN | 139 | LEU |
| 41 | HN | 147 | MET |
| 41 | HN | 149 | THR |
| 41 | HN | 153 | SER |
| 41 | HN | 156 | ARG |
| 41 | HN | 158 | GLU |
| 41 | HN | 161 | ASP |
| 41 | HN | 162 | ARG |
| 41 | HN | 163 | ILE |
| 41 | HN | 165 | ASN |
| 41 | HN | 166 | THR |
| 41 | HN | 172 | SER |
| 41 | HN | 174 | LYS |
| 41 | HN | 176 | SER |
| 41 | HN | 178 | THR |
| 41 | HN | 180 | VAL |
| 41 | HN | 192 | LEU |
| 41 | HN | 198 | GLU |
| 41 | HN | 199 | THR |
| 41 | HN | 201 | CYS |
| 41 | HN | 205 | GLU |
| 41 | HN | 209 | ASP |
| 41 | HN | 210 | ILE |
| 41 | HN | 213 | ARG |
| 41 | HN | 217 | LEU |
| 41 | HN | 218 | THR |
| 41 | HN | 221 | THR |
| 41 | HN | 222 | TYR |
| 41 | HN | 224 | ASP |
| 41 | HN | 228 | LEU |
| 41 | HN | 232 | THR |
| 41 | HN | 233 | MET |
| 41 | HN | 234 | SER |
| 41 | HN | 237 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | HN | 239 | CYS |
| 41 | HN | 240 | LEU |
| 41 | HN | 241 | ARG |
| 41 | HN | 246 | LEU |
| 41 | HN | 252 | LYS |
| 41 | HN | 255 | VAL |
| 41 | HN | 256 | ASN |
| 41 | HN | 257 | MET |
| 41 | HN | 258 | VAL |
| 41 | HN | 263 | LEU |
| 41 | HN | 267 | MET |
| 41 | HN | 270 | PHE |
| 41 | HN | 273 | LEU |
| 41 | HN | 274 | THR |
| 41 | HN | 276 | ARG |
| 41 | HN | 280 | GLN |
| 41 | HN | 282 | ARG |
| 41 | HN | 284 | LEU |
| 41 | HN | 288 | GLU |
| 41 | HN | 290 | THR |
| 41 | HN | 297 | LYS |
| 41 | HN | 299 | MET |
| 41 | HN | 316 | VAL |
| 41 | HN | 320 | ARG |
| 41 | HN | 322 | SER |
| 41 | HN | 324 | LYS |
| 41 | HN | 329 | GLN |
| 41 | HN | 330 | MET |
| 41 | HN | 334 | GLN |
| 41 | HN | 336 | LYS |
| 41 | HN | 337 | ASN |
| 41 | HN | 341 | PHE |
| 41 | HN | 344 | TRP |
| 41 | HN | 347 | ASN |
| 41 | HN | 350 | LYS |
| 41 | HN | 355 | ASP |
| 41 | HN | 359 | ARG |
| 41 | HN | 361 | LEU |
| 41 | HN | 362 | LYS |
| 41 | HN | 364 | SER |
| 41 | HN | 367 | PHE |
| 41 | HN | 368 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | HN | 379 | LYS |
| 41 | HN | 380 | ARG |
| 41 | HN | 388 | MET |
| 41 | HN | 391 | ARG |
| 41 | HN | 392 | LYS |
| 41 | HN | 395 | LEU |
| 41 | HN | 409 | THR |
| 41 | HN | 413 | SER |
| 41 | HN | 415 | MET |
| 41 | HN | 423 | VAL |
| 41 | HN | 424 | THR |
| 41 | HO | 306 | ARG |
| 41 | HQ | 306 | ARG |
| 40 | IA | 256 | GLN |
| 41 | IB | 2 | ARG |
| 41 | IB | 162 | ARG |
| 40 | IE | 2 | ARG |
| 40 | IE | 258 | ASN |
| 40 | IF | 308 | ARG |
| 40 | IH | 256 | GLN |
| 40 | IH | 329 | ASN |
| 40 | II | 308 | ARG |
| 41 | IN | 122 | LYS |
| 41 | IN | 359 | ARG |
| 41 | IP | 291 | GLN |
| 41 | IQ | 174 | LYS |
| 41 | IQ | 256 | ASN |
| 40 | JD | 128 | GLN |
| 40 | JD | 342 | GLN |
| 40 | JD | 372 | ARG |
| 40 | JF | 308 | ARG |
| 40 | JF | 429 | LYS |
| 40 | JG | 308 | ARG |
| 40 | JG | 329 | ASN |
| 40 | JG | 338 | LYS |
| 40 | JG | 392 | HIS |
| 41 | JM | 1 | MET |
| 41 | JM | 7 | LEU |
| 41 | JM | 8 | GLN |
| 41 | JM | 12 | CYS |
| 41 | JM | 19 | LYS |
| 41 | JM | 26 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | JM | 27 | GLU |
| 41 | JM | 28 | HIS |
| 41 | JM | 31 | ASP |
| 41 | JM | 33 | THR |
| 41 | JM | 40 | SER |
| 41 | JM | 42 | LEU |
| 41 | JM | 43 | GLN |
| 41 | JM | 44 | LEU |
| 41 | JM | 46 | ARG |
| 41 | JM | 50 | TYR |
| 41 | JM | 52 | ASN |
| 41 | JM | 53 | GLU |
| 41 | JM | 55 | THR |
| 41 | JM | 58 | LYS |
| 41 | JM | 60 | VAL |
| 41 | JM | 74 | ASP |
| 41 | JM | 78 | SER |
| 41 | JM | 84 | ILE |
| 41 | JM | 86 | ARG |
| 41 | JM | 88 | ASP |
| 41 | JM | 91 | VAL |
| 41 | JM | 100 | ASN |
| 41 | JM | 103 | LYS |
| 41 | JM | 108 | GLU |
| 41 | JM | 114 | ASP |
| 41 | JM | 117 | LEU |
| 41 | JM | 121 | ARG |
| 41 | JM | 131 | GLN |
| 41 | JM | 134 | GLN |
| 41 | JM | 137 | HIS |
| 41 | JM | 145 | SER |
| 41 | JM | 147 | MET |
| 41 | JM | 151 | LEU |
| 41 | JM | 153 | SER |
| 41 | JM | 154 | LYS |
| 41 | JM | 156 | ARG |
| 41 | JM | 157 | GLU |
| 41 | JM | 158 | GLU |
| 41 | JM | 162 | ARG |
| 41 | JM | 164 | MET |
| 41 | JM | 165 | ASN |
| 41 | JM | 166 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | JM | 174 | LYS |
| 41 | JM | 180 | VAL |
| 41 | JM | 182 | PRO |
| 41 | JM | 187 | LEU |
| 41 | JM | 192 | LEU |
| 41 | JM | 194 | GLU |
| 41 | JM | 195 | ASN |
| 41 | JM | 197 | ASP |
| 41 | JM | 198 | GLU |
| 41 | JM | 199 | THR |
| 41 | JM | 200 | TYR |
| 41 | JM | 202 | ILE |
| 41 | JM | 208 | TYR |
| 41 | JM | 209 | ASP |
| 41 | JM | 211 | CYS |
| 41 | JM | 214 | THR |
| 41 | JM | 216 | LYS |
| 41 | JM | 217 | LEU |
| 41 | JM | 218 | THR |
| 41 | JM | 221 | THR |
| 41 | JM | 226 | ASN |
| 41 | JM | 233 | MET |
| 41 | JM | 237 | THR |
| 41 | JM | 249 | ASP |
| 41 | JM | 253 | LEU |
| 41 | JM | 255 | VAL |
| 41 | JM | 257 | MET |
| 41 | JM | 258 | VAL |
| 41 | JM | 273 | LEU |
| 41 | JM | 274 | THR |
| 41 | JM | 275 | SER |
| 41 | JM | 276 | ARG |
| 41 | JM | 279 | GLN |
| 41 | JM | 288 | GLU |
| 41 | JM | 289 | LEU |
| 41 | JM | 290 | THR |
| 41 | JM | 297 | LYS |
| 41 | JM | 299 | MET |
| 41 | JM | 300 | MET |
| 41 | JM | 306 | ARG |
| 41 | JM | 309 | ARG |
| 41 | JM | 310 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | JM | 311 | LEU |
| 41 | JM | 312 | THR |
| 41 | JM | 316 | VAL |
| 41 | JM | 318 | ARG |
| 41 | JM | 320 | ARG |
| 41 | JM | 322 | SER |
| 41 | JM | 325 | GLU |
| 41 | JM | 329 | GLN |
| 41 | JM | 338 | SER |
| 41 | JM | 345 | ILE |
| 41 | JM | 347 | ASN |
| 41 | JM | 348 | ASN |
| 41 | JM | 349 | VAL |
| 41 | JM | 350 | LYS |
| 41 | JM | 353 | VAL |
| 41 | JM | 355 | ASP |
| 41 | JM | 356 | ILE |
| 41 | JM | 362 | LYS |
| 41 | JM | 363 | MET |
| 41 | JM | 372 | THR |
| 41 | JM | 374 | ILE |
| 41 | JM | 375 | GLN |
| 41 | JM | 376 | GLU |
| 41 | JM | 377 | LEU |
| 41 | JM | 381 | ILE |
| 41 | JM | 388 | MET |
| 41 | JM | 389 | PHE |
| 41 | JM | 391 | ARG |
| 41 | JM | 392 | LYS |
| 41 | JM | 395 | LEU |
| 41 | JM | 399 | THR |
| 41 | JM | 401 | GLU |
| 41 | JM | 403 | MET |
| 41 | JM | 406 | MET |
| 41 | JM | 410 | GLU |
| 41 | JM | 415 | MET |
| 41 | JM | 418 | LEU |
| 41 | JM | 422 | VAL |
| 41 | JM | 425 | ARG |
| 41 | JM | 428 | CYS |
| 41 | JN | 2 | ARG |
| 41 | JN | 99 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | KA | 50 | ASN |
| 40 | KA | 308 | ARG |
| 40 | KD | 221 | ARG |
| 40 | KD | 326 | LYS |
| 40 | KE | 221 | ARG |
| 40 | KF | 372 | ARG |
| 40 | KH | 88 | HIS |
| 41 | KL | 1 | MET |
| 41 | KL | 2 | ARG |
| 41 | KL | 7 | LEU |
| 41 | KL | 12 | CYS |
| 41 | KL | 16 | ILE |
| 41 | KL | 19 | LYS |
| 41 | KL | 22 | GLU |
| 41 | KL | 33 | THR |
| 41 | KL | 39 | ASP |
| 41 | KL | 40 | SER |
| 41 | KL | 46 | ARG |
| 41 | KL | 47 | ILE |
| 41 | KL | 48 | ASN |
| 41 | KL | 53 | GLU |
| 41 | KL | 62 | ARG |
| 41 | KL | 68 | LEU |
| 41 | KL | 74 | ASP |
| 41 | KL | 77 | ARG |
| 41 | KL | 83 | GLN |
| 41 | KL | 88 | ASP |
| 41 | KL | 91 | VAL |
| 41 | KL | 103 | LYS |
| 41 | KL | 107 | THR |
| 41 | KL | 111 | GLU |
| 41 | KL | 114 | ASP |
| 41 | KL | 115 | SER |
| 41 | KL | 117 | LEU |
| 41 | KL | 128 | ASP |
| 41 | KL | 129 | CYS |
| 41 | KL | 131 | GLN |
| 41 | KL | 139 | LEU |
| 41 | KL | 145 | SER |
| 41 | KL | 147 | MET |
| 41 | KL | 156 | ARG |
| 41 | KL | 157 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | KL | 164 | MET |
| 41 | KL | 166 | THR |
| 41 | KL | 172 | SER |
| 41 | KL | 178 | THR |
| 41 | KL | 179 | VAL |
| 41 | KL | 181 | GLU |
| 41 | KL | 182 | PRO |
| 41 | KL | 186 | THR |
| 41 | KL | 188 | SER |
| 41 | KL | 194 | GLU |
| 41 | KL | 199 | THR |
| 41 | KL | 213 | ARG |
| 41 | KL | 214 | THR |
| 41 | KL | 216 | LYS |
| 41 | KL | 217 | LEU |
| 41 | KL | 218 | THR |
| 41 | KL | 221 | THR |
| 41 | KL | 222 | TYR |
| 41 | KL | 224 | ASP |
| 41 | KL | 233 | MET |
| 41 | KL | 236 | VAL |
| 41 | KL | 240 | LEU |
| 41 | KL | 241 | ARG |
| 41 | KL | 245 | GLN |
| 41 | KL | 252 | LYS |
| 41 | KL | 257 | MET |
| 41 | KL | 262 | ARG |
| 41 | KL | 264 | HIS |
| 41 | KL | 267 | MET |
| 41 | KL | 273 | LEU |
| 41 | KL | 275 | SER |
| 41 | KL | 282 | ARG |
| 41 | KL | 289 | LEU |
| 41 | KL | 291 | GLN |
| 41 | KL | 292 | GLN |
| 41 | KL | 297 | LYS |
| 41 | KL | 303 | CYS |
| 41 | KL | 304 | ASP |
| 41 | KL | 306 | ARG |
| 41 | KL | 309 | ARG |
| 41 | KL | 311 | LEU |
| 41 | KL | 312 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | KL | 321 | MET |
| 41 | KL | 328 | GLU |
| 41 | KL | 333 | VAL |
| 41 | KL | 336 | LYS |
| 41 | KL | 343 | GLU |
| 41 | KL | 345 | ILE |
| 41 | KL | 347 | ASN |
| 41 | KL | 348 | ASN |
| 41 | KL | 349 | VAL |
| 41 | KL | 350 | LYS |
| 41 | KL | 351 | THR |
| 41 | KL | 353 | VAL |
| 41 | KL | 354 | CYS |
| 41 | KL | 361 | LEU |
| 41 | KL | 362 | LYS |
| 41 | KL | 364 | SER |
| 41 | KL | 372 | THR |
| 41 | KL | 375 | GLN |
| 41 | KL | 380 | ARG |
| 41 | KL | 382 | SER |
| 41 | KL | 383 | GLU |
| 41 | KL | 386 | THR |
| 41 | KL | 390 | ARG |
| 41 | KL | 391 | ARG |
| 41 | KL | 396 | HIS |
| 41 | KL | 409 | THR |
| 41 | KL | 410 | GLU |
| 41 | KL | 413 | SER |
| 41 | KL | 415 | MET |
| 41 | KL | 422 | VAL |
| 41 | KL | 423 | VAL |
| 41 | KL | 424 | THR |
| 41 | KN | 347 | ASN |
| 41 | KO | 348 | ASN |
| 40 | LA | 308 | ARG |
| 40 | LA | 339 | ARG |
| 41 | LB | 306 | ARG |
| 40 | LE | 2 | ARG |
| 40 | LE | 52 | PHE |
| 40 | LE | 54 | SER |
| 40 | LE | 55 | GLU |
| 40 | LE | 56 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | LE | 60 | LYS |
| 40 | LE | 62 | VAL |
| 40 | LF | 3 | GLU |
| 40 | LF | 4 | CYS |
| 40 | LF | 9 | VAL |
| 40 | LF | 30 | ILE |
| 40 | LF | 31 | GLN |
| 40 | LF | 33 | ASP |
| 40 | LF | 38 | SER |
| 40 | LF | 52 | PHE |
| 40 | LF | 70 | LEU |
| 40 | LF | 73 | THR |
| 40 | LF | 75 | ILE |
| 40 | LF | 78 | VAL |
| 40 | LF | 82 | THR |
| 40 | LF | 84 | ARG |
| 40 | LF | 109 | THR |
| 40 | LF | 110 | ILE |
| 40 | LF | 112 | LYS |
| 40 | LF | 116 | ASP |
| 40 | LF | 119 | LEU |
| 40 | LF | 120 | ASP |
| 40 | LF | 128 | GLN |
| 40 | LF | 130 | THR |
| 40 | LF | 137 | ILE |
| 40 | LF | 138 | PHE |
| 40 | LF | 140 | SER |
| 40 | LF | 157 | LEU |
| 40 | LF | 160 | ASP |
| 40 | LF | 163 | LYS |
| 40 | LF | 164 | LYS |
| 40 | LF | 166 | LYS |
| 40 | LF | 171 | ILE |
| 40 | LF | 177 | VAL |
| 40 | LF | 187 | SER |
| 40 | LF | 188 | ILE |
| 40 | LF | 196 | GLU |
| 40 | LF | 200 | CYS |
| 40 | LF | 203 | MET |
| 40 | LF | 204 | VAL |
| 40 | LF | 212 | ILE |
| 40 | LF | 225 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | LF | 227 | LEU |
| 40 | LF | 230 | LEU |
| 40 | LF | 238 | ILE |
| 40 | LF | 241 | SER |
| 40 | LF | 251 | ASP |
| 40 | LF | 252 | LEU |
| 40 | LF | 254 | GLU |
| 40 | LF | 256 | GLN |
| 40 | LF | 259 | LEU |
| 40 | LF | 264 | ARG |
| 40 | LF | 269 | LEU |
| 40 | LF | 271 | THR |
| 40 | LF | 276 | ILE |
| 40 | LF | 279 | GLU |
| 40 | LF | 280 | LYS |
| 40 | LF | 284 | GLU |
| 40 | LF | 285 | GLN |
| 40 | LF | 295 | CYS |
| 40 | LF | 300 | ASN |
| 40 | LF | 302 | MET |
| 40 | LF | 305 | CYS |
| 40 | LF | 308 | ARG |
| 40 | LF | 311 | LYS |
| 40 | LF | 318 | LEU |
| 40 | LF | 320 | ARG |
| 40 | LF | 323 | VAL |
| 40 | LF | 326 | LYS |
| 40 | LF | 327 | ASP |
| 40 | LF | 328 | VAL |
| 40 | LF | 339 | ARG |
| 40 | LF | 340 | SER |
| 40 | LF | 342 | GLN |
| 40 | LF | 352 | LYS |
| 40 | LF | 353 | VAL |
| 40 | LF | 362 | VAL |
| 40 | LF | 363 | VAL |
| 40 | LF | 366 | ASP |
| 40 | LF | 369 | LYS |
| 40 | LF | 372 | ARG |
| 40 | LF | 374 | VAL |
| 40 | LF | 383 | ILE |
| 40 | LF | 393 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | LF | 400 | LYS |
| 40 | LF | 401 | ARG |
| 40 | LF | 405 | HIS |
| 40 | LF | 414 | GLU |
| 40 | LF | 416 | GLU |
| 40 | LF | 421 | ARG |
| 40 | LF | 424 | MET |
| 40 | LF | 438 | SER |
| 40 | LF | 440 | GLU |
| 40 | LG | 1 | GLN |
| 40 | LG | 4 | CYS |
| 40 | LG | 6 | SER |
| 40 | LG | 9 | VAL |
| 40 | LG | 22 | GLU |
| 40 | LG | 35 | GLN |
| 40 | LG | 38 | SER |
| 40 | LG | 54 | SER |
| 40 | LG | 60 | LYS |
| 40 | LG | 68 | VAL |
| 40 | LG | 74 | VAL |
| 40 | LG | 75 | ILE |
| 40 | LG | 80 | THR |
| 40 | LG | 84 | ARG |
| 40 | LG | 94 | THR |
| 40 | LG | 105 | ARG |
| 40 | LG | 110 | ILE |
| 40 | LG | 112 | LYS |
| 40 | LG | 113 | GLU |
| 40 | LG | 116 | ASP |
| 40 | LG | 119 | LEU |
| 40 | LG | 122 | ILE |
| 40 | LG | 123 | ARG |
| 40 | LG | 124 | LYS |
| 40 | LG | 130 | THR |
| 40 | LG | 139 | HIS |
| 40 | LG | 140 | SER |
| 40 | LG | 154 | MET |
| 40 | LG | 160 | ASP |
| 40 | LG | 163 | LYS |
| 40 | LG | 164 | LYS |
| 40 | LG | 166 | LYS |
| 40 | LG | 170 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | LG | 177 | VAL |
| 40 | LG | 178 | SER |
| 40 | LG | 181 | VAL |
| 40 | LG | 190 | THR |
| 40 | LG | 193 | THR |
| 40 | LG | 195 | LEU |
| 40 | LG | 200 | CYS |
| 40 | LG | 204 | VAL |
| 40 | LG | 209 | ILE |
| 40 | LG | 211 | ASP |
| 40 | LG | 214 | ARG |
| 40 | LG | 215 | ARG |
| 40 | LG | 217 | LEU |
| 40 | LG | 235 | VAL |
| 40 | LG | 238 | ILE |
| 40 | LG | 241 | SER |
| 40 | LG | 242 | LEU |
| 40 | LG | 245 | ASP |
| 40 | LG | 250 | VAL |
| 40 | LG | 254 | GLU |
| 40 | LG | 264 | ARG |
| 40 | LG | 265 | ILE |
| 40 | LG | 271 | THR |
| 40 | LG | 274 | PRO |
| 40 | LG | 275 | VAL |
| 40 | LG | 276 | ILE |
| 40 | LG | 279 | GLU |
| 40 | LG | 280 | LYS |
| 40 | LG | 283 | HIS |
| 40 | LG | 284 | GLU |
| 40 | LG | 285 | GLN |
| 40 | LG | 286 | LEU |
| 40 | LG | 291 | ILE |
| 40 | LG | 295 | CYS |
| 40 | LG | 301 | GLN |
| 40 | LG | 303 | VAL |
| 40 | LG | 304 | LYS |
| 40 | LG | 306 | ASP |
| 40 | LG | 323 | VAL |
| 40 | LG | 326 | LYS |
| 40 | LG | 329 | ASN |
| 40 | LG | 339 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | LG | 340 | SER |
| 40 | LG | 342 | GLN |
| 40 | LG | 343 | PHE |
| 40 | LG | 349 | THR |
| 40 | LG | 352 | LYS |
| 40 | LG | 361 | THR |
| 40 | LG | 362 | VAL |
| 40 | LG | 363 | VAL |
| 40 | LG | 366 | ASP |
| 40 | LG | 367 | LEU |
| 40 | LG | 369 | LYS |
| 40 | LG | 371 | GLN |
| 40 | LG | 375 | CYS |
| 40 | LG | 376 | MET |
| 40 | LG | 389 | ARG |
| 40 | LG | 395 | ASP |
| 40 | LG | 396 | LEU |
| 40 | LG | 400 | LYS |
| 40 | LG | 410 | GLU |
| 40 | LG | 412 | MET |
| 40 | LG | 417 | PHE |
| 40 | LG | 418 | SER |
| 40 | LG | 429 | LYS |
| 40 | LG | 436 | MET |
| 40 | LG | 438 | SER |
| 40 | LH | 2 | ARG |
| 41 | LL | 37 | HIS |
| 41 | LL | 292 | GLN |
| 41 | LM | 306 | ARG |
| 41 | LN | 19 | LYS |
| 41 | LO | 100 | ASN |
| 40 | MA | 1 | GLN |
| 40 | MA | 2 | ARG |
| 40 | MA | 4 | CYS |
| 40 | MA | 7 | VAL |
| 40 | MA | 15 | GLN |
| 40 | MA | 27 | GLU |
| 40 | MA | 28 | HIS |
| 40 | MA | 36 | MET |
| 40 | MA | 46 | ASP |
| 40 | MA | 54 | SER |
| 40 | MA | 68 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MA | 82 | THR |
| 40 | MA | 93 | ILE |
| 40 | MA | 94 | THR |
| 40 | MA | 96 | LYS |
| 40 | MA | 105 | ARG |
| 40 | MA | 114 | LEU |
| 40 | MA | 120 | ASP |
| 40 | MA | 121 | ARG |
| 40 | MA | 123 | ARG |
| 40 | MA | 130 | THR |
| 40 | MA | 139 | HIS |
| 40 | MA | 140 | SER |
| 40 | MA | 141 | PHE |
| 40 | MA | 145 | THR |
| 40 | MA | 151 | SER |
| 40 | MA | 153 | LEU |
| 40 | MA | 156 | ARG |
| 40 | MA | 163 | LYS |
| 40 | MA | 170 | SER |
| 40 | MA | 171 | ILE |
| 40 | MA | 187 | SER |
| 40 | MA | 188 | ILE |
| 40 | MA | 193 | THR |
| 40 | MA | 200 | CYS |
| 40 | MA | 209 | ILE |
| 40 | MA | 211 | ASP |
| 40 | MA | 219 | ILE |
| 40 | MA | 221 | ARG |
| 40 | MA | 224 | TYR |
| 40 | MA | 230 | LEU |
| 40 | MA | 238 | ILE |
| 40 | MA | 241 | SER |
| 40 | MA | 242 | LEU |
| 40 | MA | 248 | LEU |
| 40 | MA | 249 | ASN |
| 40 | MA | 253 | THR |
| 40 | MA | 257 | THR |
| 40 | MA | 264 | ARG |
| 40 | MA | 265 | ILE |
| 40 | MA | 269 | LEU |
| 40 | MA | 271 | THR |
| 40 | MA | 276 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MA | 284 | GLU |
| 40 | MA | 302 | MET |
| 40 | MA | 303 | VAL |
| 40 | MA | 304 | LYS |
| 40 | MA | 311 | LYS |
| 40 | MA | 315 | CYS |
| 40 | MA | 316 | CYS |
| 40 | MA | 318 | LEU |
| 40 | MA | 320 | ARG |
| 40 | MA | 324 | VAL |
| 40 | MA | 329 | ASN |
| 40 | MA | 339 | ARG |
| 40 | MA | 340 | SER |
| 40 | MA | 361 | THR |
| 40 | MA | 362 | VAL |
| 40 | MA | 363 | VAL |
| 40 | MA | 366 | ASP |
| 40 | MA | 369 | LYS |
| 40 | MA | 370 | VAL |
| 40 | MA | 372 | ARG |
| 40 | MA | 375 | CYS |
| 40 | MA | 380 | THR |
| 40 | MA | 381 | THR |
| 40 | MA | 385 | GLU |
| 40 | MA | 391 | ASP |
| 40 | MA | 396 | LEU |
| 40 | MA | 400 | LYS |
| 40 | MA | 401 | ARG |
| 40 | MA | 418 | SER |
| 40 | MA | 421 | ARG |
| 40 | MA | 424 | MET |
| 40 | MA | 431 | TYR |
| 40 | MA | 438 | SER |
| 40 | MA | 439 | VAL |
| 41 | MB | 306 | ARG |
| 40 | MD | 274 | PRO |
| 40 | MD | 276 | ILE |
| 40 | MD | 280 | LYS |
| 40 | ME | 2 | ARG |
| 40 | ME | 308 | ARG |
| 40 | MF | 2 | ARG |
| 40 | MF | 3 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MF | 4 | CYS |
| 40 | MF | 6 | SER |
| 40 | MF | 9 | VAL |
| 40 | MF | 11 | GLN |
| 40 | MF | 23 | LEU |
| 40 | MF | 26 | LEU |
| 40 | MF | 51 | THR |
| 40 | MF | 54 | SER |
| 40 | MF | 60 | LYS |
| 40 | MF | 62 | VAL |
| 40 | MF | 66 | VAL |
| 40 | MF | 68 | VAL |
| 40 | MF | 71 | GLU |
| 40 | MF | 76 | ASP |
| 40 | MF | 80 | THR |
| 40 | MF | 84 | ARG |
| 40 | MF | 94 | THR |
| 40 | MF | 109 | THR |
| 40 | MF | 110 | ILE |
| 40 | MF | 112 | LYS |
| 40 | MF | 116 | ASP |
| 40 | MF | 117 | LEU |
| 40 | MF | 120 | ASP |
| 40 | MF | 123 | ARG |
| 40 | MF | 124 | LYS |
| 40 | MF | 128 | GLN |
| 40 | MF | 129 | CYS |
| 40 | MF | 130 | THR |
| 40 | MF | 137 | ILE |
| 40 | MF | 139 | HIS |
| 40 | MF | 145 | THR |
| 40 | MF | 152 | LEU |
| 40 | MF | 153 | LEU |
| 40 | MF | 154 | MET |
| 40 | MF | 160 | ASP |
| 40 | MF | 163 | LYS |
| 40 | MF | 164 | LYS |
| 40 | MF | 165 | SER |
| 40 | MF | 166 | LYS |
| 40 | MF | 171 | ILE |
| 40 | MF | 177 | VAL |
| 40 | MF | 179 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MF | 187 | SER |
| 40 | MF | 196 | GLU |
| 40 | MF | 199 | ASP |
| 40 | MF | 204 | VAL |
| 40 | MF | 205 | ASP |
| 40 | MF | 209 | ILE |
| 40 | MF | 210 | TYR |
| 40 | MF | 221 | ARG |
| 40 | MF | 225 | THR |
| 40 | MF | 231 | ILE |
| 40 | MF | 234 | ILE |
| 40 | MF | 242 | LEU |
| 40 | MF | 243 | ARG |
| 40 | MF | 245 | ASP |
| 40 | MF | 251 | ASP |
| 40 | MF | 256 | GLN |
| 40 | MF | 257 | THR |
| 40 | MF | 259 | LEU |
| 40 | MF | 271 | THR |
| 40 | MF | 275 | VAL |
| 40 | MF | 276 | ILE |
| 40 | MF | 279 | GLU |
| 40 | MF | 285 | GLN |
| 40 | MF | 295 | CYS |
| 40 | MF | 305 | CYS |
| 40 | MF | 308 | ARG |
| 40 | MF | 311 | LYS |
| 40 | MF | 317 | LEU |
| 40 | MF | 318 | LEU |
| 40 | MF | 320 | ARG |
| 40 | MF | 327 | ASP |
| 40 | MF | 340 | SER |
| 40 | MF | 352 | LYS |
| 40 | MF | 355 | ILE |
| 40 | MF | 363 | VAL |
| 40 | MF | 366 | ASP |
| 40 | MF | 367 | LEU |
| 40 | MF | 374 | VAL |
| 40 | MF | 375 | CYS |
| 40 | MF | 378 | SER |
| 40 | MF | 400 | LYS |
| 40 | MF | 401 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MF | 408 | VAL |
| 40 | MF | 424 | MET |
| 40 | MF | 436 | MET |
| 40 | MF | 438 | SER |
| 40 | MG | 1 | GLN |
| 40 | MG | 6 | SER |
| 40 | MG | 7 | VAL |
| 40 | MG | 11 | GLN |
| 40 | MG | 15 | GLN |
| 40 | MG | 23 | LEU |
| 40 | MG | 26 | LEU |
| 40 | MG | 35 | GLN |
| 40 | MG | 68 | VAL |
| 40 | MG | 71 | GLU |
| 40 | MG | 75 | ILE |
| 40 | MG | 77 | GLU |
| 40 | MG | 80 | THR |
| 40 | MG | 84 | ARG |
| 40 | MG | 85 | GLN |
| 40 | MG | 92 | LEU |
| 40 | MG | 94 | THR |
| 40 | MG | 96 | LYS |
| 40 | MG | 97 | GLU |
| 40 | MG | 98 | ASP |
| 40 | MG | 109 | THR |
| 40 | MG | 110 | ILE |
| 40 | MG | 113 | GLU |
| 40 | MG | 114 | LEU |
| 40 | MG | 116 | ASP |
| 40 | MG | 123 | ARG |
| 40 | MG | 124 | LYS |
| 40 | MG | 141 | PHE |
| 40 | MG | 158 | SER |
| 40 | MG | 160 | ASP |
| 40 | MG | 163 | LYS |
| 40 | MG | 165 | SER |
| 40 | MG | 166 | LYS |
| 40 | MG | 170 | SER |
| 40 | MG | 181 | VAL |
| 40 | MG | 187 | SER |
| 40 | MG | 188 | ILE |
| 40 | MG | 191 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MG | 193 | THR |
| 40 | MG | 198 | SER |
| 40 | MG | 200 | CYS |
| 40 | MG | 205 | ASP |
| 40 | MG | 217 | LEU |
| 40 | MG | 218 | ASP |
| 40 | MG | 238 | ILE |
| 40 | MG | 245 | ASP |
| 40 | MG | 249 | ASN |
| 40 | MG | 250 | VAL |
| 40 | MG | 256 | GLN |
| 40 | MG | 258 | ASN |
| 40 | MG | 259 | LEU |
| 40 | MG | 264 | ARG |
| 40 | MG | 271 | THR |
| 40 | MG | 274 | PRO |
| 40 | MG | 275 | VAL |
| 40 | MG | 276 | ILE |
| 40 | MG | 279 | GLU |
| 40 | MG | 280 | LYS |
| 40 | MG | 287 | SER |
| 40 | MG | 295 | CYS |
| 40 | MG | 302 | MET |
| 40 | MG | 303 | VAL |
| 40 | MG | 304 | LYS |
| 40 | MG | 305 | CYS |
| 40 | MG | 308 | ARG |
| 40 | MG | 315 | CYS |
| 40 | MG | 317 | LEU |
| 40 | MG | 323 | VAL |
| 40 | MG | 324 | VAL |
| 40 | MG | 326 | LYS |
| 40 | MG | 332 | ILE |
| 40 | MG | 340 | SER |
| 40 | MG | 341 | ILE |
| 40 | MG | 343 | PHE |
| 40 | MG | 352 | LYS |
| 40 | MG | 356 | ASN |
| 40 | MG | 362 | VAL |
| 40 | MG | 363 | VAL |
| 40 | MG | 366 | ASP |
| 40 | MG | 369 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MG | 375 | CYS |
| 40 | MG | 381 | THR |
| 40 | MG | 385 | GLU |
| 40 | MG | 390 | LEU |
| 40 | MG | 391 | ASP |
| 40 | MG | 400 | LYS |
| 40 | MG | 401 | ARG |
| 40 | MG | 412 | MET |
| 40 | MG | 416 | GLU |
| 40 | MG | 419 | GLU |
| 40 | MG | 423 | ASP |
| 40 | MG | 428 | GLU |
| 40 | MG | 429 | LYS |
| 40 | MG | 438 | SER |
| 40 | MG | 439 | VAL |
| 40 | MH | 2 | ARG |
| 40 | MH | 4 | CYS |
| 40 | MH | 7 | VAL |
| 40 | MH | 9 | VAL |
| 40 | MH | 22 | GLU |
| 40 | MH | 26 | LEU |
| 40 | MH | 36 | MET |
| 40 | MH | 54 | SER |
| 40 | MH | 56 | THR |
| 40 | MH | 60 | LYS |
| 40 | MH | 62 | VAL |
| 40 | MH | 68 | VAL |
| 40 | MH | 71 | GLU |
| 40 | MH | 73 | THR |
| 40 | MH | 74 | VAL |
| 40 | MH | 76 | ASP |
| 40 | MH | 80 | THR |
| 40 | MH | 82 | THR |
| 40 | MH | 84 | ARG |
| 40 | MH | 94 | THR |
| 40 | MH | 96 | LYS |
| 40 | MH | 97 | GLU |
| 40 | MH | 105 | ARG |
| 40 | MH | 112 | LYS |
| 40 | MH | 113 | GLU |
| 40 | MH | 117 | LEU |
| 40 | MH | 120 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MH | 121 | ARG |
| 40 | MH | 123 | ARG |
| 40 | MH | 133 | GLN |
| 40 | MH | 137 | ILE |
| 40 | MH | 139 | HIS |
| 40 | MH | 145 | THR |
| 40 | MH | 153 | LEU |
| 40 | MH | 157 | LEU |
| 40 | MH | 165 | SER |
| 40 | MH | 166 | LYS |
| 40 | MH | 168 | GLU |
| 40 | MH | 170 | SER |
| 40 | MH | 171 | ILE |
| 40 | MH | 181 | VAL |
| 40 | MH | 182 | VAL |
| 40 | MH | 187 | SER |
| 40 | MH | 193 | THR |
| 40 | MH | 200 | CYS |
| 40 | MH | 203 | MET |
| 40 | MH | 205 | ASP |
| 40 | MH | 209 | ILE |
| 40 | MH | 227 | LEU |
| 40 | MH | 228 | ASN |
| 40 | MH | 231 | ILE |
| 40 | MH | 248 | LEU |
| 40 | MH | 249 | ASN |
| 40 | MH | 251 | ASP |
| 40 | MH | 256 | GLN |
| 40 | MH | 257 | THR |
| 40 | MH | 259 | LEU |
| 40 | MH | 264 | ARG |
| 40 | MH | 271 | THR |
| 40 | MH | 276 | ILE |
| 40 | MH | 279 | GLU |
| 40 | MH | 280 | LYS |
| 40 | MH | 282 | TYR |
| 40 | MH | 285 | GLN |
| 40 | MH | 288 | VAL |
| 40 | MH | 295 | CYS |
| 40 | MH | 297 | GLU |
| 40 | MH | 302 | MET |
| 40 | MH | 303 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | MH | 305 | CYS |
| 40 | MH | 320 | ARG |
| 40 | MH | 338 | LYS |
| 40 | MH | 339 | ARG |
| 40 | MH | 341 | ILE |
| 40 | MH | 358 | GLN |
| 40 | MH | 366 | ASP |
| 40 | MH | 367 | LEU |
| 40 | MH | 369 | LYS |
| 40 | MH | 374 | VAL |
| 40 | MH | 381 | THR |
| 40 | MH | 383 | ILE |
| 40 | MH | 389 | ARG |
| 40 | MH | 391 | ASP |
| 40 | MH | 401 | ARG |
| 40 | MH | 410 | GLU |
| 40 | MH | 418 | SER |
| 40 | MH | 419 | GLU |
| 40 | MH | 421 | ARG |
| 40 | MH | 429 | LYS |
| 40 | MH | 432 | GLU |
| 40 | MH | 437 | ASP |
| 41 | MN | 354 | CYS |
| 41 | MN | 359 | ARG |
| 41 | MN | 362 | LYS |
| 41 | MN | 363 | MET |
| 41 | MN | 364 | SER |
| 41 | MO | 4 | ILE |
| 41 | MO | 7 | LEU |
| 41 | MO | 19 | LYS |
| 41 | MO | 22 | GLU |
| 41 | MO | 26 | ASP |
| 41 | MO | 31 | ASP |
| 41 | MO | 35 | THR |
| 41 | MO | 39 | ASP |
| 41 | MO | 40 | SER |
| 41 | MO | 47 | ILE |
| 41 | MO | 53 | GLU |
| 41 | MO | 55 | THR |
| 41 | MO | 58 | LYS |
| 41 | MO | 67 | ASP |
| 41 | MO | 70 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | MO | 83 | GLN |
| 41 | MO | 88 | ASP |
| 41 | MO | 91 | VAL |
| 41 | MO | 103 | LYS |
| 41 | MO | 107 | THR |
| 41 | MO | 111 | GLU |
| 41 | MO | 112 | LEU |
| 41 | MO | 114 | ASP |
| 41 | MO | 115 | SER |
| 41 | MO | 122 | LYS |
| 41 | MO | 129 | CYS |
| 41 | MO | 135 | LEU |
| 41 | MO | 137 | HIS |
| 41 | MO | 139 | LEU |
| 41 | MO | 153 | SER |
| 41 | MO | 154 | LYS |
| 41 | MO | 156 | ARG |
| 41 | MO | 159 | TYR |
| 41 | MO | 161 | ASP |
| 41 | MO | 162 | ARG |
| 41 | MO | 163 | ILE |
| 41 | MO | 166 | THR |
| 41 | MO | 168 | SER |
| 41 | MO | 170 | VAL |
| 41 | MO | 180 | VAL |
| 41 | MO | 188 | SER |
| 41 | MO | 202 | ILE |
| 41 | MO | 203 | ASP |
| 41 | MO | 205 | GLU |
| 41 | MO | 212 | PHE |
| 41 | MO | 213 | ARG |
| 41 | MO | 217 | LEU |
| 41 | MO | 219 | THR |
| 41 | MO | 222 | TYR |
| 41 | MO | 228 | LEU |
| 41 | MO | 233 | MET |
| 41 | MO | 237 | THR |
| 41 | MO | 240 | LEU |
| 41 | MO | 241 | ARG |
| 41 | MO | 245 | GLN |
| 41 | MO | 252 | LYS |
| 41 | MO | 253 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | MO | 261 | PRO |
| 41 | MO | 262 | ARG |
| 41 | MO | 264 | HIS |
| 41 | MO | 270 | PHE |
| 41 | MO | 273 | LEU |
| 41 | MO | 275 | SER |
| 41 | MO | 276 | ARG |
| 41 | MO | 282 | ARG |
| 41 | MO | 286 | VAL |
| 41 | MO | 288 | GLU |
| 41 | MO | 291 | GLN |
| 41 | MO | 295 | ASP |
| 41 | MO | 309 | ARG |
| 41 | MO | 311 | LEU |
| 41 | MO | 312 | THR |
| 41 | MO | 321 | MET |
| 41 | MO | 322 | SER |
| 41 | MO | 324 | LYS |
| 41 | MO | 333 | VAL |
| 41 | MO | 336 | LYS |
| 41 | MO | 348 | ASN |
| 41 | MO | 350 | LYS |
| 41 | MO | 353 | VAL |
| 41 | MO | 362 | LYS |
| 41 | MO | 363 | MET |
| 41 | MO | 364 | SER |
| 41 | MO | 370 | ASN |
| 41 | MO | 371 | SER |
| 41 | MO | 372 | THR |
| 41 | MO | 391 | ARG |
| 41 | MO | 397 | TRP |
| 41 | MO | 401 | GLU |
| 41 | MO | 403 | MET |
| 41 | MO | 404 | ASP |
| 41 | MO | 406 | MET |
| 41 | MO | 415 | MET |
| 41 | MO | 425 | ARG |
| 41 | MO | 428 | CYS |
| 41 | MP | 52 | ASN |
| 41 | MP | 262 | ARG |
| 41 | NB | 2 | ARG |
| 41 | NB | 83 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | NB | 306 | ARG |
| 40 | ND | 1 | GLN |
| 40 | ND | 2 | ARG |
| 40 | ND | 3 | GLU |
| 40 | ND | 7 | VAL |
| 40 | ND | 11 | GLN |
| 40 | ND | 22 | GLU |
| 40 | ND | 25 | CYS |
| 40 | ND | 26 | LEU |
| 40 | ND | 31 | GLN |
| 40 | ND | 33 | ASP |
| 40 | ND | 36 | MET |
| 40 | ND | 48 | SER |
| 40 | ND | 51 | THR |
| 40 | ND | 52 | PHE |
| 40 | ND | 54 | SER |
| 40 | ND | 56 | THR |
| 40 | ND | 61 | HIS |
| 40 | ND | 62 | VAL |
| 40 | ND | 66 | VAL |
| 40 | ND | 75 | ILE |
| 40 | ND | 79 | ARG |
| 40 | ND | 84 | ARG |
| 40 | ND | 87 | PHE |
| 40 | ND | 92 | LEU |
| 40 | ND | 93 | ILE |
| 40 | ND | 96 | LYS |
| 40 | ND | 105 | ARG |
| 40 | ND | 109 | THR |
| 40 | ND | 110 | ILE |
| 40 | ND | 112 | LYS |
| 40 | ND | 114 | LEU |
| 40 | ND | 116 | ASP |
| 40 | ND | 119 | LEU |
| 40 | ND | 120 | ASP |
| 40 | ND | 124 | LYS |
| 40 | ND | 127 | ASP |
| 40 | ND | 128 | GLN |
| 40 | ND | 129 | CYS |
| 40 | ND | 132 | LEU |
| 40 | ND | 133 | GLN |
| 40 | ND | 136 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | ND | 137 | ILE |
| 40 | ND | 139 | HIS |
| 40 | ND | 140 | SER |
| 40 | ND | 157 | LEU |
| 40 | ND | 163 | LYS |
| 40 | ND | 164 | LYS |
| 40 | ND | 166 | LYS |
| 40 | ND | 172 | TYR |
| 40 | ND | 179 | THR |
| 40 | ND | 181 | VAL |
| 40 | ND | 183 | GLU |
| 40 | ND | 186 | ASN |
| 40 | ND | 190 | THR |
| 40 | ND | 195 | LEU |
| 40 | ND | 199 | ASP |
| 40 | ND | 200 | CYS |
| 40 | ND | 203 | MET |
| 40 | ND | 205 | ASP |
| 40 | ND | 206 | ASN |
| 40 | ND | 209 | ILE |
| 40 | ND | 211 | ASP |
| 40 | ND | 220 | GLU |
| 40 | ND | 221 | ARG |
| 40 | ND | 223 | THR |
| 40 | ND | 224 | TYR |
| 40 | ND | 225 | THR |
| 40 | ND | 226 | ASN |
| 40 | ND | 229 | ARG |
| 40 | ND | 231 | ILE |
| 40 | ND | 238 | ILE |
| 40 | ND | 248 | LEU |
| 40 | ND | 252 | LEU |
| 40 | ND | 256 | GLN |
| 40 | ND | 265 | ILE |
| 40 | ND | 269 | LEU |
| 40 | ND | 274 | PRO |
| 40 | ND | 275 | VAL |
| 40 | ND | 276 | ILE |
| 40 | ND | 284 | GLU |
| 40 | ND | 285 | GLN |
| 40 | ND | 286 | LEU |
| 40 | ND | 290 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | ND | 295 | CYS |
| 40 | ND | 303 | VAL |
| 40 | ND | 305 | CYS |
| 40 | ND | 308 | ARG |
| 40 | ND | 311 | LYS |
| 40 | ND | 315 | CYS |
| 40 | ND | 316 | CYS |
| 40 | ND | 320 | ARG |
| 40 | ND | 323 | VAL |
| 40 | ND | 324 | VAL |
| 40 | ND | 326 | LYS |
| 40 | ND | 338 | LYS |
| 40 | ND | 339 | ARG |
| 40 | ND | 347 | CYS |
| 40 | ND | 349 | THR |
| 40 | ND | 352 | LYS |
| 40 | ND | 356 | ASN |
| 40 | ND | 358 | GLN |
| 40 | ND | 362 | VAL |
| 40 | ND | 363 | VAL |
| 40 | ND | 367 | LEU |
| 40 | ND | 369 | LYS |
| 40 | ND | 370 | VAL |
| 40 | ND | 375 | CYS |
| 40 | ND | 376 | MET |
| 40 | ND | 377 | LEU |
| 40 | ND | 378 | SER |
| 40 | ND | 379 | ASN |
| 40 | ND | 385 | GLU |
| 40 | ND | 395 | ASP |
| 40 | ND | 397 | MET |
| 40 | ND | 398 | TYR |
| 40 | ND | 401 | ARG |
| 40 | ND | 404 | VAL |
| 40 | ND | 413 | GLU |
| 40 | ND | 416 | GLU |
| 40 | ND | 418 | SER |
| 40 | ND | 421 | ARG |
| 40 | ND | 422 | GLU |
| 40 | ND | 428 | GLU |
| 40 | ND | 429 | LYS |
| 40 | ND | 436 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | ND | 438 | SER |
| 40 | ND | 439 | VAL |
| 40 | ND | 440 | GLU |
| 40 | NF | 226 | ASN |
| 40 | NG | 11 | GLN |
| 40 | NG | 326 | LYS |
| 41 | NL | 174 | LYS |
| 41 | NL | 306 | ARG |
| 41 | NL | 359 | ARG |
| 41 | NM | 105 | HIS |
| 41 | NM | 359 | ARG |
| 41 | NN | 2 | ARG |
| 41 | NO | 122 | LYS |
| 41 | NP | 282 | ARG |
| 41 | NP | 306 | ARG |
| 41 | NP | 359 | ARG |
| 41 | NP | 388 | MET |
| 40 | OA | 214 | ARG |
| 40 | OD | 76 | ASP |
| 40 | OD | 77 | GLU |
| 40 | OD | 79 | ARG |
| 40 | OD | 82 | THR |
| 40 | OD | 84 | ARG |
| 40 | OD | 86 | LEU |
| 40 | OD | 166 | LYS |
| 40 | OD | 429 | LYS |
| 40 | OE | 3 | GLU |
| 40 | OE | 6 | SER |
| 40 | OE | 369 | LYS |
| 40 | OF | 2 | ARG |
| 40 | OF | 285 | GLN |
| 40 | OG | 308 | ARG |
| 40 | OG | 369 | LYS |
| 40 | OH | 2 | ARG |
| 40 | OH | 3 | GLU |
| 40 | OH | 4 | CYS |
| 40 | OH | 11 | GLN |
| 40 | OH | 15 | GLN |
| 40 | OH | 20 | CYS |
| 40 | OH | 23 | LEU |
| 40 | OH | 26 | LEU |
| 40 | OH | 27 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OH | 33 | ASP |
| 40 | OH | 36 | MET |
| 40 | OH | 38 | SER |
| 40 | OH | 40 | LYS |
| 40 | OH | 51 | THR |
| 40 | OH | 55 | GLU |
| 40 | OH | 60 | LYS |
| 40 | OH | 62 | VAL |
| 40 | OH | 66 | VAL |
| 40 | OH | 68 | VAL |
| 40 | OH | 69 | ASP |
| 40 | OH | 70 | LEU |
| 40 | OH | 73 | THR |
| 40 | OH | 79 | ARG |
| 40 | OH | 84 | ARG |
| 40 | OH | 85 | GLN |
| 40 | OH | 86 | LEU |
| 40 | OH | 90 | GLU |
| 40 | OH | 91 | GLN |
| 40 | OH | 92 | LEU |
| 40 | OH | 93 | ILE |
| 40 | OH | 94 | THR |
| 40 | OH | 96 | LYS |
| 40 | OH | 97 | GLU |
| 40 | OH | 105 | ARG |
| 40 | OH | 108 | TYR |
| 40 | OH | 110 | ILE |
| 40 | OH | 112 | LYS |
| 40 | OH | 113 | GLU |
| 40 | OH | 114 | LEU |
| 40 | OH | 119 | LEU |
| 40 | OH | 120 | ASP |
| 40 | OH | 128 | GLN |
| 40 | OH | 129 | CYS |
| 40 | OH | 133 | GLN |
| 40 | OH | 151 | SER |
| 40 | OH | 152 | LEU |
| 40 | OH | 154 | MET |
| 40 | OH | 156 | ARG |
| 40 | OH | 164 | LYS |
| 40 | OH | 166 | LYS |
| 40 | OH | 167 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OH | 168 | GLU |
| 40 | OH | 170 | SER |
| 40 | OH | 176 | GLN |
| 40 | OH | 177 | VAL |
| 40 | OH | 178 | SER |
| 40 | OH | 183 | GLU |
| 40 | OH | 186 | ASN |
| 40 | OH | 187 | SER |
| 40 | OH | 190 | THR |
| 40 | OH | 192 | HIS |
| 40 | OH | 194 | THR |
| 40 | OH | 195 | LEU |
| 40 | OH | 204 | VAL |
| 40 | OH | 206 | ASN |
| 40 | OH | 209 | ILE |
| 40 | OH | 212 | ILE |
| 40 | OH | 214 | ARG |
| 40 | OH | 217 | LEU |
| 40 | OH | 218 | ASP |
| 40 | OH | 219 | ILE |
| 40 | OH | 220 | GLU |
| 40 | OH | 222 | PRO |
| 40 | OH | 223 | THR |
| 40 | OH | 224 | TYR |
| 40 | OH | 228 | ASN |
| 40 | OH | 234 | ILE |
| 40 | OH | 241 | SER |
| 40 | OH | 242 | LEU |
| 40 | OH | 243 | ARG |
| 40 | OH | 248 | LEU |
| 40 | OH | 251 | ASP |
| 40 | OH | 252 | LEU |
| 40 | OH | 253 | THR |
| 40 | OH | 254 | GLU |
| 40 | OH | 256 | GLN |
| 40 | OH | 265 | ILE |
| 40 | OH | 272 | TYR |
| 40 | OH | 275 | VAL |
| 40 | OH | 276 | ILE |
| 40 | OH | 279 | GLU |
| 40 | OH | 284 | GLU |
| 40 | OH | 285 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OH | 286 | LEU |
| 40 | OH | 287 | SER |
| 40 | OH | 288 | VAL |
| 40 | OH | 300 | ASN |
| 40 | OH | 301 | GLN |
| 40 | OH | 303 | VAL |
| 40 | OH | 304 | LYS |
| 40 | OH | 305 | CYS |
| 40 | OH | 311 | LYS |
| 40 | OH | 313 | MET |
| 40 | OH | 315 | CYS |
| 40 | OH | 316 | CYS |
| 40 | OH | 317 | LEU |
| 40 | OH | 318 | LEU |
| 40 | OH | 320 | ARG |
| 40 | OH | 323 | VAL |
| 40 | OH | 326 | LYS |
| 40 | OH | 327 | ASP |
| 40 | OH | 339 | ARG |
| 40 | OH | 344 | VAL |
| 40 | OH | 345 | ASP |
| 40 | OH | 355 | ILE |
| 40 | OH | 358 | GLN |
| 40 | OH | 362 | VAL |
| 40 | OH | 363 | VAL |
| 40 | OH | 367 | LEU |
| 40 | OH | 369 | LYS |
| 40 | OH | 370 | VAL |
| 40 | OH | 372 | ARG |
| 40 | OH | 374 | VAL |
| 40 | OH | 383 | ILE |
| 40 | OH | 389 | ARG |
| 40 | OH | 390 | LEU |
| 40 | OH | 391 | ASP |
| 40 | OH | 393 | LYS |
| 40 | OH | 396 | LEU |
| 40 | OH | 398 | TYR |
| 40 | OH | 400 | LYS |
| 40 | OH | 401 | ARG |
| 40 | OH | 404 | VAL |
| 40 | OH | 408 | VAL |
| 40 | OH | 410 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OH | 412 | MET |
| 40 | OH | 422 | GLU |
| 40 | OH | 423 | ASP |
| 40 | OH | 429 | LYS |
| 40 | OH | 432 | GLU |
| 40 | OH | 434 | VAL |
| 40 | OH | 436 | MET |
| 40 | OH | 438 | SER |
| 40 | OH | 439 | VAL |
| 40 | OH | 440 | GLU |
| 41 | OM | 162 | ARG |
| 41 | OM | 306 | ARG |
| 41 | OM | 414 | ASN |
| 41 | ON | 99 | ASN |
| 41 | ON | 204 | ASN |
| 41 | ON | 306 | ARG |
| 41 | ON | 321 | MET |
| 41 | OP | 291 | GLN |
| 41 | PB | 7 | LEU |
| 41 | PB | 8 | GLN |
| 41 | PB | 337 | ASN |
| 41 | PB | 347 | ASN |
| 40 | PD | 320 | ARG |
| 40 | PE | 226 | ASN |
| 40 | PE | 264 | ARG |
| 40 | PE | 392 | HIS |
| 41 | PL | 306 | ARG |
| 41 | PN | 276 | ARG |
| 41 | PN | 362 | LYS |
| 40 | QA | 2 | ARG |
| 40 | QA | 79 | ARG |
| 40 | QA | 389 | ARG |
| 41 | QB | 1 | MET |
| 41 | QB | 2 | ARG |
| 41 | QB | 4 | ILE |
| 41 | QB | 7 | LEU |
| 41 | QB | 8 | GLN |
| 41 | QB | 12 | CYS |
| 41 | QB | 14 | ASN |
| 41 | QB | 16 | ILE |
| 41 | QB | 19 | LYS |
| 41 | QB | 20 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QB | 21 | TRP |
| 41 | QB | 22 | GLU |
| 41 | QB | 24 | ILE |
| 41 | QB | 26 | ASP |
| 41 | QB | 27 | GLU |
| 41 | QB | 31 | ASP |
| 41 | QB | 36 | TYR |
| 41 | QB | 39 | ASP |
| 41 | QB | 40 | SER |
| 41 | QB | 42 | LEU |
| 41 | QB | 44 | LEU |
| 41 | QB | 47 | ILE |
| 41 | QB | 49 | VAL |
| 41 | QB | 62 | ARG |
| 41 | QB | 64 | VAL |
| 41 | QB | 65 | LEU |
| 41 | QB | 72 | THR |
| 41 | QB | 73 | MET |
| 41 | QB | 74 | ASP |
| 41 | QB | 75 | SER |
| 41 | QB | 77 | ARG |
| 41 | QB | 78 | SER |
| 41 | QB | 91 | VAL |
| 41 | QB | 92 | PHE |
| 41 | QB | 94 | GLN |
| 41 | QB | 101 | TRP |
| 41 | QB | 103 | LYS |
| 41 | QB | 108 | GLU |
| 41 | QB | 111 | GLU |
| 41 | QB | 112 | LEU |
| 41 | QB | 113 | VAL |
| 41 | QB | 115 | SER |
| 41 | QB | 118 | ASP |
| 41 | QB | 121 | ARG |
| 41 | QB | 122 | LYS |
| 41 | QB | 125 | GLU |
| 41 | QB | 126 | SER |
| 41 | QB | 128 | ASP |
| 41 | QB | 131 | GLN |
| 41 | QB | 135 | LEU |
| 41 | QB | 137 | HIS |
| 41 | QB | 147 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QB | 149 | THR |
| 41 | QB | 150 | LEU |
| 41 | QB | 156 | ARG |
| 41 | QB | 161 | ASP |
| 41 | QB | 162 | ARG |
| 41 | QB | 163 | ILE |
| 41 | QB | 164 | MET |
| 41 | QB | 166 | THR |
| 41 | QB | 174 | LYS |
| 41 | QB | 179 | VAL |
| 41 | QB | 182 | PRO |
| 41 | QB | 192 | LEU |
| 41 | QB | 194 | GLU |
| 41 | QB | 198 | GLU |
| 41 | QB | 200 | TYR |
| 41 | QB | 211 | CYS |
| 41 | QB | 212 | PHE |
| 41 | QB | 213 | ARG |
| 41 | QB | 216 | LYS |
| 41 | QB | 221 | THR |
| 41 | QB | 224 | ASP |
| 41 | QB | 226 | ASN |
| 41 | QB | 227 | HIS |
| 41 | QB | 229 | VAL |
| 41 | QB | 232 | THR |
| 41 | QB | 233 | MET |
| 41 | QB | 238 | THR |
| 41 | QB | 240 | LEU |
| 41 | QB | 241 | ARG |
| 41 | QB | 246 | LEU |
| 41 | QB | 249 | ASP |
| 41 | QB | 251 | ARG |
| 41 | QB | 252 | LYS |
| 41 | QB | 253 | LEU |
| 41 | QB | 262 | ARG |
| 41 | QB | 263 | LEU |
| 41 | QB | 264 | HIS |
| 41 | QB | 266 | PHE |
| 41 | QB | 270 | PHE |
| 41 | QB | 273 | LEU |
| 41 | QB | 275 | SER |
| 41 | QB | 279 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QB | 280 | GLN |
| 41 | QB | 291 | GLN |
| 41 | QB | 292 | GLN |
| 41 | QB | 293 | MET |
| 41 | QB | 294 | PHE |
| 41 | QB | 295 | ASP |
| 41 | QB | 300 | MET |
| 41 | QB | 304 | ASP |
| 41 | QB | 306 | ARG |
| 41 | QB | 309 | ARG |
| 41 | QB | 311 | LEU |
| 41 | QB | 312 | THR |
| 41 | QB | 316 | VAL |
| 41 | QB | 320 | ARG |
| 41 | QB | 321 | MET |
| 41 | QB | 324 | LYS |
| 41 | QB | 330 | MET |
| 41 | QB | 331 | LEU |
| 41 | QB | 336 | LYS |
| 41 | QB | 337 | ASN |
| 41 | QB | 343 | GLU |
| 41 | QB | 345 | ILE |
| 41 | QB | 347 | ASN |
| 41 | QB | 349 | VAL |
| 41 | QB | 350 | LYS |
| 41 | QB | 351 | THR |
| 41 | QB | 359 | ARG |
| 41 | QB | 362 | LYS |
| 41 | QB | 366 | THR |
| 41 | QB | 368 | ILE |
| 41 | QB | 375 | GLN |
| 41 | QB | 377 | LEU |
| 41 | QB | 379 | LYS |
| 41 | QB | 380 | ARG |
| 41 | QB | 383 | GLU |
| 41 | QB | 388 | MET |
| 41 | QB | 389 | PHE |
| 41 | QB | 390 | ARG |
| 41 | QB | 391 | ARG |
| 41 | QB | 392 | LYS |
| 41 | QB | 397 | TRP |
| 41 | QB | 398 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QB | 406 | MET |
| 41 | QB | 407 | GLU |
| 41 | QB | 415 | MET |
| 41 | QB | 418 | LEU |
| 41 | QB | 425 | ARG |
| 41 | QB | 428 | CYS |
| 40 | QE | 2 | ARG |
| 40 | QE | 226 | ASN |
| 40 | QF | 214 | ARG |
| 40 | QH | 221 | ARG |
| 41 | QL | 58 | LYS |
| 41 | QL | 256 | ASN |
| 41 | QL | 348 | ASN |
| 41 | QL | 359 | ARG |
| 41 | QM | 390 | ARG |
| 41 | QN | 334 | GLN |
| 41 | QP | 1 | MET |
| 41 | QP | 4 | ILE |
| 41 | QP | 7 | LEU |
| 41 | QP | 16 | ILE |
| 41 | QP | 19 | LYS |
| 41 | QP | 22 | GLU |
| 41 | QP | 25 | SER |
| 41 | QP | 33 | THR |
| 41 | QP | 40 | SER |
| 41 | QP | 42 | LEU |
| 41 | QP | 46 | ARG |
| 41 | QP | 47 | ILE |
| 41 | QP | 50 | TYR |
| 41 | QP | 53 | GLU |
| 41 | QP | 58 | LYS |
| 41 | QP | 62 | ARG |
| 41 | QP | 65 | LEU |
| 41 | QP | 68 | LEU |
| 41 | QP | 69 | GLU |
| 41 | QP | 73 | MET |
| 41 | QP | 74 | ASP |
| 41 | QP | 84 | ILE |
| 41 | QP | 86 | ARG |
| 41 | QP | 88 | ASP |
| 41 | QP | 90 | PHE |
| 41 | QP | 91 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QP | 92 | PHE |
| 41 | QP | 99 | ASN |
| 41 | QP | 103 | LYS |
| 41 | QP | 106 | TYR |
| 41 | QP | 115 | SER |
| 41 | QP | 118 | ASP |
| 41 | QP | 121 | ARG |
| 41 | QP | 123 | GLU |
| 41 | QP | 125 | GLU |
| 41 | QP | 131 | GLN |
| 41 | QP | 135 | LEU |
| 41 | QP | 138 | SER |
| 41 | QP | 139 | LEU |
| 41 | QP | 147 | MET |
| 41 | QP | 149 | THR |
| 41 | QP | 150 | LEU |
| 41 | QP | 151 | LEU |
| 41 | QP | 152 | ILE |
| 41 | QP | 154 | LYS |
| 41 | QP | 158 | GLU |
| 41 | QP | 159 | TYR |
| 41 | QP | 162 | ARG |
| 41 | QP | 165 | ASN |
| 41 | QP | 167 | PHE |
| 41 | QP | 170 | VAL |
| 41 | QP | 172 | SER |
| 41 | QP | 174 | LYS |
| 41 | QP | 179 | VAL |
| 41 | QP | 180 | VAL |
| 41 | QP | 181 | GLU |
| 41 | QP | 183 | TYR |
| 41 | QP | 184 | ASN |
| 41 | QP | 188 | SER |
| 41 | QP | 192 | LEU |
| 41 | QP | 194 | GLU |
| 41 | QP | 199 | THR |
| 41 | QP | 204 | ASN |
| 41 | QP | 207 | LEU |
| 41 | QP | 211 | CYS |
| 41 | QP | 213 | ARG |
| 41 | QP | 216 | LYS |
| 41 | QP | 225 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QP | 227 | HIS |
| 41 | QP | 232 | THR |
| 41 | QP | 236 | VAL |
| 41 | QP | 237 | THR |
| 41 | QP | 238 | THR |
| 41 | QP | 239 | CYS |
| 41 | QP | 240 | LEU |
| 41 | QP | 242 | PHE |
| 41 | QP | 250 | LEU |
| 41 | QP | 262 | ARG |
| 41 | QP | 263 | LEU |
| 41 | QP | 264 | HIS |
| 41 | QP | 266 | PHE |
| 41 | QP | 267 | MET |
| 41 | QP | 275 | SER |
| 41 | QP | 276 | ARG |
| 41 | QP | 279 | GLN |
| 41 | QP | 282 | ARG |
| 41 | QP | 284 | LEU |
| 41 | QP | 285 | THR |
| 41 | QP | 289 | LEU |
| 41 | QP | 290 | THR |
| 41 | QP | 291 | GLN |
| 41 | QP | 293 | MET |
| 41 | QP | 295 | ASP |
| 41 | QP | 297 | LYS |
| 41 | QP | 298 | ASN |
| 41 | QP | 300 | MET |
| 41 | QP | 303 | CYS |
| 41 | QP | 306 | ARG |
| 41 | QP | 311 | LEU |
| 41 | QP | 312 | THR |
| 41 | QP | 313 | VAL |
| 41 | QP | 318 | ARG |
| 41 | QP | 320 | ARG |
| 41 | QP | 323 | MET |
| 41 | QP | 324 | LYS |
| 41 | QP | 327 | ASP |
| 41 | QP | 330 | MET |
| 41 | QP | 331 | LEU |
| 41 | QP | 335 | ASN |
| 41 | QP | 336 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QP | 337 | ASN |
| 41 | QP | 342 | VAL |
| 41 | QP | 343 | GLU |
| 41 | QP | 345 | ILE |
| 41 | QP | 350 | LYS |
| 41 | QP | 353 | VAL |
| 41 | QP | 356 | ILE |
| 41 | QP | 359 | ARG |
| 41 | QP | 361 | LEU |
| 41 | QP | 362 | LYS |
| 41 | QP | 363 | MET |
| 41 | QP | 368 | ILE |
| 41 | QP | 372 | THR |
| 41 | QP | 374 | ILE |
| 41 | QP | 375 | GLN |
| 41 | QP | 376 | GLU |
| 41 | QP | 377 | LEU |
| 41 | QP | 379 | LYS |
| 41 | QP | 380 | ARG |
| 41 | QP | 381 | ILE |
| 41 | QP | 383 | GLU |
| 41 | QP | 388 | MET |
| 41 | QP | 391 | ARG |
| 41 | QP | 392 | LYS |
| 41 | QP | 406 | MET |
| 41 | QP | 410 | GLU |
| 41 | QP | 418 | LEU |
| 41 | QP | 425 | ARG |
| 40 | RA | 84 | ARG |
| 40 | RA | 233 | GLN |
| 40 | RA | 389 | ARG |
| 41 | RB | 121 | ARG |
| 41 | RB | 122 | LYS |
| 41 | RB | 359 | ARG |
| 40 | RE | 308 | ARG |
| 40 | RF | 2 | ARG |
| 40 | RG | 214 | ARG |
| 40 | RH | 308 | ARG |
| 40 | RH | 339 | ARG |
| 40 | RI | 264 | ARG |
| 40 | RI | 371 | GLN |
| 41 | RL | 2 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | RL | 216 | LYS |
| 41 | RL | 306 | ARG |
| 41 | RL | 359 | ARG |
| 41 | RN | 131 | GLN |
| 41 | RP | 306 | ARG |
| 41 | RP | 334 | GLN |
| 40 | SA | 239 | THR |
| 40 | SA | 242 | LEU |
| 40 | SA | 243 | ARG |
| 40 | SA | 244 | PHE |
| 40 | SA | 248 | LEU |
| 40 | SA | 249 | ASN |
| 40 | SA | 250 | VAL |
| 40 | SA | 256 | GLN |
| 40 | SA | 258 | ASN |
| 40 | SA | 260 | VAL |
| 40 | SA | 262 | TYR |
| 41 | SB | 276 | ARG |
| 41 | SB | 299 | MET |
| 41 | SB | 375 | GLN |
| 41 | SB | 377 | LEU |
| 41 | SB | 379 | LYS |
| 41 | SB | 383 | GLU |
| 41 | SB | 389 | PHE |
| 41 | SB | 391 | ARG |
| 41 | SB | 395 | LEU |
| 41 | SB | 401 | GLU |
| 41 | SB | 403 | MET |
| 41 | SB | 407 | GLU |
| 41 | SB | 409 | THR |
| 41 | SB | 410 | GLU |
| 41 | SB | 412 | GLU |
| 41 | SB | 415 | MET |
| 40 | SE | 342 | GLN |
| 40 | SE | 369 | LYS |
| 40 | SE | 372 | ARG |
| 40 | SF | 2 | ARG |
| 40 | SF | 128 | GLN |
| 40 | SF | 308 | ARG |
| 40 | SG | 249 | ASN |
| 40 | SG | 320 | ARG |
| 40 | SG | 372 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | SH | 372 | ARG |
| 41 | SL | 2 | ARG |
| 41 | SL | 276 | ARG |
| 41 | SM | 2 | ARG |
| 41 | SN | 337 | ASN |
| 41 | SO | 1 | MET |
| 41 | SO | 2 | ARG |
| 41 | SO | 3 | GLU |
| 41 | SO | 4 | ILE |
| 41 | SO | 5 | VAL |
| 41 | SO | 7 | LEU |
| 41 | SO | 12 | CYS |
| 41 | SO | 19 | LYS |
| 41 | SO | 35 | THR |
| 41 | SO | 40 | SER |
| 41 | SO | 42 | LEU |
| 41 | SO | 46 | ARG |
| 41 | SO | 49 | VAL |
| 41 | SO | 50 | TYR |
| 41 | SO | 53 | GLU |
| 41 | SO | 68 | LEU |
| 41 | SO | 73 | MET |
| 41 | SO | 74 | ASP |
| 41 | SO | 75 | SER |
| 41 | SO | 83 | GLN |
| 41 | SO | 86 | ARG |
| 41 | SO | 90 | PHE |
| 41 | SO | 91 | VAL |
| 41 | SO | 92 | PHE |
| 41 | SO | 103 | LYS |
| 41 | SO | 106 | TYR |
| 41 | SO | 107 | THR |
| 41 | SO | 108 | GLU |
| 41 | SO | 111 | GLU |
| 41 | SO | 117 | LEU |
| 41 | SO | 119 | VAL |
| 41 | SO | 121 | ARG |
| 41 | SO | 122 | LYS |
| 41 | SO | 138 | SER |
| 41 | SO | 143 | THR |
| 41 | SO | 145 | SER |
| 41 | SO | 154 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | SO | 156 | ARG |
| 41 | SO | 158 | GLU |
| 41 | SO | 164 | MET |
| 41 | SO | 170 | VAL |
| 41 | SO | 174 | LYS |
| 41 | SO | 176 | SER |
| 41 | SO | 177 | ASP |
| 41 | SO | 179 | VAL |
| 41 | SO | 180 | VAL |
| 41 | SO | 187 | LEU |
| 41 | SO | 192 | LEU |
| 41 | SO | 199 | THR |
| 41 | SO | 202 | ILE |
| 41 | SO | 203 | ASP |
| 41 | SO | 205 | GLU |
| 41 | SO | 208 | TYR |
| 41 | SO | 212 | PHE |
| 41 | SO | 213 | ARG |
| 41 | SO | 216 | LYS |
| 41 | SO | 217 | LEU |
| 41 | SO | 219 | THR |
| 41 | SO | 221 | THR |
| 41 | SO | 228 | LEU |
| 41 | SO | 233 | MET |
| 41 | SO | 238 | THR |
| 41 | SO | 240 | LEU |
| 41 | SO | 245 | GLN |
| 41 | SO | 246 | LEU |
| 41 | SO | 251 | ARG |
| 41 | SO | 252 | LYS |
| 41 | SO | 255 | VAL |
| 41 | SO | 258 | VAL |
| 41 | SO | 262 | ARG |
| 41 | SO | 267 | MET |
| 41 | SO | 274 | THR |
| 41 | SO | 275 | SER |
| 41 | SO | 276 | ARG |
| 41 | SO | 280 | GLN |
| 41 | SO | 288 | GLU |
| 41 | SO | 293 | MET |
| 41 | SO | 297 | LYS |
| 41 | SO | 299 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | SO | 306 | ARG |
| 41 | SO | 309 | ARG |
| 41 | SO | 310 | TYR |
| 41 | SO | 312 | THR |
| 41 | SO | 318 | ARG |
| 41 | SO | 320 | ARG |
| 41 | SO | 321 | MET |
| 41 | SO | 323 | MET |
| 41 | SO | 324 | LYS |
| 41 | SO | 331 | LEU |
| 41 | SO | 332 | ASN |
| 41 | SO | 334 | GLN |
| 41 | SO | 338 | SER |
| 41 | SO | 340 | TYR |
| 41 | SO | 341 | PHE |
| 41 | SO | 348 | ASN |
| 41 | SO | 349 | VAL |
| 41 | SO | 351 | THR |
| 41 | SO | 359 | ARG |
| 41 | SO | 362 | LYS |
| 41 | SO | 364 | SER |
| 41 | SO | 367 | PHE |
| 41 | SO | 380 | ARG |
| 41 | SO | 388 | MET |
| 41 | SO | 392 | LYS |
| 41 | SO | 396 | HIS |
| 41 | SO | 401 | GLU |
| 41 | SO | 404 | ASP |
| 41 | SO | 405 | GLU |
| 41 | SO | 406 | MET |
| 41 | SO | 409 | THR |
| 41 | SO | 410 | GLU |
| 41 | SO | 420 | ASN |
| 41 | SO | 425 | ARG |
| 41 | SP | 122 | LYS |
| 41 | SP | 359 | ARG |
| 40 | TA | 326 | LYS |
| 41 | TB | 52 | ASN |
| 41 | TB | 359 | ARG |
| 40 | TF | 2 | ARG |
| 40 | TF | 101 | ASN |
| 40 | TF | 429 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | TG | 124 | LYS |
| 40 | TG | 342 | GLN |
| 40 | TI | 2 | ARG |
| 40 | TI | 369 | LYS |
| 41 | TL | 306 | ARG |
| 41 | TL | 320 | ARG |
| 41 | TM | 2 | ARG |
| 41 | TM | 15 | GLN |
| 41 | TM | 280 | GLN |
| 41 | TM | 359 | ARG |
| 41 | TN | 2 | ARG |
| 41 | TN | 174 | LYS |
| 41 | TN | 329 | GLN |
| 41 | TN | 359 | ARG |
| 41 | TO | 2 | ARG |
| 40 | UA | 372 | ARG |
| 40 | UE | 326 | LYS |
| 40 | UE | 339 | ARG |
| 40 | UE | 372 | ARG |
| 40 | UF | 2 | ARG |
| 40 | UF | 7 | VAL |
| 40 | UF | 22 | GLU |
| 40 | UF | 23 | LEU |
| 40 | UF | 25 | CYS |
| 40 | UF | 26 | LEU |
| 40 | UF | 27 | GLU |
| 40 | UF | 30 | ILE |
| 40 | UF | 31 | GLN |
| 40 | UF | 33 | ASP |
| 40 | UF | 39 | ASP |
| 40 | UF | 46 | ASP |
| 40 | UF | 62 | VAL |
| 40 | UF | 64 | ARG |
| 40 | UF | 66 | VAL |
| 40 | UF | 70 | LEU |
| 40 | UF | 77 | GLU |
| 40 | UF | 79 | ARG |
| 40 | UF | 82 | THR |
| 40 | UF | 84 | ARG |
| 40 | UF | 92 | LEU |
| 40 | UF | 93 | ILE |
| 40 | UF | 96 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | UF | 97 | GLU |
| 40 | UF | 102 | ASN |
| 40 | UF | 110 | ILE |
| 40 | UF | 112 | LYS |
| 40 | UF | 114 | LEU |
| 40 | UF | 122 | ILE |
| 40 | UF | 133 | GLN |
| 40 | UF | 136 | LEU |
| 40 | UF | 137 | ILE |
| 40 | UF | 140 | SER |
| 40 | UF | 141 | PHE |
| 40 | UF | 145 | THR |
| 40 | UF | 149 | PHE |
| 40 | UF | 155 | GLU |
| 40 | UF | 156 | ARG |
| 40 | UF | 159 | VAL |
| 40 | UF | 160 | ASP |
| 40 | UF | 163 | LYS |
| 40 | UF | 164 | LYS |
| 40 | UF | 165 | SER |
| 40 | UF | 166 | LYS |
| 40 | UF | 171 | ILE |
| 40 | UF | 176 | GLN |
| 40 | UF | 177 | VAL |
| 40 | UF | 186 | ASN |
| 40 | UF | 190 | THR |
| 40 | UF | 195 | LEU |
| 40 | UF | 200 | CYS |
| 40 | UF | 203 | MET |
| 40 | UF | 204 | VAL |
| 40 | UF | 207 | GLU |
| 40 | UF | 212 | ILE |
| 40 | UF | 214 | ARG |
| 40 | UF | 215 | ARG |
| 40 | UF | 216 | ASN |
| 40 | UF | 217 | LEU |
| 40 | UF | 218 | ASP |
| 40 | UF | 219 | ILE |
| 40 | UF | 221 | ARG |
| 40 | UF | 228 | ASN |
| 40 | UF | 229 | ARG |
| 40 | UF | 232 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | UF | 238 | ILE |
| 40 | UF | 241 | SER |
| 40 | UF | 242 | LEU |
| 40 | UF | 248 | LEU |
| 40 | UF | 250 | VAL |
| 40 | UF | 257 | THR |
| 40 | UF | 264 | ARG |
| 40 | UF | 272 | TYR |
| 40 | UF | 275 | VAL |
| 40 | UF | 276 | ILE |
| 40 | UF | 277 | SER |
| 40 | UF | 279 | GLU |
| 40 | UF | 280 | LYS |
| 40 | UF | 286 | LEU |
| 40 | UF | 288 | VAL |
| 40 | UF | 291 | ILE |
| 40 | UF | 297 | GLU |
| 40 | UF | 303 | VAL |
| 40 | UF | 304 | LYS |
| 40 | UF | 311 | LYS |
| 40 | UF | 315 | CYS |
| 40 | UF | 316 | CYS |
| 40 | UF | 323 | VAL |
| 40 | UF | 326 | LYS |
| 40 | UF | 339 | ARG |
| 40 | UF | 344 | VAL |
| 40 | UF | 345 | ASP |
| 40 | UF | 347 | CYS |
| 40 | UF | 352 | LYS |
| 40 | UF | 358 | GLN |
| 40 | UF | 361 | THR |
| 40 | UF | 363 | VAL |
| 40 | UF | 366 | ASP |
| 40 | UF | 367 | LEU |
| 40 | UF | 372 | ARG |
| 40 | UF | 374 | VAL |
| 40 | UF | 376 | MET |
| 40 | UF | 380 | THR |
| 40 | UF | 389 | ARG |
| 40 | UF | 400 | LYS |
| 40 | UF | 404 | VAL |
| 40 | UF | 406 | TRP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | UF | 408 | VAL |
| 40 | UF | 412 | MET |
| 40 | UF | 421 | ARG |
| 40 | UF | 423 | ASP |
| 40 | UF | 424 | MET |
| 40 | UF | 429 | LYS |
| 40 | UF | 433 | GLU |
| 40 | UF | 434 | VAL |
| 40 | UF | 436 | MET |
| 40 | UF | 439 | VAL |
| 40 | UF | 440 | GLU |
| 40 | UG | 2 | ARG |
| 40 | UG | 308 | ARG |
| 40 | UG | 329 | ASN |
| 40 | UI | 2 | ARG |
| 40 | UI | 4 | CYS |
| 40 | UI | 20 | CYS |
| 40 | UI | 22 | GLU |
| 40 | UI | 23 | LEU |
| 40 | UI | 28 | HIS |
| 40 | UI | 31 | GLN |
| 40 | UI | 35 | GLN |
| 40 | UI | 36 | MET |
| 40 | UI | 39 | ASP |
| 40 | UI | 62 | VAL |
| 40 | UI | 70 | LEU |
| 40 | UI | 79 | ARG |
| 40 | UI | 92 | LEU |
| 40 | UI | 93 | ILE |
| 40 | UI | 96 | LYS |
| 40 | UI | 109 | THR |
| 40 | UI | 112 | LYS |
| 40 | UI | 113 | GLU |
| 40 | UI | 114 | LEU |
| 40 | UI | 115 | ILE |
| 40 | UI | 116 | ASP |
| 40 | UI | 117 | LEU |
| 40 | UI | 119 | LEU |
| 40 | UI | 120 | ASP |
| 40 | UI | 121 | ARG |
| 40 | UI | 122 | ILE |
| 40 | UI | 123 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | UI | 125 | LEU |
| 40 | UI | 129 | CYS |
| 40 | UI | 132 | LEU |
| 40 | UI | 133 | GLN |
| 40 | UI | 136 | LEU |
| 40 | UI | 137 | ILE |
| 40 | UI | 140 | SER |
| 40 | UI | 141 | PHE |
| 40 | UI | 145 | THR |
| 40 | UI | 149 | PHE |
| 40 | UI | 152 | LEU |
| 40 | UI | 153 | LEU |
| 40 | UI | 155 | GLU |
| 40 | UI | 156 | ARG |
| 40 | UI | 158 | SER |
| 40 | UI | 160 | ASP |
| 40 | UI | 163 | LYS |
| 40 | UI | 165 | SER |
| 40 | UI | 166 | LYS |
| 40 | UI | 167 | LEU |
| 40 | UI | 170 | SER |
| 40 | UI | 171 | ILE |
| 40 | UI | 176 | GLN |
| 40 | UI | 182 | VAL |
| 40 | UI | 187 | SER |
| 40 | UI | 188 | ILE |
| 40 | UI | 189 | LEU |
| 40 | UI | 196 | GLU |
| 40 | UI | 198 | SER |
| 40 | UI | 199 | ASP |
| 40 | UI | 200 | CYS |
| 40 | UI | 205 | ASP |
| 40 | UI | 211 | ASP |
| 40 | UI | 214 | ARG |
| 40 | UI | 217 | LEU |
| 40 | UI | 219 | ILE |
| 40 | UI | 221 | ARG |
| 40 | UI | 229 | ARG |
| 40 | UI | 231 | ILE |
| 40 | UI | 237 | SER |
| 40 | UI | 238 | ILE |
| 40 | UI | 241 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | UI | 243 | ARG |
| 40 | UI | 248 | LEU |
| 40 | UI | 250 | VAL |
| 40 | UI | 252 | LEU |
| 40 | UI | 256 | GLN |
| 40 | UI | 259 | LEU |
| 40 | UI | 264 | ARG |
| 40 | UI | 266 | HIS |
| 40 | UI | 269 | LEU |
| 40 | UI | 271 | THR |
| 40 | UI | 272 | TYR |
| 40 | UI | 275 | VAL |
| 40 | UI | 276 | ILE |
| 40 | UI | 279 | GLU |
| 40 | UI | 284 | GLU |
| 40 | UI | 285 | GLN |
| 40 | UI | 286 | LEU |
| 40 | UI | 304 | LYS |
| 40 | UI | 308 | ARG |
| 40 | UI | 309 | HIS |
| 40 | UI | 312 | TYR |
| 40 | UI | 316 | CYS |
| 40 | UI | 317 | LEU |
| 40 | UI | 318 | LEU |
| 40 | UI | 323 | VAL |
| 40 | UI | 327 | ASP |
| 40 | UI | 332 | ILE |
| 40 | UI | 338 | LYS |
| 40 | UI | 339 | ARG |
| 40 | UI | 341 | ILE |
| 40 | UI | 347 | CYS |
| 40 | UI | 357 | TYR |
| 40 | UI | 362 | VAL |
| 40 | UI | 363 | VAL |
| 40 | UI | 366 | ASP |
| 40 | UI | 367 | LEU |
| 40 | UI | 369 | LYS |
| 40 | UI | 371 | GLN |
| 40 | UI | 372 | ARG |
| 40 | UI | 375 | CYS |
| 40 | UI | 376 | MET |
| 40 | UI | 378 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | UI | 383 | ILE |
| 40 | UI | 389 | ARG |
| 40 | UI | 397 | MET |
| 40 | UI | 400 | LYS |
| 40 | UI | 401 | ARG |
| 40 | UI | 404 | VAL |
| 40 | UI | 413 | GLU |
| 40 | UI | 416 | GLU |
| 40 | UI | 421 | ARG |
| 40 | UI | 427 | LEU |
| 40 | UI | 428 | GLU |
| 40 | UI | 429 | LYS |
| 40 | UI | 433 | GLU |
| 40 | UI | 436 | MET |
| 40 | UI | 437 | ASP |
| 40 | UI | 439 | VAL |
| 41 | UM | 306 | ARG |
| 41 | UM | 359 | ARG |
| 41 | UO | 306 | ARG |
| 41 | UP | 1 | MET |
| 41 | UP | 2 | ARG |
| 41 | UP | 7 | LEU |
| 41 | UP | 8 | GLN |
| 41 | UP | 12 | CYS |
| 41 | UP | 19 | LYS |
| 41 | UP | 24 | ILE |
| 41 | UP | 30 | ILE |
| 41 | UP | 31 | ASP |
| 41 | UP | 40 | SER |
| 41 | UP | 41 | ASP |
| 41 | UP | 42 | LEU |
| 41 | UP | 44 | LEU |
| 41 | UP | 45 | GLU |
| 41 | UP | 52 | ASN |
| 41 | UP | 60 | VAL |
| 41 | UP | 62 | ARG |
| 41 | UP | 65 | LEU |
| 41 | UP | 68 | LEU |
| 41 | UP | 69 | GLU |
| 41 | UP | 73 | MET |
| 41 | UP | 75 | SER |
| 41 | UP | 78 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | UP | 84 | ILE |
| 41 | UP | 88 | ASP |
| 41 | UP | 90 | PHE |
| 41 | UP | 91 | VAL |
| 41 | UP | 92 | PHE |
| 41 | UP | 94 | GLN |
| 41 | UP | 105 | HIS |
| 41 | UP | 111 | GLU |
| 41 | UP | 113 | VAL |
| 41 | UP | 119 | VAL |
| 41 | UP | 121 | ARG |
| 41 | UP | 130 | LEU |
| 41 | UP | 131 | GLN |
| 41 | UP | 135 | LEU |
| 41 | UP | 137 | HIS |
| 41 | UP | 139 | LEU |
| 41 | UP | 143 | THR |
| 41 | UP | 147 | MET |
| 41 | UP | 155 | ILE |
| 41 | UP | 156 | ARG |
| 41 | UP | 162 | ARG |
| 41 | UP | 163 | ILE |
| 41 | UP | 166 | THR |
| 41 | UP | 170 | VAL |
| 41 | UP | 172 | SER |
| 41 | UP | 174 | LYS |
| 41 | UP | 175 | VAL |
| 41 | UP | 177 | ASP |
| 41 | UP | 178 | THR |
| 41 | UP | 191 | GLN |
| 41 | UP | 192 | LEU |
| 41 | UP | 194 | GLU |
| 41 | UP | 199 | THR |
| 41 | UP | 202 | ILE |
| 41 | UP | 203 | ASP |
| 41 | UP | 204 | ASN |
| 41 | UP | 207 | LEU |
| 41 | UP | 211 | CYS |
| 41 | UP | 213 | ARG |
| 41 | UP | 214 | THR |
| 41 | UP | 215 | LEU |
| 41 | UP | 217 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | UP | 218 | THR |
| 41 | UP | 222 | TYR |
| 41 | UP | 224 | ASP |
| 41 | UP | 225 | LEU |
| 41 | UP | 228 | LEU |
| 41 | UP | 236 | VAL |
| 41 | UP | 241 | ARG |
| 41 | UP | 242 | PHE |
| 41 | UP | 249 | ASP |
| 41 | UP | 256 | ASN |
| 41 | UP | 262 | ARG |
| 41 | UP | 263 | LEU |
| 41 | UP | 264 | HIS |
| 41 | UP | 267 | MET |
| 41 | UP | 274 | THR |
| 41 | UP | 276 | ARG |
| 41 | UP | 279 | GLN |
| 41 | UP | 282 | ARG |
| 41 | UP | 286 | VAL |
| 41 | UP | 288 | GLU |
| 41 | UP | 289 | LEU |
| 41 | UP | 291 | GLN |
| 41 | UP | 292 | GLN |
| 41 | UP | 293 | MET |
| 41 | UP | 295 | ASP |
| 41 | UP | 297 | LYS |
| 41 | UP | 298 | ASN |
| 41 | UP | 299 | MET |
| 41 | UP | 300 | MET |
| 41 | UP | 303 | CYS |
| 41 | UP | 304 | ASP |
| 41 | UP | 309 | ARG |
| 41 | UP | 312 | THR |
| 41 | UP | 316 | VAL |
| 41 | UP | 318 | ARG |
| 41 | UP | 320 | ARG |
| 41 | UP | 321 | MET |
| 41 | UP | 324 | LYS |
| 41 | UP | 330 | MET |
| 41 | UP | 336 | LYS |
| 41 | UP | 337 | ASN |
| 41 | UP | 338 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | UP | 339 | SER |
| 41 | UP | 347 | ASN |
| 41 | UP | 350 | LYS |
| 41 | UP | 351 | THR |
| 41 | UP | 356 | ILE |
| 41 | UP | 359 | ARG |
| 41 | UP | 361 | LEU |
| 41 | UP | 362 | LYS |
| 41 | UP | 364 | SER |
| 41 | UP | 367 | PHE |
| 41 | UP | 372 | THR |
| 41 | UP | 375 | GLN |
| 41 | UP | 377 | LEU |
| 41 | UP | 379 | LYS |
| 41 | UP | 380 | ARG |
| 41 | UP | 383 | GLU |
| 41 | UP | 390 | ARG |
| 41 | UP | 391 | ARG |
| 41 | UP | 392 | LYS |
| 41 | UP | 395 | LEU |
| 41 | UP | 396 | HIS |
| 41 | UP | 403 | MET |
| 41 | UP | 409 | THR |
| 41 | UP | 422 | VAL |
| 41 | UP | 423 | VAL |
| 41 | UP | 425 | ARG |
| 40 | VA | 339 | ARG |
| 41 | VB | 332 | ASN |
| 40 | VF | 133 | GLN |
| 40 | VH | 369 | LYS |
| 40 | VI | 214 | ARG |
| 40 | VI | 256 | GLN |
| 40 | VI | 369 | LYS |
| 40 | VJ | 369 | LYS |
| 41 | VN | 2 | ARG |
| 41 | VN | 306 | ARG |
| 41 | VN | 359 | ARG |
| 41 | VO | 307 | HIS |
| 41 | VP | 83 | GLN |
| 41 | VQ | 306 | ARG |
| 40 | WA | 2 | ARG |
| 40 | WA | 308 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | WB | 204 | ASN |
| 41 | WB | 306 | ARG |
| 40 | WE | 308 | ARG |
| 40 | WE | 339 | ARG |
| 40 | WF | 372 | ARG |
| 40 | WH | 2 | ARG |
| 40 | WI | 163 | LYS |
| 40 | WI | 308 | ARG |
| 41 | WM | 1 | MET |
| 41 | WM | 2 | ARG |
| 41 | WM | 7 | LEU |
| 41 | WM | 8 | GLN |
| 41 | WM | 11 | GLN |
| 41 | WM | 12 | CYS |
| 41 | WM | 19 | LYS |
| 41 | WM | 22 | GLU |
| 41 | WM | 25 | SER |
| 41 | WM | 30 | ILE |
| 41 | WM | 35 | THR |
| 41 | WM | 40 | SER |
| 41 | WM | 46 | ARG |
| 41 | WM | 65 | LEU |
| 41 | WM | 66 | VAL |
| 41 | WM | 77 | ARG |
| 41 | WM | 78 | SER |
| 41 | WM | 83 | GLN |
| 41 | WM | 86 | ARG |
| 41 | WM | 88 | ASP |
| 41 | WM | 99 | ASN |
| 41 | WM | 101 | TRP |
| 41 | WM | 103 | LYS |
| 41 | WM | 107 | THR |
| 41 | WM | 111 | GLU |
| 41 | WM | 113 | VAL |
| 41 | WM | 114 | ASP |
| 41 | WM | 117 | LEU |
| 41 | WM | 129 | CYS |
| 41 | WM | 130 | LEU |
| 41 | WM | 135 | LEU |
| 41 | WM | 136 | THR |
| 41 | WM | 139 | LEU |
| 41 | WM | 147 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | WM | 151 | LEU |
| 41 | WM | 152 | ILE |
| 41 | WM | 153 | SER |
| 41 | WM | 155 | ILE |
| 41 | WM | 156 | ARG |
| 41 | WM | 159 | TYR |
| 41 | WM | 160 | PRO |
| 41 | WM | 162 | ARG |
| 41 | WM | 168 | SER |
| 41 | WM | 169 | VAL |
| 41 | WM | 170 | VAL |
| 41 | WM | 172 | SER |
| 41 | WM | 174 | LYS |
| 41 | WM | 177 | ASP |
| 41 | WM | 180 | VAL |
| 41 | WM | 191 | GLN |
| 41 | WM | 193 | VAL |
| 41 | WM | 194 | GLU |
| 41 | WM | 195 | ASN |
| 41 | WM | 199 | THR |
| 41 | WM | 202 | ILE |
| 41 | WM | 207 | LEU |
| 41 | WM | 211 | CYS |
| 41 | WM | 212 | PHE |
| 41 | WM | 213 | ARG |
| 41 | WM | 214 | THR |
| 41 | WM | 215 | LEU |
| 41 | WM | 216 | LYS |
| 41 | WM | 218 | THR |
| 41 | WM | 221 | THR |
| 41 | WM | 224 | ASP |
| 41 | WM | 225 | LEU |
| 41 | WM | 226 | ASN |
| 41 | WM | 227 | HIS |
| 41 | WM | 232 | THR |
| 41 | WM | 237 | THR |
| 41 | WM | 241 | ARG |
| 41 | WM | 242 | PHE |
| 41 | WM | 245 | GLN |
| 41 | WM | 246 | LEU |
| 41 | WM | 252 | LYS |
| 41 | WM | 255 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | WM | 257 | MET |
| 41 | WM | 258 | VAL |
| 41 | WM | 262 | ARG |
| 41 | WM | 263 | LEU |
| 41 | WM | 274 | THR |
| 41 | WM | 275 | SER |
| 41 | WM | 278 | SER |
| 41 | WM | 280 | GLN |
| 41 | WM | 282 | ARG |
| 41 | WM | 289 | LEU |
| 41 | WM | 293 | MET |
| 41 | WM | 295 | ASP |
| 41 | WM | 297 | LYS |
| 41 | WM | 299 | MET |
| 41 | WM | 300 | MET |
| 41 | WM | 303 | CYS |
| 41 | WM | 309 | ARG |
| 41 | WM | 310 | TYR |
| 41 | WM | 311 | LEU |
| 41 | WM | 316 | VAL |
| 41 | WM | 324 | LYS |
| 41 | WM | 327 | ASP |
| 41 | WM | 330 | MET |
| 41 | WM | 331 | LEU |
| 41 | WM | 342 | VAL |
| 41 | WM | 345 | ILE |
| 41 | WM | 348 | ASN |
| 41 | WM | 350 | LYS |
| 41 | WM | 364 | SER |
| 41 | WM | 372 | THR |
| 41 | WM | 374 | ILE |
| 41 | WM | 376 | GLU |
| 41 | WM | 377 | LEU |
| 41 | WM | 379 | LYS |
| 41 | WM | 380 | ARG |
| 41 | WM | 388 | MET |
| 41 | WM | 389 | PHE |
| 41 | WM | 390 | ARG |
| 41 | WM | 391 | ARG |
| 41 | WM | 392 | LYS |
| 41 | WM | 395 | LEU |
| 41 | WM | 396 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | WM | 404 | ASP |
| 41 | WM | 406 | MET |
| 41 | WM | 415 | MET |
| 41 | WM | 423 | VAL |
| 41 | WM | 424 | THR |
| 41 | WM | 425 | ARG |
| 41 | WN | 1 | MET |
| 41 | WN | 7 | LEU |
| 41 | WN | 11 | GLN |
| 41 | WN | 12 | CYS |
| 41 | WN | 19 | LYS |
| 41 | WN | 22 | GLU |
| 41 | WN | 30 | ILE |
| 41 | WN | 31 | ASP |
| 41 | WN | 33 | THR |
| 41 | WN | 37 | HIS |
| 41 | WN | 39 | ASP |
| 41 | WN | 40 | SER |
| 41 | WN | 42 | LEU |
| 41 | WN | 44 | LEU |
| 41 | WN | 46 | ARG |
| 41 | WN | 47 | ILE |
| 41 | WN | 48 | ASN |
| 41 | WN | 49 | VAL |
| 41 | WN | 50 | TYR |
| 41 | WN | 51 | TYR |
| 41 | WN | 58 | LYS |
| 41 | WN | 60 | VAL |
| 41 | WN | 65 | LEU |
| 41 | WN | 66 | VAL |
| 41 | WN | 68 | LEU |
| 41 | WN | 74 | ASP |
| 41 | WN | 78 | SER |
| 41 | WN | 84 | ILE |
| 41 | WN | 86 | ARG |
| 41 | WN | 89 | ASN |
| 41 | WN | 90 | PHE |
| 41 | WN | 91 | VAL |
| 41 | WN | 94 | GLN |
| 41 | WN | 101 | TRP |
| 41 | WN | 103 | LYS |
| 41 | WN | 107 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | WN | 108 | GLU |
| 41 | WN | 111 | GLU |
| 41 | WN | 112 | LEU |
| 41 | WN | 113 | VAL |
| 41 | WN | 114 | ASP |
| 41 | WN | 117 | LEU |
| 41 | WN | 118 | ASP |
| 41 | WN | 119 | VAL |
| 41 | WN | 122 | LYS |
| 41 | WN | 131 | GLN |
| 41 | WN | 135 | LEU |
| 41 | WN | 136 | THR |
| 41 | WN | 139 | LEU |
| 41 | WN | 147 | MET |
| 41 | WN | 153 | SER |
| 41 | WN | 154 | LYS |
| 41 | WN | 155 | ILE |
| 41 | WN | 157 | GLU |
| 41 | WN | 162 | ARG |
| 41 | WN | 166 | THR |
| 41 | WN | 168 | SER |
| 41 | WN | 170 | VAL |
| 41 | WN | 174 | LYS |
| 41 | WN | 175 | VAL |
| 41 | WN | 176 | SER |
| 41 | WN | 180 | VAL |
| 41 | WN | 193 | VAL |
| 41 | WN | 194 | GLU |
| 41 | WN | 197 | ASP |
| 41 | WN | 199 | THR |
| 41 | WN | 202 | ILE |
| 41 | WN | 204 | ASN |
| 41 | WN | 205 | GLU |
| 41 | WN | 211 | CYS |
| 41 | WN | 213 | ARG |
| 41 | WN | 217 | LEU |
| 41 | WN | 218 | THR |
| 41 | WN | 221 | THR |
| 41 | WN | 224 | ASP |
| 41 | WN | 226 | ASN |
| 41 | WN | 227 | HIS |
| 41 | WN | 228 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | WN | 236 | VAL |
| 41 | WN | 245 | GLN |
| 41 | WN | 249 | ASP |
| 41 | WN | 251 | ARG |
| 41 | WN | 253 | LEU |
| 41 | WN | 255 | VAL |
| 41 | WN | 262 | ARG |
| 41 | WN | 267 | MET |
| 41 | WN | 274 | THR |
| 41 | WN | 275 | SER |
| 41 | WN | 276 | ARG |
| 41 | WN | 282 | ARG |
| 41 | WN | 292 | GLN |
| 41 | WN | 293 | MET |
| 41 | WN | 297 | LYS |
| 41 | WN | 298 | ASN |
| 41 | WN | 299 | MET |
| 41 | WN | 300 | MET |
| 41 | WN | 303 | CYS |
| 41 | WN | 304 | ASP |
| 41 | WN | 309 | ARG |
| 41 | WN | 310 | TYR |
| 41 | WN | 316 | VAL |
| 41 | WN | 318 | ARG |
| 41 | WN | 320 | ARG |
| 41 | WN | 321 | MET |
| 41 | WN | 324 | LYS |
| 41 | WN | 325 | GLU |
| 41 | WN | 326 | VAL |
| 41 | WN | 328 | GLU |
| 41 | WN | 331 | LEU |
| 41 | WN | 337 | ASN |
| 41 | WN | 338 | SER |
| 41 | WN | 342 | VAL |
| 41 | WN | 345 | ILE |
| 41 | WN | 347 | ASN |
| 41 | WN | 348 | ASN |
| 41 | WN | 350 | LYS |
| 41 | WN | 351 | THR |
| 41 | WN | 355 | ASP |
| 41 | WN | 359 | ARG |
| 41 | WN | 361 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | WN | 362 | LYS |
| 41 | WN | 364 | SER |
| 41 | WN | 366 | THR |
| 41 | WN | 372 | THR |
| 41 | WN | 374 | ILE |
| 41 | WN | 376 | GLU |
| 41 | WN | 377 | LEU |
| 41 | WN | 379 | LYS |
| 41 | WN | 380 | ARG |
| 41 | WN | 386 | THR |
| 41 | WN | 388 | MET |
| 41 | WN | 392 | LYS |
| 41 | WN | 395 | LEU |
| 41 | WN | 397 | TRP |
| 41 | WN | 403 | MET |
| 41 | WN | 404 | ASP |
| 41 | WN | 406 | MET |
| 41 | WN | 410 | GLU |
| 41 | WN | 413 | SER |
| 41 | WN | 423 | VAL |
| 41 | WO | 306 | ARG |
| 41 | WP | 195 | ASN |
| 41 | WP | 306 | ARG |
| 41 | WQ | 204 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (942) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 534 | ASN |
| 1 | 1A | 650 | GLN |
| 1 | 1A | 918 | ASN |
| 1 | 1A | 1025 | GLN |
| 3 | 1G | 71 | ASN |
| 3 | 1G | 109 | HIS |
| 3 | 1G | 245 | GLN |
| 4 | 1H | 173 | ASN |
| 4 | 1I | 73 | GLN |
| 5 | 1L | 281 | GLN |
| 5 | 1M | 98 | GLN |
| 5 | 1M | 269 | GLN |
| 7 | 1S | 567 | HIS |
| 7 | 1T | 55 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 1T | 58 | ASN |
| 7 | 1T | 61 | HIS |
| 7 | 1T | 191 | ASN |
| 7 | 1T | 290 | GLN |
| 7 | 1T | 303 | HIS |
| 7 | 1T | 304 | GLN |
| 7 | 1T | 378 | HIS |
| 7 | 1T | 445 | GLN |
| 7 | 1T | 451 | GLN |
| 7 | 1T | 506 | GLN |
| 7 | 1T | 586 | HIS |
| 7 | 1U | 65 | ASN |
| 8 | 1W | 320 | ASN |
| 8 | 1X | 149 | GLN |
| 8 | 1X | 180 | GLN |
| 8 | 1X | 185 | GLN |
| 9 | 2B | 245 | GLN |
| 9 | 2B | 369 | ASN |
| 9 | 2C | 447 | GLN |
| 10 | 2E | 104 | HIS |
| 10 | 2F | 41 | GLN |
| 11 | 2I | 104 | ASN |
| 11 | 2I | 174 | ASN |
| 11 | 2I | 179 | ASN |
| 11 | 2K | 112 | ASN |
| 12 | 2O | 158 | ASN |
| 12 | 2P | 220 | ASN |
| 12 | 2Q | 215 | GLN |
| 12 | 2R | 192 | GLN |
| 13 | 2U | 33 | HIS |
| 13 | 2U | 43 | GLN |
| 13 | 2U | 131 | GLN |
| 13 | 2U | 133 | GLN |
| 13 | 2V | 82 | ASN |
| 13 | 2V | 130 | ASN |
| 13 | 2V | 131 | GLN |
| 13 | 2V | 133 | GLN |
| 13 | 2W | 31 | ASN |
| 13 | 2W | 43 | GLN |
| 13 | 2W | 109 | GLN |
| 13 | 2W | 131 | GLN |
| 13 | 2W | 133 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | 2X | 7 | GLN |
| 13 | 2X | 109 | GLN |
| 13 | 2X | 130 | ASN |
| 13 | 2X | 131 | GLN |
| 13 | 2X | 133 | GLN |
| 13 | 2X | 159 | ASN |
| 14 | 3B | 8 | ASN |
| 14 | 3B | 9 | GLN |
| 14 | 3C | 9 | GLN |
| 14 | 3C | 20 | GLN |
| 15 | 3H | 194 | ASN |
| 16 | 3J | 10 | GLN |
| 16 | 3J | 31 | GLN |
| 16 | 3J | 333 | GLN |
| 16 | 3K | 107 | ASN |
| 16 | 3K | 344 | GLN |
| 16 | 3M | 217 | GLN |
| 17 | 3O | 349 | ASN |
| 17 | 3O | 397 | GLN |
| 17 | 3P | 129 | GLN |
| 17 | 3P | 134 | GLN |
| 17 | 3P | 243 | GLN |
| 17 | 3P | 326 | GLN |
| 17 | 3P | 470 | GLN |
| 17 | 3Q | 435 | GLN |
| 17 | 3Q | 446 | GLN |
| 17 | 3Q | 470 | GLN |
| 17 | 3R | 129 | GLN |
| 17 | 3R | 133 | GLN |
| 17 | 3R | 145 | ASN |
| 17 | 3R | 151 | ASN |
| 17 | 3R | 172 | ASN |
| 17 | 3R | 193 | GLN |
| 17 | 3R | 243 | GLN |
| 17 | 3R | 251 | GLN |
| 17 | 3R | 334 | ASN |
| 17 | 3R | 338 | ASN |
| 17 | 3R | 341 | ASN |
| 19 | 3Z | 378 | ASN |
| 20 | 4A | 70 | GLN |
| 20 | 4A | 152 | HIS |
| 20 | 4A | 157 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | 4A | 167 | GLN |
| 20 | 4A | 173 | GLN |
| 20 | 4A | 198 | GLN |
| 20 | 4A | 234 | GLN |
| 20 | 4B | 237 | GLN |
| 20 | 4B | 258 | GLN |
| 20 | 4B | 289 | GLN |
| 20 | 4B | 344 | GLN |
| 20 | 4B | 345 | GLN |
| 20 | 4B | 354 | HIS |
| 21 | 4D | 26 | HIS |
| 21 | 4D | 458 | ASN |
| 21 | 4D | 532 | GLN |
| 21 | 4D | 533 | ASN |
| 21 | 4E | 458 | ASN |
| 21 | 4F | 119 | GLN |
| 21 | 4F | 307 | ASN |
| 21 | 4F | 415 | ASN |
| 21 | 4F | 481 | ASN |
| 21 | 4F | 532 | GLN |
| 22 | 4H | 9 | ASN |
| 22 | 4H | 14 | ASN |
| 22 | 4H | 297 | GLN |
| 22 | 4I | 698 | ASN |
| 22 | 4J | 670 | ASN |
| 22 | 4J | 687 | GLN |
| 23 | 4M | 25 | HIS |
| 23 | 4M | 39 | GLN |
| 23 | 4M | 102 | GLN |
| 23 | 4M | 110 | ASN |
| 23 | 4M | 111 | GLN |
| 23 | 4M | 207 | ASN |
| 23 | 4M | 208 | GLN |
| 23 | 4M | 211 | GLN |
| 23 | 4M | 215 | GLN |
| 23 | 4M | 256 | GLN |
| 23 | 4N | 35 | GLN |
| 23 | 4N | 43 | GLN |
| 23 | 4N | 57 | HIS |
| 23 | 4N | 102 | GLN |
| 23 | 4N | 110 | ASN |
| 23 | 4N | 208 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | 4N | 211 | GLN |
| 23 | 4N | 239 | ASN |
| 23 | 4N | 256 | GLN |
| 24 | 4O | 208 | GLN |
| 24 | 4O | 256 | GLN |
| 23 | 4P | 208 | GLN |
| 23 | 4P | 239 | ASN |
| 23 | 4P | 256 | GLN |
| 23 | 4Q | 17 | HIS |
| 23 | 4Q | 35 | GLN |
| 23 | 4Q | 39 | GLN |
| 23 | 4Q | 43 | GLN |
| 23 | 4Q | 256 | GLN |
| 23 | 4R | 39 | GLN |
| 23 | 4R | 102 | GLN |
| 23 | 4R | 110 | ASN |
| 23 | 4R | 208 | GLN |
| 26 | 4V | 140 | HIS |
| 26 | 4W | 336 | HIS |
| 26 | 4W | 353 | ASN |
| 28 | 5B | 212 | ASN |
| 30 | 5G | 33 | ASN |
| 30 | 5G | 85 | GLN |
| 33 | 5O | 41 | GLN |
| 34 | 5Q | 183 | GLN |
| 34 | 5R | 310 | ASN |
| 34 | 5R | 322 | GLN |
| 34 | 5R | 391 | ASN |
| 34 | 5R | 402 | GLN |
| 34 | 5R | 460 | GLN |
| 34 | 5R | 502 | HIS |
| 36 | 5W | 122 | ASN |
| 36 | 5X | 192 | GLN |
| 36 | 5X | 198 | GLN |
| 36 | 5X | 221 | GLN |
| 39 | 6F | 121 | HIS |
| 39 | 6G | 24 | GLN |
| 40 | AA | 1 | GLN |
| 40 | AA | 258 | ASN |
| 41 | AB | 100 | ASN |
| 41 | AB | 184 | ASN |
| 41 | AB | 292 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | AB | 298 | ASN |
| 41 | AB | 334 | GLN |
| 41 | AB | 347 | ASN |
| 40 | AG | 186 | ASN |
| 40 | AH | 11 | GLN |
| 40 | AH | 101 | ASN |
| 40 | AH | 283 | HIS |
| 41 | AL | 347 | ASN |
| 41 | AM | 334 | GLN |
| 41 | AN | 6 | HIS |
| 41 | AN | 14 | ASN |
| 41 | AN | 134 | GLN |
| 41 | AN | 347 | ASN |
| 41 | AO | 83 | GLN |
| 41 | AO | 100 | ASN |
| 41 | AO | 131 | GLN |
| 41 | AO | 165 | ASN |
| 41 | AO | 335 | ASN |
| 41 | AO | 347 | ASN |
| 41 | AO | 370 | ASN |
| 41 | AP | 134 | GLN |
| 40 | BA | 258 | ASN |
| 40 | BA | 358 | GLN |
| 41 | BB | 131 | GLN |
| 41 | BB | 134 | GLN |
| 41 | BB | 165 | ASN |
| 41 | BB | 190 | HIS |
| 41 | BB | 245 | GLN |
| 41 | BB | 329 | GLN |
| 41 | BB | 334 | GLN |
| 41 | BB | 348 | ASN |
| 41 | BB | 384 | GLN |
| 41 | BB | 396 | HIS |
| 40 | BE | 15 | GLN |
| 40 | BE | 206 | ASN |
| 40 | BE | 301 | GLN |
| 40 | BF | 11 | GLN |
| 40 | BF | 18 | ASN |
| 40 | BF | 101 | ASN |
| 40 | BG | 256 | GLN |
| 40 | BG | 405 | HIS |
| 40 | BH | 15 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | BH | 128 | GLN |
| 40 | BH | 133 | GLN |
| 40 | BH | 206 | ASN |
| 40 | BH | 256 | GLN |
| 40 | BH | 392 | HIS |
| 40 | BI | 91 | GLN |
| 40 | BI | 102 | ASN |
| 40 | BI | 133 | GLN |
| 40 | BI | 206 | ASN |
| 40 | BI | 226 | ASN |
| 40 | BI | 256 | GLN |
| 40 | BI | 300 | ASN |
| 40 | BI | 371 | GLN |
| 41 | BL | 131 | GLN |
| 41 | BL | 204 | ASN |
| 41 | BL | 334 | GLN |
| 41 | BL | 347 | ASN |
| 41 | BM | 11 | GLN |
| 41 | BM | 14 | ASN |
| 41 | BM | 191 | GLN |
| 41 | BM | 195 | ASN |
| 41 | BM | 204 | ASN |
| 41 | BM | 245 | GLN |
| 41 | BM | 247 | ASN |
| 41 | BM | 329 | GLN |
| 41 | BM | 384 | GLN |
| 41 | BM | 414 | ASN |
| 41 | BM | 420 | ASN |
| 41 | BN | 48 | ASN |
| 41 | BN | 131 | GLN |
| 41 | BN | 347 | ASN |
| 41 | BO | 6 | HIS |
| 41 | BO | 184 | ASN |
| 41 | BO | 190 | HIS |
| 41 | BO | 247 | ASN |
| 41 | BO | 279 | GLN |
| 41 | BO | 298 | ASN |
| 41 | BO | 370 | ASN |
| 41 | BO | 375 | GLN |
| 41 | BP | 94 | GLN |
| 41 | BP | 131 | GLN |
| 41 | BP | 134 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | BP | 191 | GLN |
| 41 | BP | 334 | GLN |
| 41 | BP | 335 | ASN |
| 41 | BP | 370 | ASN |
| 41 | BP | 420 | ASN |
| 40 | CA | 301 | GLN |
| 41 | CB | 6 | HIS |
| 41 | CB | 256 | ASN |
| 41 | CB | 375 | GLN |
| 40 | CE | 128 | GLN |
| 40 | CE | 176 | GLN |
| 40 | CF | 1 | GLN |
| 40 | CF | 206 | ASN |
| 40 | CG | 101 | ASN |
| 40 | CG | 293 | ASN |
| 40 | CH | 85 | GLN |
| 40 | CH | 206 | ASN |
| 40 | CH | 285 | GLN |
| 40 | CH | 293 | ASN |
| 40 | CH | 329 | ASN |
| 40 | CI | 228 | ASN |
| 41 | CL | 8 | GLN |
| 41 | CL | 14 | ASN |
| 41 | CL | 48 | ASN |
| 41 | CL | 100 | ASN |
| 41 | CL | 191 | GLN |
| 41 | CL | 256 | ASN |
| 41 | CL | 279 | GLN |
| 41 | CL | 291 | GLN |
| 41 | CL | 329 | GLN |
| 41 | CL | 335 | ASN |
| 41 | CL | 375 | GLN |
| 41 | CL | 416 | ASN |
| 41 | CL | 420 | ASN |
| 41 | CM | 8 | GLN |
| 41 | CM | 11 | GLN |
| 41 | CM | 43 | GLN |
| 41 | CM | 94 | GLN |
| 41 | CM | 105 | HIS |
| 41 | CM | 131 | GLN |
| 41 | CM | 184 | ASN |
| 41 | CM | 280 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | CM | 334 | GLN |
| 41 | CM | 335 | ASN |
| 41 | CM | 347 | ASN |
| 41 | CM | 396 | HIS |
| 41 | CN | 6 | HIS |
| 41 | CN | 8 | GLN |
| 41 | CN | 94 | GLN |
| 41 | CN | 134 | GLN |
| 41 | CN | 184 | ASN |
| 41 | CN | 191 | GLN |
| 41 | CN | 204 | ASN |
| 41 | CN | 307 | HIS |
| 41 | CN | 347 | ASN |
| 41 | CN | 420 | ASN |
| 41 | CO | 15 | GLN |
| 41 | CO | 184 | ASN |
| 41 | CO | 191 | GLN |
| 41 | CO | 204 | ASN |
| 41 | CO | 292 | GLN |
| 41 | CO | 329 | GLN |
| 41 | CO | 334 | GLN |
| 41 | CO | 337 | ASN |
| 41 | CO | 416 | ASN |
| 41 | CO | 420 | ASN |
| 41 | CP | 8 | GLN |
| 41 | CP | 11 | GLN |
| 41 | CP | 14 | ASN |
| 41 | CP | 48 | ASN |
| 41 | CP | 89 | ASN |
| 41 | CP | 99 | ASN |
| 41 | CP | 204 | ASN |
| 41 | CP | 256 | ASN |
| 41 | CP | 298 | ASN |
| 41 | CP | 335 | ASN |
| 41 | CP | 347 | ASN |
| 41 | CP | 420 | ASN |
| 40 | DA | 1 | GLN |
| 40 | DA | 35 | GLN |
| 40 | DA | 101 | ASN |
| 40 | DA | 226 | ASN |
| 40 | DA | 249 | ASN |
| 40 | DA | 256 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | DA | 342 | GLN |
| 40 | DA | 356 | ASN |
| 40 | DA | 371 | GLN |
| 41 | DB | 11 | GLN |
| 41 | DB | 48 | ASN |
| 41 | DB | 131 | GLN |
| 41 | DB | 134 | GLN |
| 41 | DB | 226 | ASN |
| 41 | DB | 420 | ASN |
| 40 | DE | 1 | GLN |
| 40 | DE | 11 | GLN |
| 40 | DE | 85 | GLN |
| 40 | DE | 176 | GLN |
| 40 | DE | 206 | ASN |
| 40 | DE | 226 | ASN |
| 40 | DE | 285 | GLN |
| 40 | DE | 358 | GLN |
| 40 | DE | 392 | HIS |
| 40 | DF | 61 | HIS |
| 40 | DF | 128 | GLN |
| 40 | DF | 133 | GLN |
| 40 | DF | 206 | ASN |
| 40 | DF | 293 | ASN |
| 40 | DG | 101 | ASN |
| 40 | DG | 258 | ASN |
| 40 | DH | 15 | GLN |
| 40 | DH | 102 | ASN |
| 40 | DH | 107 | HIS |
| 40 | DH | 128 | GLN |
| 40 | DH | 197 | HIS |
| 40 | DH | 206 | ASN |
| 40 | DH | 216 | ASN |
| 40 | DH | 233 | GLN |
| 40 | DH | 285 | GLN |
| 40 | DI | 11 | GLN |
| 40 | DI | 85 | GLN |
| 40 | DI | 139 | HIS |
| 40 | DI | 176 | GLN |
| 40 | DI | 206 | ASN |
| 40 | DI | 249 | ASN |
| 40 | DI | 356 | ASN |
| 41 | DL | 15 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DL | 43 | GLN |
| 41 | DL | 184 | ASN |
| 41 | DL | 247 | ASN |
| 41 | DL | 347 | ASN |
| 41 | DL | 420 | ASN |
| 41 | DM | 15 | GLN |
| 41 | DM | 48 | ASN |
| 41 | DM | 99 | ASN |
| 41 | DM | 100 | ASN |
| 41 | DM | 131 | GLN |
| 41 | DM | 134 | GLN |
| 41 | DM | 165 | ASN |
| 41 | DM | 226 | ASN |
| 41 | DM | 227 | HIS |
| 41 | DM | 332 | ASN |
| 41 | DM | 337 | ASN |
| 41 | DM | 416 | ASN |
| 41 | DN | 8 | GLN |
| 41 | DN | 14 | ASN |
| 41 | DN | 15 | GLN |
| 41 | DN | 83 | GLN |
| 41 | DN | 105 | HIS |
| 41 | DN | 131 | GLN |
| 41 | DN | 165 | ASN |
| 41 | DN | 190 | HIS |
| 41 | DN | 247 | ASN |
| 41 | DN | 256 | ASN |
| 41 | DN | 292 | GLN |
| 41 | DN | 298 | ASN |
| 41 | DN | 414 | ASN |
| 41 | DO | 99 | ASN |
| 41 | DO | 131 | GLN |
| 41 | DO | 134 | GLN |
| 41 | DO | 190 | HIS |
| 41 | DO | 375 | GLN |
| 41 | DO | 414 | ASN |
| 41 | DP | 6 | HIS |
| 41 | DP | 8 | GLN |
| 41 | DP | 43 | GLN |
| 41 | DP | 99 | ASN |
| 41 | DP | 131 | GLN |
| 41 | DP | 134 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | DP | 190 | HIS |
| 41 | DP | 226 | ASN |
| 41 | DP | 247 | ASN |
| 41 | DP | 292 | GLN |
| 41 | DP | 298 | ASN |
| 41 | DP | 416 | ASN |
| 40 | EA | 61 | HIS |
| 40 | EA | 101 | ASN |
| 41 | EB | 6 | HIS |
| 41 | EB | 8 | GLN |
| 41 | EB | 256 | ASN |
| 40 | EE | 256 | GLN |
| 40 | EH | 197 | HIS |
| 40 | EH | 258 | ASN |
| 40 | EH | 329 | ASN |
| 40 | EI | 18 | ASN |
| 40 | EI | 197 | HIS |
| 40 | EI | 342 | GLN |
| 40 | EI | 358 | GLN |
| 41 | EL | 165 | ASN |
| 41 | EL | 256 | ASN |
| 41 | EM | 43 | GLN |
| 41 | EM | 94 | GLN |
| 41 | EM | 165 | ASN |
| 41 | EM | 245 | GLN |
| 41 | EM | 280 | GLN |
| 41 | EM | 335 | ASN |
| 41 | EN | 256 | ASN |
| 41 | EO | 165 | ASN |
| 41 | EP | 8 | GLN |
| 41 | EP | 191 | GLN |
| 41 | EP | 195 | ASN |
| 41 | EP | 204 | ASN |
| 41 | EP | 280 | GLN |
| 41 | EP | 420 | ASN |
| 40 | FA | 107 | HIS |
| 40 | FA | 258 | ASN |
| 40 | FA | 293 | ASN |
| 40 | FA | 358 | GLN |
| 41 | FB | 396 | HIS |
| 40 | FG | 31 | GLN |
| 41 | FM | 334 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | FN | 8 | GLN |
| 41 | FN | 247 | ASN |
| 41 | FP | 131 | GLN |
| 41 | FP | 334 | GLN |
| 41 | FP | 347 | ASN |
| 40 | GA | 11 | GLN |
| 40 | GA | 15 | GLN |
| 40 | GA | 61 | HIS |
| 40 | GA | 101 | ASN |
| 40 | GA | 102 | ASN |
| 40 | GA | 228 | ASN |
| 41 | GB | 131 | GLN |
| 41 | GB | 247 | ASN |
| 40 | GE | 18 | ASN |
| 40 | GE | 91 | GLN |
| 40 | GE | 139 | HIS |
| 40 | GE | 206 | ASN |
| 40 | GF | 15 | GLN |
| 40 | GF | 371 | GLN |
| 40 | GG | 258 | ASN |
| 40 | GH | 283 | HIS |
| 40 | GI | 31 | GLN |
| 40 | GI | 186 | ASN |
| 40 | GI | 216 | ASN |
| 40 | GI | 228 | ASN |
| 40 | GI | 356 | ASN |
| 40 | GI | 405 | HIS |
| 41 | GM | 6 | HIS |
| 41 | GM | 8 | GLN |
| 41 | GM | 191 | GLN |
| 41 | GM | 195 | ASN |
| 41 | GM | 384 | GLN |
| 41 | GM | 396 | HIS |
| 41 | GN | 6 | HIS |
| 41 | GN | 8 | GLN |
| 41 | GN | 83 | GLN |
| 41 | GN | 94 | GLN |
| 41 | GN | 105 | HIS |
| 41 | GN | 134 | GLN |
| 41 | GN | 204 | ASN |
| 41 | GN | 227 | HIS |
| 41 | GN | 245 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | GN | 264 | HIS |
| 41 | GN | 307 | HIS |
| 41 | GN | 334 | GLN |
| 41 | GN | 370 | ASN |
| 41 | GN | 375 | GLN |
| 41 | GN | 384 | GLN |
| 41 | GN | 414 | ASN |
| 41 | GO | 6 | HIS |
| 41 | GO | 8 | GLN |
| 41 | GO | 131 | GLN |
| 41 | GP | 247 | ASN |
| 41 | GP | 329 | GLN |
| 41 | GP | 334 | GLN |
| 41 | GP | 347 | ASN |
| 40 | HA | 11 | GLN |
| 40 | HA | 342 | GLN |
| 41 | HB | 337 | ASN |
| 40 | HE | 8 | HIS |
| 40 | HE | 50 | ASN |
| 40 | HE | 85 | GLN |
| 40 | HE | 128 | GLN |
| 40 | HE | 249 | ASN |
| 40 | HE | 371 | GLN |
| 40 | HG | 88 | HIS |
| 41 | HM | 8 | GLN |
| 41 | HM | 99 | ASN |
| 41 | HM | 105 | HIS |
| 41 | HN | 89 | ASN |
| 41 | HN | 134 | GLN |
| 41 | HN | 279 | GLN |
| 41 | HN | 334 | GLN |
| 41 | HN | 337 | ASN |
| 41 | HO | 14 | ASN |
| 41 | HO | 131 | GLN |
| 41 | HO | 184 | ASN |
| 41 | HO | 256 | ASN |
| 41 | HP | 298 | ASN |
| 41 | HQ | 131 | GLN |
| 41 | HQ | 334 | GLN |
| 41 | HQ | 335 | ASN |
| 40 | IE | 88 | HIS |
| 40 | IE | 285 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | IF | 11 | GLN |
| 40 | IH | 11 | GLN |
| 40 | IH | 15 | GLN |
| 40 | IH | 91 | GLN |
| 40 | IH | 256 | GLN |
| 40 | IH | 283 | HIS |
| 40 | II | 101 | ASN |
| 41 | IM | 83 | GLN |
| 41 | IN | 184 | ASN |
| 41 | IO | 8 | GLN |
| 41 | IO | 14 | ASN |
| 41 | IO | 247 | ASN |
| 41 | IO | 347 | ASN |
| 41 | IP | 11 | GLN |
| 41 | IP | 184 | ASN |
| 41 | IP | 256 | ASN |
| 41 | IP | 347 | ASN |
| 41 | IQ | 6 | HIS |
| 41 | IQ | 14 | ASN |
| 41 | IQ | 191 | GLN |
| 41 | IQ | 334 | GLN |
| 40 | JA | 91 | GLN |
| 40 | JA | 101 | ASN |
| 40 | JA | 329 | ASN |
| 41 | JB | 99 | ASN |
| 41 | JB | 204 | ASN |
| 40 | JD | 256 | GLN |
| 40 | JF | 11 | GLN |
| 40 | JF | 15 | GLN |
| 40 | JF | 18 | ASN |
| 40 | JF | 258 | ASN |
| 40 | JG | 91 | GLN |
| 40 | JG | 228 | ASN |
| 40 | JG | 329 | ASN |
| 41 | JL | 99 | ASN |
| 41 | JM | 99 | ASN |
| 41 | JM | 131 | GLN |
| 41 | JM | 190 | HIS |
| 41 | JM | 226 | ASN |
| 41 | JM | 329 | GLN |
| 41 | JM | 420 | ASN |
| 41 | JN | 83 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | JN | 256 | ASN |
| 41 | JO | 8 | GLN |
| 41 | JO | 131 | GLN |
| 41 | JO | 298 | ASN |
| 41 | KB | 184 | ASN |
| 41 | KB | 375 | GLN |
| 40 | KD | 258 | ASN |
| 40 | KF | 139 | HIS |
| 40 | KF | 228 | ASN |
| 40 | KH | 285 | GLN |
| 41 | KL | 105 | HIS |
| 41 | KL | 131 | GLN |
| 41 | KL | 279 | GLN |
| 41 | KM | 14 | ASN |
| 41 | KM | 256 | ASN |
| 41 | KM | 334 | GLN |
| 41 | KM | 348 | ASN |
| 41 | KN | 165 | ASN |
| 41 | KN | 291 | GLN |
| 41 | KO | 184 | ASN |
| 41 | KO | 256 | ASN |
| 41 | KO | 334 | GLN |
| 41 | KO | 348 | ASN |
| 41 | LB | 94 | GLN |
| 41 | LB | 184 | ASN |
| 40 | LD | 31 | GLN |
| 40 | LD | 88 | HIS |
| 40 | LE | 15 | GLN |
| 40 | LE | 258 | ASN |
| 40 | LF | 15 | GLN |
| 40 | LF | 226 | ASN |
| 40 | LF | 233 | GLN |
| 40 | LF | 309 | HIS |
| 40 | LF | 371 | GLN |
| 40 | LG | 15 | GLN |
| 40 | LG | 206 | ASN |
| 40 | LG | 301 | GLN |
| 40 | LG | 342 | GLN |
| 41 | LL | 291 | GLN |
| 41 | LL | 334 | GLN |
| 41 | LL | 347 | ASN |
| 41 | LM | 8 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | LM | 14 | ASN |
| 41 | LM | 134 | GLN |
| 41 | LO | 43 | GLN |
| 41 | LO | 347 | ASN |
| 41 | LP | 334 | GLN |
| 40 | MA | 18 | ASN |
| 40 | MA | 133 | GLN |
| 40 | MA | 206 | ASN |
| 40 | MA | 249 | ASN |
| 40 | MA | 283 | HIS |
| 40 | MA | 356 | ASN |
| 41 | MB | 184 | ASN |
| 41 | MB | 292 | GLN |
| 41 | MB | 298 | ASN |
| 41 | MB | 347 | ASN |
| 40 | MD | 258 | ASN |
| 40 | MF | 91 | GLN |
| 40 | MF | 139 | HIS |
| 40 | MF | 256 | GLN |
| 40 | MF | 356 | ASN |
| 40 | MG | 206 | ASN |
| 40 | MG | 249 | ASN |
| 40 | MG | 342 | GLN |
| 40 | MG | 356 | ASN |
| 40 | MH | 101 | ASN |
| 40 | MH | 102 | ASN |
| 40 | MH | 206 | ASN |
| 40 | MH | 249 | ASN |
| 40 | MH | 256 | GLN |
| 40 | MH | 258 | ASN |
| 40 | MH | 285 | GLN |
| 40 | MH | 358 | GLN |
| 41 | ML | 334 | GLN |
| 41 | ML | 396 | HIS |
| 41 | MM | 256 | ASN |
| 41 | MM | 298 | ASN |
| 41 | MM | 334 | GLN |
| 41 | MN | 256 | ASN |
| 41 | MO | 11 | GLN |
| 41 | MO | 99 | ASN |
| 41 | MO | 292 | GLN |
| 41 | MO | 334 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | MO | 348 | ASN |
| 41 | MO | 370 | ASN |
| 41 | MO | 375 | GLN |
| 41 | MP | 99 | ASN |
| 41 | MP | 298 | ASN |
| 41 | MP | 334 | GLN |
| 40 | NA | 8 | HIS |
| 40 | NA | 258 | ASN |
| 41 | NB | 332 | ASN |
| 40 | ND | 8 | HIS |
| 40 | ND | 88 | HIS |
| 40 | ND | 206 | ASN |
| 40 | ND | 300 | ASN |
| 40 | NE | 91 | GLN |
| 40 | NF | 358 | GLN |
| 40 | NG | 8 | HIS |
| 40 | NH | 91 | GLN |
| 40 | NH | 139 | HIS |
| 41 | NL | 99 | ASN |
| 41 | NL | 245 | GLN |
| 41 | NL | 334 | GLN |
| 41 | NL | 347 | ASN |
| 41 | NM | 292 | GLN |
| 41 | NM | 334 | GLN |
| 41 | NM | 348 | ASN |
| 41 | NN | 6 | HIS |
| 41 | NN | 105 | HIS |
| 41 | NN | 334 | GLN |
| 41 | NN | 347 | ASN |
| 41 | NO | 347 | ASN |
| 41 | NP | 195 | ASN |
| 41 | NP | 291 | GLN |
| 40 | OA | 85 | GLN |
| 40 | OA | 186 | ASN |
| 41 | OB | 43 | GLN |
| 41 | OB | 131 | GLN |
| 40 | OD | 300 | ASN |
| 40 | OD | 379 | ASN |
| 40 | OF | 228 | ASN |
| 40 | OF | 258 | ASN |
| 40 | OF | 285 | GLN |
| 40 | OH | 31 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | OH | 101 | ASN |
| 40 | OH | 176 | GLN |
| 40 | OH | 226 | ASN |
| 40 | OH | 300 | ASN |
| 41 | OL | 334 | GLN |
| 41 | OM | 94 | GLN |
| 41 | OM | 99 | ASN |
| 41 | ON | 99 | ASN |
| 41 | ON | 137 | HIS |
| 41 | ON | 256 | ASN |
| 41 | ON | 348 | ASN |
| 41 | OO | 256 | ASN |
| 41 | OO | 334 | GLN |
| 41 | OP | 8 | GLN |
| 40 | PA | 128 | GLN |
| 40 | PA | 258 | ASN |
| 41 | PB | 165 | ASN |
| 41 | PB | 348 | ASN |
| 40 | PD | 293 | ASN |
| 40 | PE | 139 | HIS |
| 40 | PF | 293 | ASN |
| 40 | PG | 128 | GLN |
| 40 | PG | 197 | HIS |
| 40 | PH | 285 | GLN |
| 41 | PL | 8 | GLN |
| 41 | PL | 14 | ASN |
| 41 | PL | 334 | GLN |
| 41 | PM | 137 | HIS |
| 41 | PN | 131 | GLN |
| 41 | PN | 190 | HIS |
| 41 | PN | 332 | ASN |
| 41 | PN | 348 | ASN |
| 41 | PO | 6 | HIS |
| 41 | PO | 8 | GLN |
| 41 | PO | 11 | GLN |
| 41 | PO | 190 | HIS |
| 41 | PO | 298 | ASN |
| 41 | PO | 329 | GLN |
| 41 | PP | 15 | GLN |
| 41 | PP | 204 | ASN |
| 41 | QB | 14 | ASN |
| 41 | QB | 94 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | QB | 99 | ASN |
| 41 | QB | 245 | GLN |
| 41 | QB | 280 | GLN |
| 41 | QB | 298 | ASN |
| 41 | QB | 414 | ASN |
| 41 | QB | 416 | ASN |
| 41 | QB | 420 | ASN |
| 40 | QE | 31 | GLN |
| 40 | QE | 35 | GLN |
| 40 | QE | 91 | GLN |
| 40 | QE | 228 | ASN |
| 40 | QF | 228 | ASN |
| 40 | QF | 258 | ASN |
| 40 | QG | 233 | GLN |
| 41 | QL | 348 | ASN |
| 41 | QM | 165 | ASN |
| 41 | QN | 137 | HIS |
| 41 | QN | 292 | GLN |
| 41 | QN | 375 | GLN |
| 41 | QO | 137 | HIS |
| 41 | QP | 28 | HIS |
| 41 | QP | 89 | ASN |
| 41 | QP | 204 | ASN |
| 41 | QP | 414 | ASN |
| 41 | RB | 137 | HIS |
| 40 | RE | 15 | GLN |
| 40 | RF | 15 | GLN |
| 40 | RF | 228 | ASN |
| 40 | RF | 233 | GLN |
| 40 | RG | 206 | ASN |
| 40 | RH | 15 | GLN |
| 40 | RI | 88 | HIS |
| 41 | RM | 6 | HIS |
| 41 | RM | 191 | GLN |
| 41 | RM | 195 | ASN |
| 41 | RM | 292 | GLN |
| 41 | RN | 165 | ASN |
| 41 | RN | 190 | HIS |
| 41 | RO | 8 | GLN |
| 41 | RO | 14 | ASN |
| 41 | RP | 8 | GLN |
| 41 | RP | 131 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | SA | 15 | GLN |
| 40 | SA | 228 | ASN |
| 41 | SB | 191 | GLN |
| 41 | SB | 195 | ASN |
| 41 | SB | 347 | ASN |
| 40 | SE | 228 | ASN |
| 40 | SE | 283 | HIS |
| 40 | SF | 379 | ASN |
| 40 | SG | 11 | GLN |
| 40 | SG | 15 | GLN |
| 40 | SG | 249 | ASN |
| 40 | SH | 11 | GLN |
| 40 | SH | 128 | GLN |
| 40 | SI | 11 | GLN |
| 41 | SL | 334 | GLN |
| 41 | SL | 347 | ASN |
| 41 | SO | 8 | GLN |
| 41 | SO | 43 | GLN |
| 41 | SO | 131 | GLN |
| 41 | SO | 165 | ASN |
| 41 | SO | 280 | GLN |
| 41 | SO | 370 | ASN |
| 41 | SO | 416 | ASN |
| 41 | SP | 43 | GLN |
| 41 | SP | 256 | ASN |
| 41 | SP | 416 | ASN |
| 41 | TB | 131 | GLN |
| 41 | TB | 195 | ASN |
| 41 | TB | 226 | ASN |
| 41 | TB | 256 | ASN |
| 40 | TE | 379 | ASN |
| 40 | TF | 228 | ASN |
| 40 | TF | 342 | GLN |
| 40 | TH | 15 | GLN |
| 40 | TH | 206 | ASN |
| 40 | TH | 285 | GLN |
| 41 | TL | 6 | HIS |
| 41 | TL | 14 | ASN |
| 41 | TL | 184 | ASN |
| 41 | TM | 184 | ASN |
| 41 | TM | 335 | ASN |
| 41 | TN | 131 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | TO | 190 | HIS |
| 41 | TO | 245 | GLN |
| 41 | TO | 414 | ASN |
| 41 | TP | 6 | HIS |
| 41 | TP | 245 | GLN |
| 40 | UA | 101 | ASN |
| 40 | UA | 228 | ASN |
| 41 | UB | 99 | ASN |
| 41 | UB | 131 | GLN |
| 41 | UB | 329 | GLN |
| 40 | UF | 31 | GLN |
| 40 | UF | 35 | GLN |
| 40 | UF | 102 | ASN |
| 40 | UF | 228 | ASN |
| 40 | UF | 233 | GLN |
| 40 | UF | 293 | ASN |
| 40 | UF | 392 | HIS |
| 40 | UF | 405 | HIS |
| 40 | UG | 88 | HIS |
| 40 | UG | 101 | ASN |
| 40 | UH | 1 | GLN |
| 40 | UH | 88 | HIS |
| 40 | UI | 15 | GLN |
| 40 | UI | 35 | GLN |
| 40 | UI | 176 | GLN |
| 40 | UI | 256 | GLN |
| 41 | UM | 165 | ASN |
| 41 | UM | 329 | GLN |
| 41 | UM | 375 | GLN |
| 41 | UO | 256 | ASN |
| 41 | UO | 375 | GLN |
| 41 | UP | 52 | ASN |
| 41 | UP | 131 | GLN |
| 41 | UP | 134 | GLN |
| 41 | UP | 184 | ASN |
| 41 | UP | 190 | HIS |
| 41 | UP | 191 | GLN |
| 41 | UP | 329 | GLN |
| 41 | UP | 335 | ASN |
| 41 | UP | 347 | ASN |
| 41 | UP | 375 | GLN |
| 41 | UP | 420 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 40 | VA | 133 | GLN |
| 40 | VA | 329 | ASN |
| 41 | VB | 8 | GLN |
| 41 | VB | 131 | GLN |
| 40 | VF | 371 | GLN |
| 40 | VH | 11 | GLN |
| 40 | VH | 256 | GLN |
| 40 | VI | 11 | GLN |
| 41 | VN | 28 | HIS |
| 41 | VO | 256 | ASN |
| 41 | VP | 99 | ASN |
| 41 | VP | 256 | ASN |
| 41 | VP | 375 | GLN |
| 41 | VQ | 8 | GLN |
| 41 | VQ | 256 | ASN |
| 40 | WA | 8 | HIS |
| 40 | WA | 11 | GLN |
| 40 | WA | 258 | ASN |
| 41 | WB | 11 | GLN |
| 41 | WB | 204 | ASN |
| 40 | WF | 101 | ASN |
| 40 | WH | 228 | ASN |
| 40 | WI | 258 | ASN |
| 41 | WM | 184 | ASN |
| 41 | WM | 204 | ASN |
| 41 | WM | 245 | GLN |
| 41 | WM | 280 | GLN |
| 41 | WM | 370 | ASN |
| 41 | WM | 384 | GLN |
| 41 | WM | 396 | HIS |
| 41 | WM | 414 | ASN |
| 41 | WM | 420 | ASN |
| 41 | WN | 14 | ASN |
| 41 | WN | 89 | ASN |
| 41 | WN | 134 | GLN |
| 41 | WN | 292 | GLN |
| 41 | WN | 298 | ASN |
| 41 | WN | 384 | GLN |
| 41 | WO | 165 | ASN |
| 41 | WO | 190 | HIS |
| 41 | WO | 334 | GLN |
| 41 | WP | 204 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | WP | 256 | ASN |
| 41 | WQ | 99 | ASN |
| 41 | WQ | 105 | HIS |
| 41 | WQ | 191 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

269 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 43 | GDP | KM | 502 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.33 | 4 (13%) |
| 42 | GTP | PD | 501 | - | 29,34,34 | 1.29 | 2 (6%) | 35,54,54 | 1.28 | 5 (14%) |
| 43 | GDP | LL | 502 | - | 25,30,30 | 0.90 | 1 (4%) | 30,47,47 | 1.23 | 3 (10%) |
| 43 | GDP | OP | 501 | - | 25,30,30 | 0.92 | 1 (4%) | 30,47,47 | 1.17 | 4 (13%) |
| 43 | GDP | IB | 501 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.35 | 5 (16%) |
| 43 | GDP | WM | 501 | - | 25,30,30 | 0.89 | 1 (4%) | 30,47,47 | 1.50 | 4 (13%) |
| 43 | GDP | LP | 501 | - | 25,30,30 | 0.87 | 0 | 30,47,47 | 1.26 | 4 (13%) |
| 42 | GTP | BF | 501 | - | 29,34,34 | 1.33 | 3 (10%) | 35,54,54 | 1.36 | 7 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 43 | GDP | HQ | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.19 | 4 (13%) |
| 42 | GTP | KB | 502 | - | 29,34,34 | 1.37 | 2 (6%) | 35,54,54 | 1.44 | 8 (22%) |
| 42 | GTP | CH | 501 | - | 29,34,34 | 1.31 | 2 (6%) | 35,54,54 | 1.33 | 6 (17%) |
| 42 | GTP | FN | 501 | - | 29,34,34 | 1.36 | 5 (17%) | 35,54,54 | 1.33 | 7 (20%) |
| 42 | GTP | HA | 501 | - | 29,34,34 | 1.31 | 3 (10%) | 35,54,54 | 1.39 | 7 (20%) |
| 42 | GTP | JO | 501 | - | 29,34,34 | 1.42 | 2 (6%) | 35,54,54 | 1.41 | 7 (20%) |
| 42 | GTP | IF | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.35 | 7 (20%) |
| 42 | GTP | SL | 501 | - | 29,34,34 | 1.40 | 4 (13%) | 35,54,54 | 1.52 | 8 (22%) |
| 42 | GTP | FO | 501 | - | 29,34,34 | 1.42 | 4 (13%) | 35,54,54 | 1.54 | 7 (20%) |
| 42 | GTP | JD | 501 | - | 29,34,34 | 1.39 | 4 (13%) | 35,54,54 | 1.37 | 6 (17%) |
| 43 | GDP | BB | 501 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.35 | 4 (13%) |
| 43 | GDP | NN | 502 | - | 25,30,30 | 1.01 | 1 (4%) | 30,47,47 | 2.21 | 6 (20%) |
| 42 | GTP | JA | 501 | - | 29,34,34 | 1.59 | 4 (13%) | 35,54,54 | 1.42 | 8 (22%) |
| 43 | GDP | SP | 502 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.11 | 1 (3%) |
| 42 | GTP | LM | 501 | - | 29,34,34 | 1.38 | 2 (6%) | 35,54,54 | 1.34 | 7 (20%) |
| 42 | GTP | LL | 501 | - | 29,34,34 | 1.46 | 3 (10%) | 35,54,54 | 1.64 | 6 (17%) |
| 42 | GTP | PE | 501 | - | 29,34,34 | 1.36 | 2 (6%) | 35,54,54 | 1.40 | 7 (20%) |
| 43 | GDP | KL | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.28 | 4 (13%) |
| 43 | GDP | ML | 502 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.32 | 4 (13%) |
| 43 | GDP | TP | 501 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 2.44 | 6 (20%) |
| 42 | GTP | FE | 501 | - | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.34 | 5 (14%) |
| 43 | GDP | UB | 501 | - | 25,30,30 | 0.86 | 0 | 30,47,47 | 1.32 | 4 (13%) |
| 42 | GTP | II | 501 | - | 29,34,34 | 1.35 | 2 (6%) | 35,54,54 | 1.43 | 7 (20%) |
| 43 | GDP | TO | 501 | - | 25,30,30 | 0.83 | 0 | 30,47,47 | 1.86 | 6 (20%) |
| 42 | GTP | GF | 501 | - | 29,34,34 | 1.46 | 5 (17%) | 35,54,54 | 1.47 | 8 (22%) |
| 42 | GTP | VQ | 501 | - | 29,34,34 | 1.31 | 3 (10%) | 35,54,54 | 1.32 | 7 (20%) |
| 43 | GDP | HB | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.29 | 4 (13%) |
| 42 | GTP | DF | 501 | - | 29,34,34 | 1.40 | 4 (13%) | 35,54,54 | 1.47 | 6 (17%) |
| 42 | GTP | OD | 501 | - | 29,34,34 | 1.33 | 4 (13%) | 35,54,54 | 1.37 | 6 (17%) |
| 42 | GTP | UB | 502 | - | 29,34,34 | 1.34 | 2 (6%) | 35,54,54 | 1.38 | 6 (17%) |
| 42 | GTP | NO | 501 | - | 29,34,34 | 1.30 | 2 (6%) | 35,54,54 | 1.29 | 6 (17%) |
| 43 | GDP | QP | 501 | - | 25,30,30 | 1.03 | 1 (4%) | 30,47,47 | 2.42 | 7 (23%) |
| 43 | GDP | HP | 502 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.22 | 4 (13%) |
| 43 | GDP | GP | 502 | - | 25,30,30 | 1.06 | 2 (8%) | 30,47,47 | 2.27 | 8 (26%) |
| 42 | GTP | IG | 501 | - | 29,34,34 | 1.36 | 2 (6%) | 35,54,54 | 1.35 | 7 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 42 | GTP | TN | 501 | - | 29,34,34 | 1.38 | 4 (13%) | 35,54,54 | 1.32 | 5 (14%) |
| 42 | GTP | LD | 501 | - | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.29 | 5 (14%) |
| 42 | GTP | RE | 501 | - | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.40 | 6 (17%) |
| 43 | GDP | DN | 501 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.39 | 4 (13%) |
| 43 | GDP | WN | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.34 | 4 (13%) |
| 43 | GDP | PL | 501 | - | 25,30,30 | 0.93 | 0 | 30,47,47 | 1.30 | 4 (13%) |
| 42 | GTP | EI | 501 | - | 29,34,34 | 1.37 | 4 (13%) | 35,54,54 | 1.45 | 6 (17%) |
| 43 | GDP | JO | 502 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.26 | 4 (13%) |
| 42 | GTP | KD | 501 | - | 29,34,34 | 1.36 | 2 (6%) | 35,54,54 | 1.40 | 5 (14%) |
| 43 | GDP | WO | 502 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.41 | 5 (16%) |
| 42 | GTP | BH | 501 | - | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.38 | 6 (17%) |
| 42 | GTP | TH | 501 | - | 29,34,34 | 1.36 | 3 (10%) | 35,54,54 | 1.25 | 5 (14%) |
| 42 | GTP | VP | 501 | - | 29,34,34 | 1.30 | 3 (10%) | 35,54,54 | 1.44 | 7 (20%) |
| 42 | GTP | HE | 501 | - | 29,34,34 | 1.36 | 2 (6%) | 35,54,54 | 1.39 | 7 (20%) |
| 43 | GDP | SN | 502 | - | 25,30,30 | 0.94 | 2 (8%) | 30,47,47 | 2.74 | 7 (23%) |
| 42 | GTP | SM | 501 | - | 29,34,34 | 1.29 | 2 (6%) | 35,54,54 | 1.38 | 7 (20%) |
| 42 | GTP | UM | 501 | - | 29,34,34 | 1.30 | 2 (6%) | 35,54,54 | 1.43 | 6 (17%) |
| 43 | GDP | PN | 502 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.35 | 4 (13%) |
| 43 | GDP | EL | 502 | - | 25,30,30 | 0.93 | 0 | 30,47,47 | 1.16 | 4 (13%) |
| 42 | GTP | WG | 501 | - | 29,34,34 | 1.33 | 3 (10%) | 35,54,54 | 1.38 | 7 (20%) |
| 42 | GTP | RN | 501 | - | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.36 | 6 (17%) |
| 42 | GTP | VN | 501 | - | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.37 | 7 (20%) |
| 43 | GDP | EO | 501 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.23 | 4 (13%) |
| 43 | GDP | QO | 502 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.35 | 4 (13%) |
| 42 | GTP | OL | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.40 | 7 (20%) |
| 43 | GDP | DL | 501 | - | 25,30,30 | 1.12 | 3 (12%) | 30,47,47 | 2.61 | 7 (23%) |
| 43 | GDP | SL | 502 | - | 25,30,30 | 0.95 | 0 | 30,47,47 | 1.92 | 6 (20%) |
| 43 | GDP | VQ | 502 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.48 | 4 (13%) |
| 43 | GDP | FB | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.35 | 4 (13%) |
| 42 | GTP | SN | 501 | - | 29,34,34 | 1.46 | 4 (13%) | 35,54,54 | 1.46 | 8 (22%) |
| 42 | GTP | GE | 501 | - | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.27 | 4 (11%) |
| 43 | GDP | GO | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.31 | 4 (13%) |
| 42 | GTP | MN | 501 | - | 29,34,34 | 1.34 | 4 (13%) | 35,54,54 | 1.34 | 5 (14%) |
| 42 | GTP | LA | 501 | - | 29,34,34 | 1.29 | 2 (6%) | 35,54,54 | 1.38 | 6 (17%) |
| 43 | GDP | HM | 502 | - | 25,30,30 | 0.87 | 0 | 30,47,47 | 1.51 | 4 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 42 | GTP | MH | 501 | - | 29,34,34 | 1.38 | 3 (10%) | 35,54,54 | 1.38 | 7 (20%) |
| 42 | GTP | RO | 501 | - | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.40 | 7 (20%) |
| 42 | GTP | TF | 501 | - | 29,34,34 | 1.43 | 3 (10%) | 35,54,54 | 1.59 | 8 (22%) |
| 43 | GDP | AO | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.32 | 4 (13%) |
| 43 | GDP | IP | 501 | - | 25,30,30 | 0.94 | 0 | 30,47,47 | 1.26 | 4 (13%) |
| 43 | GDP | BL | 502 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.32 | 4 (13%) |
| 42 | GTP | IH | 501 | - | 29,34,34 | 1.42 | 3 (10%) | 35,54,54 | 1.50 | 8 (22%) |
| 42 | GTP | QG | 501 | - | 29,34,34 | 1.36 | 3 (10%) | 35,54,54 | 1.39 | 7 (20%) |
| 43 | GDP | MN | 502 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.32 | 4 (13%) |
| 42 | GTP | DH | 501 | - | 29,34,34 | 1.70 | 5 (17%) | 35,54,54 | 1.99 | 8 (22%) |
| 43 | GDP | AM | 501 | - | 25,30,30 | 0.87 | 1 (4%) | 30,47,47 | 1.54 | 4 (13%) |
| 42 | GTP | PM | 501 | - | 29,34,34 | 1.29 | 2 (6%) | 35,54,54 | 1.37 | 5 (14%) |
| 42 | GTP | MM | 501 | - | 29,34,34 | 1.41 | 3 (10%) | 35,54,54 | 1.63 | 8 (22%) |
| 42 | GTP | SP | 501 | - | 29,34,34 | 1.29 | 4 (13%) | 35,54,54 | 1.35 | 5 (14%) |
| 42 | GTP | GP | 501 | - | 29,34,34 | 1.48 | 4 (13%) | 35,54,54 | 1.71 | 7 (20%) |
| 42 | GTP | JE | 501 | - | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.27 | 7 (20%) |
| 42 | GTP | OB | 502 | - | 29,34,34 | 1.36 | 3 (10%) | 35,54,54 | 1.45 | 7 (20%) |
| 43 | GDP | AN | 501 | - | 25,30,30 | 0.89 | 1 (4%) | 30,47,47 | 1.45 | 4 (13%) |
| 42 | GTP | PB | 502 | - | 29,34,34 | 1.34 | 4 (13%) | 35,54,54 | 1.34 | 7 (20%) |
| 43 | GDP | FP | 501 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 2.43 | 7 (23%) |
| 43 | GDP | VO | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.37 | 4 (13%) |
| 43 | GDP | KB | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.25 | 4 (13%) |
| 42 | GTP | AE | 501 | - | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.28 | 3 (8%) |
| 42 | GTP | CA | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.32 | 6 (17%) |
| 43 | GDP | UM | 502 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.15 | 2 (6%) |
| 42 | GTP | BI | 501 | - | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.45 | 6 (17%) |
| 42 | GTP | CE | 501 | - | 29,34,34 | 1.45 | 3 (10%) | 35,54,54 | 1.33 | 7 (20%) |
| 42 | GTP | JB | 502 | - | 29,34,34 | 1.64 | 3 (10%) | 35,54,54 | 2.00 | 9 (25%) |
| 43 | GDP | PO | 502 | - | 25,30,30 | 0.92 | 0 | 30,47,47 | 1.34 | 4 (13%) |
| 43 | GDP | UP | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.26 | 5 (16%) |
| 42 | GTP | AG | 501 | - | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.37 | 6 (17%) |
| 42 | GTP | AF | 501 | - | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.36 | 6 (17%) |
| 42 | GTP | OO | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.36 | 6 (17%) |
| 43 | GDP | PM | 502 | - | 25,30,30 | 0.93 | 0 | 30,47,47 | 1.23 | 4 (13%) |
| 43 | GDP | NL | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.20 | 4 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 42 | GTP | EG | 501 | - | 29,34,34 | 1.66 | 4 (13%) | 35,54,54 | 1.71 | 9 (25%) |
| 42 | GTP | EA | 501 | - | 29,34,34 | 1.36 | 3 (10%) | 35,54,54 | 1.38 | 7 (20%) |
| 42 | GTP | ON | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.37 | 7 (20%) |
| 42 | GTP | QO | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.32 | 5 (14%) |
| 43 | GDP | LB | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.28 | 4 (13%) |
| 43 | GDP | AB | 501 | - | 25,30,30 | 0.88 | 1 (4%) | 30,47,47 | 1.45 | 4 (13%) |
| 42 | GTP | FM | 501 | - | 29,34,34 | 1.45 | 4 (13%) | 35,54,54 | 1.43 | 8 (22%) |
| 42 | GTP | GA | 501 | - | 29,34,34 | 1.65 | 5 (17%) | 35,54,54 | 1.55 | 8 (22%) |
| 42 | GTP | TL | 501 | - | 29,34,34 | 1.43 | 4 (13%) | 35,54,54 | 1.42 | 7 (20%) |
| 42 | GTP | EL | 501 | - | 29,34,34 | 1.32 | 3 (10%) | 35,54,54 | 1.30 | 7 (20%) |
| 42 | GTP | DI | 501 | - | 29,34,34 | 1.48 | 3 (10%) | 35,54,54 | 1.79 | 7 (20%) |
| 42 | GTP | HM | 501 | - | 29,34,34 | 1.38 | 3 (10%) | 35,54,54 | 1.42 | 7 (20%) |
| 42 | GTP | TG | 501 | - | 29,34,34 | 1.30 | 4 (13%) | 35,54,54 | 1.52 | 5 (14%) |
| 42 | GTP | KN | 501 | - | 29,34,34 | 1.40 | 5 (17%) | 35,54,54 | 1.79 | 8 (22%) |
| 43 | GDP | TM | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.34 | 4 (13%) |
| 43 | GDP | CB | 501 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.40 | 4 (13%) |
| 42 | GTP | WE | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.42 | 6 (17%) |
| 43 | GDP | BM | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.38 | 4 (13%) |
| 42 | GTP | WF | 501 | - | 29,34,34 | 1.37 | 4 (13%) | 35,54,54 | 1.37 | 7 (20%) |
| 43 | GDP | IQ | 501 | - | 25,30,30 | 0.93 | 0 | 30,47,47 | 1.16 | 4 (13%) |
| 43 | GDP | SO | 501 | - | 25,30,30 | 0.84 | 0 | 30,47,47 | 1.66 | 5 (16%) |
| 43 | GDP | QM | 501 | - | 25,30,30 | 0.91 | 1 (4%) | 30,47,47 | 1.53 | 4 (13%) |
| 42 | GTP | IA | 501 | - | 29,34,34 | 1.32 | 2 (6%) | 35,54,54 | 1.32 | 6 (17%) |
| 42 | GTP | AA | 501 | - | 29,34,34 | 1.33 | 5 (17%) | 35,54,54 | 1.35 | 5 (14%) |
| 42 | GTP | RG | 501 | - | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.38 | 5 (14%) |
| 42 | GTP | CF | 501 | - | 29,34,34 | 1.36 | 4 (13%) | 35,54,54 | 1.34 | 6 (17%) |
| 43 | GDP | EN | 501 | - | 25,30,30 | 0.88 | 2 (8%) | 30,47,47 | 2.07 | 7 (23%) |
| 43 | GDP | OL | 502 | - | 25,30,30 | 0.93 | 0 | 30,47,47 | 1.24 | 4 (13%) |
| 43 | GDP | FO | 502 | - | 25,30,30 | 0.87 | 0 | 30,47,47 | 1.34 | 4 (13%) |
| 43 | GDP | BN | 501 | - | 25,30,30 | 0.87 | 0 | 30,47,47 | 1.50 | 4 (13%) |
| 42 | GTP | MB | 502 | - | 29,34,34 | 1.54 | 5 (17%) | 35,54,54 | 1.40 | 5 (14%) |
| 42 | GTP | ML | 501 | - | 29,34,34 | 1.44 | 3 (10%) | 35,54,54 | 1.52 | 7 (20%) |
| 43 | GDP | OB | 501 | - | 25,30,30 | 0.92 | 0 | 30,47,47 | 1.34 | 4 (13%) |
| 42 | GTP | SH | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.46 | 7 (20%) |
| 43 | GDP | BP | 501 | - | 25,30,30 | 0.90 | 1 (4%) | 30,47,47 | 1.46 | 4 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 43 | GDP | DB | 501 | - | 25,30,30 | 0.86 | 0 | 30,47,47 | 1.64 | 6 (20%) |
| 42 | GTP | ND | 501 | - | 29,34,34 | 1.26 | 3 (10%) | 35,54,54 | 1.24 | 3 (8%) |
| 42 | GTP | DE | 501 | - | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.37 | 5 (14%) |
| 43 | GDP | FM | 502 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.20 | 4 (13%) |
| 42 | GTP | KE | 501 | - | 29,34,34 | 1.33 | 4 (13%) | 35,54,54 | 1.35 | 5 (14%) |
| 42 | GTP | HP | 501 | - | 29,34,34 | 1.38 | 5 (17%) | 35,54,54 | 1.39 | 6 (17%) |
| 42 | GTP | VB | 502 | - | 29,34,34 | 1.35 | 2 (6%) | 35,54,54 | 1.32 | 7 (20%) |
| 43 | GDP | BO | 501 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.25 | 4 (13%) |
| 43 | GDP | CM | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.36 | 4 (13%) |
| 43 | GDP | HN | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.30 | 4 (13%) |
| 42 | GTP | PO | 501 | - | 29,34,34 | 1.39 | 2 (6%) | 35,54,54 | 1.40 | 8 (22%) |
| 43 | GDP | LN | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.26 | 4 (13%) |
| 43 | GDP | NB | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.29 | 4 (13%) |
| 43 | GDP | RO | 502 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.35 | 4 (13%) |
| 43 | GDP | GN | 501 | - | 25,30,30 | 0.88 | 1 (4%) | 30,47,47 | 1.63 | 6 (20%) |
| 43 | GDP | IN | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.24 | 4 (13%) |
| 42 | GTP | WO | 501 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.42 | 7 (20%) |
| 43 | GDP | NM | 502 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.46 | 5 (16%) |
| 43 | GDP | CL | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.30 | 4 (13%) |
| 43 | GDP | QL | 502 | - | 25,30,30 | 0.93 | 0 | 30,47,47 | 1.22 | 4 (13%) |
| 43 | GDP | VB | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.27 | 4 (13%) |
| 43 | GDP | FN | 502 | - | 25,30,30 | 0.85 | 1 (4%) | 30,47,47 | 2.07 | 6 (20%) |
| 42 | GTP | IE | 501 | - | 29,34,34 | 1.31 | 3 (10%) | 35,54,54 | 1.28 | 5 (14%) |
| 42 | GTP | DG | 501 | - | 29,34,34 | 1.47 | 4 (13%) | 35,54,54 | 1.47 | 8 (22%) |
| 43 | GDP | GM | 501 | - | 25,30,30 | 0.90 | 1 (4%) | 30,47,47 | 1.46 | 4 (13%) |
| 43 | GDP | RB | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.39 | 5 (16%) |
| 42 | GTP | PN | 501 | - | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.34 | 5 (14%) |
| 43 | GDP | WB | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.28 | 4 (13%) |
| 43 | GDP | HO | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.24 | 4 (13%) |
| 42 | GTP | NG | 501 | - | 29,34,34 | 1.36 | 2 (6%) | 35,54,54 | 1.34 | 5 (14%) |
| 42 | GTP | AH | 501 | - | 29,34,34 | 1.31 | 3 (10%) | 35,54,54 | 1.34 | 5 (14%) |
| 43 | GDP | RM | 501 | - | 25,30,30 | 0.89 | 1 (4%) | 30,47,47 | 1.78 | 8 (26%) |
| 42 | GTP | FB | 502 | - | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.43 | 7 (20%) |
| 42 | GTP | SG | 501 | - | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.39 | 7 (20%) |
| 43 | GDP | RN | 502 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 2.58 | 6 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 42 | GTP | KO | 501 | - | 29,34,34 | 1.77 | 5 (17%) | 35,54,54 | 1.80 | 7 (20%) |
| 43 | GDP | GB | 501 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.28 | 4 (13%) |
| 43 | GDP | CN | 501 | - | 25,30,30 | 0.87 | 1 (4%) | 30,47,47 | 1.50 | 4 (13%) |
| 42 | GTP | DA | 501 | - | 29,34,34 | 1.35 | 4 (13%) | 35,54,54 | 1.43 | 8 (22%) |
| 43 | GDP | JN | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.27 | 4 (13%) |
| 42 | GTP | GH | 501 | - | 29,34,34 | 1.31 | 2 (6%) | 35,54,54 | 1.47 | 8 (22%) |
| 42 | GTP | KM | 501 | - | 29,34,34 | 1.57 | 3 (10%) | 35,54,54 | 1.67 | 8 (22%) |
| 42 | GTP | BL | 501 | - | 29,34,34 | 1.29 | 2 (6%) | 35,54,54 | 1.40 | 5 (14%) |
| 43 | GDP | EP | 501 | - | 25,30,30 | 0.85 | 1 (4%) | 30,47,47 | 2.41 | 8 (26%) |
| 42 | GTP | VF | 501 | - | 29,34,34 | 1.30 | 4 (13%) | 35,54,54 | 1.31 | 6 (17%) |
| 43 | GDP | UO | 502 | - | 25,30,30 | 0.87 | 0 | 30,47,47 | 1.39 | 5 (16%) |
| 42 | GTP | WI | 501 | - | 29,34,34 | 1.30 | 2 (6%) | 35,54,54 | 1.48 | 7 (20%) |
| 43 | GDP | CP | 501 | - | 25,30,30 | 0.93 | 0 | 30,47,47 | 1.31 | 4 (13%) |
| 42 | GTP | CG | 501 | - | 29,34,34 | 1.39 | 3 (10%) | 35,54,54 | 1.45 | 7 (20%) |
| 42 | GTP | CI | 501 | - | 29,34,34 | 1.26 | 1 (3%) | 35,54,54 | 1.33 | 5 (14%) |
| 43 | GDP | VP | 502 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.39 | 4 (13%) |
| 43 | GDP | MO | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.33 | 4 (13%) |
| 43 | GDP | TL | 502 | - | 25,30,30 | 0.97 | 2 (8%) | 30,47,47 | 2.69 | 6 (20%) |
| 42 | GTP | QF | 501 | - | 29,34,34 | 1.36 | 4 (13%) | 35,54,54 | 1.42 | 7 (20%) |
| 42 | GTP | UA | 501 | - | 29,34,34 | 1.74 | 6 (20%) | 35,54,54 | 2.01 | 9 (25%) |
| 42 | GTP | OM | 501 | - | 29,34,34 | 1.28 | 4 (13%) | 35,54,54 | 1.29 | 4 (11%) |
| 43 | GDP | DM | 501 | - | 25,30,30 | 0.82 | 0 | 30,47,47 | 1.70 | 6 (20%) |
| 43 | GDP | SM | 502 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.40 | 6 (20%) |
| 43 | GDP | TN | 502 | - | 25,30,30 | 0.90 | 1 (4%) | 30,47,47 | 1.31 | 4 (13%) |
| 42 | GTP | MD | 501 | - | 29,34,34 | 1.43 | 4 (13%) | 35,54,54 | 1.55 | 8 (22%) |
| 43 | GDP | AP | 501 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 42 | GTP | JF | 501 | - | 29,34,34 | 1.31 | 2 (6%) | 35,54,54 | 1.42 | 8 (22%) |
| 42 | GTP | UO | 501 | - | 29,34,34 | 1.31 | 2 (6%) | 35,54,54 | 1.36 | 6 (17%) |
| 43 | GDP | QB | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.21 | 4 (13%) |
| 43 | GDP | VN | 502 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.27 | 4 (13%) |
| 42 | GTP | HB | 502 | - | 29,34,34 | 1.30 | 3 (10%) | 35,54,54 | 1.36 | 5 (14%) |
| 42 | GTP | NE | 501 | - | 29,34,34 | 1.32 | 2 (6%) | 35,54,54 | 1.44 | 7 (20%) |
| 43 | GDP | SB | 501 | - | 25,30,30 | 0.86 | 1 (4%) | 30,47,47 | 2.02 | 6 (20%) |
| 42 | GTP | TI | 501 | - | 29,34,34 | 1.66 | 2 (6%) | 35,54,54 | 1.72 | 6 (17%) |
| 43 | GDP | JM | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.34 | 4 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 42 | GTP | VA | 501 | - | 29,34,34 | 1.38 | 3 (10%) | 35,54,54 | 1.40 | 9 (25%) |
| 43 | GDP | EB | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.37 | 4 (13%) |
| 43 | GDP | CO | 501 | - | 25,30,30 | 0.90 | 1 (4%) | 30,47,47 | 1.51 | 4 (13%) |
| 43 | GDP | OO | 502 | - | 25,30,30 | 0.92 | 0 | 30,47,47 | 1.23 | 4 (13%) |
| 43 | GDP | QN | 502 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.42 | 5 (16%) |
| 43 | GDP | UN | 501 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.23 | 4 (13%) |
| 42 | GTP | WA | 501 | - | 29,34,34 | 1.31 | 3 (10%) | 35,54,54 | 1.37 | 7 (20%) |
| 43 | GDP | LO | 502 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.31 | 4 (13%) |
| 42 | GTP | LB | 502 | - | 29,34,34 | 1.35 | 2 (6%) | 35,54,54 | 1.37 | 7 (20%) |
| 42 | GTP | EF | 501 | - | 29,34,34 | 1.32 | 2 (6%) | 35,54,54 | 1.38 | 6 (17%) |
| 42 | GTP | EH | 501 | - | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.28 | 5 (14%) |
| 42 | GTP | NM | 501 | - | 29,34,34 | 1.32 | 3 (10%) | 35,54,54 | 1.27 | 5 (14%) |
| 42 | GTP | UE | 501 | - | 29,34,34 | 1.37 | 5 (17%) | 35,54,54 | 1.28 | 6 (17%) |
| 43 | GDP | DO | 501 | - | 25,30,30 | 0.86 | 0 | 30,47,47 | 1.40 | 4 (13%) |
| 43 | GDP | DP | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.21 | 4 (13%) |
| 43 | GDP | JL | 501 | - | 25,30,30 | 0.95 | 2 (8%) | 30,47,47 | 2.36 | 7 (23%) |
| 43 | GDP | MP | 501 | - | 25,30,30 | 0.90 | 1 (4%) | 30,47,47 | 1.49 | 4 (13%) |
| 43 | GDP | EM | 501 | - | 25,30,30 | 0.91 | 2 (8%) | 30,47,47 | 1.99 | 7 (23%) |
| 43 | GDP | ON | 502 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.43 | 4 (13%) |
| 42 | GTP | UI | 501 | - | 29,34,34 | 1.39 | 4 (13%) | 35,54,54 | 1.45 | 7 (20%) |
| 43 | GDP | RL | 501 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.23 | 4 (13%) |
| 43 | GDP | NP | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 1.21 | 4 (13%) |
| 42 | GTP | RP | 501 | - | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.38 | 5 (14%) |
| 43 | GDP | KN | 502 | - | 25,30,30 | 0.85 | 0 | 30,47,47 | 1.39 | 4 (13%) |
| 42 | GTP | GB | 502 | - | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.43 | 7 (20%) |
| 43 | GDP | AL | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.19 | 4 (13%) |
| 43 | GDP | MB | 501 | - | 25,30,30 | 0.89 | 1 (4%) | 30,47,47 | 1.41 | 4 (13%) |
| 43 | GDP | IO | 501 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.27 | 4 (13%) |
| 43 | GDP | KP | 501 | - | 25,30,30 | 0.86 | 0 | 30,47,47 | 1.47 | 4 (13%) |
| 43 | GDP | LM | 502 | - | 25,30,30 | 0.88 | 1 (4%) | 30,47,47 | 1.50 | 4 (13%) |
| 43 | GDP | WQ | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.21 | 4 (13%) |
| 43 | GDP | NO | 502 | - | 25,30,30 | 0.92 | 0 | 30,47,47 | 1.30 | 4 (13%) |
| 43 | GDP | PB | 501 | - | 25,30,30 | 0.91 | 0 | 30,47,47 | 1.34 | 4 (13%) |
| 42 | GTP | BA | 501 | - | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.35 | 5 (14%) |
| 42 | GTP | BG | 501 | - | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.35 | 4 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 43 | GDP | OM | 502 | - | 25,30,30 | 0.93 | 0 | 30,47,47 | 1.23 | 4 (13%) |
| 42 | GTP | HH | 501 | - | 29,34,34 | 1.32 | 3 (10%) | 35,54,54 | 1.46 | 6 (17%) |
| 43 | GDP | TB | 501 | - | 25,30,30 | 0.89 | 0 | 30,47,47 | 2.07 | 9 (30%) |
| 43 | GDP | RP | 502 | - | 25,30,30 | 0.80 | 2 (8%) | 30,47,47 | 2.69 | 8 (26%) |
| 43 | GDP | JB | 501 | - | 25,30,30 | 0.88 | 0 | 30,47,47 | 1.44 | 4 (13%) |
| 43 | GDP | IM | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.31 | 4 (13%) |
| 42 | GTP | NN | 501 | - | 29,34,34 | 1.34 | 2 (6%) | 35,54,54 | 1.37 | 4 (11%) |
| 42 | GTP | QN | 501 | - | 29,34,34 | 1.53 | 5 (17%) | 35,54,54 | 1.42 | 6 (17%) |
| 43 | GDP | WP | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.25 | 4 (13%) |
| 42 | GTP | QL | 501 | - | 29,34,34 | 1.75 | 7 (24%) | 35,54,54 | 1.86 | 12 (34%) |
| 42 | GTP | RF | 501 | - | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.31 | 6 (17%) |
| 43 | GDP | PP | 501 | - | 25,30,30 | 0.90 | 0 | 30,47,47 | 1.35 | 4 (13%) |
| 43 | GDP | KO | 502 | - | 25,30,30 | 0.89 | 2 (8%) | 30,47,47 | 2.05 | 7 (23%) |
| 42 | GTP | LO | 501 | - | 29,34,34 | 1.35 | 3 (10%) | 35,54,54 | 1.40 | 6 (17%) |
| 43 | GDP | MM | 502 | - | 25,30,30 | 0.87 | 0 | 30,47,47 | 1.32 | 4 (13%) |
| 42 | GTP | FI | 501 | - | 29,34,34 | 1.32 | 2 (6%) | 35,54,54 | 1.49 | 7 (20%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 43 | GDP | KM | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | PD | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 43 | GDP | LL | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | OP | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | IB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | WM | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | LP | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | BF | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | HQ | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | KB | 502 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | CH | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | FN | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | HA | 501 | - | - | 9/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 42 | GTP | JO | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | IF | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | SL | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | FO | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 42 | GTP | JD | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 43 | GDP | BB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | NN | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | JA | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | SP | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | LM | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 42 | GTP | LL | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | PE | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | KL | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | ML | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | TP | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | FE | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 43 | GDP | UB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | II | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | TO | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | GF | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | VQ | 501 | - | - | 9/18/38/38 | 0/3/3/3 |
| 43 | GDP | HB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | DF | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 42 | GTP | OD | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | UB | 502 | - | - | 3/18/38/38 | 0/3/3/3 |
| 42 | GTP | NO | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 43 | GDP | QP | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | HP | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | GP | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | IG | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | TN | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | LD | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | RE | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | DN | 501 | - | - | 3/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 43 | GDP | WN | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | PL | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | EI | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 43 | GDP | JO | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | KD | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | WO | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | BH | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | TH | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 42 | GTP | VP | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 42 | GTP | HE | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 43 | GDP | SN | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | SM | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 42 | GTP | UM | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 43 | GDP | PN | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | EL | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | WG | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | RN | 501 | - | - | 9/18/38/38 | 0/3/3/3 |
| 42 | GTP | VN | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | EO | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | QO | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | OL | 501 | - | - | 10/18/38/38 | 0/3/3/3 |
| 43 | GDP | DL | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | SL | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | VQ | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | FB | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 42 | GTP | SN | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | GE | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | GO | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | MN | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | LA | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | HM | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | MH | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | RO | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | TF | 501 | - | - | 6/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 43 | GDP | AO | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | IP | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | BL | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | IH | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | QG | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 43 | GDP | MN | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | DH | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | AM | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | PM | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | MM | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | SP | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 42 | GTP | GP | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | JE | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | OB | 502 | - | - | 8/18/38/38 | 0/3/3/3 |
| 43 | GDP | AN | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | PB | 502 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | FP | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | VO | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | KB | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | AE | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | CA | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 43 | GDP | UM | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | BI | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | CE | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | JB | 502 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | PO | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | UP | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | AG | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | AF | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | OO | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | PM | 502 | - | - | 5/12/32/32 | 0/3/3/3 |
| 43 | GDP | NL | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | EG | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | EA | 501 | - | - | 5/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 42 | GTP | ON | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | QO | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 43 | GDP | LB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | AB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | FM | 501 | - | - | 9/18/38/38 | 0/3/3/3 |
| 42 | GTP | GA | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 42 | GTP | TL | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 42 | GTP | EL | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | DI | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | HM | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | TG | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | KN | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | TM | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | CB | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 42 | GTP | WE | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | BM | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | WF | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | IQ | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | SO | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | QM | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | IA | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 42 | GTP | AA | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 42 | GTP | RG | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | CF | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 43 | GDP | EN | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | OL | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | FO | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | BN | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | MB | 502 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | ML | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | OB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | SH | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 43 | GDP | BP | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | DB | 501 | - | - | 3/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 42 | GTP | ND | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | DE | 501 | - | - | 9/18/38/38 | 0/3/3/3 |
| 43 | GDP | FM | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 42 | GTP | KE | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | HP | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | VB | 502 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | BO | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | CM | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | HN | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 42 | GTP | PO | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | LN | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | NB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | RO | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | GN | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | IN | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | WO | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | NM | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | CL | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | QL | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | VB | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | FN | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 42 | GTP | IE | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | DG | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 43 | GDP | GM | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | RB | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | PN | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 43 | GDP | WB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | HO | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | NG | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 42 | GTP | AH | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | RM | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 42 | GTP | FB | 502 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | SG | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | RN | 502 | - | - | 2/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 42 | GTP | KO | 501 | - | - | 10/18/38/38 | 0/3/3/3 |
| 43 | GDP | GB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | CN | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | DA | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 43 | GDP | JN | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | GH | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 42 | GTP | KM | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | BL | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 43 | GDP | EP | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 42 | GTP | VF | 501 | - | - | 10/18/38/38 | 0/3/3/3 |
| 43 | GDP | UO | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | WI | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | CP | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | CG | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | CI | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | VP | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | MO | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | TL | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | QF | 501 | - | - | 9/18/38/38 | 0/3/3/3 |
| 42 | GTP | UA | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 42 | GTP | OM | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | DM | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | SM | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | TN | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 42 | GTP | MD | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | AP | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | JF | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 42 | GTP | UO | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | QB | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | VN | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | HB | 502 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | NE | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 43 | GDP | SB | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 42 | GTP | TI | 501 | - | - | 7/18/38/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 43 | GDP | JM | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | VA | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | EB | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | CO | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | OO | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | QN | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | UN | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | WA | 501 | - | - | 9/18/38/38 | 0/3/3/3 |
| 43 | GDP | LO | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | LB | 502 | - | - | 4/18/38/38 | 0/3/3/3 |
| 42 | GTP | EF | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | EH | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | NM | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | UE | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | DO | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | DP | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | JL | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | MP | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | EM | 501 | - | - | 2/12/32/32 | 0/3/3/3 |
| 43 | GDP | ON | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | UI | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 43 | GDP | RL | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | NP | 501 | - | - | 5/12/32/32 | 0/3/3/3 |
| 42 | GTP | RP | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | KN | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | GB | 502 | - | - | 9/18/38/38 | 0/3/3/3 |
| 43 | GDP | AL | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | MB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | IO | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | KP | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | LM | 502 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | WQ | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | NO | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | PB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 42 | GTP | BA | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 42 | GTP | BG | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | OM | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | HH | 501 | - | - | 4/18/38/38 | 0/3/3/3 |
| 43 | GDP | TB | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | RP | 502 | - | - | 1/12/32/32 | 0/3/3/3 |
| 43 | GDP | JB | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 43 | GDP | IM | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | NN | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 42 | GTP | QN | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 43 | GDP | WP | 501 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | QL | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 42 | GTP | RF | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 43 | GDP | PP | 501 | - | - | 3/12/32/32 | 0/3/3/3 |
| 43 | GDP | KO | 502 | - | - | 2/12/32/32 | 0/3/3/3 |
| 42 | GTP | LO | 501 | - | - | 9/18/38/38 | 0/3/3/3 |
| 43 | GDP | MM | 502 | - | - | 4/12/32/32 | 0/3/3/3 |
| 42 | GTP | FI | 501 | - | - | 6/18/38/38 | 0/3/3/3 |

All (452) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | TI | 501 | GTP | C5-C6 | -5.97 | 1.35 | 1.47 |
| 42 | JB | 502 | GTP | C5-C6 | -5.87 | 1.35 | 1.47 |
| 42 | KO | 501 | GTP | C5-C6 | -5.67 | 1.36 | 1.47 |
| 42 | EG | 501 | GTP | C5-C6 | -5.64 | 1.36 | 1.47 |
| 42 | UA | 501 | GTP | C5-C6 | -5.47 | 1.36 | 1.47 |
| 42 | DH | 501 | GTP | C5-C6 | -5.39 | 1.36 | 1.47 |
| 42 | FM | 501 | GTP | C5-C6 | -5.19 | 1.37 | 1.47 |
| 42 | PO | 501 | GTP | C5-C6 | -5.17 | 1.37 | 1.47 |
| 42 | KM | 501 | GTP | C5-C6 | -5.16 | 1.37 | 1.47 |
| 42 | DG | 501 | GTP | C5-C6 | -5.14 | 1.37 | 1.47 |
| 42 | FO | 501 | GTP | C5-C6 | -5.12 | 1.37 | 1.47 |
| 42 | JO | 501 | GTP | C5-C6 | -5.10 | 1.37 | 1.47 |
| 42 | ML | 501 | GTP | C5-C6 | -5.09 | 1.37 | 1.47 |
| 42 | TF | 501 | GTP | C5-C6 | -5.05 | 1.37 | 1.47 |
| 42 | GP | 501 | GTP | C5-C6 | -5.05 | 1.37 | 1.47 |
| 42 | QL | 501 | GTP | C5-C6 | -5.04 | 1.37 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | EA | 501 | GTP | C5-C6 | -5.03 | 1.37 | 1.47 |
| 42 | DI | 501 | GTP | C5-C6 | -5.03 | 1.37 | 1.47 |
| 42 | LL | 501 | GTP | C5-C6 | -5.02 | 1.37 | 1.47 |
| 42 | LB | 502 | GTP | C5-C6 | -5.01 | 1.37 | 1.47 |
| 42 | IG | 501 | GTP | C5-C6 | -5.00 | 1.37 | 1.47 |
| 42 | CG | 501 | GTP | C5-C6 | -4.99 | 1.37 | 1.47 |
| 42 | CE | 501 | GTP | C5-C6 | -4.99 | 1.37 | 1.47 |
| 42 | GF | 501 | GTP | C5-C6 | -4.98 | 1.37 | 1.47 |
| 42 | VB | 502 | GTP | C5-C6 | -4.95 | 1.37 | 1.47 |
| 42 | DF | 501 | GTP | C5-C6 | -4.94 | 1.37 | 1.47 |
| 42 | HE | 501 | GTP | C5-C6 | -4.94 | 1.37 | 1.47 |
| 42 | KB | 502 | GTP | C5-C6 | -4.93 | 1.37 | 1.47 |
| 42 | FI | 501 | GTP | C5-C6 | -4.91 | 1.37 | 1.47 |
| 42 | JF | 501 | GTP | C5-C6 | -4.90 | 1.37 | 1.47 |
| 42 | PE | 501 | GTP | C5-C6 | -4.90 | 1.37 | 1.47 |
| 42 | IH | 501 | GTP | C5-C6 | -4.90 | 1.37 | 1.47 |
| 42 | LM | 501 | GTP | C5-C6 | -4.89 | 1.37 | 1.47 |
| 42 | II | 501 | GTP | C5-C6 | -4.88 | 1.37 | 1.47 |
| 42 | KD | 501 | GTP | C5-C6 | -4.88 | 1.37 | 1.47 |
| 42 | HH | 501 | GTP | C5-C6 | -4.87 | 1.37 | 1.47 |
| 42 | GH | 501 | GTP | C5-C6 | -4.86 | 1.37 | 1.47 |
| 42 | UO | 501 | GTP | C5-C6 | -4.84 | 1.37 | 1.47 |
| 42 | LO | 501 | GTP | C5-C6 | -4.84 | 1.37 | 1.47 |
| 42 | UB | 502 | GTP | C5-C6 | -4.83 | 1.37 | 1.47 |
| 42 | JA | 501 | GTP | C5-C6 | -4.82 | 1.37 | 1.47 |
| 42 | HM | 501 | GTP | C5-C6 | -4.82 | 1.37 | 1.47 |
| 42 | UI | 501 | GTP | C5-C6 | -4.81 | 1.37 | 1.47 |
| 42 | WF | 501 | GTP | C5-C6 | -4.80 | 1.37 | 1.47 |
| 42 | CF | 501 | GTP | C5-C6 | -4.80 | 1.38 | 1.47 |
| 42 | EF | 501 | GTP | C5-C6 | -4.80 | 1.38 | 1.47 |
| 42 | SL | 501 | GTP | C5-C6 | -4.79 | 1.38 | 1.47 |
| 42 | WG | 501 | GTP | C5-C6 | -4.78 | 1.38 | 1.47 |
| 42 | EI | 501 | GTP | C5-C6 | -4.78 | 1.38 | 1.47 |
| 42 | QG | 501 | GTP | C5-C6 | -4.77 | 1.38 | 1.47 |
| 42 | QF | 501 | GTP | C5-C6 | -4.77 | 1.38 | 1.47 |
| 42 | MH | 501 | GTP | C5-C6 | -4.76 | 1.38 | 1.47 |
| 42 | CH | 501 | GTP | C5-C6 | -4.76 | 1.38 | 1.47 |
| 42 | WA | 501 | GTP | C5-C6 | -4.75 | 1.38 | 1.47 |
| 42 | GB | 502 | GTP | C5-C6 | -4.74 | 1.38 | 1.47 |
| 42 | RF | 501 | GTP | C5-C6 | -4.74 | 1.38 | 1.47 |
| 42 | NG | 501 | GTP | C5-C6 | -4.73 | 1.38 | 1.47 |
| 42 | NE | 501 | GTP | C5-C6 | -4.72 | 1.38 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | IA | 501 | GTP | C5-C6 | -4.70 | 1.38 | 1.47 |
| 42 | QN | 501 | GTP | C5-C6 | -4.70 | 1.38 | 1.47 |
| 42 | CA | 501 | GTP | C5-C6 | -4.68 | 1.38 | 1.47 |
| 42 | VA | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 42 | JA | 501 | GTP | PB-O3B | 4.67 | 1.64 | 1.59 |
| 42 | GA | 501 | GTP | C5-C6 | -4.67 | 1.38 | 1.47 |
| 42 | PB | 502 | GTP | C5-C6 | -4.66 | 1.38 | 1.47 |
| 42 | KE | 501 | GTP | C5-C6 | -4.65 | 1.38 | 1.47 |
| 42 | TH | 501 | GTP | C5-C6 | -4.65 | 1.38 | 1.47 |
| 42 | WE | 501 | GTP | C5-C6 | -4.64 | 1.38 | 1.47 |
| 42 | LA | 501 | GTP | C5-C6 | -4.64 | 1.38 | 1.47 |
| 42 | BF | 501 | GTP | C5-C6 | -4.63 | 1.38 | 1.47 |
| 42 | SH | 501 | GTP | C5-C6 | -4.63 | 1.38 | 1.47 |
| 42 | WI | 501 | GTP | C5-C6 | -4.62 | 1.38 | 1.47 |
| 42 | UM | 501 | GTP | C5-C6 | -4.61 | 1.38 | 1.47 |
| 42 | OO | 501 | GTP | C5-C6 | -4.60 | 1.38 | 1.47 |
| 42 | OB | 502 | GTP | C5-C6 | -4.60 | 1.38 | 1.47 |
| 42 | EL | 501 | GTP | C5-C6 | -4.59 | 1.38 | 1.47 |
| 42 | NN | 501 | GTP | C5-C6 | -4.59 | 1.38 | 1.47 |
| 42 | WO | 501 | GTP | C5-C6 | -4.59 | 1.38 | 1.47 |
| 42 | ON | 501 | GTP | C5-C6 | -4.58 | 1.38 | 1.47 |
| 42 | TL | 501 | GTP | C5-C6 | -4.57 | 1.38 | 1.47 |
| 42 | SN | 501 | GTP | C5-C6 | -4.57 | 1.38 | 1.47 |
| 42 | MD | 501 | GTP | C5-C6 | -4.57 | 1.38 | 1.47 |
| 42 | SM | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |
| 42 | NM | 501 | GTP | C5-C6 | -4.56 | 1.38 | 1.47 |
| 42 | VN | 501 | GTP | C5-C6 | -4.55 | 1.38 | 1.47 |
| 42 | IF | 501 | GTP | C5-C6 | -4.55 | 1.38 | 1.47 |
| 42 | HP | 501 | GTP | C5-C6 | -4.55 | 1.38 | 1.47 |
| 42 | OD | 501 | GTP | C5-C6 | -4.55 | 1.38 | 1.47 |
| 42 | IE | 501 | GTP | C5-C6 | -4.55 | 1.38 | 1.47 |
| 42 | RO | 501 | GTP | C5-C6 | -4.54 | 1.38 | 1.47 |
| 42 | RG | 501 | GTP | C5-C6 | -4.54 | 1.38 | 1.47 |
| 42 | JE | 501 | GTP | C5-C6 | -4.54 | 1.38 | 1.47 |
| 42 | MB | 502 | GTP | C5-C6 | -4.53 | 1.38 | 1.47 |
| 42 | SG | 501 | GTP | C5-C6 | -4.52 | 1.38 | 1.47 |
| 42 | NO | 501 | GTP | C5-C6 | -4.50 | 1.38 | 1.47 |
| 42 | QO | 501 | GTP | C5-C6 | -4.49 | 1.38 | 1.47 |
| 42 | FE | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 42 | FN | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 42 | VQ | 501 | GTP | C5-C6 | -4.48 | 1.38 | 1.47 |
| 42 | VP | 501 | GTP | C5-C6 | -4.46 | 1.38 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | OL | 501 | GTP | C5-C6 | -4.45 | 1.38 | 1.47 |
| 42 | HA | 501 | GTP | C5-C6 | -4.44 | 1.38 | 1.47 |
| 42 | PM | 501 | GTP | C5-C6 | -4.44 | 1.38 | 1.47 |
| 42 | VF | 501 | GTP | C5-C6 | -4.43 | 1.38 | 1.47 |
| 42 | TN | 501 | GTP | C5-C6 | -4.43 | 1.38 | 1.47 |
| 42 | UE | 501 | GTP | C5-C6 | -4.42 | 1.38 | 1.47 |
| 42 | PD | 501 | GTP | C5-C6 | -4.41 | 1.38 | 1.47 |
| 42 | MM | 501 | GTP | C5-C6 | -4.41 | 1.38 | 1.47 |
| 42 | MN | 501 | GTP | C5-C6 | -4.41 | 1.38 | 1.47 |
| 42 | BI | 501 | GTP | C5-C6 | -4.40 | 1.38 | 1.47 |
| 42 | RE | 501 | GTP | C5-C6 | -4.40 | 1.38 | 1.47 |
| 42 | HB | 502 | GTP | C5-C6 | -4.40 | 1.38 | 1.47 |
| 42 | FB | 502 | GTP | C5-C6 | -4.40 | 1.38 | 1.47 |
| 42 | BL | 501 | GTP | C5-C6 | -4.36 | 1.38 | 1.47 |
| 42 | RN | 501 | GTP | C5-C6 | -4.36 | 1.38 | 1.47 |
| 42 | EH | 501 | GTP | C5-C6 | -4.36 | 1.38 | 1.47 |
| 42 | DE | 501 | GTP | C5-C6 | -4.35 | 1.38 | 1.47 |
| 42 | AA | 501 | GTP | C5-C6 | -4.35 | 1.38 | 1.47 |
| 42 | KO | 501 | GTP | C2-N3 | 4.31 | 1.43 | 1.33 |
| 42 | LD | 501 | GTP | C5-C6 | -4.30 | 1.38 | 1.47 |
| 42 | PN | 501 | GTP | C5-C6 | -4.30 | 1.38 | 1.47 |
| 42 | DA | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 42 | AH | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 42 | CI | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 42 | AG | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 42 | GE | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 42 | BG | 501 | GTP | C5-C6 | -4.27 | 1.39 | 1.47 |
| 42 | BH | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 42 | EG | 501 | GTP | PB-O3B | 4.25 | 1.64 | 1.59 |
| 42 | BA | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 42 | ND | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 42 | SP | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 42 | AF | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 42 | RP | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 42 | AE | 501 | GTP | C5-C6 | -4.17 | 1.39 | 1.47 |
| 42 | KN | 501 | GTP | C5-C6 | -4.15 | 1.39 | 1.47 |
| 42 | DH | 501 | GTP | C2-N3 | 4.14 | 1.43 | 1.33 |
| 42 | JD | 501 | GTP | C5-C6 | -4.12 | 1.39 | 1.47 |
| 42 | QL | 501 | GTP | C2-N3 | 4.12 | 1.43 | 1.33 |
| 42 | UA | 501 | GTP | C2-N3 | 4.07 | 1.43 | 1.33 |
| 42 | OM | 501 | GTP | C5-C6 | -4.06 | 1.39 | 1.47 |
| 42 | GA | 501 | GTP | PB-O3B | 4.05 | 1.63 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | TI | 501 | GTP | C2-N3 | 3.83 | 1.42 | 1.33 |
| 42 | KM | 501 | GTP | C2-N3 | 3.75 | 1.42 | 1.33 |
| 42 | JB | 502 | GTP | C2-N3 | 3.71 | 1.42 | 1.33 |
| 42 | SN | 501 | GTP | C2-N3 | 3.63 | 1.42 | 1.33 |
| 42 | DI | 501 | GTP | C2-N3 | 3.37 | 1.41 | 1.33 |
| 42 | GA | 501 | GTP | C2-N3 | 3.35 | 1.41 | 1.33 |
| 42 | GA | 501 | GTP | PB-O3A | 3.33 | 1.63 | 1.59 |
| 42 | QN | 501 | GTP | PB-O3B | 3.32 | 1.63 | 1.59 |
| 42 | MD | 501 | GTP | C2-N3 | 3.32 | 1.41 | 1.33 |
| 42 | TF | 501 | GTP | C2-N3 | 3.31 | 1.41 | 1.33 |
| 42 | MM | 501 | GTP | C2-N3 | 3.30 | 1.41 | 1.33 |
| 42 | GP | 501 | GTP | C2-N3 | 3.30 | 1.41 | 1.33 |
| 42 | ML | 501 | GTP | C2-N3 | 3.26 | 1.41 | 1.33 |
| 42 | KN | 501 | GTP | C2-N3 | 3.26 | 1.41 | 1.33 |
| 42 | LL | 501 | GTP | C2-N3 | 3.20 | 1.41 | 1.33 |
| 42 | MB | 502 | GTP | PB-O3A | 3.19 | 1.62 | 1.59 |
| 42 | DA | 501 | GTP | C2-N3 | 3.13 | 1.40 | 1.33 |
| 42 | JD | 501 | GTP | C2-N3 | 3.12 | 1.40 | 1.33 |
| 42 | MB | 502 | GTP | C2-N3 | 3.11 | 1.40 | 1.33 |
| 42 | FO | 501 | GTP | C2-N3 | 3.07 | 1.40 | 1.33 |
| 42 | SL | 501 | GTP | C2-N3 | 3.06 | 1.40 | 1.33 |
| 42 | QL | 501 | GTP | PA-O3A | 3.00 | 1.62 | 1.59 |
| 42 | FM | 501 | GTP | C2-N3 | 2.99 | 1.40 | 1.33 |
| 42 | QL | 501 | GTP | PB-O3A | 2.96 | 1.62 | 1.59 |
| 42 | MH | 501 | GTP | C2-N3 | 2.95 | 1.40 | 1.33 |
| 42 | MB | 502 | GTP | PB-O3B | 2.94 | 1.62 | 1.59 |
| 42 | QN | 501 | GTP | PB-O3A | 2.92 | 1.62 | 1.59 |
| 42 | JO | 501 | GTP | C2-N3 | 2.88 | 1.40 | 1.33 |
| 42 | CE | 501 | GTP | PB-O3B | 2.85 | 1.62 | 1.59 |
| 42 | KD | 501 | GTP | C2-N3 | 2.85 | 1.40 | 1.33 |
| 42 | FI | 501 | GTP | C2-N3 | 2.85 | 1.40 | 1.33 |
| 42 | CG | 501 | GTP | C2-N3 | 2.82 | 1.40 | 1.33 |
| 42 | KB | 502 | GTP | C2-N3 | 2.81 | 1.40 | 1.33 |
| 42 | TL | 501 | GTP | C2-N3 | 2.81 | 1.40 | 1.33 |
| 42 | QN | 501 | GTP | PA-O3A | 2.79 | 1.62 | 1.59 |
| 42 | PE | 501 | GTP | C2-N3 | 2.77 | 1.39 | 1.33 |
| 42 | TL | 501 | GTP | PA-O3A | 2.76 | 1.62 | 1.59 |
| 42 | EG | 501 | GTP | C2-N3 | 2.75 | 1.39 | 1.33 |
| 42 | JA | 501 | GTP | C2-N3 | 2.74 | 1.39 | 1.33 |
| 42 | NE | 501 | GTP | C2-N3 | 2.74 | 1.39 | 1.33 |
| 42 | GB | 502 | GTP | C2-N3 | 2.74 | 1.39 | 1.33 |
| 42 | TG | 501 | GTP | C2-N3 | 2.74 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | CE | 501 | GTP | C2-N3 | 2.74 | 1.39 | 1.33 |
| 42 | AH | 501 | GTP | PB-O3B | 2.74 | 1.62 | 1.59 |
| 42 | TN | 501 | GTP | C2-N3 | 2.74 | 1.39 | 1.33 |
| 42 | GH | 501 | GTP | C2-N3 | 2.74 | 1.39 | 1.33 |
| 42 | WF | 501 | GTP | C2-N3 | 2.73 | 1.39 | 1.33 |
| 42 | JF | 501 | GTP | C2-N3 | 2.72 | 1.39 | 1.33 |
| 42 | TG | 501 | GTP | C5-C6 | -2.71 | 1.42 | 1.47 |
| 42 | PB | 502 | GTP | C2-N3 | 2.71 | 1.39 | 1.33 |
| 42 | UA | 501 | GTP | C2-N2 | 2.71 | 1.40 | 1.34 |
| 42 | PO | 501 | GTP | C2-N3 | 2.71 | 1.39 | 1.33 |
| 42 | DG | 501 | GTP | PB-O3A | 2.71 | 1.62 | 1.59 |
| 42 | DG | 501 | GTP | C2-N3 | 2.70 | 1.39 | 1.33 |
| 42 | SM | 501 | GTP | C2-N3 | 2.70 | 1.39 | 1.33 |
| 42 | TG | 501 | GTP | PB-O3A | 2.70 | 1.62 | 1.59 |
| 42 | II | 501 | GTP | C2-N3 | 2.70 | 1.39 | 1.33 |
| 42 | LM | 501 | GTP | C2-N3 | 2.70 | 1.39 | 1.33 |
| 42 | VA | 501 | GTP | PB-O3B | 2.69 | 1.62 | 1.59 |
| 42 | HM | 501 | GTP | C2-N3 | 2.69 | 1.39 | 1.33 |
| 43 | RL | 501 | GDP | C6-N1 | -2.68 | 1.33 | 1.37 |
| 43 | GP | 502 | GDP | O4'-C1' | 2.68 | 1.44 | 1.40 |
| 42 | GF | 501 | GTP | C2-N3 | 2.67 | 1.39 | 1.33 |
| 42 | DH | 501 | GTP | PB-O3A | 2.67 | 1.62 | 1.59 |
| 42 | MN | 501 | GTP | C2-N3 | 2.66 | 1.39 | 1.33 |
| 42 | TG | 501 | GTP | PA-O3A | 2.65 | 1.62 | 1.59 |
| 42 | UI | 501 | GTP | C2-N3 | 2.65 | 1.39 | 1.33 |
| 42 | JD | 501 | GTP | PB-O3A | 2.65 | 1.62 | 1.59 |
| 42 | IG | 501 | GTP | C2-N3 | 2.65 | 1.39 | 1.33 |
| 42 | EG | 501 | GTP | PB-O3A | 2.65 | 1.62 | 1.59 |
| 42 | CF | 501 | GTP | C2-N3 | 2.64 | 1.39 | 1.33 |
| 42 | BF | 501 | GTP | C2-N3 | 2.63 | 1.39 | 1.33 |
| 42 | JA | 501 | GTP | PB-O3A | 2.62 | 1.62 | 1.59 |
| 42 | CH | 501 | GTP | C2-N3 | 2.62 | 1.39 | 1.33 |
| 42 | KO | 501 | GTP | PB-O3A | 2.62 | 1.62 | 1.59 |
| 42 | OL | 501 | GTP | C2-N3 | 2.62 | 1.39 | 1.33 |
| 42 | VP | 501 | GTP | C2-N3 | 2.62 | 1.39 | 1.33 |
| 42 | OB | 502 | GTP | C2-N3 | 2.61 | 1.39 | 1.33 |
| 42 | UO | 501 | GTP | C2-N3 | 2.61 | 1.39 | 1.33 |
| 42 | IE | 501 | GTP | C2-N3 | 2.60 | 1.39 | 1.33 |
| 42 | QG | 501 | GTP | PB-O3B | 2.60 | 1.62 | 1.59 |
| 42 | HP | 501 | GTP | C2-N3 | 2.59 | 1.39 | 1.33 |
| 42 | LO | 501 | GTP | C2-N3 | 2.59 | 1.39 | 1.33 |
| 42 | UA | 501 | GTP | PB-O3B | 2.59 | 1.62 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | PM | 501 | GTP | C2-N3 | 2.59 | 1.39 | 1.33 |
| 42 | HA | 501 | GTP | PG-O1G | 2.58 | 1.58 | 1.50 |
| 42 | EI | 501 | GTP | C2-N3 | 2.58 | 1.39 | 1.33 |
| 42 | EF | 501 | GTP | C2-N3 | 2.58 | 1.39 | 1.33 |
| 42 | JB | 502 | GTP | PB-O3B | 2.58 | 1.62 | 1.59 |
| 42 | TH | 501 | GTP | C2-N3 | 2.58 | 1.39 | 1.33 |
| 42 | RE | 501 | GTP | C2-N3 | 2.57 | 1.39 | 1.33 |
| 42 | DE | 501 | GTP | C2-N3 | 2.57 | 1.39 | 1.33 |
| 42 | NG | 501 | GTP | C2-N3 | 2.57 | 1.39 | 1.33 |
| 42 | OO | 501 | GTP | C2-N3 | 2.57 | 1.39 | 1.33 |
| 42 | TL | 501 | GTP | PB-O3A | 2.57 | 1.62 | 1.59 |
| 42 | JD | 501 | GTP | PA-O3A | 2.57 | 1.62 | 1.59 |
| 42 | VB | 502 | GTP | C2-N3 | 2.56 | 1.39 | 1.33 |
| 42 | DF | 501 | GTP | C2-N3 | 2.56 | 1.39 | 1.33 |
| 42 | LB | 502 | GTP | C2-N3 | 2.56 | 1.39 | 1.33 |
| 42 | IH | 501 | GTP | PB-O3B | 2.56 | 1.62 | 1.59 |
| 42 | HE | 501 | GTP | C2-N3 | 2.56 | 1.39 | 1.33 |
| 42 | QN | 501 | GTP | C2-N3 | 2.56 | 1.39 | 1.33 |
| 42 | SH | 501 | GTP | C2-N3 | 2.55 | 1.39 | 1.33 |
| 42 | QO | 501 | GTP | C2-N3 | 2.55 | 1.39 | 1.33 |
| 42 | IH | 501 | GTP | C2-N3 | 2.55 | 1.39 | 1.33 |
| 42 | JE | 501 | GTP | C2-N3 | 2.55 | 1.39 | 1.33 |
| 42 | DH | 501 | GTP | PA-O3A | 2.54 | 1.62 | 1.59 |
| 42 | RO | 501 | GTP | C2-N3 | 2.53 | 1.39 | 1.33 |
| 42 | DI | 501 | GTP | PB-O3A | 2.53 | 1.62 | 1.59 |
| 42 | SP | 501 | GTP | C2-N3 | 2.53 | 1.39 | 1.33 |
| 42 | WI | 501 | GTP | C2-N3 | 2.53 | 1.39 | 1.33 |
| 42 | UB | 502 | GTP | C2-N3 | 2.53 | 1.39 | 1.33 |
| 42 | NM | 501 | GTP | C2-N3 | 2.53 | 1.39 | 1.33 |
| 43 | RN | 502 | GDP | C2-N3 | 2.52 | 1.39 | 1.33 |
| 42 | CA | 501 | GTP | C2-N3 | 2.51 | 1.39 | 1.33 |
| 42 | EL | 501 | GTP | C2-N3 | 2.50 | 1.39 | 1.33 |
| 42 | UE | 501 | GTP | PA-O3A | 2.50 | 1.62 | 1.59 |
| 42 | OD | 501 | GTP | C2-N3 | 2.49 | 1.39 | 1.33 |
| 42 | DG | 501 | GTP | PA-O3A | 2.49 | 1.62 | 1.59 |
| 42 | ON | 501 | GTP | C2-N3 | 2.48 | 1.39 | 1.33 |
| 42 | IF | 501 | GTP | C2-N3 | 2.48 | 1.39 | 1.33 |
| 42 | TH | 501 | GTP | PB-O3B | 2.48 | 1.62 | 1.59 |
| 42 | NN | 501 | GTP | C2-N3 | 2.48 | 1.39 | 1.33 |
| 42 | RP | 501 | GTP | C2-N3 | 2.48 | 1.39 | 1.33 |
| 42 | HP | 501 | GTP | PB-O3A | 2.48 | 1.62 | 1.59 |
| 42 | SG | 501 | GTP | C2-N3 | 2.47 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | LA | 501 | GTP | C2-N3 | 2.47 | 1.39 | 1.33 |
| 42 | MM | 501 | GTP | PB-O3A | 2.46 | 1.62 | 1.59 |
| 42 | WO | 501 | GTP | C2-N3 | 2.45 | 1.39 | 1.33 |
| 42 | WG | 501 | GTP | C2-N3 | 2.45 | 1.39 | 1.33 |
| 42 | TN | 501 | GTP | PB-O3A | 2.45 | 1.62 | 1.59 |
| 42 | DH | 501 | GTP | C2-N2 | 2.44 | 1.39 | 1.34 |
| 42 | NO | 501 | GTP | C2-N3 | 2.44 | 1.39 | 1.33 |
| 42 | IA | 501 | GTP | C2-N3 | 2.44 | 1.39 | 1.33 |
| 42 | EA | 501 | GTP | C2-N3 | 2.44 | 1.39 | 1.33 |
| 42 | KE | 501 | GTP | C2-N3 | 2.44 | 1.39 | 1.33 |
| 43 | JL | 501 | GDP | O4'-C1' | 2.44 | 1.44 | 1.40 |
| 42 | LD | 501 | GTP | C2-N3 | 2.43 | 1.39 | 1.33 |
| 42 | UI | 501 | GTP | PB-O3A | 2.43 | 1.62 | 1.59 |
| 42 | FN | 501 | GTP | C2-N3 | 2.43 | 1.39 | 1.33 |
| 42 | GF | 501 | GTP | PA-O3A | 2.43 | 1.62 | 1.59 |
| 42 | WA | 501 | GTP | C2-N3 | 2.42 | 1.39 | 1.33 |
| 42 | HH | 501 | GTP | C2-N3 | 2.41 | 1.39 | 1.33 |
| 42 | SL | 501 | GTP | PB-O3A | 2.40 | 1.62 | 1.59 |
| 42 | UA | 501 | GTP | PB-O3A | 2.40 | 1.62 | 1.59 |
| 42 | VQ | 501 | GTP | C2-N3 | 2.40 | 1.39 | 1.33 |
| 42 | PD | 501 | GTP | C2-N3 | 2.40 | 1.39 | 1.33 |
| 43 | TL | 502 | GDP | C2-N3 | 2.40 | 1.39 | 1.33 |
| 42 | GP | 501 | GTP | PB-O3A | 2.39 | 1.62 | 1.59 |
| 42 | UE | 501 | GTP | PB-O3A | 2.39 | 1.62 | 1.59 |
| 42 | QG | 501 | GTP | C2-N3 | 2.39 | 1.39 | 1.33 |
| 42 | KM | 501 | GTP | PB-O3A | 2.38 | 1.62 | 1.59 |
| 43 | TP | 501 | GDP | C2-N3 | 2.38 | 1.39 | 1.33 |
| 42 | MB | 502 | GTP | PA-O3A | 2.38 | 1.62 | 1.59 |
| 43 | SN | 502 | GDP | C2-N3 | 2.37 | 1.39 | 1.33 |
| 42 | VF | 501 | GTP | C2-N3 | 2.37 | 1.39 | 1.33 |
| 42 | UE | 501 | GTP | C2-N3 | 2.37 | 1.39 | 1.33 |
| 42 | WE | 501 | GTP | C2-N3 | 2.37 | 1.39 | 1.33 |
| 42 | QF | 501 | GTP | PB-O3A | 2.36 | 1.62 | 1.59 |
| 42 | RN | 501 | GTP | C2-N3 | 2.36 | 1.38 | 1.33 |
| 43 | AP | 501 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 42 | RG | 501 | GTP | C2-N3 | 2.35 | 1.38 | 1.33 |
| 42 | QF | 501 | GTP | PA-O3A | 2.35 | 1.62 | 1.59 |
| 43 | SN | 502 | GDP | O4'-C1' | 2.35 | 1.44 | 1.40 |
| 42 | VN | 501 | GTP | C2-N3 | 2.35 | 1.38 | 1.33 |
| 42 | VA | 501 | GTP | C2-N3 | 2.34 | 1.38 | 1.33 |
| 42 | MD | 501 | GTP | PA-O3A | 2.32 | 1.62 | 1.59 |
| 42 | QL | 501 | GTP | O4'-C1' | 2.31 | 1.43 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 43 | JL | 501 | GDP | C2-N3 | 2.31 | 1.38 | 1.33 |
| 43 | EM | 501 | GDP | O4'-C1' | 2.31 | 1.43 | 1.40 |
| 42 | GF | 501 | GTP | PB-O3A | 2.31 | 1.62 | 1.59 |
| 42 | OM | 501 | GTP | C2-N3 | 2.31 | 1.38 | 1.33 |
| 43 | KO | 502 | GDP | O4'-C1' | 2.30 | 1.43 | 1.40 |
| 42 | QF | 501 | GTP | C2-N3 | 2.30 | 1.38 | 1.33 |
| 43 | DL | 501 | GDP | C5-C6 | 2.29 | 1.52 | 1.47 |
| 42 | UM | 501 | GTP | C2-N3 | 2.29 | 1.38 | 1.33 |
| 42 | DA | 501 | GTP | PB-O3A | 2.29 | 1.62 | 1.59 |
| 42 | QL | 501 | GTP | PB-O3B | 2.28 | 1.62 | 1.59 |
| 42 | HA | 501 | GTP | C2-N3 | 2.28 | 1.38 | 1.33 |
| 42 | TN | 501 | GTP | PA-O3A | 2.27 | 1.61 | 1.59 |
| 42 | EI | 501 | GTP | PB-O3A | 2.27 | 1.61 | 1.59 |
| 42 | FB | 502 | GTP | C2-N3 | 2.27 | 1.38 | 1.33 |
| 42 | WF | 501 | GTP | PB-O3A | 2.27 | 1.61 | 1.59 |
| 42 | GF | 501 | GTP | PB-O3B | 2.26 | 1.61 | 1.59 |
| 42 | SN | 501 | GTP | PA-O3A | 2.26 | 1.61 | 1.59 |
| 42 | VF | 501 | GTP | PB-O3A | 2.26 | 1.61 | 1.59 |
| 43 | TL | 502 | GDP | O4'-C1' | 2.26 | 1.43 | 1.40 |
| 42 | FN | 501 | GTP | PB-O3B | 2.26 | 1.61 | 1.59 |
| 42 | CF | 501 | GTP | PB-O3A | 2.25 | 1.61 | 1.59 |
| 42 | HP | 501 | GTP | PA-O3A | 2.25 | 1.61 | 1.59 |
| 42 | RF | 501 | GTP | C2-N3 | 2.25 | 1.38 | 1.33 |
| 42 | AA | 501 | GTP | PB-O3A | 2.25 | 1.61 | 1.59 |
| 42 | GP | 501 | GTP | PA-O3A | 2.24 | 1.61 | 1.59 |
| 42 | UI | 501 | GTP | PA-O3A | 2.24 | 1.61 | 1.59 |
| 42 | DF | 501 | GTP | PB-O3B | 2.24 | 1.61 | 1.59 |
| 42 | EL | 501 | GTP | PB-O3A | 2.23 | 1.61 | 1.59 |
| 42 | LL | 501 | GTP | PB-O3A | 2.23 | 1.61 | 1.59 |
| 42 | FN | 501 | GTP | PB-O3A | 2.23 | 1.61 | 1.59 |
| 42 | MH | 501 | GTP | PB-O3A | 2.23 | 1.61 | 1.59 |
| 42 | GE | 501 | GTP | PA-O3A | 2.23 | 1.61 | 1.59 |
| 42 | SL | 501 | GTP | PA-O3A | 2.23 | 1.61 | 1.59 |
| 42 | FM | 501 | GTP | PB-O3A | 2.22 | 1.61 | 1.59 |
| 42 | FM | 501 | GTP | PA-O3A | 2.22 | 1.61 | 1.59 |
| 42 | DE | 501 | GTP | PB-O3A | 2.22 | 1.61 | 1.59 |
| 42 | KN | 501 | GTP | PB-O3A | 2.22 | 1.61 | 1.59 |
| 43 | MP | 501 | GDP | O4'-C1' | 2.21 | 1.43 | 1.40 |
| 42 | QL | 501 | GTP | C2-N2 | 2.20 | 1.39 | 1.34 |
| 43 | QP | 501 | GDP | O4'-C1' | 2.20 | 1.43 | 1.40 |
| 42 | KO | 501 | GTP | PA-O3A | 2.20 | 1.61 | 1.59 |
| 43 | SP | 502 | GDP | O4'-C1' | 2.20 | 1.43 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | EA | 501 | GTP | PB-O3B | 2.20 | 1.61 | 1.59 |
| 43 | LM | 502 | GDP | O4'-C1' | 2.19 | 1.43 | 1.40 |
| 43 | DL | 501 | GDP | C4-N3 | -2.19 | 1.32 | 1.37 |
| 42 | MD | 501 | GTP | PB-O3A | 2.19 | 1.61 | 1.59 |
| 42 | KN | 501 | GTP | PB-O3B | 2.18 | 1.61 | 1.59 |
| 42 | SN | 501 | GTP | PB-O3A | 2.18 | 1.61 | 1.59 |
| 42 | UA | 501 | GTP | PA-O3A | 2.17 | 1.61 | 1.59 |
| 42 | BI | 501 | GTP | C2-N3 | 2.17 | 1.38 | 1.33 |
| 43 | UM | 502 | GDP | C6-N1 | -2.17 | 1.34 | 1.37 |
| 42 | BH | 501 | GTP | C2-N3 | 2.17 | 1.38 | 1.33 |
| 43 | CO | 501 | GDP | O4'-C1' | 2.17 | 1.43 | 1.40 |
| 43 | GP | 502 | GDP | C5-C6 | 2.16 | 1.51 | 1.47 |
| 42 | KN | 501 | GTP | PA-O3A | 2.15 | 1.61 | 1.59 |
| 42 | FN | 501 | GTP | PA-O3A | 2.15 | 1.61 | 1.59 |
| 43 | GM | 501 | GDP | O4'-C1' | 2.15 | 1.43 | 1.40 |
| 42 | GA | 501 | GTP | PA-O3A | 2.14 | 1.61 | 1.59 |
| 42 | BH | 501 | GTP | PB-O3A | 2.14 | 1.61 | 1.59 |
| 42 | FO | 501 | GTP | PB-O3A | 2.13 | 1.61 | 1.59 |
| 42 | AF | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 43 | MB | 501 | GDP | O4'-C1' | 2.13 | 1.43 | 1.40 |
| 42 | AG | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 43 | RP | 502 | GDP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 42 | DA | 501 | GTP | PA-O3A | 2.13 | 1.61 | 1.59 |
| 42 | OD | 501 | GTP | PA-O3A | 2.13 | 1.61 | 1.59 |
| 42 | FE | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 43 | EM | 501 | GDP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 42 | AH | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 43 | SB | 501 | GDP | O4'-C1' | 2.12 | 1.43 | 1.40 |
| 42 | CF | 501 | GTP | PA-O3A | 2.12 | 1.61 | 1.59 |
| 42 | EH | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 42 | HB | 502 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 42 | UE | 501 | GTP | PB-O3B | 2.11 | 1.61 | 1.59 |
| 43 | QM | 501 | GDP | O4'-C1' | 2.11 | 1.43 | 1.40 |
| 42 | ND | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 42 | LO | 501 | GTP | PB-O3A | 2.10 | 1.61 | 1.59 |
| 42 | MN | 501 | GTP | PB-O3A | 2.10 | 1.61 | 1.59 |
| 42 | AA | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 43 | TN | 502 | GDP | C6-N1 | -2.10 | 1.34 | 1.37 |
| 43 | BP | 501 | GDP | O4'-C1' | 2.10 | 1.43 | 1.40 |
| 42 | VQ | 501 | GTP | PB-O3A | 2.10 | 1.61 | 1.59 |
| 42 | BF | 501 | GTP | PB-O3A | 2.10 | 1.61 | 1.59 |
| 42 | BL | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 43 | FN | 502 | GDP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 43 | NN | 502 | GDP | O4'-C1' | 2.09 | 1.43 | 1.40 |
| 42 | PB | 502 | GTP | PB-O3A | 2.09 | 1.61 | 1.59 |
| 42 | EI | 501 | GTP | PA-O3A | 2.09 | 1.61 | 1.59 |
| 43 | RM | 501 | GDP | O4'-C1' | 2.09 | 1.43 | 1.40 |
| 42 | KE | 501 | GTP | PB-O3A | 2.08 | 1.61 | 1.59 |
| 43 | KO | 502 | GDP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 42 | OM | 501 | GTP | PB-O3A | 2.08 | 1.61 | 1.59 |
| 43 | LL | 502 | GDP | C6-N1 | -2.07 | 1.34 | 1.37 |
| 42 | PN | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 42 | WA | 501 | GTP | PB-O3A | 2.07 | 1.61 | 1.59 |
| 42 | HB | 502 | GTP | PB-O3A | 2.07 | 1.61 | 1.59 |
| 42 | KO | 501 | GTP | C2-N2 | 2.07 | 1.39 | 1.34 |
| 43 | FP | 501 | GDP | O4'-C1' | 2.07 | 1.43 | 1.40 |
| 42 | DF | 501 | GTP | PB-O3A | 2.06 | 1.61 | 1.59 |
| 43 | EP | 501 | GDP | O4'-C1' | 2.06 | 1.43 | 1.40 |
| 42 | HP | 501 | GTP | PB-O3B | 2.06 | 1.61 | 1.59 |
| 42 | OD | 501 | GTP | PB-O3A | 2.06 | 1.61 | 1.59 |
| 42 | WG | 501 | GTP | PB-O3A | 2.06 | 1.61 | 1.59 |
| 42 | BA | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 42 | AA | 501 | GTP | PA-O3A | 2.05 | 1.61 | 1.59 |
| 42 | BG | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 43 | AM | 501 | GDP | O4'-C1' | 2.05 | 1.43 | 1.40 |
| 43 | CB | 501 | GDP | O4'-C1' | 2.05 | 1.43 | 1.40 |
| 43 | CN | 501 | GDP | O4'-C1' | 2.05 | 1.43 | 1.40 |
| 42 | TF | 501 | GTP | PG-O1G | 2.05 | 1.56 | 1.50 |
| 42 | AE | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 42 | AA | 501 | GTP | PB-O3B | 2.04 | 1.61 | 1.59 |
| 42 | HM | 501 | GTP | PB-O3B | 2.04 | 1.61 | 1.59 |
| 42 | SP | 501 | GTP | PB-O3A | 2.04 | 1.61 | 1.59 |
| 42 | ML | 501 | GTP | PB-O3A | 2.04 | 1.61 | 1.59 |
| 43 | BB | 501 | GDP | O4'-C1' | 2.04 | 1.43 | 1.40 |
| 43 | AN | 501 | GDP | O4'-C1' | 2.04 | 1.43 | 1.40 |
| 42 | OB | 502 | GTP | PB-O3B | 2.04 | 1.61 | 1.59 |
| 42 | IE | 501 | GTP | PA-O3A | 2.03 | 1.61 | 1.59 |
| 42 | NM | 501 | GTP | PB-O3B | 2.03 | 1.61 | 1.59 |
| 42 | WF | 501 | GTP | PA-O3A | 2.03 | 1.61 | 1.59 |
| 42 | KE | 501 | GTP | PA-O3A | 2.03 | 1.61 | 1.59 |
| 42 | ND | 501 | GTP | PA-O3A | 2.03 | 1.61 | 1.59 |
| 43 | EN | 501 | GDP | C2-N3 | 2.03 | 1.38 | 1.33 |
| 42 | VP | 501 | GTP | PB-O3B | 2.03 | 1.61 | 1.59 |
| 42 | CG | 501 | GTP | PB-O3A | 2.02 | 1.61 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | PB | 502 | GTP | PA-O3A | 2.02 | 1.61 | 1.59 |
| 43 | WM | 501 | GDP | O4'-C1' | 2.02 | 1.43 | 1.40 |
| 43 | AB | 501 | GDP | O4'-C1' | 2.02 | 1.43 | 1.40 |
| 42 | RN | 501 | GTP | PA-O3A | 2.02 | 1.61 | 1.59 |
| 42 | MN | 501 | GTP | PB-O3B | 2.02 | 1.61 | 1.59 |
| 42 | SP | 501 | GTP | PA-O3A | 2.02 | 1.61 | 1.59 |
| 43 | RP | 502 | GDP | O4'-C1' | 2.02 | 1.43 | 1.40 |
| 42 | OM | 501 | GTP | PA-O3A | 2.01 | 1.61 | 1.59 |
| 43 | OP | 501 | GDP | C6-N1 | -2.01 | 1.34 | 1.37 |
| 43 | DL | 501 | GDP | C2-N1 | 2.01 | 1.42 | 1.37 |
| 42 | FO | 501 | GTP | PA-O3A | 2.01 | 1.61 | 1.59 |
| 43 | GN | 501 | GDP | O4'-C1' | 2.01 | 1.43 | 1.40 |
| 42 | GE | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 43 | EN | 501 | GDP | O4'-C1' | 2.01 | 1.43 | 1.40 |
| 42 | HH | 501 | GTP | PB-O3B | 2.00 | 1.61 | 1.59 |
| 42 | VF | 501 | GTP | PA-O3A | 2.00 | 1.61 | 1.59 |

All (1480) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | SN | 502 | GDP | O6-C6-C5 | -8.40 | 107.66 | 124.32 |
| 43 | DL | 501 | GDP | N2-C2-N3 | -8.23 | 103.62 | 119.67 |
| 43 | TL | 502 | GDP | O6-C6-C5 | -8.08 | 108.31 | 124.32 |
| 43 | RN | 502 | GDP | O6-C6-C5 | -7.61 | 109.23 | 124.32 |
| 43 | RP | 502 | GDP | C2-N1-C6 | -7.58 | 111.25 | 125.11 |
| 43 | RP | 502 | GDP | O6-C6-C5 | -7.28 | 109.90 | 124.32 |
| 43 | RN | 502 | GDP | O6-C6-N1 | 7.16 | 129.12 | 120.62 |
| 43 | TP | 501 | GDP | O6-C6-C5 | -7.00 | 110.45 | 124.32 |
| 43 | QP | 501 | GDP | C2-N1-C6 | -6.89 | 112.49 | 125.11 |
| 43 | FP | 501 | GDP | N2-C2-N3 | -6.85 | 106.31 | 119.67 |
| 43 | JL | 501 | GDP | C2-N1-C6 | -6.82 | 112.62 | 125.11 |
| 43 | SN | 502 | GDP | C2-N1-C6 | -6.79 | 112.68 | 125.11 |
| 43 | DL | 501 | GDP | C2-N1-C6 | -6.77 | 112.72 | 125.11 |
| 43 | TL | 502 | GDP | C2-N1-C6 | -6.55 | 113.12 | 125.11 |
| 43 | TL | 502 | GDP | O6-C6-N1 | 6.53 | 128.37 | 120.62 |
| 43 | TP | 501 | GDP | C2-N1-C6 | -6.48 | 113.26 | 125.11 |
| 42 | DH | 501 | GTP | C4'-O4'-C1' | 6.38 | 115.77 | 109.92 |
| 43 | EP | 501 | GDP | C2-N1-C6 | -6.36 | 113.47 | 125.11 |
| 43 | EP | 501 | GDP | O6-C6-C5 | -6.24 | 111.95 | 124.32 |
| 43 | NN | 502 | GDP | N2-C2-N3 | -6.20 | 107.58 | 119.67 |
| 43 | TB | 501 | GDP | O4'-C1'-N9 | 6.16 | 116.92 | 108.75 |
| 42 | UA | 501 | GTP | C4'-O4'-C1' | 6.10 | 115.51 | 109.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | TG | 501 | GTP | C8-N7-C5 | 6.05 | 112.85 | 102.55 |
| 43 | QP | 501 | GDP | N2-C2-N3 | -6.03 | 107.91 | 119.67 |
| 43 | FN | 502 | GDP | O6-C6-C5 | -5.94 | 112.54 | 124.32 |
| 43 | GP | 502 | GDP | N2-C2-N3 | -5.92 | 108.12 | 119.67 |
| 43 | RN | 502 | GDP | C2-N1-C6 | -5.89 | 114.33 | 125.11 |
| 43 | SN | 502 | GDP | O6-C6-N1 | 5.83 | 127.54 | 120.62 |
| 43 | EN | 501 | GDP | O6-C6-C5 | -5.81 | 112.79 | 124.32 |
| 43 | JL | 501 | GDP | O6-C6-C5 | -5.78 | 112.87 | 124.32 |
| 43 | SB | 501 | GDP | O6-C6-C5 | -5.73 | 112.96 | 124.32 |
| 43 | FP | 501 | GDP | C2-N1-C6 | -5.66 | 114.75 | 125.11 |
| 43 | KO | 502 | GDP | O6-C6-C5 | -5.63 | 113.17 | 124.32 |
| 43 | SN | 502 | GDP | C5-C6-N1 | 5.62 | 124.80 | 114.07 |
| 43 | NN | 502 | GDP | C2-N1-C6 | -5.60 | 114.85 | 125.11 |
| 42 | DI | 501 | GTP | C4'-O4'-C1' | 5.55 | 115.01 | 109.92 |
| 43 | RP | 502 | GDP | C5-C6-N1 | 5.53 | 124.63 | 114.07 |
| 43 | JL | 501 | GDP | C5-C6-N1 | 5.45 | 124.48 | 114.07 |
| 42 | JB | 502 | GTP | C4'-O4'-C1' | 5.34 | 114.81 | 109.92 |
| 43 | EM | 501 | GDP | O6-C6-C5 | -5.34 | 113.74 | 124.32 |
| 42 | KO | 501 | GTP | N2-C2-N3 | 5.28 | 129.98 | 119.67 |
| 43 | FN | 502 | GDP | C2-N1-C6 | -5.23 | 115.54 | 125.11 |
| 43 | TO | 501 | GDP | O6-C6-C5 | -5.19 | 114.04 | 124.32 |
| 43 | SL | 502 | GDP | N2-C2-N3 | -5.16 | 109.60 | 119.67 |
| 43 | DL | 501 | GDP | N2-C2-N1 | 5.16 | 127.64 | 116.76 |
| 43 | TB | 501 | GDP | C8-N7-C5 | 5.13 | 111.29 | 102.55 |
| 43 | GP | 502 | GDP | C2-N1-C6 | -5.12 | 115.74 | 125.11 |
| 43 | TP | 501 | GDP | O6-C6-N1 | 5.10 | 126.67 | 120.62 |
| 43 | FP | 501 | GDP | N2-C2-N1 | 5.10 | 127.52 | 116.76 |
| 43 | SB | 501 | GDP | C2-N1-C6 | -5.06 | 115.84 | 125.11 |
| 43 | DL | 501 | GDP | C8-N7-C5 | 5.05 | 111.15 | 102.55 |
| 43 | EN | 501 | GDP | C2-N1-C6 | -5.03 | 115.90 | 125.11 |
| 43 | GP | 502 | GDP | C8-N7-C5 | 5.02 | 111.10 | 102.55 |
| 43 | KO | 502 | GDP | C2-N1-C6 | -5.00 | 115.97 | 125.11 |
| 42 | KO | 501 | GTP | N1-C2-N3 | -4.99 | 114.18 | 123.32 |
| 42 | UA | 501 | GTP | O6-C6-C5 | -4.96 | 114.50 | 124.32 |
| 43 | TL | 502 | GDP | C5-C6-N1 | 4.84 | 123.31 | 114.07 |
| 43 | FP | 501 | GDP | C8-N7-C5 | 4.81 | 110.73 | 102.55 |
| 43 | EM | 501 | GDP | C2-N1-C6 | -4.80 | 116.32 | 125.11 |
| 42 | JB | 502 | GTP | O6-C6-C5 | -4.79 | 114.83 | 124.32 |
| 43 | GP | 502 | GDP | N2-C2-N1 | 4.78 | 126.86 | 116.76 |
| 43 | RM | 501 | GDP | O6-C6-C5 | -4.68 | 115.04 | 124.32 |
| 43 | TP | 501 | GDP | C5-C6-N1 | 4.61 | 122.87 | 114.07 |
| 43 | SL | 502 | GDP | C2-N1-C6 | -4.55 | 116.77 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | TI | 501 | GTP | N1-C2-N3 | -4.55 | 114.98 | 123.32 |
| 43 | QP | 501 | GDP | C8-N7-C5 | 4.55 | 110.30 | 102.55 |
| 42 | GP | 501 | GTP | C4'-O4'-C1' | 4.52 | 114.07 | 109.92 |
| 43 | EP | 501 | GDP | C5-C6-N1 | 4.52 | 122.69 | 114.07 |
| 43 | TO | 501 | GDP | C2-N1-C6 | -4.49 | 116.89 | 125.11 |
| 43 | DM | 501 | GDP | O6-C6-C5 | -4.48 | 115.43 | 124.32 |
| 43 | SO | 501 | GDP | O6-C6-C5 | -4.47 | 115.45 | 124.32 |
| 43 | NN | 502 | GDP | N2-C2-N1 | 4.47 | 126.20 | 116.76 |
| 42 | KN | 501 | GTP | C4'-O4'-C1' | 4.45 | 114.00 | 109.92 |
| 43 | SB | 501 | GDP | O6-C6-N1 | 4.43 | 125.88 | 120.62 |
| 43 | DB | 501 | GDP | N2-C2-N3 | -4.43 | 111.03 | 119.67 |
| 42 | FO | 501 | GTP | C4'-O4'-C1' | 4.43 | 113.98 | 109.92 |
| 43 | NN | 502 | GDP | C8-N7-C5 | 4.37 | 110.00 | 102.55 |
| 42 | KN | 501 | GTP | N2-C2-N3 | 4.36 | 128.18 | 119.67 |
| 42 | QL | 501 | GTP | C4'-O4'-C1' | 4.32 | 113.88 | 109.92 |
| 43 | QP | 501 | GDP | C5-C6-N1 | 4.30 | 122.27 | 114.07 |
| 43 | DM | 501 | GDP | C2-N1-C6 | -4.29 | 117.25 | 125.11 |
| 42 | TI | 501 | GTP | N2-C2-N3 | 4.19 | 127.85 | 119.67 |
| 43 | FN | 502 | GDP | O6-C6-N1 | 4.14 | 125.53 | 120.62 |
| 43 | FN | 502 | GDP | C5-C6-N1 | 4.11 | 121.92 | 114.07 |
| 43 | RP | 502 | GDP | O6-C6-N1 | 4.09 | 125.47 | 120.62 |
| 43 | EN | 501 | GDP | O6-C6-N1 | 4.08 | 125.45 | 120.62 |
| 43 | TO | 501 | GDP | O6-C6-N1 | 4.06 | 125.44 | 120.62 |
| 43 | KO | 502 | GDP | O6-C6-N1 | 4.06 | 125.43 | 120.62 |
| 42 | OM | 501 | GTP | C8-N7-C5 | 4.05 | 109.45 | 102.55 |
| 43 | AM | 501 | GDP | C2-N1-C6 | -4.05 | 117.70 | 125.11 |
| 42 | MM | 501 | GTP | N2-C2-N3 | 4.03 | 127.54 | 119.67 |
| 43 | EN | 501 | GDP | C5-C6-N1 | 4.02 | 121.75 | 114.07 |
| 42 | GP | 501 | GTP | O6-C6-C5 | -4.02 | 116.36 | 124.32 |
| 43 | BN | 501 | GDP | C2-N1-C6 | -4.01 | 117.76 | 125.11 |
| 42 | QL | 501 | GTP | N2-C2-N3 | 4.00 | 127.49 | 119.67 |
| 43 | EP | 501 | GDP | O6-C6-N1 | 4.00 | 125.36 | 120.62 |
| 42 | DH | 501 | GTP | N2-C2-N3 | 4.00 | 127.47 | 119.67 |
| 43 | GN | 501 | GDP | O6-C6-C5 | -4.00 | 116.40 | 124.32 |
| 42 | DG | 501 | GTP | C4'-O4'-C1' | 3.98 | 113.57 | 109.92 |
| 43 | RN | 502 | GDP | C5-C6-N1 | 3.97 | 121.65 | 114.07 |
| 43 | QP | 501 | GDP | N2-C2-N1 | 3.97 | 125.13 | 116.76 |
| 43 | SL | 502 | GDP | N2-C2-N1 | 3.95 | 125.09 | 116.76 |
| 42 | TF | 501 | GTP | C4'-O4'-C1' | 3.94 | 113.53 | 109.92 |
| 42 | EG | 501 | GTP | O6-C6-C5 | -3.93 | 116.53 | 124.32 |
| 43 | SL | 502 | GDP | C8-N7-C5 | 3.91 | 109.20 | 102.55 |
| 43 | VQ | 502 | GDP | C2-N1-C6 | -3.91 | 117.96 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | KO | 501 | GTP | C4'-O4'-C1' | 3.88 | 113.48 | 109.92 |
| 43 | WM | 501 | GDP | C2-N1-C6 | -3.88 | 118.01 | 125.11 |
| 42 | LL | 501 | GTP | C4'-O4'-C1' | 3.87 | 113.47 | 109.92 |
| 43 | KO | 502 | GDP | C5-C6-N1 | 3.84 | 121.40 | 114.07 |
| 42 | KM | 501 | GTP | C4'-O4'-C1' | 3.84 | 113.44 | 109.92 |
| 43 | EP | 501 | GDP | N2-C2-N3 | -3.84 | 112.19 | 119.67 |
| 43 | LM | 502 | GDP | C2-N1-C6 | -3.83 | 118.11 | 125.11 |
| 42 | FI | 501 | GTP | C4'-O4'-C1' | 3.82 | 113.42 | 109.92 |
| 43 | BN | 501 | GDP | C5-C6-N1 | 3.81 | 121.34 | 114.07 |
| 42 | KM | 501 | GTP | O6-C6-C5 | -3.81 | 116.77 | 124.32 |
| 43 | AM | 501 | GDP | C5-C6-N1 | 3.80 | 121.33 | 114.07 |
| 42 | LL | 501 | GTP | C5-C6-N1 | 3.80 | 121.32 | 114.07 |
| 43 | CN | 501 | GDP | C2-N1-C6 | -3.79 | 118.17 | 125.11 |
| 43 | QM | 501 | GDP | C2-N1-C6 | -3.78 | 118.18 | 125.11 |
| 42 | DH | 501 | GTP | C5-C6-N1 | 3.78 | 121.28 | 114.07 |
| 42 | TI | 501 | GTP | C4'-O4'-C1' | 3.77 | 113.38 | 109.92 |
| 43 | HM | 502 | GDP | C2-N1-C6 | -3.77 | 118.22 | 125.11 |
| 43 | CO | 501 | GDP | C2-N1-C6 | -3.77 | 118.22 | 125.11 |
| 43 | AM | 501 | GDP | O6-C6-C5 | -3.76 | 116.87 | 124.32 |
| 43 | EM | 501 | GDP | C5-C6-N1 | 3.75 | 121.23 | 114.07 |
| 43 | ON | 502 | GDP | C2-N1-C6 | -3.74 | 118.27 | 125.11 |
| 42 | KN | 501 | GTP | O6-C6-N1 | -3.74 | 116.19 | 120.62 |
| 42 | JB | 502 | GTP | C5-C6-N1 | 3.74 | 121.20 | 114.07 |
| 43 | KP | 501 | GDP | C2-N1-C6 | -3.74 | 118.27 | 125.11 |
| 43 | FP | 501 | GDP | O6-C6-C5 | -3.73 | 116.92 | 124.32 |
| 43 | HM | 502 | GDP | C5-C6-N1 | 3.73 | 121.18 | 114.07 |
| 42 | MM | 501 | GTP | C4'-O4'-C1' | 3.72 | 113.33 | 109.92 |
| 43 | SB | 501 | GDP | C5-C6-N1 | 3.72 | 121.16 | 114.07 |
| 43 | EM | 501 | GDP | O6-C6-N1 | 3.71 | 125.03 | 120.62 |
| 43 | RM | 501 | GDP | C2-N1-C6 | -3.71 | 118.32 | 125.11 |
| 43 | SO | 501 | GDP | O6-C6-N1 | 3.70 | 125.01 | 120.62 |
| 43 | TB | 501 | GDP | N2-C2-N1 | 3.66 | 124.49 | 116.76 |
| 42 | AE | 501 | GTP | C8-N7-C5 | 3.66 | 108.79 | 102.55 |
| 43 | LM | 502 | GDP | O6-C6-C5 | -3.66 | 117.06 | 124.32 |
| 43 | MP | 501 | GDP | C2-N1-C6 | -3.65 | 118.42 | 125.11 |
| 42 | BA | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 42 | DH | 501 | GTP | O6-C6-C5 | -3.64 | 117.10 | 124.32 |
| 42 | JD | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 43 | GM | 501 | GDP | C5-C6-N1 | 3.64 | 121.01 | 114.07 |
| 43 | RP | 502 | GDP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 43 | GM | 501 | GDP | C2-N1-C6 | -3.63 | 118.47 | 125.11 |
| 42 | DI | 501 | GTP | N2-C2-N3 | 3.63 | 126.75 | 119.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | DM | 501 | GDP | C5-C6-N1 | 3.62 | 120.98 | 114.07 |
| 43 | CO | 501 | GDP | O6-C6-C5 | -3.62 | 117.15 | 124.32 |
| 43 | CN | 501 | GDP | O6-C6-C5 | -3.62 | 117.15 | 124.32 |
| 43 | CO | 501 | GDP | C5-C6-N1 | 3.62 | 120.97 | 114.07 |
| 43 | VQ | 502 | GDP | C5-C6-N1 | 3.62 | 120.97 | 114.07 |
| 42 | WI | 501 | GTP | C4'-O4'-C1' | 3.61 | 113.23 | 109.92 |
| 42 | HM | 501 | GTP | C4'-O4'-C1' | 3.61 | 113.23 | 109.92 |
| 42 | AG | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 42 | AH | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 43 | KP | 501 | GDP | O6-C6-C5 | -3.60 | 117.17 | 124.32 |
| 42 | BH | 501 | GTP | C8-N7-C5 | 3.60 | 108.68 | 102.55 |
| 42 | NE | 501 | GTP | C4'-O4'-C1' | 3.59 | 113.22 | 109.92 |
| 42 | AF | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 43 | BP | 501 | GDP | O6-C6-C5 | -3.58 | 117.21 | 124.32 |
| 42 | II | 501 | GTP | C4'-O4'-C1' | 3.58 | 113.20 | 109.92 |
| 42 | SN | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 42 | DI | 501 | GTP | C5-C6-N1 | 3.58 | 120.90 | 114.07 |
| 42 | UA | 501 | GTP | C5-C6-N1 | 3.57 | 120.89 | 114.07 |
| 43 | AB | 501 | GDP | C2-N1-C6 | -3.56 | 118.59 | 125.11 |
| 42 | CI | 501 | GTP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 43 | TP | 501 | GDP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 42 | SP | 501 | GTP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 43 | LM | 502 | GDP | C5-C6-N1 | 3.56 | 120.86 | 114.07 |
| 43 | AN | 501 | GDP | C2-N1-C6 | -3.54 | 118.62 | 125.11 |
| 42 | SL | 501 | GTP | C5-C6-N1 | 3.54 | 120.83 | 114.07 |
| 42 | BI | 501 | GTP | C8-N7-C5 | 3.54 | 108.58 | 102.55 |
| 42 | BL | 501 | GTP | C8-N7-C5 | 3.54 | 108.57 | 102.55 |
| 42 | ND | 501 | GTP | C8-N7-C5 | 3.54 | 108.57 | 102.55 |
| 42 | GA | 501 | GTP | C5-C6-N1 | 3.54 | 120.82 | 114.07 |
| 42 | UE | 501 | GTP | C8-N7-C5 | 3.54 | 108.57 | 102.55 |
| 42 | BG | 501 | GTP | C8-N7-C5 | 3.53 | 108.57 | 102.55 |
| 43 | MP | 501 | GDP | C5-C6-N1 | 3.53 | 120.81 | 114.07 |
| 43 | CN | 501 | GDP | C5-C6-N1 | 3.53 | 120.81 | 114.07 |
| 43 | QM | 501 | GDP | C5-C6-N1 | 3.53 | 120.81 | 114.07 |
| 42 | TF | 501 | GTP | C8-N7-C5 | 3.53 | 108.56 | 102.55 |
| 42 | ML | 501 | GTP | C5-C6-N1 | 3.53 | 120.81 | 114.07 |
| 42 | PN | 501 | GTP | C8-N7-C5 | 3.52 | 108.55 | 102.55 |
| 43 | KP | 501 | GDP | C5-C6-N1 | 3.52 | 120.78 | 114.07 |
| 43 | JB | 501 | GDP | O6-C6-C5 | -3.51 | 117.36 | 124.32 |
| 43 | BN | 501 | GDP | O6-C6-C5 | -3.51 | 117.36 | 124.32 |
| 42 | ML | 501 | GTP | N2-C2-N3 | 3.51 | 126.52 | 119.67 |
| 42 | VF | 501 | GTP | C8-N7-C5 | 3.51 | 108.52 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | EI | 501 | GTP | C4'-O4'-C1' | 3.50 | 113.13 | 109.92 |
| 43 | BP | 501 | GDP | C2-N1-C6 | -3.50 | 118.70 | 125.11 |
| 42 | RP | 501 | GTP | C8-N7-C5 | 3.50 | 108.51 | 102.55 |
| 42 | AA | 501 | GTP | C8-N7-C5 | 3.50 | 108.50 | 102.55 |
| 43 | WM | 501 | GDP | C5-C6-N1 | 3.50 | 120.74 | 114.07 |
| 42 | MB | 502 | GTP | C8-N7-C5 | 3.50 | 108.50 | 102.55 |
| 42 | KN | 501 | GTP | C8-N7-C5 | 3.49 | 108.50 | 102.55 |
| 43 | QM | 501 | GDP | O6-C6-C5 | -3.49 | 117.40 | 124.32 |
| 42 | EH | 501 | GTP | C8-N7-C5 | 3.49 | 108.49 | 102.55 |
| 43 | WM | 501 | GDP | O6-C6-C5 | -3.48 | 117.42 | 124.32 |
| 42 | GE | 501 | GTP | C8-N7-C5 | 3.48 | 108.48 | 102.55 |
| 43 | MB | 501 | GDP | C2-N1-C6 | -3.48 | 118.74 | 125.11 |
| 42 | EG | 501 | GTP | O2B-PB-O3B | 3.48 | 116.67 | 107.27 |
| 42 | FN | 501 | GTP | C8-N7-C5 | 3.47 | 108.46 | 102.55 |
| 43 | VQ | 502 | GDP | O6-C6-C5 | -3.47 | 117.44 | 124.32 |
| 42 | MD | 501 | GTP | N2-C2-N3 | 3.47 | 126.44 | 119.67 |
| 42 | QN | 501 | GTP | C4'-O4'-C1' | 3.46 | 113.10 | 109.92 |
| 42 | SL | 501 | GTP | C4'-O4'-C1' | 3.46 | 113.09 | 109.92 |
| 42 | GH | 501 | GTP | C4'-O4'-C1' | 3.46 | 113.09 | 109.92 |
| 42 | VP | 501 | GTP | C8-N7-C5 | 3.46 | 108.43 | 102.55 |
| 43 | RM | 501 | GDP | C5-C6-N1 | 3.45 | 120.66 | 114.07 |
| 43 | JB | 501 | GDP | C2-N1-C6 | -3.45 | 118.80 | 125.11 |
| 42 | FE | 501 | GTP | C8-N7-C5 | 3.45 | 108.42 | 102.55 |
| 42 | DA | 501 | GTP | C8-N7-C5 | 3.44 | 108.41 | 102.55 |
| 42 | NO | 501 | GTP | C8-N7-C5 | 3.44 | 108.41 | 102.55 |
| 42 | UM | 501 | GTP | C8-N7-C5 | 3.43 | 108.39 | 102.55 |
| 42 | HB | 502 | GTP | C8-N7-C5 | 3.43 | 108.39 | 102.55 |
| 43 | AN | 501 | GDP | C5-C6-N1 | 3.43 | 120.61 | 114.07 |
| 43 | VP | 502 | GDP | C2-N1-C6 | -3.42 | 118.85 | 125.11 |
| 42 | LD | 501 | GTP | C8-N7-C5 | 3.41 | 108.36 | 102.55 |
| 42 | TH | 501 | GTP | C8-N7-C5 | 3.40 | 108.34 | 102.55 |
| 42 | FB | 502 | GTP | C8-N7-C5 | 3.40 | 108.34 | 102.55 |
| 42 | MN | 501 | GTP | C8-N7-C5 | 3.40 | 108.34 | 102.55 |
| 42 | SG | 501 | GTP | C8-N7-C5 | 3.40 | 108.33 | 102.55 |
| 43 | JL | 501 | GDP | O4'-C1'-N9 | -3.40 | 104.24 | 108.75 |
| 43 | HM | 502 | GDP | O6-C6-C5 | -3.39 | 117.59 | 124.32 |
| 42 | DE | 501 | GTP | C8-N7-C5 | 3.39 | 108.32 | 102.55 |
| 42 | MM | 501 | GTP | C8-N7-C5 | 3.38 | 108.31 | 102.55 |
| 42 | NM | 501 | GTP | C8-N7-C5 | 3.38 | 108.31 | 102.55 |
| 42 | HA | 501 | GTP | C8-N7-C5 | 3.38 | 108.31 | 102.55 |
| 43 | TO | 501 | GDP | C5-C6-N1 | 3.38 | 120.51 | 114.07 |
| 42 | BF | 501 | GTP | C8-N7-C5 | 3.37 | 108.30 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | VQ | 501 | GTP | C8-N7-C5 | 3.37 | 108.30 | 102.55 |
| 43 | DB | 501 | GDP | N2-C2-N1 | 3.37 | 123.88 | 116.76 |
| 42 | PD | 501 | GTP | C8-N7-C5 | 3.37 | 108.29 | 102.55 |
| 43 | GM | 501 | GDP | O6-C6-C5 | -3.37 | 117.64 | 124.32 |
| 42 | SM | 501 | GTP | C8-N7-C5 | 3.37 | 108.29 | 102.55 |
| 42 | RE | 501 | GTP | C8-N7-C5 | 3.37 | 108.28 | 102.55 |
| 42 | UA | 501 | GTP | O6-C6-N1 | 3.36 | 124.61 | 120.62 |
| 42 | OL | 501 | GTP | C8-N7-C5 | 3.36 | 108.27 | 102.55 |
| 42 | TI | 501 | GTP | C8-N7-C5 | 3.36 | 108.27 | 102.55 |
| 42 | KN | 501 | GTP | C5-C6-N1 | 3.35 | 120.47 | 114.07 |
| 43 | MP | 501 | GDP | O6-C6-C5 | -3.35 | 117.67 | 124.32 |
| 42 | WE | 501 | GTP | C4'-O4'-C1' | 3.35 | 112.99 | 109.92 |
| 42 | EG | 501 | GTP | C5-C6-N1 | 3.35 | 120.46 | 114.07 |
| 43 | JL | 501 | GDP | C8-N7-C5 | 3.35 | 108.25 | 102.55 |
| 42 | PM | 501 | GTP | C8-N7-C5 | 3.35 | 108.25 | 102.55 |
| 42 | TN | 501 | GTP | C8-N7-C5 | 3.35 | 108.25 | 102.55 |
| 42 | MD | 501 | GTP | C8-N7-C5 | 3.35 | 108.25 | 102.55 |
| 43 | GN | 501 | GDP | C2-N1-C6 | -3.34 | 118.99 | 125.11 |
| 42 | HE | 501 | GTP | C4'-O4'-C1' | 3.34 | 112.99 | 109.92 |
| 42 | MD | 501 | GTP | C4'-O4'-C1' | 3.34 | 112.98 | 109.92 |
| 43 | KN | 502 | GDP | C2-N1-C6 | -3.34 | 119.00 | 125.11 |
| 42 | ML | 501 | GTP | O6-C6-C5 | -3.34 | 117.70 | 124.32 |
| 43 | JB | 501 | GDP | C5-C6-N1 | 3.34 | 120.44 | 114.07 |
| 42 | NN | 501 | GTP | C8-N7-C5 | 3.33 | 108.23 | 102.55 |
| 42 | HH | 501 | GTP | C4'-O4'-C1' | 3.33 | 112.98 | 109.92 |
| 42 | ON | 501 | GTP | C4'-O4'-C1' | 3.33 | 112.97 | 109.92 |
| 43 | SO | 501 | GDP | C2-N1-C6 | -3.33 | 119.02 | 125.11 |
| 42 | OO | 501 | GTP | C8-N7-C5 | 3.33 | 108.21 | 102.55 |
| 43 | AB | 501 | GDP | C5-C6-N1 | 3.33 | 120.42 | 114.07 |
| 42 | PM | 501 | GTP | C4'-O4'-C1' | 3.32 | 112.97 | 109.92 |
| 42 | IE | 501 | GTP | C8-N7-C5 | 3.32 | 108.21 | 102.55 |
| 42 | QL | 501 | GTP | C8-N7-C5 | 3.32 | 108.21 | 102.55 |
| 42 | LL | 501 | GTP | O6-C6-C5 | -3.32 | 117.73 | 124.32 |
| 42 | CA | 501 | GTP | C4'-O4'-C1' | 3.32 | 112.97 | 109.92 |
| 42 | JB | 502 | GTP | C2-N1-C6 | -3.32 | 119.03 | 125.11 |
| 42 | SL | 501 | GTP | C8-N7-C5 | 3.32 | 108.20 | 102.55 |
| 43 | AB | 501 | GDP | O6-C6-C5 | -3.32 | 117.74 | 124.32 |
| 42 | IH | 501 | GTP | C4'-O4'-C1' | 3.32 | 112.96 | 109.92 |
| 43 | CM | 501 | GDP | C2-N1-C6 | -3.31 | 119.05 | 125.11 |
| 42 | VN | 501 | GTP | C8-N7-C5 | 3.31 | 108.18 | 102.55 |
| 42 | GH | 501 | GTP | C8-N7-C5 | 3.30 | 108.17 | 102.55 |
| 42 | KE | 501 | GTP | C8-N7-C5 | 3.30 | 108.17 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | JE | 501 | GTP | C8-N7-C5 | 3.30 | 108.17 | 102.55 |
| 43 | MB | 501 | GDP | O6-C6-C5 | -3.30 | 117.78 | 124.32 |
| 42 | GF | 501 | GTP | C5-C6-N1 | 3.30 | 120.37 | 114.07 |
| 42 | RG | 501 | GTP | C8-N7-C5 | 3.30 | 108.17 | 102.55 |
| 43 | PP | 501 | GDP | O6-C6-C5 | -3.30 | 117.78 | 124.32 |
| 42 | IA | 501 | GTP | C8-N7-C5 | 3.30 | 108.17 | 102.55 |
| 43 | VO | 501 | GDP | C5-C6-N1 | 3.30 | 120.37 | 114.07 |
| 42 | QO | 501 | GTP | C4'-O4'-C1' | 3.30 | 112.95 | 109.92 |
| 42 | LA | 501 | GTP | C8-N7-C5 | 3.30 | 108.16 | 102.55 |
| 43 | GP | 502 | GDP | O6-C6-C5 | -3.29 | 117.80 | 124.32 |
| 42 | NN | 501 | GTP | C5-C6-N1 | 3.29 | 120.34 | 114.07 |
| 42 | UO | 501 | GTP | C4'-O4'-C1' | 3.28 | 112.93 | 109.92 |
| 42 | HP | 501 | GTP | C8-N7-C5 | 3.28 | 108.14 | 102.55 |
| 43 | MB | 501 | GDP | C5-C6-N1 | 3.28 | 120.33 | 114.07 |
| 42 | QO | 501 | GTP | C8-N7-C5 | 3.28 | 108.13 | 102.55 |
| 42 | EL | 501 | GTP | C8-N7-C5 | 3.28 | 108.13 | 102.55 |
| 42 | TL | 501 | GTP | C8-N7-C5 | 3.28 | 108.13 | 102.55 |
| 42 | WI | 501 | GTP | C8-N7-C5 | 3.28 | 108.13 | 102.55 |
| 42 | IF | 501 | GTP | C8-N7-C5 | 3.28 | 108.13 | 102.55 |
| 42 | WF | 501 | GTP | C4'-O4'-C1' | 3.27 | 112.92 | 109.92 |
| 43 | DB | 501 | GDP | C2-N1-C6 | -3.27 | 119.12 | 125.11 |
| 42 | BI | 501 | GTP | C4'-O4'-C1' | 3.27 | 112.92 | 109.92 |
| 42 | VP | 501 | GTP | C4'-O4'-C1' | 3.27 | 112.92 | 109.92 |
| 42 | QN | 501 | GTP | C8-N7-C5 | 3.27 | 108.11 | 102.55 |
| 42 | GP | 501 | GTP | O2B-PB-O3A | 3.26 | 116.10 | 107.27 |
| 43 | CB | 501 | GDP | C2-N1-C6 | -3.26 | 119.14 | 125.11 |
| 43 | BM | 501 | GDP | C5-C6-N1 | 3.26 | 120.30 | 114.07 |
| 42 | ON | 501 | GTP | C8-N7-C5 | 3.26 | 108.10 | 102.55 |
| 42 | SH | 501 | GTP | C8-N7-C5 | 3.26 | 108.10 | 102.55 |
| 42 | GF | 501 | GTP | C4'-O4'-C1' | 3.26 | 112.91 | 109.92 |
| 43 | EM | 501 | GDP | C4'-O4'-C1' | 3.26 | 112.91 | 109.92 |
| 43 | PO | 502 | GDP | C2-N1-C6 | -3.26 | 119.14 | 125.11 |
| 43 | CM | 501 | GDP | O6-C6-C5 | -3.26 | 117.86 | 124.32 |
| 42 | GA | 501 | GTP | C8-N7-C5 | 3.26 | 108.10 | 102.55 |
| 42 | OD | 501 | GTP | C8-N7-C5 | 3.26 | 108.10 | 102.55 |
| 42 | DE | 501 | GTP | C4'-O4'-C1' | 3.26 | 112.91 | 109.92 |
| 43 | ON | 502 | GDP | C5-C6-N1 | 3.25 | 120.28 | 114.07 |
| 43 | RN | 502 | GDP | C8-N7-C5 | 3.25 | 108.09 | 102.55 |
| 42 | DF | 501 | GTP | N1-C2-N3 | -3.25 | 117.36 | 123.32 |
| 42 | FM | 501 | GTP | C4'-O4'-C1' | 3.25 | 112.90 | 109.92 |
| 42 | MH | 501 | GTP | C8-N7-C5 | 3.25 | 108.08 | 102.55 |
| 43 | NM | 502 | GDP | C5-C6-N1 | 3.25 | 120.27 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | UO | 502 | GDP | C5-C6-N1 | 3.25 | 120.27 | 114.07 |
| 43 | BM | 501 | GDP | C2-N1-C6 | -3.25 | 119.17 | 125.11 |
| 43 | QP | 501 | GDP | O6-C6-C5 | -3.25 | 117.88 | 124.32 |
| 43 | WO | 502 | GDP | C2-N1-C6 | -3.25 | 119.17 | 125.11 |
| 42 | WO | 501 | GTP | C8-N7-C5 | 3.24 | 108.07 | 102.55 |
| 42 | RN | 501 | GTP | C8-N7-C5 | 3.24 | 108.07 | 102.55 |
| 42 | FO | 501 | GTP | C5-C6-N1 | 3.24 | 120.26 | 114.07 |
| 42 | CG | 501 | GTP | C4'-O4'-C1' | 3.24 | 112.89 | 109.92 |
| 42 | NG | 501 | GTP | C8-N7-C5 | 3.24 | 108.06 | 102.55 |
| 43 | CB | 501 | GDP | O6-C6-C5 | -3.24 | 117.90 | 124.32 |
| 43 | TM | 501 | GDP | C2-N1-C6 | -3.24 | 119.18 | 125.11 |
| 42 | GB | 502 | GTP | C5-C6-N1 | 3.24 | 120.25 | 114.07 |
| 42 | DG | 501 | GTP | C5-C6-N1 | 3.24 | 120.25 | 114.07 |
| 43 | WN | 501 | GDP | C5-C6-N1 | 3.24 | 120.25 | 114.07 |
| 42 | CH | 501 | GTP | C8-N7-C5 | 3.23 | 108.05 | 102.55 |
| 42 | DF | 501 | GTP | O4'-C1'-N9 | -3.23 | 104.46 | 108.75 |
| 42 | CF | 501 | GTP | C8-N7-C5 | 3.23 | 108.04 | 102.55 |
| 43 | PN | 502 | GDP | C2-N1-C6 | -3.23 | 119.21 | 125.11 |
| 43 | VP | 502 | GDP | C5-C6-N1 | 3.22 | 120.22 | 114.07 |
| 42 | JO | 501 | GTP | C4'-O4'-C1' | 3.22 | 112.88 | 109.92 |
| 43 | WO | 502 | GDP | O6-C6-C5 | -3.22 | 117.94 | 124.32 |
| 43 | TO | 501 | GDP | C8-N7-C5 | 3.22 | 108.03 | 102.55 |
| 43 | WN | 501 | GDP | C2-N1-C6 | -3.22 | 119.22 | 125.11 |
| 42 | KD | 501 | GTP | N2-C2-N3 | 3.22 | 125.95 | 119.67 |
| 42 | WE | 501 | GTP | C8-N7-C5 | 3.22 | 108.03 | 102.55 |
| 42 | CA | 501 | GTP | C8-N7-C5 | 3.22 | 108.02 | 102.55 |
| 43 | AN | 501 | GDP | O6-C6-C5 | -3.21 | 117.95 | 124.32 |
| 42 | CE | 501 | GTP | C4'-O4'-C1' | 3.21 | 112.87 | 109.92 |
| 43 | VO | 501 | GDP | C2-N1-C6 | -3.21 | 119.23 | 125.11 |
| 42 | UI | 501 | GTP | C8-N7-C5 | 3.21 | 108.02 | 102.55 |
| 42 | KD | 501 | GTP | C4'-O4'-C1' | 3.21 | 112.86 | 109.92 |
| 42 | OB | 502 | GTP | C8-N7-C5 | 3.21 | 108.01 | 102.55 |
| 42 | BI | 501 | GTP | C5-C6-N1 | 3.21 | 120.19 | 114.07 |
| 42 | KB | 502 | GTP | C5-C6-N1 | 3.21 | 120.19 | 114.07 |
| 43 | NM | 502 | GDP | C2-N1-C6 | -3.20 | 119.25 | 125.11 |
| 43 | PP | 501 | GDP | C5-C6-N1 | 3.20 | 120.17 | 114.07 |
| 42 | VA | 501 | GTP | C8-N7-C5 | 3.20 | 107.99 | 102.55 |
| 43 | CM | 501 | GDP | C5-C6-N1 | 3.20 | 120.17 | 114.07 |
| 42 | QL | 501 | GTP | N1-C2-N3 | -3.19 | 117.47 | 123.32 |
| 43 | WO | 502 | GDP | C5-C6-N1 | 3.19 | 120.16 | 114.07 |
| 42 | HM | 501 | GTP | C8-N7-C5 | 3.19 | 107.98 | 102.55 |
| 42 | QG | 501 | GTP | C8-N7-C5 | 3.19 | 107.98 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | LO | 502 | GDP | C2-N1-C6 | -3.19 | 119.27 | 125.11 |
| 42 | TF | 501 | GTP | O6-C6-C5 | -3.19 | 118.00 | 124.32 |
| 42 | GA | 501 | GTP | C4'-O4'-C1' | 3.19 | 112.84 | 109.92 |
| 42 | EF | 501 | GTP | C8-N7-C5 | 3.19 | 107.97 | 102.55 |
| 43 | JM | 501 | GDP | O6-C6-C5 | -3.19 | 118.00 | 124.32 |
| 42 | EI | 501 | GTP | C8-N7-C5 | 3.19 | 107.97 | 102.55 |
| 42 | KB | 502 | GTP | C8-N7-C5 | 3.18 | 107.97 | 102.55 |
| 42 | UA | 501 | GTP | N2-C2-N3 | 3.18 | 125.89 | 119.67 |
| 42 | GP | 501 | GTP | C5-C6-N1 | 3.18 | 120.14 | 114.07 |
| 42 | NE | 501 | GTP | C8-N7-C5 | 3.18 | 107.97 | 102.55 |
| 42 | MD | 501 | GTP | C5-C6-N1 | 3.18 | 120.14 | 114.07 |
| 42 | LO | 501 | GTP | C8-N7-C5 | 3.18 | 107.96 | 102.55 |
| 42 | LL | 501 | GTP | C2-N1-C6 | -3.18 | 119.29 | 125.11 |
| 42 | KO | 501 | GTP | C8-N7-C5 | 3.18 | 107.96 | 102.55 |
| 43 | BP | 501 | GDP | C5-C6-N1 | 3.17 | 120.12 | 114.07 |
| 42 | OB | 502 | GTP | C5-C6-N1 | 3.17 | 120.12 | 114.07 |
| 42 | GB | 502 | GTP | C8-N7-C5 | 3.17 | 107.94 | 102.55 |
| 42 | UI | 501 | GTP | C5-C6-N1 | 3.16 | 120.11 | 114.07 |
| 42 | PB | 502 | GTP | C8-N7-C5 | 3.16 | 107.94 | 102.55 |
| 42 | WF | 501 | GTP | C8-N7-C5 | 3.16 | 107.93 | 102.55 |
| 42 | JB | 502 | GTP | O4'-C1'-N9 | -3.16 | 104.56 | 108.75 |
| 42 | BL | 501 | GTP | C5-C6-N1 | 3.16 | 120.09 | 114.07 |
| 42 | IH | 501 | GTP | C8-N7-C5 | 3.16 | 107.92 | 102.55 |
| 43 | OB | 501 | GDP | C2-N1-C6 | -3.16 | 119.33 | 125.11 |
| 42 | MM | 501 | GTP | C5-C6-N1 | 3.15 | 120.09 | 114.07 |
| 42 | FI | 501 | GTP | C8-N7-C5 | 3.15 | 107.92 | 102.55 |
| 43 | SP | 502 | GDP | C8-N7-C5 | 3.15 | 107.92 | 102.55 |
| 42 | RO | 501 | GTP | C8-N7-C5 | 3.15 | 107.92 | 102.55 |
| 42 | DI | 501 | GTP | C8-N7-C5 | 3.15 | 107.92 | 102.55 |
| 43 | OB | 501 | GDP | C5-C6-N1 | 3.15 | 120.08 | 114.07 |
| 42 | JF | 501 | GTP | C8-N7-C5 | 3.15 | 107.91 | 102.55 |
| 43 | GO | 501 | GDP | C2-N1-C6 | -3.15 | 119.35 | 125.11 |
| 43 | BB | 501 | GDP | C2-N1-C6 | -3.14 | 119.35 | 125.11 |
| 43 | MO | 501 | GDP | C2-N1-C6 | -3.14 | 119.36 | 125.11 |
| 43 | ON | 502 | GDP | O6-C6-C5 | -3.14 | 118.09 | 124.32 |
| 42 | CG | 501 | GTP | C5-C6-N1 | 3.14 | 120.06 | 114.07 |
| 42 | LB | 502 | GTP | C4'-O4'-C1' | 3.14 | 112.80 | 109.92 |
| 42 | VB | 502 | GTP | C8-N7-C5 | 3.14 | 107.89 | 102.55 |
| 43 | PB | 501 | GDP | C2-N1-C6 | -3.14 | 119.37 | 125.11 |
| 42 | QF | 501 | GTP | C4'-O4'-C1' | 3.14 | 112.80 | 109.92 |
| 42 | MB | 502 | GTP | C5-C6-N1 | 3.14 | 120.06 | 114.07 |
| 42 | SN | 501 | GTP | C4'-O4'-C1' | 3.14 | 112.80 | 109.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | VP | 502 | GDP | O6-C6-C5 | -3.14 | 118.11 | 124.32 |
| 42 | OL | 501 | GTP | C4'-O4'-C1' | 3.13 | 112.80 | 109.92 |
| 43 | BB | 501 | GDP | C5-C6-N1 | 3.13 | 120.05 | 114.07 |
| 42 | MH | 501 | GTP | C5-C6-N1 | 3.13 | 120.05 | 114.07 |
| 43 | CB | 501 | GDP | C5-C6-N1 | 3.13 | 120.05 | 114.07 |
| 42 | KM | 501 | GTP | C8-N7-C5 | 3.13 | 107.88 | 102.55 |
| 42 | WA | 501 | GTP | C8-N7-C5 | 3.13 | 107.88 | 102.55 |
| 42 | JF | 501 | GTP | C4'-O4'-C1' | 3.13 | 112.79 | 109.92 |
| 42 | JD | 501 | GTP | C5-C6-N1 | 3.13 | 120.04 | 114.07 |
| 43 | KN | 502 | GDP | C5-C6-N1 | 3.12 | 120.03 | 114.07 |
| 43 | MM | 502 | GDP | C2-N1-C6 | -3.12 | 119.39 | 125.11 |
| 43 | TB | 501 | GDP | N2-C2-N3 | -3.12 | 113.59 | 119.67 |
| 42 | DI | 501 | GTP | C2-N1-C6 | -3.12 | 119.40 | 125.11 |
| 42 | JA | 501 | GTP | C8-N7-C5 | 3.12 | 107.86 | 102.55 |
| 43 | FB | 501 | GDP | C2-N1-C6 | -3.12 | 119.40 | 125.11 |
| 42 | QG | 501 | GTP | C4'-O4'-C1' | 3.12 | 112.78 | 109.92 |
| 43 | PN | 502 | GDP | C5-C6-N1 | 3.12 | 120.02 | 114.07 |
| 42 | MB | 502 | GTP | C2-N1-C6 | -3.11 | 119.41 | 125.11 |
| 43 | RP | 502 | GDP | O4'-C1'-N9 | -3.11 | 104.62 | 108.75 |
| 42 | DH | 501 | GTP | C8-N7-C5 | 3.11 | 107.84 | 102.55 |
| 42 | LO | 501 | GTP | C5-C6-N1 | 3.11 | 120.00 | 114.07 |
| 42 | SH | 501 | GTP | C5-C6-N1 | 3.11 | 120.00 | 114.07 |
| 42 | VB | 502 | GTP | C5-C6-N1 | 3.11 | 120.00 | 114.07 |
| 43 | RM | 501 | GDP | O6-C6-N1 | 3.11 | 124.31 | 120.62 |
| 42 | BI | 501 | GTP | C2-N1-C6 | -3.10 | 119.43 | 125.11 |
| 42 | UB | 502 | GTP | C8-N7-C5 | 3.10 | 107.83 | 102.55 |
| 42 | WG | 501 | GTP | C8-N7-C5 | 3.10 | 107.83 | 102.55 |
| 42 | WO | 501 | GTP | C4'-O4'-C1' | 3.10 | 112.76 | 109.92 |
| 42 | DA | 501 | GTP | C5-C6-N1 | 3.10 | 119.98 | 114.07 |
| 42 | GF | 501 | GTP | C8-N7-C5 | 3.10 | 107.83 | 102.55 |
| 42 | RF | 501 | GTP | C8-N7-C5 | 3.09 | 107.81 | 102.55 |
| 42 | BL | 501 | GTP | C2-N1-C6 | -3.09 | 119.45 | 125.11 |
| 42 | AA | 501 | GTP | C5-C6-N1 | 3.09 | 119.96 | 114.07 |
| 42 | TL | 501 | GTP | C5-C6-N1 | 3.09 | 119.96 | 114.07 |
| 42 | QF | 501 | GTP | C8-N7-C5 | 3.08 | 107.80 | 102.55 |
| 43 | PB | 501 | GDP | C5-C6-N1 | 3.08 | 119.95 | 114.07 |
| 43 | IB | 501 | GDP | C2-N1-C6 | -3.08 | 119.47 | 125.11 |
| 43 | GO | 501 | GDP | C5-C6-N1 | 3.08 | 119.95 | 114.07 |
| 43 | DO | 501 | GDP | C5-C6-N1 | 3.08 | 119.94 | 114.07 |
| 43 | PP | 501 | GDP | C2-N1-C6 | -3.08 | 119.48 | 125.11 |
| 42 | KM | 501 | GTP | C5-C6-N1 | 3.08 | 119.94 | 114.07 |
| 42 | RG | 501 | GTP | C4'-O4'-C1' | 3.07 | 112.74 | 109.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | MN | 502 | GDP | O6-C6-C5 | -3.07 | 118.23 | 124.32 |
| 42 | CG | 501 | GTP | O6-C6-C5 | -3.07 | 118.23 | 124.32 |
| 43 | TM | 501 | GDP | C5-C6-N1 | 3.07 | 119.93 | 114.07 |
| 43 | PO | 502 | GDP | C5-C6-N1 | 3.07 | 119.93 | 114.07 |
| 42 | PB | 502 | GTP | C4'-O4'-C1' | 3.07 | 112.74 | 109.92 |
| 42 | RO | 501 | GTP | C4'-O4'-C1' | 3.07 | 112.73 | 109.92 |
| 42 | UM | 501 | GTP | C5-C6-N1 | 3.07 | 119.92 | 114.07 |
| 42 | EA | 501 | GTP | C4'-O4'-C1' | 3.07 | 112.73 | 109.92 |
| 42 | WG | 501 | GTP | C4'-O4'-C1' | 3.07 | 112.73 | 109.92 |
| 42 | PE | 501 | GTP | C8-N7-C5 | 3.06 | 107.77 | 102.55 |
| 42 | GP | 501 | GTP | C8-N7-C5 | 3.06 | 107.77 | 102.55 |
| 43 | RB | 501 | GDP | O6-C6-C5 | -3.06 | 118.25 | 124.32 |
| 43 | TM | 501 | GDP | O6-C6-C5 | -3.06 | 118.25 | 124.32 |
| 43 | NM | 502 | GDP | O6-C6-C5 | -3.06 | 118.25 | 124.32 |
| 43 | IB | 501 | GDP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 43 | CL | 501 | GDP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 43 | CP | 501 | GDP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 43 | FB | 501 | GDP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 42 | LA | 501 | GTP | C5-C6-N1 | 3.06 | 119.91 | 114.07 |
| 43 | MO | 501 | GDP | C5-C6-N1 | 3.06 | 119.90 | 114.07 |
| 43 | NN | 502 | GDP | C5-C6-N1 | 3.06 | 119.90 | 114.07 |
| 43 | KN | 502 | GDP | O6-C6-C5 | -3.06 | 118.26 | 124.32 |
| 42 | ML | 501 | GTP | C8-N7-C5 | 3.06 | 107.75 | 102.55 |
| 42 | GH | 501 | GTP | C5-C6-N1 | 3.06 | 119.90 | 114.07 |
| 42 | SM | 501 | GTP | C5-C6-N1 | 3.05 | 119.90 | 114.07 |
| 42 | CG | 501 | GTP | C8-N7-C5 | 3.05 | 107.75 | 102.55 |
| 42 | HB | 502 | GTP | C2-N1-C6 | -3.05 | 119.52 | 125.11 |
| 42 | SH | 501 | GTP | C4'-O4'-C1' | 3.05 | 112.72 | 109.92 |
| 43 | JM | 501 | GDP | C5-C6-N1 | 3.05 | 119.89 | 114.07 |
| 42 | GP | 501 | GTP | C2-N1-C6 | -3.05 | 119.53 | 125.11 |
| 43 | QN | 502 | GDP | O6-C6-C5 | -3.05 | 118.28 | 124.32 |
| 43 | ON | 502 | GDP | C8-N7-C5 | 3.05 | 107.74 | 102.55 |
| 42 | MB | 502 | GTP | C4'-O4'-C1' | 3.05 | 112.72 | 109.92 |
| 42 | UA | 501 | GTP | C8-N7-C5 | 3.05 | 107.74 | 102.55 |
| 42 | CF | 501 | GTP | C4'-O4'-C1' | 3.05 | 112.72 | 109.92 |
| 43 | BB | 501 | GDP | O6-C6-C5 | -3.05 | 118.28 | 124.32 |
| 42 | HB | 502 | GTP | C5-C6-N1 | 3.04 | 119.88 | 114.07 |
| 43 | UO | 502 | GDP | O6-C6-C5 | -3.04 | 118.29 | 124.32 |
| 42 | KD | 501 | GTP | C8-N7-C5 | 3.04 | 107.72 | 102.55 |
| 42 | UB | 502 | GTP | C4'-O4'-C1' | 3.04 | 112.71 | 109.92 |
| 43 | QN | 502 | GDP | C5-C6-N1 | 3.04 | 119.87 | 114.07 |
| 43 | TL | 502 | GDP | C8-N7-C5 | 3.04 | 107.72 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | CP | 501 | GDP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 42 | TI | 501 | GTP | O6-C6-C5 | -3.04 | 118.30 | 124.32 |
| 42 | OL | 501 | GTP | O2B-PB-O3A | 3.04 | 115.48 | 107.27 |
| 42 | EF | 501 | GTP | C5-C6-N1 | 3.04 | 119.86 | 114.07 |
| 43 | LO | 502 | GDP | C5-C6-N1 | 3.04 | 119.86 | 114.07 |
| 43 | UO | 502 | GDP | C2-N1-C6 | -3.04 | 119.55 | 125.11 |
| 43 | TN | 502 | GDP | C8-N7-C5 | 3.03 | 107.71 | 102.55 |
| 43 | QN | 502 | GDP | C2-N1-C6 | -3.03 | 119.56 | 125.11 |
| 43 | EP | 501 | GDP | C4'-O4'-C1' | 3.03 | 112.70 | 109.92 |
| 42 | RE | 501 | GTP | O4'-C1'-N9 | -3.03 | 104.73 | 108.75 |
| 42 | AE | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 42 | LM | 501 | GTP | C8-N7-C5 | 3.03 | 107.71 | 102.55 |
| 42 | FO | 501 | GTP | O6-C6-C5 | -3.03 | 118.32 | 124.32 |
| 42 | HP | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 43 | GP | 502 | GDP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 42 | AA | 501 | GTP | C2-N1-C6 | -3.03 | 119.57 | 125.11 |
| 43 | NO | 502 | GDP | C8-N7-C5 | 3.03 | 107.70 | 102.55 |
| 42 | JA | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 42 | OO | 501 | GTP | C4'-O4'-C1' | 3.03 | 112.70 | 109.92 |
| 42 | MN | 501 | GTP | C5-C6-N1 | 3.03 | 119.84 | 114.07 |
| 43 | FO | 502 | GDP | O6-C6-C5 | -3.03 | 118.32 | 124.32 |
| 42 | AG | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 42 | BH | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 42 | UO | 501 | GTP | C8-N7-C5 | 3.02 | 107.69 | 102.55 |
| 43 | FO | 502 | GDP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 43 | EP | 501 | GDP | C8-N7-C5 | 3.02 | 107.69 | 102.55 |
| 42 | FI | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 43 | OB | 501 | GDP | C8-N7-C5 | 3.02 | 107.68 | 102.55 |
| 42 | LL | 501 | GTP | C8-N7-C5 | 3.01 | 107.68 | 102.55 |
| 42 | JO | 501 | GTP | C8-N7-C5 | 3.01 | 107.68 | 102.55 |
| 43 | DN | 501 | GDP | O6-C6-C5 | -3.01 | 118.35 | 124.32 |
| 43 | BO | 501 | GDP | C8-N7-C5 | 3.01 | 107.67 | 102.55 |
| 43 | LL | 502 | GDP | C8-N7-C5 | 3.01 | 107.67 | 102.55 |
| 43 | MM | 502 | GDP | C5-C6-N1 | 3.01 | 119.81 | 114.07 |
| 42 | HH | 501 | GTP | C8-N7-C5 | 3.01 | 107.67 | 102.55 |
| 43 | PN | 502 | GDP | O6-C6-C5 | -3.01 | 118.36 | 124.32 |
| 42 | DE | 501 | GTP | C5-C6-N1 | 3.01 | 119.81 | 114.07 |
| 43 | AO | 501 | GDP | C2-N1-C6 | -3.01 | 119.61 | 125.11 |
| 42 | FM | 501 | GTP | O6-C6-C5 | -3.01 | 118.36 | 124.32 |
| 43 | KO | 502 | GDP | C4'-O4'-C1' | 3.00 | 112.68 | 109.92 |
| 43 | HN | 501 | GDP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 42 | AF | 501 | GTP | C2-N1-C6 | -3.00 | 119.61 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | WB | 501 | GDP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 43 | WN | 501 | GDP | O6-C6-C5 | -3.00 | 118.37 | 124.32 |
| 43 | ML | 502 | GDP | C2-N1-C6 | -3.00 | 119.62 | 125.11 |
| 42 | AF | 501 | GTP | C5-C6-N1 | 3.00 | 119.79 | 114.07 |
| 42 | BF | 501 | GTP | C4'-O4'-C1' | 3.00 | 112.67 | 109.92 |
| 42 | BH | 501 | GTP | C2-N1-C6 | -2.99 | 119.63 | 125.11 |
| 43 | DO | 501 | GDP | O6-C6-C5 | -2.99 | 118.39 | 124.32 |
| 43 | NB | 501 | GDP | C2-N1-C6 | -2.99 | 119.64 | 125.11 |
| 42 | GA | 501 | GTP | N2-C2-N3 | 2.99 | 125.51 | 119.67 |
| 43 | AO | 501 | GDP | C5-C6-N1 | 2.99 | 119.77 | 114.07 |
| 42 | ML | 501 | GTP | C4'-O4'-C1' | 2.99 | 112.66 | 109.92 |
| 43 | EB | 501 | GDP | C5-C6-N1 | 2.99 | 119.77 | 114.07 |
| 43 | IM | 501 | GDP | O6-C6-C5 | -2.99 | 118.40 | 124.32 |
| 43 | EO | 501 | GDP | C8-N7-C5 | 2.98 | 107.63 | 102.55 |
| 43 | OM | 502 | GDP | C8-N7-C5 | 2.98 | 107.63 | 102.55 |
| 43 | FO | 502 | GDP | C2-N1-C6 | -2.98 | 119.65 | 125.11 |
| 43 | MN | 502 | GDP | C2-N1-C6 | -2.98 | 119.66 | 125.11 |
| 43 | MM | 502 | GDP | O6-C6-C5 | -2.98 | 118.41 | 124.32 |
| 42 | BA | 501 | GTP | C2-N1-C6 | -2.98 | 119.66 | 125.11 |
| 43 | SM | 502 | GDP | O6-C6-C5 | -2.98 | 118.42 | 124.32 |
| 42 | PN | 501 | GTP | C2-N1-C6 | -2.98 | 119.66 | 125.11 |
| 42 | FB | 502 | GTP | C4'-O4'-C1' | 2.98 | 112.65 | 109.92 |
| 42 | GB | 502 | GTP | C4'-O4'-C1' | 2.97 | 112.65 | 109.92 |
| 43 | TB | 501 | GDP | O6-C6-C5 | -2.97 | 118.42 | 124.32 |
| 42 | FB | 502 | GTP | C5-C6-N1 | 2.97 | 119.75 | 114.07 |
| 42 | LB | 502 | GTP | C8-N7-C5 | 2.97 | 107.61 | 102.55 |
| 42 | OO | 501 | GTP | C5-C6-N1 | 2.97 | 119.74 | 114.07 |
| 42 | SP | 501 | GTP | C5-C6-N1 | 2.97 | 119.74 | 114.07 |
| 42 | SP | 501 | GTP | C2-N1-C6 | -2.97 | 119.67 | 125.11 |
| 42 | SL | 501 | GTP | O2B-PB-O3A | 2.97 | 115.31 | 107.27 |
| 43 | OL | 502 | GDP | C8-N7-C5 | 2.97 | 107.60 | 102.55 |
| 42 | GB | 502 | GTP | O6-C6-C5 | -2.97 | 118.44 | 124.32 |
| 42 | KB | 502 | GTP | C4'-O4'-C1' | 2.97 | 112.64 | 109.92 |
| 42 | CE | 501 | GTP | C8-N7-C5 | 2.96 | 107.59 | 102.55 |
| 43 | EB | 501 | GDP | O6-C6-C5 | -2.96 | 118.45 | 124.32 |
| 43 | OP | 501 | GDP | C8-N7-C5 | 2.96 | 107.59 | 102.55 |
| 42 | HH | 501 | GTP | O4'-C1'-N9 | -2.96 | 104.82 | 108.75 |
| 43 | GN | 501 | GDP | O4'-C1'-N9 | 2.96 | 112.67 | 108.75 |
| 42 | LM | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 42 | AG | 501 | GTP | C2-N1-C6 | -2.96 | 119.70 | 125.11 |
| 42 | II | 501 | GTP | C8-N7-C5 | 2.96 | 107.58 | 102.55 |
| 43 | BM | 501 | GDP | O6-C6-C5 | -2.96 | 118.46 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | JF | 501 | GTP | C5-C6-N1 | 2.96 | 119.71 | 114.07 |
| 42 | CH | 501 | GTP | C4'-O4'-C1' | 2.95 | 112.63 | 109.92 |
| 42 | BA | 501 | GTP | C5-C6-N1 | 2.95 | 119.71 | 114.07 |
| 43 | VB | 501 | GDP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |
| 43 | BL | 502 | GDP | C8-N7-C5 | 2.95 | 107.58 | 102.55 |
| 43 | BP | 501 | GDP | C8-N7-C5 | 2.95 | 107.58 | 102.55 |
| 42 | PO | 501 | GTP | C8-N7-C5 | 2.95 | 107.57 | 102.55 |
| 43 | OO | 502 | GDP | C8-N7-C5 | 2.95 | 107.57 | 102.55 |
| 43 | SB | 501 | GDP | C8-N7-C5 | 2.95 | 107.57 | 102.55 |
| 43 | WP | 501 | GDP | C8-N7-C5 | 2.95 | 107.56 | 102.55 |
| 43 | WB | 501 | GDP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 43 | RO | 502 | GDP | O6-C6-C5 | -2.94 | 118.48 | 124.32 |
| 43 | DN | 501 | GDP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 43 | AO | 501 | GDP | O6-C6-C5 | -2.94 | 118.49 | 124.32 |
| 42 | NN | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 43 | GO | 501 | GDP | O6-C6-C5 | -2.94 | 118.50 | 124.32 |
| 43 | VQ | 502 | GDP | C8-N7-C5 | 2.94 | 107.55 | 102.55 |
| 43 | JM | 501 | GDP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 43 | KM | 502 | GDP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 42 | FN | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 42 | WI | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 43 | FP | 501 | GDP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 42 | BG | 501 | GTP | C4'-O4'-C1' | 2.93 | 112.61 | 109.92 |
| 43 | PL | 501 | GDP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 42 | FM | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 42 | SN | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 43 | KM | 502 | GDP | O6-C6-C5 | -2.93 | 118.51 | 124.32 |
| 42 | PO | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 43 | BM | 501 | GDP | C8-N7-C5 | 2.93 | 107.54 | 102.55 |
| 43 | UP | 501 | GDP | C8-N7-C5 | 2.93 | 107.54 | 102.55 |
| 42 | KM | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 43 | MO | 501 | GDP | O6-C6-C5 | -2.93 | 118.51 | 124.32 |
| 43 | NB | 501 | GDP | C8-N7-C5 | 2.93 | 107.54 | 102.55 |
| 42 | AH | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 43 | WQ | 501 | GDP | C8-N7-C5 | 2.93 | 107.54 | 102.55 |
| 43 | GN | 501 | GDP | C8-N7-C5 | 2.93 | 107.53 | 102.55 |
| 42 | QF | 501 | GTP | O2B-PB-O3A | 2.92 | 115.18 | 107.27 |
| 43 | ML | 502 | GDP | C5-C6-N1 | 2.92 | 119.65 | 114.07 |
| 43 | NN | 502 | GDP | O6-C6-C5 | -2.92 | 118.53 | 124.32 |
| 42 | HH | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 42 | NO | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 43 | TN | 502 | GDP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | VN | 501 | GTP | C4'-O4'-C1' | 2.92 | 112.60 | 109.92 |
| 43 | MM | 502 | GDP | C8-N7-C5 | 2.92 | 107.52 | 102.55 |
| 42 | PO | 501 | GTP | C4'-O4'-C1' | 2.92 | 112.60 | 109.92 |
| 43 | HP | 502 | GDP | C8-N7-C5 | 2.92 | 107.51 | 102.55 |
| 43 | RP | 502 | GDP | N2-C2-N3 | -2.92 | 113.99 | 119.67 |
| 42 | WA | 501 | GTP | C5-C6-N1 | 2.92 | 119.63 | 114.07 |
| 42 | DF | 501 | GTP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 43 | TM | 501 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 42 | QL | 501 | GTP | O4'-C4'-C5' | 2.91 | 118.67 | 109.33 |
| 42 | GA | 501 | GTP | O6-C6-C5 | -2.91 | 118.55 | 124.32 |
| 43 | SN | 502 | GDP | C4'-O4'-C1' | 2.91 | 112.59 | 109.92 |
| 43 | DB | 501 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 42 | QL | 501 | GTP | C5-C6-N1 | 2.91 | 119.63 | 114.07 |
| 43 | NL | 501 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 43 | WM | 501 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 43 | MB | 501 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 43 | IM | 501 | GDP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |
| 42 | HE | 501 | GTP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 43 | KM | 502 | GDP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 42 | SG | 501 | GTP | C4'-O4'-C1' | 2.91 | 112.59 | 109.92 |
| 43 | IP | 501 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 43 | UP | 501 | GDP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |
| 42 | ML | 501 | GTP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |
| 42 | PE | 501 | GTP | C5-C6-N1 | 2.91 | 119.61 | 114.07 |
| 43 | CM | 501 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 42 | GE | 501 | GTP | C2-N1-C6 | -2.90 | 119.79 | 125.11 |
| 43 | PL | 501 | GDP | C5-C6-N1 | 2.90 | 119.61 | 114.07 |
| 42 | TN | 501 | GTP | C5-C6-N1 | 2.90 | 119.61 | 114.07 |
| 42 | TH | 501 | GTP | C5-C6-N1 | 2.90 | 119.61 | 114.07 |
| 43 | NB | 501 | GDP | C5-C6-N1 | 2.90 | 119.61 | 114.07 |
| 43 | RB | 501 | GDP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 42 | DF | 501 | GTP | C4'-O4'-C1' | 2.90 | 112.58 | 109.92 |
| 42 | DE | 501 | GTP | C2-N1-C6 | -2.90 | 119.80 | 125.11 |
| 42 | JO | 501 | GTP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 42 | HE | 501 | GTP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 42 | NE | 501 | GTP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 42 | UB | 502 | GTP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 43 | PO | 502 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 42 | EA | 501 | GTP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 43 | HB | 501 | GDP | O6-C6-C5 | -2.90 | 118.58 | 124.32 |
| 43 | IM | 501 | GDP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 43 | NM | 502 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | IN | 501 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 43 | TN | 502 | GDP | C2-N1-C6 | -2.89 | 119.81 | 125.11 |
| 42 | IG | 501 | GTP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 42 | EH | 501 | GTP | C2-N1-C6 | -2.89 | 119.81 | 125.11 |
| 43 | HB | 501 | GDP | C5-C6-N1 | 2.89 | 119.59 | 114.07 |
| 43 | VP | 502 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 43 | PB | 501 | GDP | O6-C6-C5 | -2.89 | 118.59 | 124.32 |
| 43 | NP | 501 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 43 | PB | 501 | GDP | C8-N7-C5 | 2.89 | 107.46 | 102.55 |
| 42 | QL | 501 | GTP | O4'-C1'-N9 | -2.89 | 104.92 | 108.75 |
| 43 | BL | 502 | GDP | C5-C6-N1 | 2.89 | 119.58 | 114.07 |
| 43 | IB | 501 | GDP | C8-N7-C5 | 2.89 | 107.46 | 102.55 |
| 43 | LB | 501 | GDP | C5-C6-N1 | 2.89 | 119.58 | 114.07 |
| 43 | HN | 501 | GDP | C2-N1-C6 | -2.88 | 119.83 | 125.11 |
| 42 | VP | 501 | GTP | C5-C6-N1 | 2.88 | 119.57 | 114.07 |
| 42 | JB | 502 | GTP | N2-C2-N3 | 2.88 | 125.30 | 119.67 |
| 42 | GE | 501 | GTP | C5-C6-N1 | 2.88 | 119.57 | 114.07 |
| 43 | GN | 501 | GDP | C5-C6-N1 | 2.88 | 119.57 | 114.07 |
| 43 | DL | 501 | GDP | C5-C6-N1 | 2.88 | 119.57 | 114.07 |
| 42 | SG | 501 | GTP | C5-C6-N1 | 2.88 | 119.57 | 114.07 |
| 42 | VA | 501 | GTP | C5-C6-N1 | 2.88 | 119.57 | 114.07 |
| 42 | RP | 501 | GTP | C4'-O4'-C1' | 2.88 | 112.56 | 109.92 |
| 43 | ML | 502 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 43 | LB | 501 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 43 | MN | 502 | GDP | C5-C6-N1 | 2.88 | 119.56 | 114.07 |
| 42 | UA | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 43 | QO | 502 | GDP | O6-C6-C5 | -2.88 | 118.62 | 124.32 |
| 42 | UO | 501 | GTP | C5-C6-N1 | 2.88 | 119.56 | 114.07 |
| 42 | UM | 501 | GTP | C4'-O4'-C1' | 2.88 | 112.56 | 109.92 |
| 43 | UB | 501 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 42 | VP | 501 | GTP | O4'-C1'-N9 | -2.87 | 104.94 | 108.75 |
| 42 | RE | 501 | GTP | C5-C6-N1 | 2.87 | 119.55 | 114.07 |
| 43 | GN | 501 | GDP | O6-C6-N1 | 2.87 | 124.03 | 120.62 |
| 43 | RO | 502 | GDP | C5-C6-N1 | 2.87 | 119.55 | 114.07 |
| 42 | HP | 501 | GTP | C4'-O4'-C1' | 2.87 | 112.55 | 109.92 |
| 42 | AE | 501 | GTP | C2-N1-C6 | -2.87 | 119.86 | 125.11 |
| 42 | AH | 501 | GTP | C2-N1-C6 | -2.87 | 119.86 | 125.11 |
| 43 | AP | 501 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 43 | VO | 501 | GDP | O6-C6-C5 | -2.87 | 118.63 | 124.32 |
| 43 | SO | 501 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 42 | EH | 501 | GTP | C5-C6-N1 | 2.87 | 119.55 | 114.07 |
| 43 | IB | 501 | GDP | O6-C6-C5 | -2.87 | 118.63 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | PO | 502 | GDP | O6-C6-C5 | -2.87 | 118.63 | 124.32 |
| 43 | FN | 502 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 43 | PL | 501 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 43 | LO | 502 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 43 | SO | 501 | GDP | C5-C6-N1 | 2.87 | 119.54 | 114.07 |
| 43 | BL | 502 | GDP | C2-N1-C6 | -2.87 | 119.86 | 125.11 |
| 43 | HB | 501 | GDP | C2-N1-C6 | -2.87 | 119.86 | 125.11 |
| 43 | BB | 501 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 43 | KO | 502 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 42 | MH | 501 | GTP | N2-C2-N3 | 2.86 | 125.25 | 119.67 |
| 42 | NG | 501 | GTP | C5-C6-N1 | 2.86 | 119.52 | 114.07 |
| 43 | AN | 501 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 43 | CL | 501 | GDP | O6-C6-C5 | -2.85 | 118.66 | 124.32 |
| 42 | GF | 501 | GTP | O6-C6-C5 | -2.85 | 118.66 | 124.32 |
| 43 | CB | 501 | GDP | C8-N7-C5 | 2.85 | 107.41 | 102.55 |
| 43 | AL | 501 | GDP | C8-N7-C5 | 2.85 | 107.41 | 102.55 |
| 42 | OD | 501 | GTP | C4'-O4'-C1' | 2.85 | 112.54 | 109.92 |
| 42 | PM | 501 | GTP | C5-C6-N1 | 2.85 | 119.51 | 114.07 |
| 43 | CL | 501 | GDP | C2-N1-C6 | -2.85 | 119.89 | 125.11 |
| 43 | RO | 502 | GDP | C2-N1-C6 | -2.85 | 119.89 | 125.11 |
| 43 | AB | 501 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 43 | BN | 501 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 43 | CN | 501 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 43 | LB | 501 | GDP | C2-N1-C6 | -2.85 | 119.89 | 125.11 |
| 43 | BO | 501 | GDP | C5-C6-N1 | 2.85 | 119.50 | 114.07 |
| 43 | GB | 501 | GDP | C5-C6-N1 | 2.85 | 119.50 | 114.07 |
| 42 | NM | 501 | GTP | C5-C6-N1 | 2.85 | 119.50 | 114.07 |
| 43 | HB | 501 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 43 | ML | 502 | GDP | O6-C6-C5 | -2.85 | 118.68 | 124.32 |
| 42 | IH | 501 | GTP | C5-C6-N1 | 2.85 | 119.50 | 114.07 |
| 43 | UM | 502 | GDP | C8-N7-C5 | 2.85 | 107.39 | 102.55 |
| 43 | VO | 501 | GDP | C8-N7-C5 | 2.85 | 107.39 | 102.55 |
| 42 | CI | 501 | GTP | C5-C6-N1 | 2.85 | 119.50 | 114.07 |
| 43 | HQ | 501 | GDP | C8-N7-C5 | 2.85 | 107.39 | 102.55 |
| 43 | DN | 501 | GDP | C5-C6-N1 | 2.85 | 119.50 | 114.07 |
| 43 | EL | 502 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 42 | LA | 501 | GTP | C4'-O4'-C1' | 2.84 | 112.53 | 109.92 |
| 42 | NG | 501 | GTP | C4'-O4'-C1' | 2.84 | 112.53 | 109.92 |
| 43 | KP | 501 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 42 | PE | 501 | GTP | C4'-O4'-C1' | 2.84 | 112.53 | 109.92 |
| 43 | KB | 501 | GDP | C2-N1-C6 | -2.84 | 119.91 | 125.11 |
| 42 | IF | 501 | GTP | C4'-O4'-C1' | 2.84 | 112.53 | 109.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | SL | 502 | GDP | C5-C6-N1 | 2.84 | 119.49 | 114.07 |
| 42 | EG | 501 | GTP | C2-N1-C6 | -2.84 | 119.91 | 125.11 |
| 43 | DO | 501 | GDP | C2-N1-C6 | -2.84 | 119.91 | 125.11 |
| 42 | UI | 501 | GTP | C4'-O4'-C1' | 2.84 | 112.52 | 109.92 |
| 42 | OL | 501 | GTP | C5-C6-N1 | 2.84 | 119.48 | 114.07 |
| 42 | CH | 501 | GTP | C5-C6-N1 | 2.84 | 119.48 | 114.07 |
| 43 | DP | 501 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 42 | MN | 501 | GTP | C2-N1-C6 | -2.84 | 119.92 | 125.11 |
| 43 | JN | 501 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 43 | MP | 501 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 42 | LD | 501 | GTP | C5-C6-N1 | 2.83 | 119.48 | 114.07 |
| 43 | KM | 502 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 43 | TN | 502 | GDP | O6-C6-C5 | -2.83 | 118.70 | 124.32 |
| 42 | OB | 502 | GTP | N2-C2-N3 | 2.83 | 125.20 | 119.67 |
| 42 | HM | 501 | GTP | C5-C6-N1 | 2.83 | 119.47 | 114.07 |
| 43 | AO | 501 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 43 | JO | 502 | GDP | C5-C6-N1 | 2.83 | 119.47 | 114.07 |
| 43 | GO | 501 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 43 | QL | 502 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 43 | IQ | 501 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 43 | WB | 501 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 42 | CE | 501 | GTP | C5-C6-N1 | 2.83 | 119.46 | 114.07 |
| 43 | GB | 501 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 43 | NO | 502 | GDP | C5-C6-N1 | 2.82 | 119.46 | 114.07 |
| 43 | PL | 501 | GDP | O6-C6-C5 | -2.82 | 118.73 | 124.32 |
| 43 | WB | 501 | GDP | O6-C6-C5 | -2.82 | 118.73 | 124.32 |
| 43 | QO | 502 | GDP | C2-N1-C6 | -2.82 | 119.94 | 125.11 |
| 43 | CO | 501 | GDP | C8-N7-C5 | 2.82 | 107.35 | 102.55 |
| 42 | DG | 501 | GTP | N2-C2-N3 | 2.82 | 125.18 | 119.67 |
| 42 | LO | 501 | GTP | C4'-O4'-C1' | 2.82 | 112.51 | 109.92 |
| 43 | FB | 501 | GDP | O6-C6-C5 | -2.82 | 118.73 | 124.32 |
| 43 | EB | 501 | GDP | C2-N1-C6 | -2.82 | 119.95 | 125.11 |
| 42 | WE | 501 | GTP | C5-C6-N1 | 2.82 | 119.45 | 114.07 |
| 43 | JO | 502 | GDP | C8-N7-C5 | 2.82 | 107.34 | 102.55 |
| 42 | IA | 501 | GTP | C5-C6-N1 | 2.82 | 119.44 | 114.07 |
| 43 | KB | 501 | GDP | C5-C6-N1 | 2.82 | 119.44 | 114.07 |
| 42 | FB | 502 | GTP | C2-N1-C6 | -2.82 | 119.95 | 125.11 |
| 43 | IM | 501 | GDP | C8-N7-C5 | 2.82 | 107.34 | 102.55 |
| 42 | CF | 501 | GTP | C5-C6-N1 | 2.81 | 119.44 | 114.07 |
| 42 | HA | 501 | GTP | C4'-O4'-C1' | 2.81 | 112.50 | 109.92 |
| 43 | JN | 501 | GDP | C5-C6-N1 | 2.81 | 119.44 | 114.07 |
| 42 | IG | 501 | GTP | C4'-O4'-C1' | 2.81 | 112.50 | 109.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | MO | 501 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 43 | UN | 501 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 42 | BF | 501 | GTP | C5-C6-N1 | 2.81 | 119.43 | 114.07 |
| 43 | EM | 501 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 43 | IN | 501 | GDP | C2-N1-C6 | -2.81 | 119.97 | 125.11 |
| 42 | RN | 501 | GTP | C5-C6-N1 | 2.81 | 119.42 | 114.07 |
| 42 | ON | 501 | GTP | C5-C6-N1 | 2.81 | 119.42 | 114.07 |
| 43 | CP | 501 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 42 | SL | 501 | GTP | C2-N1-C6 | -2.80 | 119.98 | 125.11 |
| 43 | HO | 501 | GDP | C8-N7-C5 | 2.80 | 107.32 | 102.55 |
| 43 | HN | 501 | GDP | O6-C6-C5 | -2.80 | 118.77 | 124.32 |
| 42 | UM | 501 | GTP | C2-N1-C6 | -2.80 | 119.98 | 125.11 |
| 43 | PN | 502 | GDP | C8-N7-C5 | 2.80 | 107.32 | 102.55 |
| 42 | VF | 501 | GTP | C5-C6-N1 | 2.80 | 119.41 | 114.07 |
| 42 | DH | 501 | GTP | N1-C2-N3 | -2.80 | 118.19 | 123.32 |
| 43 | LP | 501 | GDP | C5-C6-N1 | 2.80 | 119.41 | 114.07 |
| 43 | CL | 501 | GDP | C8-N7-C5 | 2.80 | 107.31 | 102.55 |
| 43 | UP | 501 | GDP | C5-C6-N1 | 2.80 | 119.41 | 114.07 |
| 43 | LP | 501 | GDP | C8-N7-C5 | 2.80 | 107.31 | 102.55 |
| 43 | UB | 501 | GDP | O6-C6-C5 | -2.80 | 118.78 | 124.32 |
| 42 | VN | 501 | GTP | C5-C6-N1 | 2.80 | 119.41 | 114.07 |
| 42 | RN | 501 | GTP | C2-N1-C6 | -2.80 | 119.99 | 125.11 |
| 43 | KL | 501 | GDP | C8-N7-C5 | 2.80 | 107.31 | 102.55 |
| 43 | LP | 501 | GDP | C2-N1-C6 | -2.80 | 119.99 | 125.11 |
| 42 | UE | 501 | GTP | C5-C6-N1 | 2.79 | 119.40 | 114.07 |
| 42 | DA | 501 | GTP | C4'-O4'-C1' | 2.79 | 112.48 | 109.92 |
| 42 | UA | 501 | GTP | N1-C2-N3 | -2.79 | 118.21 | 123.32 |
| 43 | KB | 501 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 43 | LO | 502 | GDP | O6-C6-C5 | -2.79 | 118.79 | 124.32 |
| 43 | KN | 502 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 42 | GF | 501 | GTP | C2-N1-C6 | -2.79 | 120.01 | 125.11 |
| 43 | FM | 502 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 43 | HM | 502 | GDP | C8-N7-C5 | 2.79 | 107.29 | 102.55 |
| 43 | RB | 501 | GDP | C2-N1-C6 | -2.79 | 120.01 | 125.11 |
| 42 | WO | 501 | GTP | C5-C6-N1 | 2.78 | 119.38 | 114.07 |
| 43 | LB | 501 | GDP | O6-C6-C5 | -2.78 | 118.80 | 124.32 |
| 43 | IO | 501 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 43 | PM | 502 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 43 | FB | 501 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 43 | QO | 502 | GDP | C8-N7-C5 | 2.78 | 107.28 | 102.55 |
| 42 | FE | 501 | GTP | C5-C6-N1 | 2.78 | 119.37 | 114.07 |
| 43 | CP | 501 | GDP | O6-C6-C5 | -2.78 | 118.82 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | IO | 501 | GDP | C5-C6-N1 | 2.78 | 119.37 | 114.07 |
| 42 | EG | 501 | GTP | C4'-O4'-C1' | 2.77 | 112.46 | 109.92 |
| 43 | NO | 502 | GDP | C2-N1-C6 | -2.77 | 120.03 | 125.11 |
| 42 | WG | 501 | GTP | C5-C6-N1 | 2.77 | 119.36 | 114.07 |
| 43 | TL | 502 | GDP | N2-C2-N3 | -2.77 | 114.27 | 119.67 |
| 43 | OO | 502 | GDP | C5-C6-N1 | 2.77 | 119.35 | 114.07 |
| 43 | KL | 501 | GDP | C2-N1-C6 | -2.77 | 120.04 | 125.11 |
| 43 | IN | 501 | GDP | C5-C6-N1 | 2.77 | 119.35 | 114.07 |
| 43 | SL | 502 | GDP | O6-C6-C5 | -2.77 | 118.83 | 124.32 |
| 42 | OB | 502 | GTP | N1-C2-N3 | -2.77 | 118.25 | 123.32 |
| 43 | QB | 501 | GDP | C8-N7-C5 | 2.77 | 107.26 | 102.55 |
| 42 | IG | 501 | GTP | C5-C6-N1 | 2.77 | 119.35 | 114.07 |
| 42 | EA | 501 | GTP | C5-C6-N1 | 2.76 | 119.34 | 114.07 |
| 43 | RO | 502 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 43 | UO | 502 | GDP | C8-N7-C5 | 2.76 | 107.25 | 102.55 |
| 42 | EI | 501 | GTP | C5-C6-N1 | 2.76 | 119.34 | 114.07 |
| 42 | KD | 501 | GTP | C5-C6-N1 | 2.76 | 119.33 | 114.07 |
| 42 | PD | 501 | GTP | C5-C6-N1 | 2.76 | 119.33 | 114.07 |
| 42 | PN | 501 | GTP | C5-C6-N1 | 2.76 | 119.33 | 114.07 |
| 43 | GM | 501 | GDP | C8-N7-C5 | 2.76 | 107.24 | 102.55 |
| 42 | JB | 502 | GTP | C8-N7-C5 | 2.76 | 107.24 | 102.55 |
| 43 | QO | 502 | GDP | C5-C6-N1 | 2.76 | 119.33 | 114.07 |
| 42 | PB | 502 | GTP | C5-C6-N1 | 2.75 | 119.33 | 114.07 |
| 43 | LM | 502 | GDP | C8-N7-C5 | 2.75 | 107.24 | 102.55 |
| 42 | UI | 501 | GTP | O6-C6-C5 | -2.75 | 118.86 | 124.32 |
| 43 | SM | 502 | GDP | C2-N1-C6 | -2.75 | 120.07 | 125.11 |
| 42 | EI | 501 | GTP | O4'-C1'-N9 | -2.75 | 105.09 | 108.75 |
| 43 | KB | 501 | GDP | O6-C6-C5 | -2.75 | 118.86 | 124.32 |
| 42 | RF | 501 | GTP | C4'-O4'-C1' | 2.75 | 112.44 | 109.92 |
| 43 | WN | 501 | GDP | C8-N7-C5 | 2.75 | 107.23 | 102.55 |
| 42 | SL | 501 | GTP | O6-C6-C5 | -2.75 | 118.87 | 124.32 |
| 42 | DA | 501 | GTP | N2-C2-N3 | 2.75 | 125.04 | 119.67 |
| 43 | BO | 501 | GDP | C2-N1-C6 | -2.75 | 120.08 | 125.11 |
| 42 | TN | 501 | GTP | C2-N1-C6 | -2.75 | 120.08 | 125.11 |
| 43 | GB | 501 | GDP | O6-C6-C5 | -2.74 | 118.88 | 124.32 |
| 42 | KO | 501 | GTP | C5-C6-N1 | 2.74 | 119.31 | 114.07 |
| 43 | UN | 501 | GDP | C5-C6-N1 | 2.74 | 119.31 | 114.07 |
| 42 | PN | 501 | GTP | C4'-O4'-C1' | 2.74 | 112.44 | 109.92 |
| 43 | SM | 502 | GDP | C8-N7-C5 | 2.74 | 107.21 | 102.55 |
| 43 | IO | 501 | GDP | C2-N1-C6 | -2.74 | 120.10 | 125.11 |
| 43 | JB | 501 | GDP | C8-N7-C5 | 2.74 | 107.21 | 102.55 |
| 42 | ND | 501 | GTP | C5-C6-N1 | 2.74 | 119.29 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | VB | 501 | GDP | O6-C6-C5 | -2.74 | 118.89 | 124.32 |
| 42 | VQ | 501 | GTP | C5-C6-N1 | 2.73 | 119.29 | 114.07 |
| 43 | LP | 501 | GDP | O6-C6-C5 | -2.73 | 118.90 | 124.32 |
| 42 | EL | 501 | GTP | C5-C6-N1 | 2.73 | 119.29 | 114.07 |
| 43 | VN | 502 | GDP | C8-N7-C5 | 2.73 | 107.20 | 102.55 |
| 43 | SM | 502 | GDP | C5-C6-N1 | 2.73 | 119.28 | 114.07 |
| 42 | CA | 501 | GTP | C5-C6-N1 | 2.73 | 119.28 | 114.07 |
| 42 | KN | 501 | GTP | C2-N1-C6 | -2.73 | 120.11 | 125.11 |
| 42 | QO | 501 | GTP | C5-C6-N1 | 2.73 | 119.28 | 114.07 |
| 43 | HN | 501 | GDP | C8-N7-C5 | 2.73 | 107.20 | 102.55 |
| 42 | OD | 501 | GTP | C5-C6-N1 | 2.73 | 119.28 | 114.07 |
| 42 | LM | 501 | GTP | C4'-O4'-C1' | 2.73 | 112.42 | 109.92 |
| 42 | BG | 501 | GTP | C5-C6-N1 | 2.73 | 119.27 | 114.07 |
| 43 | FM | 502 | GDP | C5-C6-N1 | 2.73 | 119.27 | 114.07 |
| 42 | JB | 502 | GTP | O6-C6-N1 | 2.73 | 123.85 | 120.62 |
| 42 | FI | 501 | GTP | N2-C2-N3 | 2.72 | 124.99 | 119.67 |
| 42 | IH | 501 | GTP | O3G-PG-O3B | 2.72 | 113.76 | 104.64 |
| 43 | WP | 501 | GDP | C5-C6-N1 | 2.72 | 119.26 | 114.07 |
| 43 | OL | 502 | GDP | C5-C6-N1 | 2.72 | 119.26 | 114.07 |
| 43 | WO | 502 | GDP | C8-N7-C5 | 2.72 | 107.18 | 102.55 |
| 42 | FO | 501 | GTP | N2-C2-N3 | 2.72 | 124.98 | 119.67 |
| 42 | HP | 501 | GTP | C2-N1-C6 | -2.72 | 120.13 | 125.11 |
| 43 | UB | 501 | GDP | C2-N1-C6 | -2.72 | 120.14 | 125.11 |
| 43 | NP | 501 | GDP | C5-C6-N1 | 2.72 | 119.25 | 114.07 |
| 43 | DN | 501 | GDP | C8-N7-C5 | 2.72 | 107.17 | 102.55 |
| 43 | IO | 501 | GDP | O6-C6-C5 | -2.71 | 118.94 | 124.32 |
| 42 | FO | 501 | GTP | C8-N7-C5 | 2.71 | 107.17 | 102.55 |
| 42 | JE | 501 | GTP | C5-C6-N1 | 2.71 | 119.25 | 114.07 |
| 43 | KL | 501 | GDP | C5-C6-N1 | 2.71 | 119.24 | 114.07 |
| 43 | LN | 501 | GDP | C5-C6-N1 | 2.71 | 119.24 | 114.07 |
| 43 | TB | 501 | GDP | C2-N1-C6 | -2.71 | 120.15 | 125.11 |
| 42 | TF | 501 | GTP | C5-C6-N1 | 2.71 | 119.24 | 114.07 |
| 42 | KE | 501 | GTP | C4'-O4'-C1' | 2.71 | 112.41 | 109.92 |
| 43 | QN | 502 | GDP | C8-N7-C5 | 2.71 | 107.16 | 102.55 |
| 43 | DL | 501 | GDP | N1-C2-N3 | 2.71 | 128.28 | 123.32 |
| 43 | LN | 501 | GDP | O6-C6-C5 | -2.71 | 118.96 | 124.32 |
| 42 | RO | 501 | GTP | C5-C6-N1 | 2.70 | 119.23 | 114.07 |
| 42 | KM | 501 | GTP | N2-C2-N3 | 2.70 | 124.95 | 119.67 |
| 43 | HO | 501 | GDP | C5-C6-N1 | 2.70 | 119.23 | 114.07 |
| 43 | RB | 501 | GDP | C8-N7-C5 | 2.70 | 107.15 | 102.55 |
| 43 | QM | 501 | GDP | C8-N7-C5 | 2.70 | 107.15 | 102.55 |
| 42 | IE | 501 | GTP | C5-C6-N1 | 2.70 | 119.22 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | PP | 501 | GDP | C8-N7-C5 | 2.70 | 107.14 | 102.55 |
| 42 | WF | 501 | GTP | C5-C6-N1 | 2.70 | 119.22 | 114.07 |
| 42 | HA | 501 | GTP | C5-C6-N1 | 2.70 | 119.21 | 114.07 |
| 42 | JO | 501 | GTP | N2-C2-N3 | 2.69 | 124.93 | 119.67 |
| 43 | OL | 502 | GDP | C2-N1-C6 | -2.69 | 120.18 | 125.11 |
| 43 | AM | 501 | GDP | C8-N7-C5 | 2.69 | 107.13 | 102.55 |
| 43 | LN | 501 | GDP | C8-N7-C5 | 2.69 | 107.13 | 102.55 |
| 43 | BL | 502 | GDP | O6-C6-C5 | -2.69 | 118.99 | 124.32 |
| 42 | JA | 501 | GTP | C4'-O4'-C1' | 2.69 | 112.39 | 109.92 |
| 43 | IP | 501 | GDP | C5-C6-N1 | 2.69 | 119.20 | 114.07 |
| 43 | WQ | 501 | GDP | C5-C6-N1 | 2.69 | 119.20 | 114.07 |
| 43 | JN | 501 | GDP | O6-C6-C5 | -2.69 | 118.99 | 124.32 |
| 43 | OB | 501 | GDP | O6-C6-C5 | -2.69 | 119.00 | 124.32 |
| 42 | WA | 501 | GTP | C4'-O4'-C1' | 2.68 | 112.38 | 109.92 |
| 43 | VN | 502 | GDP | C5-C6-N1 | 2.68 | 119.19 | 114.07 |
| 43 | VN | 502 | GDP | O6-C6-C5 | -2.68 | 119.00 | 124.32 |
| 43 | NB | 501 | GDP | O6-C6-C5 | -2.68 | 119.00 | 124.32 |
| 42 | RN | 501 | GTP | C4'-O4'-C1' | 2.68 | 112.38 | 109.92 |
| 43 | QB | 501 | GDP | O6-C6-C5 | -2.68 | 119.01 | 124.32 |
| 43 | EN | 501 | GDP | C8-N7-C5 | 2.68 | 107.11 | 102.55 |
| 42 | LB | 502 | GTP | C5-C6-N1 | 2.67 | 119.17 | 114.07 |
| 42 | TL | 501 | GTP | C2-N1-C6 | -2.67 | 120.22 | 125.11 |
| 42 | UM | 501 | GTP | O4'-C1'-N9 | -2.67 | 105.20 | 108.75 |
| 42 | KD | 501 | GTP | N1-C2-N3 | -2.67 | 118.43 | 123.32 |
| 43 | GB | 501 | GDP | C2-N1-C6 | -2.67 | 120.22 | 125.11 |
| 42 | GA | 501 | GTP | C2-N1-C6 | -2.67 | 120.22 | 125.11 |
| 43 | JO | 502 | GDP | C2-N1-C6 | -2.67 | 120.22 | 125.11 |
| 42 | FM | 501 | GTP | C8-N7-C5 | 2.67 | 107.09 | 102.55 |
| 42 | SN | 501 | GTP | O6-C6-C5 | -2.67 | 119.03 | 124.32 |
| 43 | JN | 501 | GDP | C2-N1-C6 | -2.67 | 120.22 | 125.11 |
| 42 | TL | 501 | GTP | C4'-O4'-C1' | 2.67 | 112.37 | 109.92 |
| 42 | WA | 501 | GTP | O6-C6-C5 | -2.67 | 119.03 | 124.32 |
| 43 | OO | 502 | GDP | C2-N1-C6 | -2.66 | 120.23 | 125.11 |
| 43 | IP | 501 | GDP | C2-N1-C6 | -2.66 | 120.23 | 125.11 |
| 42 | BH | 501 | GTP | C4'-O4'-C1' | 2.66 | 112.36 | 109.92 |
| 42 | SH | 501 | GTP | O6-C6-C5 | -2.66 | 119.05 | 124.32 |
| 42 | KN | 501 | GTP | N2-C2-N1 | -2.66 | 111.15 | 116.76 |
| 43 | DL | 501 | GDP | O6-C6-C5 | -2.66 | 119.05 | 124.32 |
| 42 | EF | 501 | GTP | C4'-O4'-C1' | 2.66 | 112.36 | 109.92 |
| 43 | RL | 501 | GDP | C5-C6-N1 | 2.65 | 119.13 | 114.07 |
| 43 | KL | 501 | GDP | O6-C6-C5 | -2.65 | 119.07 | 124.32 |
| 43 | DP | 501 | GDP | C5-C6-N1 | 2.65 | 119.12 | 114.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | SH | 501 | GTP | C2-N1-C6 | -2.65 | 120.26 | 125.11 |
| 42 | II | 501 | GTP | C5-C6-N1 | 2.65 | 119.12 | 114.07 |
| 42 | LL | 501 | GTP | N2-C2-N3 | 2.65 | 124.84 | 119.67 |
| 42 | GB | 502 | GTP | C2-N1-C6 | -2.65 | 120.27 | 125.11 |
| 42 | TL | 501 | GTP | O6-C6-C5 | -2.64 | 119.08 | 124.32 |
| 42 | UI | 501 | GTP | O2B-PB-O3A | 2.64 | 114.42 | 107.27 |
| 42 | HH | 501 | GTP | O6-C6-C5 | -2.64 | 119.09 | 124.32 |
| 43 | HP | 502 | GDP | C5-C6-N1 | 2.64 | 119.11 | 114.07 |
| 42 | LO | 501 | GTP | O6-C6-C5 | -2.64 | 119.09 | 124.32 |
| 42 | UI | 501 | GTP | C2-N1-C6 | -2.64 | 120.28 | 125.11 |
| 42 | JA | 501 | GTP | O2B-PB-O3B | 2.64 | 114.40 | 107.27 |
| 42 | EF | 501 | GTP | O6-C6-C5 | -2.64 | 119.10 | 124.32 |
| 43 | OP | 501 | GDP | C5-C6-N1 | 2.63 | 119.09 | 114.07 |
| 43 | JO | 502 | GDP | O6-C6-C5 | -2.63 | 119.10 | 124.32 |
| 43 | SN | 502 | GDP | N2-C2-N3 | -2.63 | 114.54 | 119.67 |
| 43 | PM | 502 | GDP | C5-C6-N1 | 2.63 | 119.09 | 114.07 |
| 43 | JM | 501 | GDP | C8-N7-C5 | 2.63 | 107.02 | 102.55 |
| 42 | IF | 501 | GTP | C5-C6-N1 | 2.63 | 119.08 | 114.07 |
| 42 | ND | 501 | GTP | C2-N1-C6 | -2.63 | 120.30 | 125.11 |
| 42 | CI | 501 | GTP | C2-N1-C6 | -2.62 | 120.31 | 125.11 |
| 42 | MM | 501 | GTP | C2-N1-C6 | -2.62 | 120.31 | 125.11 |
| 43 | DO | 501 | GDP | C8-N7-C5 | 2.62 | 107.01 | 102.55 |
| 43 | FO | 502 | GDP | C8-N7-C5 | 2.62 | 107.01 | 102.55 |
| 42 | CG | 501 | GTP | C2-N1-C6 | -2.62 | 120.32 | 125.11 |
| 42 | DH | 501 | GTP | C2-N1-C6 | -2.62 | 120.32 | 125.11 |
| 42 | MN | 501 | GTP | C4'-O4'-C1' | 2.62 | 112.32 | 109.92 |
| 42 | RN | 501 | GTP | O2B-PB-O3A | 2.62 | 114.34 | 107.27 |
| 42 | JD | 501 | GTP | C2-N1-C6 | -2.61 | 120.32 | 125.11 |
| 43 | DM | 501 | GDP | C8-N7-C5 | 2.61 | 107.00 | 102.55 |
| 43 | RL | 501 | GDP | C8-N7-C5 | 2.61 | 107.00 | 102.55 |
| 43 | WP | 501 | GDP | C2-N1-C6 | -2.61 | 120.33 | 125.11 |
| 42 | MD | 501 | GTP | C2-N1-C6 | -2.61 | 120.33 | 125.11 |
| 43 | WQ | 501 | GDP | C2-N1-C6 | -2.61 | 120.33 | 125.11 |
| 43 | GP | 502 | GDP | O5'-C5'-C4' | 2.61 | 117.88 | 108.99 |
| 42 | WI | 501 | GTP | O4'-C1'-N9 | -2.61 | 105.29 | 108.75 |
| 42 | RF | 501 | GTP | O4'-C1'-N9 | -2.60 | 105.29 | 108.75 |
| 43 | EB | 501 | GDP | C8-N7-C5 | 2.60 | 106.98 | 102.55 |
| 43 | UB | 501 | GDP | C5-C6-N1 | 2.60 | 119.04 | 114.07 |
| 43 | OL | 502 | GDP | O6-C6-C5 | -2.60 | 119.16 | 124.32 |
| 43 | AL | 501 | GDP | C5-C6-N1 | 2.60 | 119.03 | 114.07 |
| 43 | OM | 502 | GDP | C5-C6-N1 | 2.60 | 119.03 | 114.07 |
| 42 | IA | 501 | GTP | C4'-O4'-C1' | 2.60 | 112.31 | 109.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | KE | 501 | GTP | C5-C6-N1 | 2.60 | 119.02 | 114.07 |
| 43 | UN | 501 | GDP | C2-N1-C6 | -2.59 | 120.36 | 125.11 |
| 43 | MN | 502 | GDP | C8-N7-C5 | 2.59 | 106.96 | 102.55 |
| 42 | GF | 501 | GTP | O4'-C1'-N9 | -2.59 | 105.31 | 108.75 |
| 42 | PM | 501 | GTP | C2-N1-C6 | -2.59 | 120.37 | 125.11 |
| 43 | EN | 501 | GDP | C4'-O4'-C1' | 2.59 | 112.30 | 109.92 |
| 42 | VA | 501 | GTP | O3G-PG-O3B | 2.59 | 113.31 | 104.64 |
| 42 | QG | 501 | GTP | C5-C6-N1 | 2.58 | 119.00 | 114.07 |
| 42 | FO | 501 | GTP | N1-C2-N3 | -2.58 | 118.59 | 123.32 |
| 43 | LN | 501 | GDP | C2-N1-C6 | -2.58 | 120.38 | 125.11 |
| 42 | RP | 501 | GTP | C5-C6-N1 | 2.58 | 118.99 | 114.07 |
| 42 | HH | 501 | GTP | C2-N1-C6 | -2.57 | 120.40 | 125.11 |
| 42 | KB | 502 | GTP | N2-C2-N3 | 2.57 | 124.69 | 119.67 |
| 42 | EG | 501 | GTP | C8-N7-C5 | 2.57 | 106.93 | 102.55 |
| 42 | TF | 501 | GTP | N2-C2-N3 | 2.57 | 124.69 | 119.67 |
| 43 | VN | 502 | GDP | C2-N1-C6 | -2.57 | 120.40 | 125.11 |
| 43 | SM | 502 | GDP | C4'-O4'-C1' | 2.57 | 112.28 | 109.92 |
| 43 | VB | 501 | GDP | C8-N7-C5 | 2.57 | 106.92 | 102.55 |
| 43 | IP | 501 | GDP | O6-C6-C5 | -2.57 | 119.23 | 124.32 |
| 42 | TG | 501 | GTP | O2B-PB-O3A | 2.57 | 114.22 | 107.27 |
| 43 | EL | 502 | GDP | C5-C6-N1 | 2.57 | 118.97 | 114.07 |
| 42 | OM | 501 | GTP | C4'-O4'-C1' | 2.56 | 112.27 | 109.92 |
| 43 | IN | 501 | GDP | O6-C6-C5 | -2.56 | 119.24 | 124.32 |
| 42 | VB | 502 | GTP | O6-C6-C5 | -2.56 | 119.25 | 124.32 |
| 43 | HQ | 501 | GDP | C5-C6-N1 | 2.56 | 118.95 | 114.07 |
| 42 | QF | 501 | GTP | C5-C6-N1 | 2.56 | 118.95 | 114.07 |
| 43 | PM | 502 | GDP | O6-C6-C5 | -2.56 | 119.25 | 124.32 |
| 42 | VQ | 501 | GTP | C4'-O4'-C1' | 2.55 | 112.26 | 109.92 |
| 43 | UM | 502 | GDP | C5-C6-N1 | 2.55 | 118.93 | 114.07 |
| 42 | UO | 501 | GTP | O6-C6-C5 | -2.55 | 119.27 | 124.32 |
| 42 | PD | 501 | GTP | C4'-O4'-C1' | 2.55 | 112.26 | 109.92 |
| 42 | LA | 501 | GTP | C2-N1-C6 | -2.55 | 120.45 | 125.11 |
| 43 | RM | 501 | GDP | C8-N7-C5 | 2.54 | 106.88 | 102.55 |
| 42 | BG | 501 | GTP | C2-N1-C6 | -2.54 | 120.45 | 125.11 |
| 43 | RB | 501 | GDP | C4'-O4'-C1' | 2.54 | 112.25 | 109.92 |
| 43 | HO | 501 | GDP | C2-N1-C6 | -2.54 | 120.45 | 125.11 |
| 42 | GH | 501 | GTP | O6-C6-C5 | -2.54 | 119.28 | 124.32 |
| 42 | UB | 502 | GTP | O6-C6-C5 | -2.54 | 119.28 | 124.32 |
| 42 | RE | 501 | GTP | C4'-O4'-C1' | 2.54 | 112.25 | 109.92 |
| 42 | EF | 501 | GTP | C2-N1-C6 | -2.54 | 120.46 | 125.11 |
| 42 | WO | 501 | GTP | O6-C6-C5 | -2.54 | 119.28 | 124.32 |
| 42 | UO | 501 | GTP | N1-C2-N3 | -2.54 | 118.67 | 123.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 42 | PO | 501 | GTP | O6-C6-C5 | -2.54 | 119.28 | 124.32 |
| 42 | EL | 501 | GTP | C4'-O4'-C1' | 2.54 | 112.25 | 109.92 |
| 42 | IG | 501 | GTP | O6-C6-C5 | -2.54 | 119.29 | 124.32 |
| 43 | BO | 501 | GDP | O6-C6-C5 | -2.54 | 119.29 | 124.32 |
| 42 | FN | 501 | GTP | C2-N1-C6 | -2.54 | 120.47 | 125.11 |
| 43 | DP | 501 | GDP | C2-N1-C6 | -2.54 | 120.47 | 125.11 |
| 42 | LD | 501 | GTP | C2-N1-C6 | -2.53 | 120.47 | 125.11 |
| 43 | NO | 502 | GDP | O6-C6-C5 | -2.53 | 119.30 | 124.32 |
| 42 | LA | 501 | GTP | O6-C6-C5 | -2.53 | 119.31 | 124.32 |
| 43 | HO | 501 | GDP | O6-C6-C5 | -2.53 | 119.31 | 124.32 |
| 42 | FM | 501 | GTP | N1-C2-N3 | -2.53 | 118.69 | 123.32 |
| 43 | UN | 501 | GDP | O6-C6-C5 | -2.53 | 119.31 | 124.32 |
| 43 | NL | 501 | GDP | C5-C6-N1 | 2.53 | 118.89 | 114.07 |
| 42 | WE | 501 | GTP | O4'-C1'-N9 | -2.52 | 105.40 | 108.75 |
| 42 | QL | 501 | GTP | O6-C6-C5 | -2.52 | 119.32 | 124.32 |
| 43 | WP | 501 | GDP | O6-C6-C5 | -2.52 | 119.32 | 124.32 |
| 43 | QB | 501 | GDP | C5-C6-N1 | 2.52 | 118.88 | 114.07 |
| 42 | WE | 501 | GTP | C2-N1-C6 | -2.52 | 120.50 | 125.11 |
| 42 | OO | 501 | GTP | C2-N1-C6 | -2.52 | 120.50 | 125.11 |
| 43 | PM | 502 | GDP | C2-N1-C6 | -2.51 | 120.51 | 125.11 |
| 42 | RG | 501 | GTP | O4'-C1'-N9 | -2.51 | 105.42 | 108.75 |
| 43 | QP | 501 | GDP | O4'-C1'-N9 | 2.51 | 112.08 | 108.75 |
| 42 | SN | 501 | GTP | N2-C2-N3 | 2.51 | 124.57 | 119.67 |
| 42 | DA | 501 | GTP | C2-N1-C6 | -2.51 | 120.52 | 125.11 |
| 42 | FE | 501 | GTP | C2-N1-C6 | -2.51 | 120.52 | 125.11 |
| 43 | FN | 502 | GDP | C4'-O4'-C1' | 2.50 | 112.22 | 109.92 |
| 42 | JF | 501 | GTP | N1-C2-N3 | -2.50 | 118.74 | 123.32 |
| 42 | TG | 501 | GTP | C2-N1-C6 | -2.50 | 120.53 | 125.11 |
| 42 | JF | 501 | GTP | O6-C6-C5 | -2.50 | 119.36 | 124.32 |
| 43 | RM | 501 | GDP | C4'-O4'-C1' | 2.50 | 112.22 | 109.92 |
| 43 | DM | 501 | GDP | O6-C6-N1 | 2.50 | 123.58 | 120.62 |
| 43 | TP | 501 | GDP | N2-C2-N3 | -2.50 | 114.80 | 119.67 |
| 43 | DP | 501 | GDP | O6-C6-C5 | -2.50 | 119.37 | 124.32 |
| 43 | OO | 502 | GDP | O6-C6-C5 | -2.50 | 119.37 | 124.32 |
| 42 | IH | 501 | GTP | O4'-C1'-N9 | -2.50 | 105.44 | 108.75 |
| 42 | RP | 501 | GTP | C2-N1-C6 | -2.49 | 120.54 | 125.11 |
| 42 | TI | 501 | GTP | C5-C6-N1 | 2.49 | 118.82 | 114.07 |
| 42 | RG | 501 | GTP | C5-C6-N1 | 2.49 | 118.82 | 114.07 |
| 42 | OB | 502 | GTP | C4'-O4'-C1' | 2.49 | 112.20 | 109.92 |
| 42 | SG | 501 | GTP | C2-N1-C6 | -2.49 | 120.55 | 125.11 |
| 43 | FM | 502 | GDP | C2-N1-C6 | -2.49 | 120.56 | 125.11 |
| 42 | GA | 501 | GTP | N1-C2-N3 | -2.48 | 118.77 | 123.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | PE | 501 | GTP | N1-C2-N3 | -2.48 | 118.77 | 123.32 |
| 43 | QL | 502 | GDP | O6-C6-C5 | -2.48 | 119.40 | 124.32 |
| 42 | NG | 501 | GTP | O6-C6-C5 | -2.48 | 119.41 | 124.32 |
| 42 | BI | 501 | GTP | O6-C6-C5 | -2.48 | 119.41 | 124.32 |
| 42 | HB | 502 | GTP | O6-C6-C5 | -2.48 | 119.41 | 124.32 |
| 43 | HP | 502 | GDP | C2-N1-C6 | -2.48 | 120.58 | 125.11 |
| 42 | VP | 501 | GTP | C2-N1-C6 | -2.48 | 120.58 | 125.11 |
| 42 | DI | 501 | GTP | O6-C6-C5 | -2.47 | 119.42 | 124.32 |
| 43 | DB | 501 | GDP | O6-C6-C5 | -2.47 | 119.42 | 124.32 |
| 43 | NP | 501 | GDP | C2-N1-C6 | -2.47 | 120.59 | 125.11 |
| 42 | TF | 501 | GTP | C2-N1-C6 | -2.47 | 120.59 | 125.11 |
| 42 | RF | 501 | GTP | N1-C2-N3 | -2.47 | 118.80 | 123.32 |
| 42 | WG | 501 | GTP | O6-C6-C5 | -2.47 | 119.43 | 124.32 |
| 43 | HP | 502 | GDP | O6-C6-C5 | -2.47 | 119.43 | 124.32 |
| 42 | VA | 501 | GTP | C4'-O4'-C1' | 2.47 | 112.18 | 109.92 |
| 43 | WQ | 501 | GDP | O6-C6-C5 | -2.46 | 119.43 | 124.32 |
| 42 | SN | 501 | GTP | N1-C2-N3 | -2.46 | 118.81 | 123.32 |
| 42 | UB | 502 | GTP | C2-N1-C6 | -2.46 | 120.60 | 125.11 |
| 42 | IE | 501 | GTP | C4'-O4'-C1' | 2.46 | 112.18 | 109.92 |
| 42 | HE | 501 | GTP | O6-C6-C5 | -2.46 | 119.44 | 124.32 |
| 42 | FE | 501 | GTP | C4'-O4'-C1' | 2.46 | 112.18 | 109.92 |
| 42 | MH | 501 | GTP | N1-C2-N3 | -2.46 | 118.82 | 123.32 |
| 42 | NG | 501 | GTP | C2-N1-C6 | -2.46 | 120.61 | 125.11 |
| 42 | LD | 501 | GTP | C4'-O4'-C1' | 2.45 | 112.17 | 109.92 |
| 43 | NM | 502 | GDP | O4'-C1'-N9 | 2.45 | 112.00 | 108.75 |
| 42 | SM | 501 | GTP | O6-C6-C5 | -2.45 | 119.46 | 124.32 |
| 42 | HP | 501 | GTP | O6-C6-C5 | -2.45 | 119.46 | 124.32 |
| 43 | EL | 502 | GDP | O6-C6-C5 | -2.45 | 119.46 | 124.32 |
| 42 | MH | 501 | GTP | O6-C6-C5 | -2.45 | 119.47 | 124.32 |
| 43 | QL | 502 | GDP | C5-C6-N1 | 2.45 | 118.74 | 114.07 |
| 42 | FB | 502 | GTP | O4'-C1'-N9 | -2.45 | 105.50 | 108.75 |
| 43 | NP | 501 | GDP | O6-C6-C5 | -2.45 | 119.47 | 124.32 |
| 42 | FM | 501 | GTP | N2-C2-N3 | 2.45 | 124.45 | 119.67 |
| 42 | JO | 501 | GTP | N1-C2-N3 | -2.44 | 118.84 | 123.32 |
| 42 | OB | 502 | GTP | O3G-PG-O3B | 2.44 | 112.83 | 104.64 |
| 43 | NL | 501 | GDP | O6-C6-C5 | -2.44 | 119.48 | 124.32 |
| 42 | PO | 501 | GTP | N2-C2-N3 | 2.44 | 124.44 | 119.67 |
| 42 | SM | 501 | GTP | C2-N1-C6 | -2.44 | 120.64 | 125.11 |
| 43 | FM | 502 | GDP | O6-C6-C5 | -2.44 | 119.49 | 124.32 |
| 42 | WF | 501 | GTP | N1-C2-N3 | -2.44 | 118.86 | 123.32 |
| 42 | II | 501 | GTP | O6-C6-C5 | -2.43 | 119.49 | 124.32 |
| 42 | KB | 502 | GTP | O6-C6-C5 | -2.43 | 119.50 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | JO | 501 | GTP | O6-C6-C5 | -2.43 | 119.50 | 124.32 |
| 42 | MD | 501 | GTP | O6-C6-C5 | -2.43 | 119.50 | 124.32 |
| 42 | DF | 501 | GTP | C5-C6-N1 | 2.43 | 118.70 | 114.07 |
| 42 | NM | 501 | GTP | C2-N1-C6 | -2.43 | 120.67 | 125.11 |
| 42 | GP | 501 | GTP | O6-C6-N1 | 2.42 | 123.50 | 120.62 |
| 42 | BL | 501 | GTP | C4'-O4'-C1' | 2.42 | 112.14 | 109.92 |
| 43 | IQ | 501 | GDP | C5-C6-N1 | 2.42 | 118.69 | 114.07 |
| 42 | VA | 501 | GTP | N1-C2-N3 | -2.42 | 118.89 | 123.32 |
| 42 | TN | 501 | GTP | N2-C2-N3 | 2.42 | 124.39 | 119.67 |
| 42 | EA | 501 | GTP | O6-C6-C5 | -2.42 | 119.53 | 124.32 |
| 42 | MN | 501 | GTP | O6-C6-C5 | -2.42 | 119.53 | 124.32 |
| 42 | LB | 502 | GTP | N1-C2-N3 | -2.42 | 118.89 | 123.32 |
| 42 | QN | 501 | GTP | C5-C6-N1 | 2.42 | 118.68 | 114.07 |
| 42 | SN | 501 | GTP | O2B-PB-O3A | 2.41 | 113.80 | 107.27 |
| 42 | IH | 501 | GTP | O6-C6-C5 | -2.41 | 119.53 | 124.32 |
| 42 | CE | 501 | GTP | N2-C2-N3 | 2.41 | 124.38 | 119.67 |
| 42 | WO | 501 | GTP | O4'-C1'-N9 | -2.41 | 105.55 | 108.75 |
| 42 | LO | 501 | GTP | N1-C2-N3 | -2.41 | 118.90 | 123.32 |
| 42 | LM | 501 | GTP | O6-C6-C5 | -2.41 | 119.55 | 124.32 |
| 42 | PD | 501 | GTP | C2-N1-C6 | -2.41 | 120.71 | 125.11 |
| 43 | AL | 501 | GDP | C2-N1-C6 | -2.40 | 120.71 | 125.11 |
| 42 | EI | 501 | GTP | C2-N1-C6 | -2.40 | 120.71 | 125.11 |
| 42 | UE | 501 | GTP | C4'-O4'-C1' | 2.40 | 112.12 | 109.92 |
| 42 | PE | 501 | GTP | N2-C2-N3 | 2.40 | 124.36 | 119.67 |
| 42 | NN | 501 | GTP | O6-C6-C5 | -2.40 | 119.56 | 124.32 |
| 42 | HB | 502 | GTP | C4'-O4'-C1' | 2.39 | 112.12 | 109.92 |
| 42 | RF | 501 | GTP | C5-C6-N1 | 2.39 | 118.63 | 114.07 |
| 42 | QL | 501 | GTP | O5'-C5'-C4' | 2.39 | 117.13 | 108.99 |
| 42 | GH | 501 | GTP | N1-C2-N3 | -2.39 | 118.94 | 123.32 |
| 43 | DB | 501 | GDP | C5-C6-N1 | 2.39 | 118.63 | 114.07 |
| 43 | EO | 501 | GDP | C2-N1-C6 | -2.39 | 120.74 | 125.11 |
| 42 | CE | 501 | GTP | O6-C6-C5 | -2.39 | 119.59 | 124.32 |
| 42 | LO | 501 | GTP | C2-N1-C6 | -2.39 | 120.74 | 125.11 |
| 42 | HP | 501 | GTP | O4'-C1'-N9 | -2.39 | 105.58 | 108.75 |
| 42 | UE | 501 | GTP | C2-N1-C6 | -2.38 | 120.75 | 125.11 |
| 42 | VB | 502 | GTP | N1-C2-N3 | -2.38 | 118.96 | 123.32 |
| 42 | LB | 502 | GTP | O3G-PG-O3B | 2.38 | 112.62 | 104.64 |
| 42 | DG | 501 | GTP | O2B-PB-O3A | 2.38 | 113.70 | 107.27 |
| 42 | VF | 501 | GTP | C2-N1-C6 | -2.38 | 120.76 | 125.11 |
| 42 | PB | 502 | GTP | N1-C2-N3 | -2.37 | 118.97 | 123.32 |
| 42 | VN | 501 | GTP | O4'-C1'-N9 | -2.37 | 105.60 | 108.75 |
| 42 | MH | 501 | GTP | C4'-O4'-C1' | 2.37 | 112.10 | 109.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | DF | 501 | GTP | N2-C2-N3 | 2.37 | 124.30 | 119.67 |
| 42 | FI | 501 | GTP | N1-C2-N3 | -2.37 | 118.98 | 123.32 |
| 42 | FB | 502 | GTP | O6-C6-C5 | -2.37 | 119.62 | 124.32 |
| 42 | WG | 501 | GTP | C2-N1-C6 | -2.37 | 120.77 | 125.11 |
| 42 | TH | 501 | GTP | N1-C2-N3 | -2.37 | 118.99 | 123.32 |
| 42 | KB | 502 | GTP | O4'-C1'-N9 | -2.36 | 105.61 | 108.75 |
| 42 | WI | 501 | GTP | C2-N1-C6 | -2.36 | 120.78 | 125.11 |
| 42 | WA | 501 | GTP | C2-N1-C6 | -2.36 | 120.78 | 125.11 |
| 42 | BL | 501 | GTP | O6-C6-C5 | -2.36 | 119.64 | 124.32 |
| 43 | RN | 502 | GDP | O4'-C1'-N9 | -2.36 | 105.61 | 108.75 |
| 42 | BA | 501 | GTP | C4'-O4'-C1' | 2.36 | 112.09 | 109.92 |
| 42 | JA | 501 | GTP | N1-C2-N3 | -2.36 | 119.00 | 123.32 |
| 42 | JA | 501 | GTP | O6-C6-C5 | -2.36 | 119.64 | 124.32 |
| 42 | II | 501 | GTP | N1-C2-N3 | -2.36 | 119.00 | 123.32 |
| 42 | OD | 501 | GTP | O2B-PB-O3A | 2.36 | 113.64 | 107.27 |
| 43 | OP | 501 | GDP | C2-N1-C6 | -2.36 | 120.80 | 125.11 |
| 42 | KB | 502 | GTP | N1-C2-N3 | -2.36 | 119.00 | 123.32 |
| 42 | HM | 501 | GTP | N2-C2-N3 | 2.36 | 124.27 | 119.67 |
| 42 | FN | 501 | GTP | C4'-O4'-C1' | 2.35 | 112.08 | 109.92 |
| 42 | MM | 501 | GTP | O2B-PB-O3A | 2.35 | 113.64 | 107.27 |
| 42 | OL | 501 | GTP | C2-N1-C6 | -2.35 | 120.80 | 125.11 |
| 43 | EL | 502 | GDP | C2-N1-C6 | -2.35 | 120.80 | 125.11 |
| 42 | SH | 501 | GTP | O4'-C1'-N9 | -2.35 | 105.63 | 108.75 |
| 43 | OM | 502 | GDP | O6-C6-C5 | -2.35 | 119.66 | 124.32 |
| 42 | DG | 501 | GTP | C8-N7-C5 | 2.35 | 106.55 | 102.55 |
| 42 | IG | 501 | GTP | N1-C2-N3 | -2.35 | 119.01 | 123.32 |
| 42 | NO | 501 | GTP | C2-N1-C6 | -2.35 | 120.81 | 125.11 |
| 42 | VF | 501 | GTP | O2B-PB-O3A | 2.35 | 113.62 | 107.27 |
| 42 | KB | 502 | GTP | C2-N1-C6 | -2.35 | 120.81 | 125.11 |
| 42 | SN | 501 | GTP | C2-N1-C6 | -2.35 | 120.81 | 125.11 |
| 42 | PO | 501 | GTP | N1-C2-N3 | -2.35 | 119.02 | 123.32 |
| 42 | PE | 501 | GTP | O4'-C1'-N9 | -2.35 | 105.63 | 108.75 |
| 42 | WO | 501 | GTP | N1-C2-N3 | -2.34 | 119.03 | 123.32 |
| 42 | PE | 501 | GTP | O6-C6-C5 | -2.34 | 119.67 | 124.32 |
| 42 | SM | 501 | GTP | O2B-PB-O3A | 2.34 | 113.61 | 107.27 |
| 42 | GB | 502 | GTP | O2B-PB-O3A | 2.34 | 113.60 | 107.27 |
| 42 | SM | 501 | GTP | C4'-O4'-C1' | 2.34 | 112.07 | 109.92 |
| 42 | SM | 501 | GTP | N1-C2-N3 | -2.34 | 119.04 | 123.32 |
| 42 | EI | 501 | GTP | O6-C6-C5 | -2.33 | 119.69 | 124.32 |
| 42 | MM | 501 | GTP | O4'-C1'-N9 | -2.33 | 105.65 | 108.75 |
| 42 | BF | 501 | GTP | N1-C2-N3 | -2.33 | 119.05 | 123.32 |
| 42 | OO | 501 | GTP | O6-C6-C5 | -2.33 | 119.70 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | WF | 501 | GTP | N2-C2-N3 | 2.33 | 124.21 | 119.67 |
| 42 | DG | 501 | GTP | N1-C2-N3 | -2.32 | 119.06 | 123.32 |
| 43 | UP | 501 | GDP | O6-C6-C5 | -2.32 | 119.71 | 124.32 |
| 42 | OD | 501 | GTP | C2-N1-C6 | -2.32 | 120.86 | 125.11 |
| 43 | AL | 501 | GDP | O6-C6-C5 | -2.32 | 119.72 | 124.32 |
| 42 | IH | 501 | GTP | C2-N1-C6 | -2.32 | 120.86 | 125.11 |
| 43 | VB | 501 | GDP | C2-N1-C6 | -2.32 | 120.86 | 125.11 |
| 42 | JA | 501 | GTP | N2-C2-N3 | 2.32 | 124.20 | 119.67 |
| 42 | II | 501 | GTP | O4'-C1'-N9 | -2.32 | 105.67 | 108.75 |
| 42 | SP | 501 | GTP | O2B-PB-O3A | 2.32 | 113.53 | 107.27 |
| 42 | CE | 501 | GTP | N1-C2-N3 | -2.31 | 119.08 | 123.32 |
| 42 | IE | 501 | GTP | N1-C2-N3 | -2.31 | 119.08 | 123.32 |
| 43 | JL | 501 | GDP | N2-C2-N3 | -2.31 | 115.16 | 119.67 |
| 42 | NO | 501 | GTP | C4'-O4'-C1' | 2.31 | 112.04 | 109.92 |
| 43 | NL | 501 | GDP | C2-N1-C6 | -2.31 | 120.88 | 125.11 |
| 42 | SL | 501 | GTP | N2-C2-N3 | 2.31 | 124.18 | 119.67 |
| 42 | JD | 501 | GTP | O6-C6-C5 | -2.31 | 119.74 | 124.32 |
| 42 | EH | 501 | GTP | O6-C6-C5 | -2.31 | 119.74 | 124.32 |
| 42 | WE | 501 | GTP | O6-C6-C5 | -2.31 | 119.74 | 124.32 |
| 43 | LL | 502 | GDP | C5-C6-N1 | 2.31 | 118.47 | 114.07 |
| 42 | VN | 501 | GTP | C2-N1-C6 | -2.31 | 120.89 | 125.11 |
| 42 | FO | 501 | GTP | C2-N1-C6 | -2.30 | 120.89 | 125.11 |
| 43 | LL | 502 | GDP | C2-N1-C6 | -2.30 | 120.89 | 125.11 |
| 42 | VB | 502 | GTP | C2-N1-C6 | -2.30 | 120.90 | 125.11 |
| 42 | IF | 501 | GTP | O4'-C1'-N9 | -2.30 | 105.69 | 108.75 |
| 42 | WI | 501 | GTP | O6-C6-C5 | -2.30 | 119.76 | 124.32 |
| 42 | IA | 501 | GTP | C2-N1-C6 | -2.30 | 120.90 | 125.11 |
| 42 | GH | 501 | GTP | C2-N1-C6 | -2.30 | 120.90 | 125.11 |
| 42 | CH | 501 | GTP | N1-C2-N3 | -2.30 | 119.11 | 123.32 |
| 42 | NM | 501 | GTP | C4'-O4'-C1' | 2.30 | 112.03 | 109.92 |
| 42 | CH | 501 | GTP | O6-C6-C5 | -2.30 | 119.77 | 124.32 |
| 42 | ON | 501 | GTP | C2-N1-C6 | -2.30 | 120.91 | 125.11 |
| 42 | RG | 501 | GTP | N1-C2-N3 | -2.30 | 119.12 | 123.32 |
| 42 | AA | 501 | GTP | O6-C6-C5 | -2.29 | 119.77 | 124.32 |
| 42 | AG | 501 | GTP | C4'-O4'-C1' | 2.29 | 112.03 | 109.92 |
| 42 | WA | 501 | GTP | N1-C2-N3 | -2.29 | 119.12 | 123.32 |
| 42 | QG | 501 | GTP | O3G-PG-O3B | 2.29 | 112.32 | 104.64 |
| 42 | NE | 501 | GTP | N2-C2-N3 | 2.29 | 124.14 | 119.67 |
| 42 | LM | 501 | GTP | N1-C2-N3 | -2.29 | 119.13 | 123.32 |
| 42 | RO | 501 | GTP | N1-C2-N3 | -2.29 | 119.13 | 123.32 |
| 42 | SG | 501 | GTP | O4'-C1'-N9 | -2.29 | 105.71 | 108.75 |
| 42 | JE | 501 | GTP | C2-N1-C6 | -2.28 | 120.93 | 125.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | WO | 501 | GTP | C2-N1-C6 | -2.28 | 120.94 | 125.11 |
| 42 | HM | 501 | GTP | O4'-C1'-N9 | -2.28 | 105.72 | 108.75 |
| 42 | MB | 502 | GTP | O6-C6-C5 | -2.28 | 119.80 | 124.32 |
| 42 | VA | 501 | GTP | O6-C6-C5 | -2.28 | 119.81 | 124.32 |
| 43 | SN | 502 | GDP | C8-N7-C5 | 2.28 | 106.42 | 102.55 |
| 42 | CF | 501 | GTP | O6-C6-C5 | -2.27 | 119.81 | 124.32 |
| 42 | AH | 501 | GTP | C4'-O4'-C1' | 2.27 | 112.01 | 109.92 |
| 42 | RO | 501 | GTP | O6-C6-C5 | -2.27 | 119.82 | 124.32 |
| 42 | HA | 501 | GTP | C2-N1-C6 | -2.27 | 120.95 | 125.11 |
| 42 | SL | 501 | GTP | N1-C2-N3 | -2.27 | 119.16 | 123.32 |
| 42 | VQ | 501 | GTP | C2-N1-C6 | -2.27 | 120.95 | 125.11 |
| 43 | QL | 502 | GDP | C2-N1-C6 | -2.27 | 120.95 | 125.11 |
| 42 | VB | 502 | GTP | C4'-O4'-C1' | 2.27 | 112.00 | 109.92 |
| 42 | JE | 501 | GTP | O6-C6-C5 | -2.27 | 119.83 | 124.32 |
| 42 | KE | 501 | GTP | N1-C2-N3 | -2.27 | 119.17 | 123.32 |
| 43 | HQ | 501 | GDP | O6-C6-C5 | -2.26 | 119.83 | 124.32 |
| 42 | WA | 501 | GTP | O2B-PB-O3A | 2.26 | 113.39 | 107.27 |
| 42 | GB | 502 | GTP | N1-C2-N3 | -2.26 | 119.17 | 123.32 |
| 43 | IQ | 501 | GDP | O6-C6-C5 | -2.26 | 119.84 | 124.32 |
| 42 | DH | 501 | GTP | O4'-C1'-N9 | -2.26 | 105.75 | 108.75 |
| 43 | OP | 501 | GDP | O6-C6-C5 | -2.25 | 119.85 | 124.32 |
| 42 | VF | 501 | GTP | C4'-O4'-C1' | 2.25 | 111.99 | 109.92 |
| 42 | NE | 501 | GTP | N1-C2-N3 | -2.25 | 119.19 | 123.32 |
| 42 | QN | 501 | GTP | O2B-PB-O3A | 2.25 | 113.36 | 107.27 |
| 43 | OM | 502 | GDP | C2-N1-C6 | -2.25 | 120.99 | 125.11 |
| 43 | RL | 501 | GDP | C2-N1-C6 | -2.25 | 120.99 | 125.11 |
| 42 | KM | 501 | GTP | O6-C6-N1 | 2.25 | 123.29 | 120.62 |
| 43 | TB | 501 | GDP | C5-C6-N1 | 2.25 | 118.36 | 114.07 |
| 43 | TB | 501 | GDP | C4'-O4'-C1' | -2.25 | 107.87 | 109.92 |
| 43 | EO | 501 | GDP | C5-C6-N1 | 2.25 | 118.35 | 114.07 |
| 42 | HE | 501 | GTP | N1-C2-N3 | -2.24 | 119.22 | 123.32 |
| 42 | QO | 501 | GTP | C2-N1-C6 | -2.24 | 121.01 | 125.11 |
| 42 | VA | 501 | GTP | C2-N1-C6 | -2.24 | 121.01 | 125.11 |
| 43 | RP | 502 | GDP | C4'-O4'-C1' | 2.24 | 111.97 | 109.92 |
| 42 | VN | 501 | GTP | O6-C6-C5 | -2.23 | 119.89 | 124.32 |
| 42 | RP | 501 | GTP | O4'-C1'-N9 | -2.23 | 105.79 | 108.75 |
| 42 | DG | 501 | GTP | C2-N1-C6 | -2.23 | 121.03 | 125.11 |
| 42 | UM | 501 | GTP | O6-C6-C5 | -2.23 | 119.90 | 124.32 |
| 42 | JE | 501 | GTP | C4'-O4'-C1' | 2.23 | 111.97 | 109.92 |
| 42 | LB | 502 | GTP | N2-C2-N3 | 2.23 | 124.03 | 119.67 |
| 42 | EA | 501 | GTP | C2-N1-C6 | -2.22 | 121.04 | 125.11 |
| 42 | HM | 501 | GTP | N1-C2-N3 | -2.22 | 119.25 | 123.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | UO | 502 | GDP | O4'-C1'-N9 | 2.22 | 111.69 | 108.75 |
| 42 | HA | 501 | GTP | O2A-PA-O3A | 2.22 | 113.27 | 107.27 |
| 42 | TF | 501 | GTP | O2B-PB-O3A | 2.22 | 113.27 | 107.27 |
| 43 | EP | 501 | GDP | N2-C2-N1 | 2.22 | 121.44 | 116.76 |
| 42 | CA | 501 | GTP | N1-C2-N3 | -2.22 | 119.26 | 123.32 |
| 42 | MH | 501 | GTP | C2-N1-C6 | -2.21 | 121.06 | 125.11 |
| 43 | RL | 501 | GDP | O6-C6-C5 | -2.21 | 119.94 | 124.32 |
| 42 | CF | 501 | GTP | N1-C2-N3 | -2.21 | 119.27 | 123.32 |
| 43 | FP | 501 | GDP | O6-C6-N1 | 2.21 | 123.24 | 120.62 |
| 42 | TG | 501 | GTP | C4'-O4'-C1' | 2.21 | 111.95 | 109.92 |
| 42 | EL | 501 | GTP | C2-N1-C6 | -2.21 | 121.07 | 125.11 |
| 43 | SB | 501 | GDP | N2-C2-N3 | -2.20 | 115.37 | 119.67 |
| 43 | QB | 501 | GDP | C2-N1-C6 | -2.20 | 121.07 | 125.11 |
| 42 | DA | 501 | GTP | N1-C2-N3 | -2.20 | 119.28 | 123.32 |
| 42 | IF | 501 | GTP | N1-C2-N3 | -2.20 | 119.28 | 123.32 |
| 42 | VQ | 501 | GTP | O4'-C1'-N9 | -2.20 | 105.82 | 108.75 |
| 42 | CI | 501 | GTP | C4'-O4'-C1' | 2.20 | 111.94 | 109.92 |
| 42 | OM | 501 | GTP | C5-C6-N1 | 2.20 | 118.27 | 114.07 |
| 42 | LM | 501 | GTP | C2-N1-C6 | -2.20 | 121.08 | 125.11 |
| 42 | NO | 501 | GTP | N1-C2-N3 | -2.20 | 119.30 | 123.32 |
| 42 | RE | 501 | GTP | N1-C2-N3 | -2.19 | 119.30 | 123.32 |
| 42 | JD | 501 | GTP | C4'-O4'-C1' | 2.19 | 111.93 | 109.92 |
| 42 | WF | 501 | GTP | O6-C6-C5 | -2.19 | 119.97 | 124.32 |
| 42 | BH | 501 | GTP | O6-C6-C5 | -2.19 | 119.98 | 124.32 |
| 42 | DA | 501 | GTP | O3G-PG-O3B | 2.19 | 111.98 | 104.64 |
| 43 | TB | 501 | GDP | O6-C6-N1 | 2.19 | 123.22 | 120.62 |
| 43 | HQ | 501 | GDP | C2-N1-C6 | -2.19 | 121.10 | 125.11 |
| 42 | KE | 501 | GTP | O2B-PB-O3A | 2.19 | 113.19 | 107.27 |
| 42 | II | 501 | GTP | N2-C2-N3 | 2.19 | 123.95 | 119.67 |
| 42 | GH | 501 | GTP | O4'-C1'-N9 | -2.18 | 105.85 | 108.75 |
| 42 | TH | 501 | GTP | C2-N1-C6 | -2.18 | 121.11 | 125.11 |
| 42 | GE | 501 | GTP | O6-C6-C5 | -2.18 | 119.99 | 124.32 |
| 43 | JL | 501 | GDP | O4'-C4'-C5' | 2.18 | 116.32 | 109.33 |
| 42 | CF | 501 | GTP | C2-N1-C6 | -2.18 | 121.12 | 125.11 |
| 42 | WF | 501 | GTP | O4'-C1'-N9 | -2.18 | 105.85 | 108.75 |
| 42 | DG | 501 | GTP | O6-C6-C5 | -2.18 | 120.00 | 124.32 |
| 42 | ON | 501 | GTP | O6-C6-C5 | -2.18 | 120.00 | 124.32 |
| 42 | SH | 501 | GTP | N1-C2-N3 | -2.18 | 119.33 | 123.32 |
| 42 | AF | 501 | GTP | O6-C6-C5 | -2.17 | 120.01 | 124.32 |
| 42 | JD | 501 | GTP | N1-C2-N3 | -2.17 | 119.34 | 123.32 |
| 42 | QN | 501 | GTP | N1-C2-N3 | -2.17 | 119.34 | 123.32 |
| 42 | LB | 502 | GTP | O6-C6-C5 | -2.17 | 120.02 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | AH | 501 | GTP | O6-C6-C5 | -2.17 | 120.03 | 124.32 |
| 42 | TG | 501 | GTP | O4'-C1'-N9 | -2.17 | 105.87 | 108.75 |
| 42 | HA | 501 | GTP | N1-C2-N3 | -2.16 | 119.36 | 123.32 |
| 42 | IA | 501 | GTP | O6-C6-C5 | -2.16 | 120.03 | 124.32 |
| 42 | VF | 501 | GTP | N1-C2-N3 | -2.16 | 119.36 | 123.32 |
| 43 | EN | 501 | GDP | C2'-C3'-C4' | 2.16 | 106.79 | 102.61 |
| 42 | OM | 501 | GTP | C2-N1-C6 | -2.16 | 121.15 | 125.11 |
| 42 | DE | 501 | GTP | O6-C6-C5 | -2.16 | 120.04 | 124.32 |
| 42 | QF | 501 | GTP | N1-C2-N3 | -2.16 | 119.36 | 123.32 |
| 42 | JA | 501 | GTP | C2-N1-C6 | -2.16 | 121.16 | 125.11 |
| 42 | CG | 501 | GTP | N1-C2-N3 | -2.16 | 119.37 | 123.32 |
| 42 | EF | 501 | GTP | N1-C2-N3 | -2.16 | 119.37 | 123.32 |
| 42 | AG | 501 | GTP | O6-C6-C5 | -2.16 | 120.04 | 124.32 |
| 42 | UI | 501 | GTP | N1-C2-N3 | -2.16 | 119.37 | 123.32 |
| 42 | RE | 501 | GTP | C2-N1-C6 | -2.16 | 121.16 | 125.11 |
| 42 | QF | 501 | GTP | O6-C6-C5 | -2.16 | 120.05 | 124.32 |
| 42 | EL | 501 | GTP | O6-C6-C5 | -2.15 | 120.05 | 124.32 |
| 42 | BF | 501 | GTP | C2-N1-C6 | -2.15 | 121.17 | 125.11 |
| 42 | EA | 501 | GTP | O4'-C1'-N9 | -2.15 | 105.89 | 108.75 |
| 42 | SP | 501 | GTP | O6-C6-C5 | -2.15 | 120.05 | 124.32 |
| 42 | CH | 501 | GTP | C2-N1-C6 | -2.15 | 121.17 | 125.11 |
| 42 | KO | 501 | GTP | O6-C6-C5 | -2.15 | 120.06 | 124.32 |
| 42 | RN | 501 | GTP | O6-C6-C5 | -2.15 | 120.06 | 124.32 |
| 42 | HE | 501 | GTP | C2-N1-C6 | -2.15 | 121.17 | 125.11 |
| 42 | ON | 501 | GTP | O4'-C1'-N9 | -2.15 | 105.90 | 108.75 |
| 42 | AF | 501 | GTP | C4'-O4'-C1' | 2.15 | 111.89 | 109.92 |
| 42 | OB | 502 | GTP | O4'-C1'-N9 | -2.15 | 105.90 | 108.75 |
| 42 | NE | 501 | GTP | C2-N1-C6 | -2.14 | 121.19 | 125.11 |
| 43 | IQ | 501 | GDP | C2-N1-C6 | -2.14 | 121.19 | 125.11 |
| 42 | JF | 501 | GTP | C2-N1-C6 | -2.14 | 121.19 | 125.11 |
| 42 | NO | 501 | GTP | O6-C6-C5 | -2.14 | 120.08 | 124.32 |
| 42 | PN | 501 | GTP | O6-C6-C5 | -2.14 | 120.08 | 124.32 |
| 42 | CA | 501 | GTP | C2-N1-C6 | -2.14 | 121.20 | 125.11 |
| 42 | FM | 501 | GTP | C2-N1-C6 | -2.14 | 121.20 | 125.11 |
| 42 | TN | 501 | GTP | O4'-C1'-N9 | -2.14 | 105.91 | 108.75 |
| 42 | TF | 501 | GTP | O3G-PG-O3B | 2.13 | 111.79 | 104.64 |
| 43 | QN | 502 | GDP | C4'-O4'-C1' | 2.13 | 111.88 | 109.92 |
| 42 | AG | 501 | GTP | O2A-PA-O3A | 2.13 | 113.04 | 107.27 |
| 42 | LM | 501 | GTP | N2-C2-N3 | 2.13 | 123.84 | 119.67 |
| 42 | CA | 501 | GTP | O6-C6-C5 | -2.13 | 120.09 | 124.32 |
| 42 | WI | 501 | GTP | N1-C2-N3 | -2.13 | 119.42 | 123.32 |
| 42 | JO | 501 | GTP | O4'-C1'-N9 | -2.13 | 105.92 | 108.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | TH | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 42 | EL | 501 | GTP | N1-C2-N3 | -2.12 | 119.43 | 123.32 |
| 43 | IB | 501 | GDP | O2B-PB-O3A | 2.12 | 111.76 | 104.64 |
| 42 | ON | 501 | GTP | N1-C2-N3 | -2.12 | 119.43 | 123.32 |
| 42 | UA | 501 | GTP | O3G-PG-O3B | 2.12 | 111.75 | 104.64 |
| 42 | FN | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 42 | LD | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 42 | RO | 501 | GTP | C2-N1-C6 | -2.12 | 121.23 | 125.11 |
| 42 | OL | 501 | GTP | N1-C2-N3 | -2.12 | 119.44 | 123.32 |
| 42 | EG | 501 | GTP | O2A-PA-O3A | 2.12 | 113.00 | 107.27 |
| 42 | JE | 501 | GTP | N1-C2-N3 | -2.12 | 119.44 | 123.32 |
| 42 | LA | 501 | GTP | N1-C2-N3 | -2.12 | 119.44 | 123.32 |
| 42 | KO | 501 | GTP | O4'-C4'-C5' | 2.12 | 116.11 | 109.33 |
| 42 | VN | 501 | GTP | N1-C2-N3 | -2.12 | 119.44 | 123.32 |
| 42 | DI | 501 | GTP | O4'-C1'-N9 | -2.11 | 105.94 | 108.75 |
| 42 | FI | 501 | GTP | C2-N1-C6 | -2.11 | 121.24 | 125.11 |
| 42 | IG | 501 | GTP | O4'-C1'-N9 | -2.11 | 105.94 | 108.75 |
| 42 | EL | 501 | GTP | O2B-PB-O3A | 2.11 | 112.98 | 107.27 |
| 42 | WG | 501 | GTP | O2B-PB-O3A | 2.11 | 112.96 | 107.27 |
| 42 | QF | 501 | GTP | C2-N1-C6 | -2.10 | 121.26 | 125.11 |
| 42 | IH | 501 | GTP | N1-C2-N3 | -2.10 | 119.47 | 123.32 |
| 42 | PB | 502 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 42 | NE | 501 | GTP | O4'-C1'-N9 | -2.10 | 105.96 | 108.75 |
| 42 | VB | 502 | GTP | N2-C2-N3 | 2.10 | 123.78 | 119.67 |
| 42 | QG | 501 | GTP | N1-C2-N3 | -2.10 | 119.47 | 123.32 |
| 42 | SG | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 43 | WO | 502 | GDP | C2'-C3'-C4' | 2.10 | 106.67 | 102.61 |
| 42 | HM | 501 | GTP | C2-N1-C6 | -2.10 | 121.27 | 125.11 |
| 42 | QL | 501 | GTP | O3G-PG-O3B | 2.10 | 111.67 | 104.64 |
| 42 | GH | 501 | GTP | N2-C2-N3 | 2.10 | 123.77 | 119.67 |
| 42 | FN | 501 | GTP | N1-C2-N3 | -2.10 | 119.48 | 123.32 |
| 42 | IA | 501 | GTP | N1-C2-N3 | -2.10 | 119.48 | 123.32 |
| 42 | QG | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 42 | AF | 501 | GTP | O2B-PB-O3A | 2.10 | 112.94 | 107.27 |
| 42 | MM | 501 | GTP | N2-C2-N1 | -2.10 | 112.34 | 116.76 |
| 43 | RM | 501 | GDP | O4'-C1'-N9 | -2.10 | 105.97 | 108.75 |
| 42 | BF | 501 | GTP | O6-C6-C5 | -2.10 | 120.17 | 124.32 |
| 42 | PM | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 42 | AA | 501 | GTP | C4'-O4'-C1' | 2.09 | 111.84 | 109.92 |
| 42 | QN | 501 | GTP | O4'-C1'-N9 | -2.09 | 105.97 | 108.75 |
| 42 | OO | 501 | GTP | N1-C2-N3 | -2.09 | 119.49 | 123.32 |
| 43 | EO | 501 | GDP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 42 | FB | 502 | GTP | C2'-C3'-C4' | 2.09 | 106.64 | 102.61 |
| 42 | DA | 501 | GTP | O6-C6-C5 | -2.09 | 120.19 | 124.32 |
| 42 | FM | 501 | GTP | O2B-PB-O3A | 2.09 | 112.91 | 107.27 |
| 42 | EA | 501 | GTP | N1-C2-N3 | -2.08 | 119.50 | 123.32 |
| 42 | FI | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 42 | IG | 501 | GTP | C2-N1-C6 | -2.08 | 121.30 | 125.11 |
| 43 | GP | 502 | GDP | O4'-C4'-C5' | 2.08 | 116.00 | 109.33 |
| 42 | EH | 501 | GTP | C4'-O4'-C1' | 2.08 | 111.83 | 109.92 |
| 42 | QL | 501 | GTP | O2'-C2'-C3' | -2.08 | 105.15 | 111.82 |
| 42 | QG | 501 | GTP | O4'-C1'-N9 | -2.08 | 105.99 | 108.75 |
| 42 | CE | 501 | GTP | C2-N1-C6 | -2.08 | 121.31 | 125.11 |
| 43 | AP | 501 | GDP | C5-C6-N1 | 2.08 | 118.03 | 114.07 |
| 42 | PB | 502 | GTP | N2-C2-N3 | 2.08 | 123.73 | 119.67 |
| 42 | VQ | 501 | GTP | N1-C2-N3 | -2.08 | 119.52 | 123.32 |
| 42 | WG | 501 | GTP | N1-C2-N3 | -2.07 | 119.52 | 123.32 |
| 42 | PO | 501 | GTP | C2-N1-C6 | -2.07 | 121.31 | 125.11 |
| 42 | QO | 501 | GTP | N1-C2-N3 | -2.07 | 119.52 | 123.32 |
| 42 | VP | 501 | GTP | N1-C2-N3 | -2.07 | 119.52 | 123.32 |
| 42 | CG | 501 | GTP | N2-C2-N3 | 2.07 | 123.72 | 119.67 |
| 42 | VP | 501 | GTP | O6-C6-C5 | -2.07 | 120.21 | 124.32 |
| 42 | UO | 501 | GTP | N2-C2-N3 | 2.07 | 123.72 | 119.67 |
| 42 | HA | 501 | GTP | O6-C6-C5 | -2.07 | 120.23 | 124.32 |
| 42 | UE | 501 | GTP | N1-C2-N3 | -2.07 | 119.54 | 123.32 |
| 42 | FN | 501 | GTP | O2B-PB-O3A | 2.06 | 112.85 | 107.27 |
| 42 | MD | 501 | GTP | N1-C2-N3 | -2.06 | 119.54 | 123.32 |
| 43 | KO | 502 | GDP | O3B-PB-O3A | 2.06 | 111.55 | 104.64 |
| 42 | OL | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 42 | ML | 501 | GTP | N1-C2-N3 | -2.06 | 119.54 | 123.32 |
| 42 | CI | 501 | GTP | O2B-PB-O3A | 2.06 | 112.85 | 107.27 |
| 42 | EG | 501 | GTP | O3G-PG-O3B | 2.06 | 111.55 | 104.64 |
| 42 | UB | 502 | GTP | N1-C2-N3 | -2.06 | 119.55 | 123.32 |
| 42 | BF | 501 | GTP | O4'-C1'-N9 | -2.06 | 106.01 | 108.75 |
| 42 | NM | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 42 | GA | 501 | GTP | O2A-PA-O3A | 2.06 | 112.83 | 107.27 |
| 43 | DM | 501 | GDP | N2-C2-N3 | -2.06 | 115.67 | 119.67 |
| 42 | BA | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 42 | KM | 501 | GTP | N1-C2-N3 | -2.05 | 119.56 | 123.32 |
| 42 | JE | 501 | GTP | O3G-PG-O3B | 2.05 | 111.52 | 104.64 |
| 42 | GF | 501 | GTP | O3G-PG-O3B | 2.05 | 111.51 | 104.64 |
| 42 | SG | 501 | GTP | N1-C2-N3 | -2.05 | 119.57 | 123.32 |
| 43 | UP | 501 | GDP | O2B-PB-O3A | 2.04 | 111.49 | 104.64 |
| 42 | FE | 501 | GTP | O6-C6-C5 | -2.04 | 120.28 | 124.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | SM | 502 | GDP | C2'-C3'-C4' | 2.04 | 106.54 | 102.61 |
| 42 | VA | 501 | GTP | O2A-PA-O3A | 2.03 | 112.77 | 107.27 |
| 42 | BI | 501 | GTP | C2'-C3'-C4' | 2.03 | 106.54 | 102.61 |
| 43 | EM | 501 | GDP | C2'-C3'-C4' | 2.03 | 106.54 | 102.61 |
| 42 | VA | 501 | GTP | O2B-PB-O3B | 2.03 | 112.77 | 107.27 |
| 42 | HE | 501 | GTP | N2-C2-N3 | 2.03 | 123.64 | 119.67 |
| 42 | IF | 501 | GTP | C2-N1-C6 | -2.03 | 121.39 | 125.11 |
| 42 | JF | 501 | GTP | N2-C2-N3 | 2.03 | 123.63 | 119.67 |
| 42 | RO | 501 | GTP | O3G-PG-O3B | 2.03 | 111.43 | 104.64 |
| 42 | BH | 501 | GTP | O2B-PB-O3A | 2.03 | 112.75 | 107.27 |
| 42 | KN | 501 | GTP | O3G-PG-O3B | 2.03 | 111.43 | 104.64 |
| 43 | TO | 501 | GDP | N2-C2-N3 | -2.02 | 115.73 | 119.67 |
| 42 | JF | 501 | GTP | O3G-PG-O3B | 2.02 | 111.40 | 104.64 |
| 42 | PD | 501 | GTP | O6-C6-C5 | -2.02 | 120.32 | 124.32 |
| 42 | OD | 501 | GTP | N1-C2-N3 | -2.01 | 119.63 | 123.32 |
| 42 | MD | 501 | GTP | O4'-C1'-N9 | -2.01 | 106.08 | 108.75 |
| 42 | IE | 501 | GTP | C2-N1-C6 | -2.01 | 121.43 | 125.11 |
| 42 | EG | 501 | GTP | O6-C6-N1 | 2.01 | 123.01 | 120.62 |
| 42 | JB | 502 | GTP | O3G-PG-O3B | 2.01 | 111.38 | 104.64 |
| 42 | UE | 501 | GTP | O6-C6-C5 | -2.01 | 120.34 | 124.32 |
| 42 | GF | 501 | GTP | N1-C2-N3 | -2.01 | 119.64 | 123.32 |
| 42 | QL | 501 | GTP | O2B-PB-O3A | 2.01 | 112.70 | 107.27 |
| 42 | TL | 501 | GTP | O2B-PB-O3A | 2.01 | 112.70 | 107.27 |
| 42 | TL | 501 | GTP | N1-C2-N3 | -2.01 | 119.64 | 123.32 |
| 42 | PB | 502 | GTP | C2-N1-C6 | -2.01 | 121.44 | 125.11 |
| 42 | VQ | 501 | GTP | O6-C6-C5 | -2.00 | 120.35 | 124.32 |
| 42 | RF | 501 | GTP | N2-C2-N3 | 2.00 | 123.59 | 119.67 |
| 43 | RM | 501 | GDP | C2'-C3'-C4' | 2.00 | 106.48 | 102.61 |
| 42 | PO | 501 | GTP | O3G-PG-O3B | 2.00 | 111.35 | 104.64 |
| 42 | IF | 501 | GTP | O6-C6-C5 | -2.00 | 120.35 | 124.32 |

There are no chirality outliers.

All (1290) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | AA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | AE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | AE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | AE | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | AF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | AF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | AF | 501 | GTP | C5'-O5'-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | AF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | AG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | AG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | AG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | AG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | AH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | BA | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | BA | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | BA | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | BA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | BA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | BF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | BF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | BF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | BF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | BG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | BG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | BG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | BG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | BH | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | BH | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | BH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | BI | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | BI | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | BI | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | BI | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | BL | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | CA | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | CA | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | CA | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | CA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | CA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | CE | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | CE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | CF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | CF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | CF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | CF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | CG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | CG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | CG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | CG | 501 | GTP | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | CG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | CH | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | CH | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | CH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | CI | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | CI | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | CI | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | DA | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | DA | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | DA | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | DA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | DF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | DG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | DG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | DG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | DH | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | DH | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | DH | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | DH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | DI | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | DI | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | DI | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | EA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | EF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | EF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | EF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | EG | 501 | GTP | PB-O3B-PG-O3G |
| 42 | EG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | EG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | EG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | EI | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | EI | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | EL | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | FB | 502 | GTP | C5'-O5'-PA-O3A |
| 42 | FB | 502 | GTP | C5'-O5'-PA-O2A |
| 42 | FB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | FB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | FE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | FI | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | FI | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | FI | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | FI | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | FM | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | FM | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | FM | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | FM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | FN | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | FN | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | FN | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | FO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | GA | 501 | GTP | PB-O3B-PG-O2G |
| 42 | GB | 502 | GTP | C5'-O5'-PA-O2A |
| 42 | GB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | GE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | GF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | GF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | GF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | GF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | GH | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | GH | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | GH | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | GH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | GH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | GP | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | GP | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | HA | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | HA | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | HA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | HA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | HB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | HE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | HE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | HE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | HH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | HM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | HM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | HP | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | HP | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | HP | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | HP | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | HP | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | IA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | IE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | IE | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | IF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | IF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | IF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | IF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | IG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | IG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | IG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | IG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | IG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | IH | 501 | GTP | PB-O3B-PG-O3G |
| 42 | IH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | II | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | II | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | II | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | II | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | JA | 501 | GTP | PB-O3B-PG-O3G |
| 42 | JA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | JB | 502 | GTP | PB-O3B-PG-O3G |
| 42 | JB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | JB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | JD | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | JD | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | JD | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | JE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | JE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | JE | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | JE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | JF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | JO | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | JO | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | JO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | KB | 502 | GTP | C5'-O5'-PA-O3A |
| 42 | KB | 502 | GTP | C5'-O5'-PA-O2A |
| 42 | KB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | KD | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | KD | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | KD | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | KD | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | KE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | KE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | KE | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | KE | 501 | GTP | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | KM | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | KM | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | KM | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | KN | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | KN | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | KO | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | KO | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | KO | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | KO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | LA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | LB | 502 | GTP | PB-O3B-PG-O3G |
| 42 | LB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | LD | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | LD | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | LD | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | LD | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | LL | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | LL | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | LL | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | LO | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | LO | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | MB | 502 | GTP | C5'-O5'-PA-O3A |
| 42 | MB | 502 | GTP | C5'-O5'-PA-O1A |
| 42 | MB | 502 | GTP | C5'-O5'-PA-O2A |
| 42 | MD | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | MD | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | MD | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | MD | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | MH | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | MH | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | MH | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | MH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | ML | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | ML | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | ML | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | MM | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | MM | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | MM | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | MN | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | MN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | MN | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | ND | 501 | GTP | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | ND | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | ND | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | ND | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | NE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | NG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | NM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | NO | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | NO | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | NO | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | NO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | OB | 502 | GTP | PB-O3B-PG-O2G |
| 42 | OB | 502 | GTP | PB-O3B-PG-O3G |
| 42 | OB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | OB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | OD | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | OD | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | OD | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | OD | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | OL | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | OL | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | OL | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | OL | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | OM | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | OM | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | OM | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | OM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | ON | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | ON | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | ON | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | ON | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | ON | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | OO | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | OO | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | OO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | PB | 502 | GTP | C5'-O5'-PA-O3A |
| 42 | PB | 502 | GTP | C5'-O5'-PA-O1A |
| 42 | PB | 502 | GTP | C5'-O5'-PA-O2A |
| 42 | PB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | PD | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | PD | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | PE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | PE | 501 | GTP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | PE | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | PE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | PE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | PM | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | PM | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | PM | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | PM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | PM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | PN | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | PN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | PN | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | PN | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | PN | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | PO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | QF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | QF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | QF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | QF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | QG | 501 | GTP | PB-O3B-PG-O3G |
| 42 | QG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | QG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | QL | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | QL | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | QL | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | QL | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | QN | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | QN | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | QO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | RE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | RE | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | RE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | RF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | RF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | RF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | RF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | RG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | RG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | RG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | RN | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | RN | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | RO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | RO | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | RP | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | SG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | SG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | SG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | SG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | SH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | SH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | SL | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | SL | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | SM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | SN | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | SN | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | SN | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | TF | 501 | GTP | PB-O3B-PG-O3G |
| 42 | TF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | TF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | TG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | TG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | TG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | TH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | TI | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | TI | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | TI | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | TN | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | TN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | TN | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | UA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | UB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | UB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | UE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | UE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | UE | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | UE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | UI | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | UI | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | UI | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | UI | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | UM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | UO | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | UO | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | UO | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | UO | 501 | GTP | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | VA | 501 | GTP | PB-O3B-PG-O3G |
| 42 | VA | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | VA | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | VA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | VB | 502 | GTP | O4'-C4'-C5'-O5' |
| 42 | VF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | VF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | VF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | VF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | VN | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | VN | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | VN | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | VN | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | VP | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | VQ | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | VQ | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | VQ | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | WA | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | WA | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | WA | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | WE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | WE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | WF | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | WF | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | WF | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | WF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | WF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | WG | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | WG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | WG | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | WG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | WI | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | WI | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | WI | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | WI | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | WI | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | WO | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | WO | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | WO | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | WO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | WO | 501 | GTP | C3'-C4'-C5'-O5' |
| 43 | AB | 501 | GDP | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | AB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | AL | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | AL | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | AM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | AN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | AN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | AN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | AN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | AO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | AP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | AP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | AP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | BB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | BL | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | BL | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | BM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | BN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | BO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | BO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | BP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | CB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | CL | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | CL | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | CL | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | CM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | CM | 501 | GDP | C5'-O5'-PA-O2A |
| 43 | CN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | CN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | CO | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | CP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | DB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | DB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | DL | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | DL | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | DN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | DO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | DO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | EB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | EL | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | EL | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | EM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | EM | 501 | GDP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | EN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | EO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | EP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | EP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | FB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | FB | 501 | GDP | C5'-O5'-PA-O2A |
| 43 | FM | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | FN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | FN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | FO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | FP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | GB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | GB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | GB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | GB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | GM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | GM | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | GM | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | GN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | GN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | GN | 501 | GDP | C5'-O5'-PA-O2A |
| 43 | GO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | GP | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | GP | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | GP | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | HB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | HB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | HB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | HB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | HM | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | HM | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | HN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | HN | 501 | GDP | C5'-O5'-PA-O2A |
| 43 | HN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | HO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | HO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | HO | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | HP | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | HP | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | HQ | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | IB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | IB | 501 | GDP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | IM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | IM | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | IN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | IO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | IO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | IP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | IQ | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | IQ | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | JB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | JB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | JB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | JL | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | JL | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | JL | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | JM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | JM | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | JN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | JN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | JN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | JO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | JO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | KB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | KL | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | KM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | KN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | KN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | KO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | KO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | KP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | KP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | LB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | LB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | LB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | LL | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | LM | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | LM | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | LN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | LO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | LP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | LP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | MB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | MB | 501 | GDP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | MB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | ML | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | ML | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | MM | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | MM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | MM | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | MM | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | MN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | MN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | MO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | MO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | MP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | NB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | NB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | NL | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | NL | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | NM | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | NN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | NN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | NN | 502 | GDP | C5'-O5'-PA-O2A |
| 43 | NO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | NO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | NO | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | NO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | NP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | NP | 501 | GDP | C5'-O5'-PA-O2A |
| 43 | OB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | OB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | OL | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | OL | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | OL | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | OM | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | OM | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | OM | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | ON | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | ON | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | OO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | OO | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | OP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | OP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | PB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | PB | 501 | GDP | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | PL | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | PM | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | PM | 502 | GDP | C5'-O5'-PA-O2A |
| 43 | PN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | PN | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | PO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | PO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | PP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | QB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | QL | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | QM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | QN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | QN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | QO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | QO | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | QP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | QP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | RB | 501 | GDP | PA-O3A-PB-O2B |
| 43 | RB | 501 | GDP | PA-O3A-PB-O3B |
| 43 | RB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | RL | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | RM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | RN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | RO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | RP | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | SB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | SB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | SL | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | SM | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | SM | 502 | GDP | C5'-O5'-PA-O2A |
| 43 | SN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | SO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | SO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | SP | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | TB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | TL | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | TL | 502 | GDP | C5'-O5'-PA-O2A |
| 43 | TM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | TM | 501 | GDP | C5'-O5'-PA-O2A |
| 43 | TN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | TN | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | TO | 501 | GDP | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | TO | 501 | GDP | C5'-O5'-PA-O2A |
| 43 | TP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | TP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | TP | 501 | GDP | C5'-O5'-PA-O2A |
| 43 | UB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | UB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | UM | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | UN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | UN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | UN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | UO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | UO | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | UO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | UP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | VB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | VB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | VN | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | VN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | VN | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | VN | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | VO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | VO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | VO | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | VP | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | VP | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | VQ | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | VQ | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | WB | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | WM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | WM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | WM | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | WM | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | WN | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | WN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | WO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | WP | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | WP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | WP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | WQ | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | WQ | 501 | GDP | C5'-O5'-PA-O1A |
| 42 | AA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | AF | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | AG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | AH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | BF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | BH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | BI | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | CE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | CH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | DA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | DE | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | DE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | DF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | DH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | DI | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | DI | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | EF | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | FE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | FN | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | FO | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | GB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | GE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | GF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | HH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | IA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | IF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | IH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | II | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | JA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | KB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | KE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | LB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | LM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | LO | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | MD | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | ND | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | NE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | NN | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | NN | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | NO | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | OD | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | OL | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | OM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | OO | 501 | GTP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | PB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | PO | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | QF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | QL | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | QO | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | RE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | RF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | RG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | RN | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | RP | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | SG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | SN | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | TL | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | TL | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | UA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | UE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | UM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | UO | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | VP | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | WA | 501 | GTP | C3'-C4'-C5'-O5' |
| 43 | AO | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | AP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | BB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | BB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | BL | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | BM | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | BM | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | BO | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | BO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | CB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | CN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | CO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | DB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | DP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | DP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | EB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | EO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | GP | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | HM | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | HN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | HO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | HP | 502 | GDP | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | HP | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | HQ | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | IB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | IB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | IM | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | IO | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | IO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | IP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | IP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | IQ | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | IQ | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | JB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | JL | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | JM | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | JN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | JO | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | JO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | KB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | KB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | KL | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | KP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | LB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | LO | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | LP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | MB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | MO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | NL | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | OB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | OB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | OL | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | ON | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | OO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | OP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | PB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | PL | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | PL | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | PM | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | PM | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | PN | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | PO | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | PO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | QB | 501 | GDP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | QL | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | QL | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | QM | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | QM | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | QN | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | QO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | RL | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | RL | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | RO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | SP | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | TN | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | UB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | UM | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | UN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | VO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | VP | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | VP | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | VQ | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | WB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | WB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | WN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | WP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | WQ | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | WQ | 501 | GDP | C3'-C4'-C5'-O5' |
| 42 | BL | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | CF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | HB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | JF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | LA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | MM | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | MM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | MN | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | TH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | VF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | WG | 501 | GTP | C3'-C4'-C5'-O5' |
| 43 | AB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | AL | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | AO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | BP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | BP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | CP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | CP | 501 | GDP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | DM | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | DM | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | EB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | EO | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | KL | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | KN | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | KN | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | LL | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | LO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | MN | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | MN | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | MO | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | NB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | NP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | NP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | OP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | PP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | PP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | QN | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | RO | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | SP | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | UP | 501 | GDP | C3'-C4'-C5'-O5' |
| 42 | EA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | EL | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | FM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | JE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | JO | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | KO | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | MN | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | NG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | NM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | SM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | UI | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | VA | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | VB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | VQ | 501 | GTP | C3'-C4'-C5'-O5' |
| 43 | AB | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | AL | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | LL | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | MP | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | NB | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | NM | 502 | GDP | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | WO | 502 | GDP | C3'-C4'-C5'-O5' |
| 42 | LL | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | LO | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | MB | 502 | GTP | C3'-C4'-C5'-O5' |
| 42 | MH | 501 | GTP | C3'-C4'-C5'-O5' |
| 43 | AM | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | BN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | IN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | KM | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | ML | 502 | GDP | C3'-C4'-C5'-O5' |
| 42 | EF | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | EH | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | LM | 501 | GTP | C3'-C4'-C5'-O5' |
| 43 | DN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | EL | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | GO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | IN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | LN | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | ML | 502 | GDP | O4'-C4'-C5'-O5' |
| 43 | UP | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | WO | 502 | GDP | O4'-C4'-C5'-O5' |
| 42 | OM | 501 | GTP | C4'-C5'-O5'-PA |
| 43 | AM | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | FO | 502 | GDP | C3'-C4'-C5'-O5' |
| 43 | KM | 502 | GDP | O4'-C4'-C5'-O5' |
| 42 | DF | 501 | GTP | PB-O3B-PG-O1G |
| 42 | IA | 501 | GTP | PB-O3B-PG-O1G |
| 42 | MB | 502 | GTP | O4'-C4'-C5'-O5' |
| 43 | FB | 501 | GDP | C3'-C4'-C5'-O5' |
| 42 | CG | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | CI | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | ON | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | PN | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | RE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | RF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | WI | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | DG | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | LL | 501 | GTP | O4'-C4'-C5'-O5' |
| 43 | BN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | EL | 502 | GDP | O4'-C4'-C5'-O5' |
| 42 | BH | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | BI | 501 | GTP | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | CA | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | GH | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | IF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | IG | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | WF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | KM | 501 | GTP | O4'-C4'-C5'-O5' |
| 43 | DN | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | LN | 501 | GDP | O4'-C4'-C5'-O5' |
| 42 | HE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | PM | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | DA | 501 | GTP | PB-O3B-PG-O3G |
| 42 | IA | 501 | GTP | PB-O3B-PG-O3G |
| 42 | GA | 501 | GTP | C3'-C4'-C5'-O5' |
| 43 | DL | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | GO | 501 | GDP | O4'-C4'-C5'-O5' |
| 42 | EI | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | FI | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | OO | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | AF | 501 | GTP | PA-O3A-PB-O2B |
| 42 | CE | 501 | GTP | PG-O3B-PB-O1B |
| 42 | DA | 501 | GTP | PA-O3A-PB-O2B |
| 42 | DE | 501 | GTP | PA-O3A-PB-O2B |
| 42 | EG | 501 | GTP | PG-O3B-PB-O1B |
| 42 | FM | 501 | GTP | PG-O3B-PB-O1B |
| 42 | FN | 501 | GTP | PA-O3A-PB-O2B |
| 42 | GP | 501 | GTP | PB-O3A-PA-O1A |
| 42 | LO | 501 | GTP | PG-O3B-PB-O1B |
| 42 | LO | 501 | GTP | PA-O3A-PB-O2B |
| 42 | OL | 501 | GTP | PB-O3A-PA-O1A |
| 42 | QN | 501 | GTP | PA-O3A-PB-O2B |
| 42 | UI | 501 | GTP | PA-O3A-PB-O2B |
| 42 | VQ | 501 | GTP | PG-O3B-PB-O1B |
| 42 | VQ | 501 | GTP | PA-O3A-PB-O2B |
| 42 | WA | 501 | GTP | PG-O3B-PB-O1B |
| 42 | BF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | CF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | CH | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | DI | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | FB | 502 | GTP | C4'-C5'-O5'-PA |
| 42 | GF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | HP | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | KD | 501 | GTP | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | KE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | RG | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | UI | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | VN | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | VP | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | WG | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | BG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | BH | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | CE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | CE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | CH | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | CI | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | DE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | DE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | DE | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | EH | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | EH | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | FB | 502 | GTP | C5'-O5'-PA-O1A |
| 42 | FE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | FE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | FI | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | FN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | GB | 502 | GTP | C5'-O5'-PA-O3A |
| 42 | GB | 502 | GTP | C5'-O5'-PA-O1A |
| 42 | GE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | GE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | HA | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | HE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | HH | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | HM | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | HM | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | HM | 501 | GTP | C5'-O5'-PA-O2A |
| 42 | IE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | IE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | JO | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | KB | 502 | GTP | C5'-O5'-PA-O1A |
| 42 | KD | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | KN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | LD | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | LO | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | NE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | NE | 501 | GTP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | NM | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | NM | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | NN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | OO | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | QN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | RE | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | RG | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | RN | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | RN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | RO | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | RO | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | SH | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | SH | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | SN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | VA | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | VB | 502 | GTP | C5'-O5'-PA-O1A |
| 42 | VN | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | VQ | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | WA | 501 | GTP | C5'-O5'-PA-O1A |
| 42 | WE | 501 | GTP | C5'-O5'-PA-O3A |
| 42 | WE | 501 | GTP | C5'-O5'-PA-O1A |
| 43 | AM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | AO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | BB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | BM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | BN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | BP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | CO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | CP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | EN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | FB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | FM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | FP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | GO | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | HM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | HN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | HQ | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | IM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | IN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | IP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | JM | 501 | GDP | C5'-O5'-PA-O3A |
| 43 | KL | 501 | GDP | C5'-O5'-PA-O3A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 43 | KM | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | LM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | LN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | LO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | LP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | NL | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | NM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | NP | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | OM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | ON | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | OO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | PB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | PL | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | PM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | PN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | QB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | QL | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | QM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | QO | 502 | GDP | C5'-O5'-PA-O3A |
| 43 | RL | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | RM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | RN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | SL | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | SM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | SN | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | SN | 502 | GDP | C5'-O5'-PA-O2A |
| 43 | SP | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | TB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | TL | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | TM | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | TO | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | UB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | UM | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | UO | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | VB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | VQ | 502 | GDP | C5'-O5'-PA-O1A |
| 43 | WB | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | WN | 501 | GDP | C5'-O5'-PA-O1A |
| 43 | WO | 502 | GDP | C5'-O5'-PA-O1A |
| 42 | AG | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | BG | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | CE | 501 | GTP | C4'-C5'-O5'-PA |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | FE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | GB | 502 | GTP | C4'-C5'-O5'-PA |
| 42 | HM | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | II | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | KB | 502 | GTP | C4'-C5'-O5'-PA |
| 42 | KO | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | MD | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | ND | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | OL | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | PB | 502 | GTP | C4'-C5'-O5'-PA |
| 42 | PE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | QF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | RN | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | SG | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | SH | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | TI | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | UE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | UO | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | VF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | WE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | WO | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | JA | 501 | GTP | PB-O3B-PG-O1G |
| 43 | DL | 501 | GDP | O4'-C4'-C5'-O5' |
| 43 | FB | 501 | GDP | O4'-C4'-C5'-O5' |
| 42 | HA | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | OD | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | AE | 501 | GTP | PB-O3A-PA-O1A |
| 42 | AH | 501 | GTP | PA-O3A-PB-O2B |
| 42 | BA | 501 | GTP | PA-O3A-PB-O2B |
| 42 | BH | 501 | GTP | PA-O3A-PB-O2B |
| 42 | CF | 501 | GTP | PA-O3A-PB-O2B |
| 42 | CG | 501 | GTP | PA-O3A-PB-O2B |
| 42 | CI | 501 | GTP | PA-O3A-PB-O2B |
| 42 | DG | 501 | GTP | PA-O3A-PB-O2B |
| 42 | EA | 501 | GTP | PA-O3A-PB-O2B |
| 42 | EF | 501 | GTP | PA-O3A-PB-O2B |
| 42 | EG | 501 | GTP | PA-O3A-PB-O2B |
| 42 | EH | 501 | GTP | PA-O3A-PB-O2B |
| 42 | EL | 501 | GTP | PA-O3A-PB-O2B |
| 42 | HA | 501 | GTP | PA-O3A-PB-O2B |
| 42 | HP | 501 | GTP | PA-O3A-PB-O2B |
| 42 | KE | 501 | GTP | PA-O3A-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | OD | 501 | GTP | PA-O3A-PB-O1B |
| 42 | PN | 501 | GTP | PA-O3A-PB-O2B |
| 42 | QF | 501 | GTP | PA-O3A-PB-O2B |
| 42 | QG | 501 | GTP | PA-O3A-PB-O2B |
| 42 | RN | 501 | GTP | PA-O3A-PB-O2B |
| 42 | RO | 501 | GTP | PA-O3A-PB-O2B |
| 42 | RP | 501 | GTP | PA-O3A-PB-O2B |
| 42 | SM | 501 | GTP | PA-O3A-PB-O2B |
| 42 | SN | 501 | GTP | PA-O3A-PB-O2B |
| 42 | SP | 501 | GTP | PA-O3A-PB-O2B |
| 42 | TI | 501 | GTP | PA-O3A-PB-O1B |
| 42 | UA | 501 | GTP | PA-O3A-PB-O2B |
| 42 | WA | 501 | GTP | PA-O3A-PB-O2B |
| 42 | WG | 501 | GTP | PA-O3A-PB-O2B |
| 42 | KM | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | SP | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | EF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | HH | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | FN | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | HB | 502 | GTP | C4'-C5'-O5'-PA |
| 42 | IE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | PO | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | UB | 502 | GTP | C4'-C5'-O5'-PA |
| 42 | GA | 501 | GTP | O4'-C4'-C5'-O5' |
| 43 | FO | 502 | GDP | O4'-C4'-C5'-O5' |
| 42 | BA | 501 | GTP | PA-O3A-PB-O1B |
| 42 | CI | 501 | GTP | PA-O3A-PB-O1B |
| 42 | EH | 501 | GTP | PA-O3A-PB-O1B |
| 42 | FM | 501 | GTP | PA-O3A-PB-O2B |
| 42 | GP | 501 | GTP | PA-O3A-PB-O2B |
| 42 | HA | 501 | GTP | PA-O3A-PB-O1B |
| 42 | JB | 502 | GTP | PG-O3B-PB-O2B |
| 42 | KD | 501 | GTP | PA-O3A-PB-O2B |
| 42 | KO | 501 | GTP | PG-O3B-PB-O1B |
| 42 | KO | 501 | GTP | PA-O3A-PB-O2B |
| 42 | LD | 501 | GTP | PA-O3A-PB-O2B |
| 42 | MB | 502 | GTP | PA-O3A-PB-O1B |
| 42 | MH | 501 | GTP | PA-O3A-PB-O2B |
| 42 | NE | 501 | GTP | PA-O3A-PB-O2B |
| 42 | NN | 501 | GTP | PG-O3B-PB-O1B |
| 42 | QF | 501 | GTP | PA-O3A-PB-O1B |
| 42 | QL | 501 | GTP | PA-O3A-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | TF | 501 | GTP | PA-O3A-PB-O2B |
| 42 | VB | 502 | GTP | PA-O3A-PB-O2B |
| 42 | WG | 501 | GTP | PA-O3A-PB-O1B |
| 42 | EL | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | MM | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | NE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | PD | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | KN | 501 | GTP | C3'-C4'-C5'-O5' |
| 43 | DO | 501 | GDP | C3'-C4'-C5'-O5' |
| 43 | TM | 501 | GDP | C3'-C4'-C5'-O5' |
| 42 | AF | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | BA | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | EH | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | DA | 501 | GTP | PB-O3B-PG-O2G |
| 42 | EG | 501 | GTP | PB-O3B-PG-O2G |
| 42 | HA | 501 | GTP | PB-O3B-PG-O2G |
| 42 | IH | 501 | GTP | PB-O3B-PG-O2G |
| 42 | JB | 502 | GTP | PB-O3B-PG-O2G |
| 42 | LB | 502 | GTP | PB-O3B-PG-O2G |
| 42 | QG | 501 | GTP | PB-O3B-PG-O2G |
| 42 | TF | 501 | GTP | PB-O3B-PG-O2G |
| 42 | VA | 501 | GTP | PB-O3B-PG-O2G |
| 43 | LL | 502 | GDP | PA-O3A-PB-O2B |
| 42 | LD | 501 | GTP | C4'-C5'-O5'-PA |
| 43 | TB | 501 | GDP | C3'-C4'-C5'-O5' |
| 42 | AE | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | ML | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | AA | 501 | GTP | PG-O3B-PB-O2B |
| 42 | AH | 501 | GTP | PA-O3A-PB-O1B |
| 42 | BG | 501 | GTP | PA-O3A-PB-O2B |
| 42 | BH | 501 | GTP | PA-O3A-PB-O1B |
| 42 | CA | 501 | GTP | PA-O3A-PB-O2B |
| 42 | CF | 501 | GTP | PA-O3A-PB-O1B |
| 42 | CG | 501 | GTP | PA-O3A-PB-O1B |
| 42 | DE | 501 | GTP | PG-O3B-PB-O2B |
| 42 | DE | 501 | GTP | PA-O3A-PB-O1B |
| 42 | DG | 501 | GTP | PG-O3B-PB-O2B |
| 42 | DG | 501 | GTP | PA-O3A-PB-O1B |
| 42 | DH | 501 | GTP | PA-O3A-PB-O2B |
| 42 | EA | 501 | GTP | PA-O3A-PB-O1B |
| 42 | EH | 501 | GTP | PG-O3B-PB-O2B |
| 42 | FM | 501 | GTP | PA-O3A-PB-O1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | FN | 501 | GTP | PG-O3B-PB-O2B |
| 42 | GB | 502 | GTP | PB-O3A-PA-O1A |
| 42 | GB | 502 | GTP | PB-O3A-PA-O2A |
| 42 | GP | 501 | GTP | PA-O3A-PB-O1B |
| 42 | HB | 502 | GTP | PA-O3A-PB-O1B |
| 42 | HB | 502 | GTP | PA-O3A-PB-O2B |
| 42 | IE | 501 | GTP | PA-O3A-PB-O1B |
| 42 | IE | 501 | GTP | PA-O3A-PB-O2B |
| 42 | IH | 501 | GTP | PG-O3B-PB-O1B |
| 42 | IH | 501 | GTP | PA-O3A-PB-O2B |
| 42 | JD | 501 | GTP | PA-O3A-PB-O2B |
| 42 | JE | 501 | GTP | PA-O3A-PB-O2B |
| 42 | KO | 501 | GTP | PA-O3A-PB-O1B |
| 42 | LA | 501 | GTP | PG-O3B-PB-O2B |
| 42 | LD | 501 | GTP | PA-O3A-PB-O1B |
| 42 | LO | 501 | GTP | PA-O3A-PB-O1B |
| 42 | MH | 501 | GTP | PA-O3A-PB-O1B |
| 42 | ML | 501 | GTP | PG-O3B-PB-O1B |
| 42 | MM | 501 | GTP | PA-O3A-PB-O2B |
| 42 | NM | 501 | GTP | PA-O3A-PB-O2B |
| 42 | NN | 501 | GTP | PB-O3A-PA-O2A |
| 42 | OB | 502 | GTP | PG-O3B-PB-O1B |
| 42 | OD | 501 | GTP | PB-O3A-PA-O2A |
| 42 | OL | 501 | GTP | PG-O3B-PB-O2B |
| 42 | QG | 501 | GTP | PG-O3B-PB-O2B |
| 42 | QN | 501 | GTP | PG-O3B-PB-O2B |
| 42 | RF | 501 | GTP | PA-O3A-PB-O2B |
| 42 | RG | 501 | GTP | PA-O3A-PB-O1B |
| 42 | RG | 501 | GTP | PA-O3A-PB-O2B |
| 42 | RN | 501 | GTP | PG-O3B-PB-O2B |
| 42 | SL | 501 | GTP | PA-O3A-PB-O1B |
| 42 | SL | 501 | GTP | PA-O3A-PB-O2B |
| 42 | SM | 501 | GTP | PG-O3B-PB-O2B |
| 42 | SN | 501 | GTP | PG-O3B-PB-O2B |
| 42 | SN | 501 | GTP | PA-O3A-PB-O1B |
| 42 | TH | 501 | GTP | PA-O3A-PB-O1B |
| 42 | TH | 501 | GTP | PA-O3A-PB-O2B |
| 42 | TI | 501 | GTP | PA-O3A-PB-O2B |
| 42 | UE | 501 | GTP | PG-O3B-PB-O1B |
| 42 | UI | 501 | GTP | PG-O3B-PB-O2B |
| 42 | VF | 501 | GTP | PG-O3B-PB-O1B |
| 42 | VF | 501 | GTP | PG-O3B-PB-O2B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | VF | 501 | GTP | PA-O3A-PB-O1B |
| 42 | VF | 501 | GTP | PA-O3A-PB-O2B |
| 43 | TL | 502 | GDP | C3'-C4'-C5'-O5' |
| 42 | OB | 502 | GTP | PB-O3B-PG-O1G |
| 42 | QG | 501 | GTP | PB-O3B-PG-O1G |
| 42 | DG | 501 | GTP | C3'-C4'-C5'-O5' |
| 42 | SP | 501 | GTP | O4'-C4'-C5'-O5' |
| 42 | JO | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | QL | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | RO | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | VQ | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | DE | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | JD | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | LA | 501 | GTP | C4'-C5'-O5'-PA |
| 42 | OB | 502 | GTP | C4'-C5'-O5'-PA |
| 42 | BF | 501 | GTP | PG-O3B-PB-O2B |
| 42 | CA | 501 | GTP | PA-O3A-PB-O1B |
| 42 | CE | 501 | GTP | PG-O3B-PB-O2B |
| 42 | DH | 501 | GTP | PA-O3A-PB-O1B |
| 42 | EA | 501 | GTP | PG-O3B-PB-O2B |
| 42 | EF | 501 | GTP | PA-O3A-PB-O1B |
| 42 | EG | 501 | GTP | PG-O3B-PB-O2B |
| 42 | EL | 501 | GTP | PA-O3A-PB-O1B |
| 42 | FM | 501 | GTP | PG-O3B-PB-O2B |
| 42 | GB | 502 | GTP | PG-O3B-PB-O2B |
| 42 | GF | 501 | GTP | PG-O3B-PB-O2B |
| 42 | GP | 501 | GTP | PB-O3A-PA-O2A |
| 42 | HP | 501 | GTP | PA-O3A-PB-O1B |
| 42 | IH | 501 | GTP | PA-O3A-PB-O1B |
| 42 | JB | 502 | GTP | PA-O3A-PB-O2B |
| 42 | KB | 502 | GTP | PA-O3A-PB-O2B |
| 42 | KE | 501 | GTP | PG-O3B-PB-O2B |
| 42 | KO | 501 | GTP | PG-O3B-PB-O2B |
| 42 | LL | 501 | GTP | PG-O3B-PB-O2B |
| 42 | LO | 501 | GTP | PG-O3B-PB-O2B |
| 42 | MB | 502 | GTP | PG-O3B-PB-O2B |
| 42 | MH | 501 | GTP | PG-O3B-PB-O2B |
| 42 | ML | 501 | GTP | PA-O3A-PB-O2B |
| 42 | OB | 502 | GTP | PG-O3B-PB-O2B |
| 42 | OL | 501 | GTP | PA-O3A-PB-O2B |
| 42 | OL | 501 | GTP | PB-O3A-PA-O2A |
| 42 | PN | 501 | GTP | PA-O3A-PB-O1B |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | PO | 501 | GTP | PA-O3A-PB-O1B |
| 42 | QF | 501 | GTP | PB-O3A-PA-O2A |
| 42 | QG | 501 | GTP | PA-O3A-PB-O1B |
| 42 | RE | 501 | GTP | PA-O3A-PB-O2B |
| 42 | RN | 501 | GTP | PA-O3A-PB-O1B |
| 42 | RO | 501 | GTP | PA-O3A-PB-O1B |
| 42 | RP | 501 | GTP | PA-O3A-PB-O1B |
| 42 | SL | 501 | GTP | PG-O3B-PB-O2B |
| 42 | SP | 501 | GTP | PA-O3A-PB-O1B |
| 42 | TF | 501 | GTP | PA-O3A-PB-O1B |
| 42 | TG | 501 | GTP | PG-O3B-PB-O2B |
| 42 | TG | 501 | GTP | PA-O3A-PB-O1B |
| 42 | TG | 501 | GTP | PA-O3A-PB-O2B |
| 42 | TI | 501 | GTP | PG-O3B-PB-O2B |
| 42 | TN | 501 | GTP | PG-O3B-PB-O1B |
| 42 | TN | 501 | GTP | PB-O3A-PA-O2A |
| 42 | UA | 501 | GTP | PA-O3A-PB-O1B |
| 42 | UO | 501 | GTP | PA-O3A-PB-O1B |
| 42 | VQ | 501 | GTP | PG-O3B-PB-O2B |
| 42 | WA | 501 | GTP | PG-O3B-PB-O2B |
| 42 | WA | 501 | GTP | PA-O3A-PB-O1B |
| 42 | WE | 501 | GTP | PA-O3A-PB-O2B |
| 42 | WO | 501 | GTP | PA-O3A-PB-O2B |

There are no ring outliers.

219 monomers are involved in 527 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 43 | KM | 502 | GDP | 1 | 0 |
| 43 | WM | 501 | GDP | 1 | 0 |
| 43 | LP | 501 | GDP | 1 | 0 |
| 42 | BF | 501 | GTP | 2 | 0 |
| 42 | KB | 502 | GTP | 3 | 0 |
| 42 | CH | 501 | GTP | 1 | 0 |
| 42 | FN | 501 | GTP | 2 | 0 |
| 42 | HA | 501 | GTP | 4 | 0 |
| 42 | JO | 501 | GTP | 5 | 0 |
| 42 | IF | 501 | GTP | 2 | 0 |
| 42 | SL | 501 | GTP | 1 | 0 |
| 42 | FO | 501 | GTP | 1 | 0 |
| 43 | BB | 501 | GDP | 3 | 0 |
| 43 | NN | 502 | GDP | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 42 | JA | 501 | GTP | 4 | 0 |
| 43 | SP | 502 | GDP | 1 | 0 |
| 42 | LM | 501 | GTP | 5 | 0 |
| 42 | LL | 501 | GTP | 3 | 0 |
| 42 | PE | 501 | GTP | 2 | 0 |
| 43 | KL | 501 | GDP | 2 | 0 |
| 43 | ML | 502 | GDP | 2 | 0 |
| 43 | TP | 501 | GDP | 1 | 0 |
| 42 | FE | 501 | GTP | 1 | 0 |
| 43 | UB | 501 | GDP | 1 | 0 |
| 42 | II | 501 | GTP | 3 | 0 |
| 43 | TO | 501 | GDP | 1 | 0 |
| 42 | GF | 501 | GTP | 1 | 0 |
| 42 | VQ | 501 | GTP | 1 | 0 |
| 42 | DF | 501 | GTP | 4 | 0 |
| 42 | OD | 501 | GTP | 5 | 0 |
| 42 | UB | 502 | GTP | 3 | 0 |
| 42 | NO | 501 | GTP | 3 | 0 |
| 43 | QP | 501 | GDP | 6 | 0 |
| 43 | GP | 502 | GDP | 2 | 0 |
| 42 | IG | 501 | GTP | 4 | 0 |
| 42 | TN | 501 | GTP | 1 | 0 |
| 42 | LD | 501 | GTP | 2 | 0 |
| 43 | DN | 501 | GDP | 3 | 0 |
| 43 | WN | 501 | GDP | 1 | 0 |
| 43 | PL | 501 | GDP | 4 | 0 |
| 43 | JO | 502 | GDP | 1 | 0 |
| 42 | KD | 501 | GTP | 3 | 0 |
| 43 | WO | 502 | GDP | 2 | 0 |
| 42 | BH | 501 | GTP | 1 | 0 |
| 42 | TH | 501 | GTP | 2 | 0 |
| 42 | VP | 501 | GTP | 1 | 0 |
| 43 | SN | 502 | GDP | 1 | 0 |
| 42 | SM | 501 | GTP | 2 | 0 |
| 42 | UM | 501 | GTP | 1 | 0 |
| 43 | PN | 502 | GDP | 1 | 0 |
| 42 | WG | 501 | GTP | 5 | 0 |
| 42 | VN | 501 | GTP | 2 | 0 |
| 43 | QO | 502 | GDP | 1 | 0 |
| 42 | OL | 501 | GTP | 2 | 0 |
| 43 | DL | 501 | GDP | 3 | 0 |
| 43 | SL | 502 | GDP | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 43 | VQ | 502 | GDP | 1 | 0 |
| 42 | SN | 501 | GTP | 3 | 0 |
| 42 | MN | 501 | GTP | 9 | 0 |
| 42 | LA | 501 | GTP | 4 | 0 |
| 43 | HM | 502 | GDP | 1 | 0 |
| 42 | MH | 501 | GTP | 1 | 0 |
| 42 | RO | 501 | GTP | 1 | 0 |
| 43 | BL | 502 | GDP | 2 | 0 |
| 42 | IH | 501 | GTP | 3 | 0 |
| 42 | QG | 501 | GTP | 2 | 0 |
| 43 | MN | 502 | GDP | 2 | 0 |
| 42 | DH | 501 | GTP | 2 | 0 |
| 43 | AM | 501 | GDP | 1 | 0 |
| 42 | MM | 501 | GTP | 8 | 0 |
| 42 | SP | 501 | GTP | 1 | 0 |
| 42 | GP | 501 | GTP | 3 | 0 |
| 42 | JE | 501 | GTP | 3 | 0 |
| 42 | OB | 502 | GTP | 4 | 0 |
| 43 | AN | 501 | GDP | 1 | 0 |
| 43 | FP | 501 | GDP | 3 | 0 |
| 43 | VO | 501 | GDP | 1 | 0 |
| 42 | AE | 501 | GTP | 2 | 0 |
| 42 | CA | 501 | GTP | 1 | 0 |
| 43 | UM | 502 | GDP | 1 | 0 |
| 42 | BI | 501 | GTP | 1 | 0 |
| 42 | CE | 501 | GTP | 5 | 0 |
| 42 | JB | 502 | GTP | 3 | 0 |
| 43 | UP | 501 | GDP | 2 | 0 |
| 42 | AG | 501 | GTP | 3 | 0 |
| 42 | OO | 501 | GTP | 3 | 0 |
| 42 | EG | 501 | GTP | 1 | 0 |
| 42 | EA | 501 | GTP | 5 | 0 |
| 42 | ON | 501 | GTP | 2 | 0 |
| 42 | QO | 501 | GTP | 1 | 0 |
| 43 | LB | 501 | GDP | 2 | 0 |
| 43 | AB | 501 | GDP | 1 | 0 |
| 42 | FM | 501 | GTP | 3 | 0 |
| 42 | GA | 501 | GTP | 4 | 0 |
| 42 | TL | 501 | GTP | 3 | 0 |
| 42 | EL | 501 | GTP | 2 | 0 |
| 42 | DI | 501 | GTP | 8 | 0 |
| 42 | HM | 501 | GTP | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 42 | TG | 501 | GTP | 5 | 0 |
| 42 | KN | 501 | GTP | 3 | 0 |
| 43 | CB | 501 | GDP | 1 | 0 |
| 42 | WE | 501 | GTP | 4 | 0 |
| 43 | BM | 501 | GDP | 2 | 0 |
| 42 | WF | 501 | GTP | 2 | 0 |
| 43 | SO | 501 | GDP | 3 | 0 |
| 43 | QM | 501 | GDP | 2 | 0 |
| 42 | IA | 501 | GTP | 2 | 0 |
| 42 | AA | 501 | GTP | 1 | 0 |
| 42 | RG | 501 | GTP | 3 | 0 |
| 42 | CF | 501 | GTP | 2 | 0 |
| 43 | OL | 502 | GDP | 2 | 0 |
| 43 | FO | 502 | GDP | 2 | 0 |
| 43 | BN | 501 | GDP | 1 | 0 |
| 42 | MB | 502 | GTP | 9 | 0 |
| 42 | ML | 501 | GTP | 2 | 0 |
| 43 | OB | 501 | GDP | 1 | 0 |
| 42 | SH | 501 | GTP | 3 | 0 |
| 43 | BP | 501 | GDP | 1 | 0 |
| 43 | DB | 501 | GDP | 4 | 0 |
| 42 | ND | 501 | GTP | 1 | 0 |
| 42 | DE | 501 | GTP | 6 | 0 |
| 42 | KE | 501 | GTP | 3 | 0 |
| 42 | HP | 501 | GTP | 2 | 0 |
| 42 | VB | 502 | GTP | 4 | 0 |
| 43 | CM | 501 | GDP | 2 | 0 |
| 43 | HN | 501 | GDP | 2 | 0 |
| 42 | PO | 501 | GTP | 2 | 0 |
| 43 | LN | 501 | GDP | 1 | 0 |
| 43 | RO | 502 | GDP | 1 | 0 |
| 43 | GN | 501 | GDP | 2 | 0 |
| 42 | WO | 501 | GTP | 1 | 0 |
| 43 | NM | 502 | GDP | 2 | 0 |
| 43 | CL | 501 | GDP | 1 | 0 |
| 43 | VB | 501 | GDP | 1 | 0 |
| 42 | IE | 501 | GTP | 3 | 0 |
| 42 | DG | 501 | GTP | 4 | 0 |
| 43 | GM | 501 | GDP | 2 | 0 |
| 42 | PN | 501 | GTP | 2 | 0 |
| 43 | WB | 501 | GDP | 1 | 0 |
| 43 | HO | 501 | GDP | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 42 | NG | 501 | GTP | 5 | 0 |
| 42 | AH | 501 | GTP | 2 | 0 |
| 43 | RM | 501 | GDP | 1 | 0 |
| 42 | FB | 502 | GTP | 3 | 0 |
| 43 | RN | 502 | GDP | 1 | 0 |
| 42 | KO | 501 | GTP | 2 | 0 |
| 43 | GB | 501 | GDP | 1 | 0 |
| 43 | CN | 501 | GDP | 4 | 0 |
| 42 | DA | 501 | GTP | 7 | 0 |
| 43 | JN | 501 | GDP | 1 | 0 |
| 42 | GH | 501 | GTP | 2 | 0 |
| 42 | KM | 501 | GTP | 2 | 0 |
| 42 | BL | 501 | GTP | 1 | 0 |
| 43 | EP | 501 | GDP | 5 | 0 |
| 42 | VF | 501 | GTP | 1 | 0 |
| 43 | UO | 502 | GDP | 2 | 0 |
| 42 | WI | 501 | GTP | 4 | 0 |
| 43 | CP | 501 | GDP | 4 | 0 |
| 42 | CG | 501 | GTP | 3 | 0 |
| 42 | CI | 501 | GTP | 4 | 0 |
| 43 | VP | 502 | GDP | 1 | 0 |
| 43 | MO | 501 | GDP | 1 | 0 |
| 42 | QF | 501 | GTP | 2 | 0 |
| 42 | UA | 501 | GTP | 2 | 0 |
| 42 | OM | 501 | GTP | 2 | 0 |
| 43 | DM | 501 | GDP | 2 | 0 |
| 43 | TN | 502 | GDP | 2 | 0 |
| 42 | MD | 501 | GTP | 2 | 0 |
| 42 | JF | 501 | GTP | 2 | 0 |
| 42 | UO | 501 | GTP | 3 | 0 |
| 43 | QB | 501 | GDP | 5 | 0 |
| 42 | HB | 502 | GTP | 1 | 0 |
| 42 | NE | 501 | GTP | 3 | 0 |
| 43 | SB | 501 | GDP | 1 | 0 |
| 42 | TI | 501 | GTP | 4 | 0 |
| 43 | JM | 501 | GDP | 6 | 0 |
| 42 | VA | 501 | GTP | 3 | 0 |
| 43 | EB | 501 | GDP | 1 | 0 |
| 43 | CO | 501 | GDP | 5 | 0 |
| 43 | QN | 502 | GDP | 1 | 0 |
| 43 | UN | 501 | GDP | 1 | 0 |
| 42 | WA | 501 | GTP | 3 | 0 |

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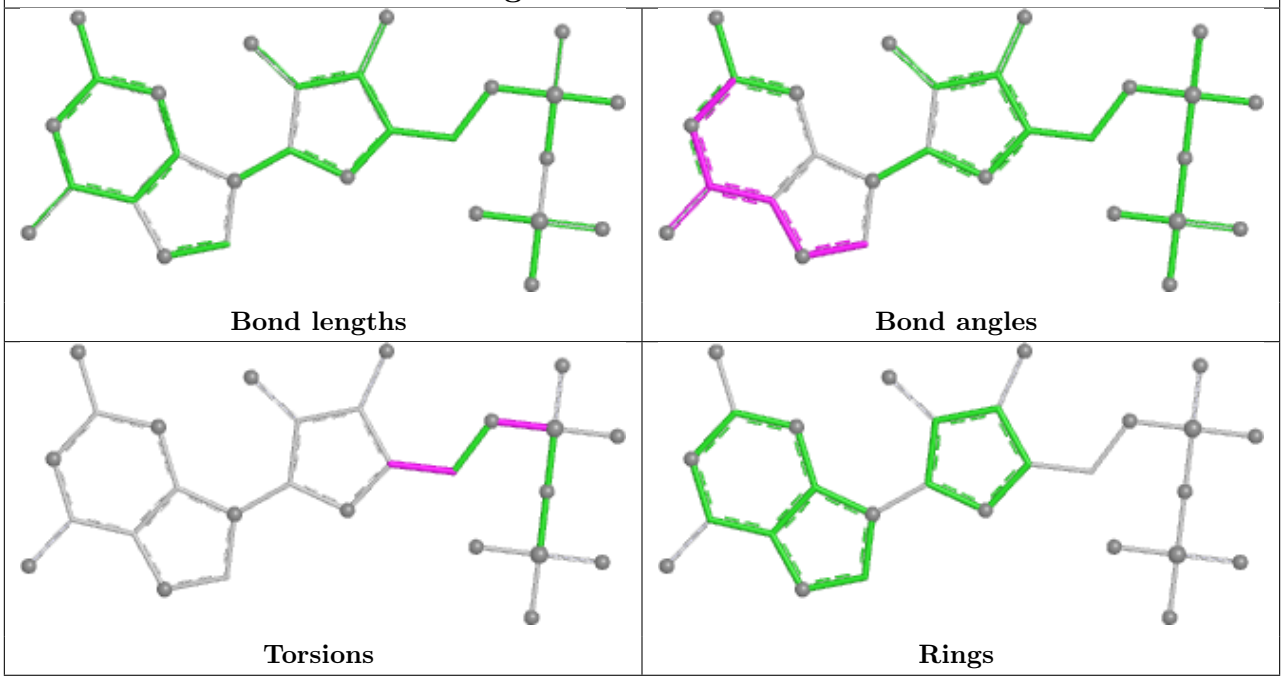
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 43 | LO | 502 | GDP | 2 | 0 |
| 42 | LB | 502 | GTP | 3 | 0 |
| 42 | EF | 501 | GTP | 2 | 0 |
| 42 | EH | 501 | GTP | 1 | 0 |
| 42 | NM | 501 | GTP | 4 | 0 |
| 42 | UE | 501 | GTP | 3 | 0 |
| 43 | DO | 501 | GDP | 1 | 0 |
| 43 | DP | 501 | GDP | 5 | 0 |
| 43 | JL | 501 | GDP | 1 | 0 |
| 43 | MP | 501 | GDP | 1 | 0 |
| 43 | EM | 501 | GDP | 4 | 0 |
| 43 | ON | 502 | GDP | 1 | 0 |
| 42 | UI | 501 | GTP | 5 | 0 |
| 43 | RL | 501 | GDP | 1 | 0 |
| 42 | RP | 501 | GTP | 4 | 0 |
| 43 | KN | 502 | GDP | 3 | 0 |
| 42 | GB | 502 | GTP | 3 | 0 |
| 43 | MB | 501 | GDP | 1 | 0 |
| 43 | IO | 501 | GDP | 1 | 0 |
| 43 | KP | 501 | GDP | 2 | 0 |
| 43 | LM | 502 | GDP | 1 | 0 |
| 43 | WQ | 501 | GDP | 1 | 0 |
| 43 | NO | 502 | GDP | 1 | 0 |
| 43 | PB | 501 | GDP | 2 | 0 |
| 42 | BG | 501 | GTP | 2 | 0 |
| 42 | HH | 501 | GTP | 2 | 0 |
| 43 | RP | 502 | GDP | 2 | 0 |
| 43 | JB | 501 | GDP | 2 | 0 |
| 42 | NN | 501 | GTP | 4 | 0 |
| 42 | QN | 501 | GTP | 2 | 0 |
| 43 | WP | 501 | GDP | 1 | 0 |
| 42 | QL | 501 | GTP | 2 | 0 |
| 42 | RF | 501 | GTP | 4 | 0 |
| 43 | PP | 501 | GDP | 3 | 0 |
| 42 | LO | 501 | GTP | 4 | 0 |
| 43 | MM | 502 | GDP | 1 | 0 |
| 42 | FI | 501 | GTP | 2 | 0 |

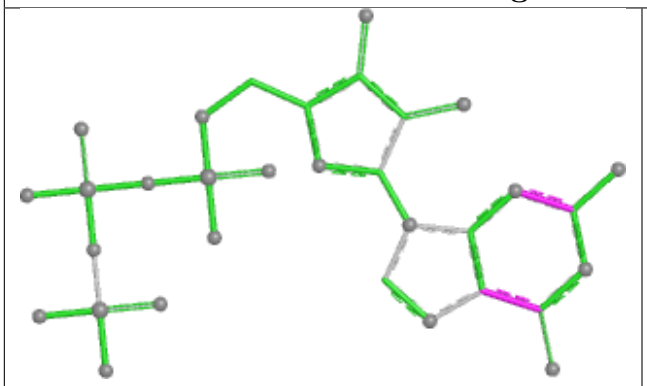
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

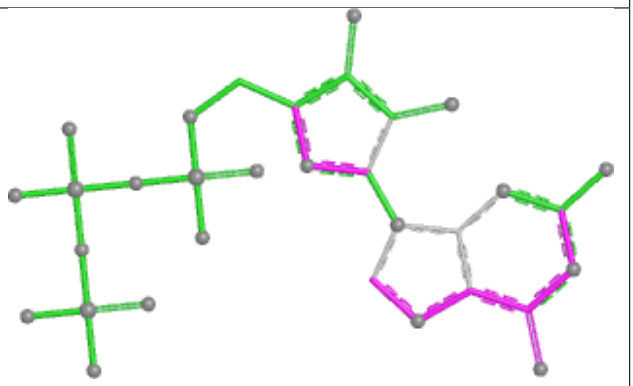
**Ligand GDP KM 502**



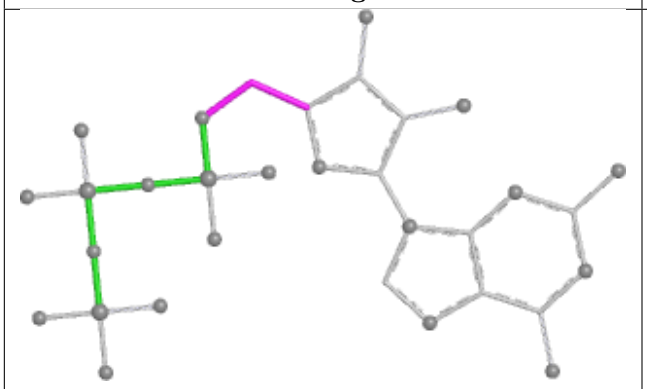
## Ligand GTP PD 501



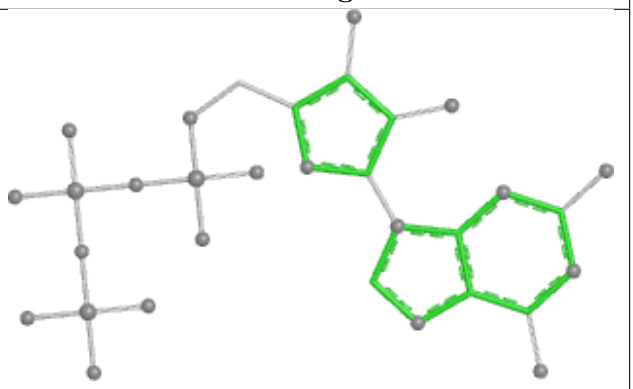
Bond lengths



Bond angles

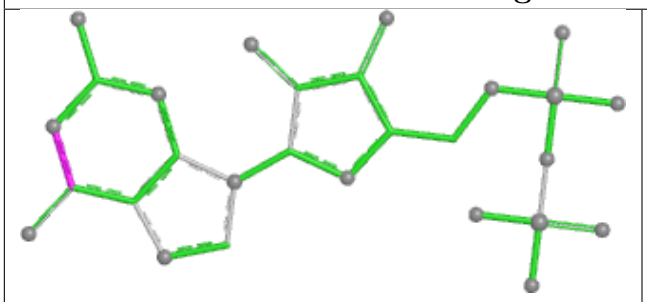


Torsions

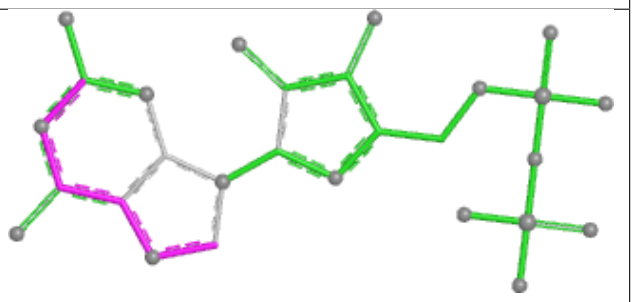


Rings

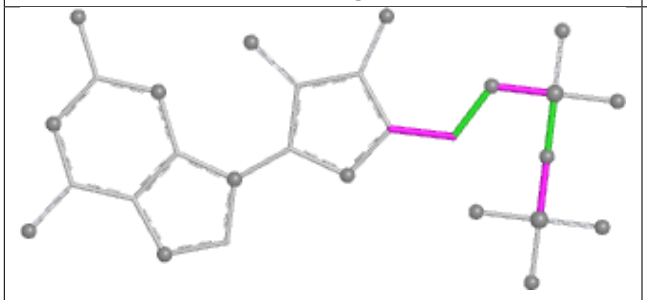
## Ligand GDP LL 502



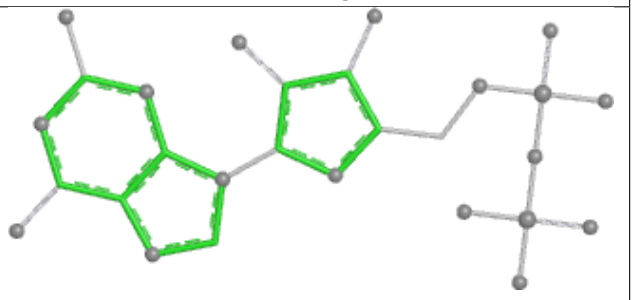
Bond lengths



Bond angles

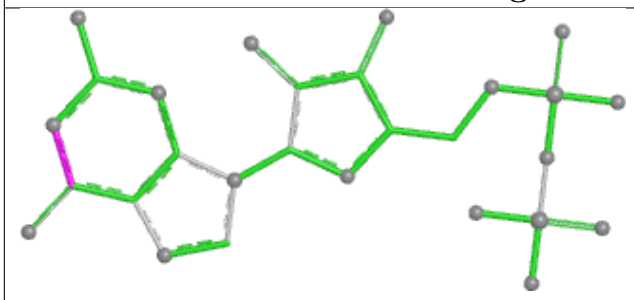


Torsions

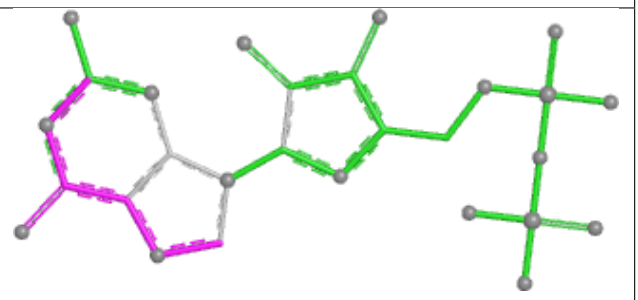


Rings

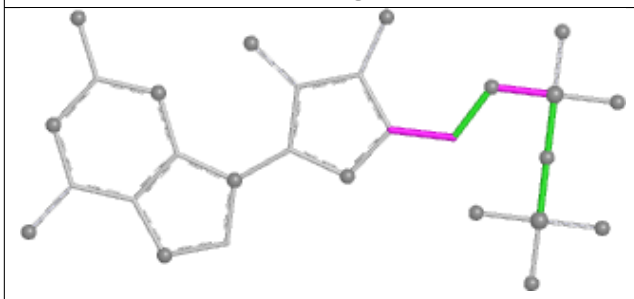
## Ligand GDP OP 501



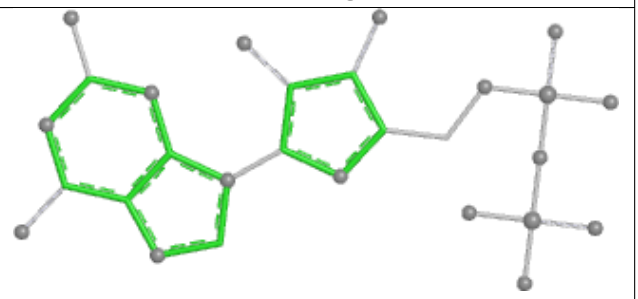
Bond lengths



Bond angles

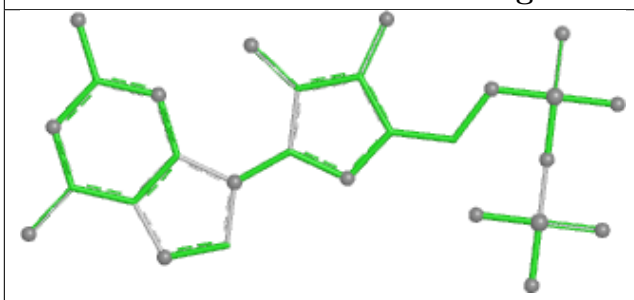


Torsions

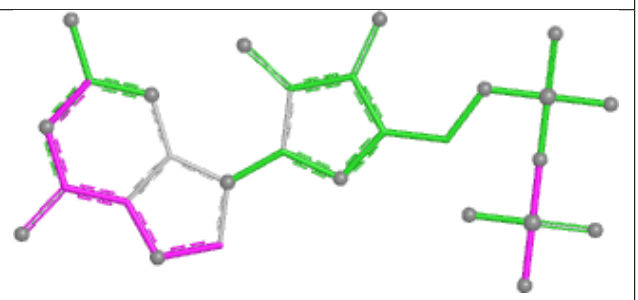


Rings

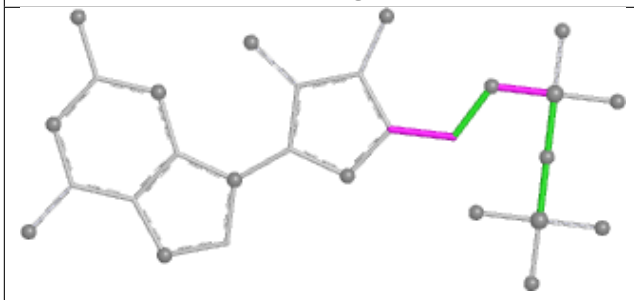
## Ligand GDP IB 501



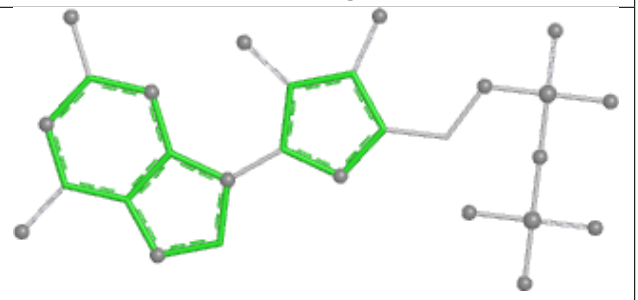
Bond lengths



Bond angles

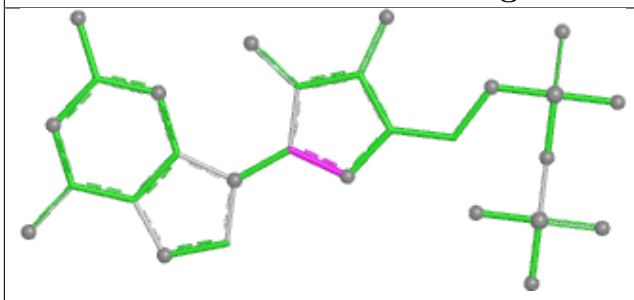


Torsions

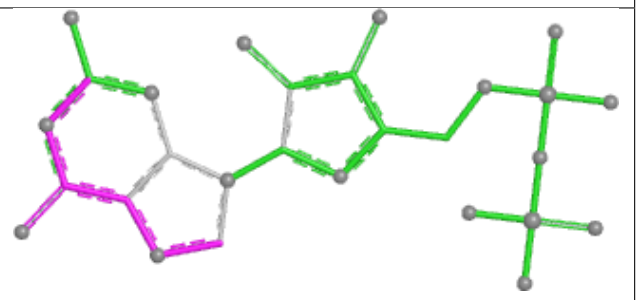


Rings

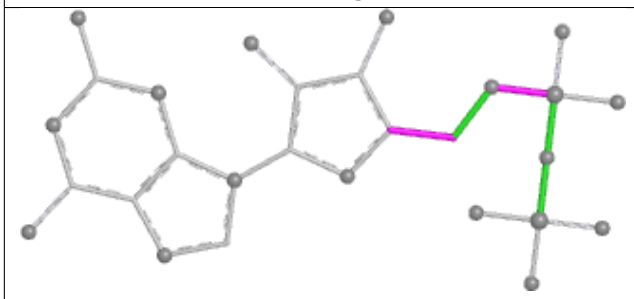
## Ligand GDP WM 501



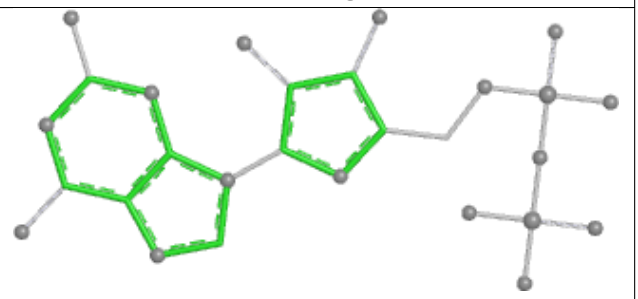
Bond lengths



Bond angles

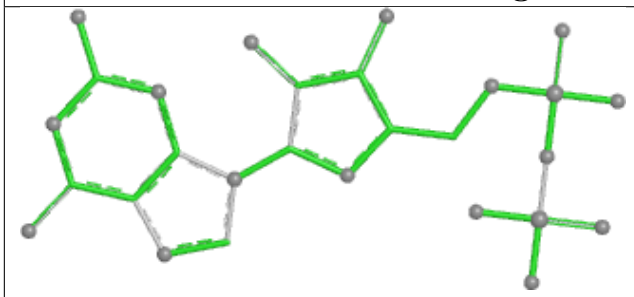


Torsions

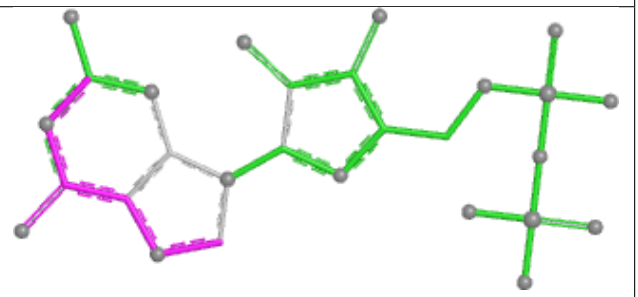


Rings

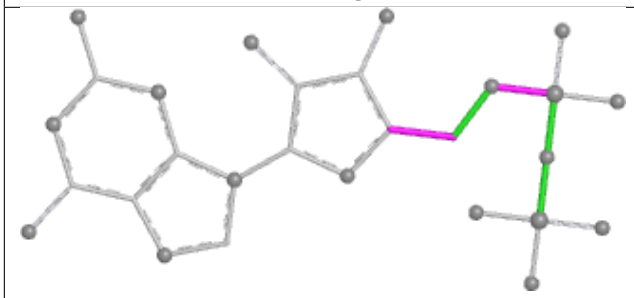
## Ligand GDP LP 501



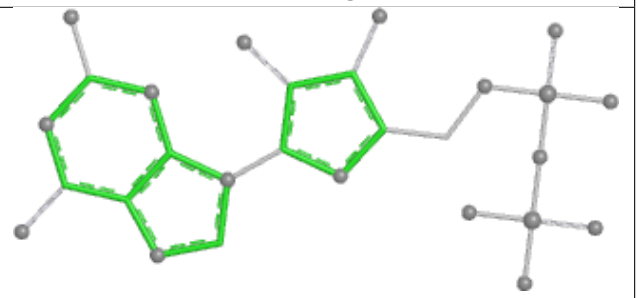
Bond lengths



Bond angles

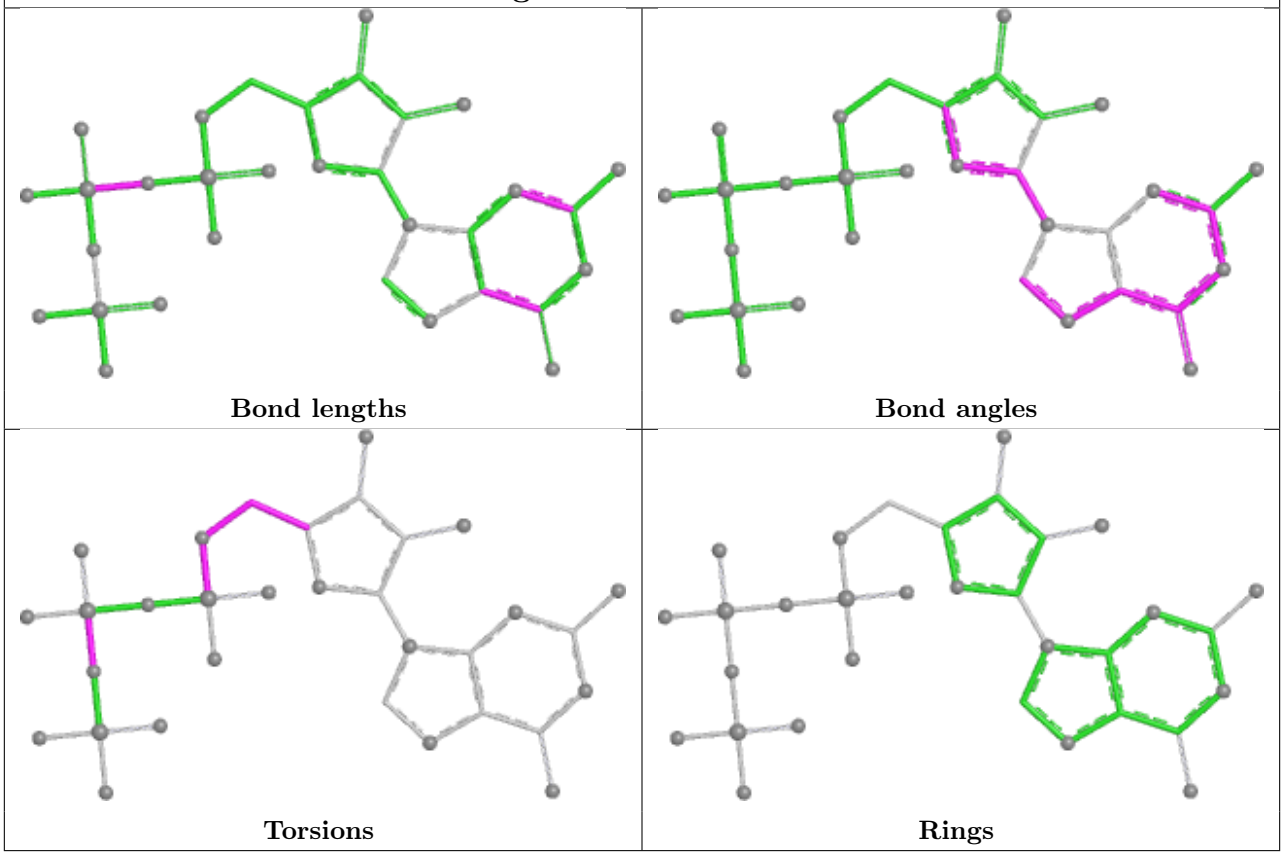


Torsions



Rings

## Ligand GTP BF 501

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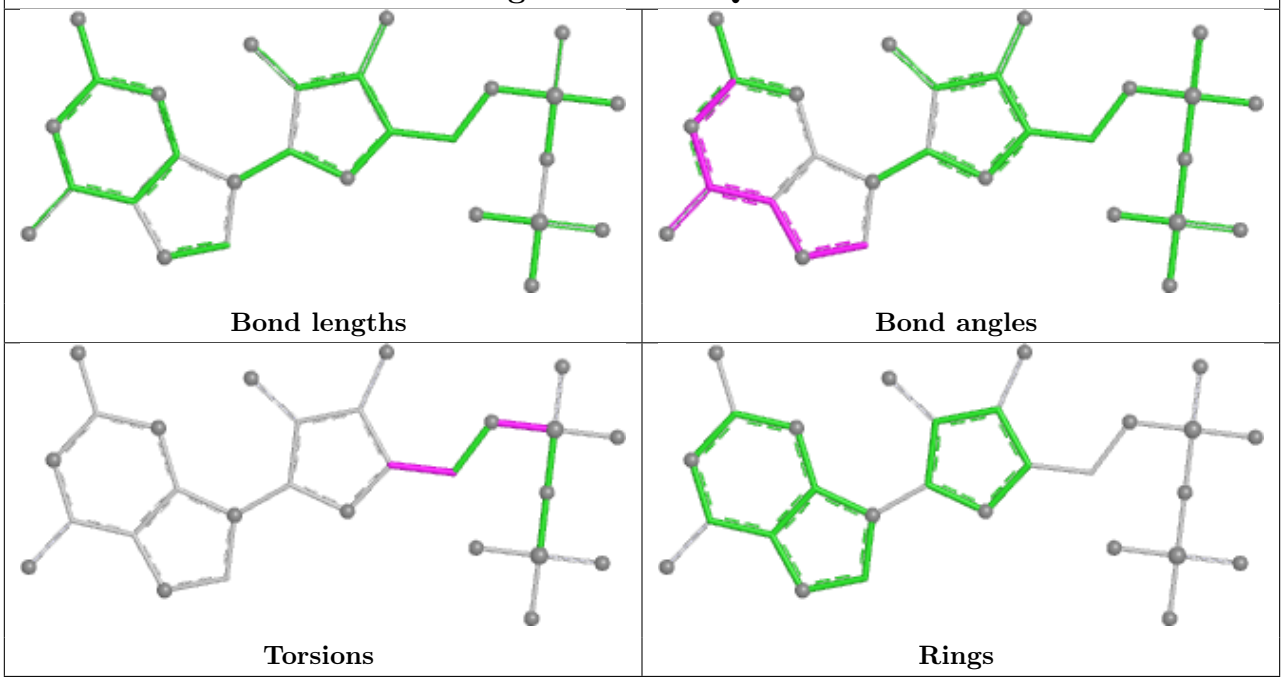

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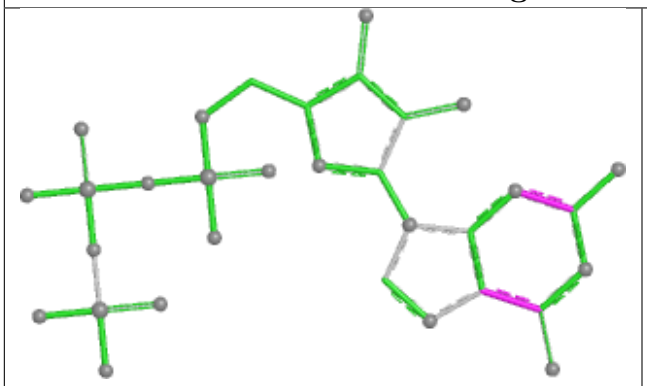

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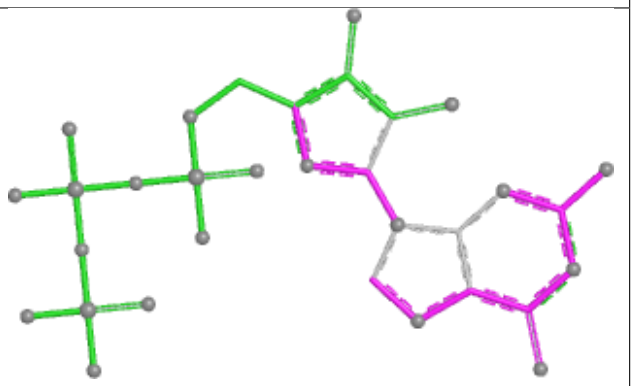

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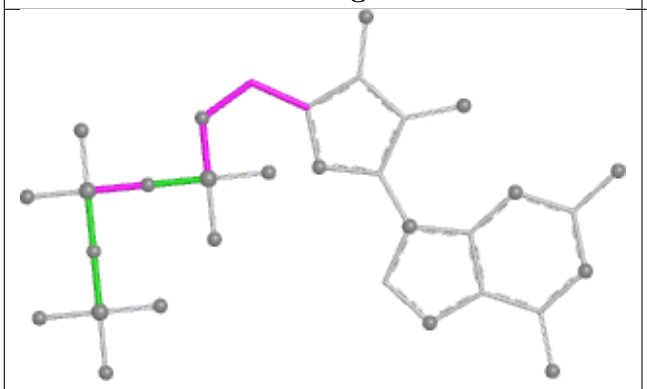

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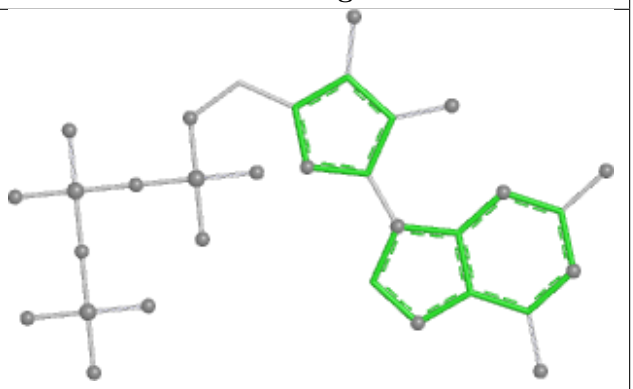

Rings

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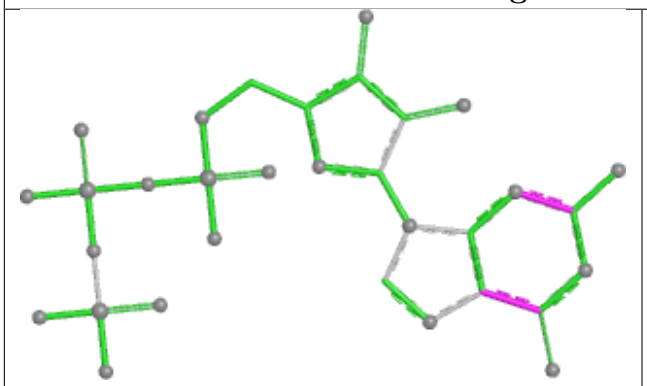

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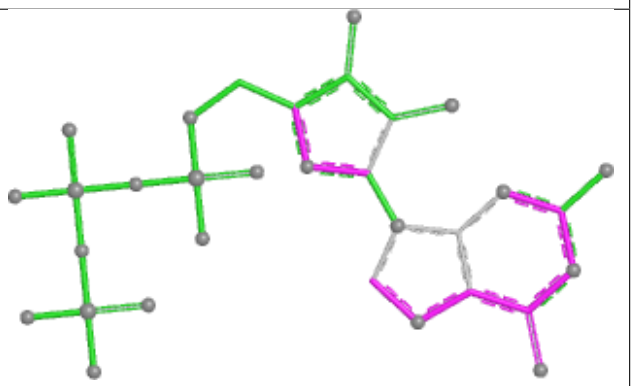

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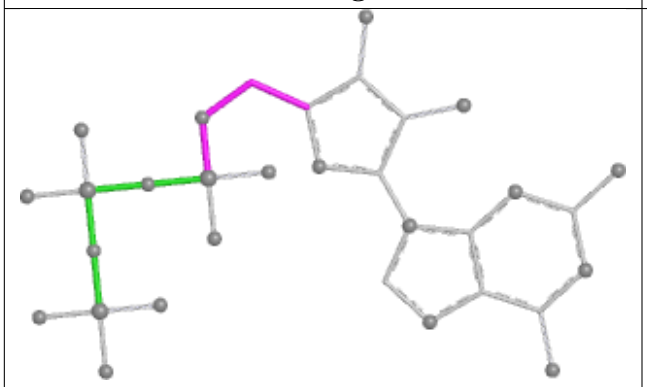

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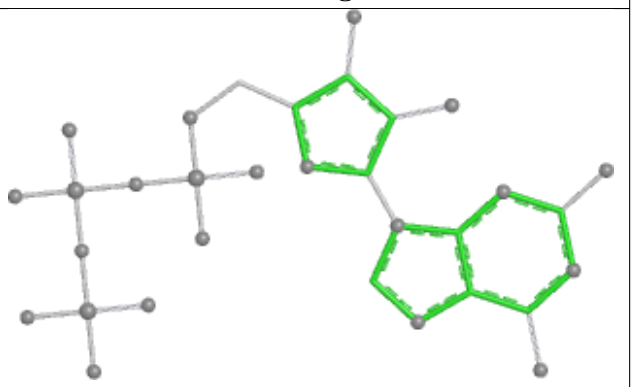

Rings

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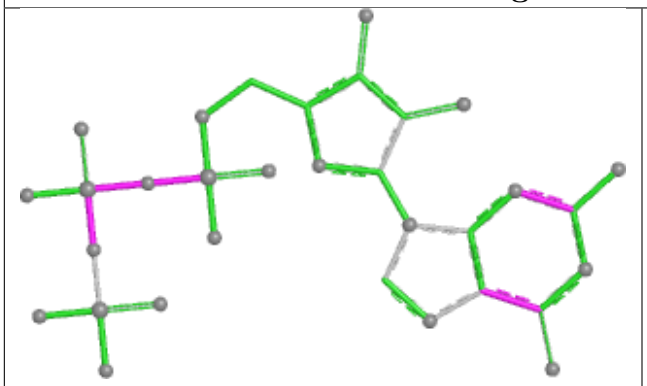

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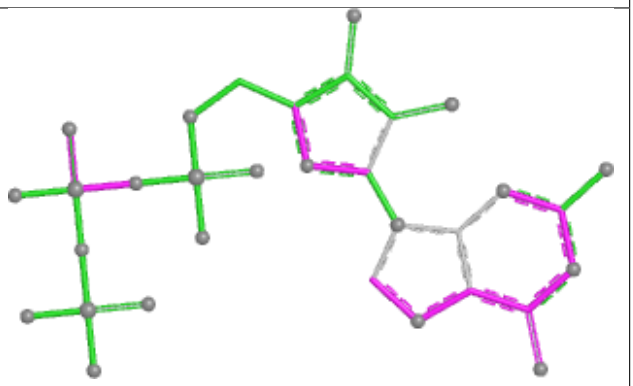

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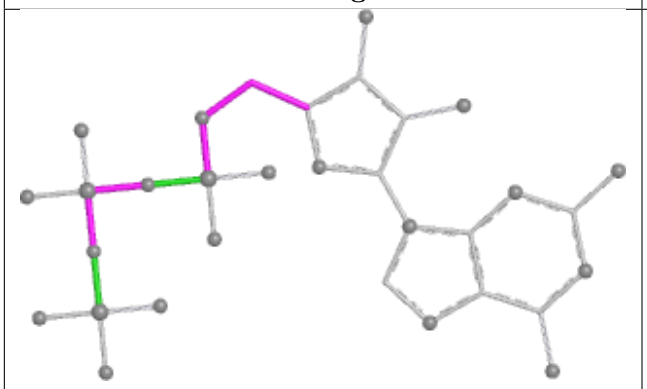

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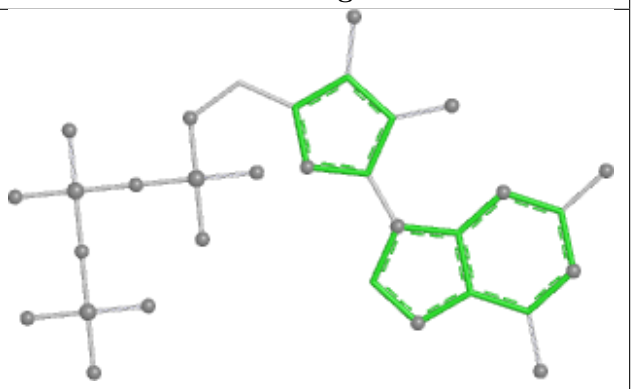

Rings

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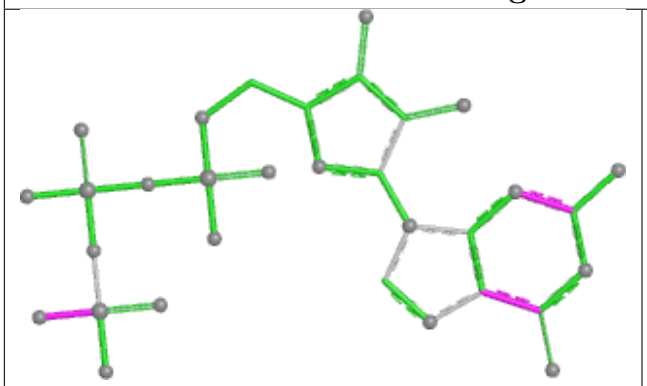

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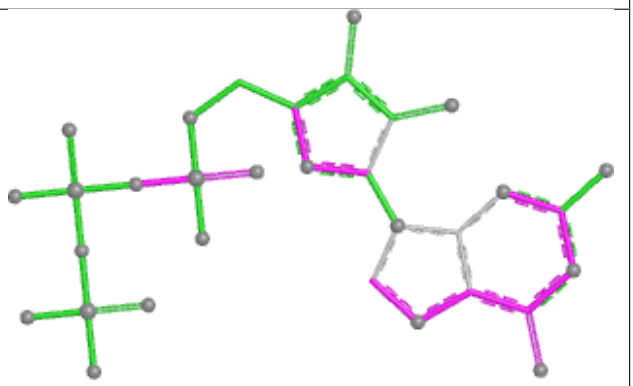

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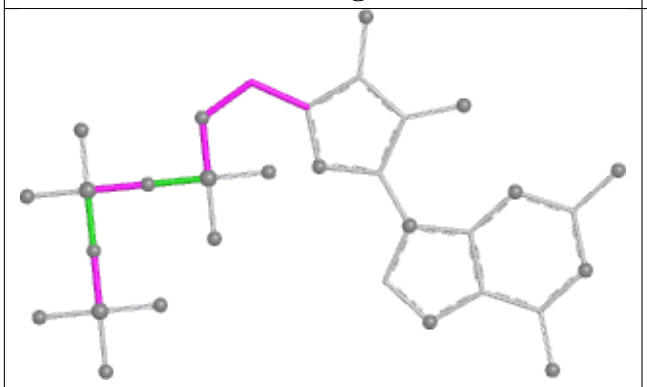

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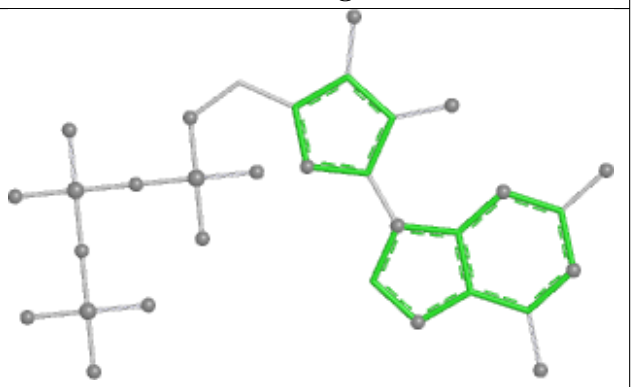

Rings

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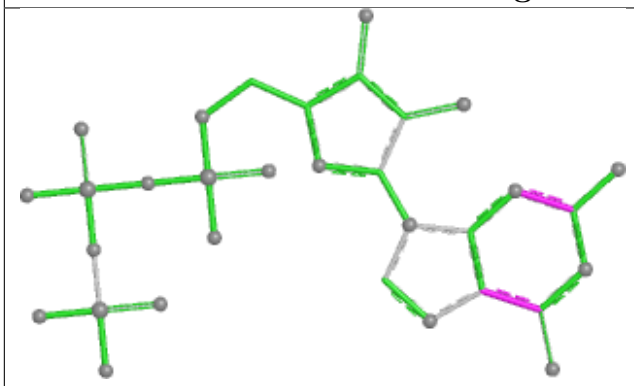

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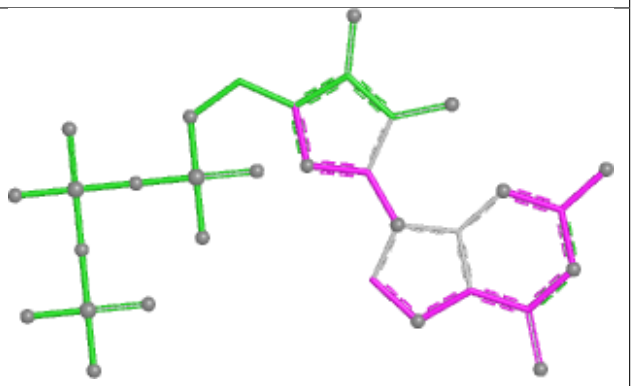

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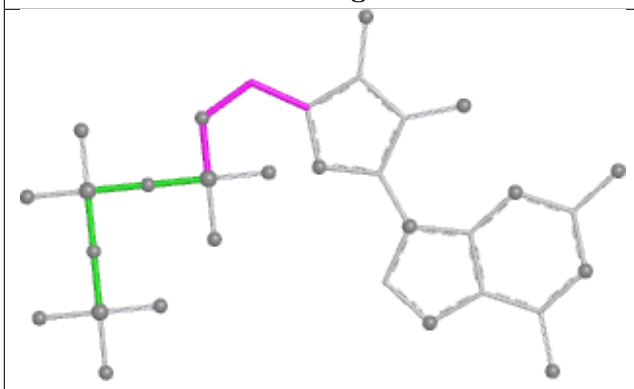

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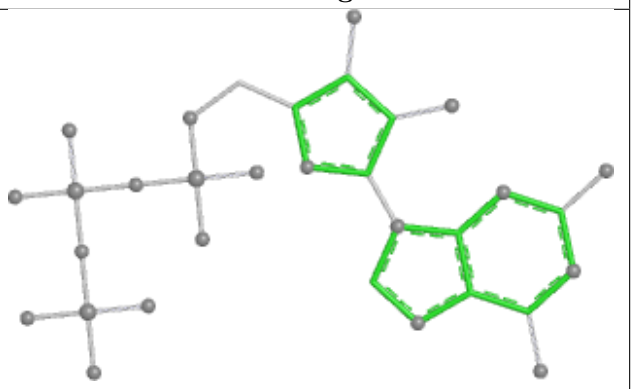

Rings

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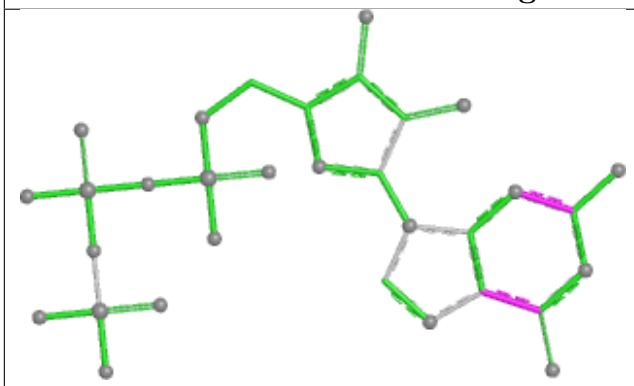

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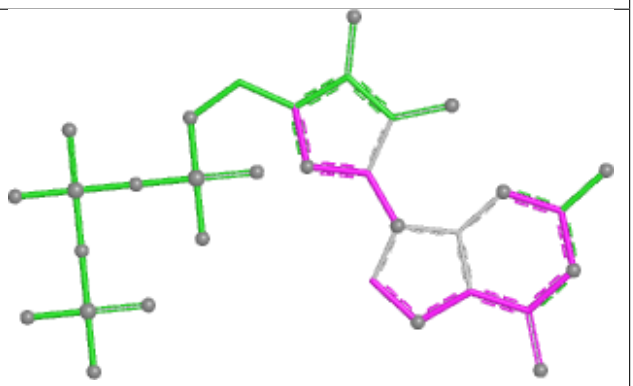

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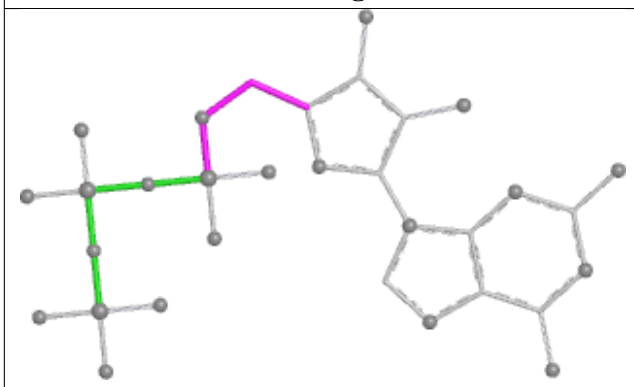

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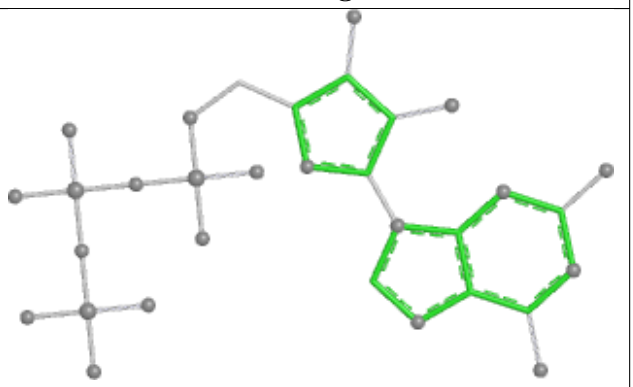

Rings

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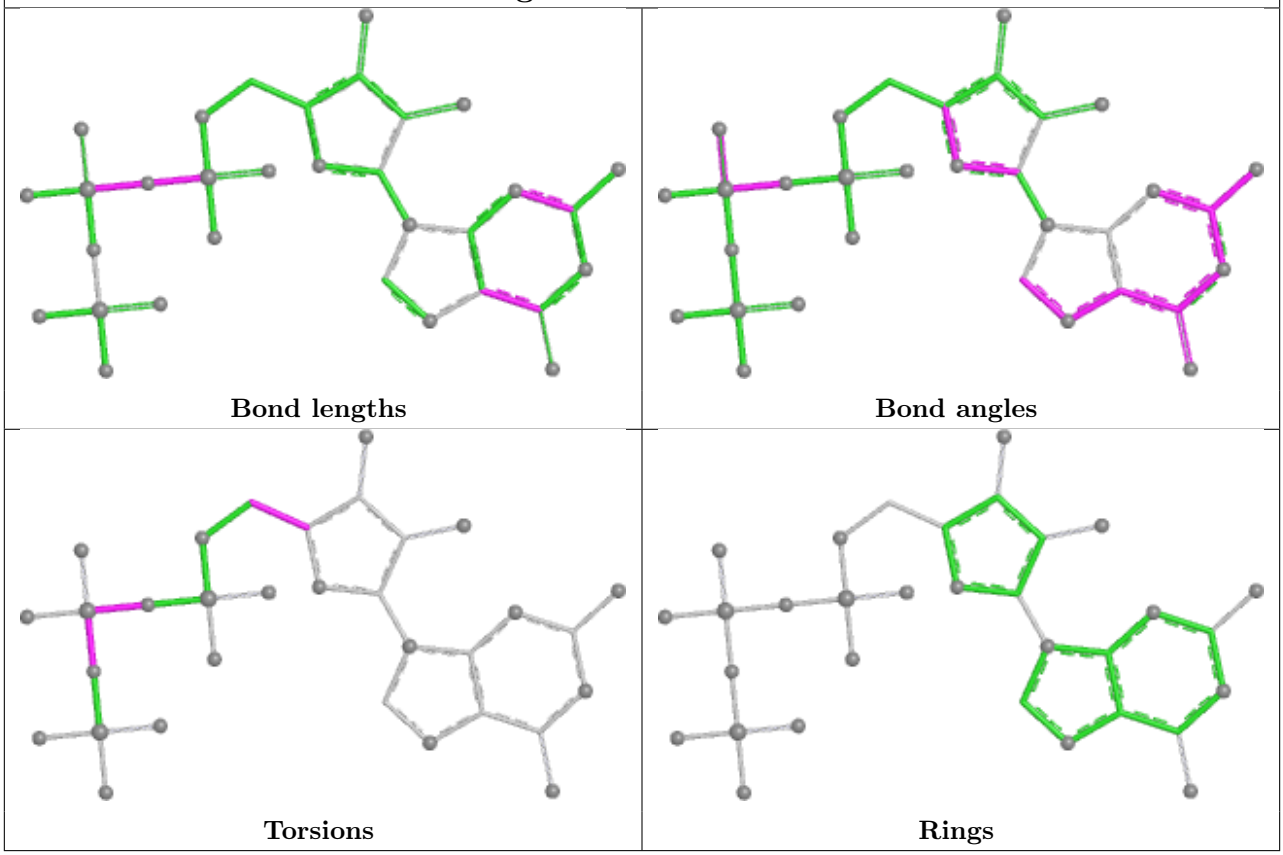


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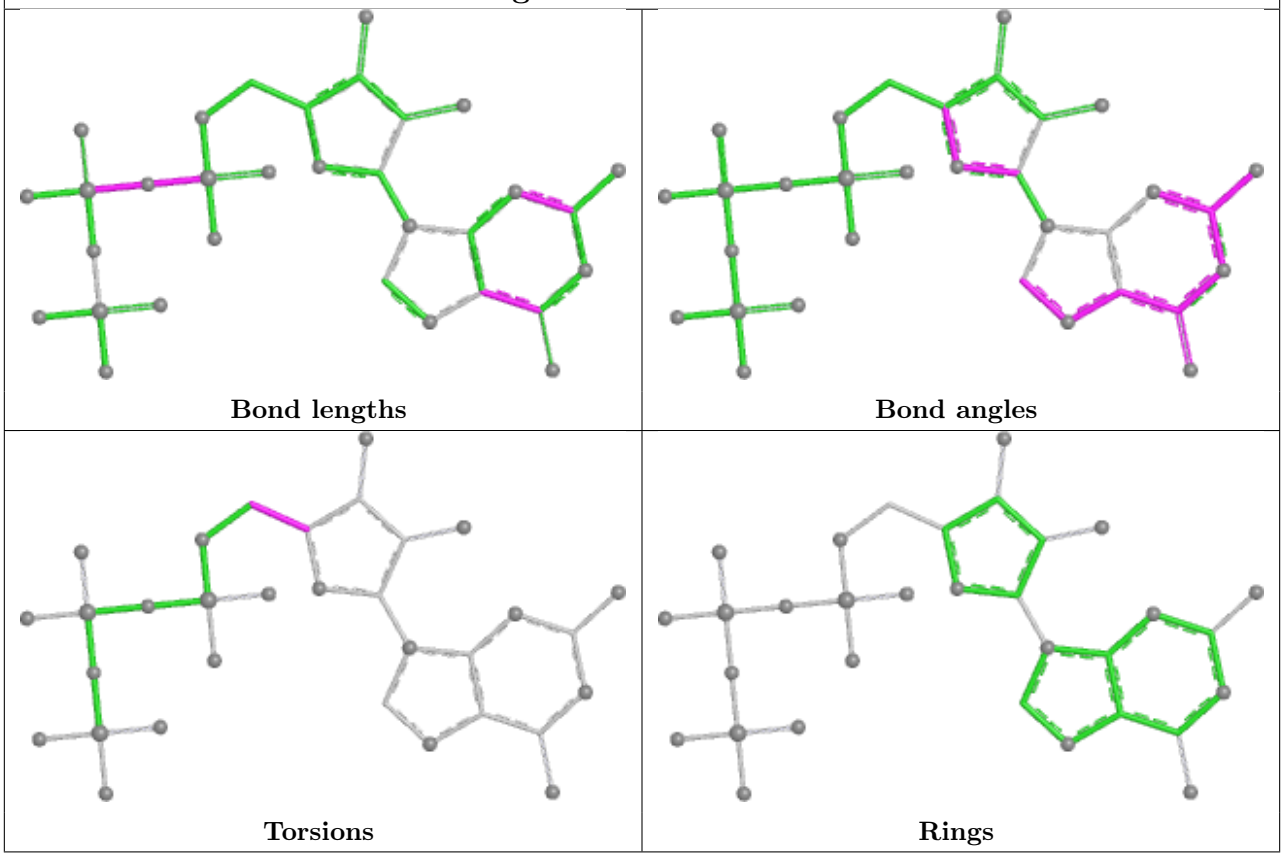

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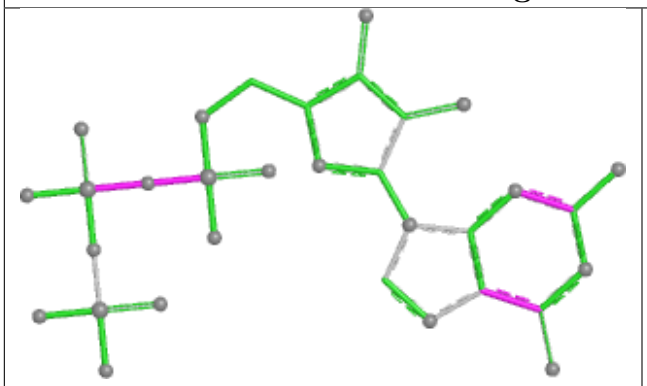

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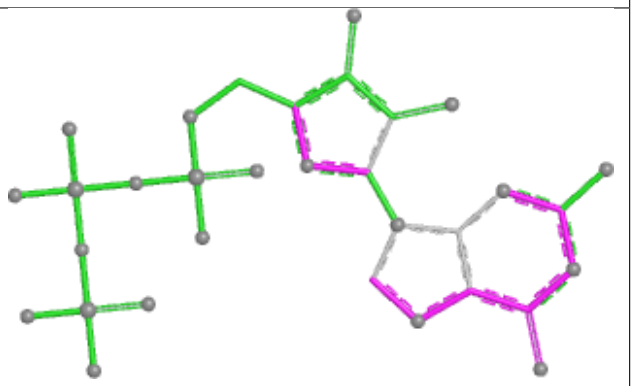

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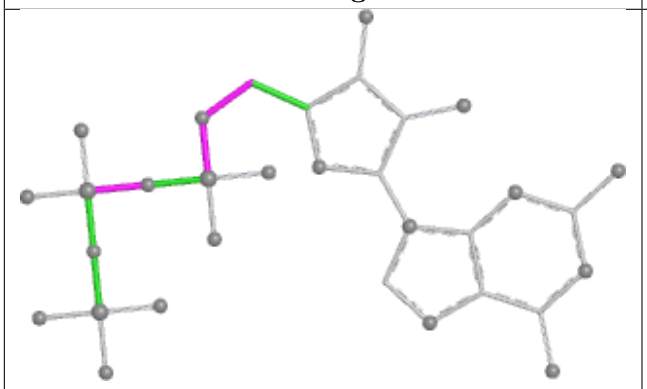

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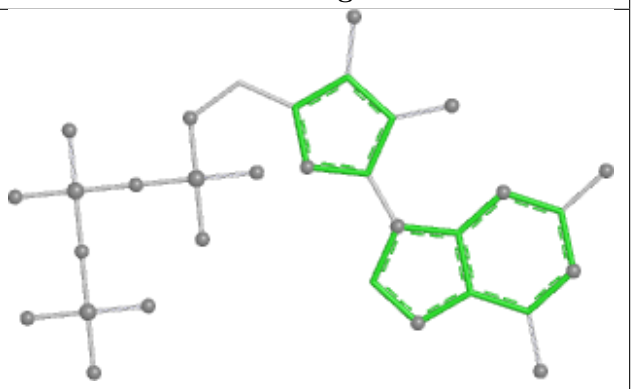
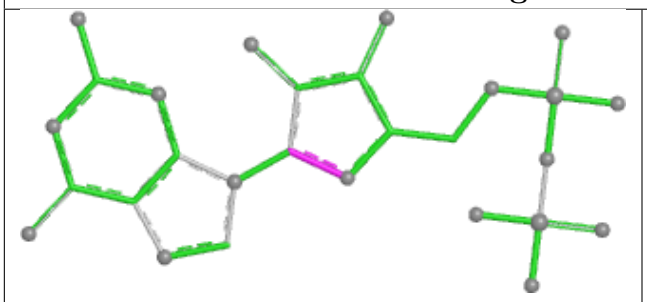


Rings

## Ligand GDP BB 501



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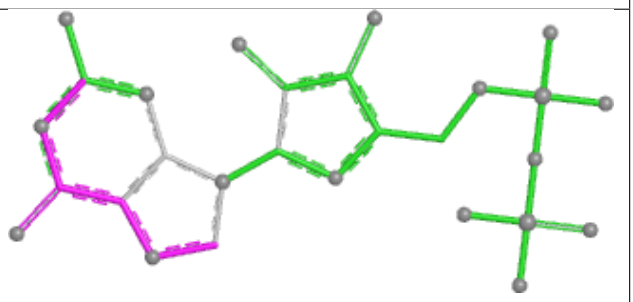

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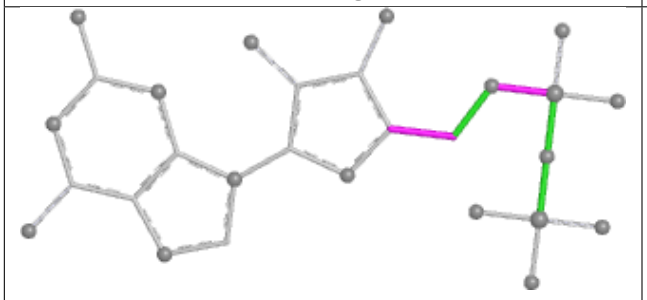

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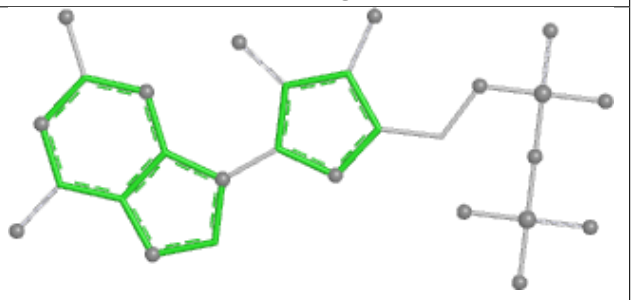

Rings

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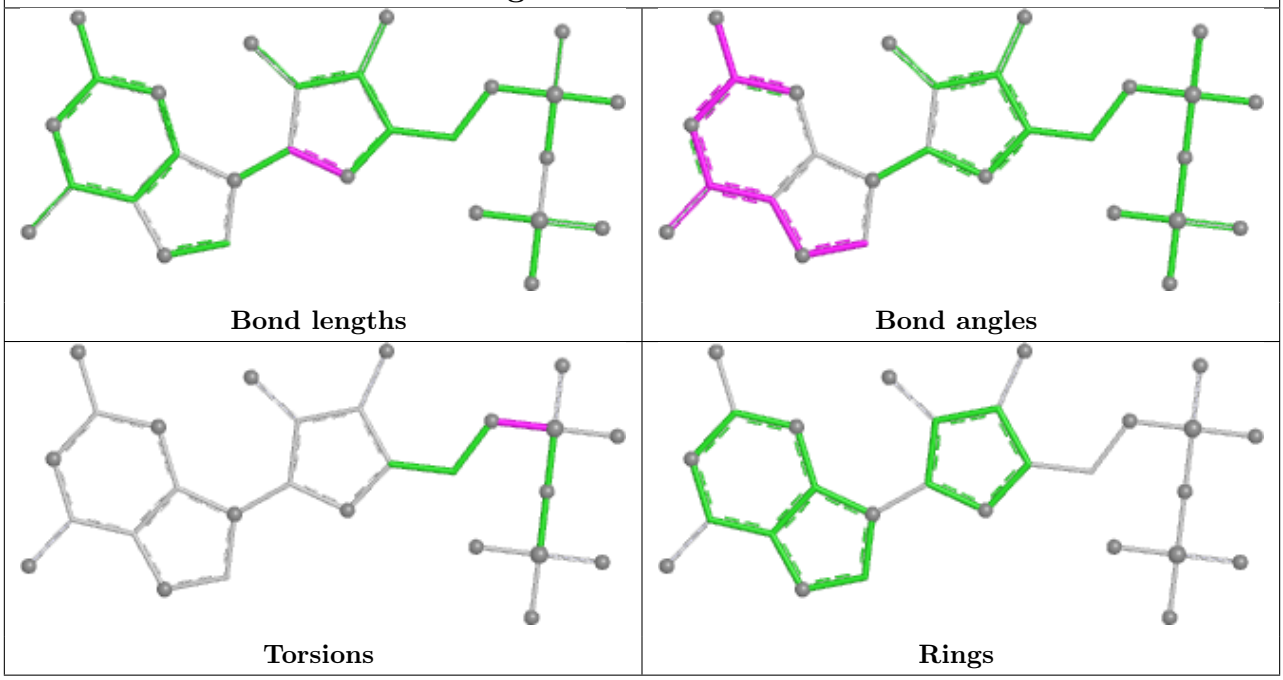


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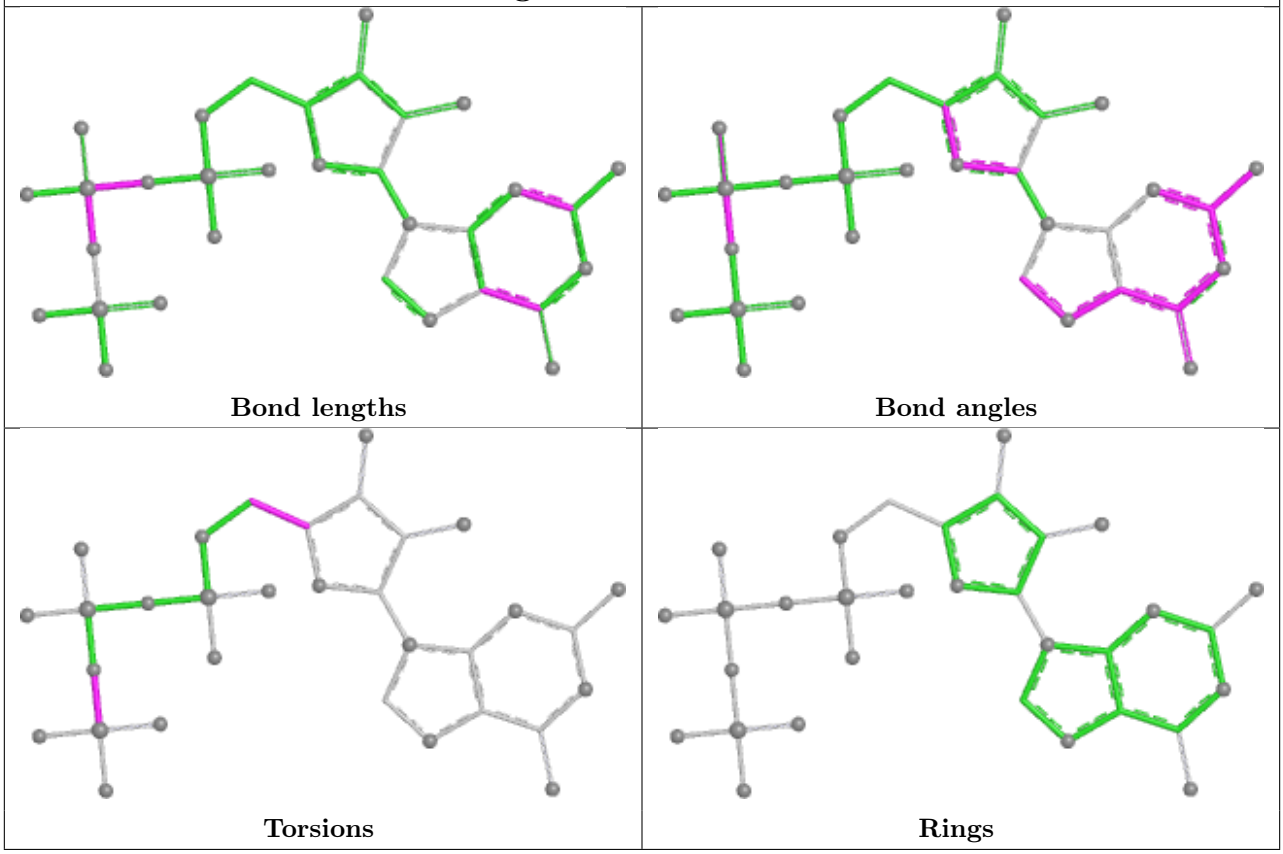

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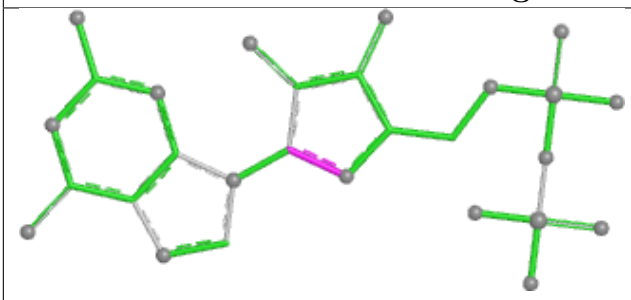

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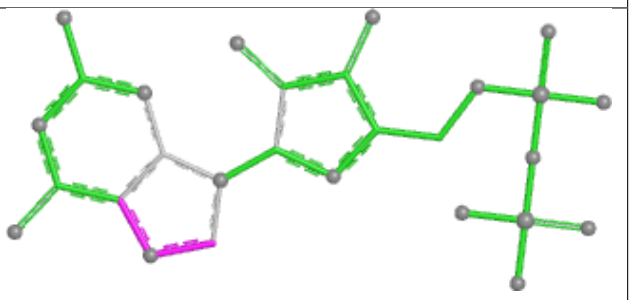

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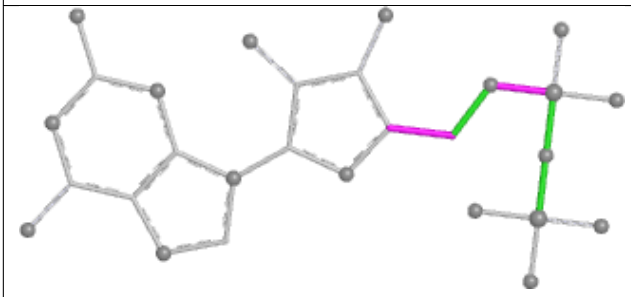

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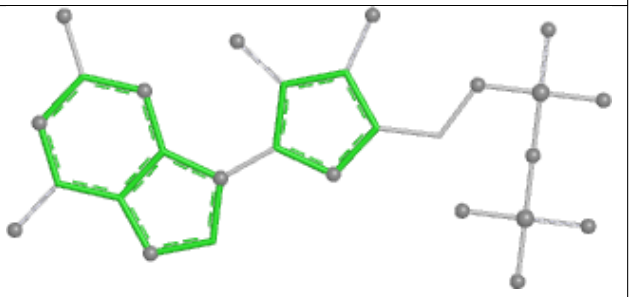
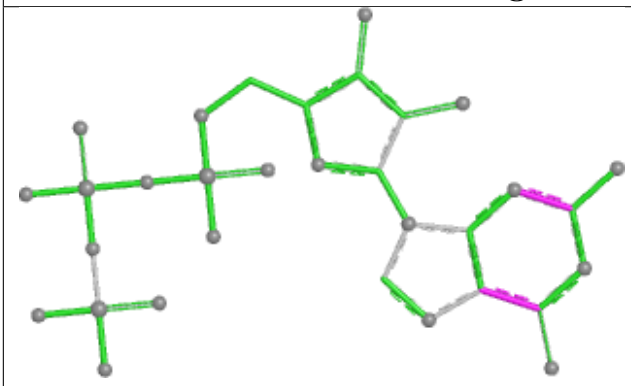


Rings

## Ligand GTP LM 501



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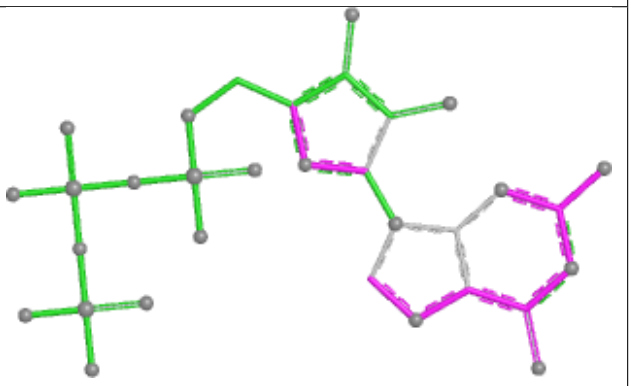

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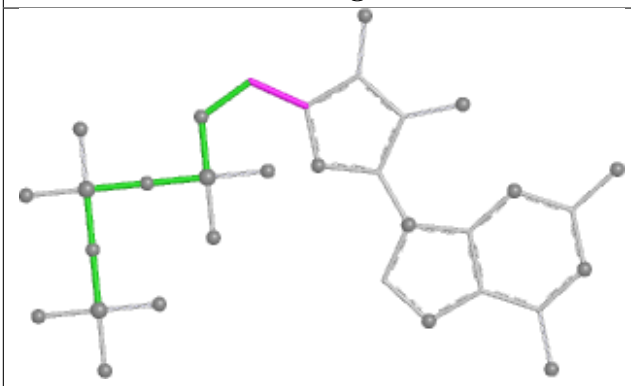

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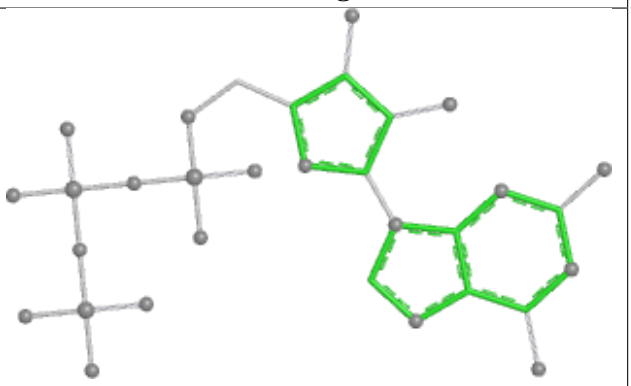
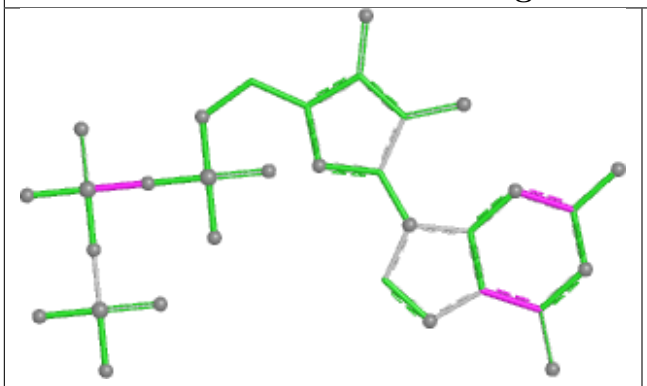


Rings

## Ligand GTP LL 501



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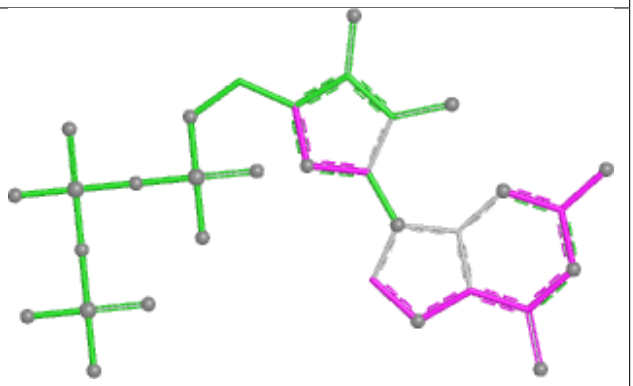
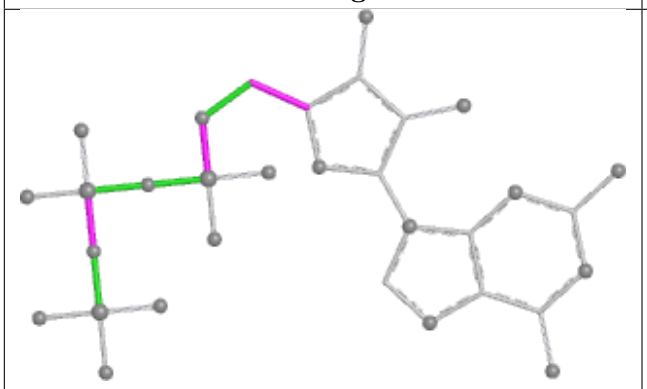


Bond angles



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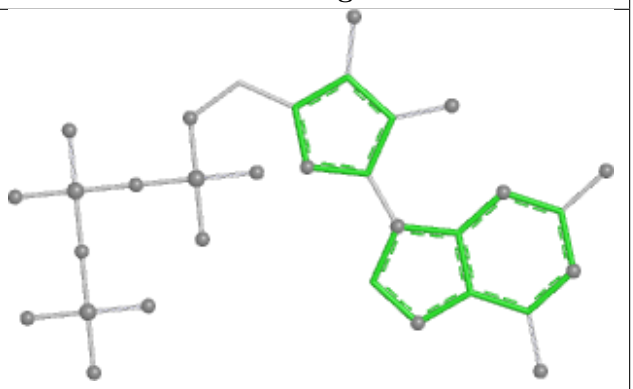
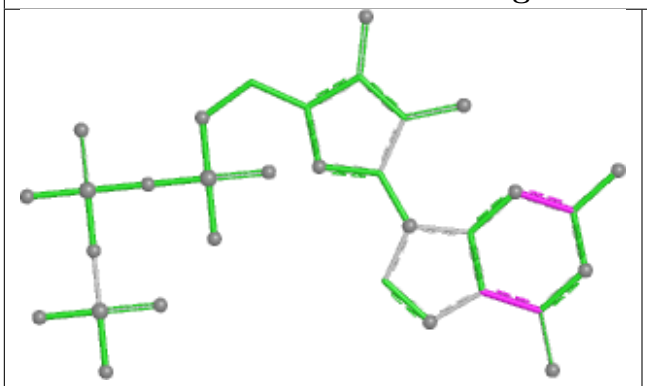


Rings

## Ligand GTP PE 501



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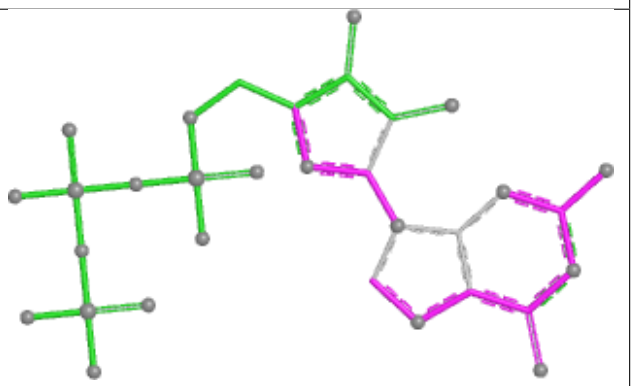
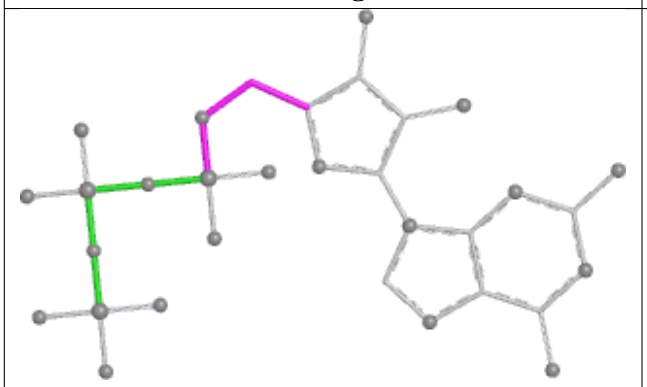
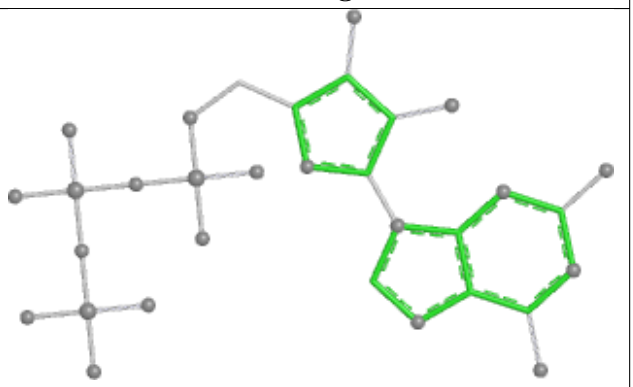


Bond angles

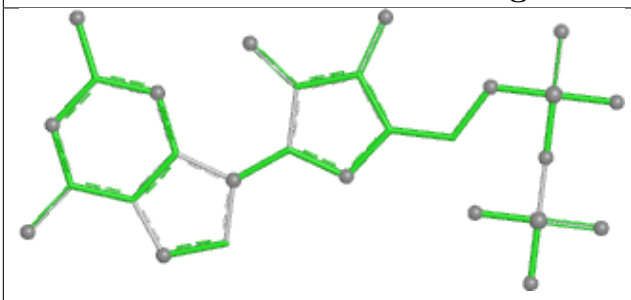


Torsions



Rings

## Ligand GDP KL 501



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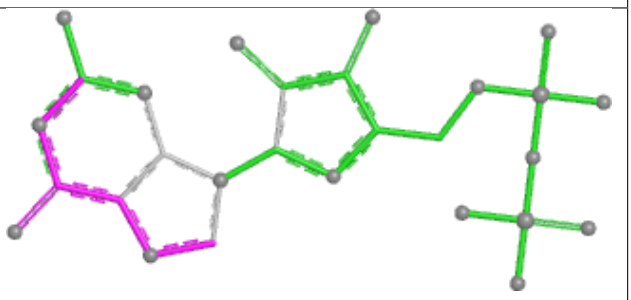
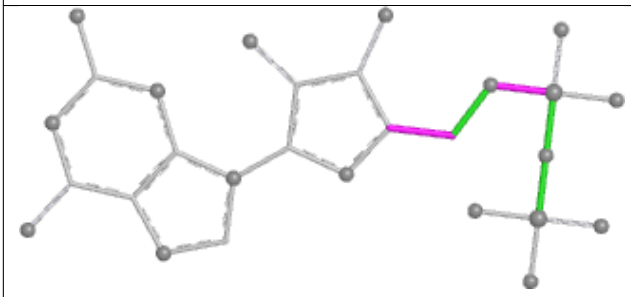


Bond angles



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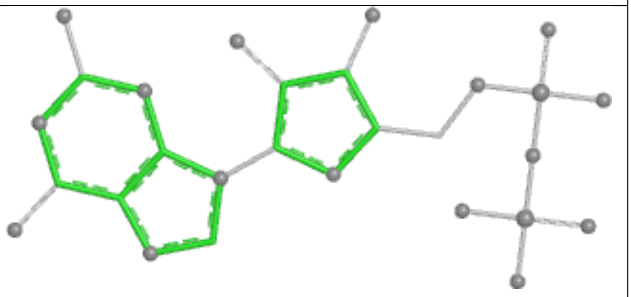
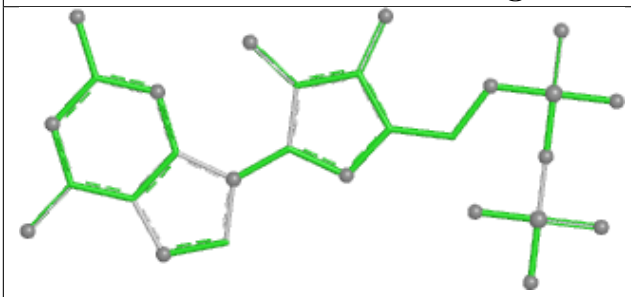


Rings

## Ligand GDP ML 502



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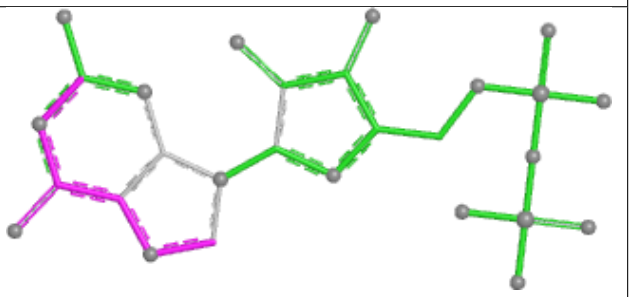
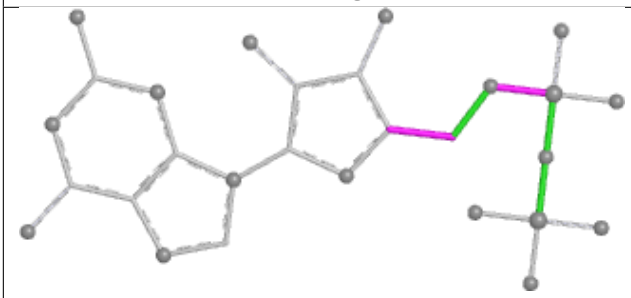


Bond angles



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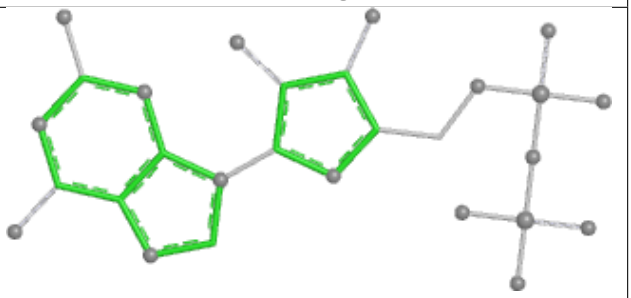

Rings

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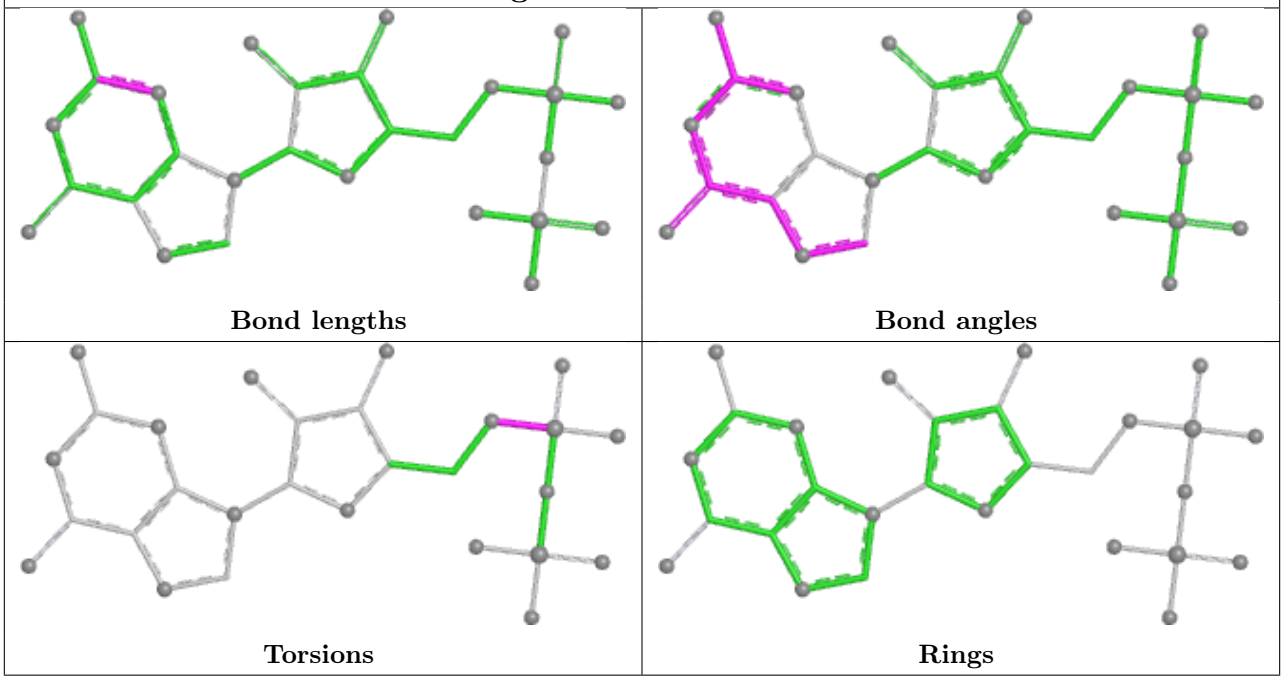
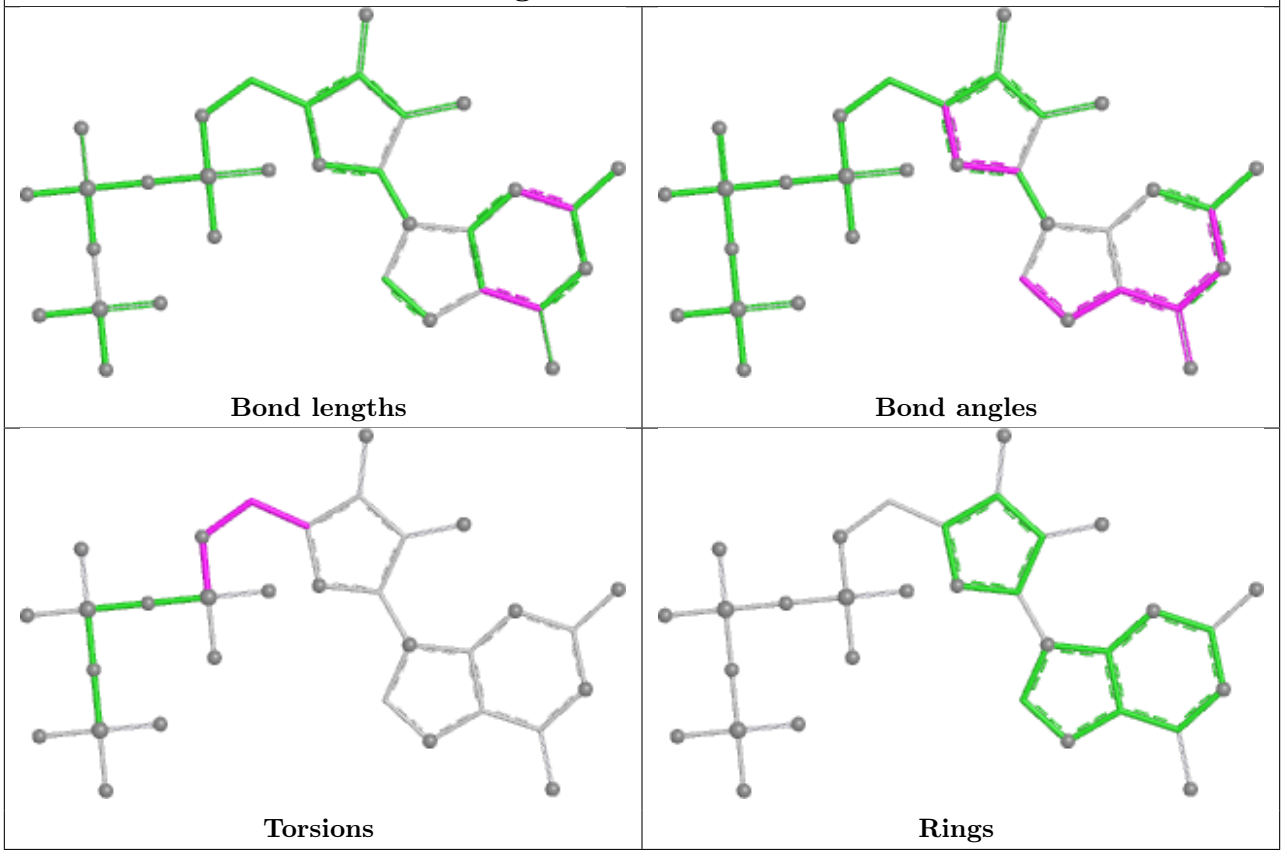
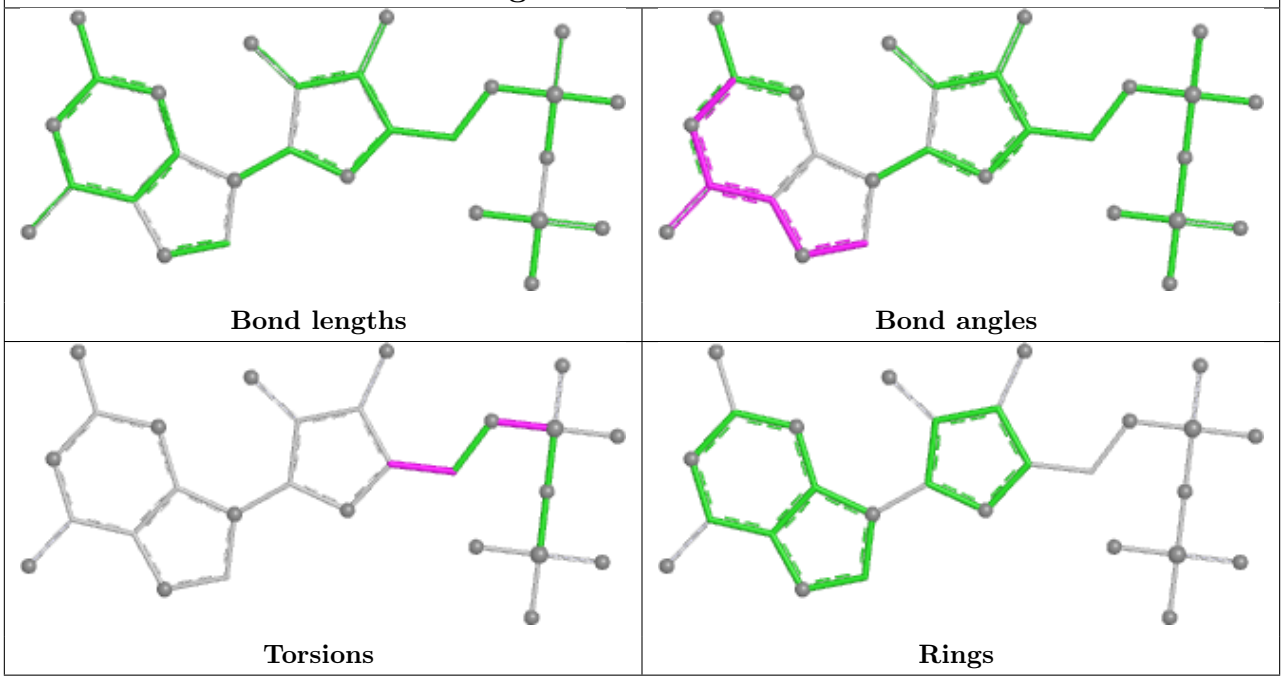


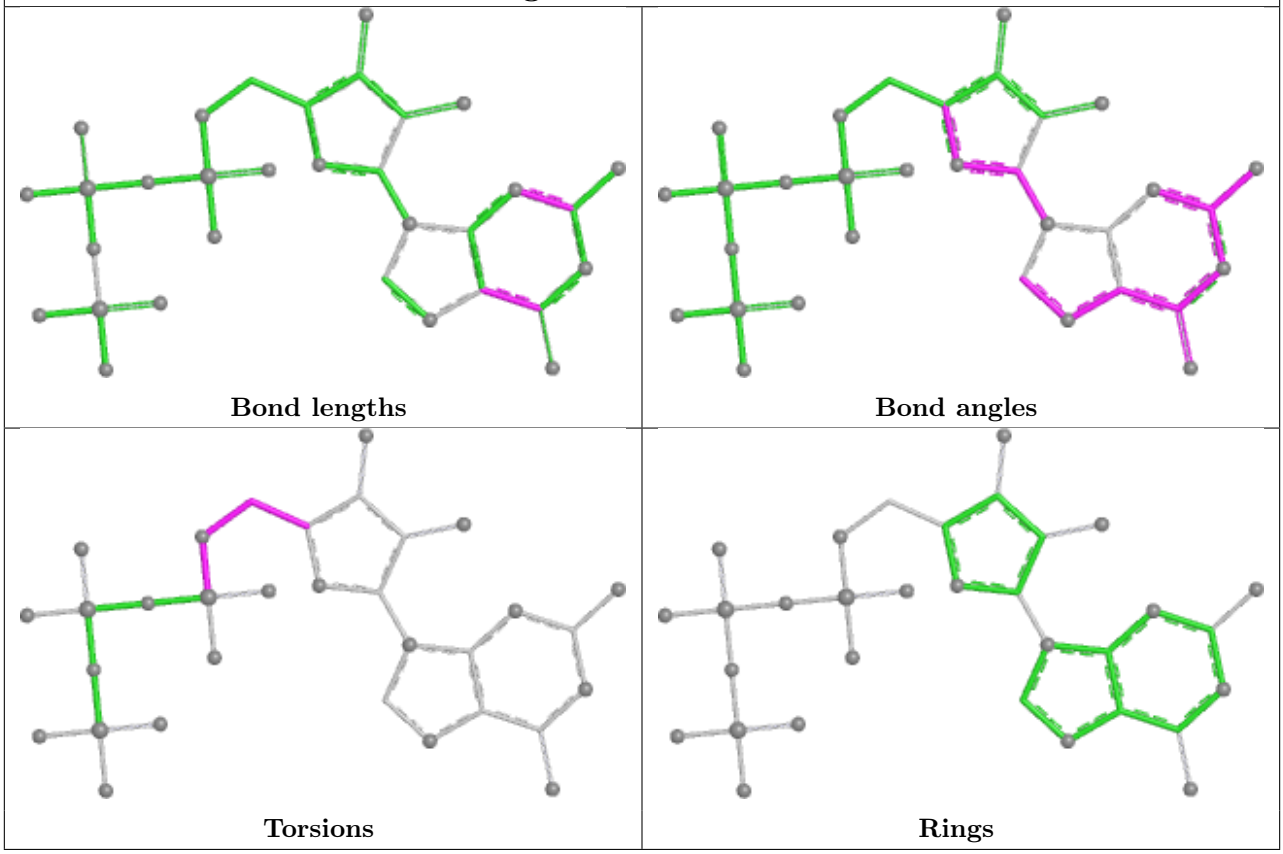

## Ligand GTP FE 501



## Ligand GDP UB 501




## Ligand GTP II 501



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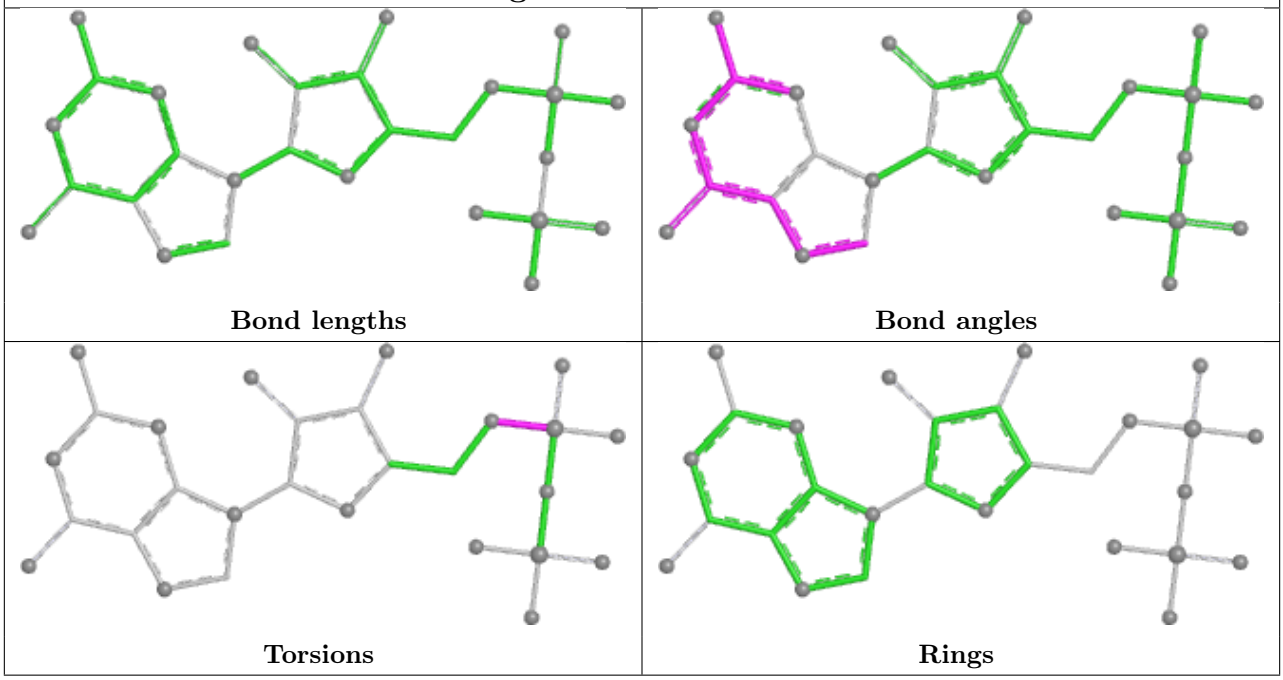


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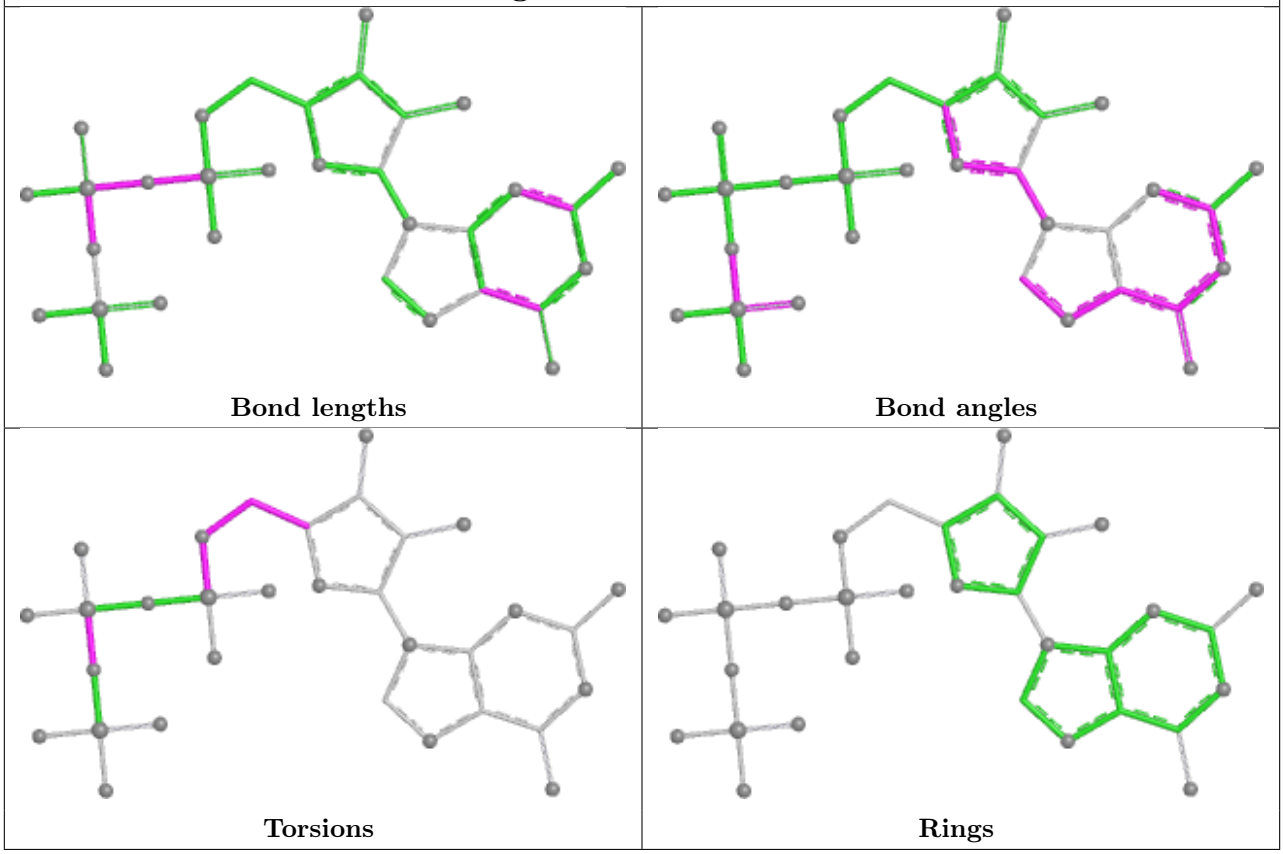

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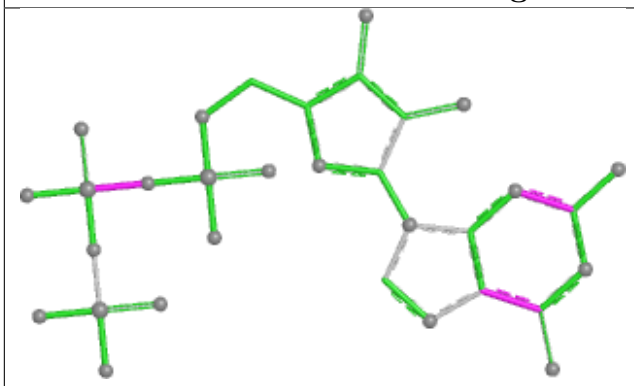
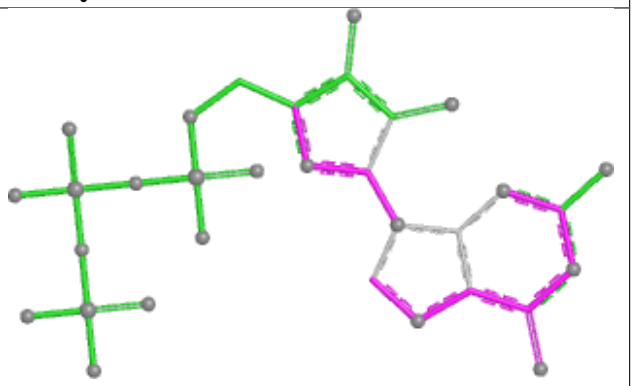
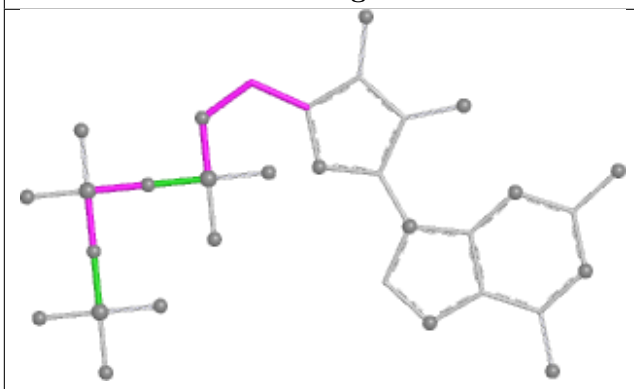


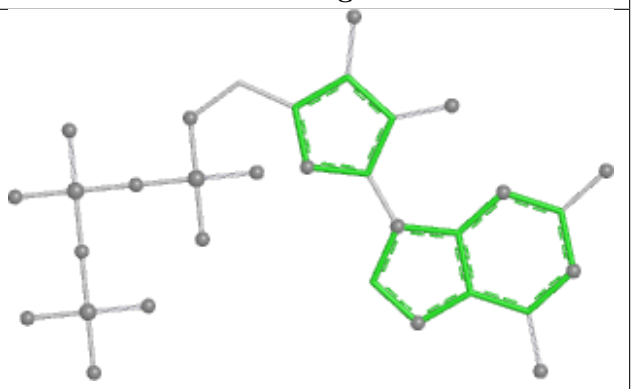
Bond lengths



Bond angles

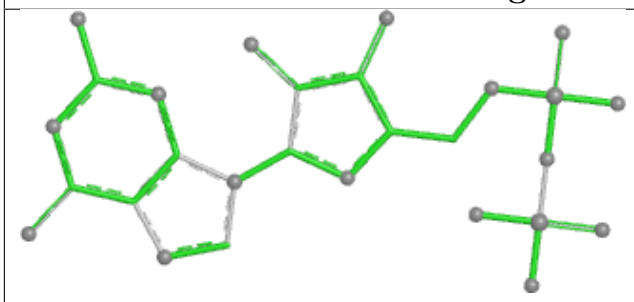


Torsions



Rings

## Ligand GDP HB 501



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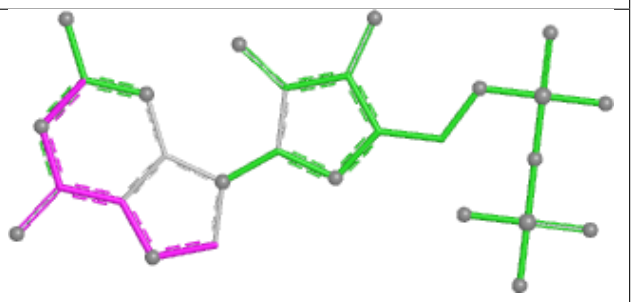
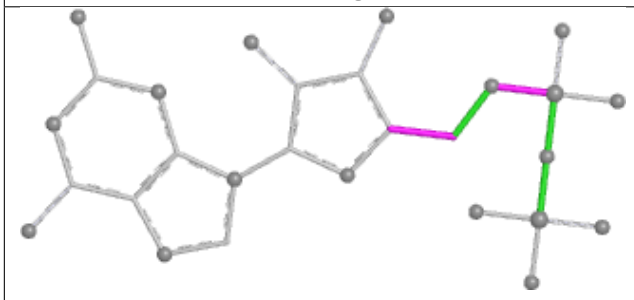


Bond angles



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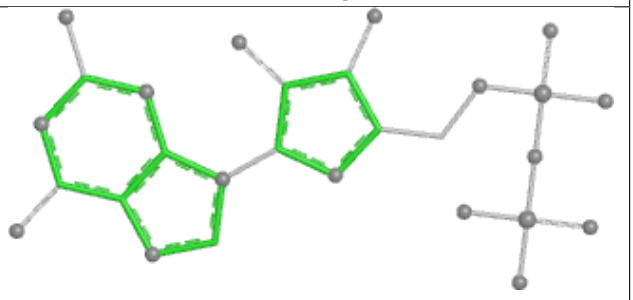

Rings

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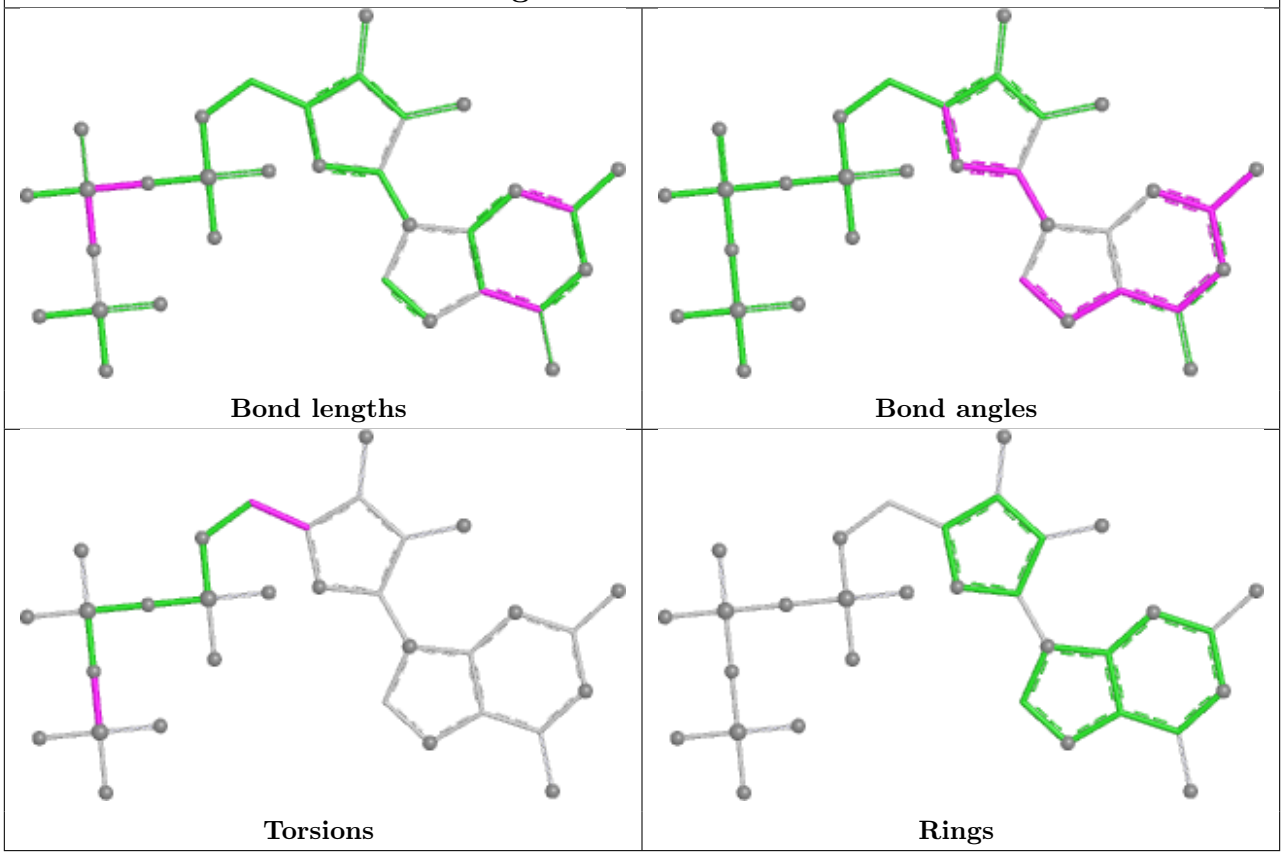


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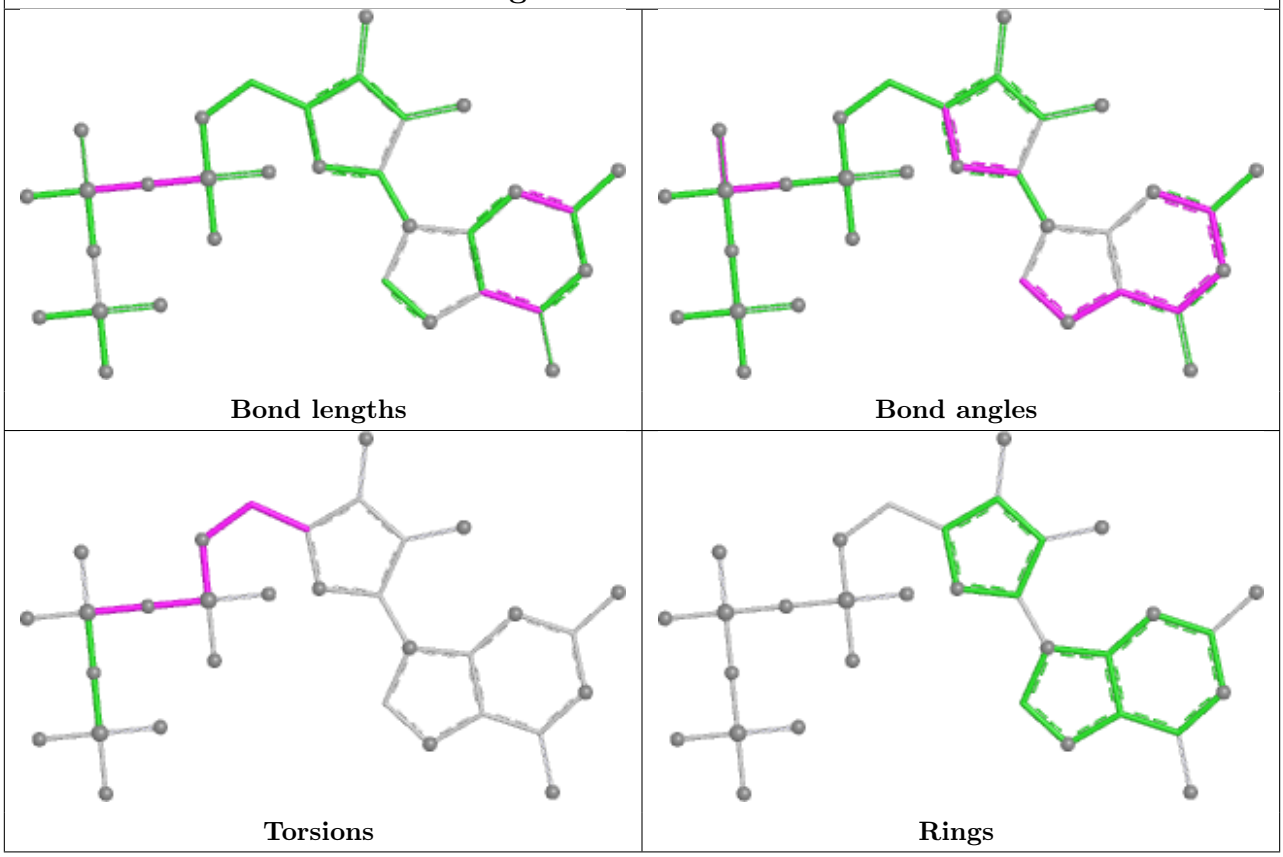

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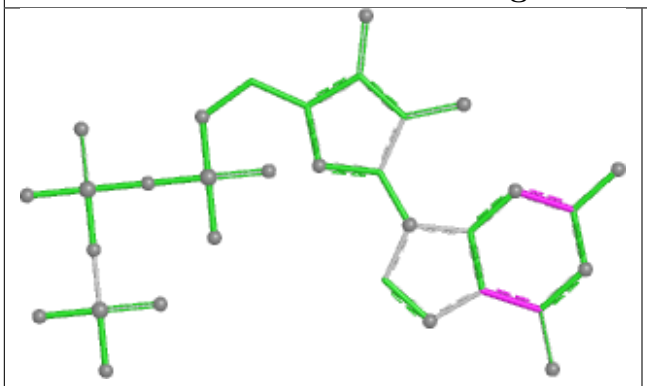

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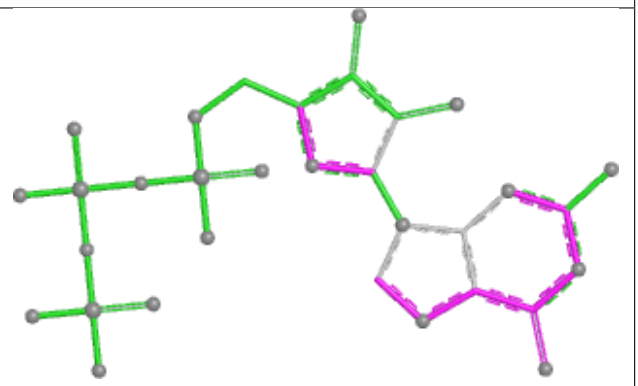
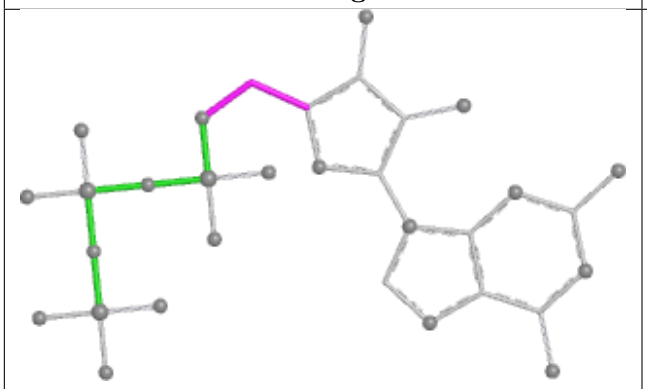


Bond angles



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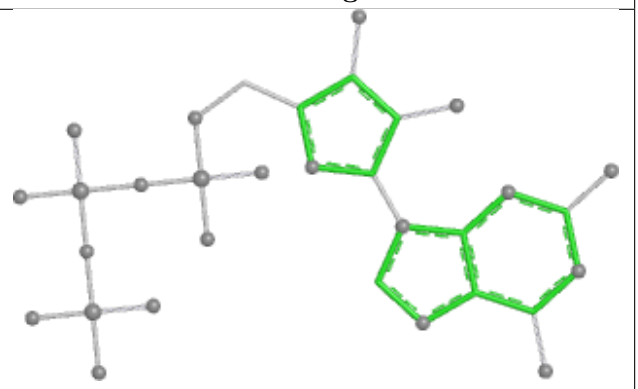
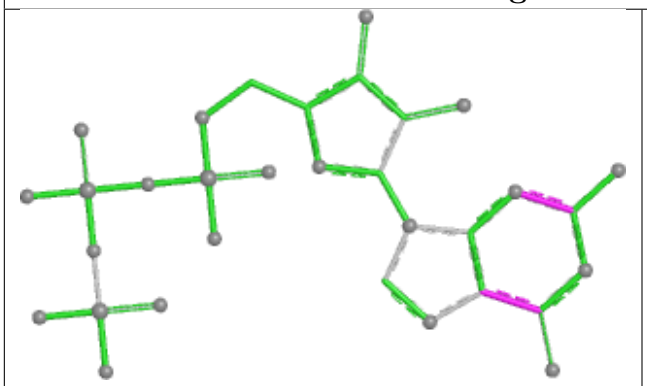


Rings

## Ligand GTP NO 501



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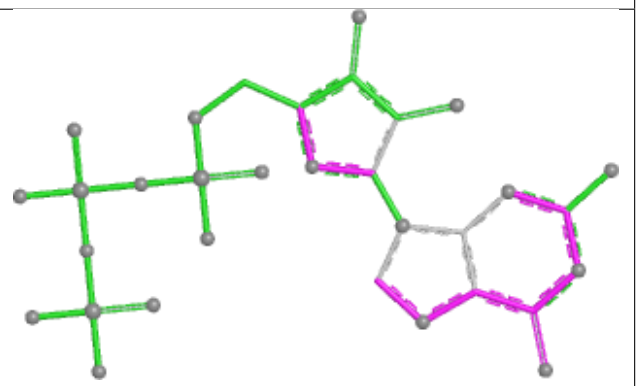

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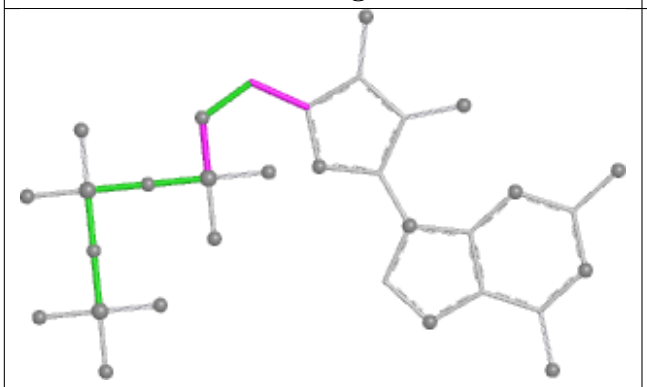

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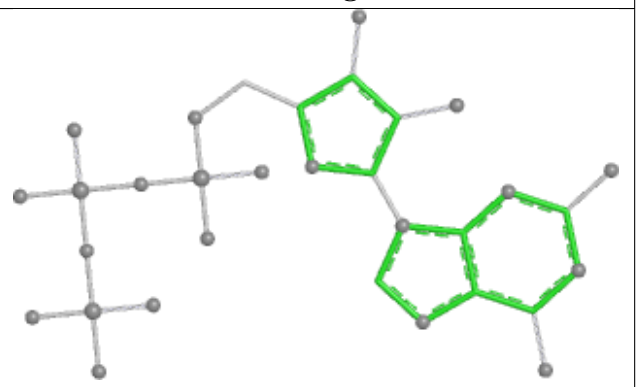
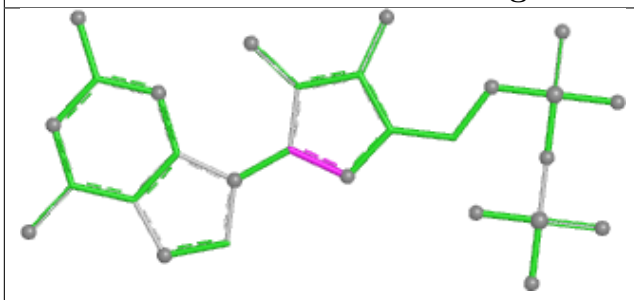


Rings

## Ligand GDP QP 501



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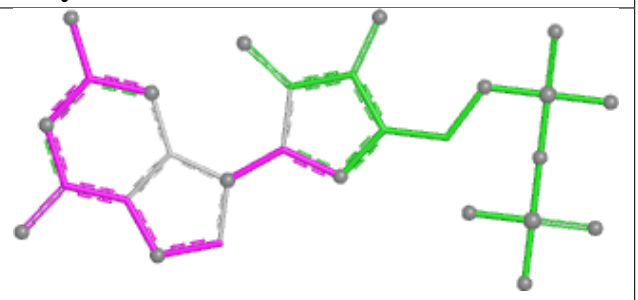

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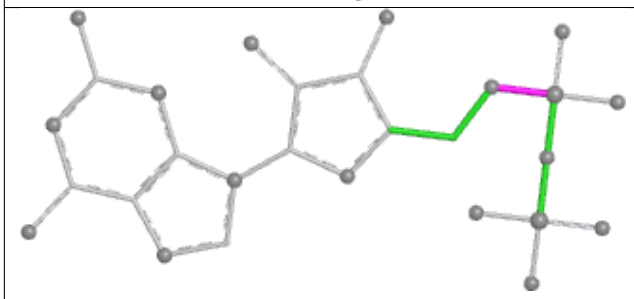

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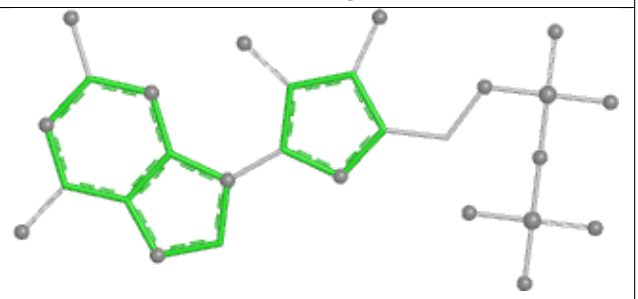

Rings

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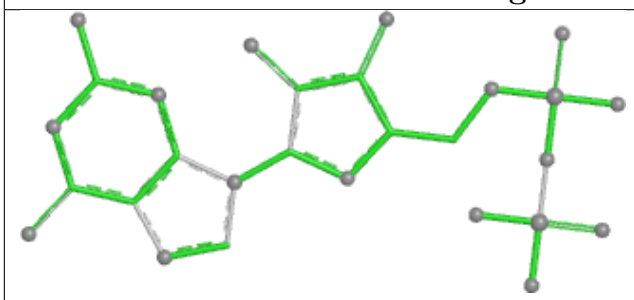

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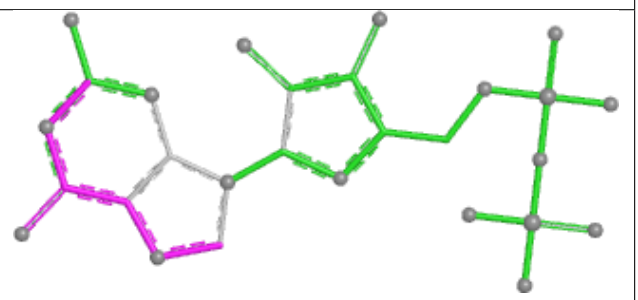
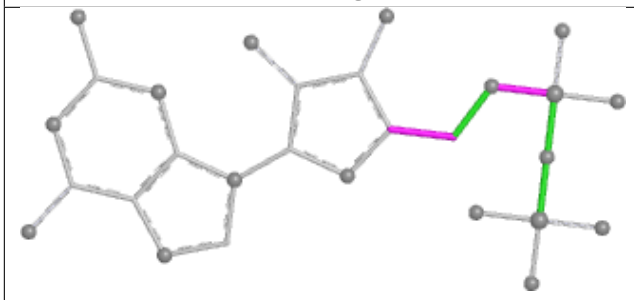


Bond angles



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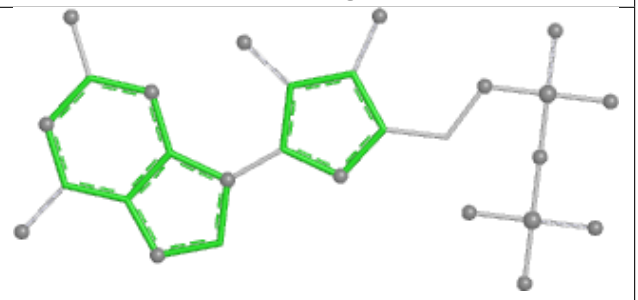
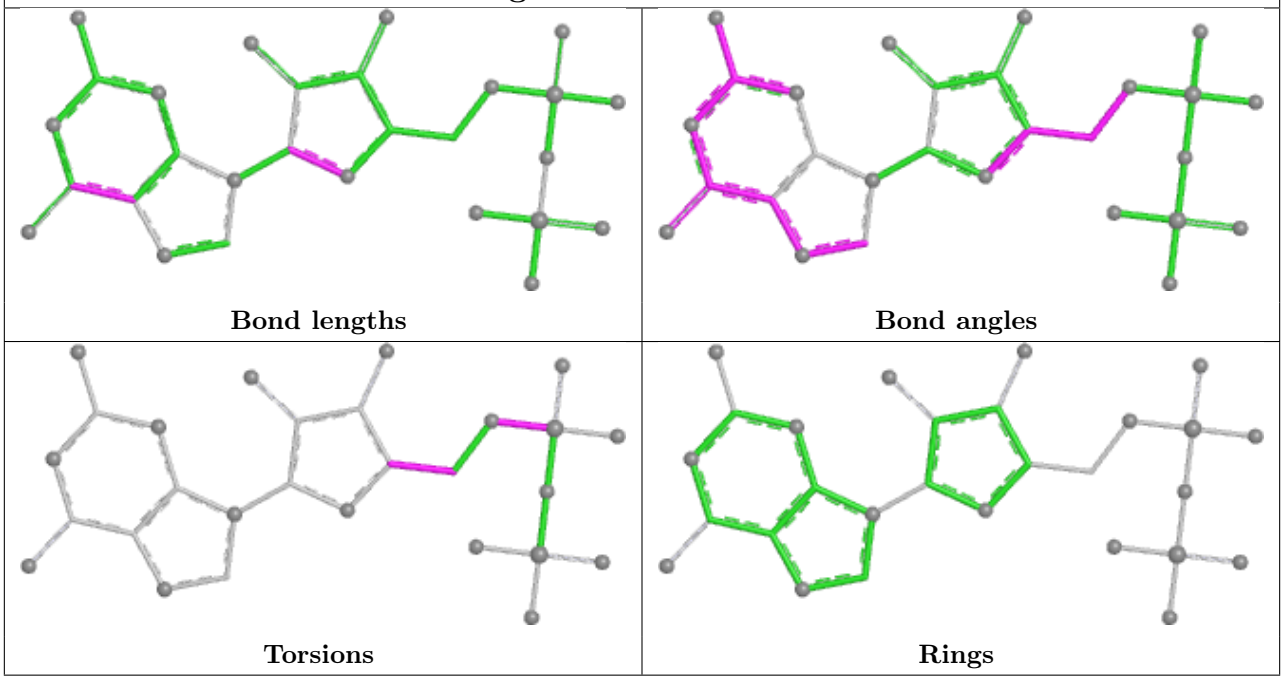


Rings

## Ligand GDP GP 502

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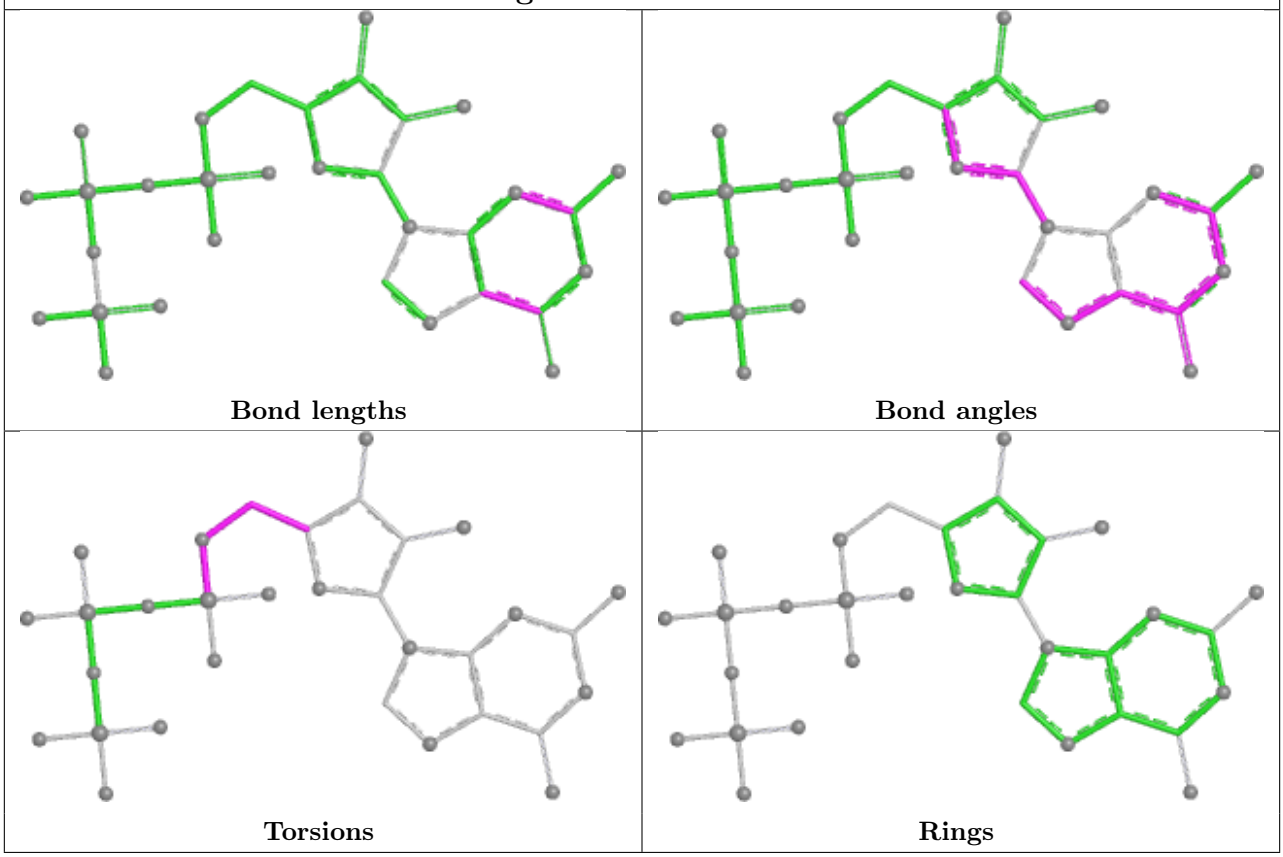

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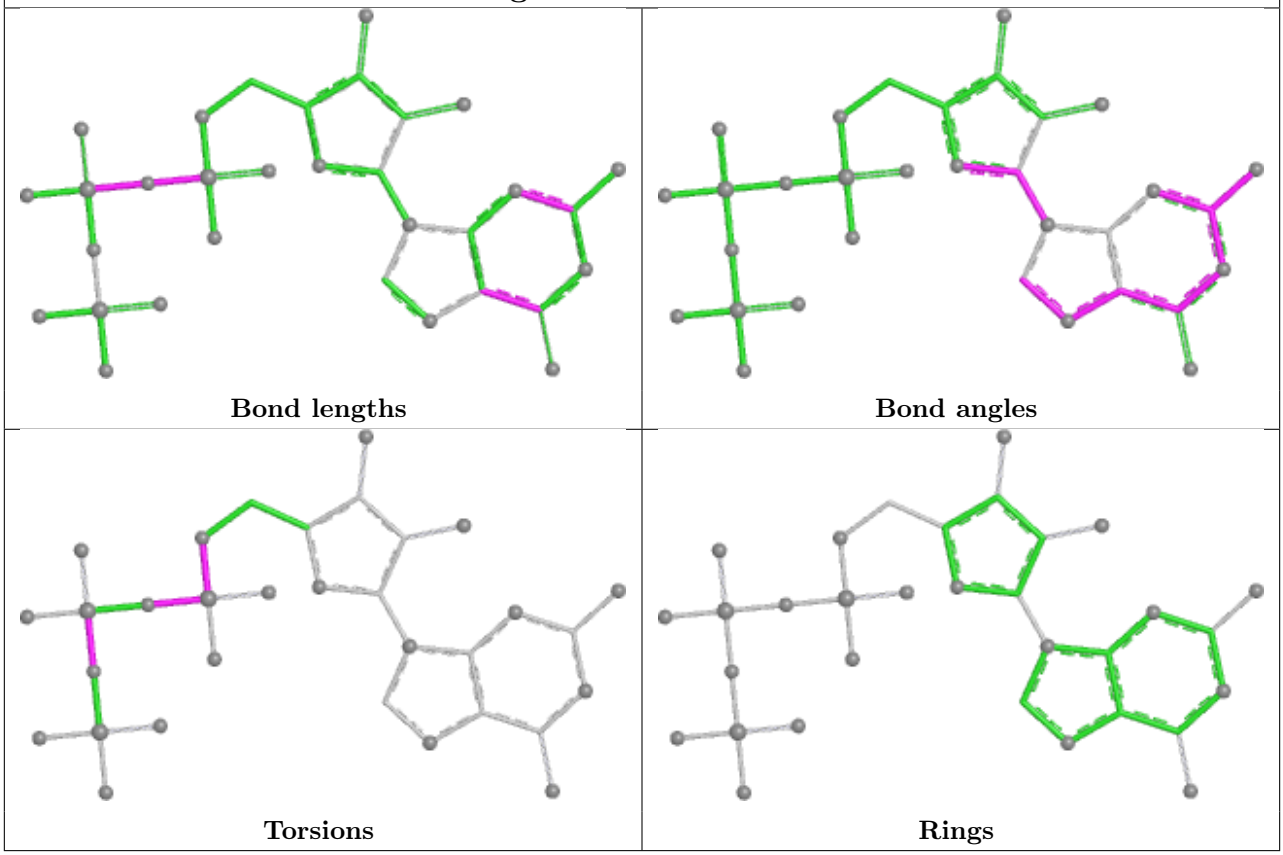


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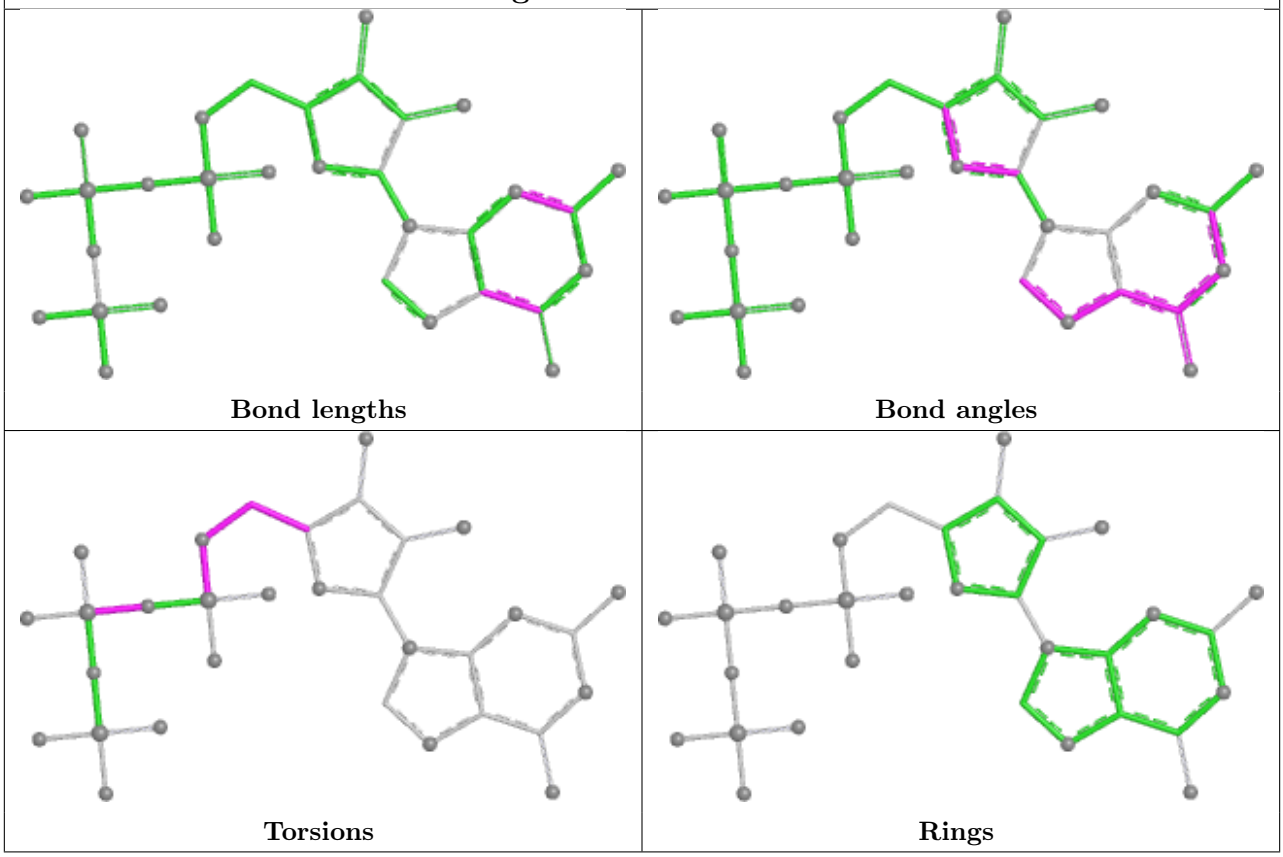

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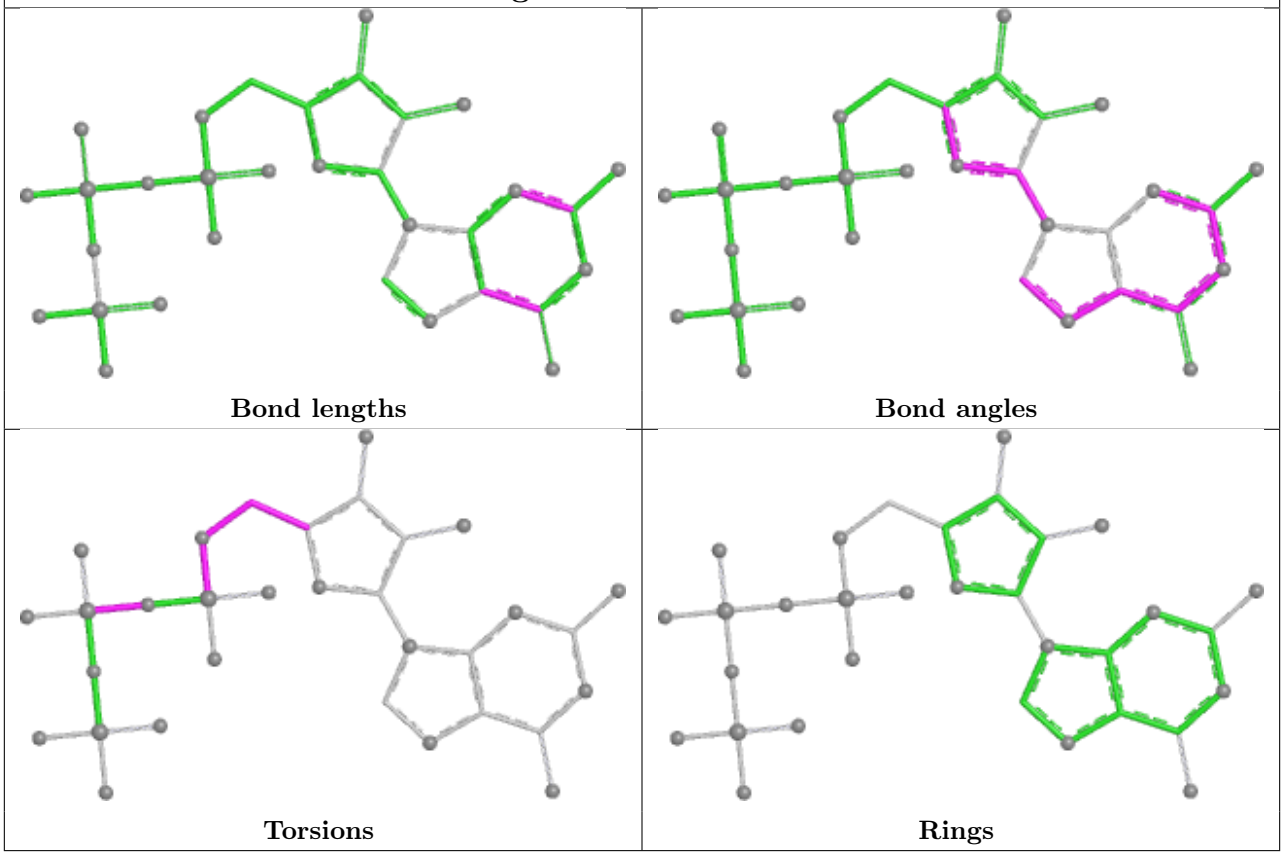


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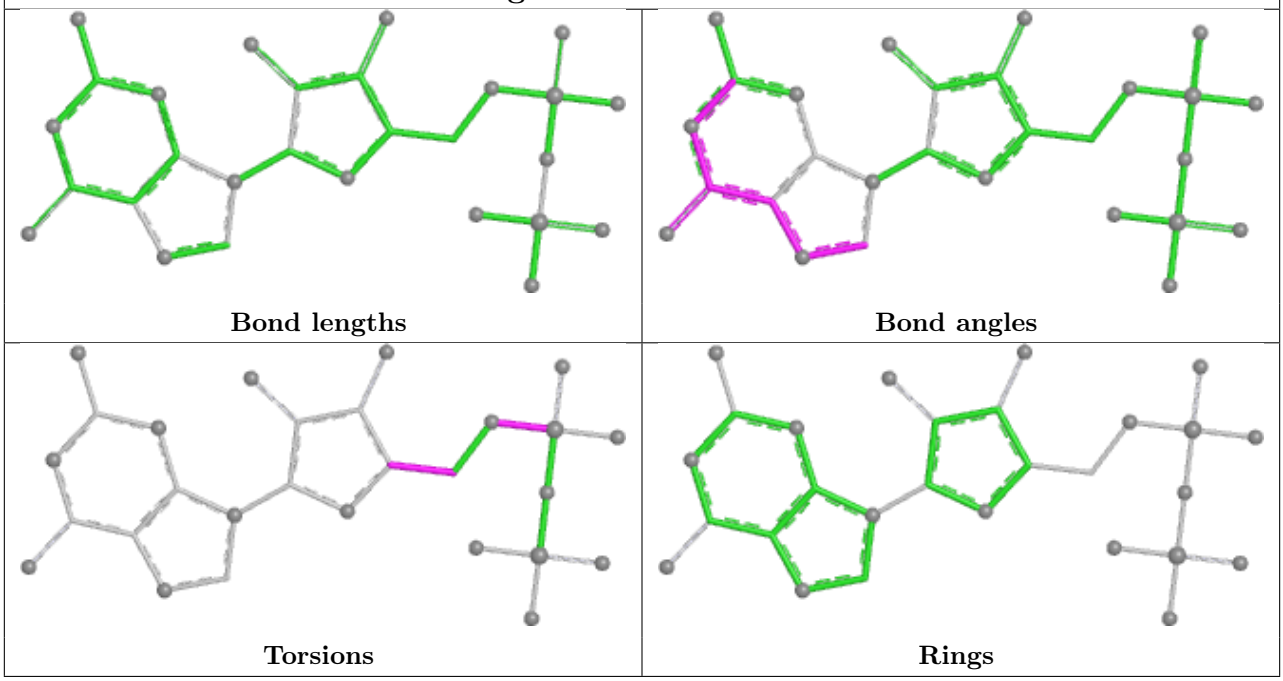
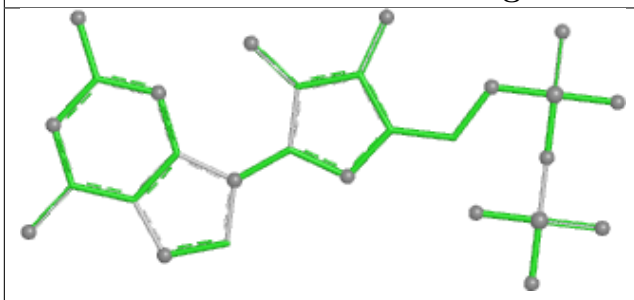
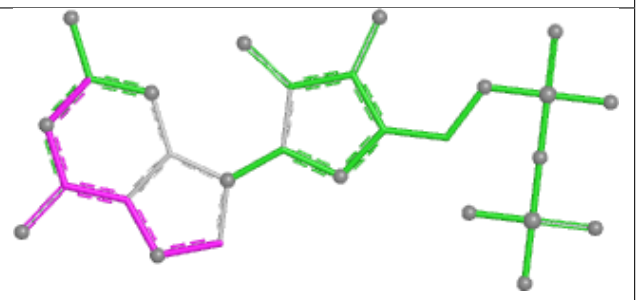


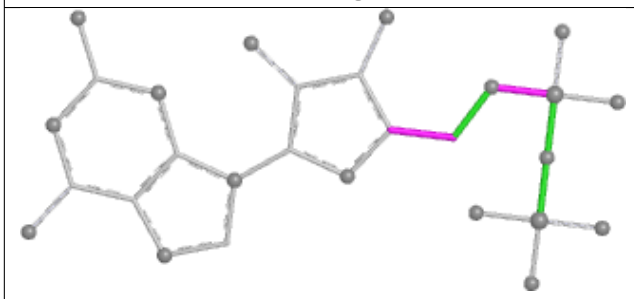
## Ligand GDP WN 501



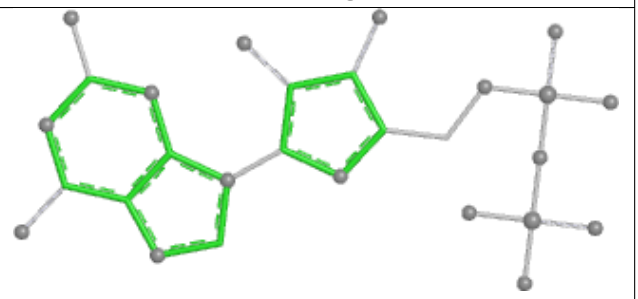
Bond lengths



Bond angles

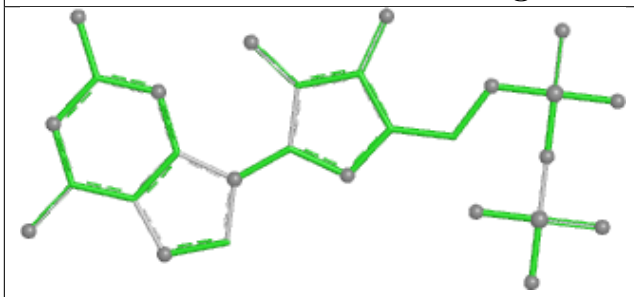


Torsions



Rings

## Ligand GDP PL 501



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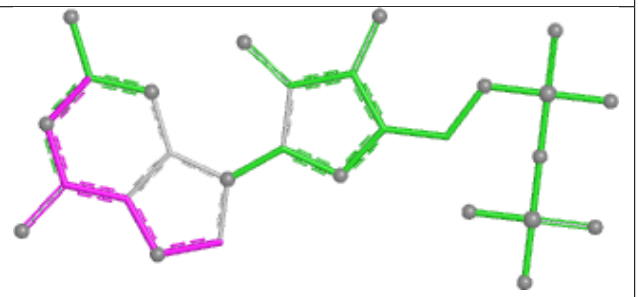
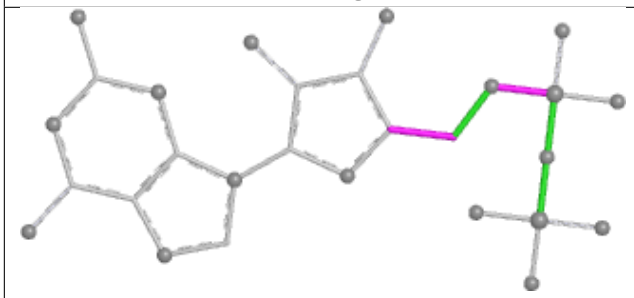
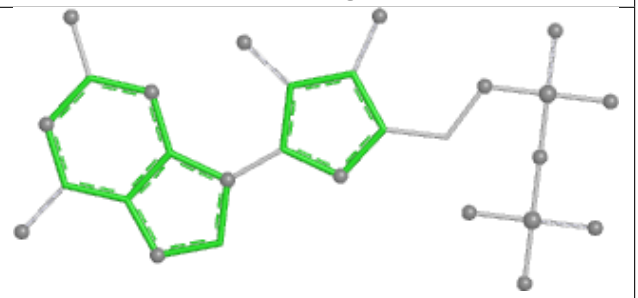


Bond angles

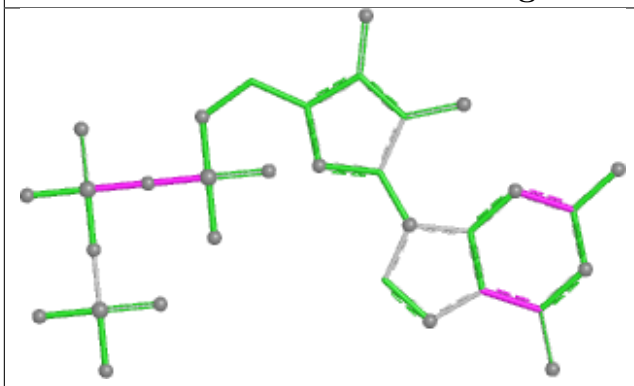


Torsions



Rings

## Ligand GTP EI 501



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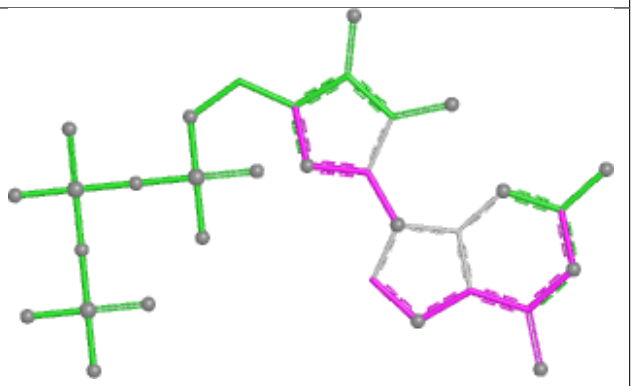

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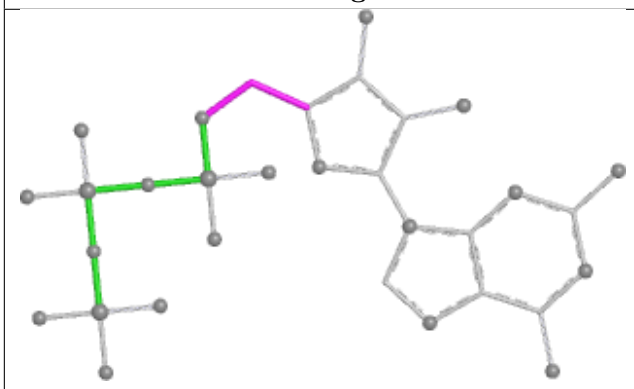

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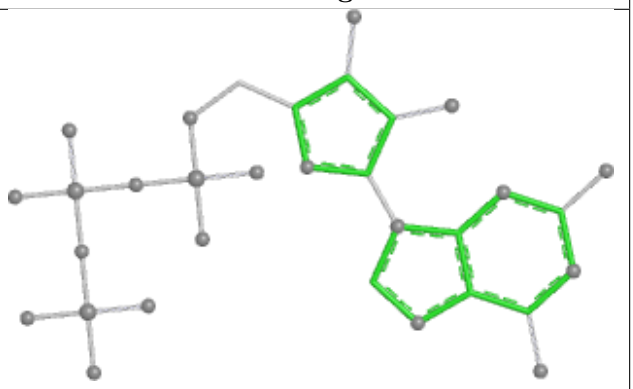
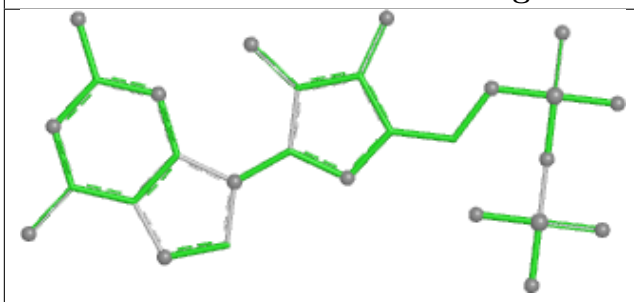


Rings

## Ligand GDP JO 502



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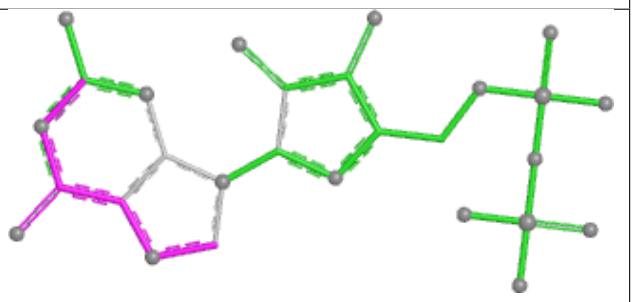

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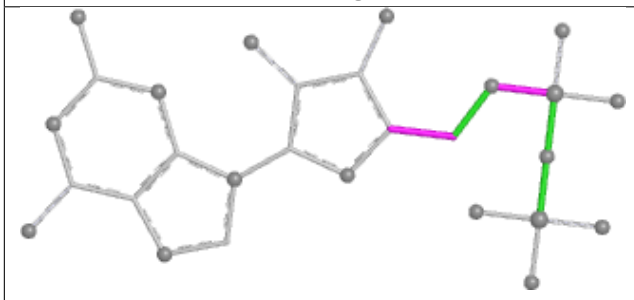

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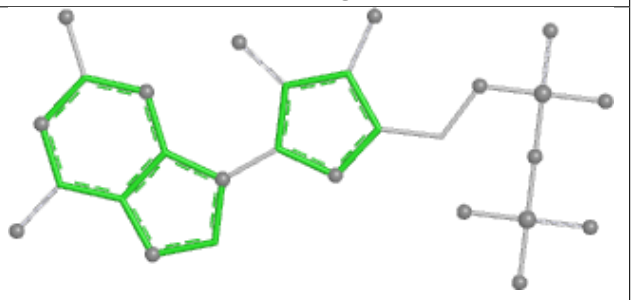

Rings

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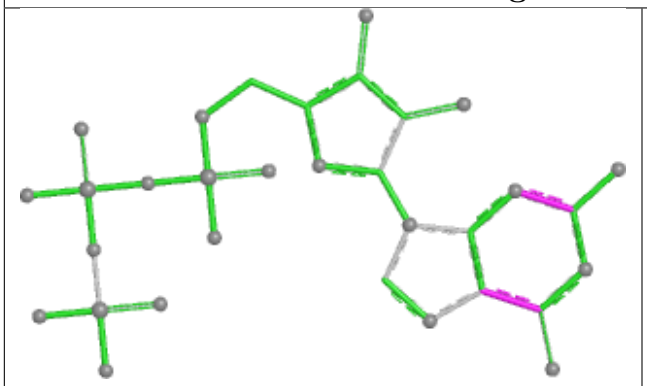

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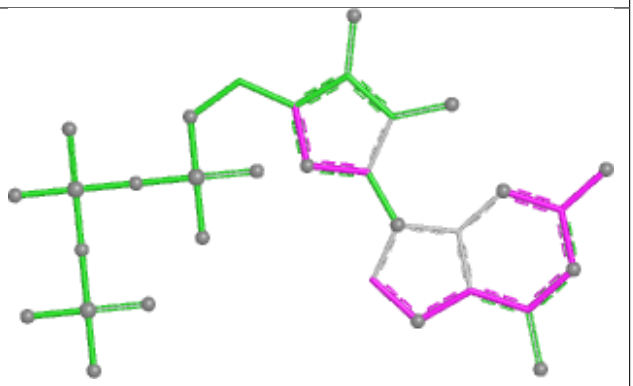

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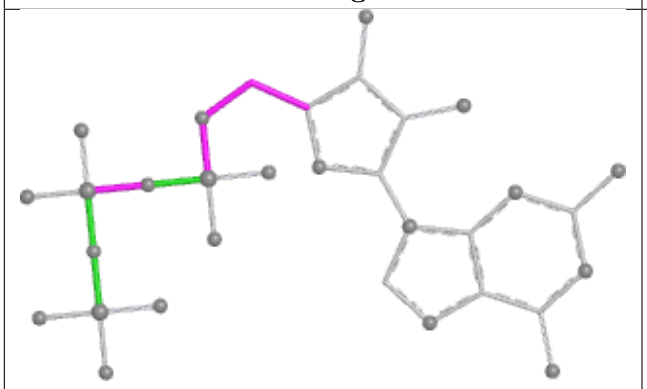

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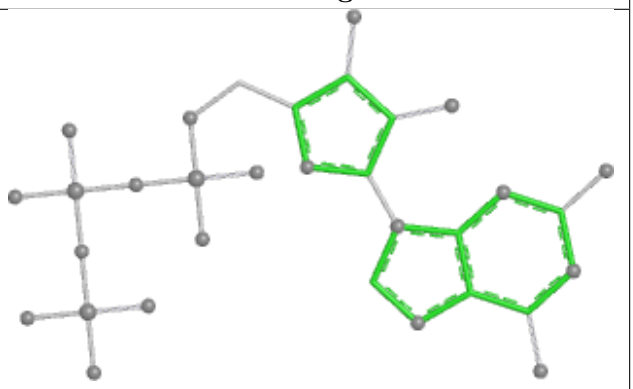
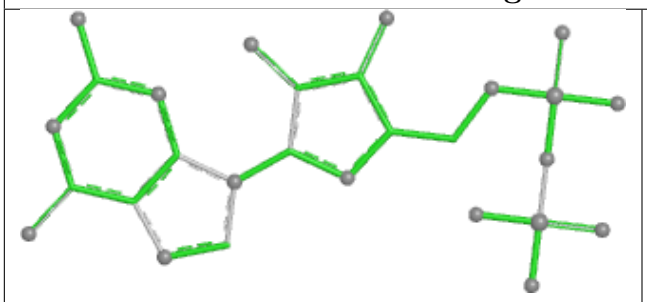


Rings

## Ligand GDP WO 502



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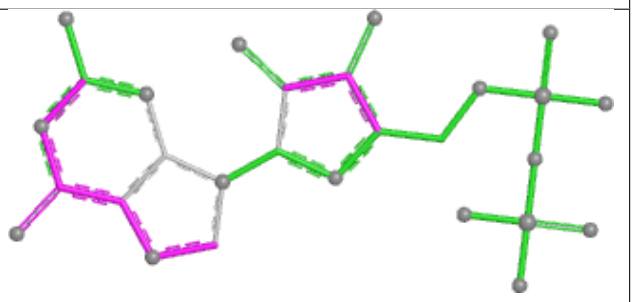

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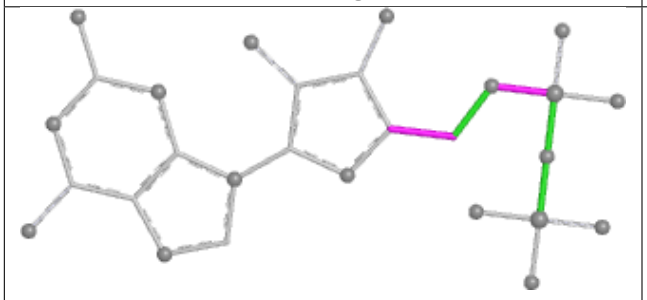

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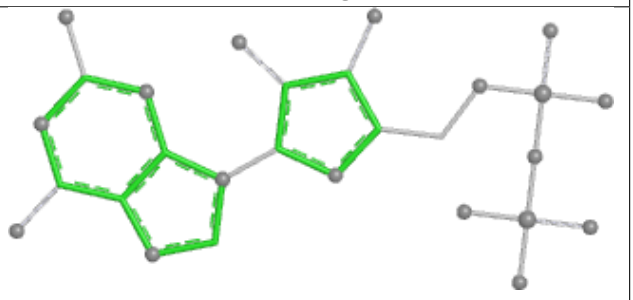
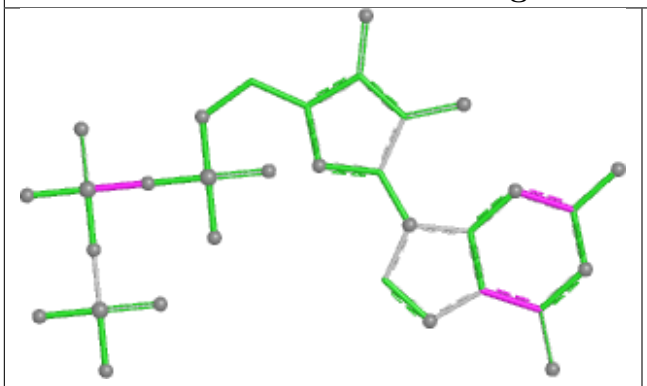


Rings

## Ligand GTP BH 501



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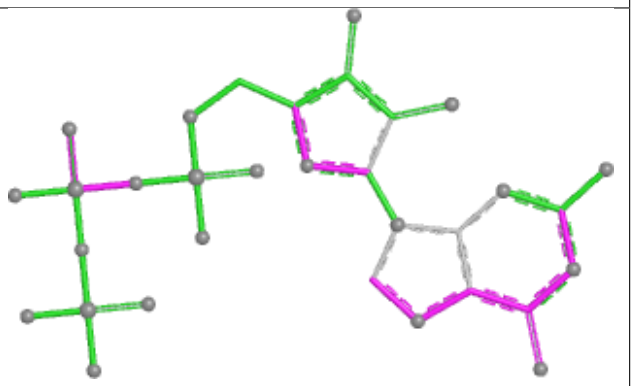

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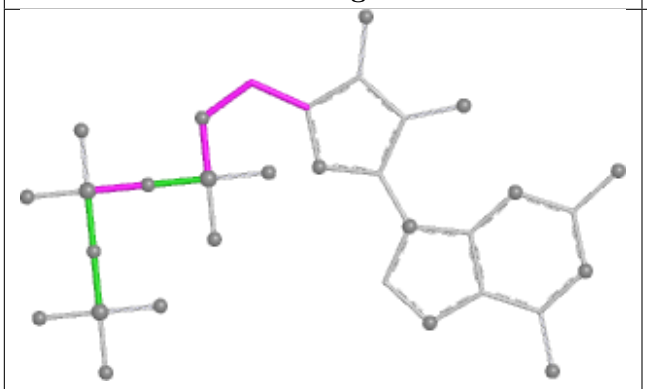

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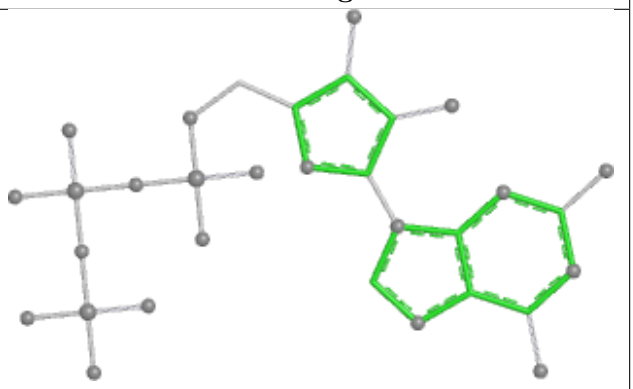
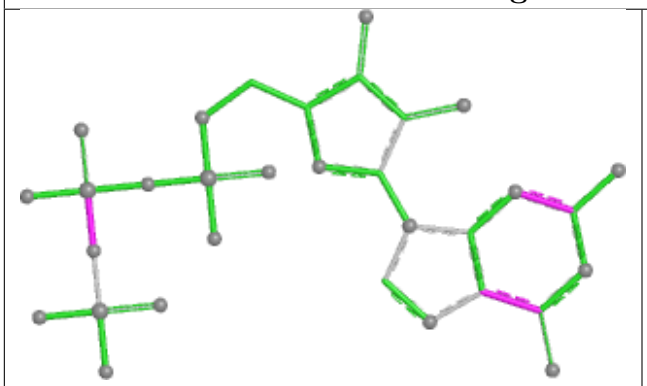


Rings

## Ligand GTP TH 501



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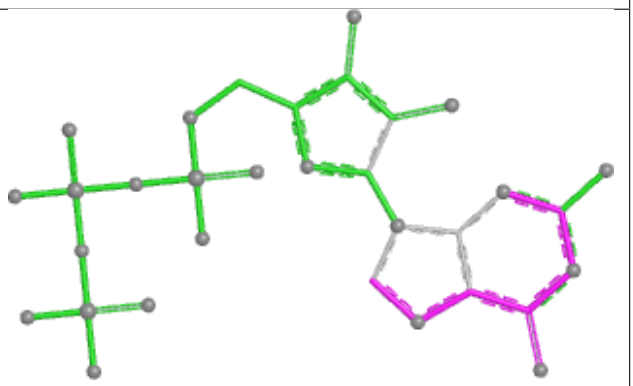

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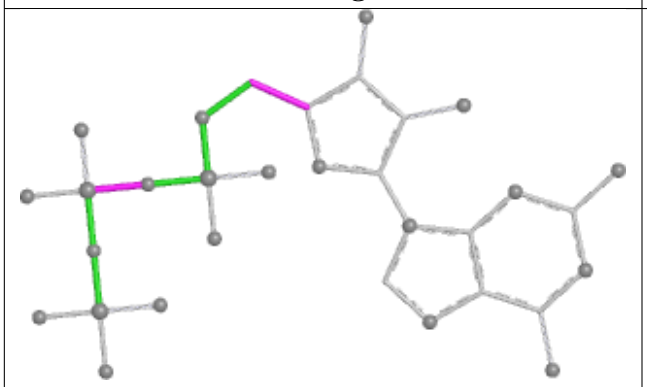

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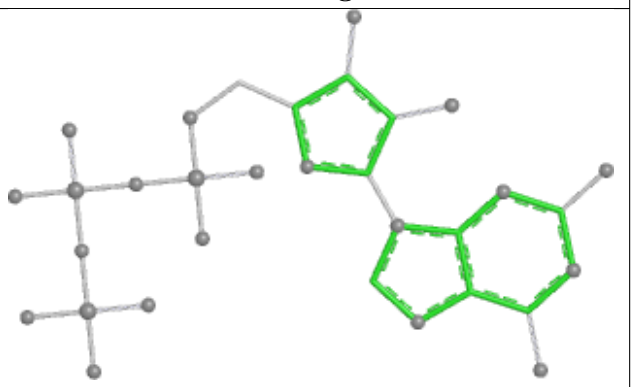

Rings

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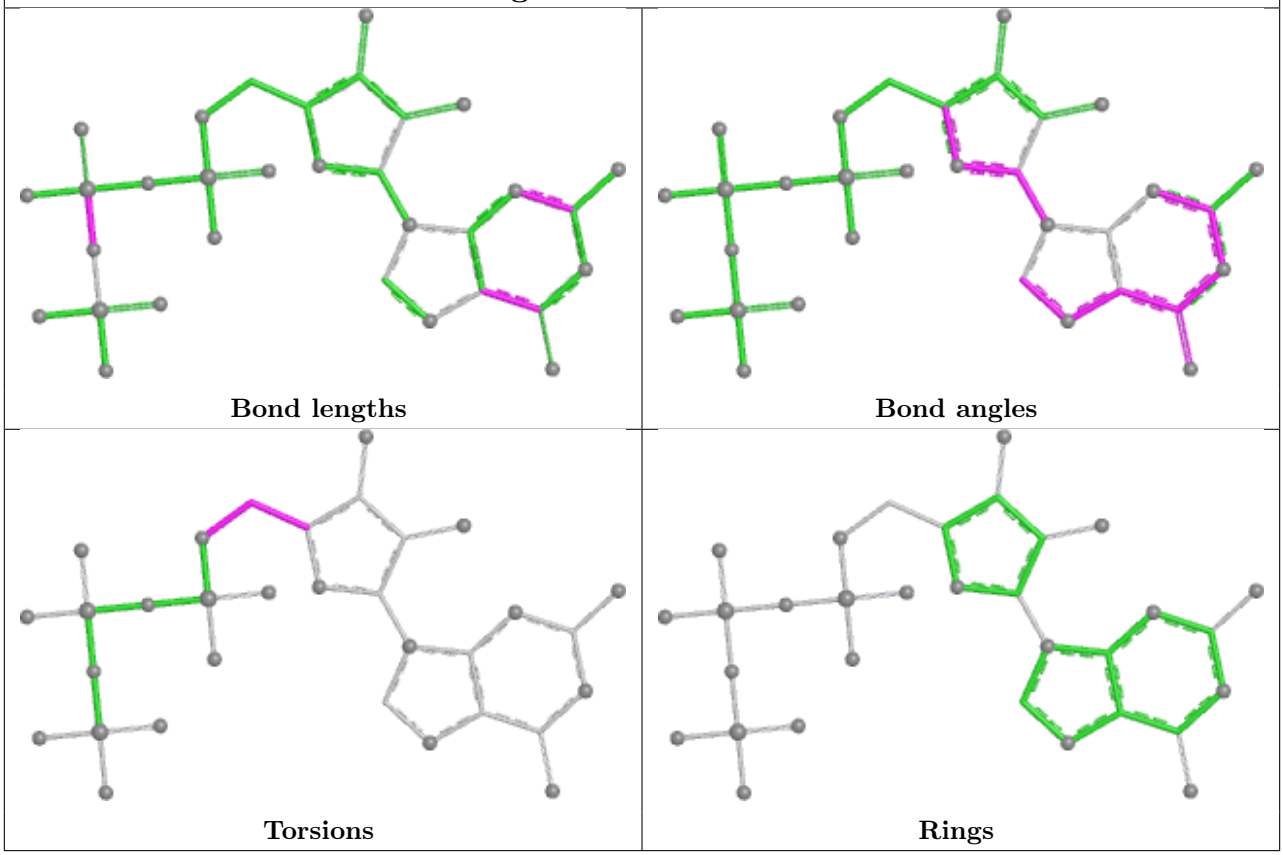


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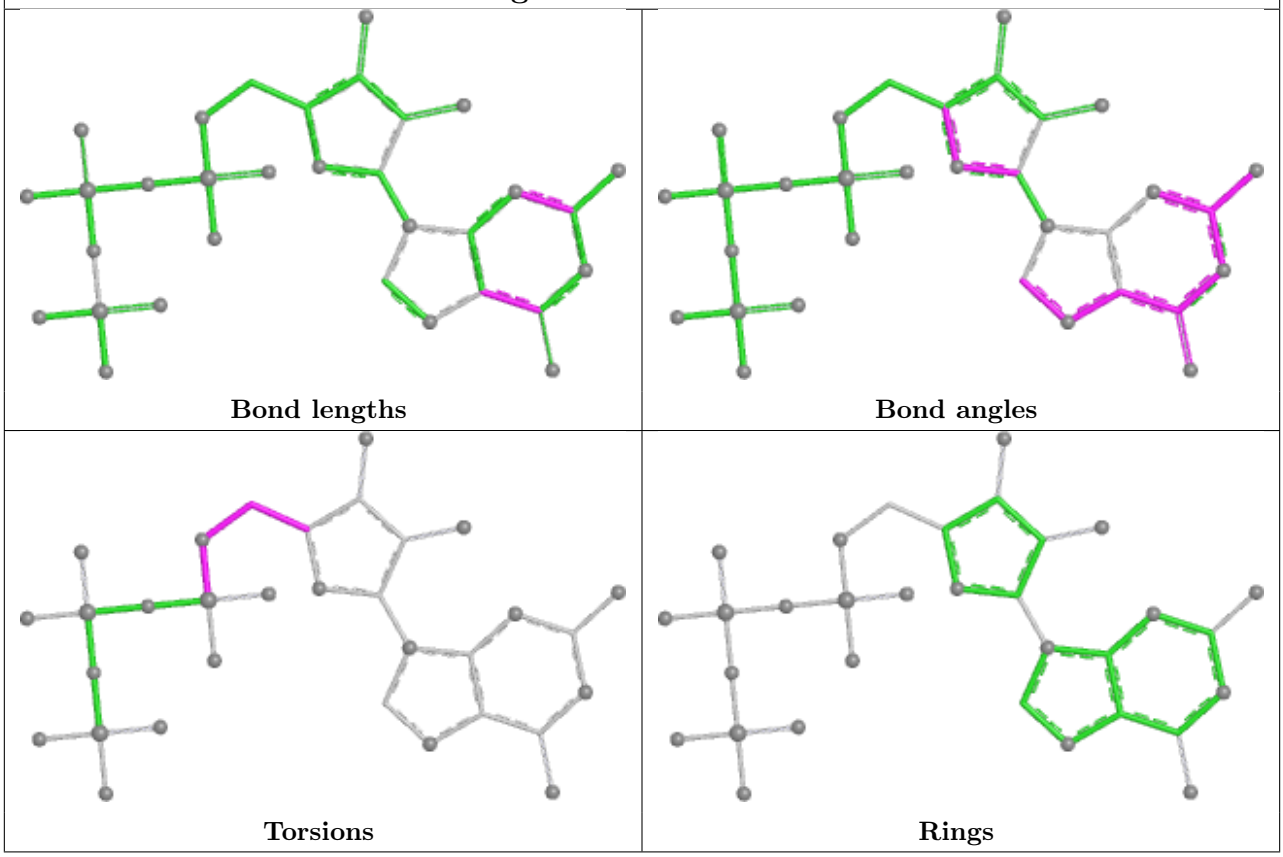

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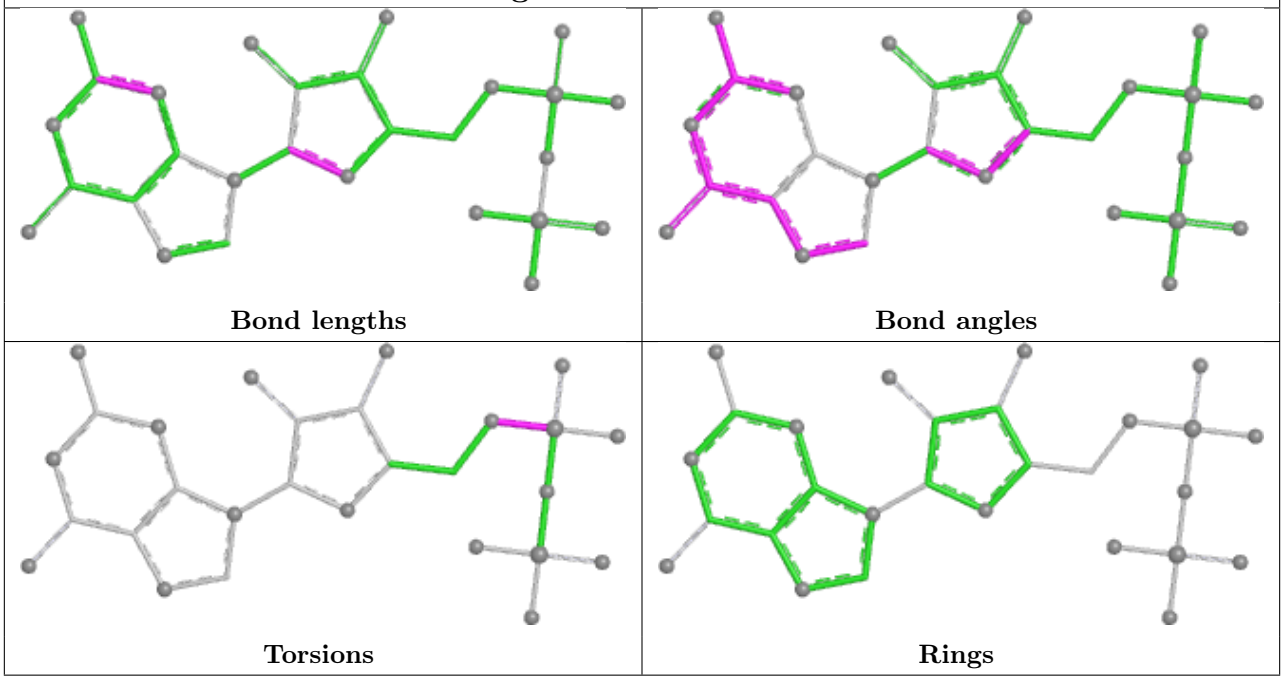


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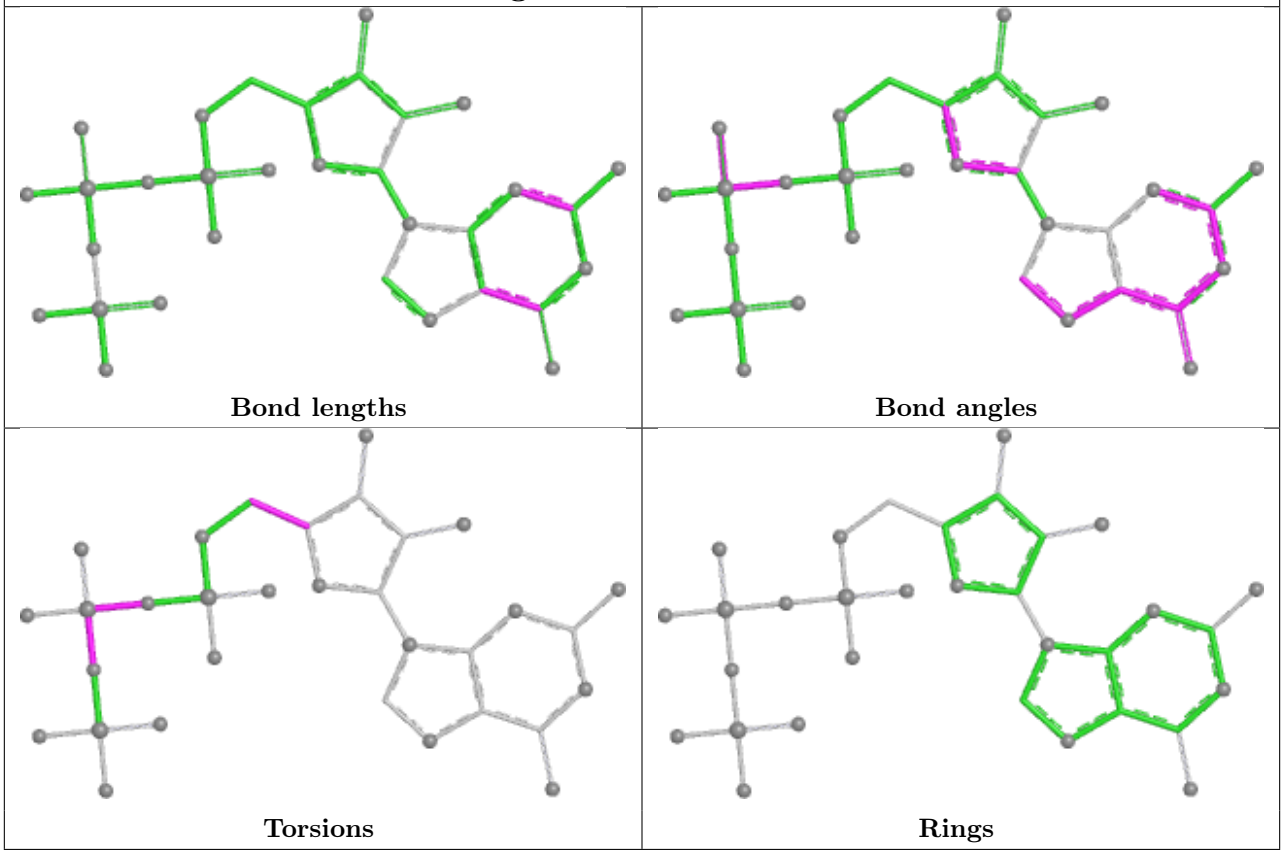

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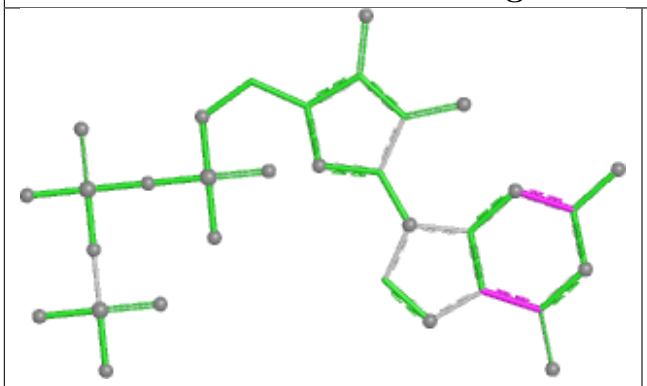

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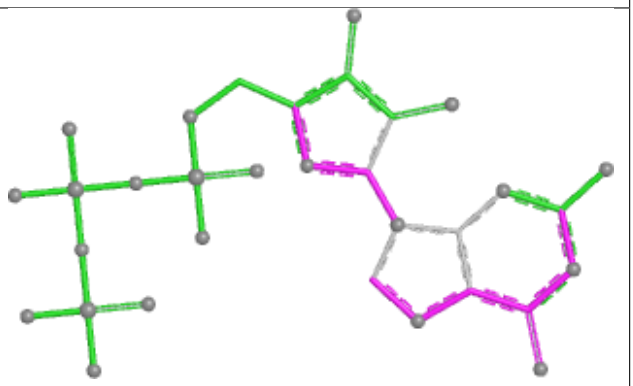
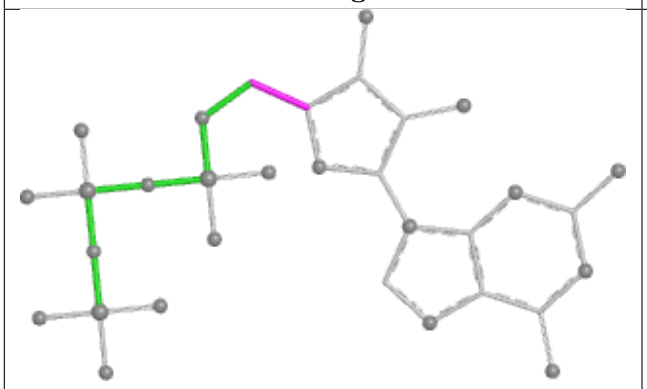
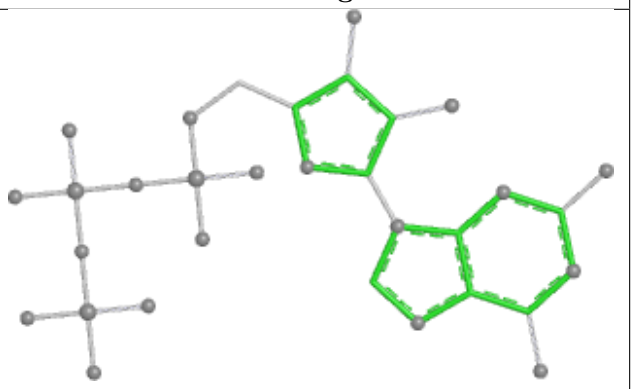


Bond angles



Torsions



Rings

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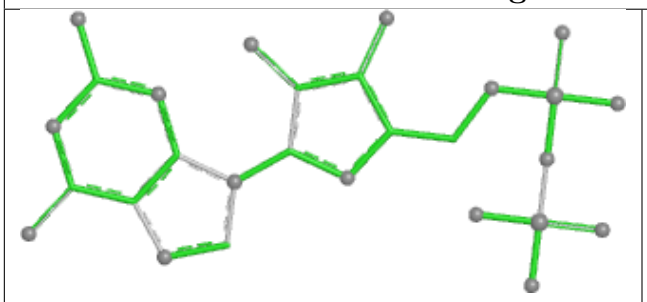

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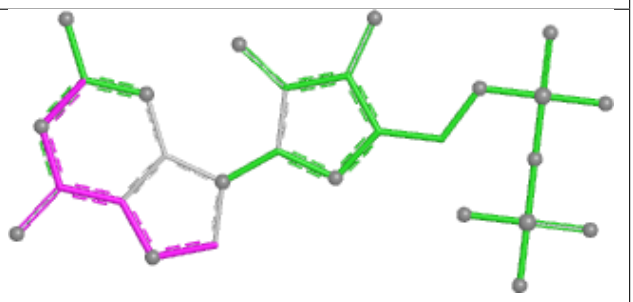

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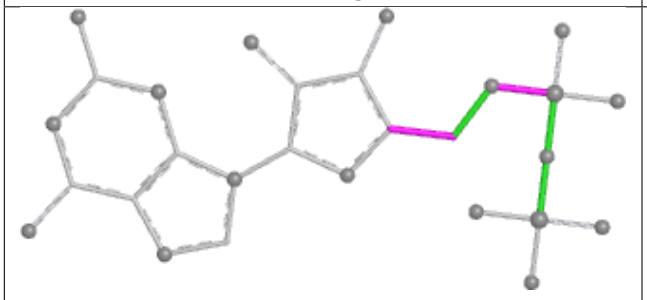

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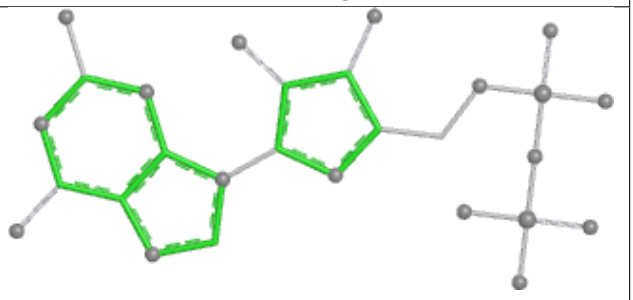

Rings

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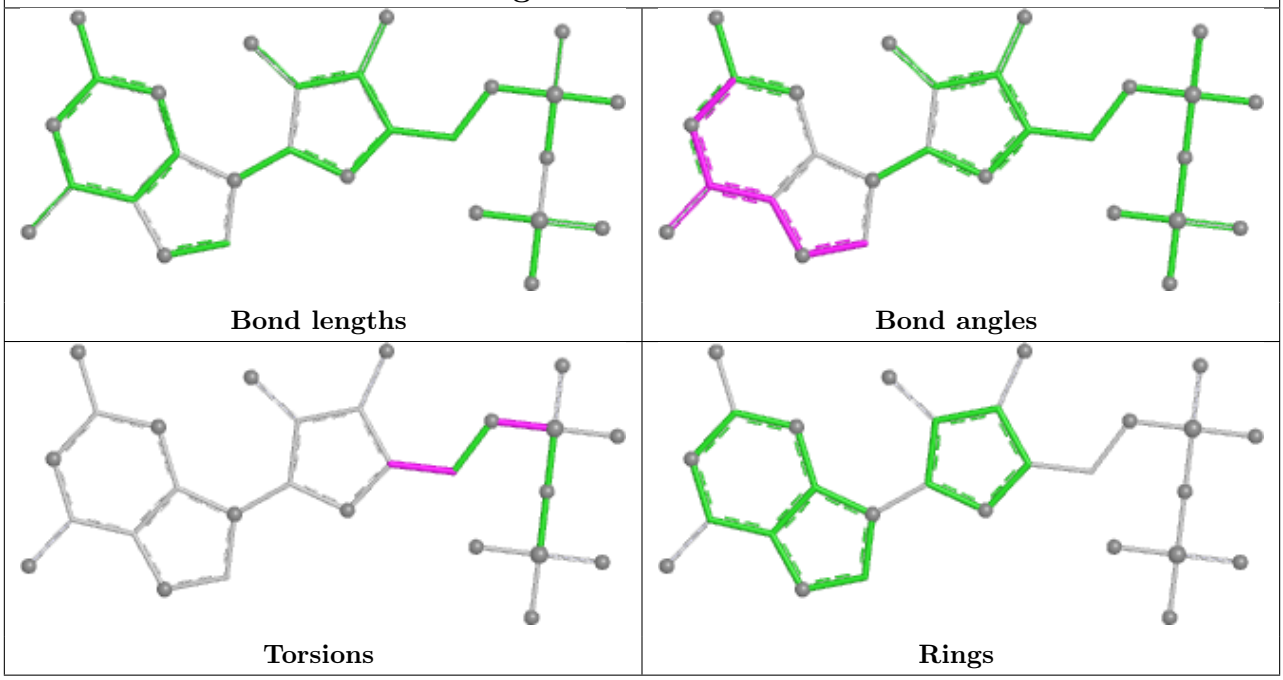


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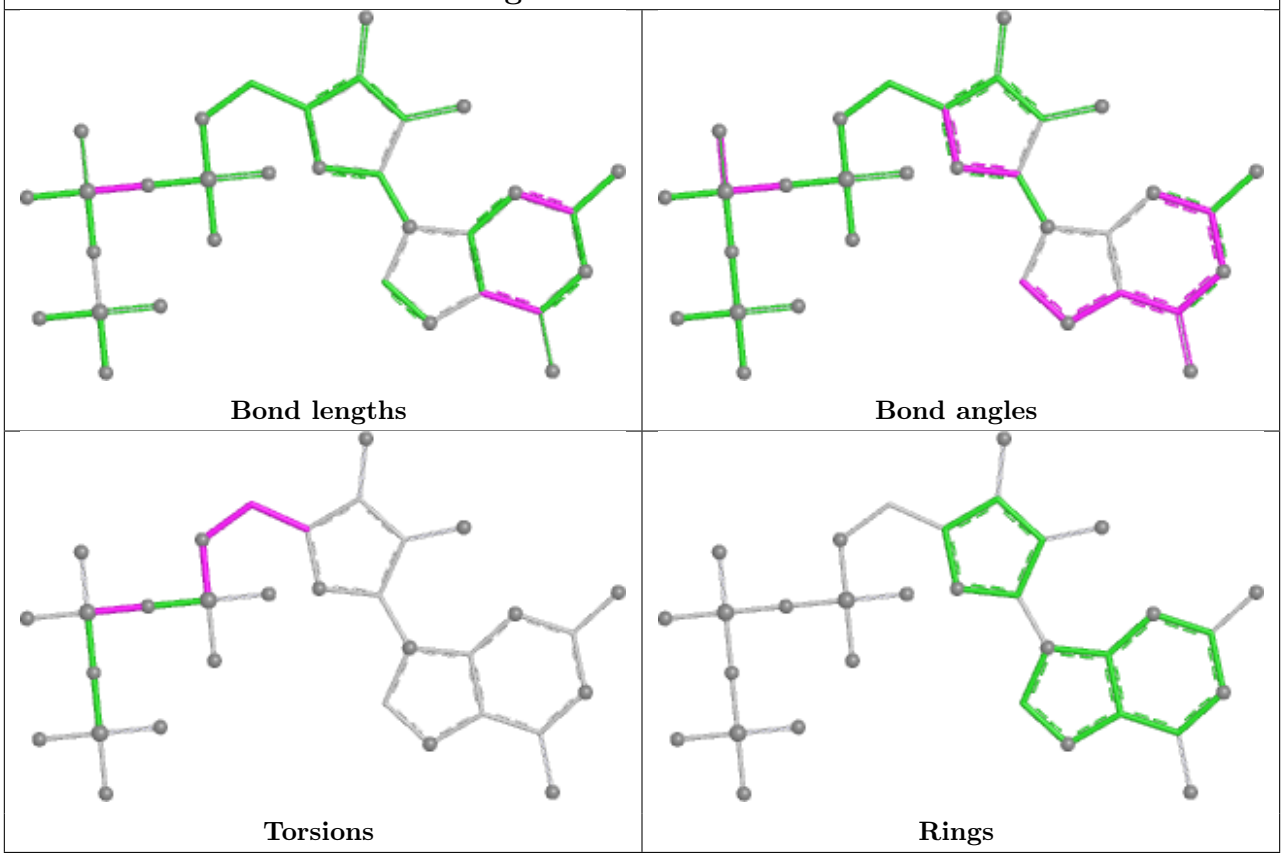

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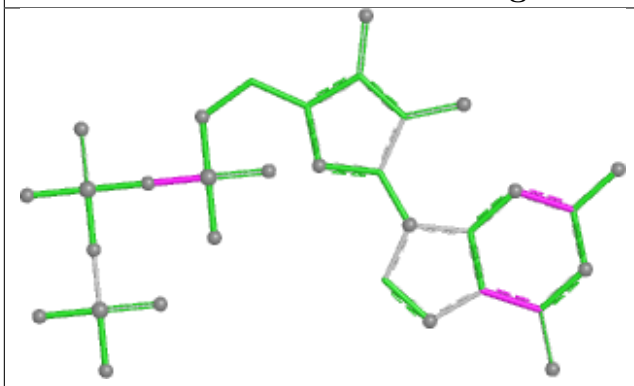

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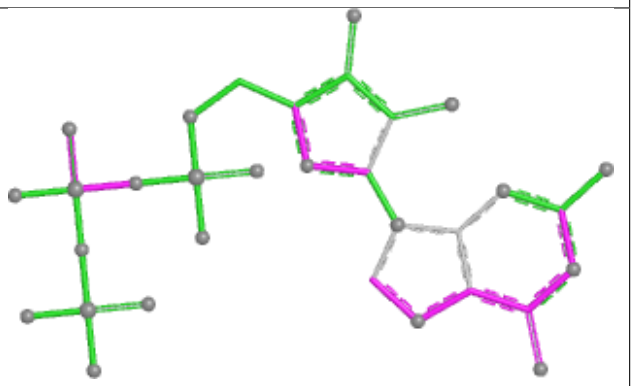

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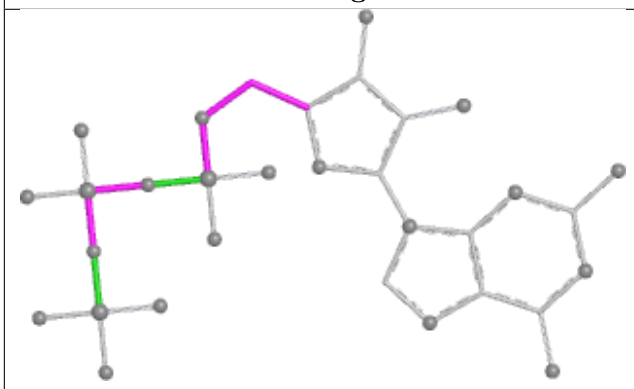

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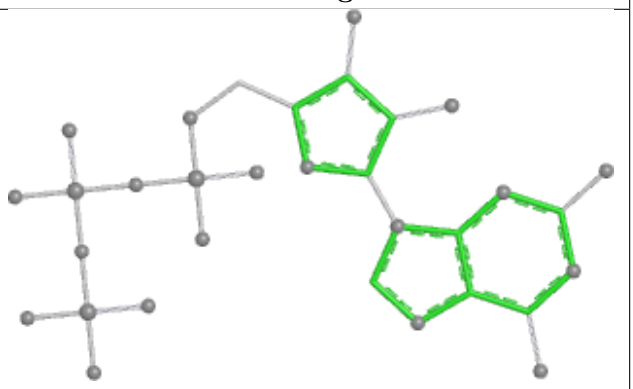
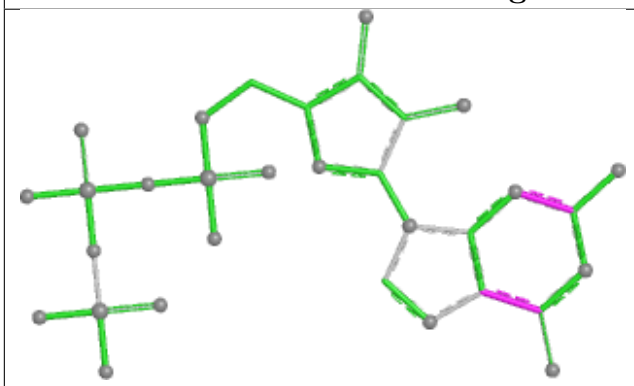


Rings

## Ligand GTP VN 501



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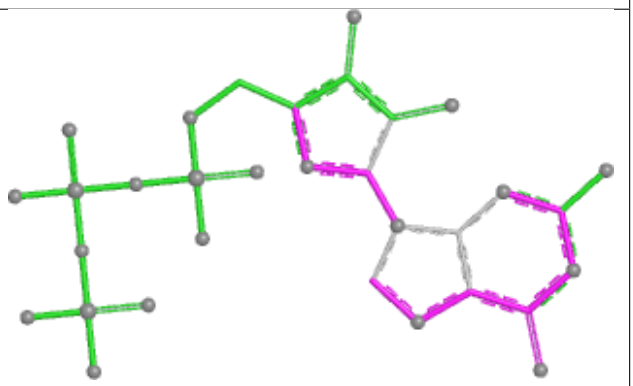

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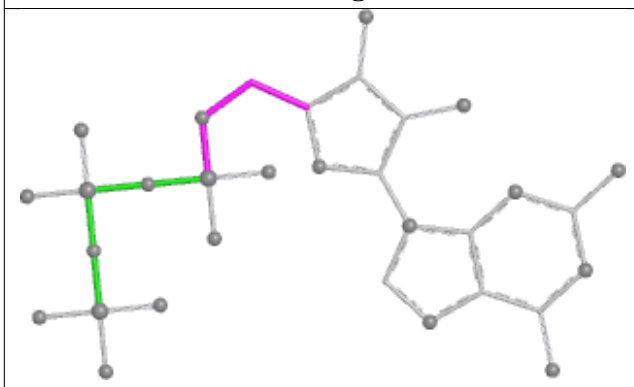

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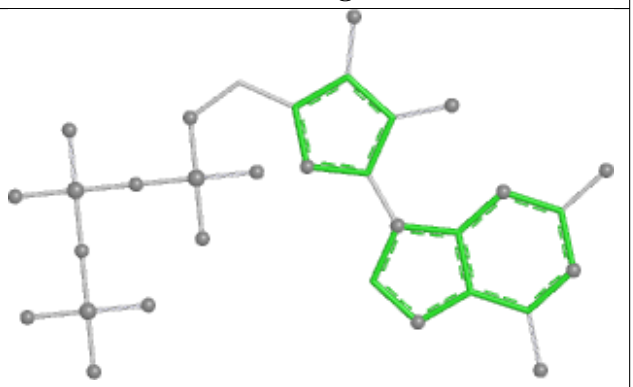
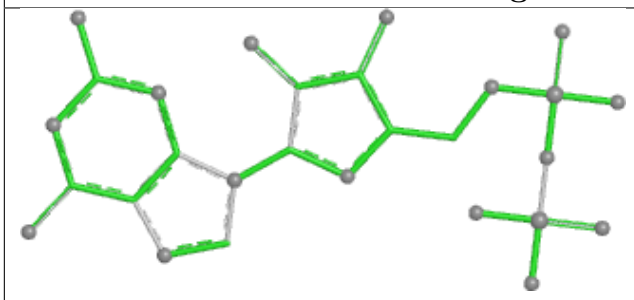


Rings

## Ligand GDP EO 501



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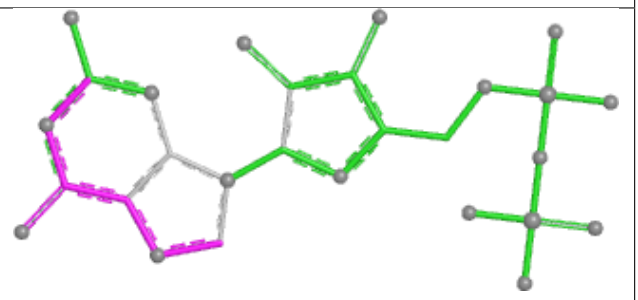

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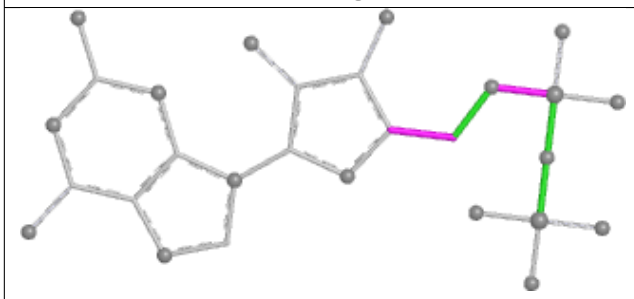

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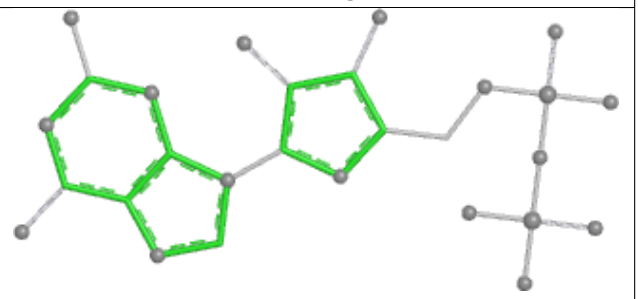
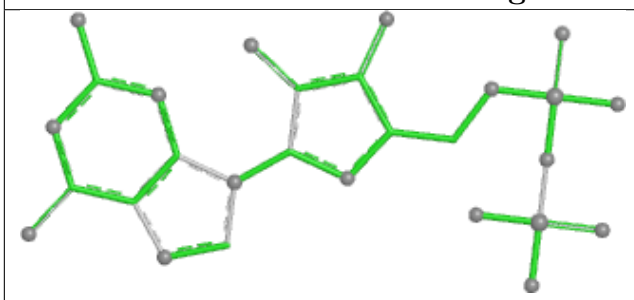


Rings

## Ligand GDP QO 502



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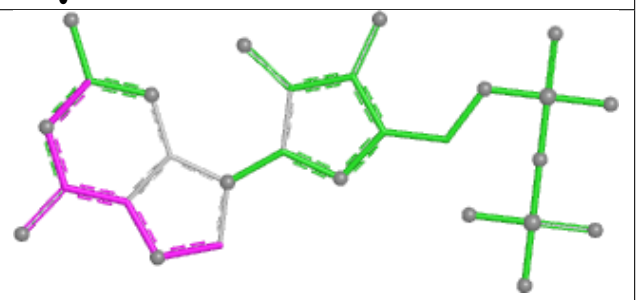
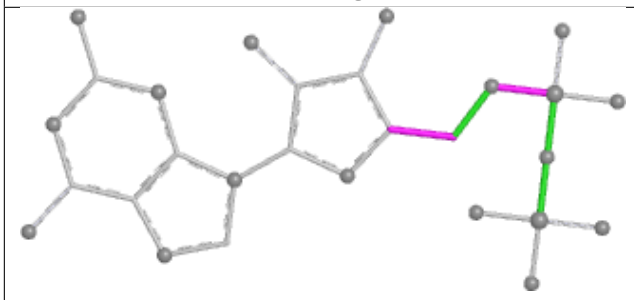


Bond angles



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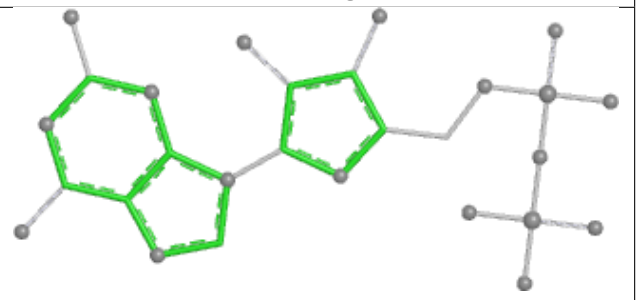
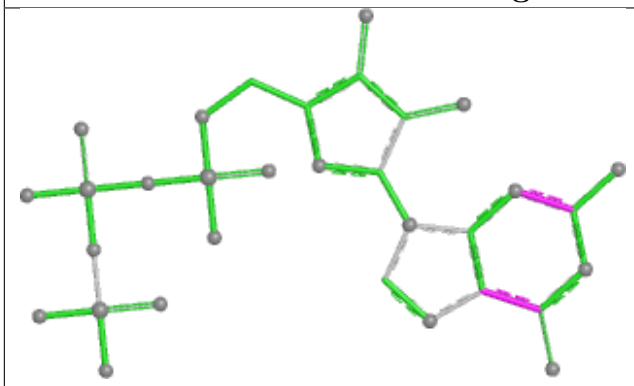


Rings

## Ligand GTP OL 501



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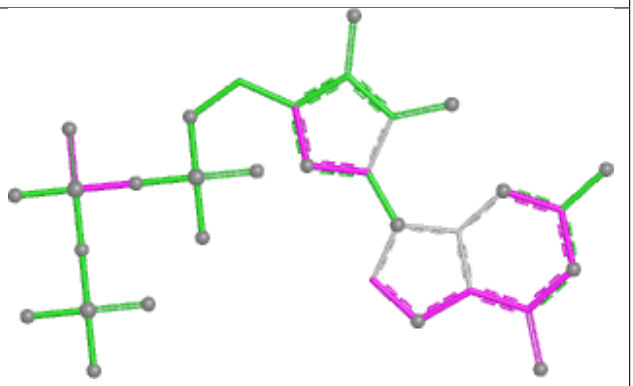

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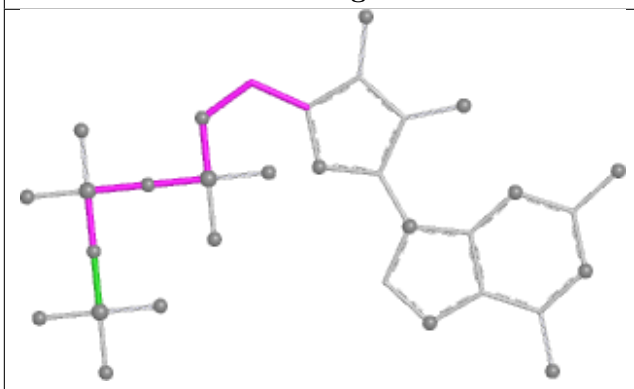

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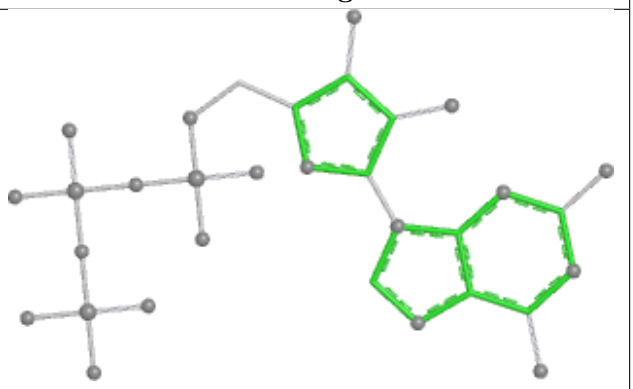

Rings

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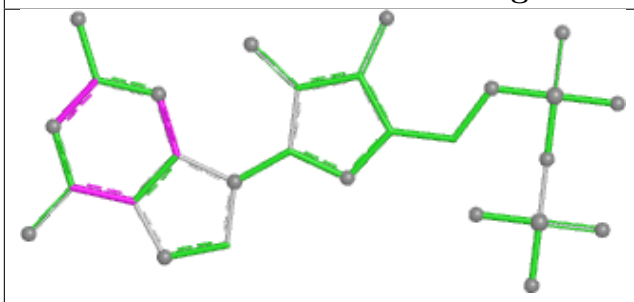

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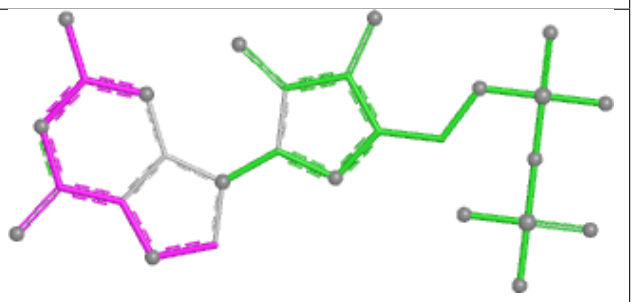

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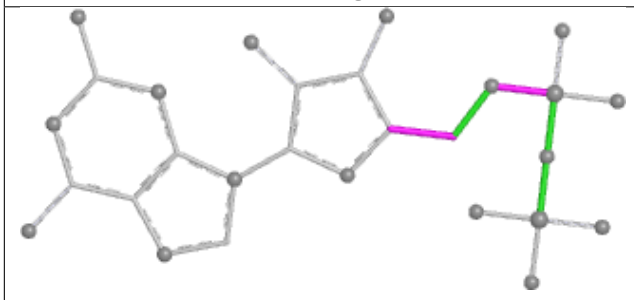

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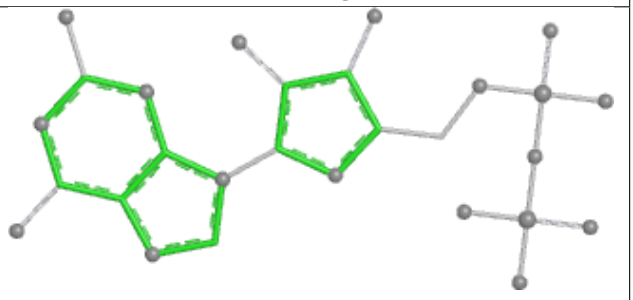

Rings

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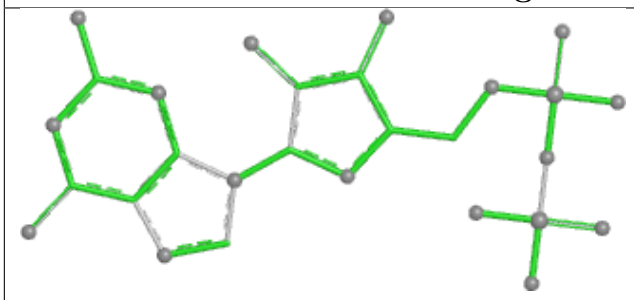

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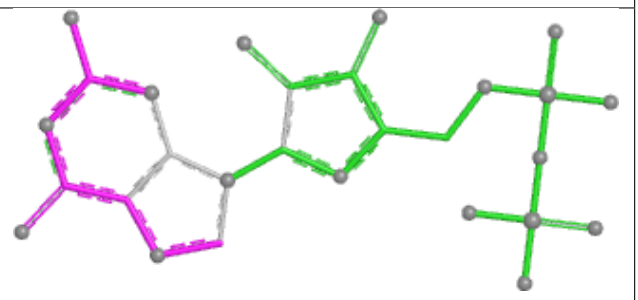

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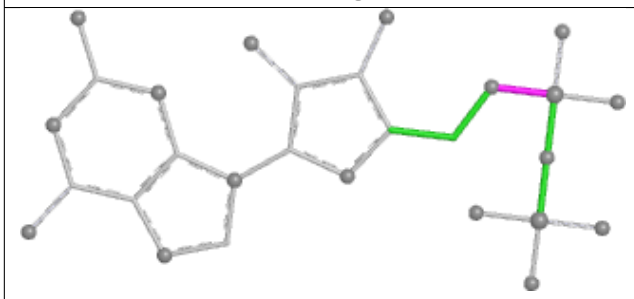

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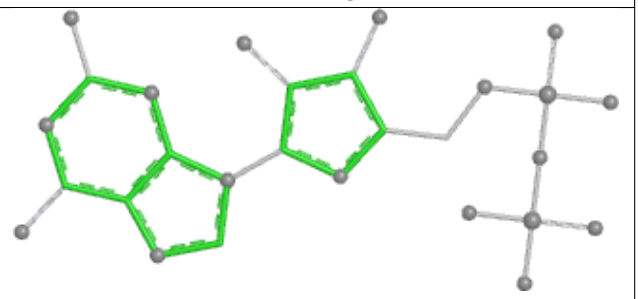

Rings

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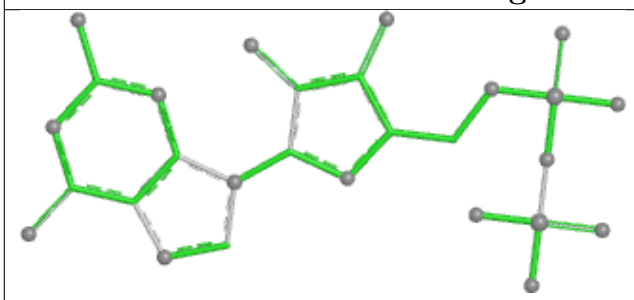

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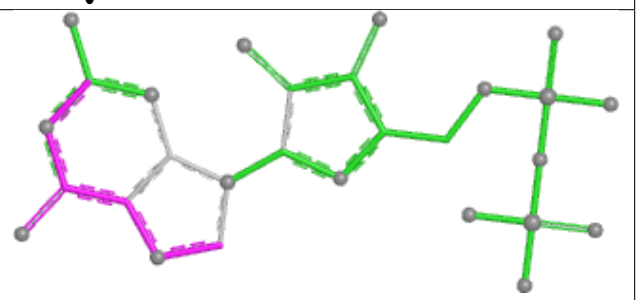

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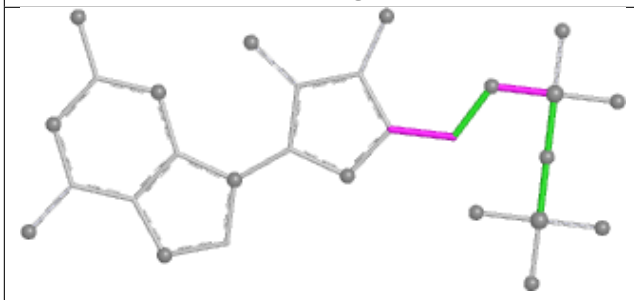

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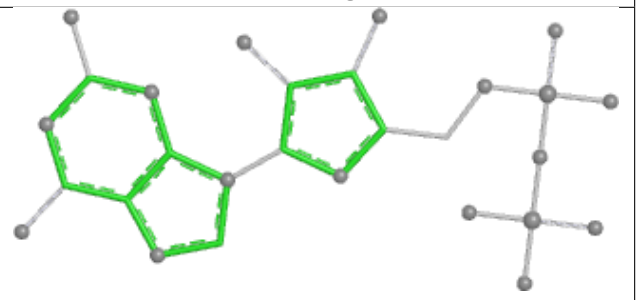
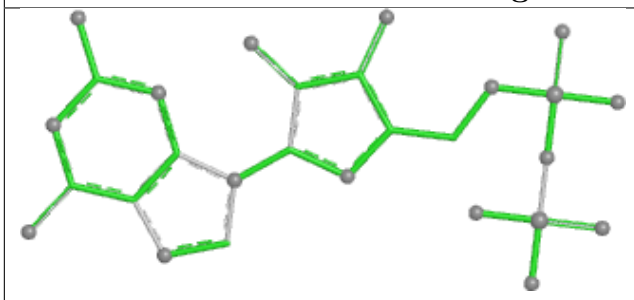


Rings

## Ligand GDP FB 501



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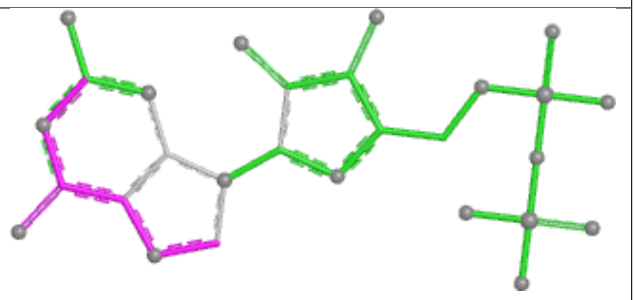

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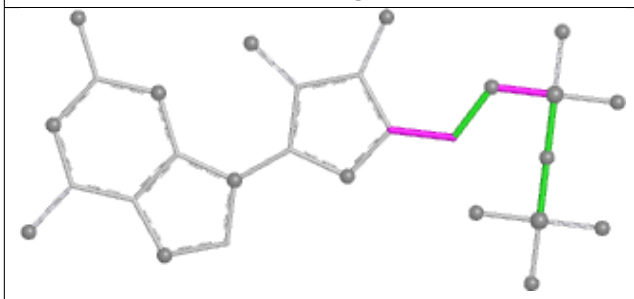

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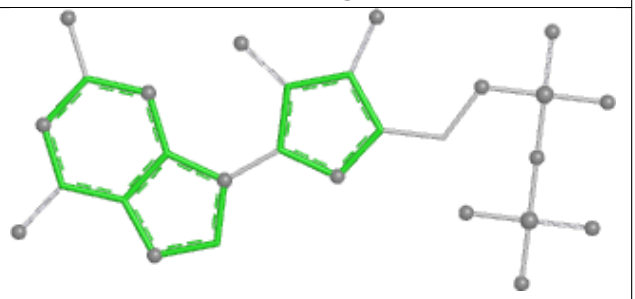
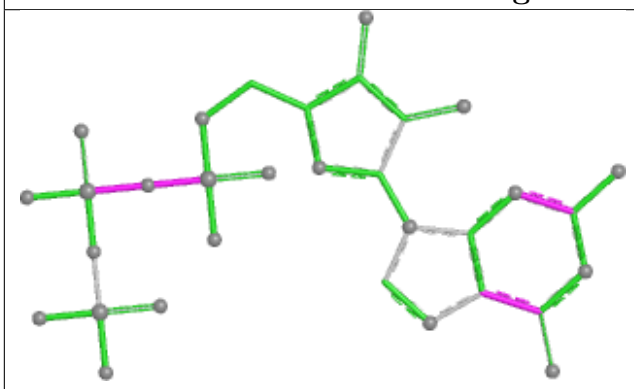


Rings

## Ligand GTP SN 501



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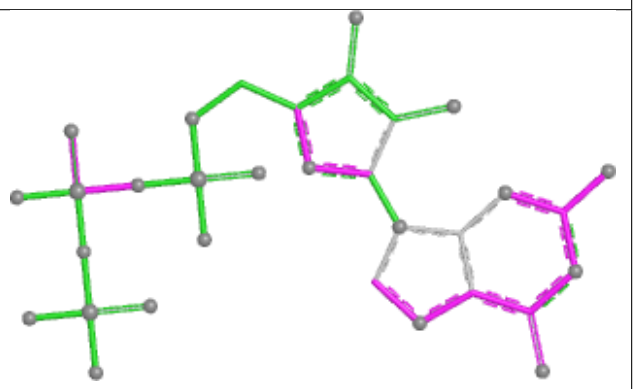

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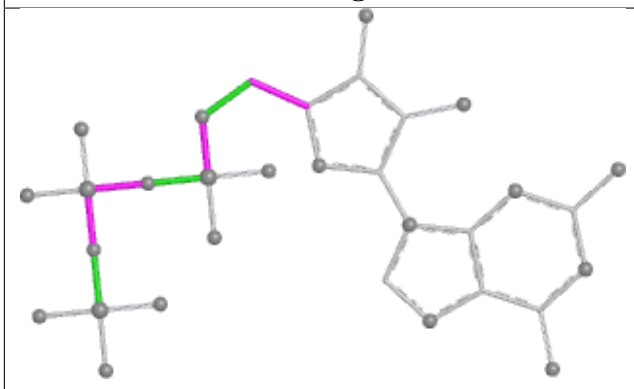

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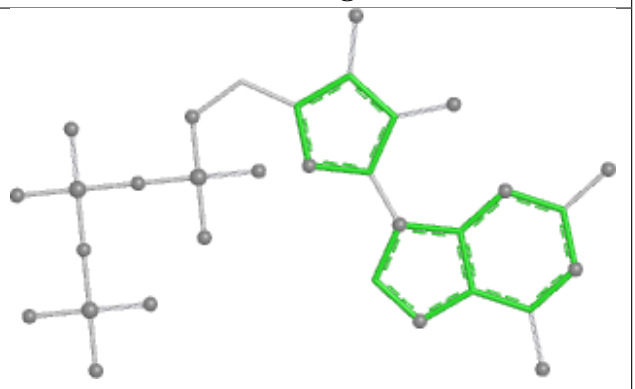

Rings

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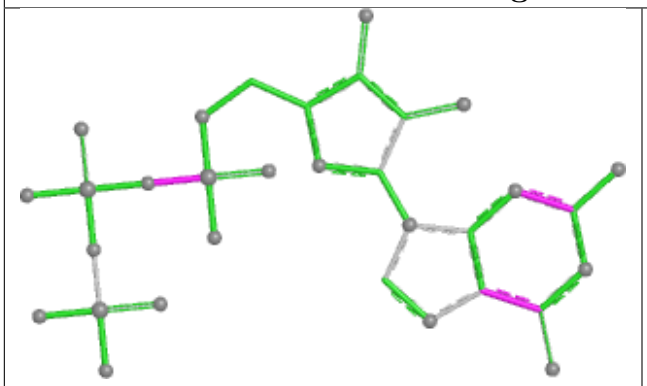

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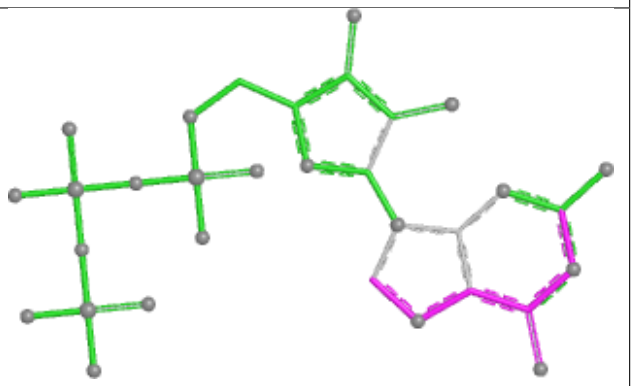

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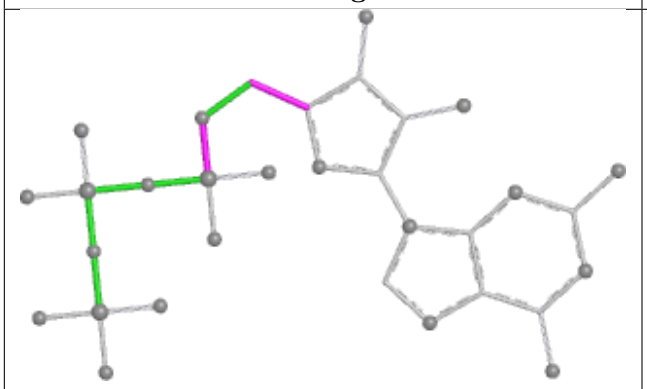

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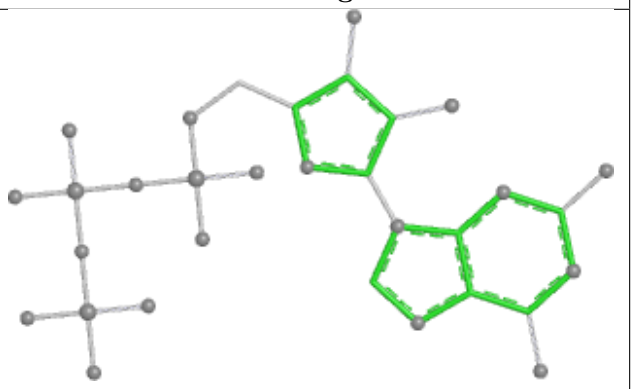
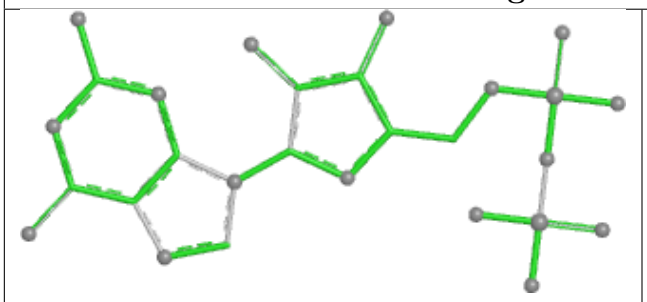


Rings

## Ligand GDP GO 501



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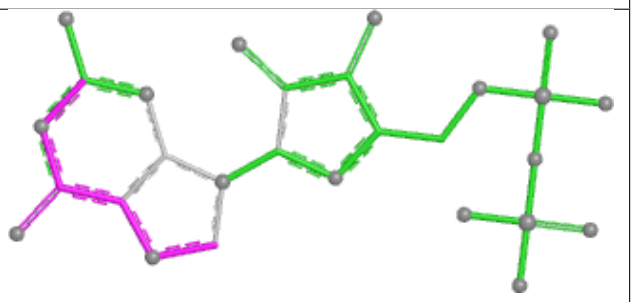

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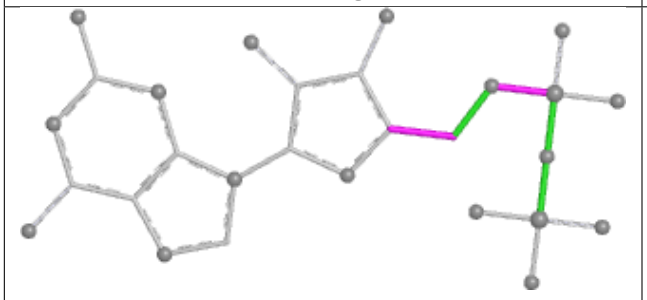

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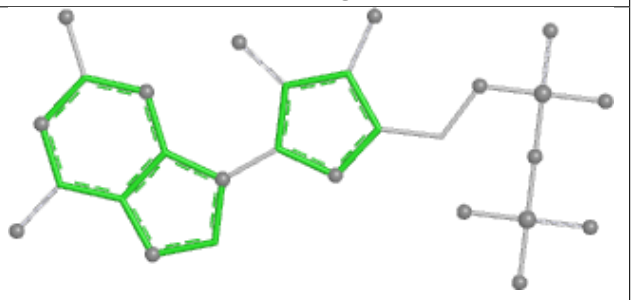
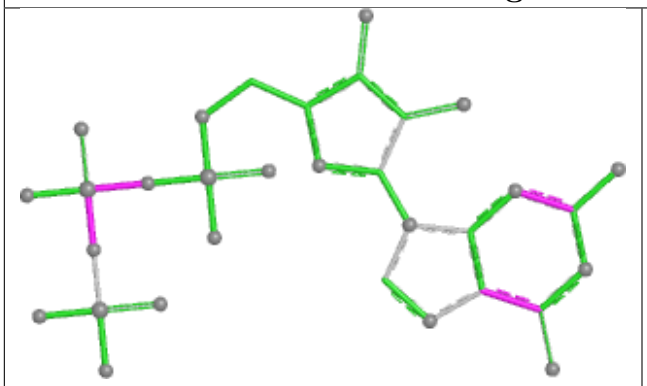


Rings

## Ligand GTP MN 501



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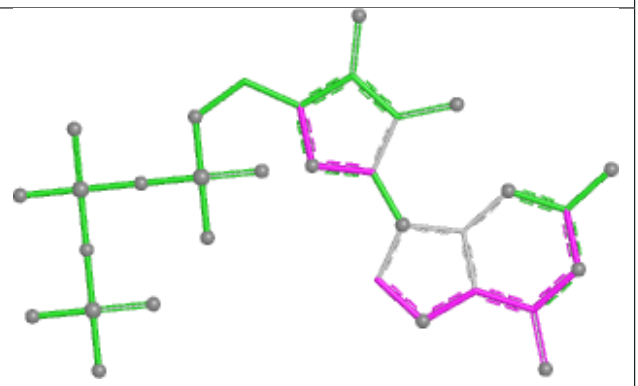

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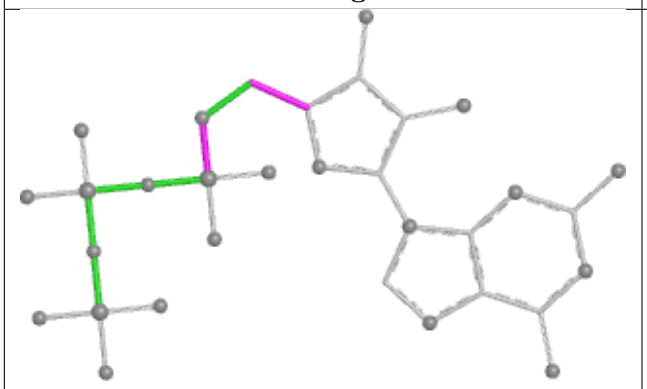

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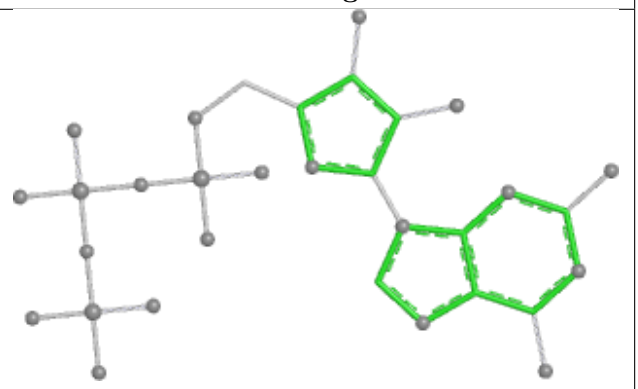

Rings

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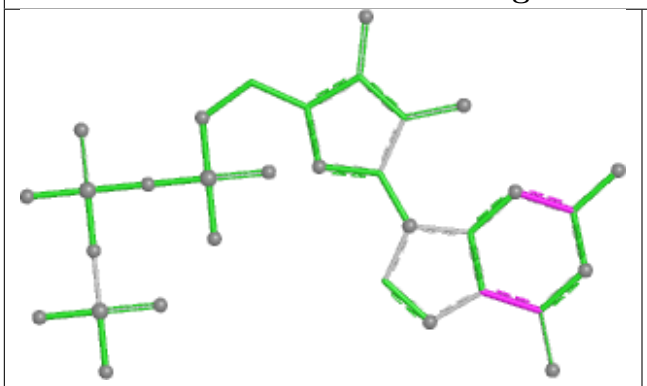

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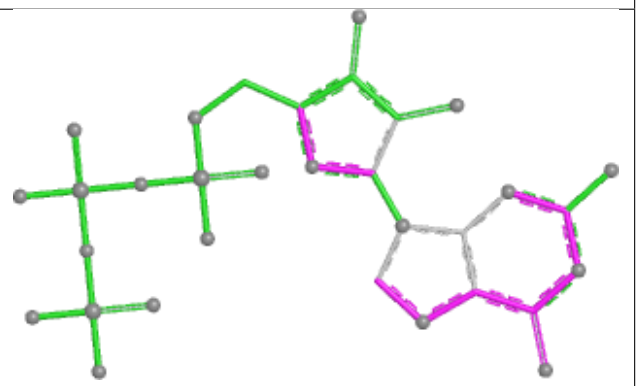

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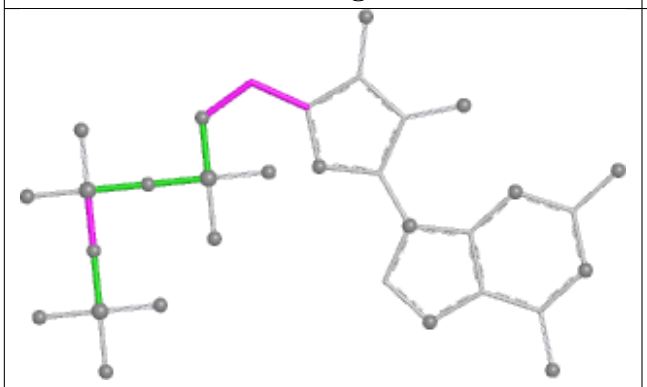

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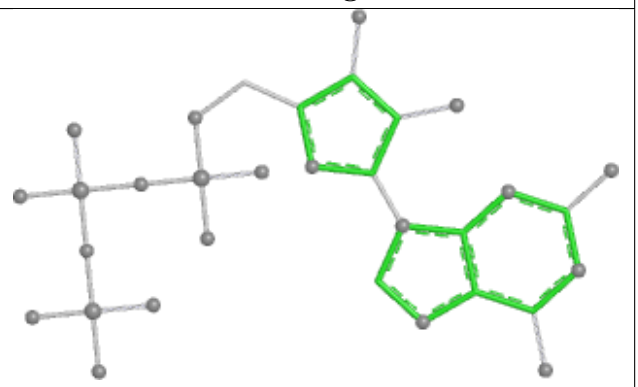
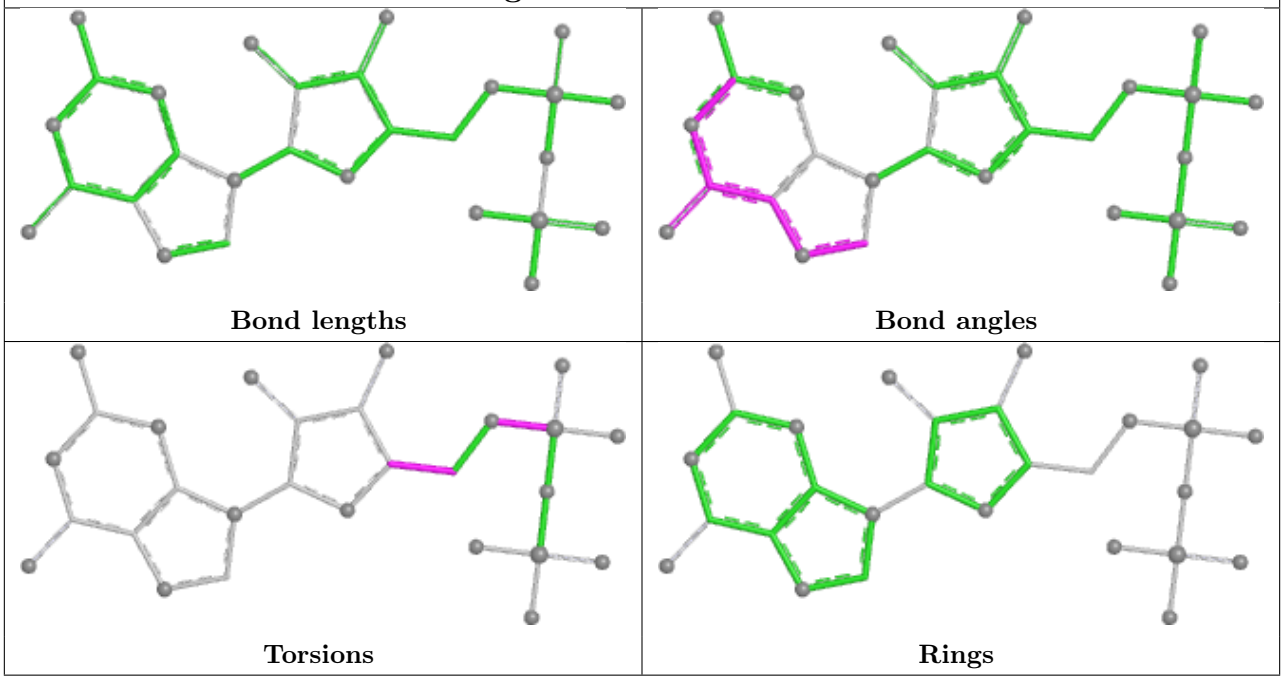


Rings

## Ligand GDP HM 502

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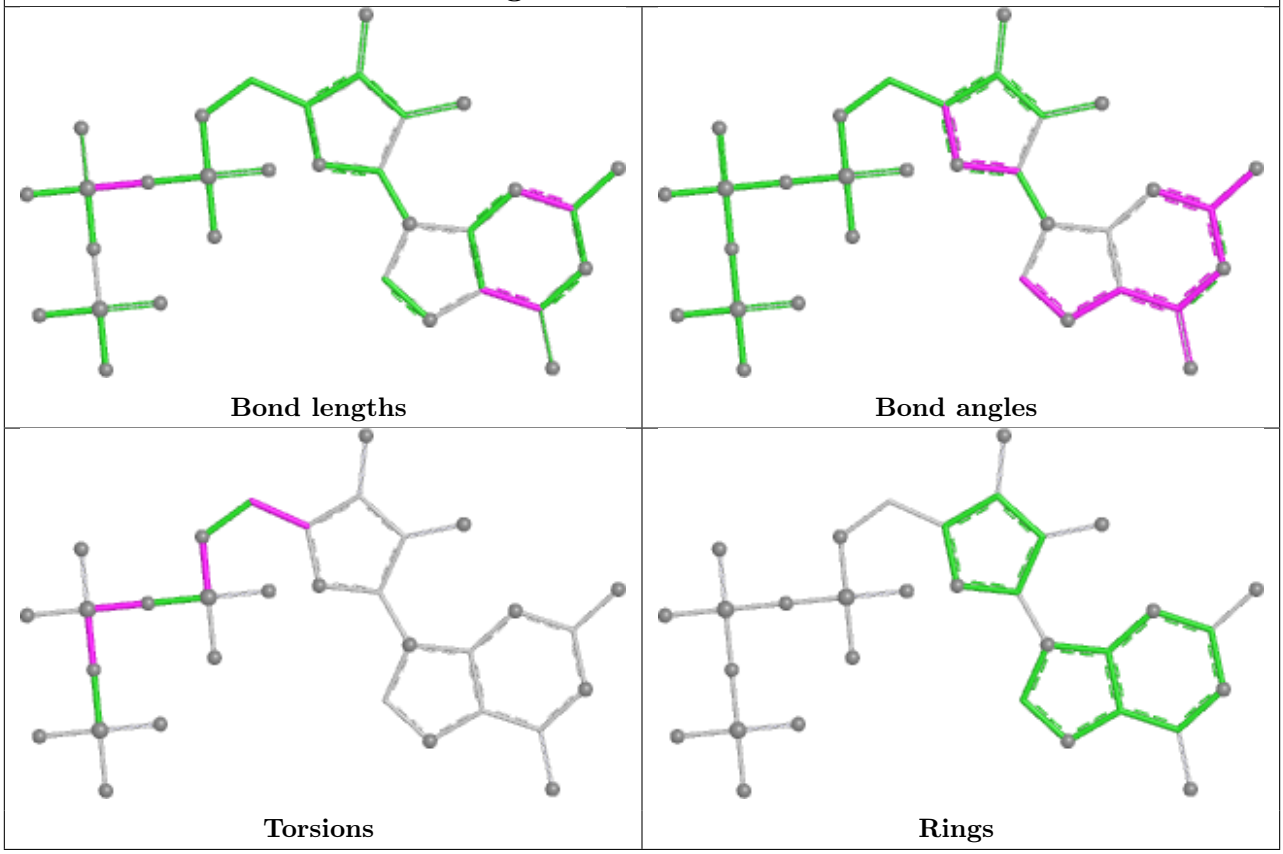

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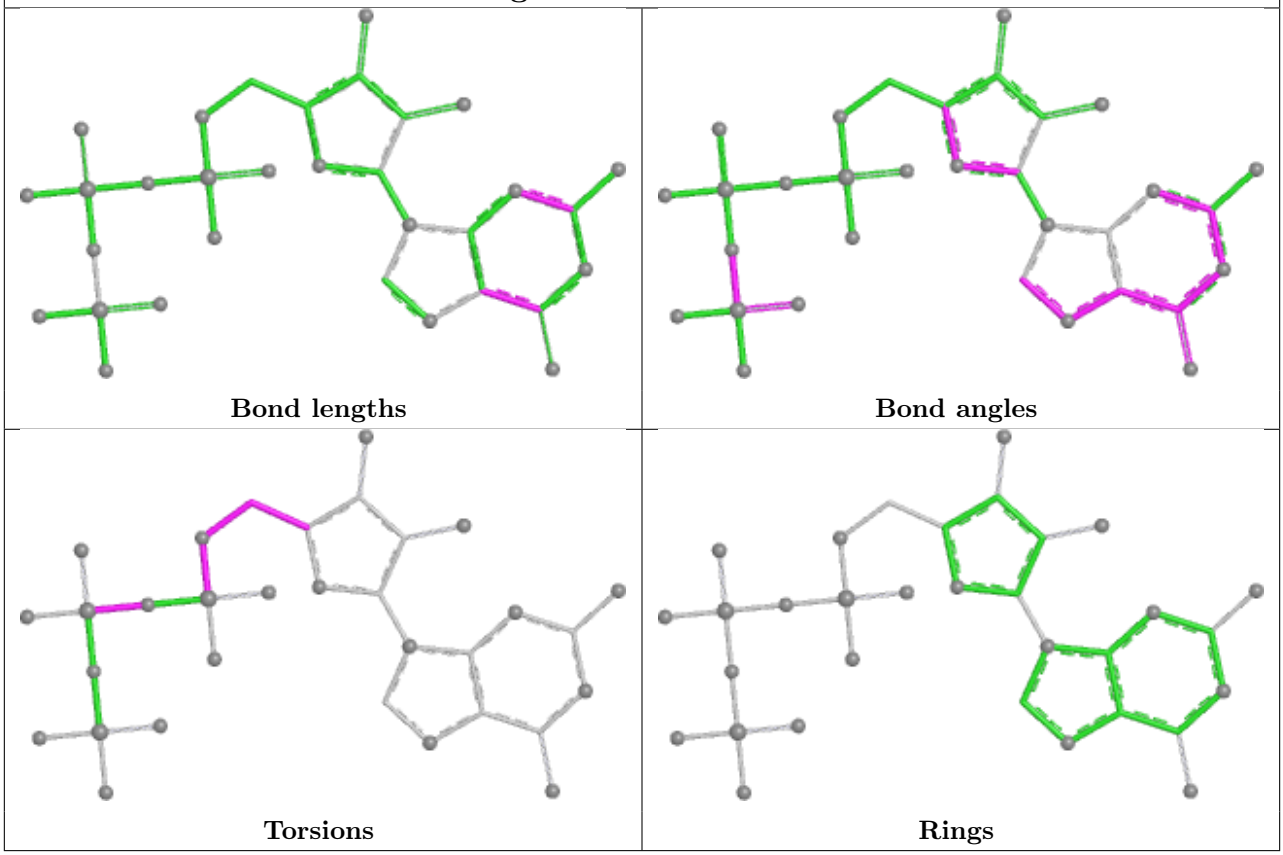


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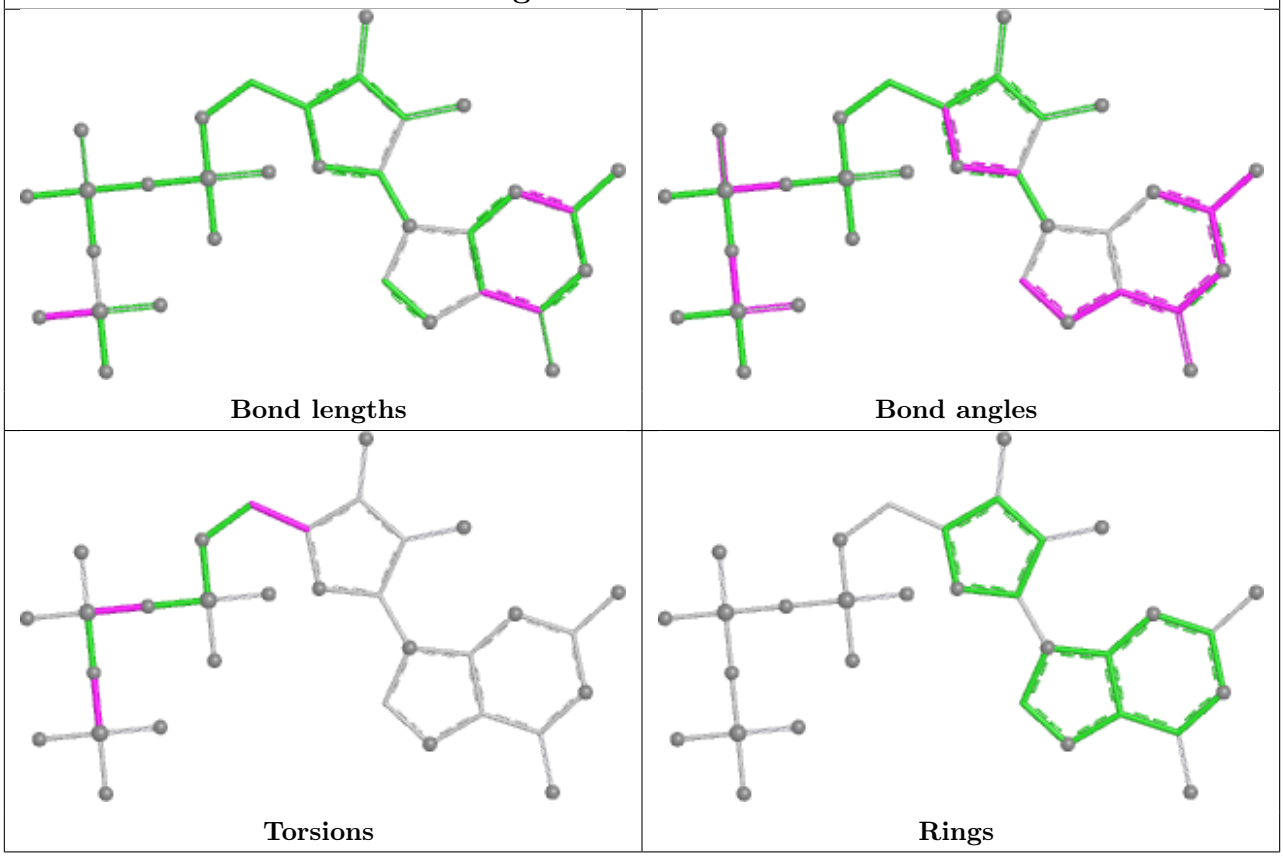

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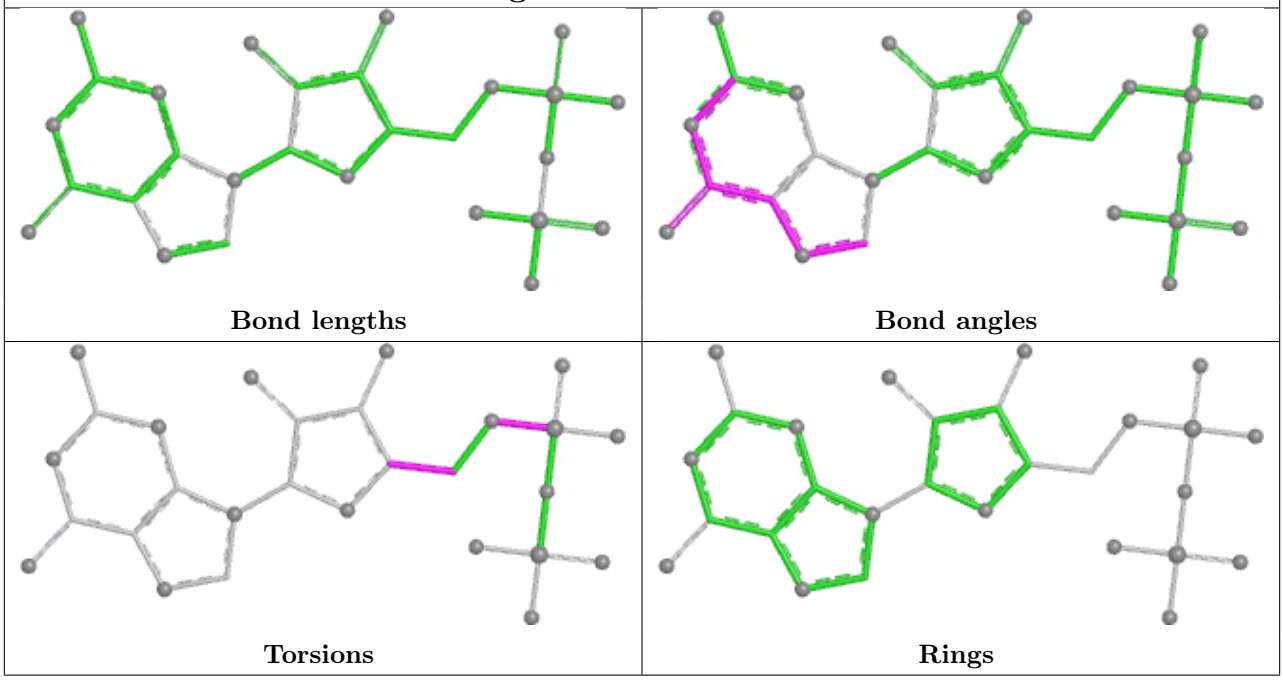


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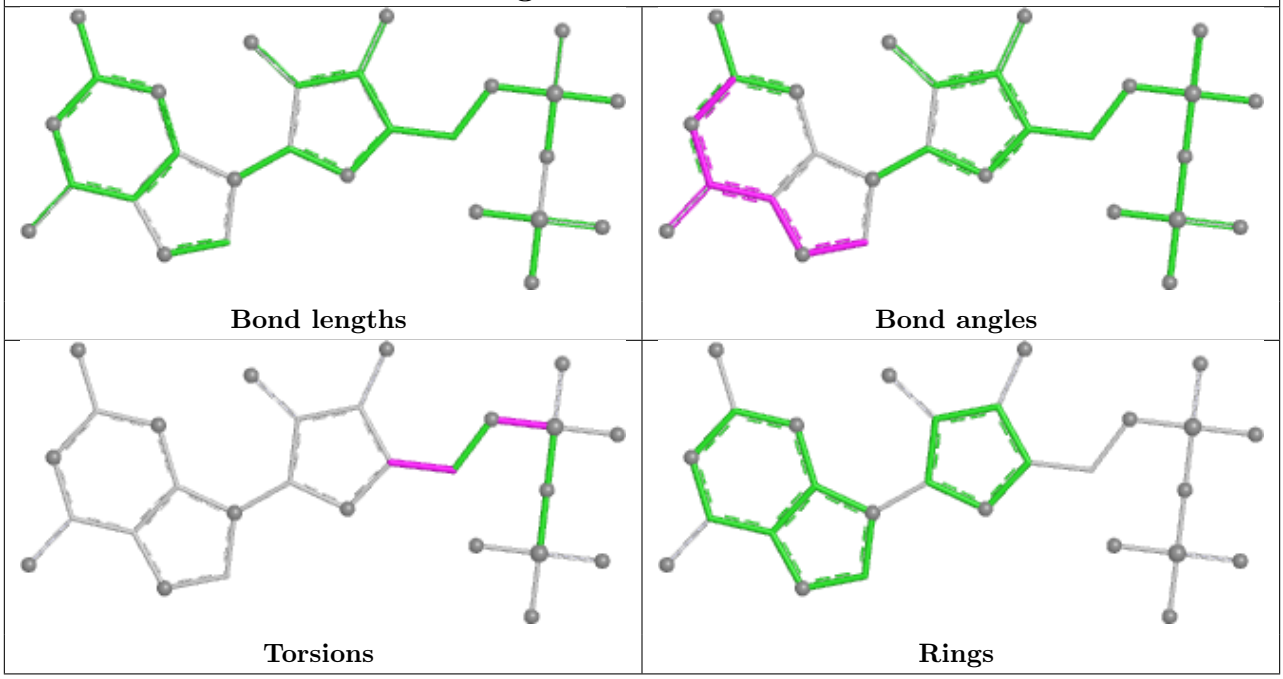

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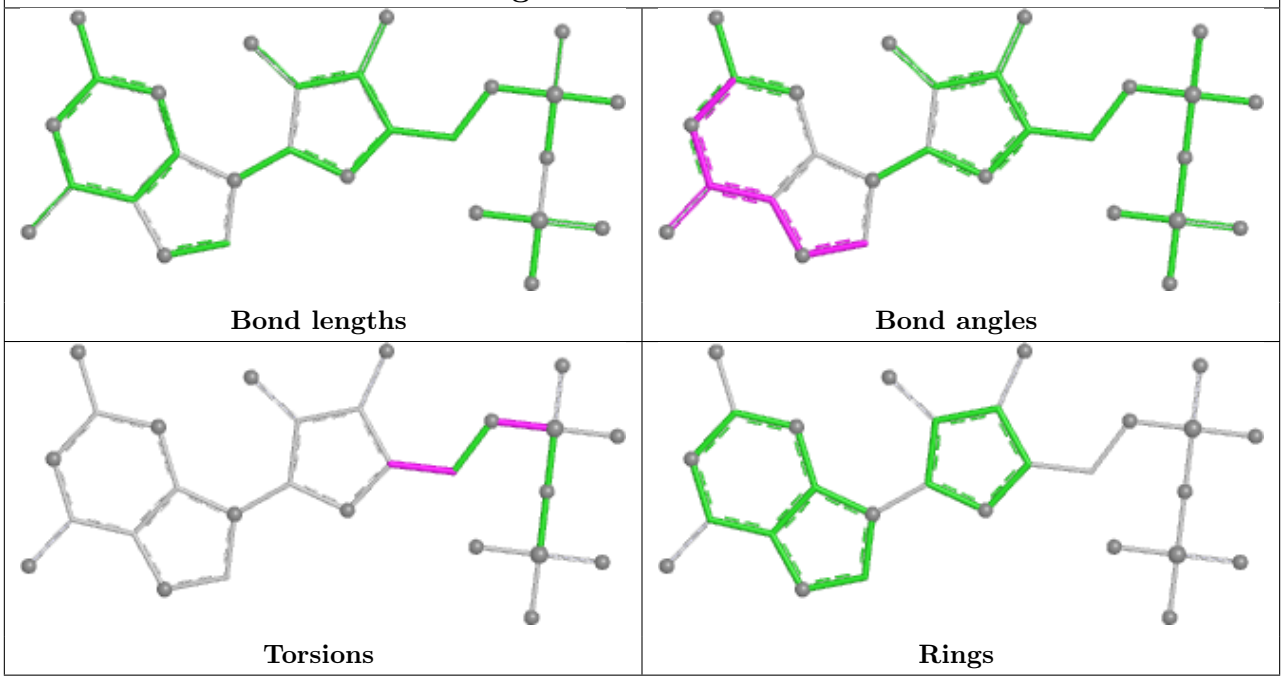


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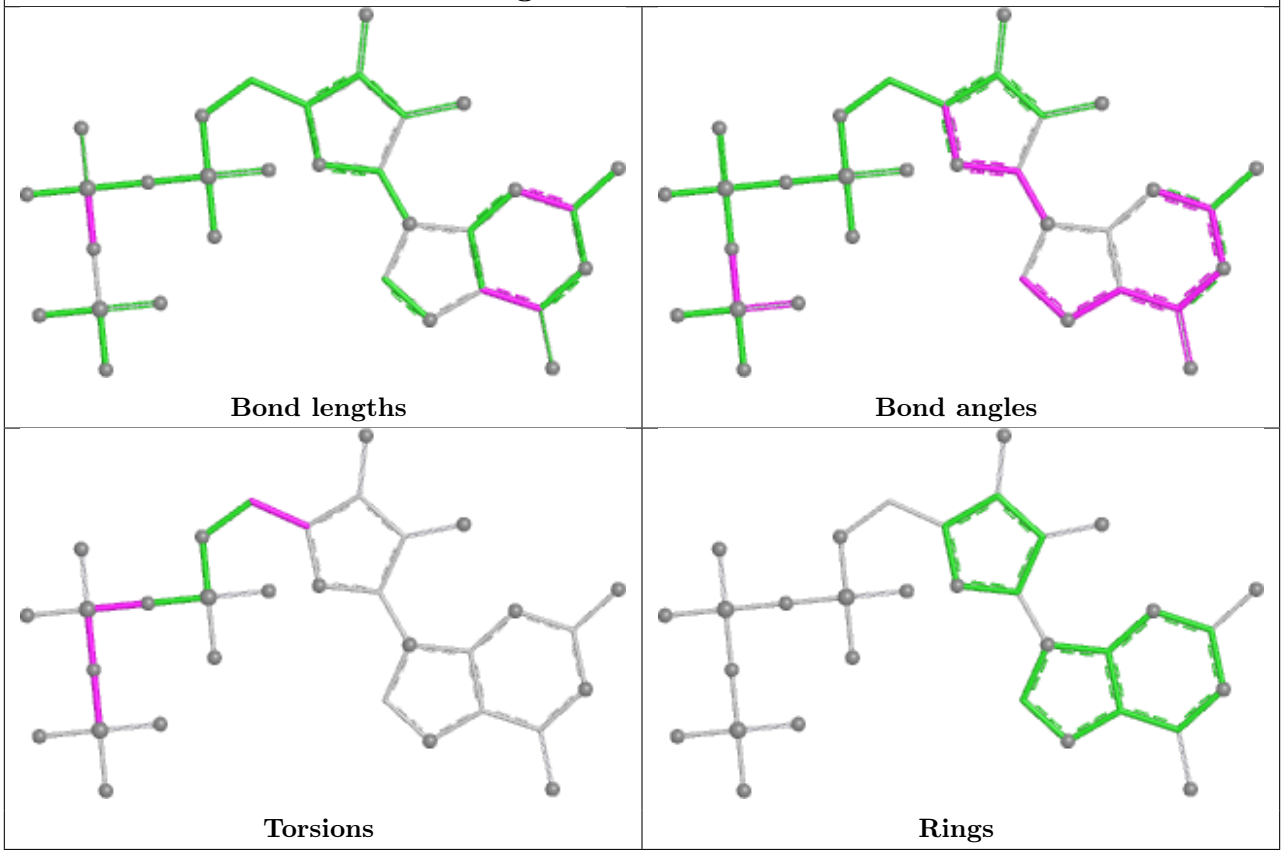

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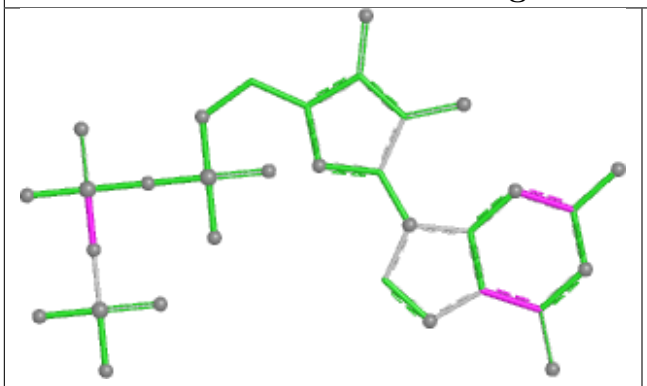
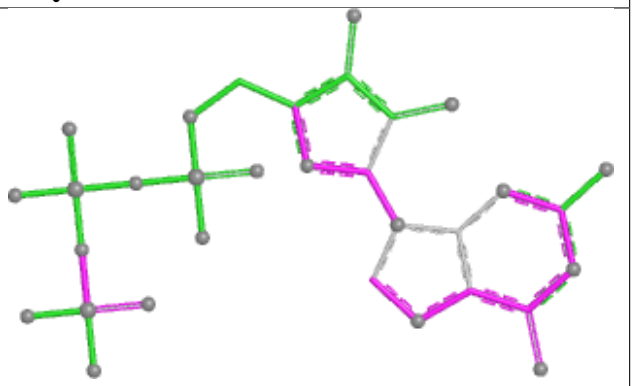
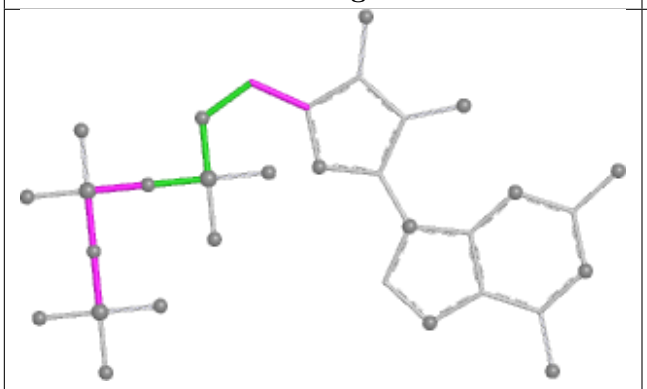


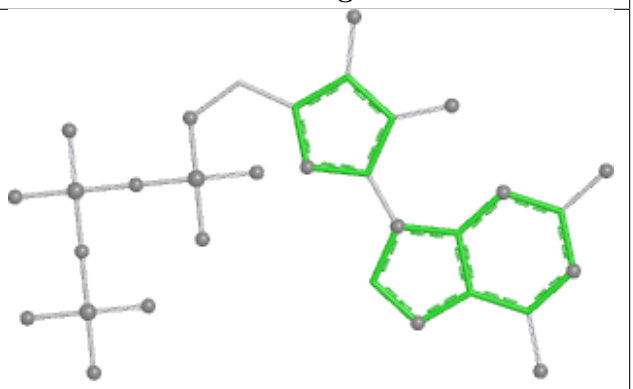
Bond lengths



Bond angles

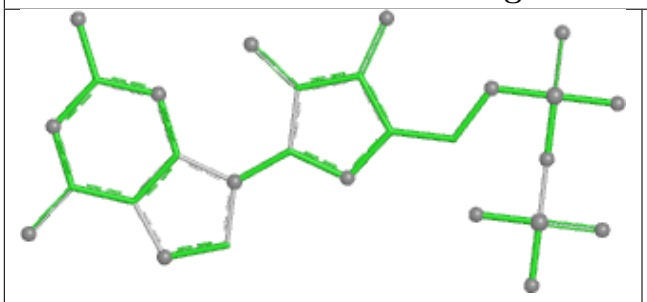


Torsions



Rings

## Ligand GDP MN 502



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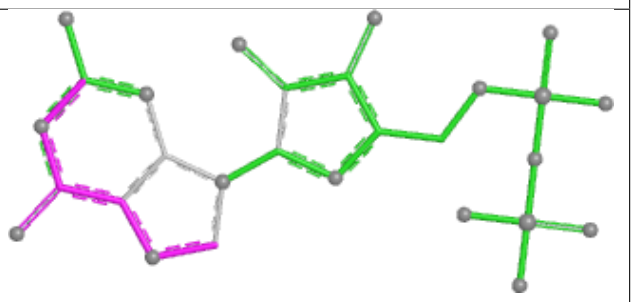

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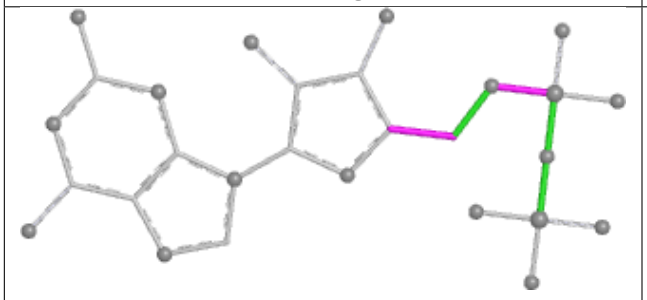
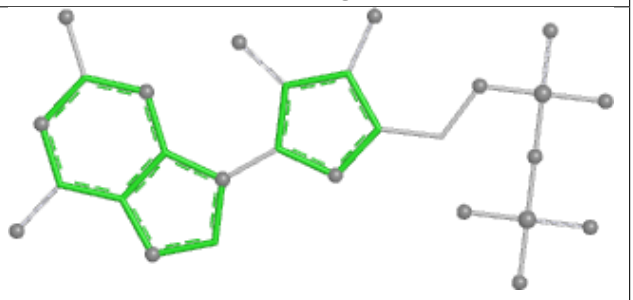
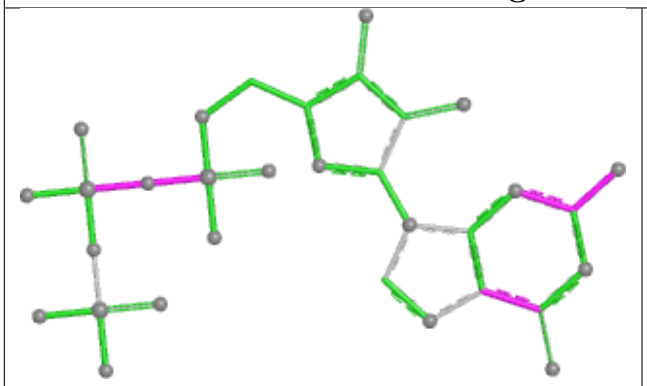


Torsions



Rings

## Ligand GTP DH 501



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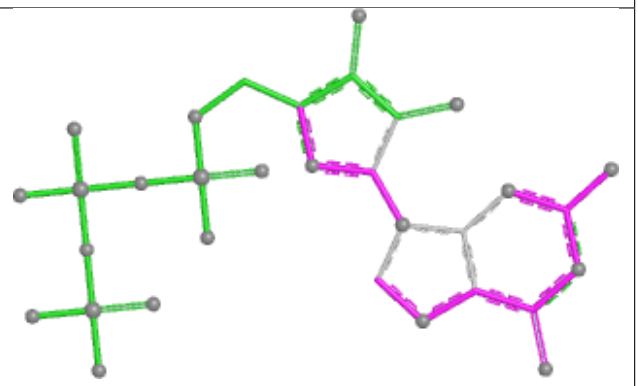

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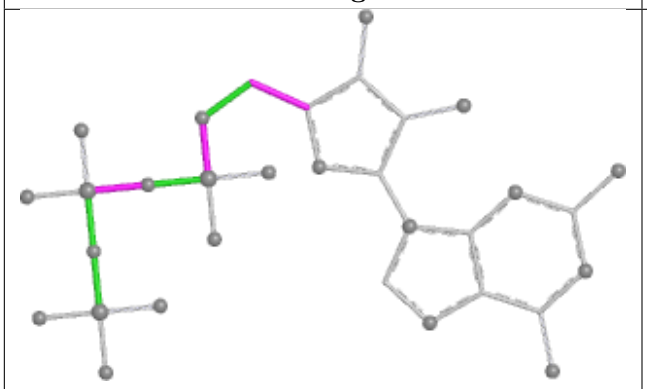

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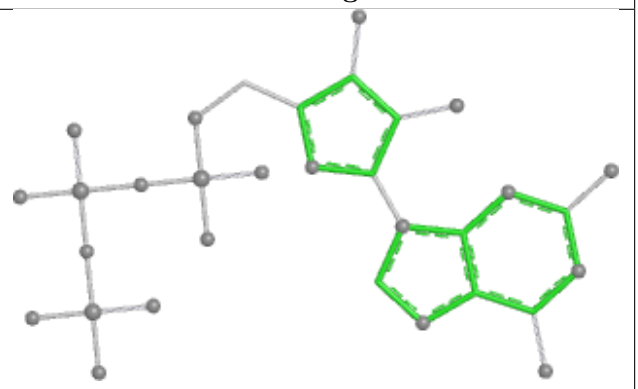
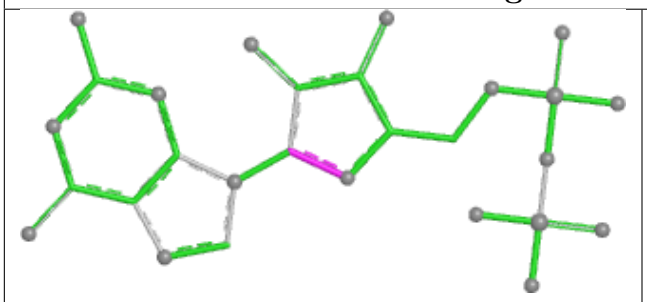


Rings

## Ligand GDP AM 501



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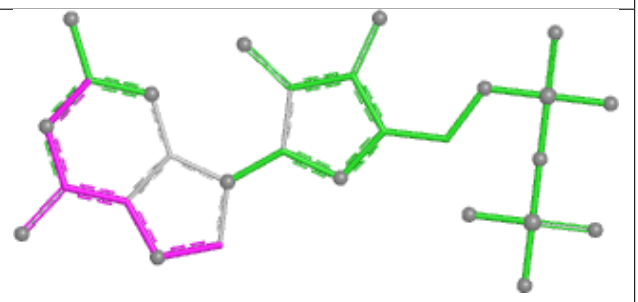

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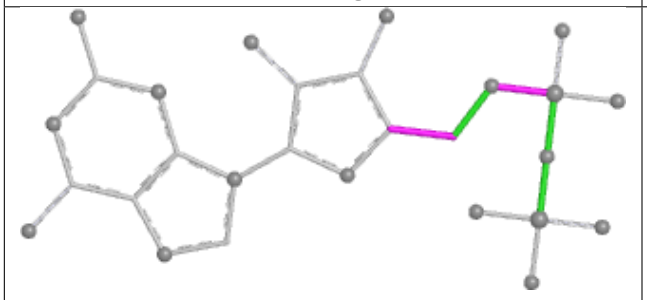

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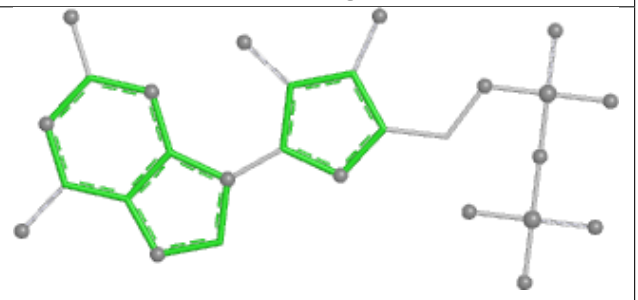
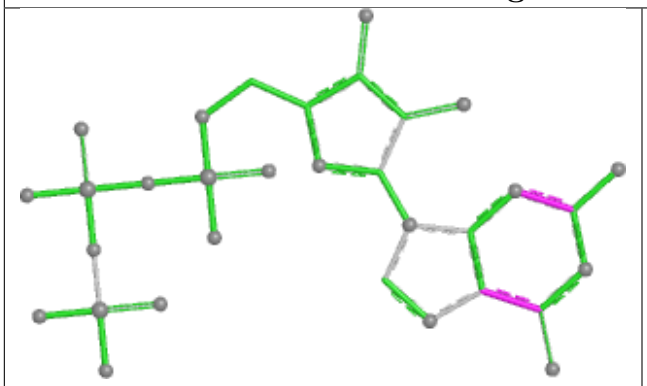


Rings

## Ligand GTP PM 501



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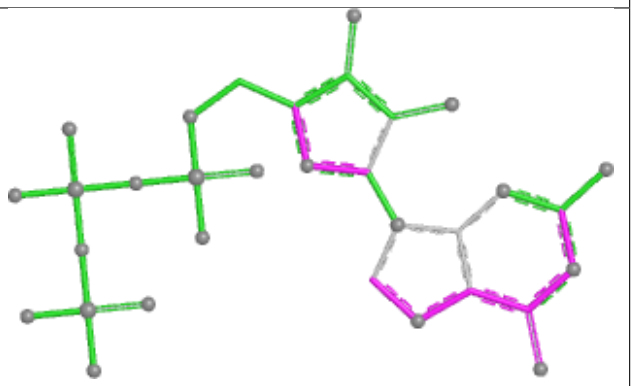

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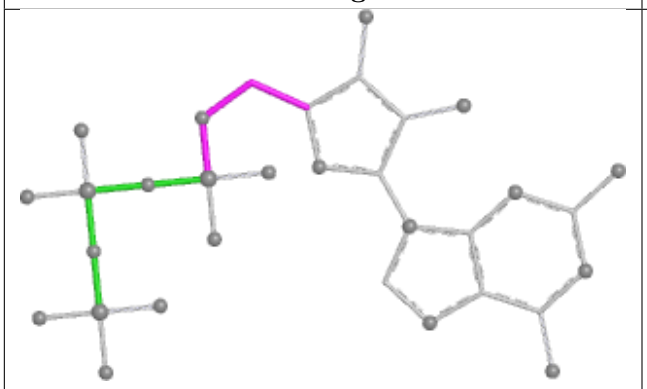

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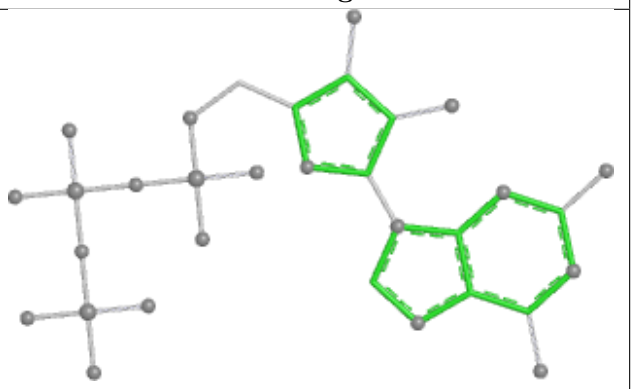
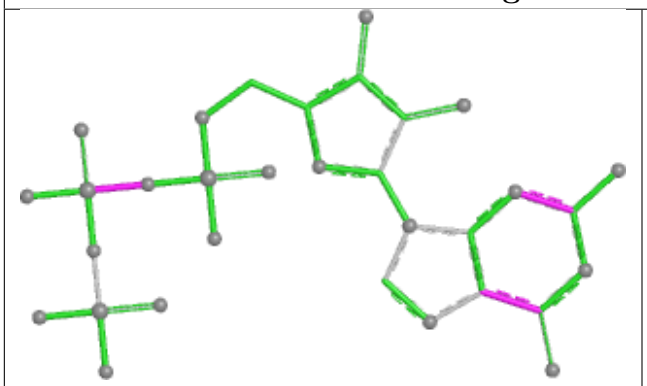


Rings

## Ligand GTP MM 501



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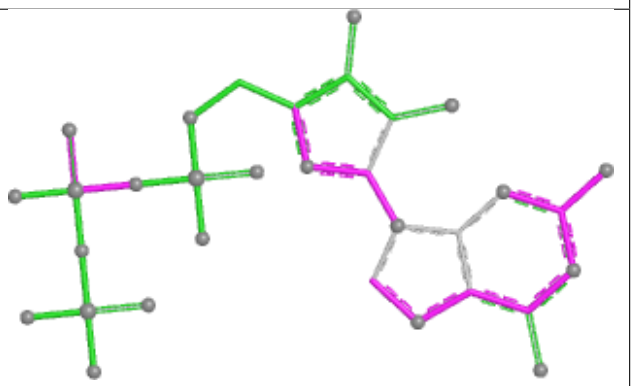

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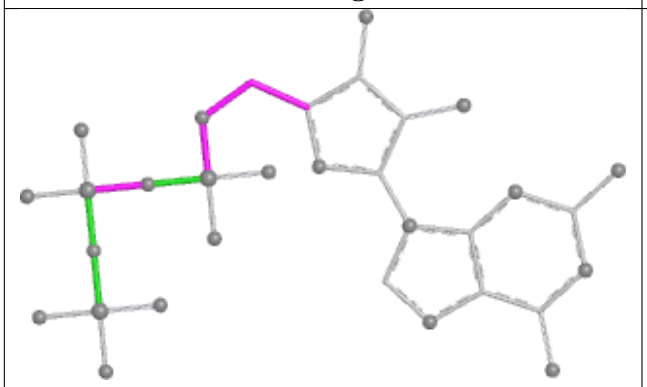

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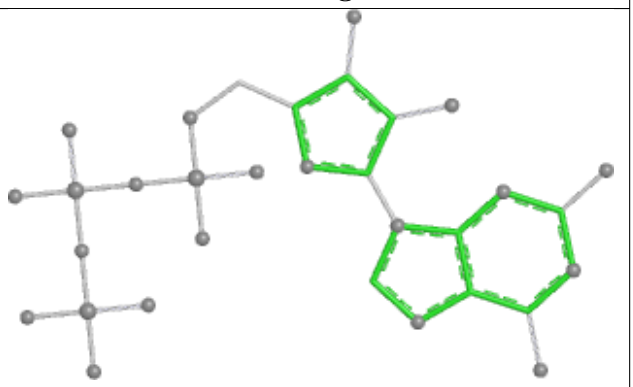
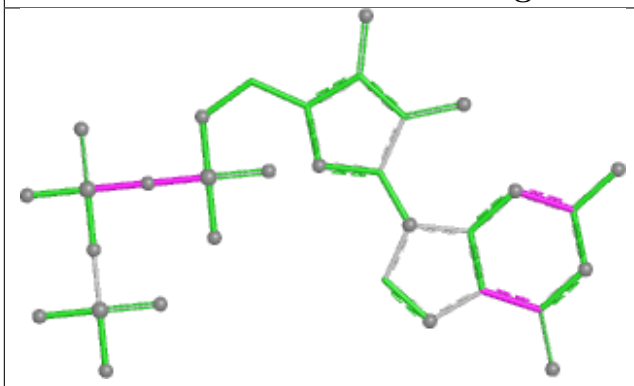


Rings

## Ligand GTP SP 501



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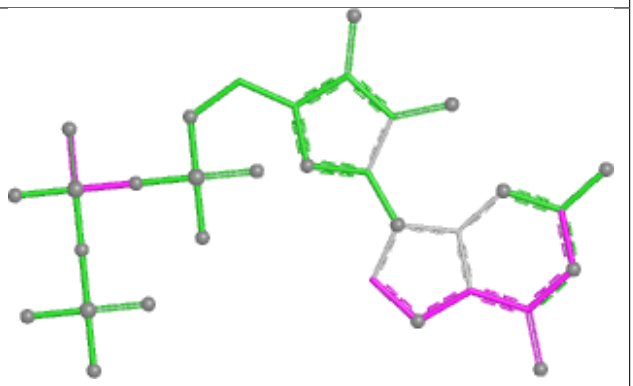

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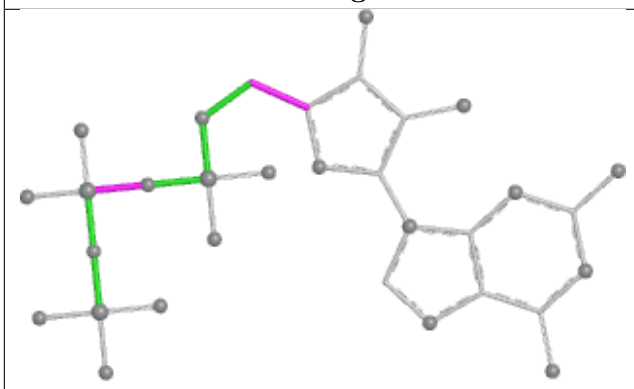

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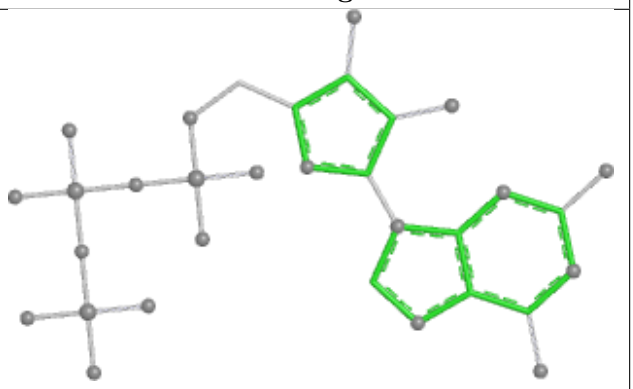
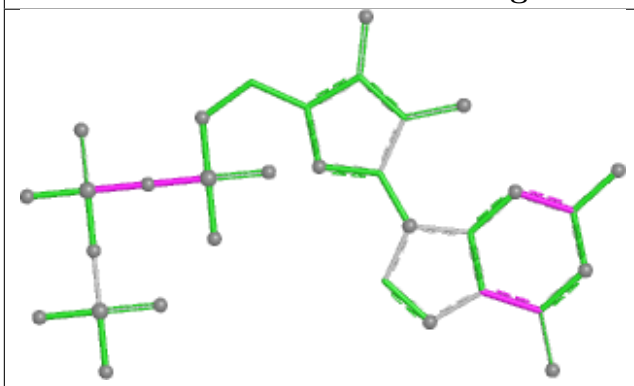


Rings

## Ligand GTP GP 501



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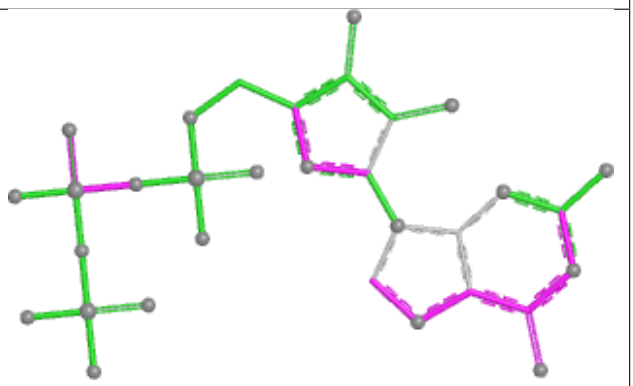

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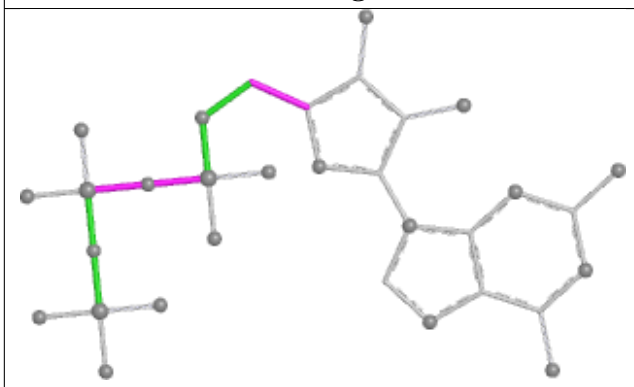

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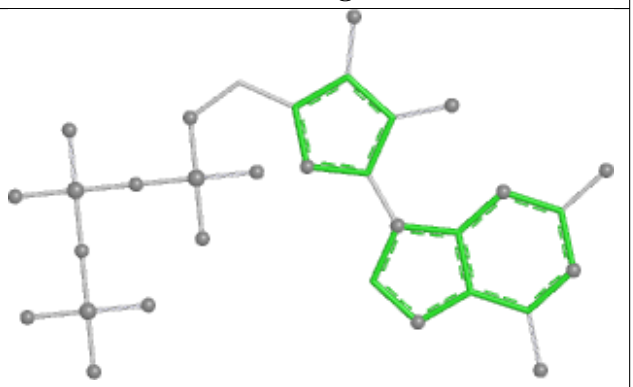
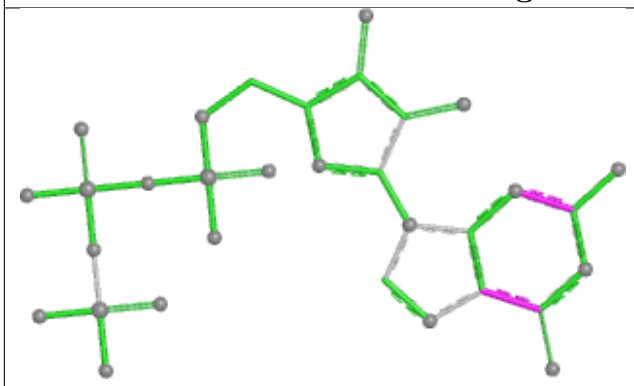


Rings

## Ligand GTP JE 501



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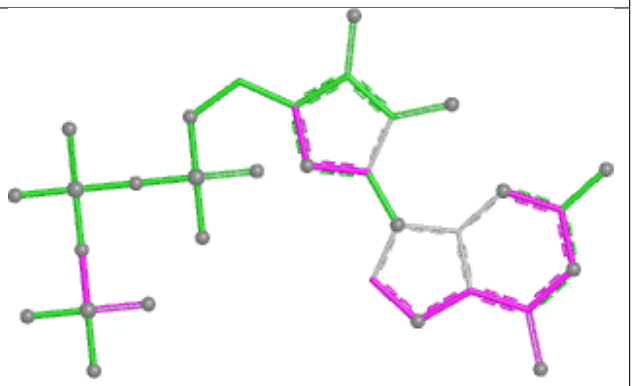

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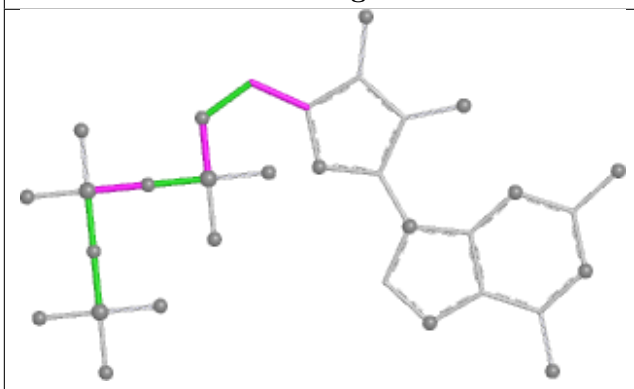

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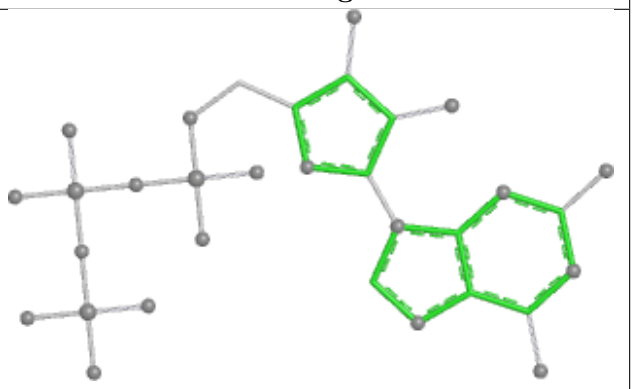
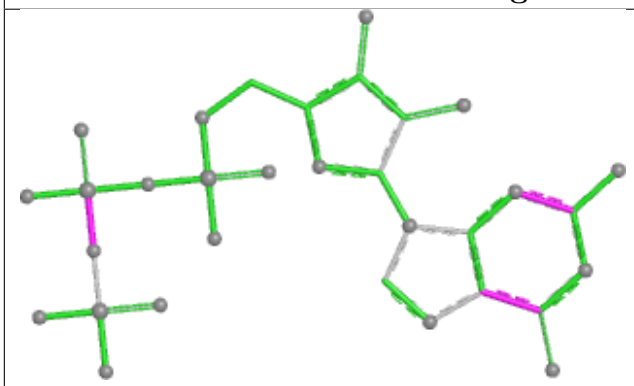


Rings

## Ligand GTP OB 502



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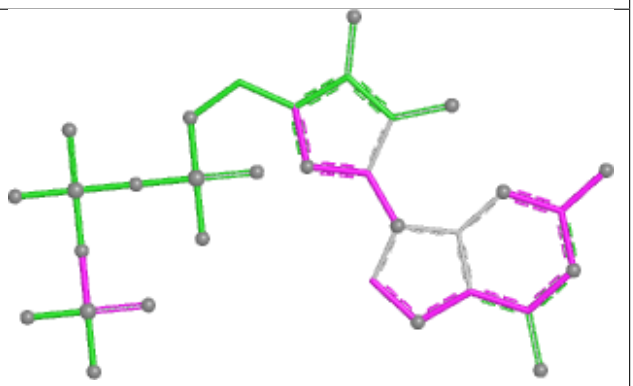

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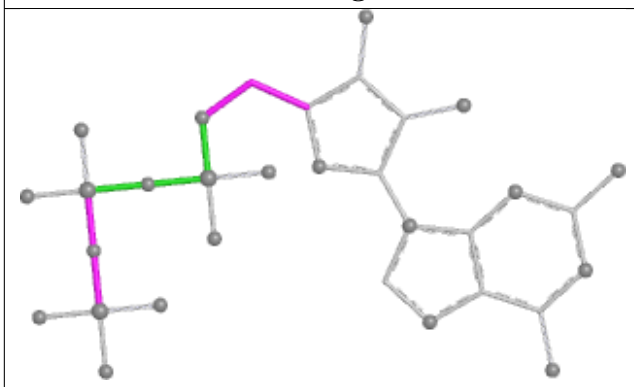

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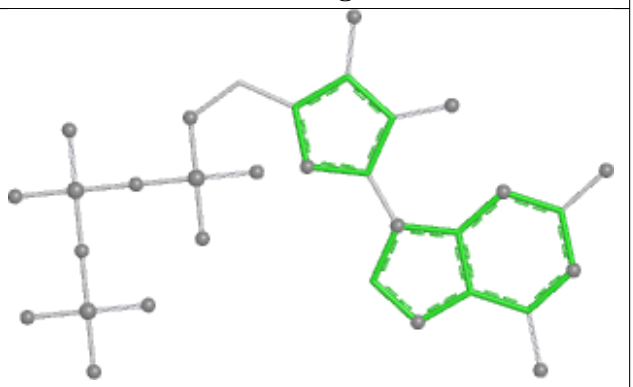
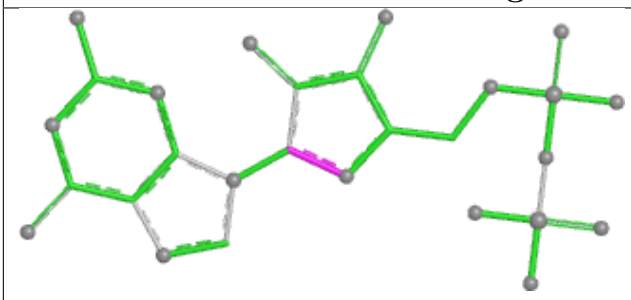


Rings

## Ligand GDP AN 501



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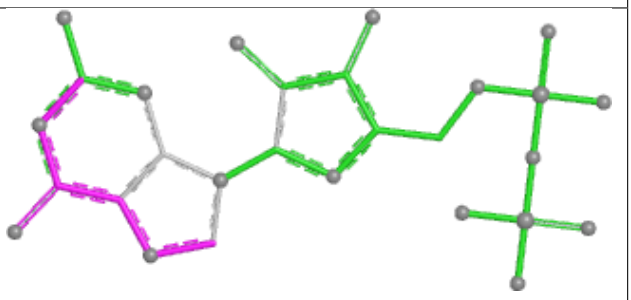

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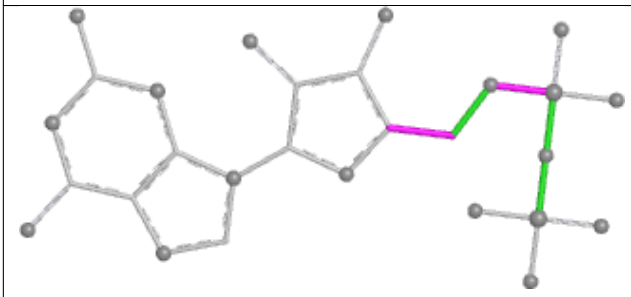

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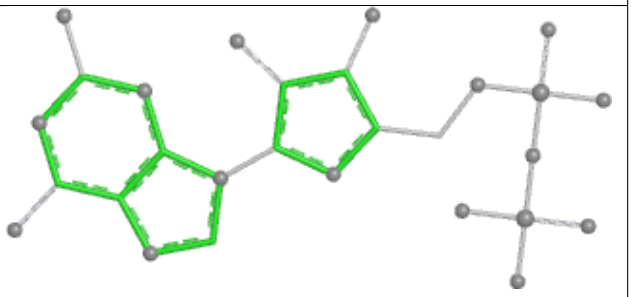
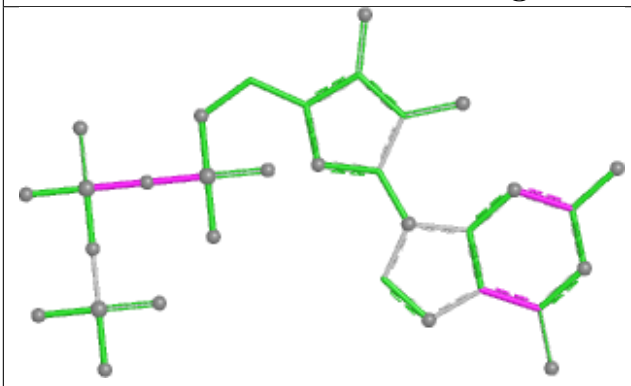


Rings

## Ligand GTP PB 502



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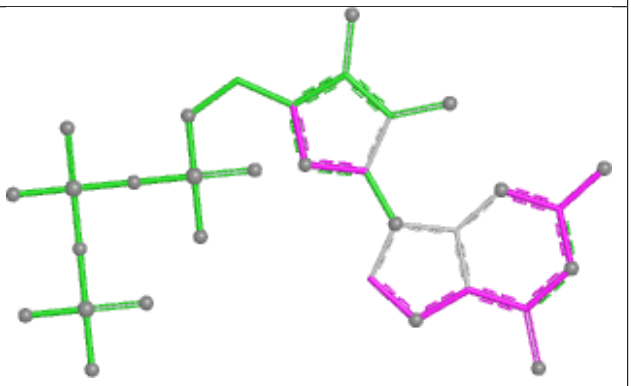

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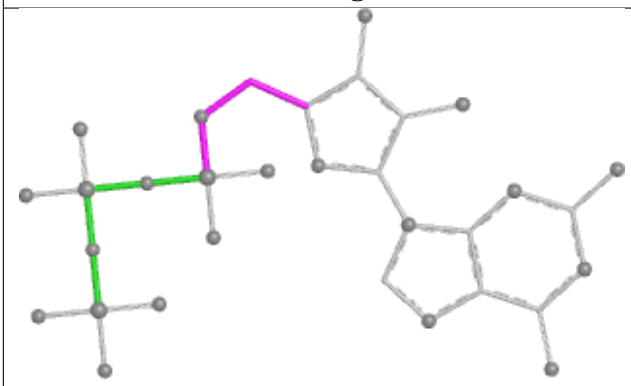

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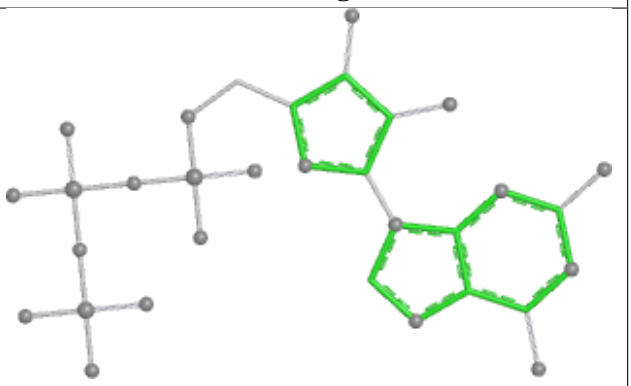
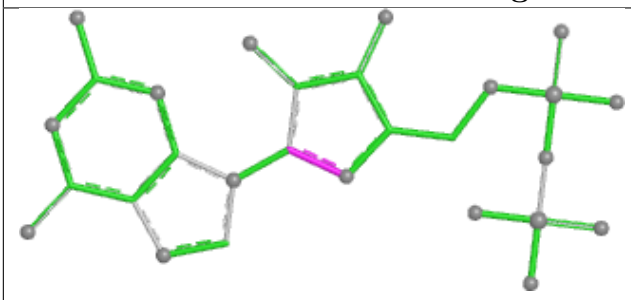


Rings

## Ligand GDP FP 501



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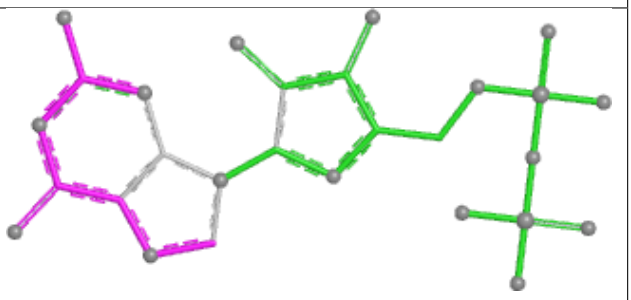
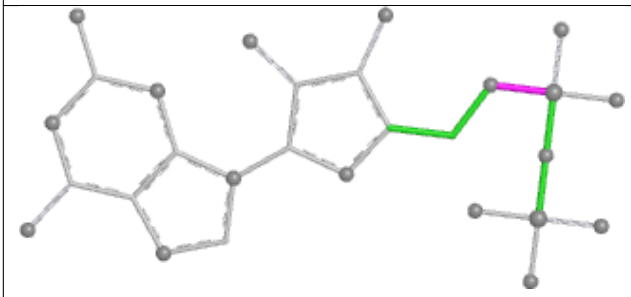


Bond angles



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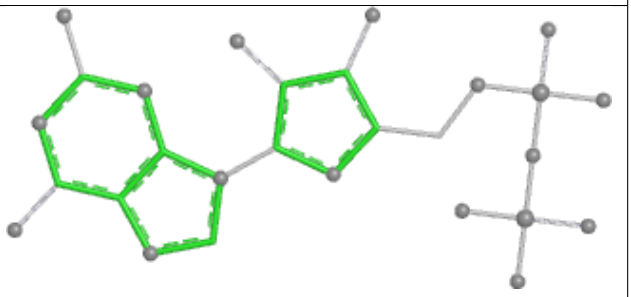
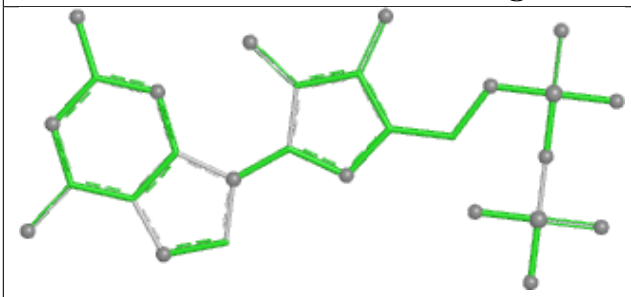


Rings

## Ligand GDP VO 501



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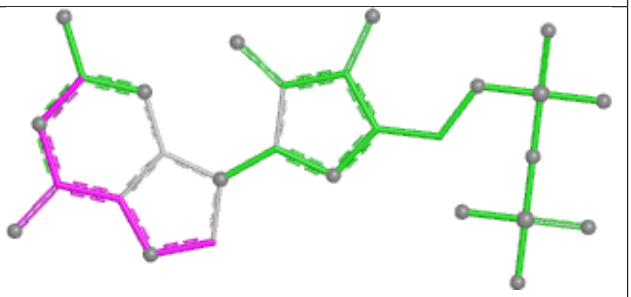
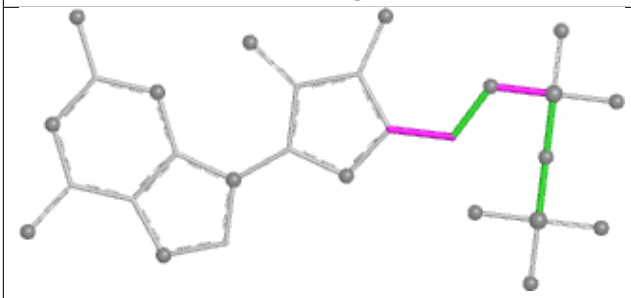


Bond angles



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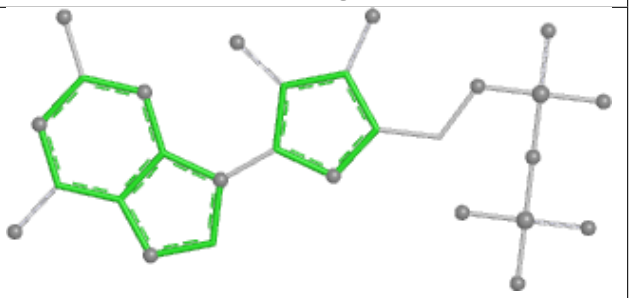

Rings

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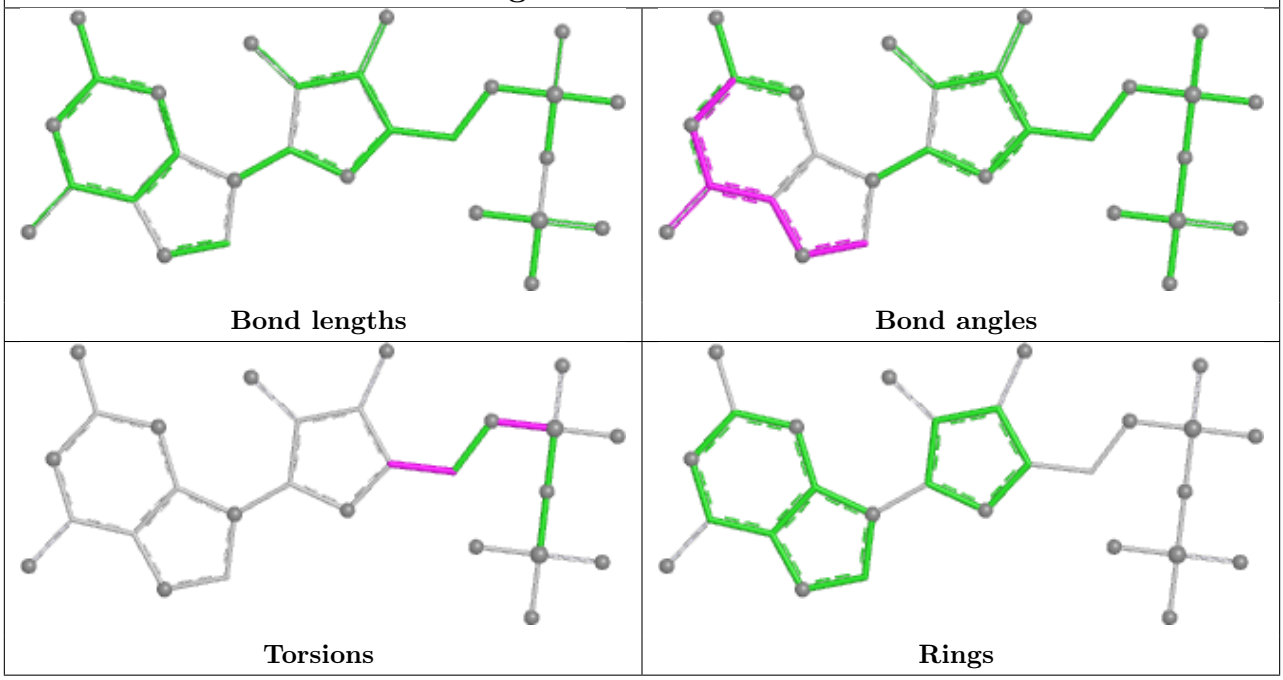


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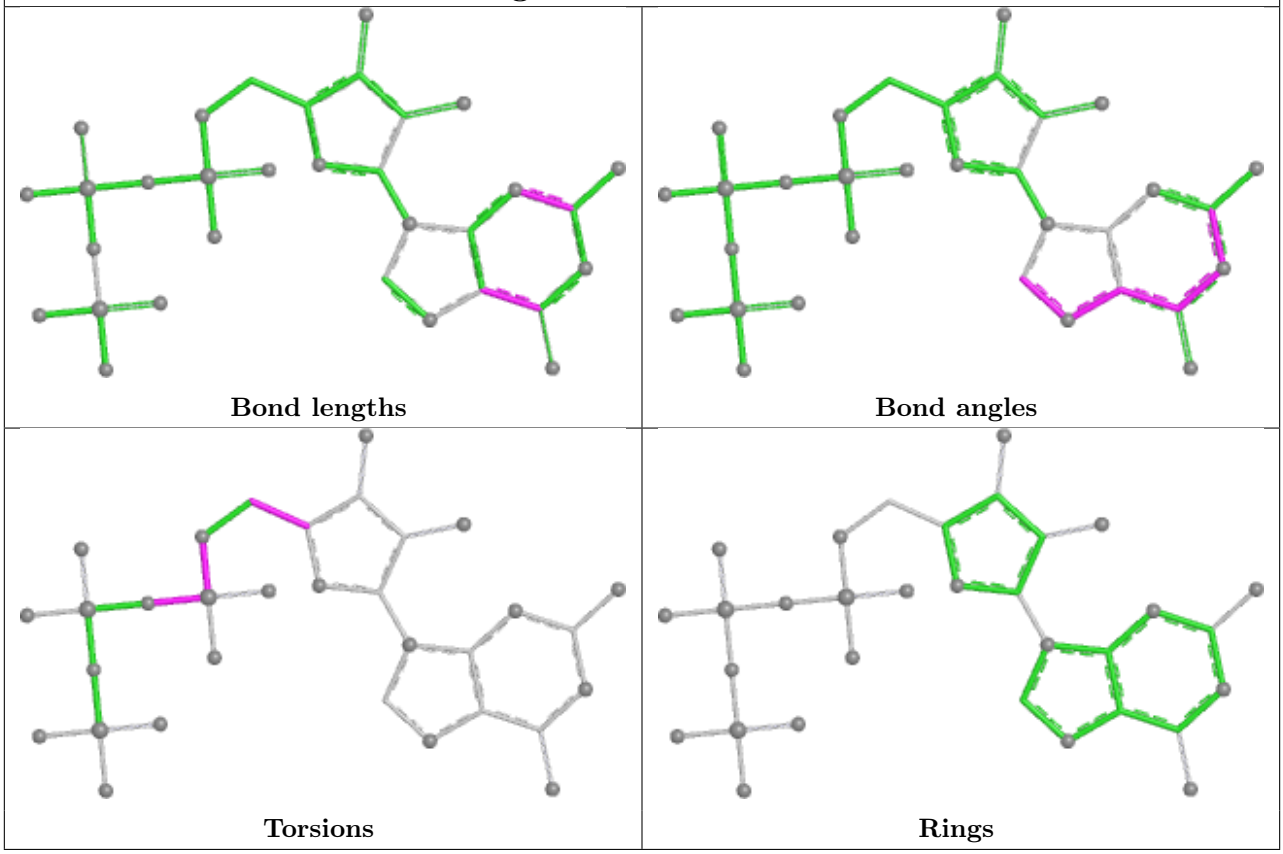
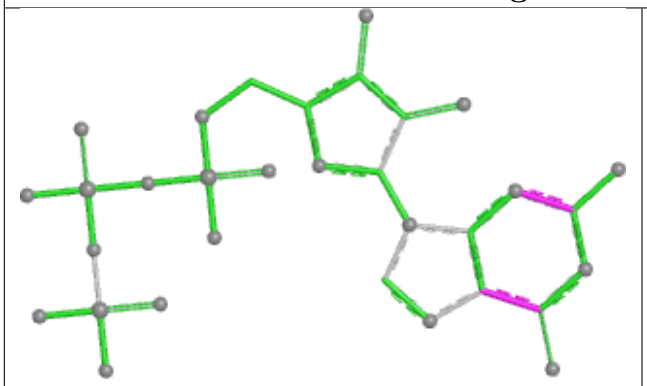
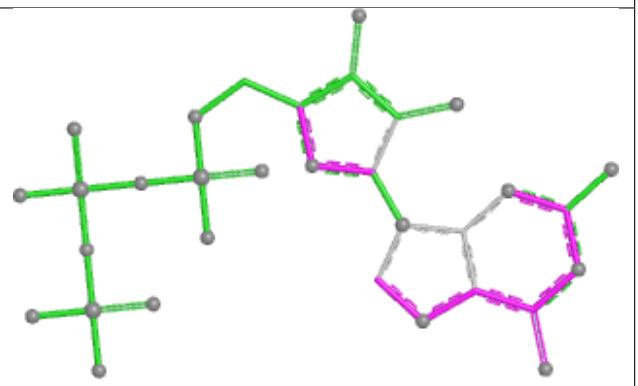


## Ligand GTP CA 501



Bond lengths



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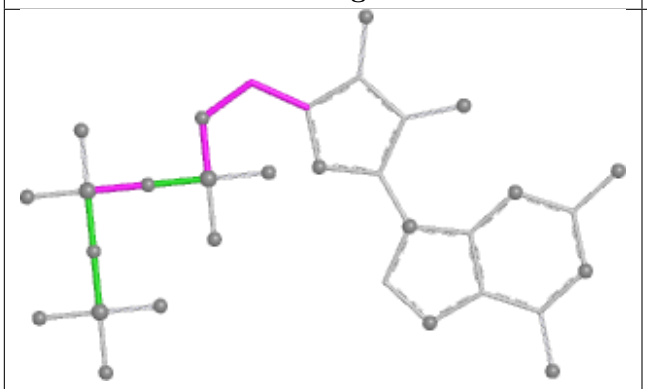
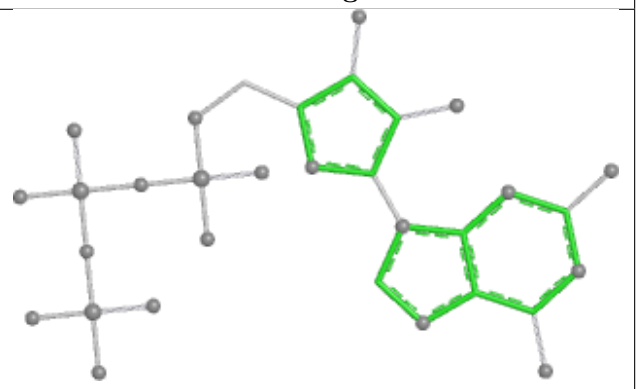


Torsions



Rings

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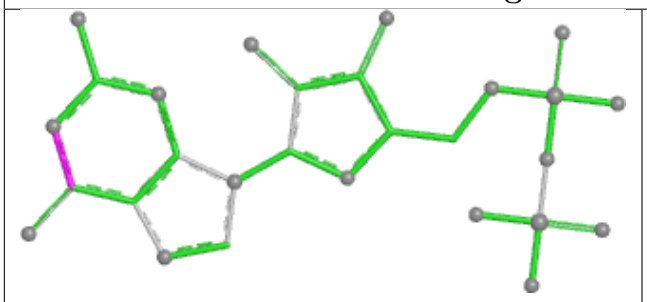

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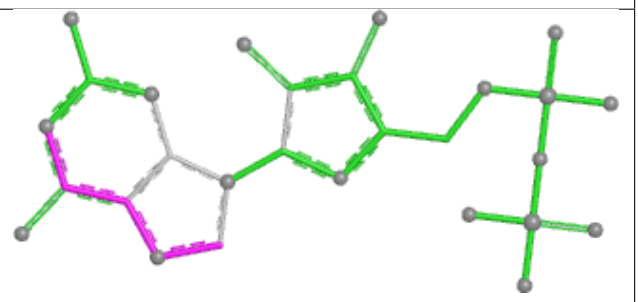

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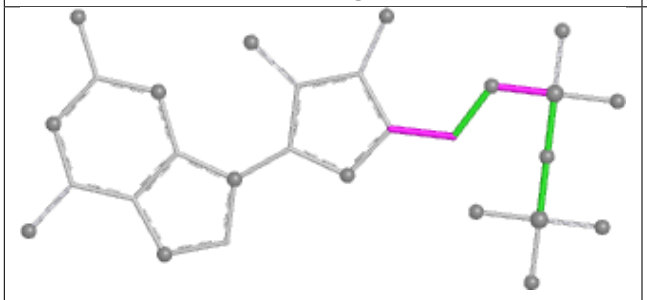

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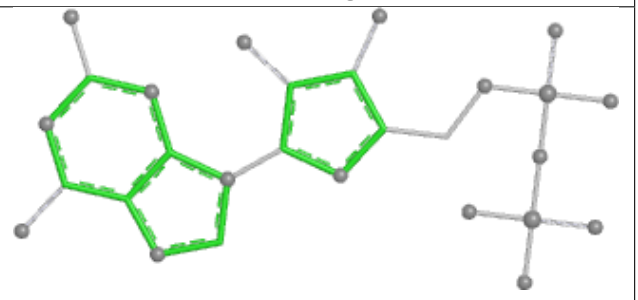

Rings

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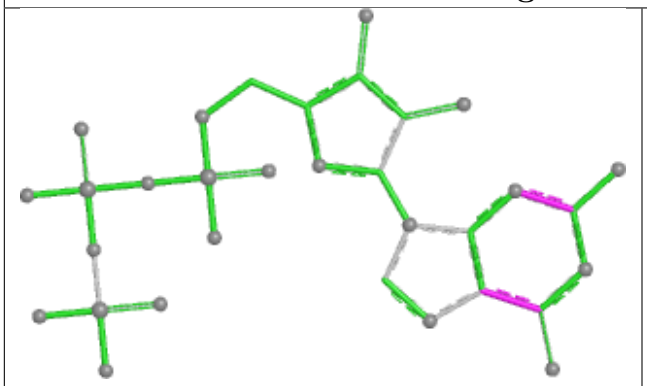

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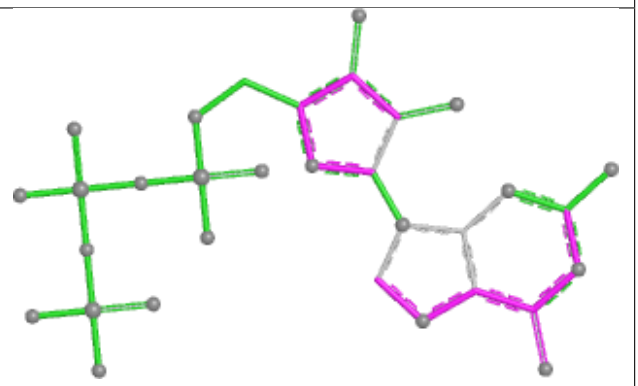

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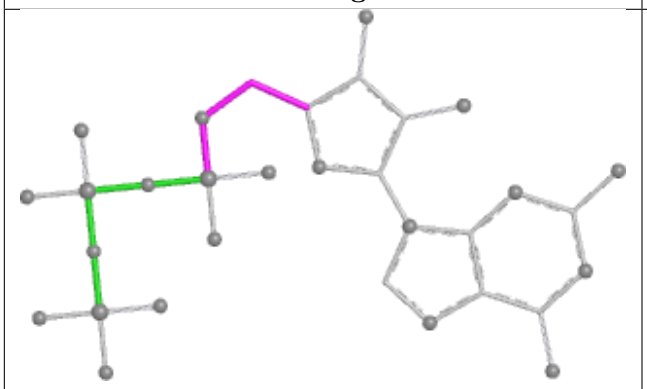

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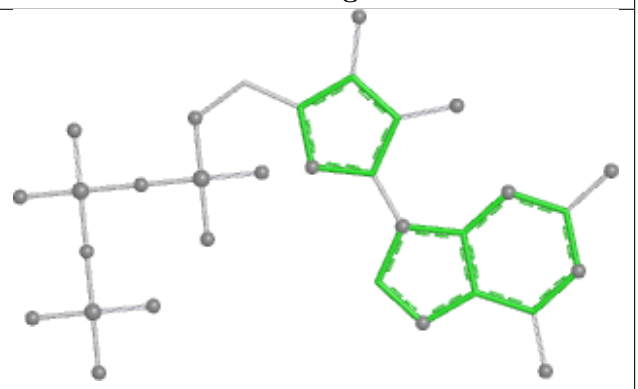

Rings

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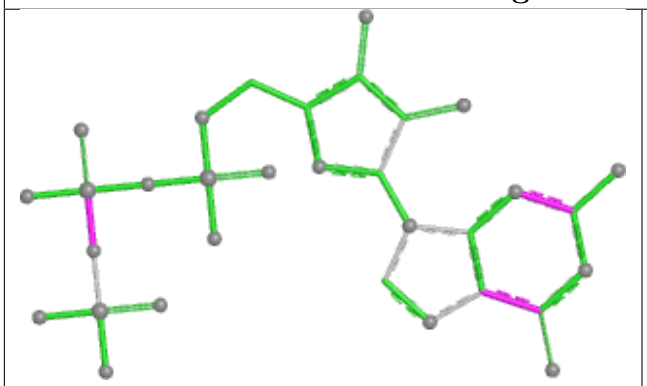

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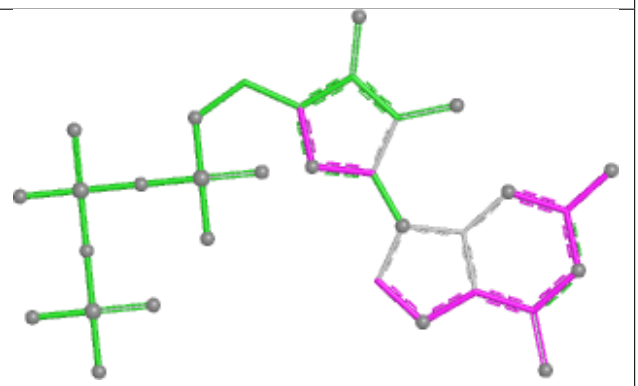

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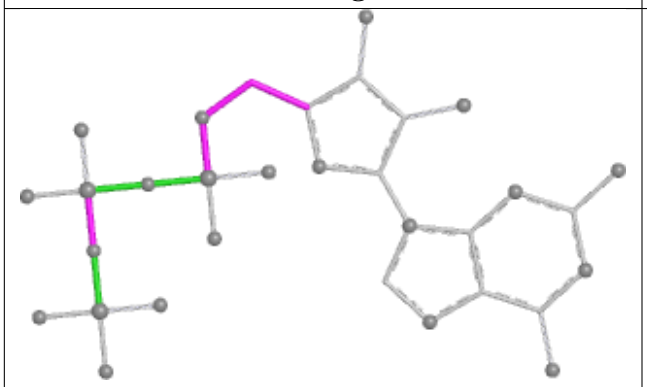

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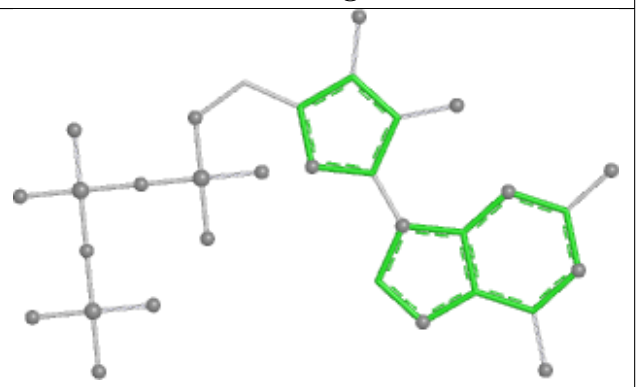

Rings

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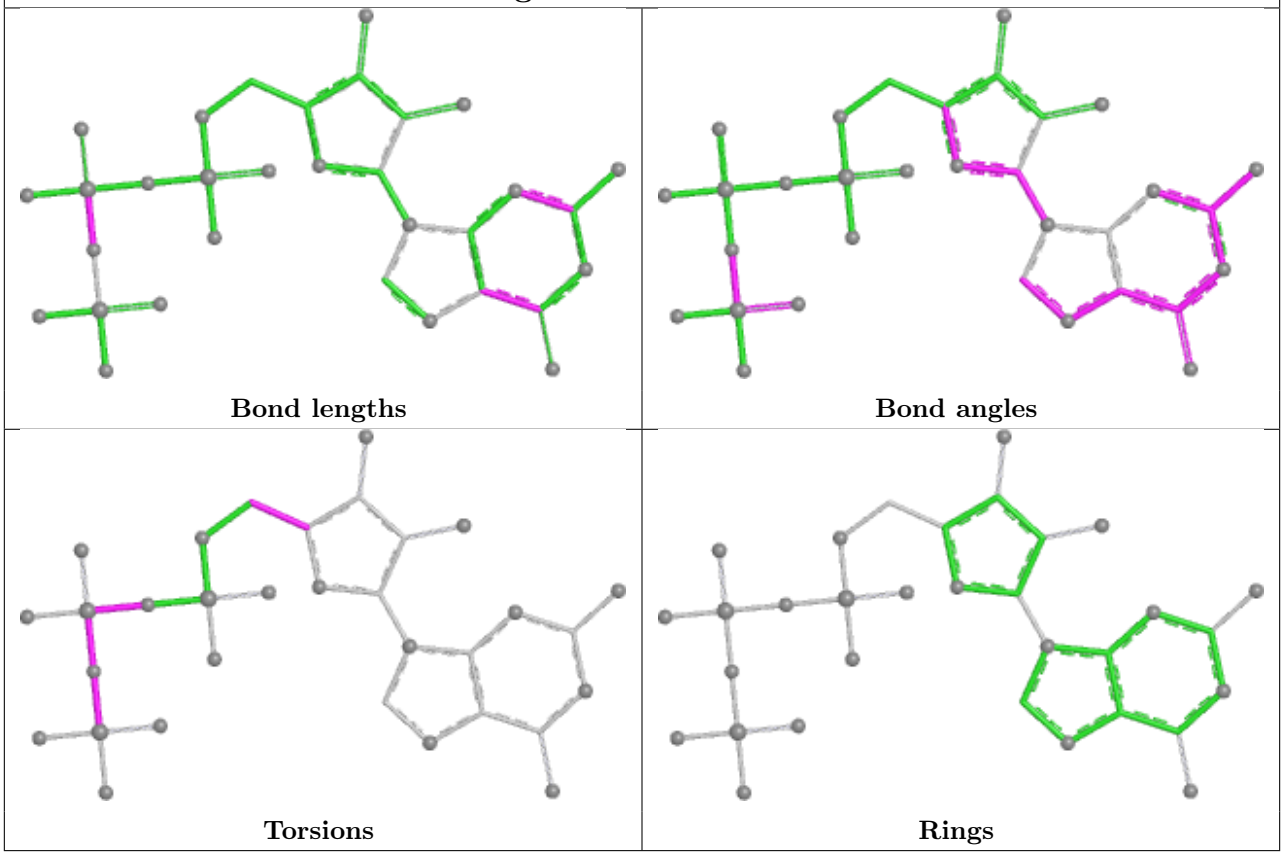


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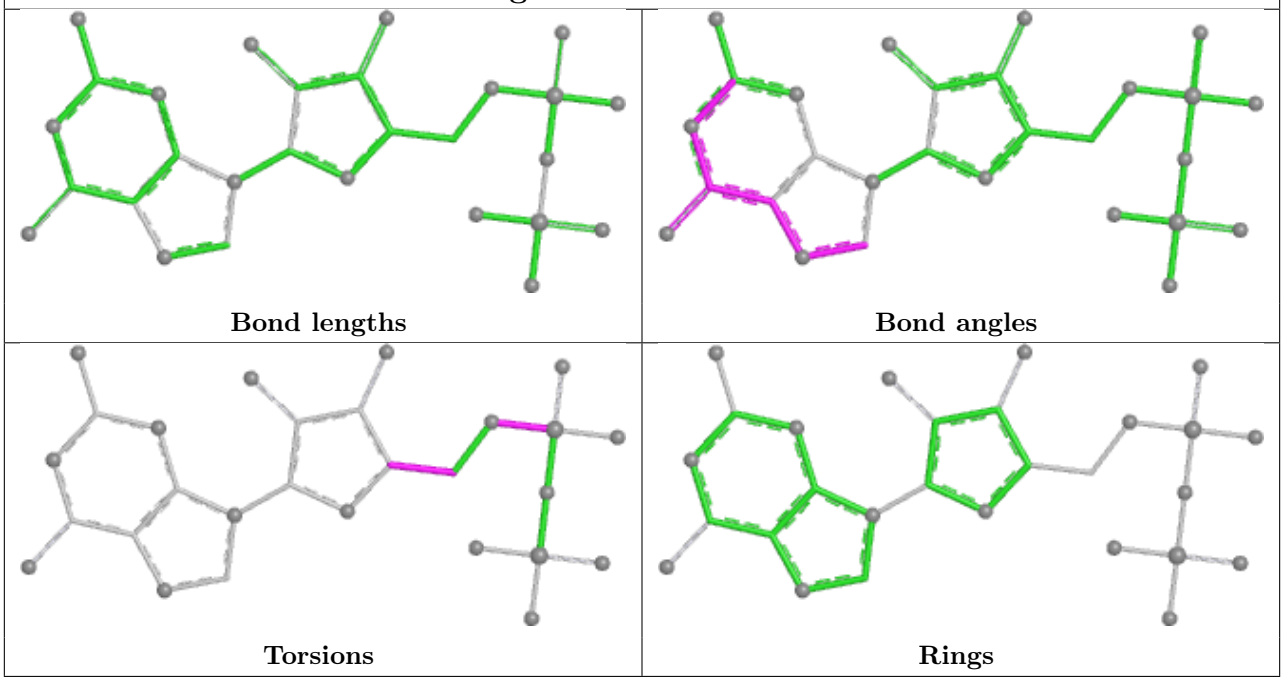

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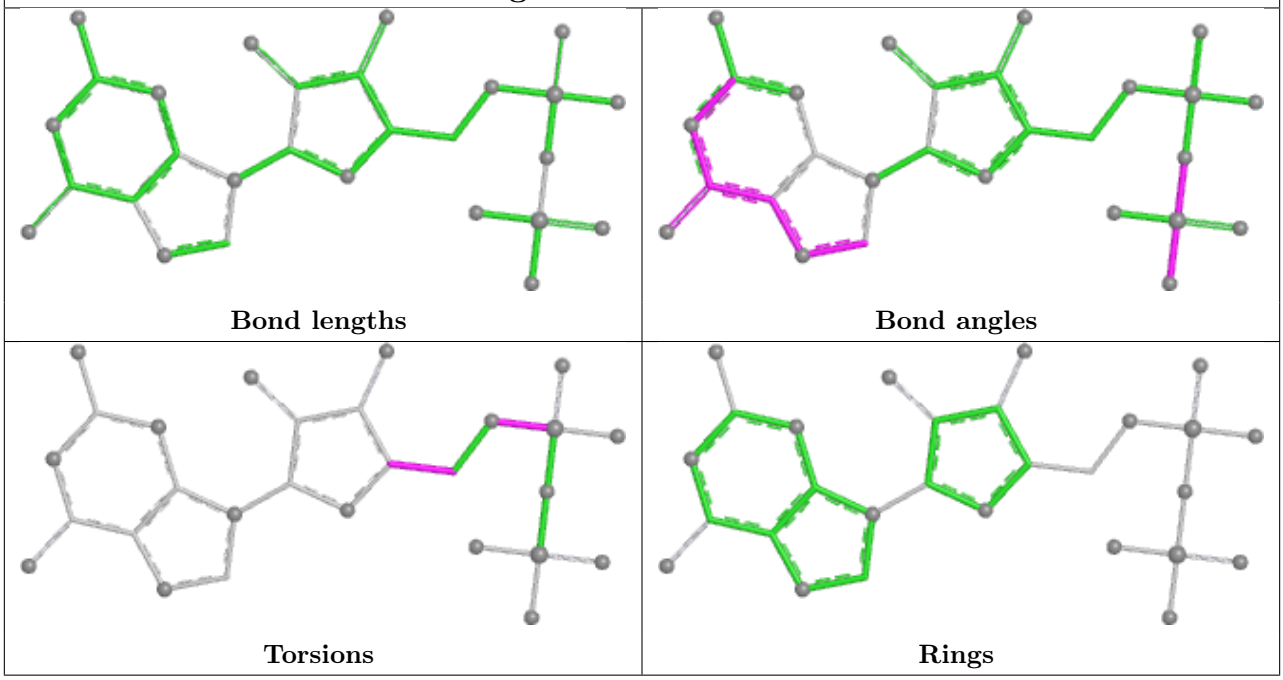


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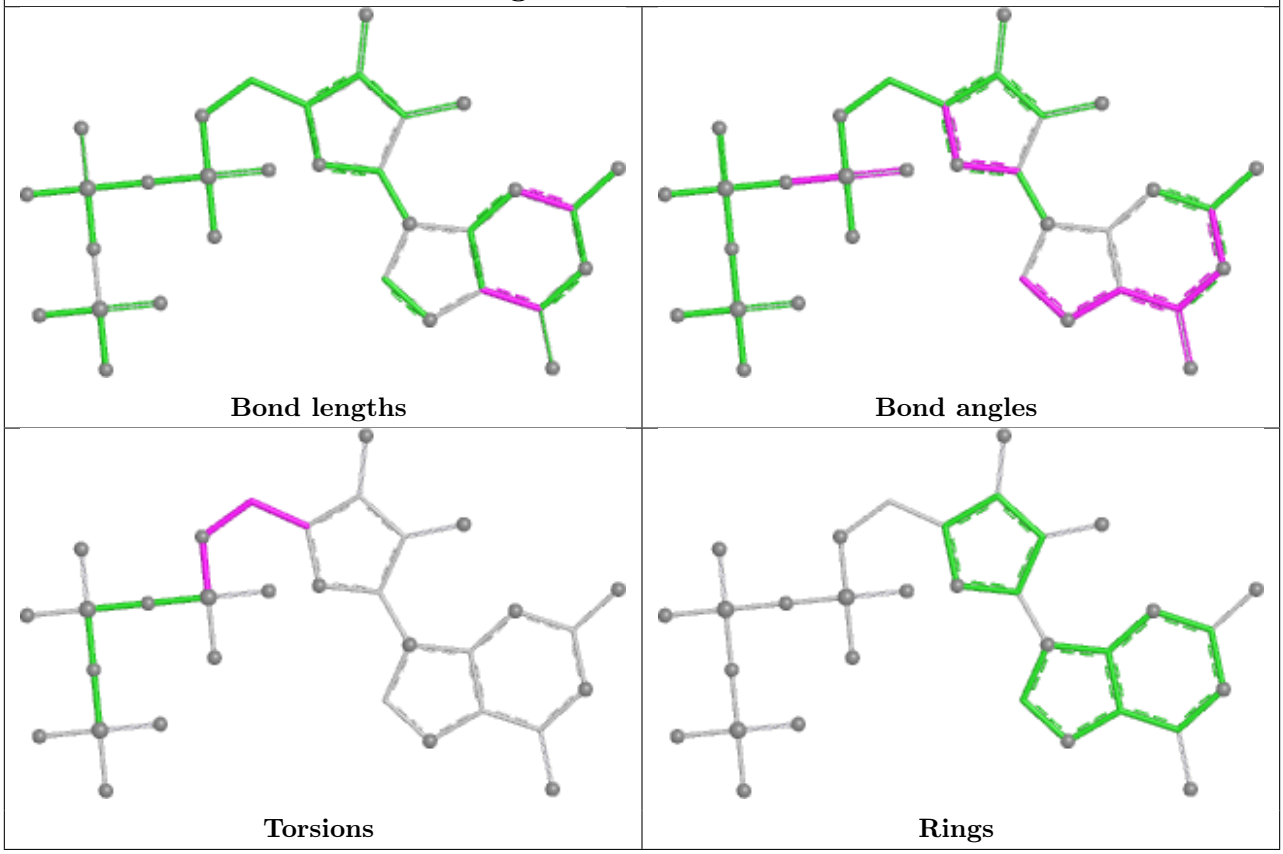

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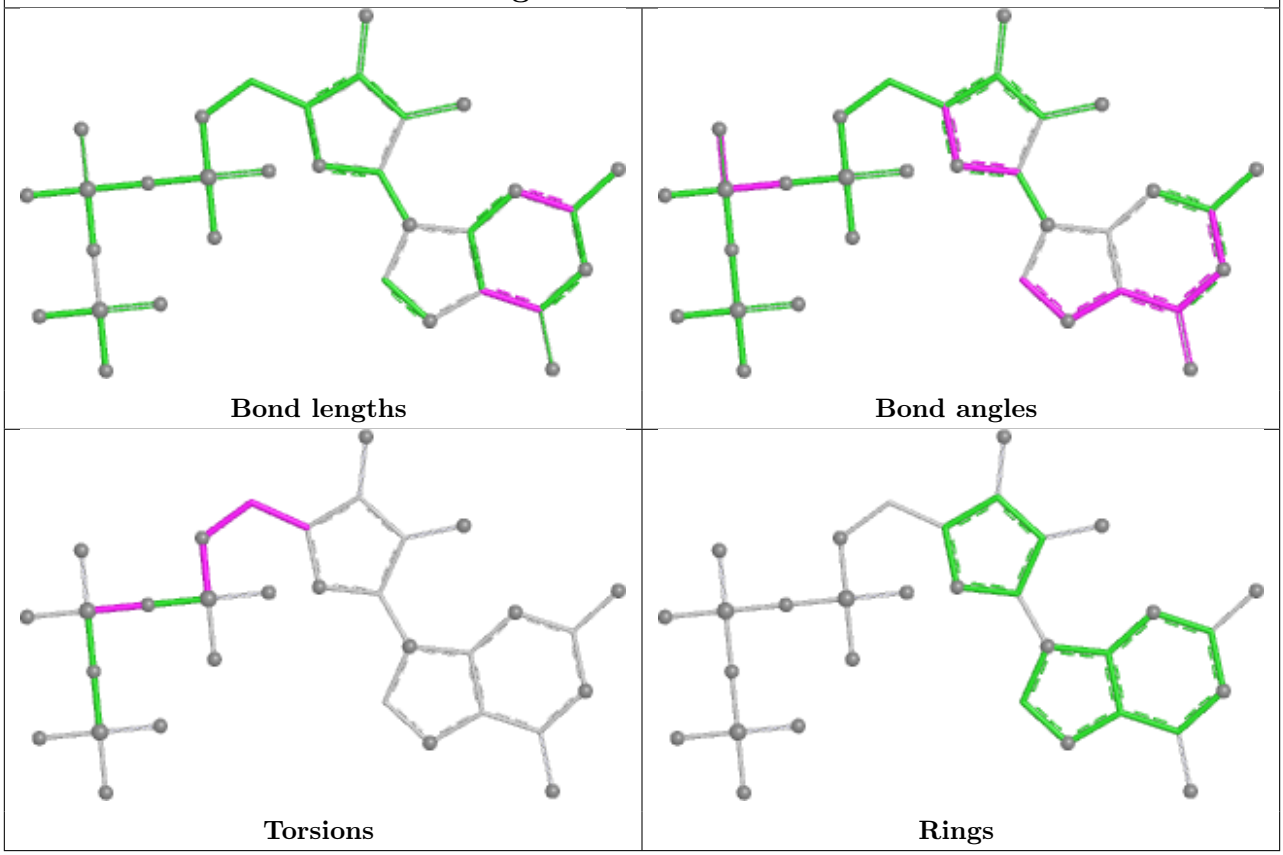


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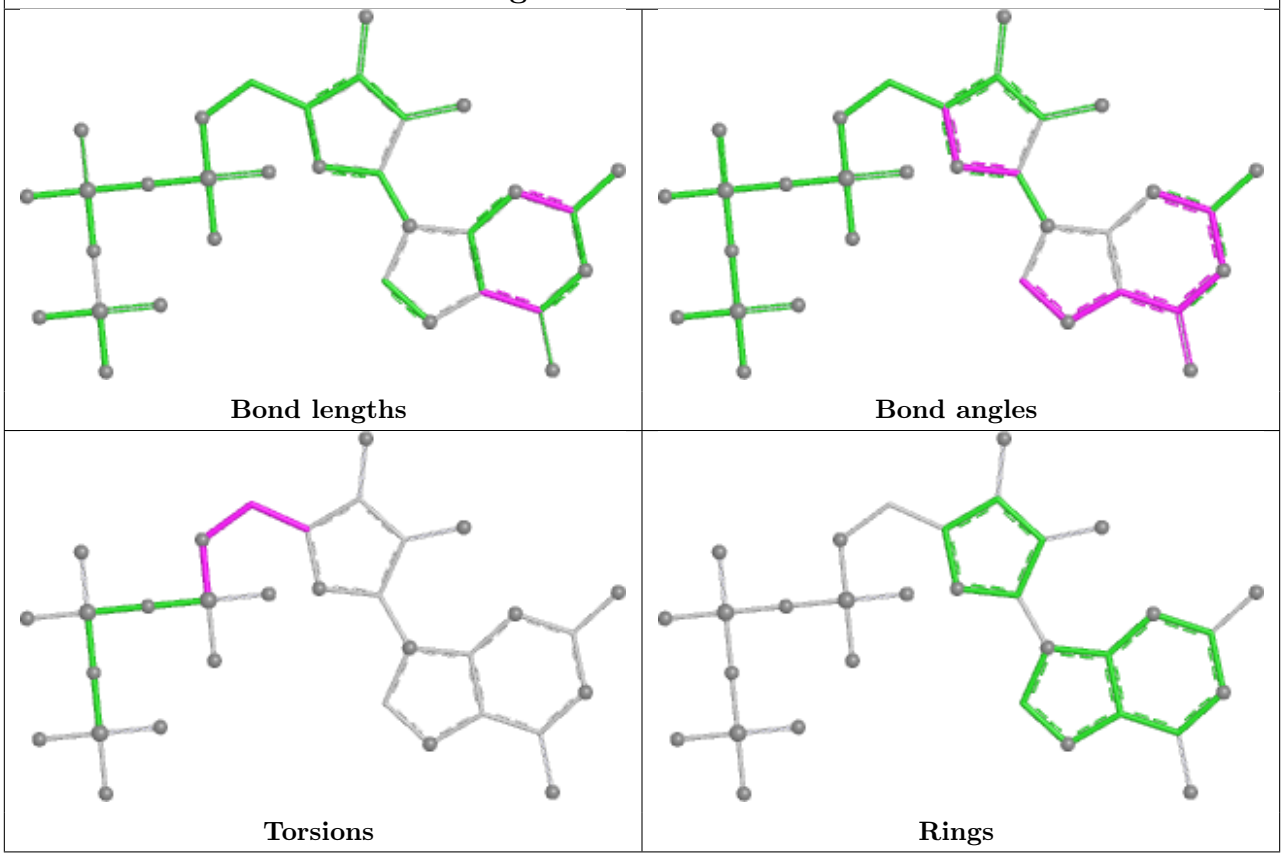

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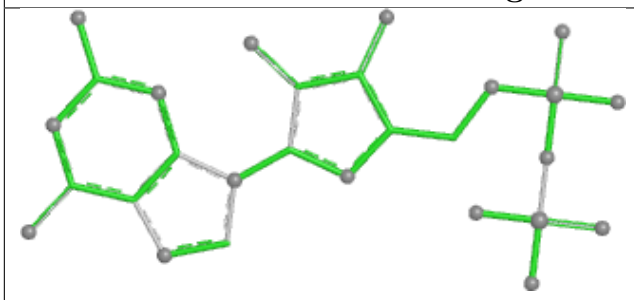
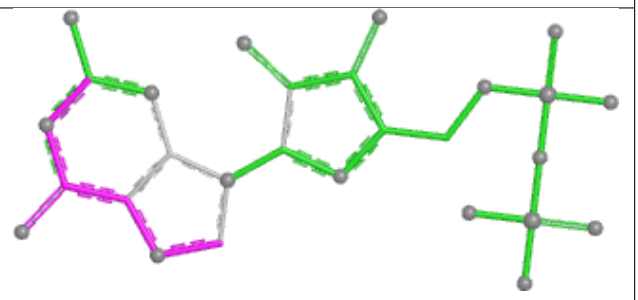
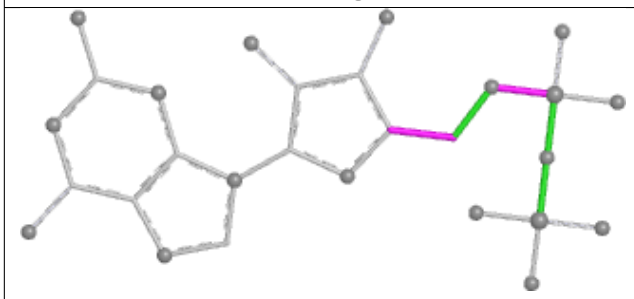


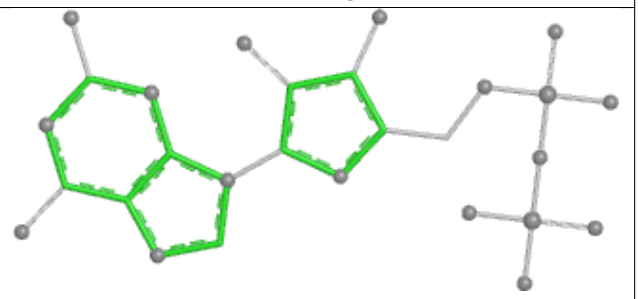
Bond lengths



Bond angles

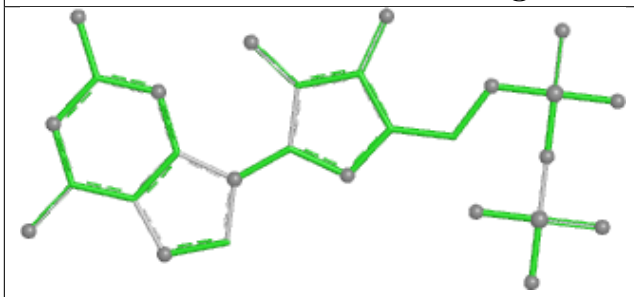


Torsions



Rings

## Ligand GDP NL 501



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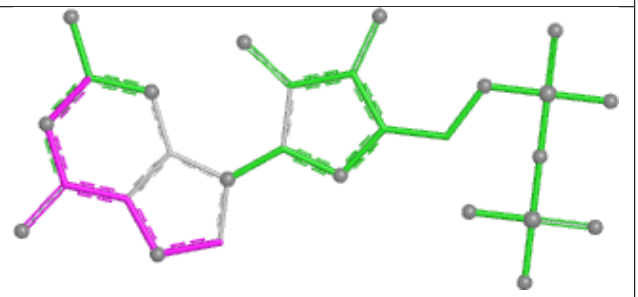

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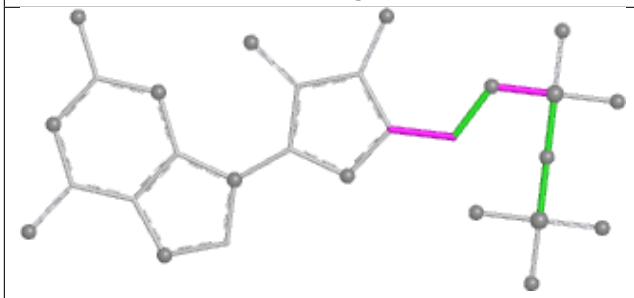

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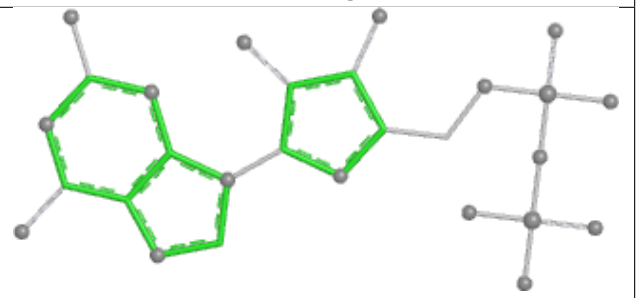

Rings

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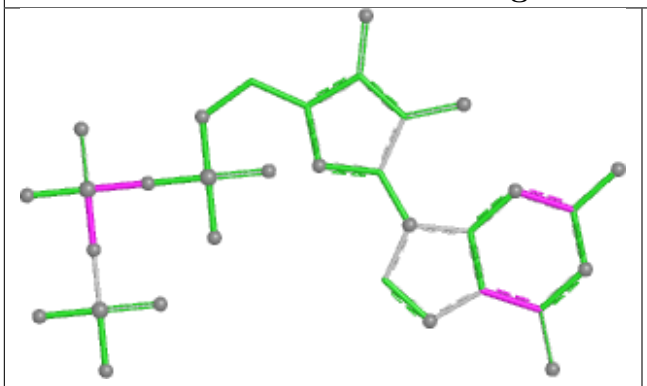

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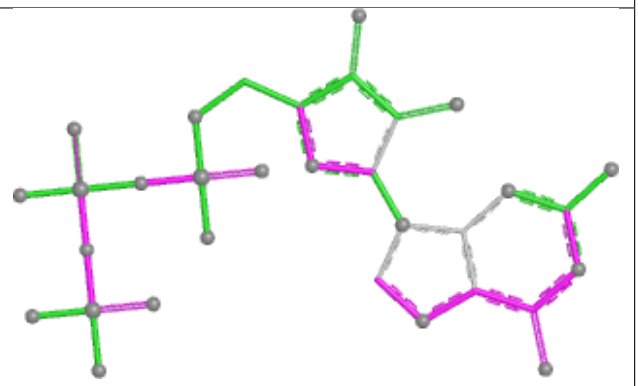

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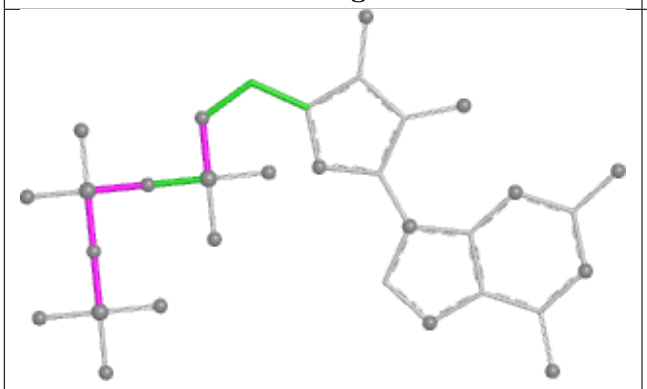

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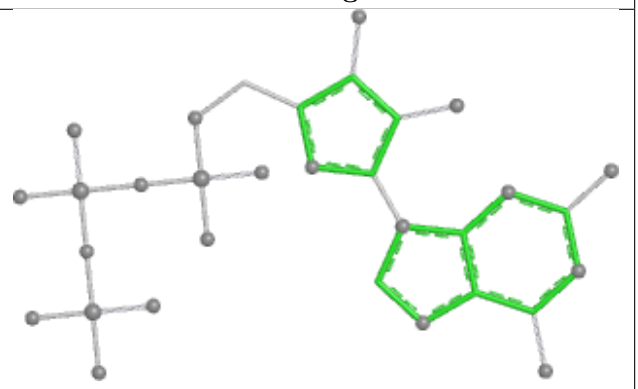

Rings

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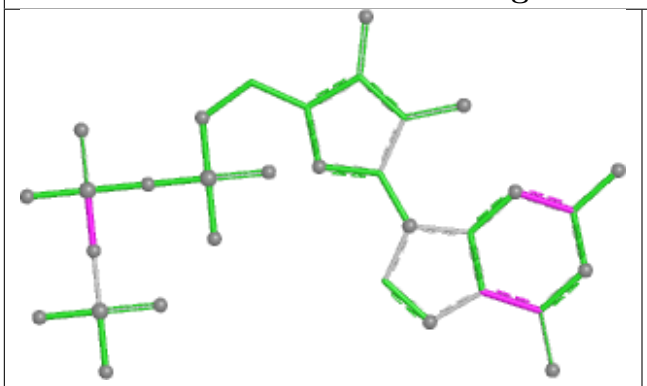

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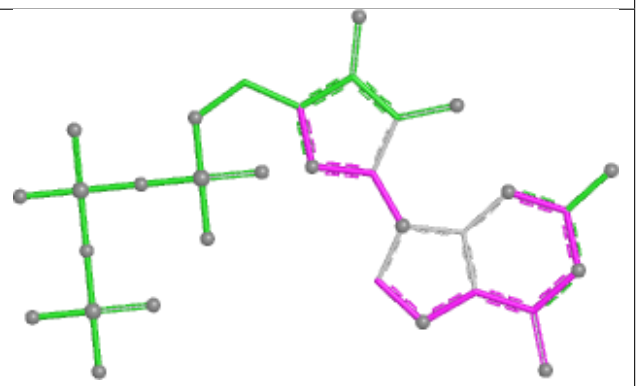

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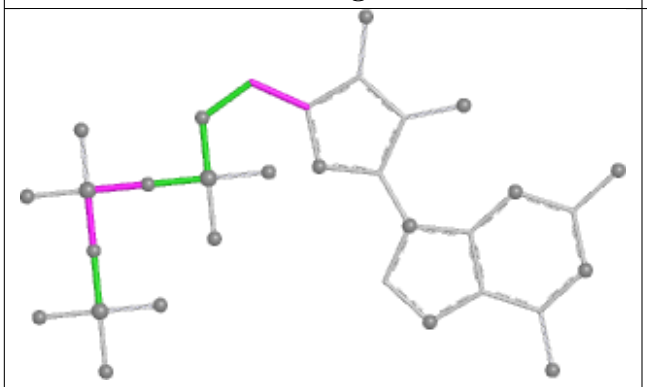

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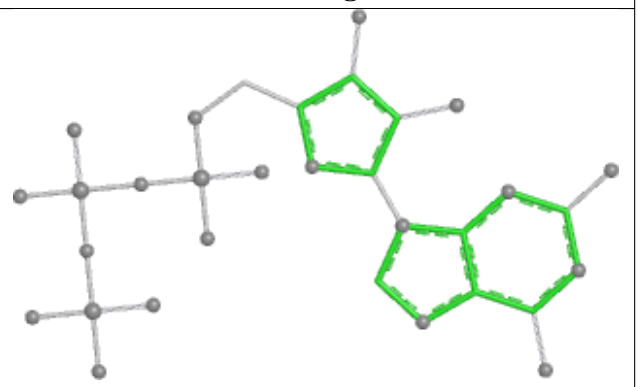

Rings

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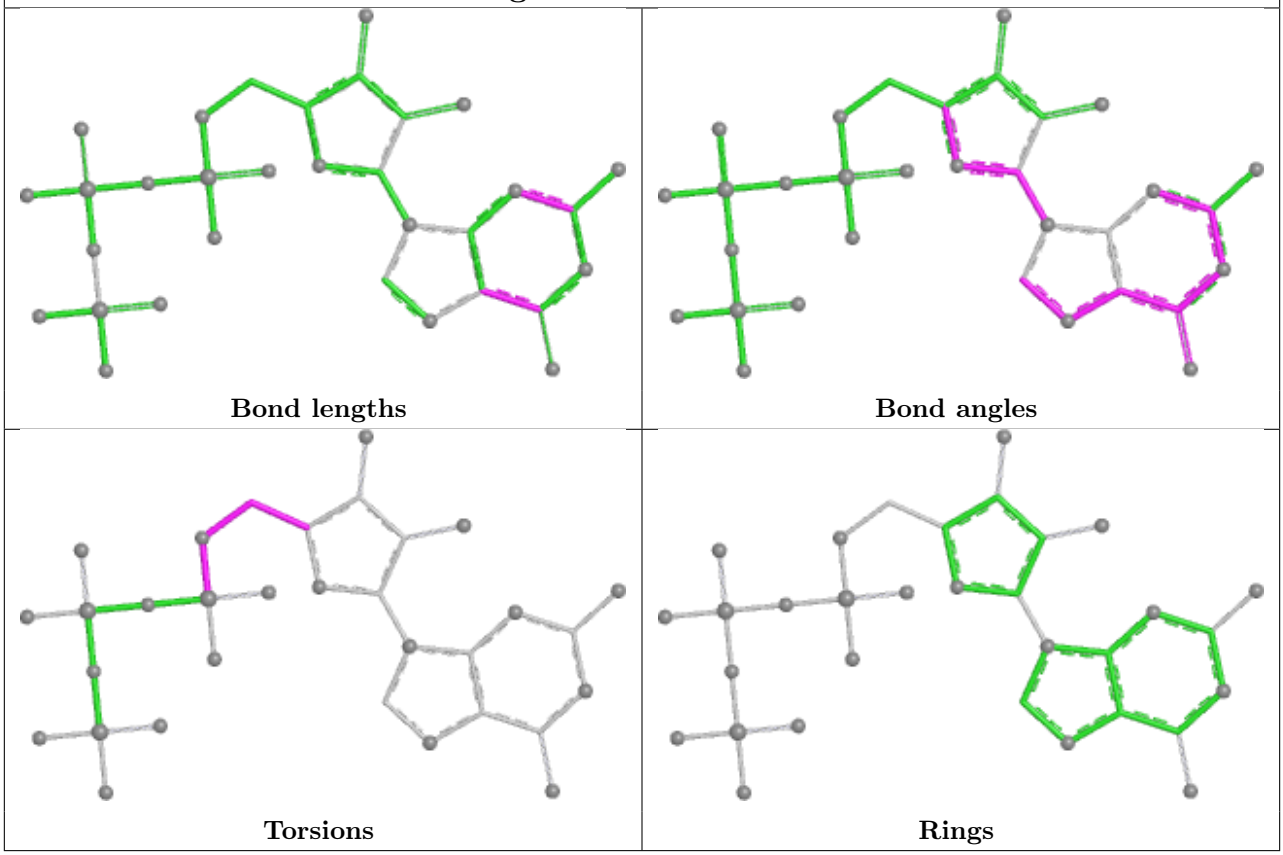


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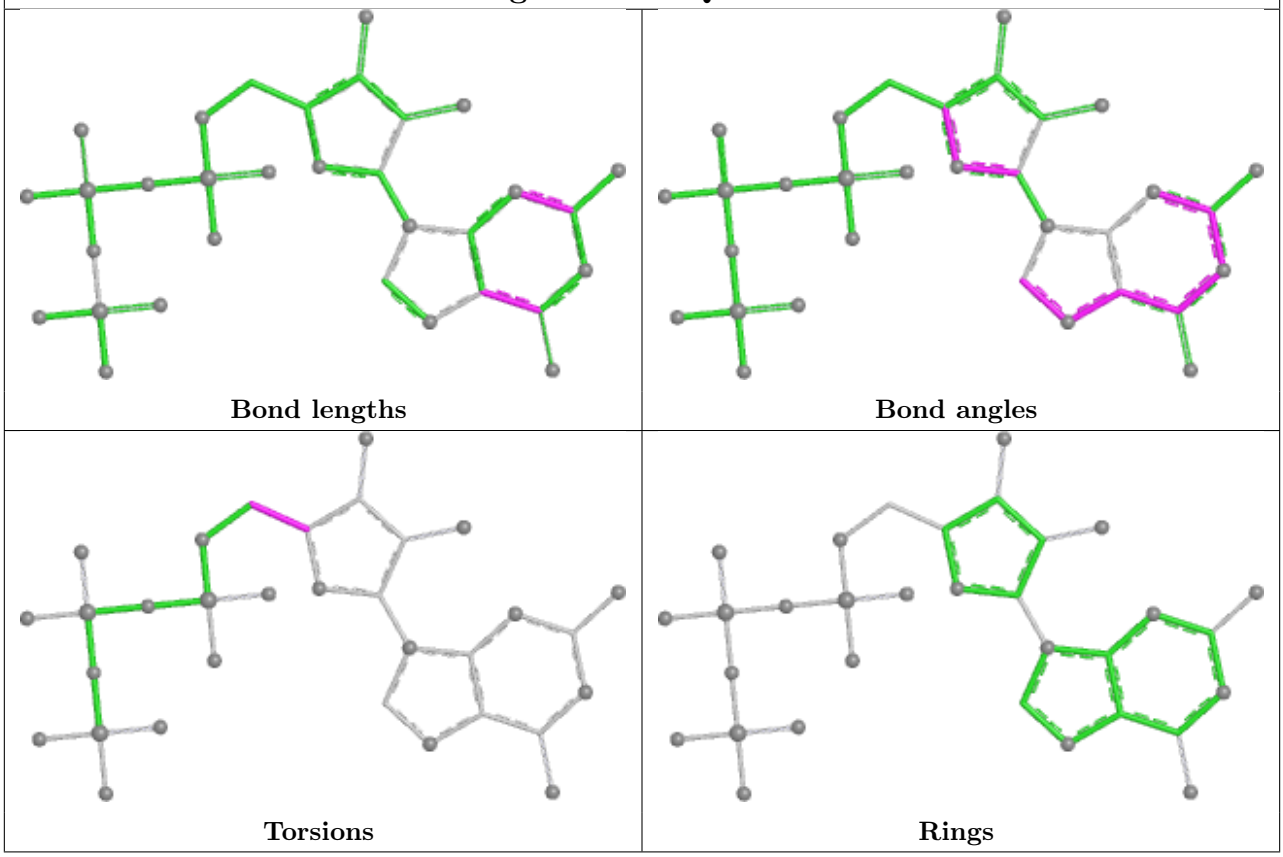

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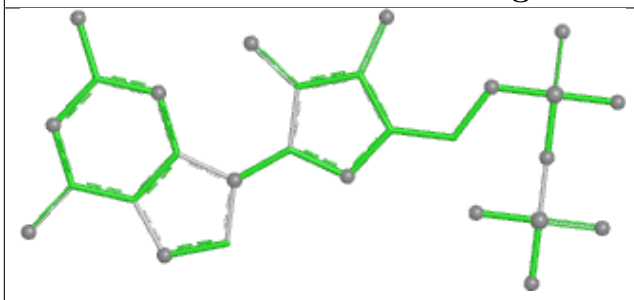

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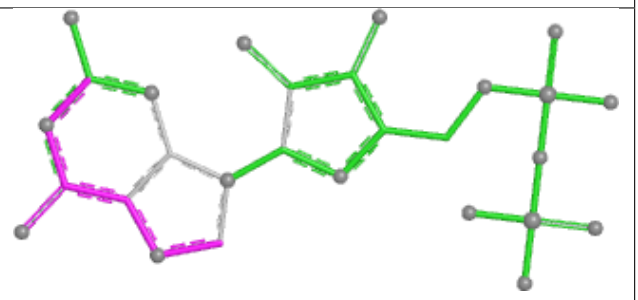

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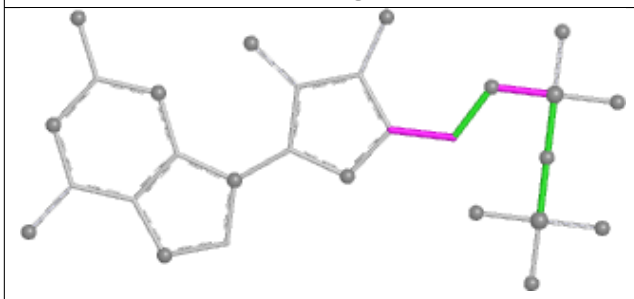

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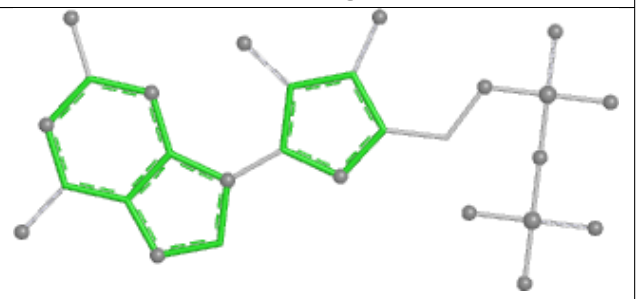

Rings

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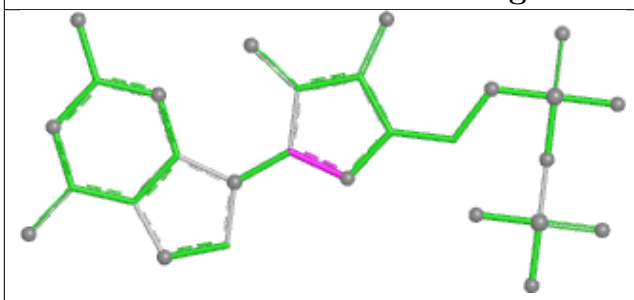

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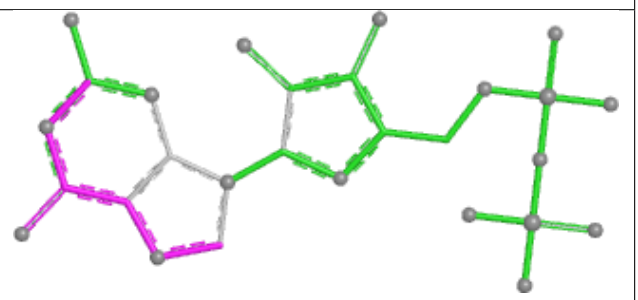
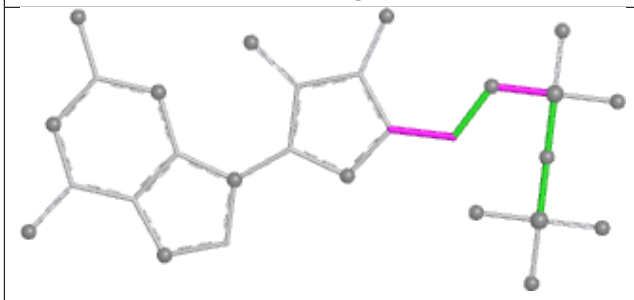


Bond angles



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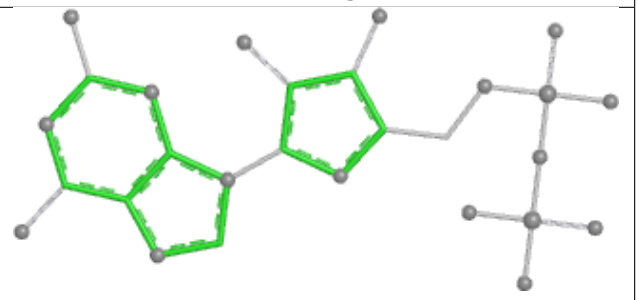

Rings

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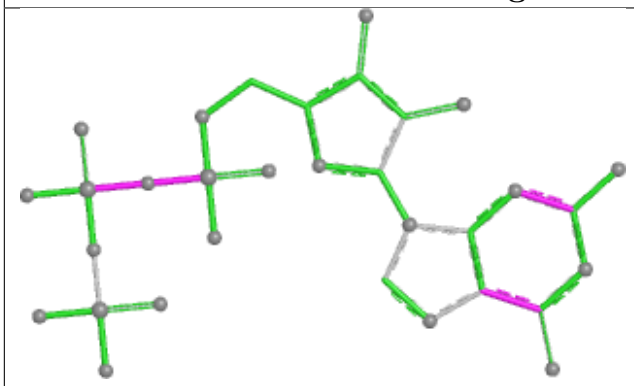

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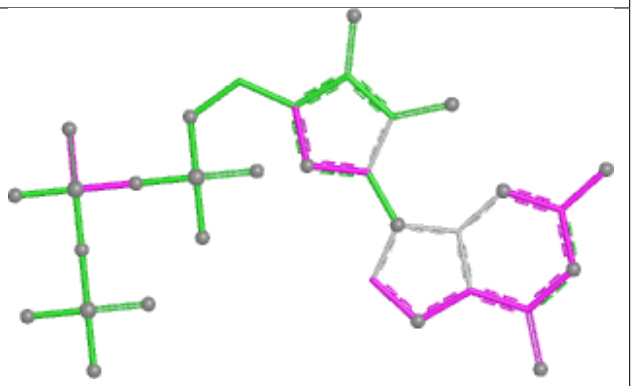

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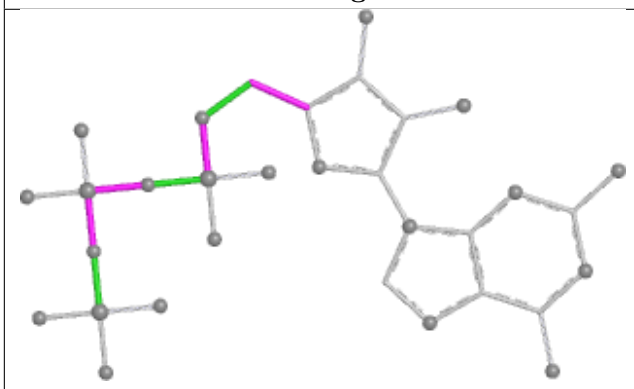

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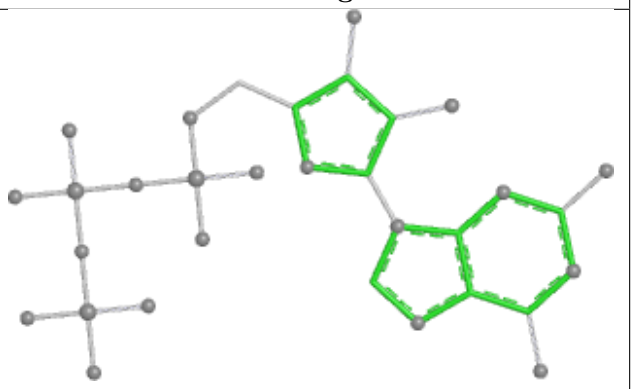

Rings

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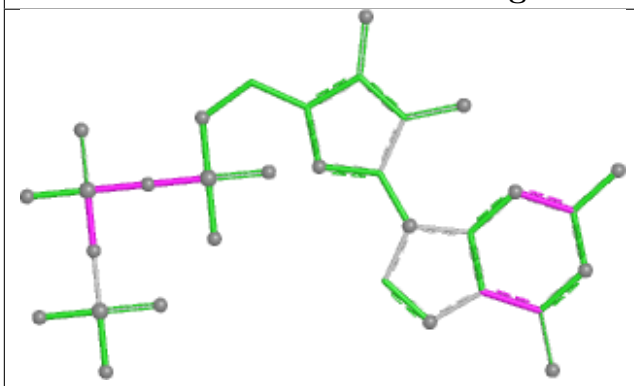

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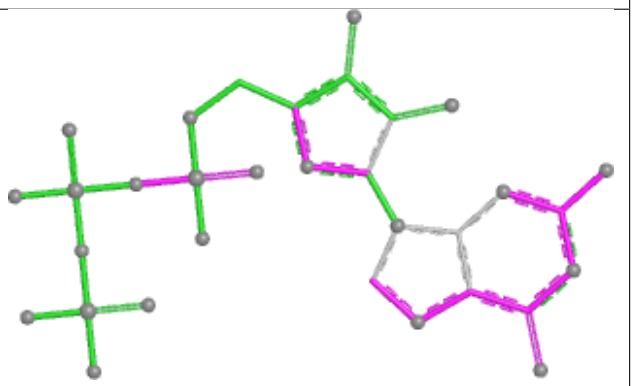
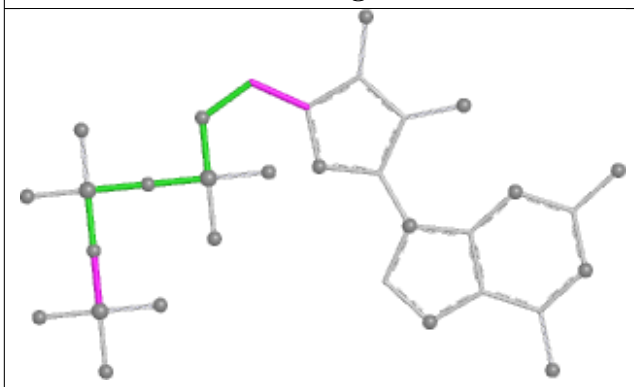
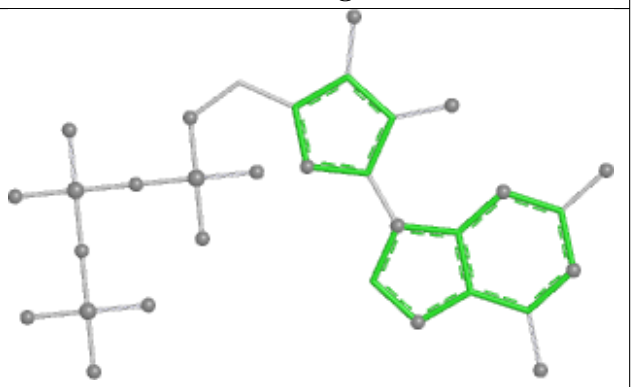


Bond angles



Torsions



Rings

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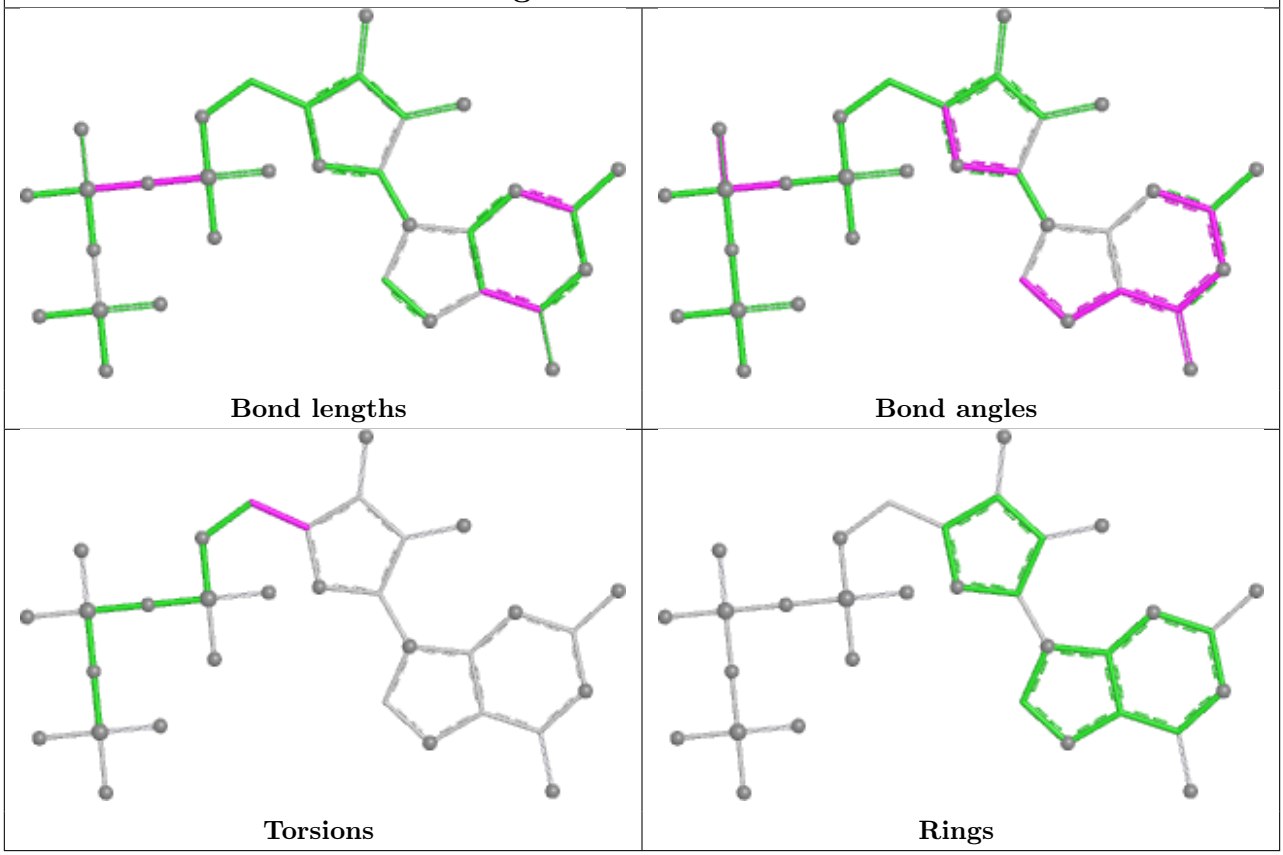


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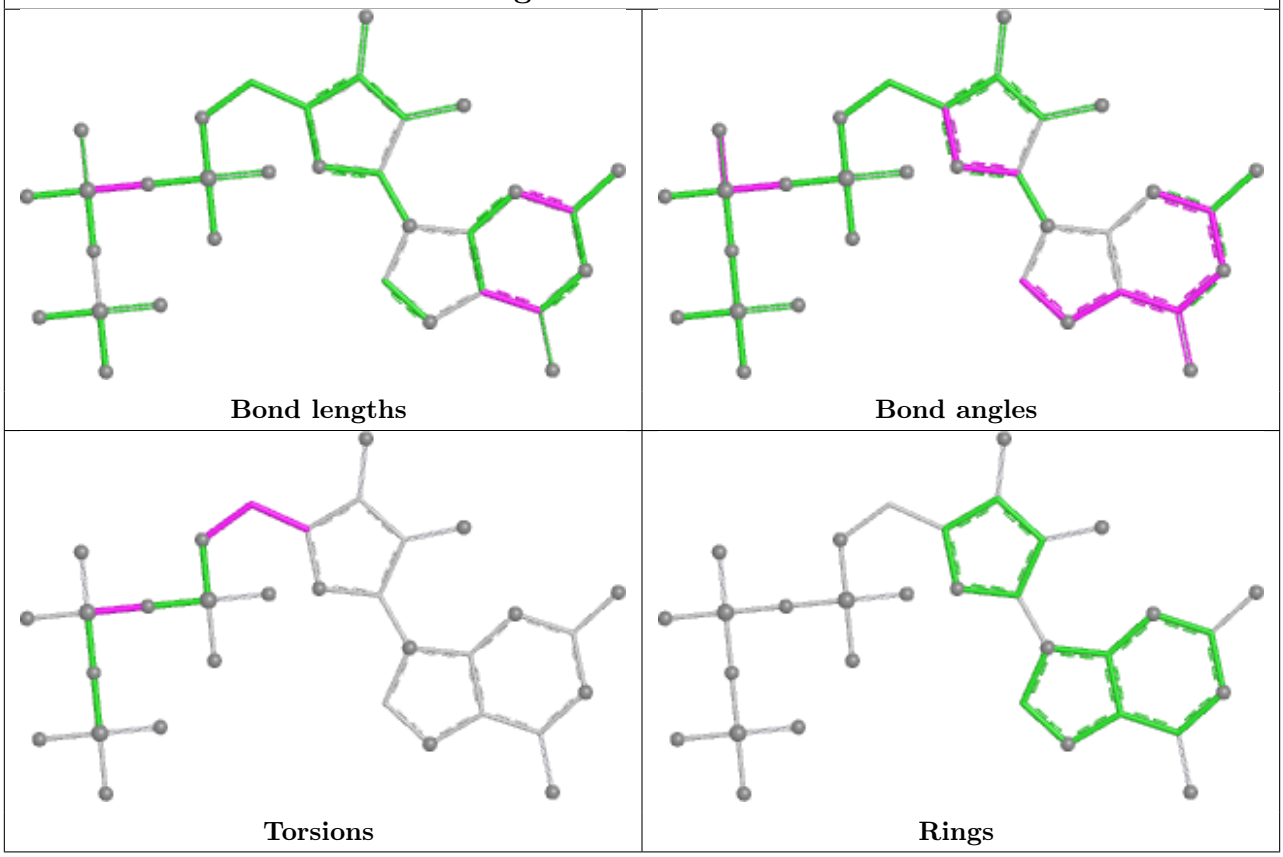

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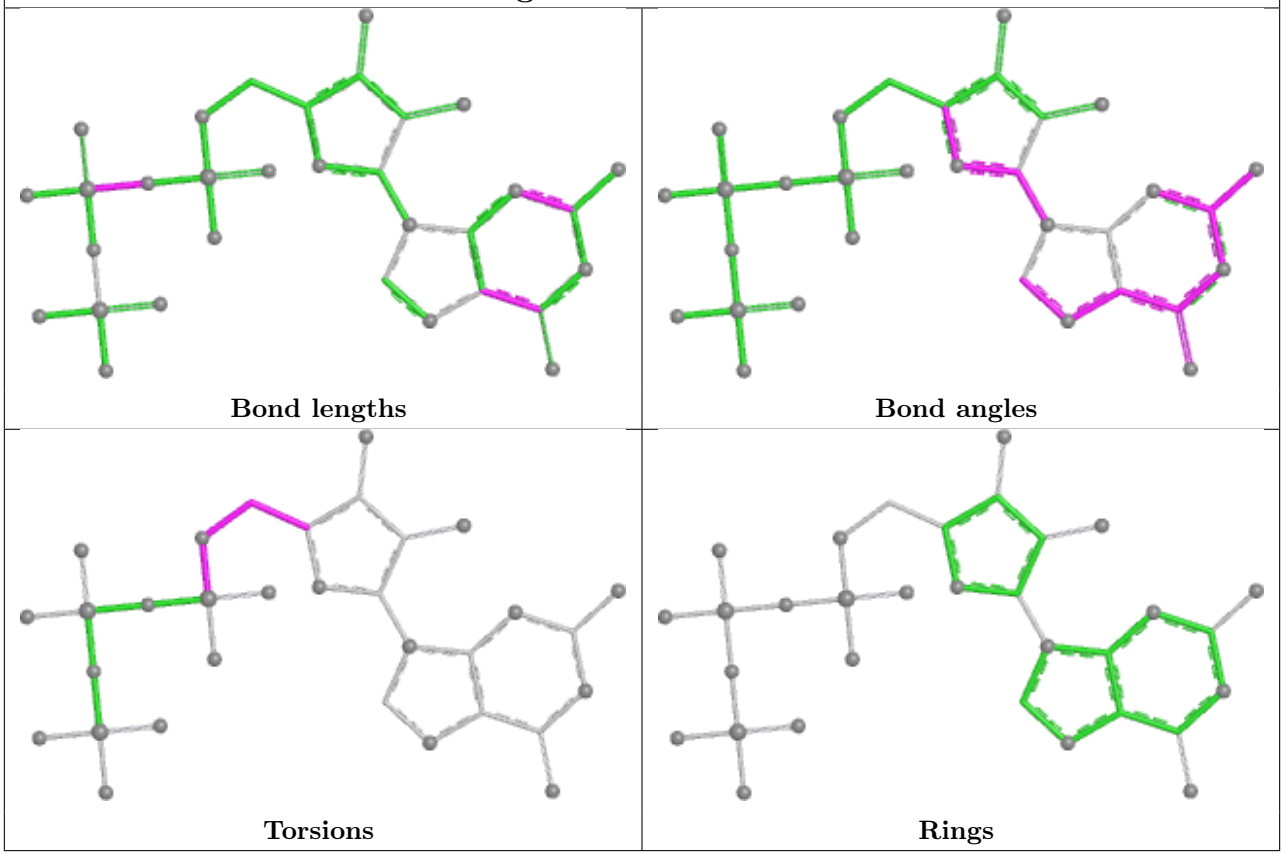


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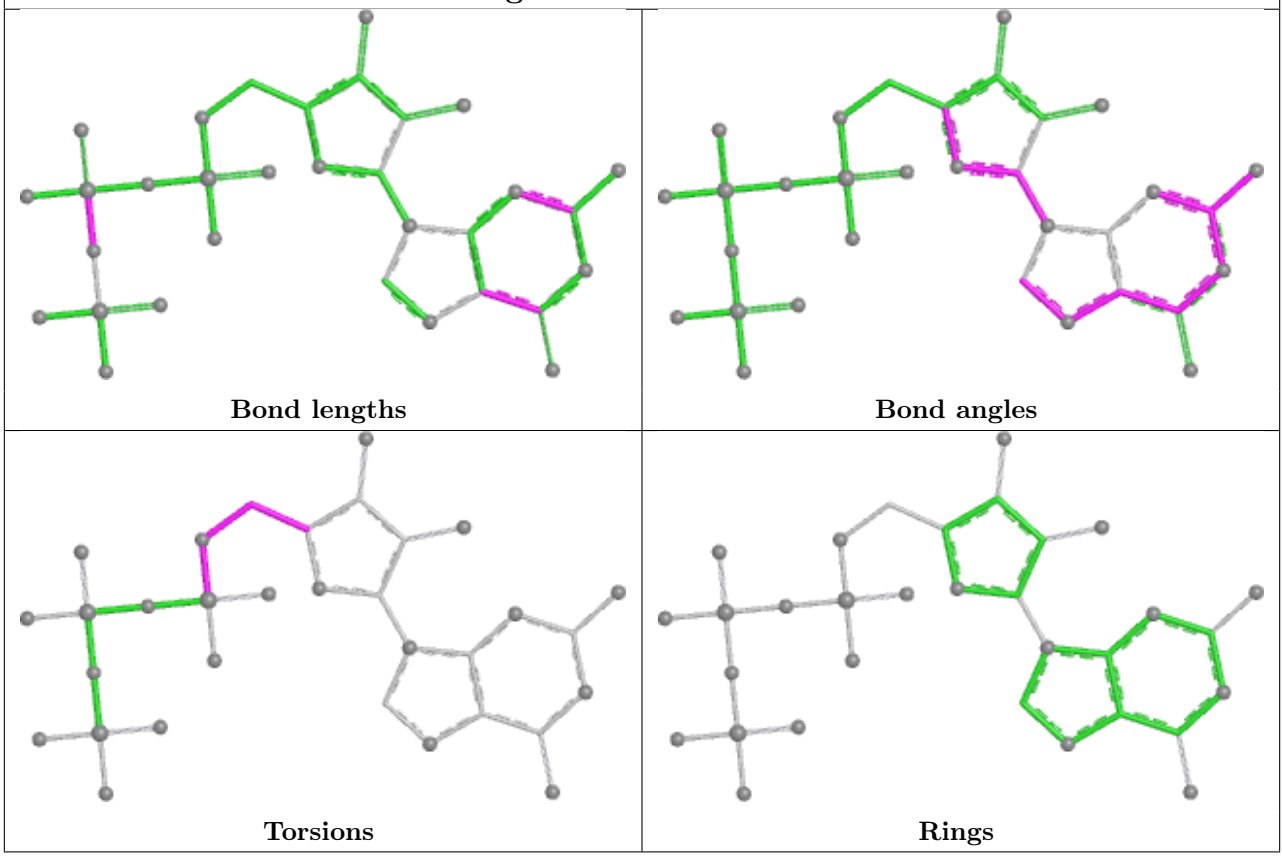

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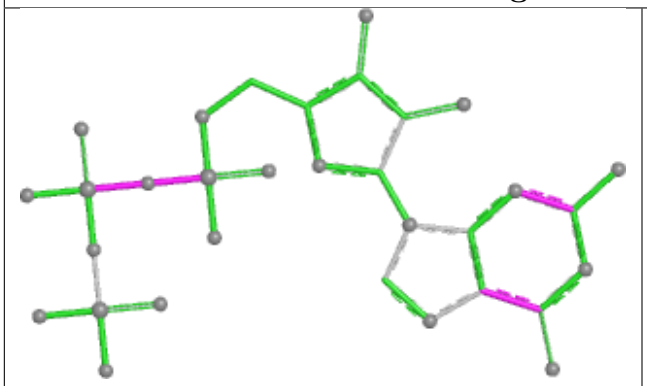

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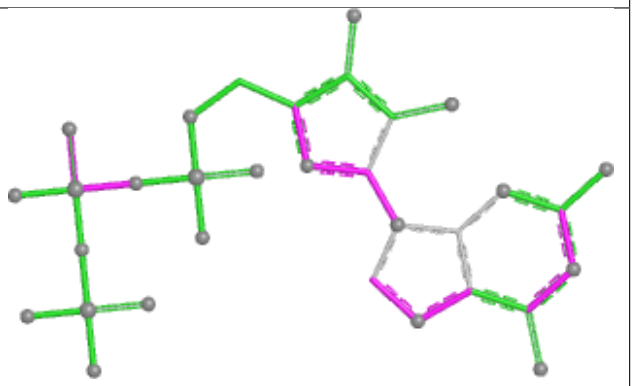

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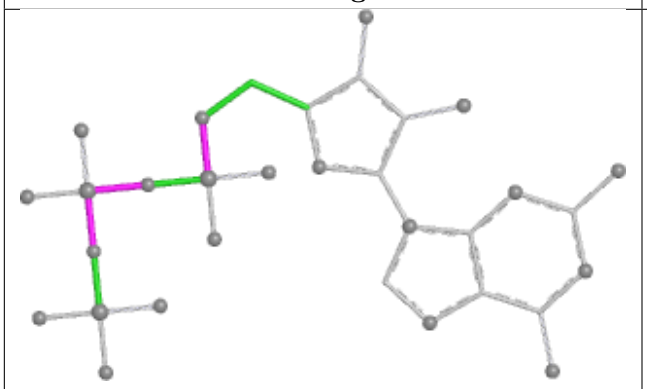

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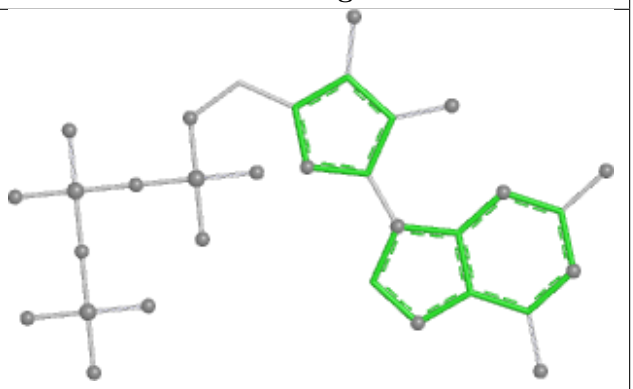

Rings

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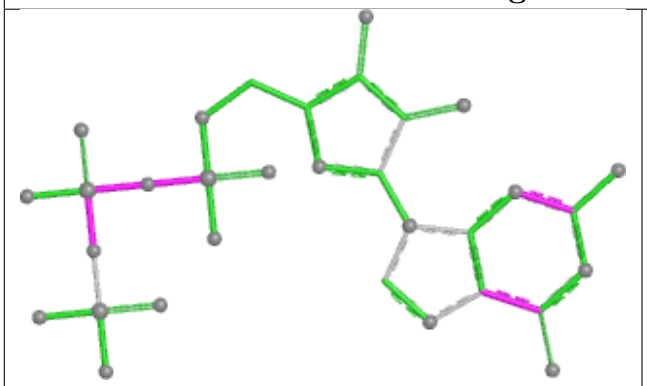

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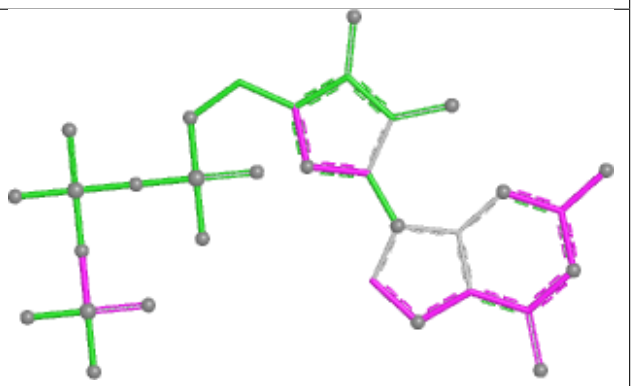

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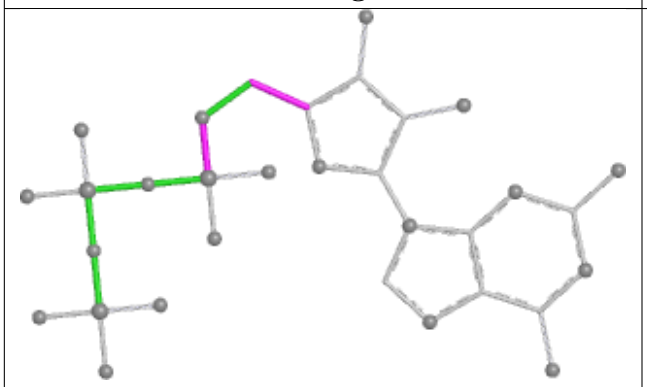

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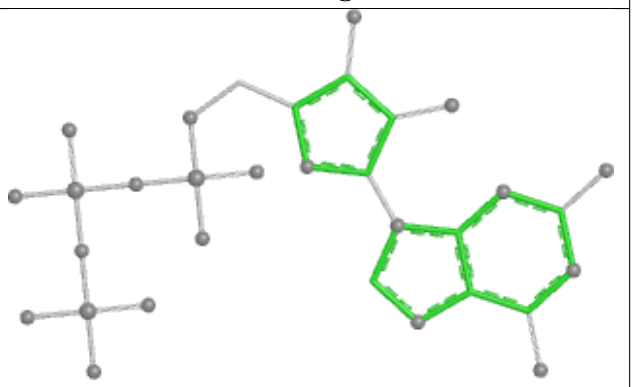

Rings

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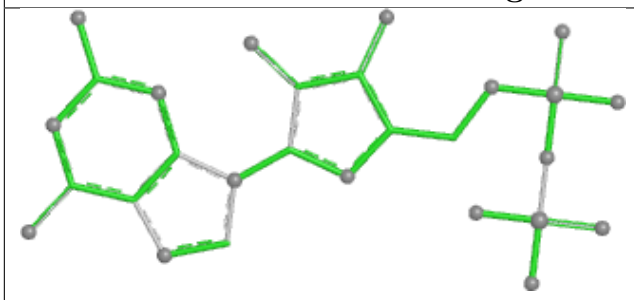

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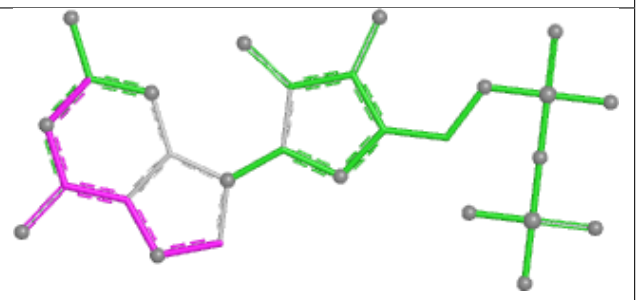

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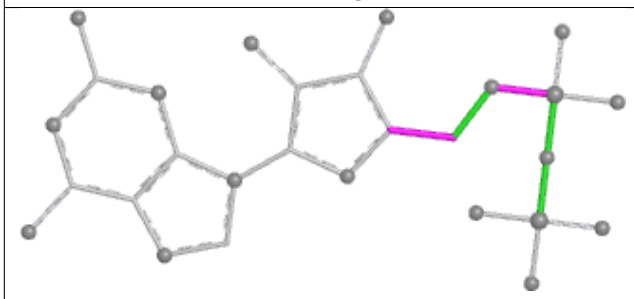

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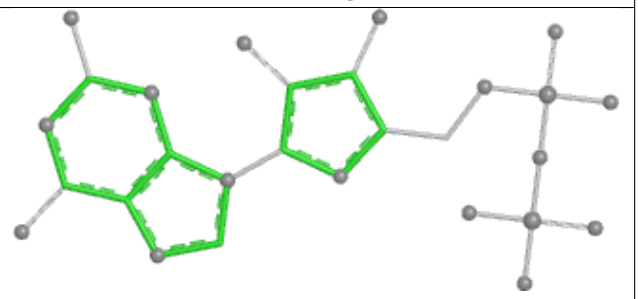
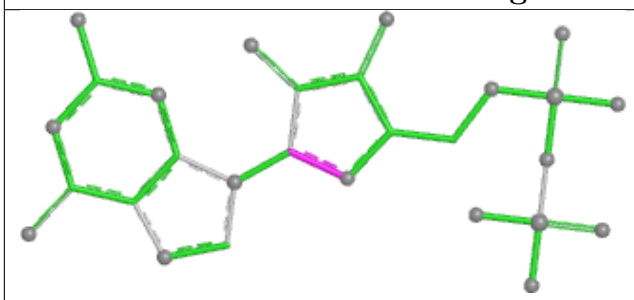


Rings

## Ligand GDP CB 501



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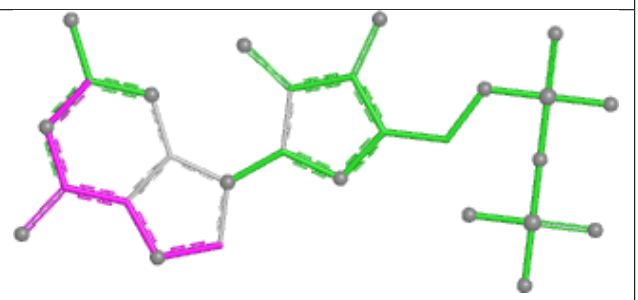

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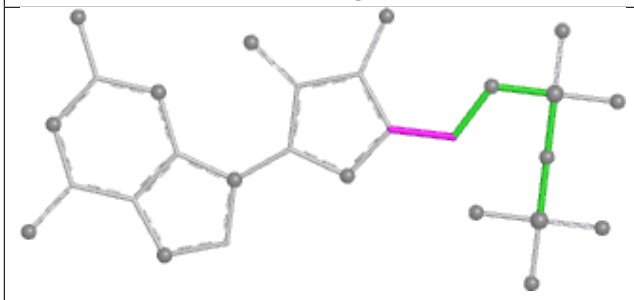

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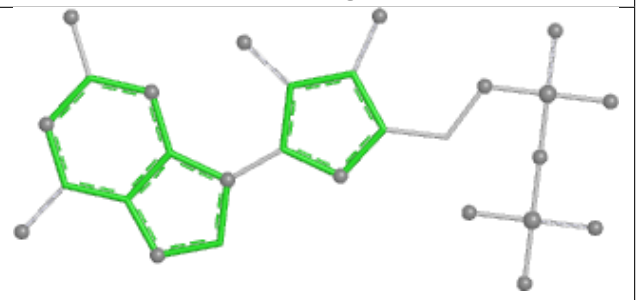

Rings

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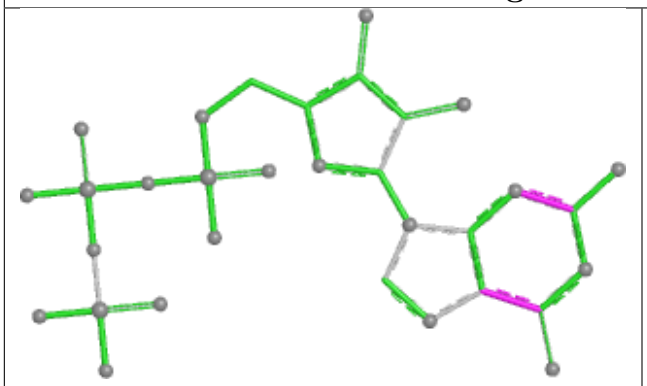

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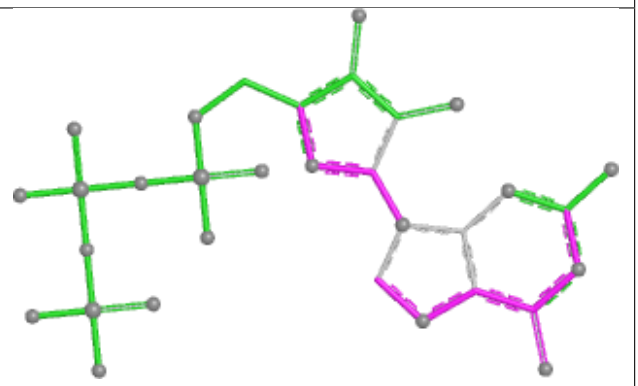

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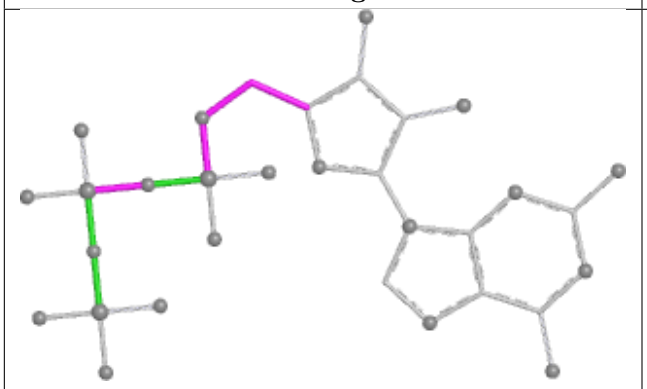

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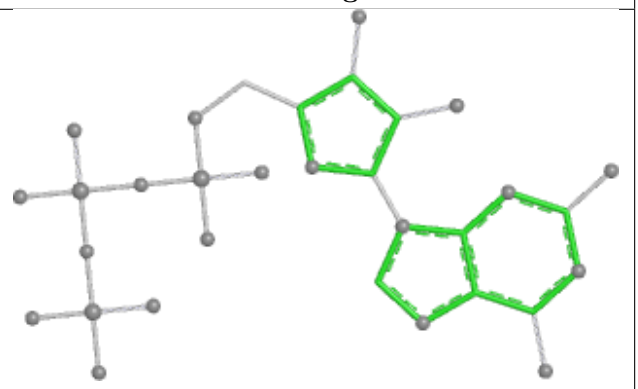
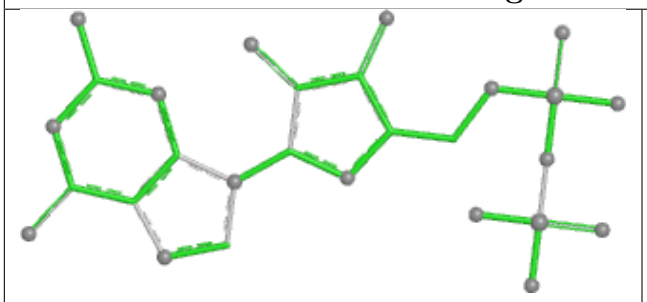


Rings

## Ligand GDP BM 501



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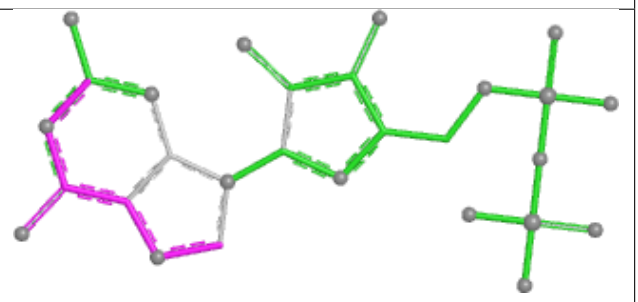

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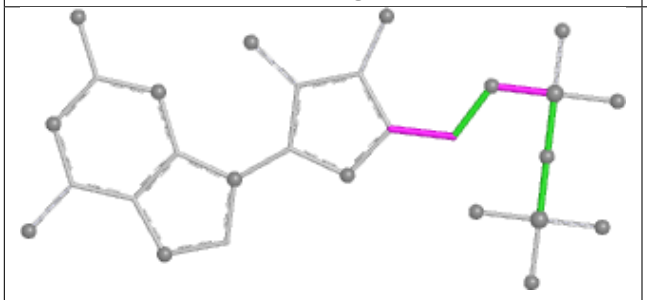

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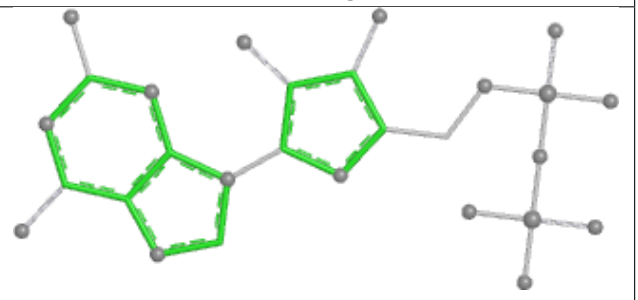

Rings

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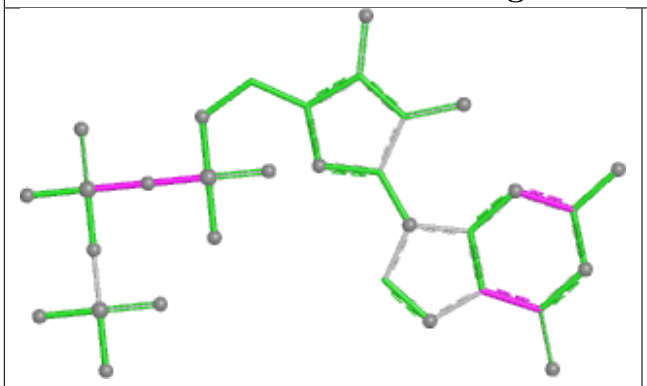

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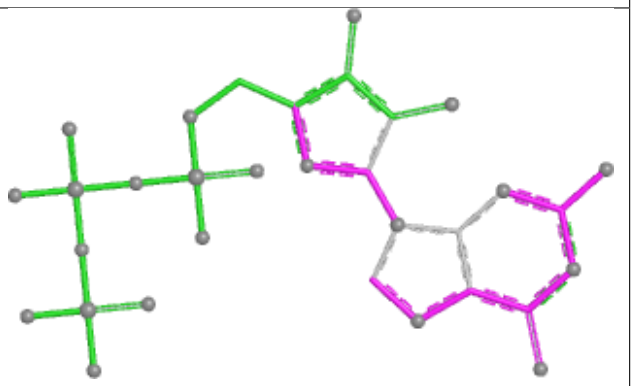

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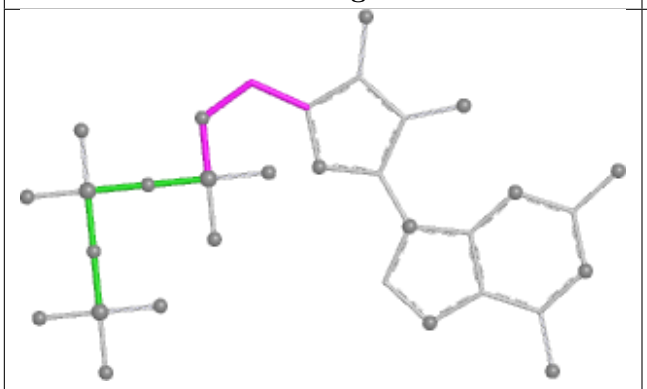

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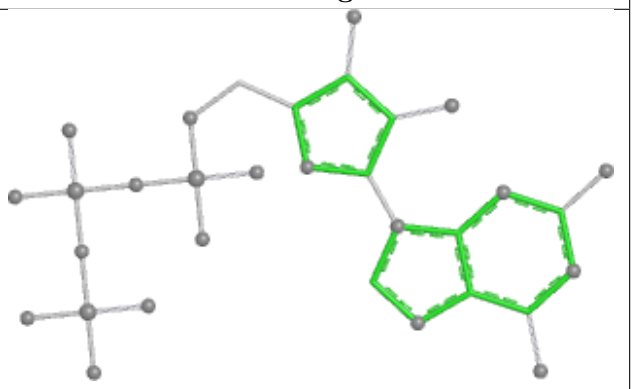

Rings

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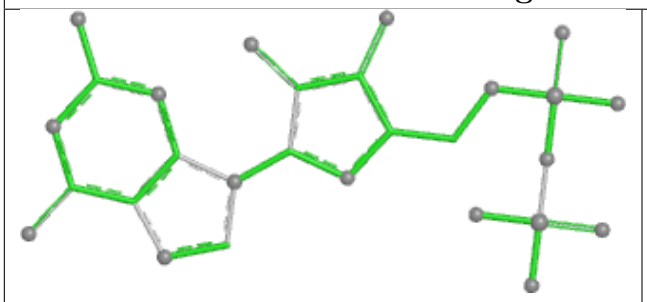

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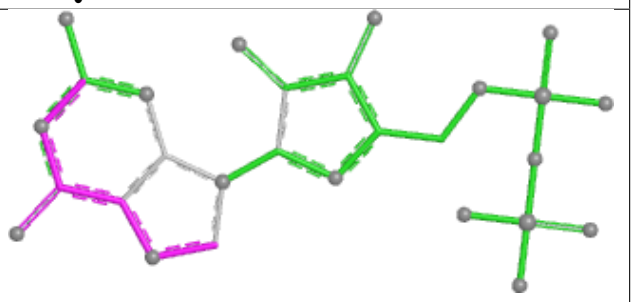

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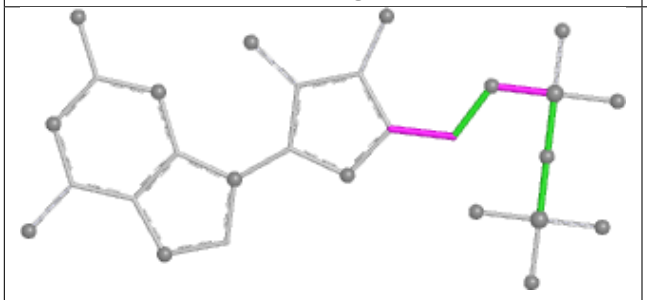

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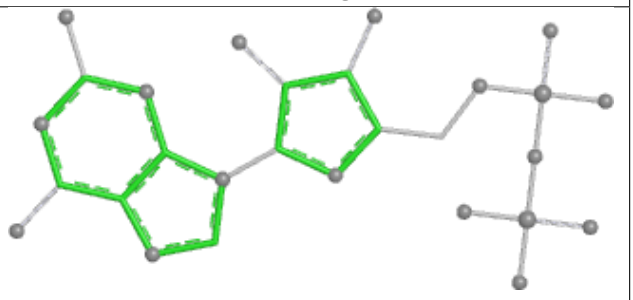

Rings

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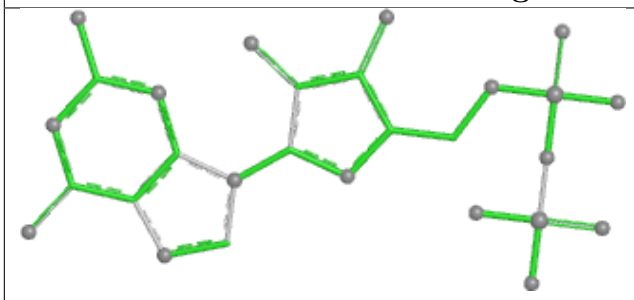

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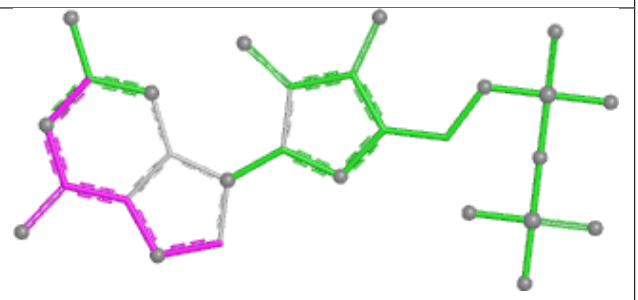

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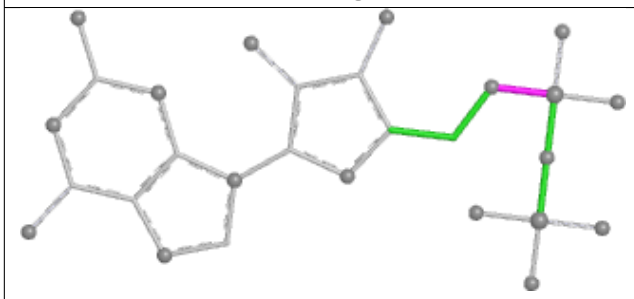

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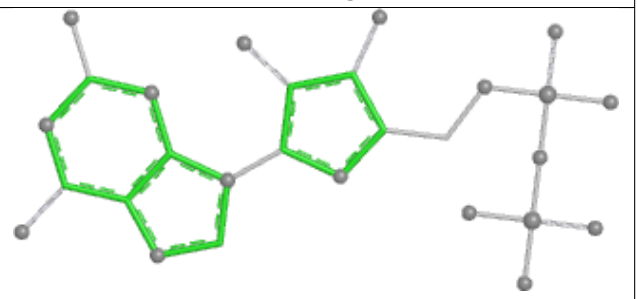

Rings

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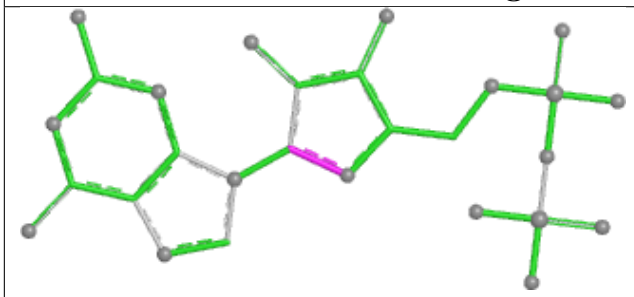

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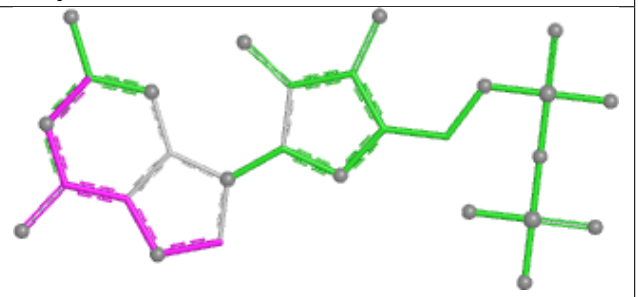

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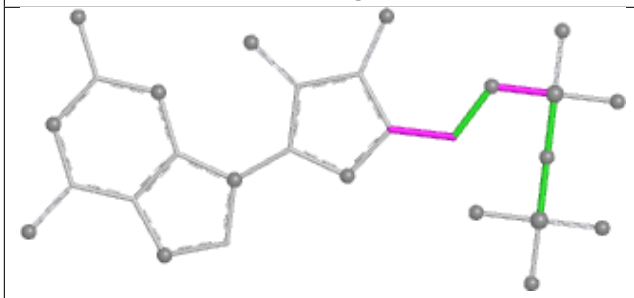

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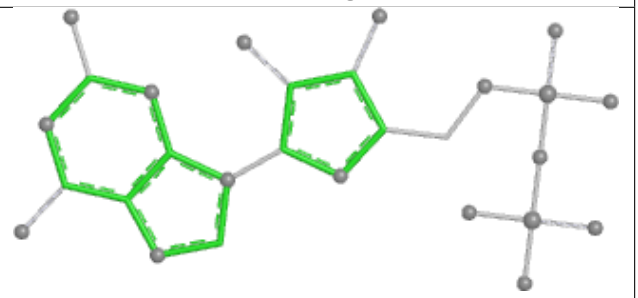
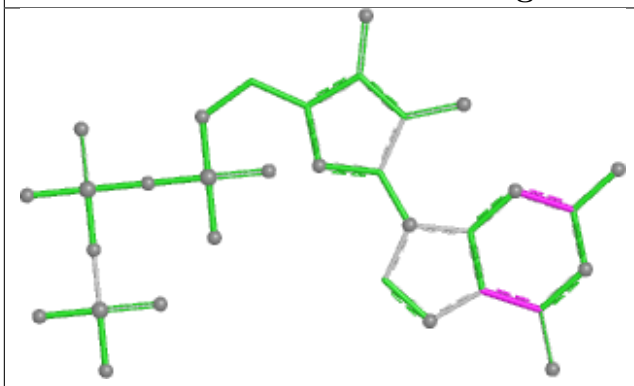


Rings

## Ligand GTP IA 501



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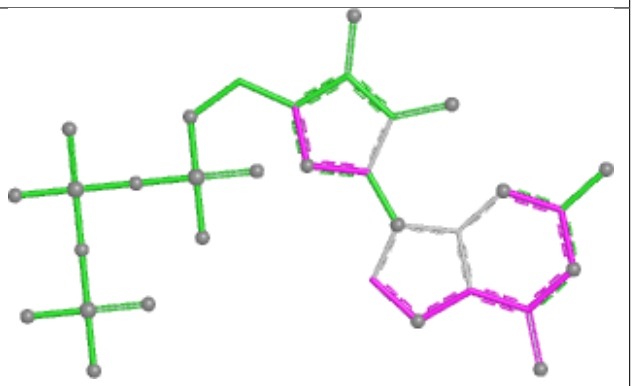

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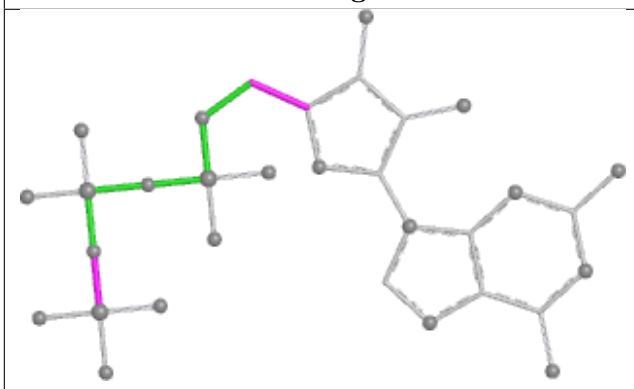

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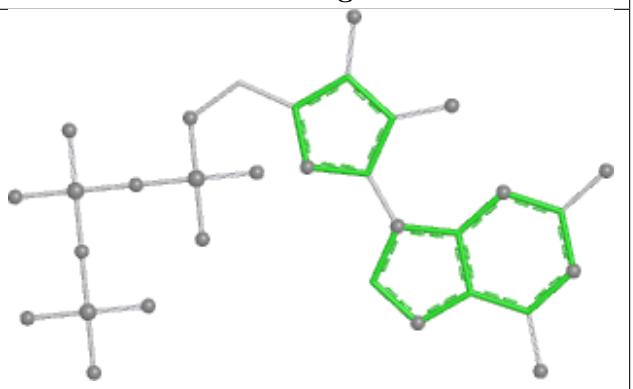

Rings

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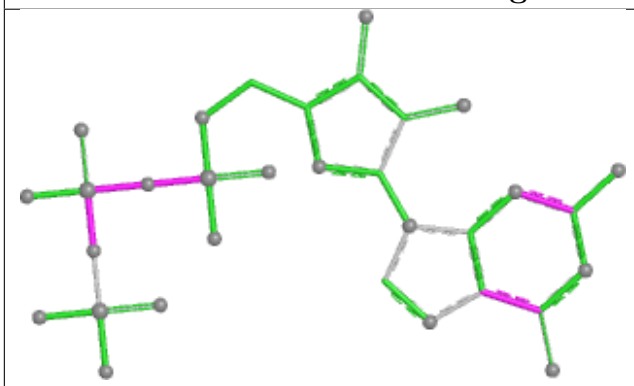

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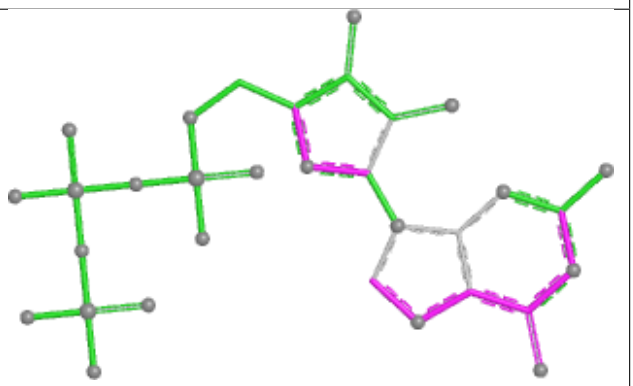

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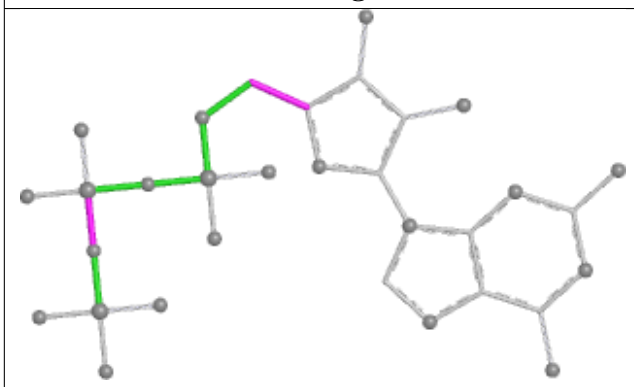

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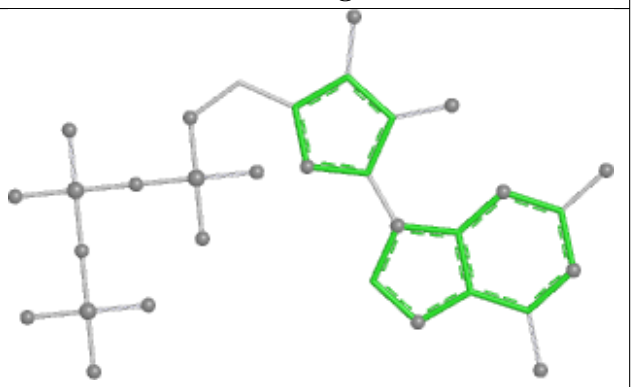
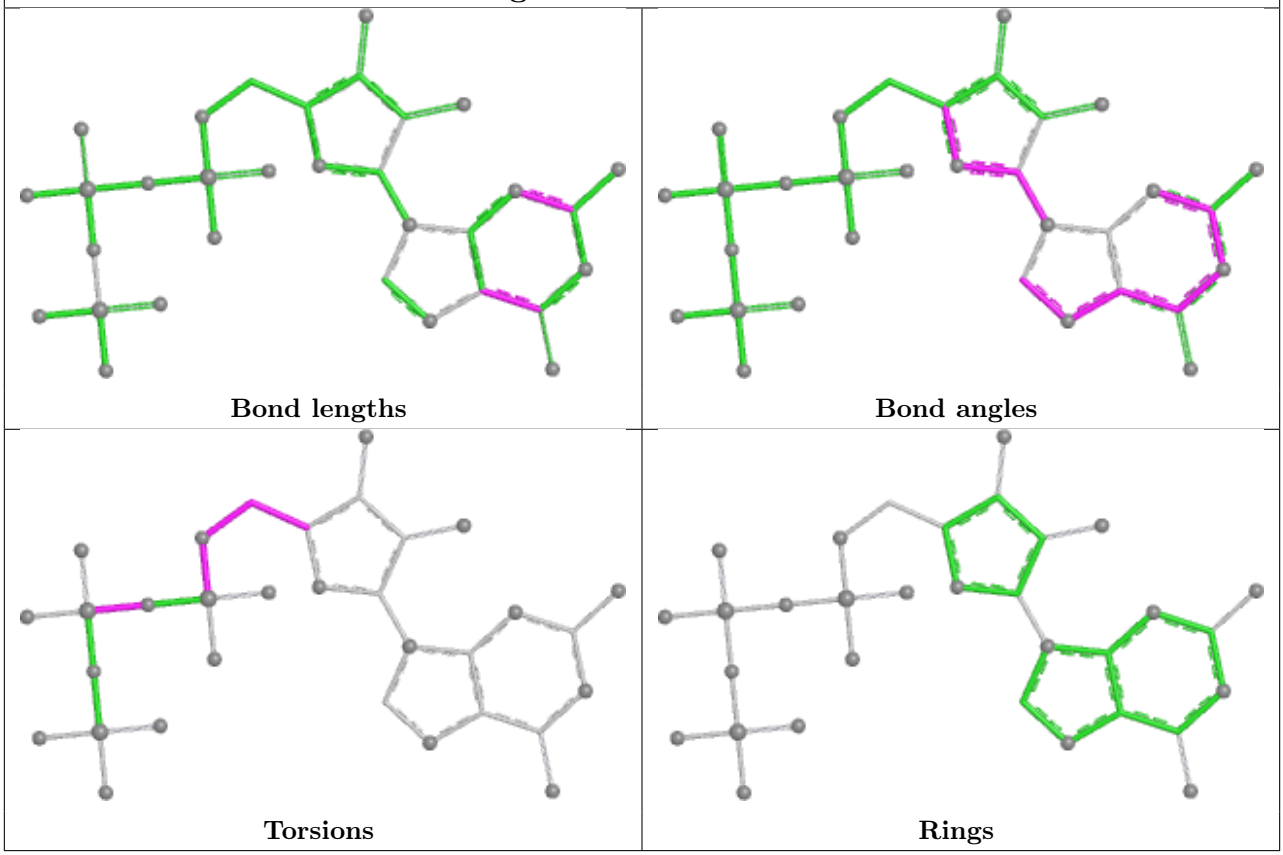
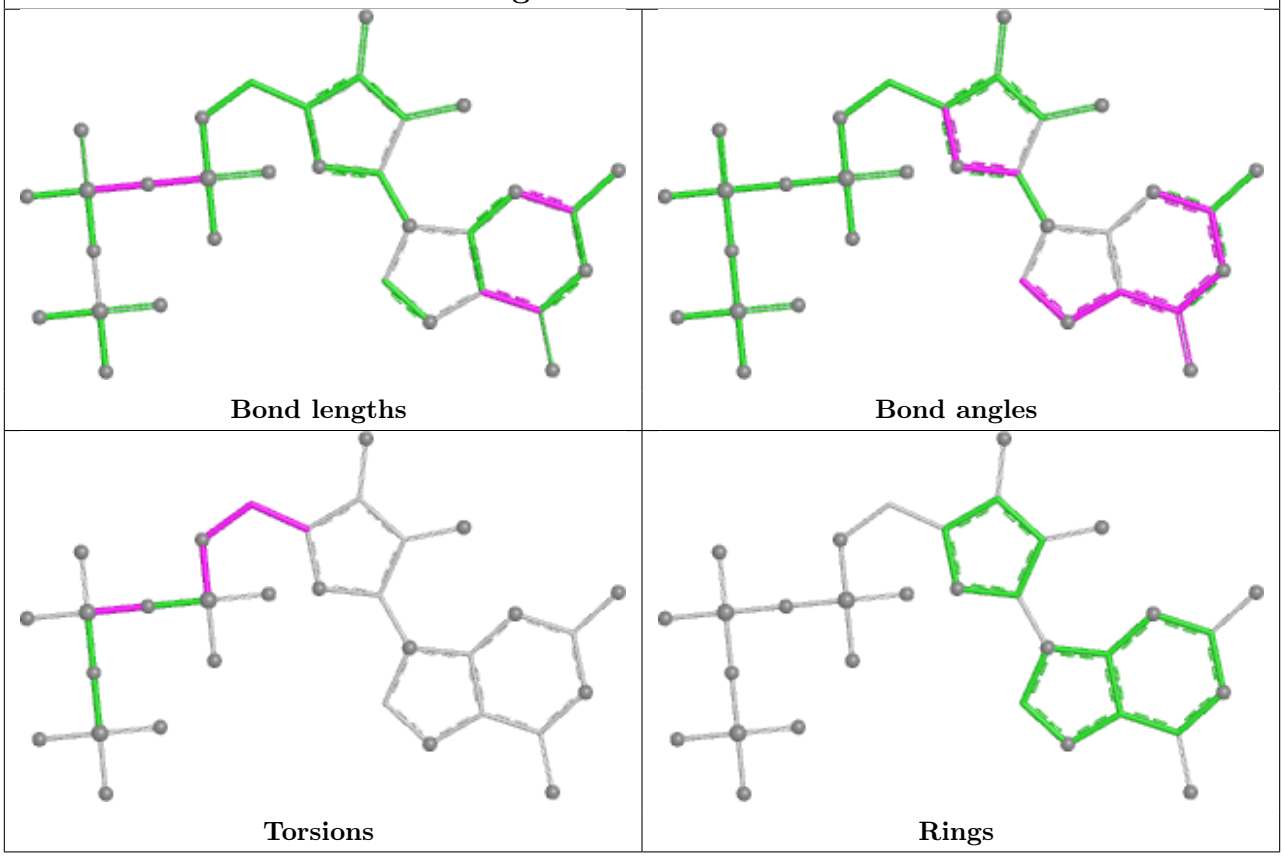


Rings

## Ligand GTP RG 501




## Ligand GTP CF 501



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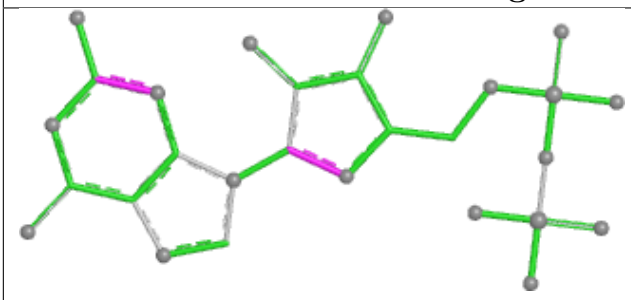

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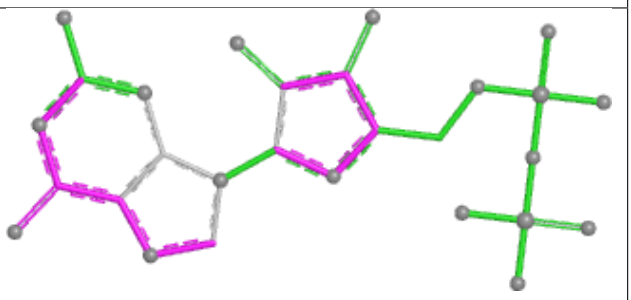

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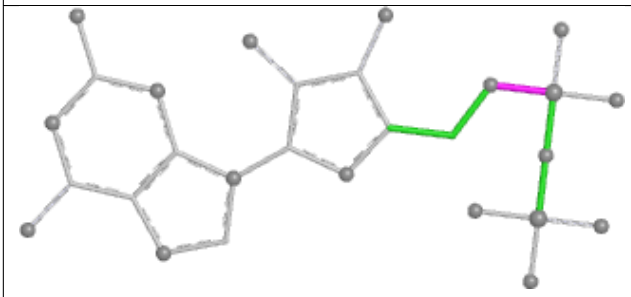
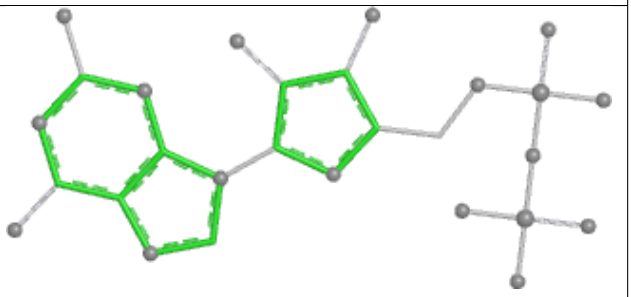
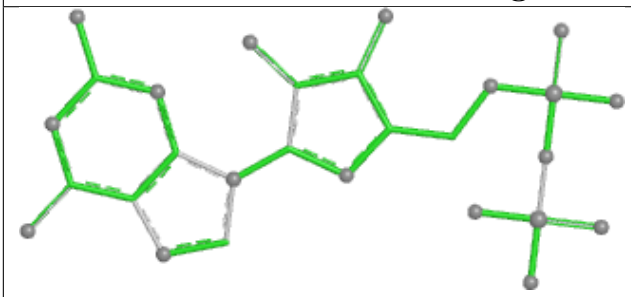


Torsions



Rings

## Ligand GDP OL 502



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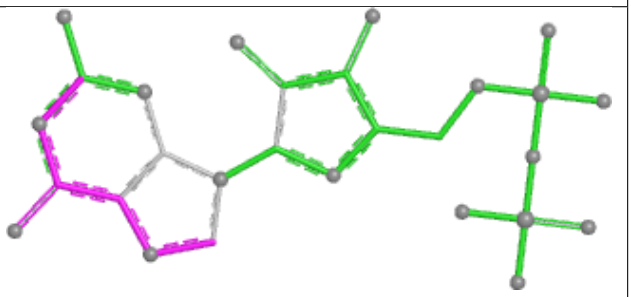

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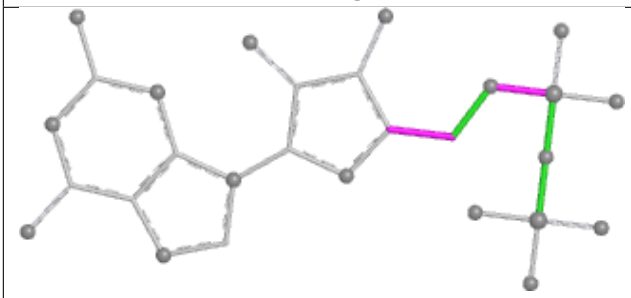

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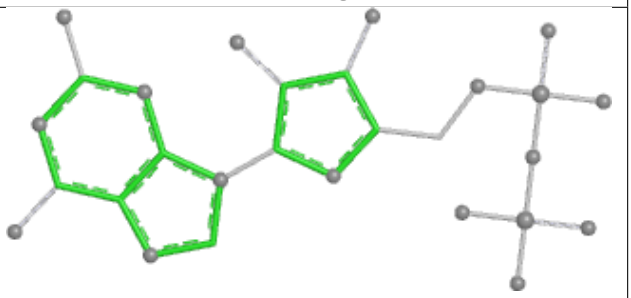

Rings

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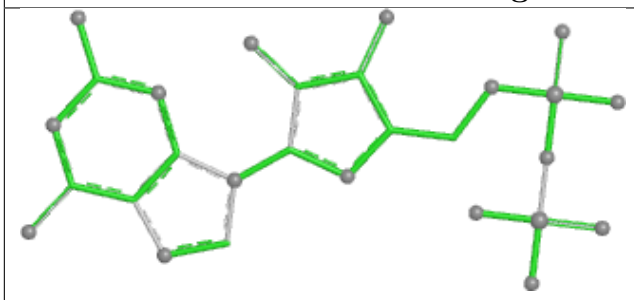

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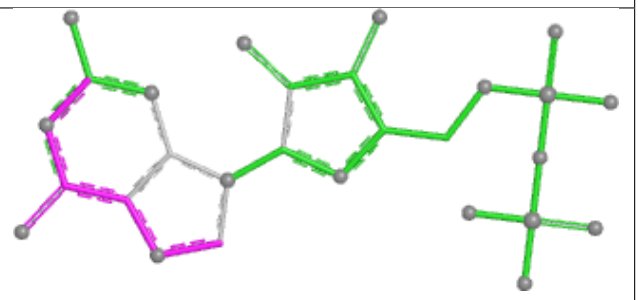

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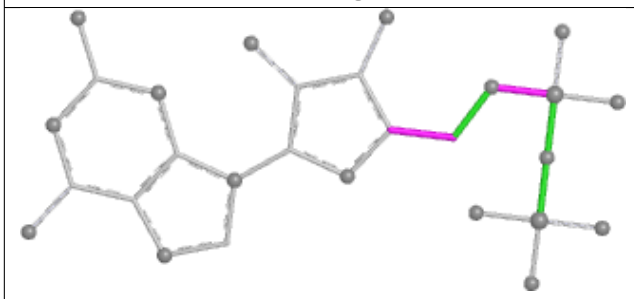

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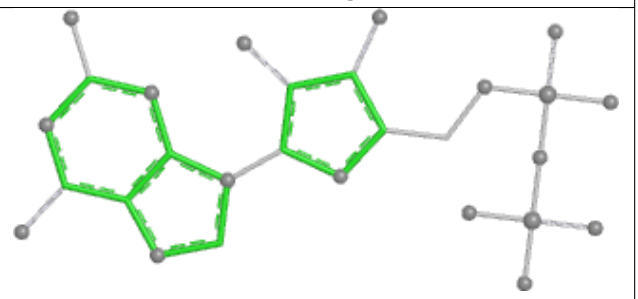

Rings

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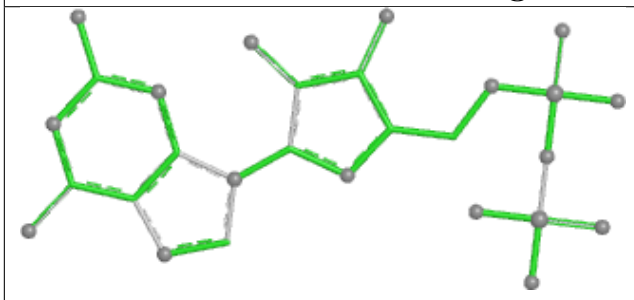

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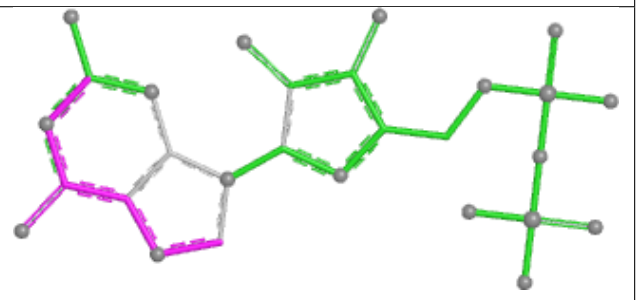

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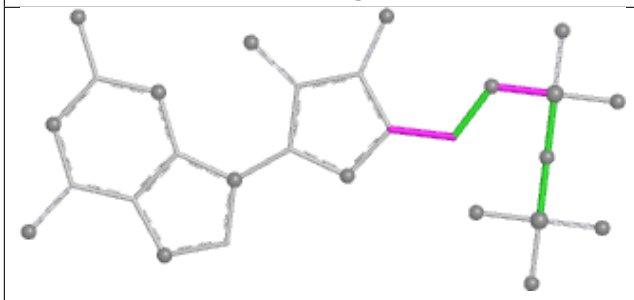

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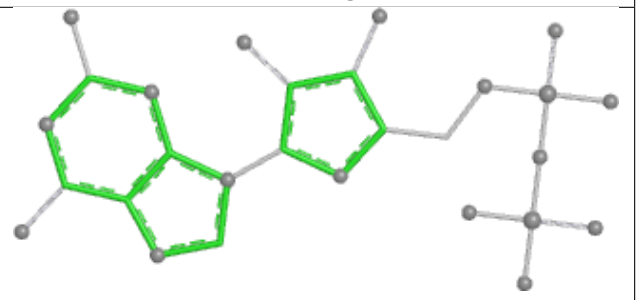

Rings

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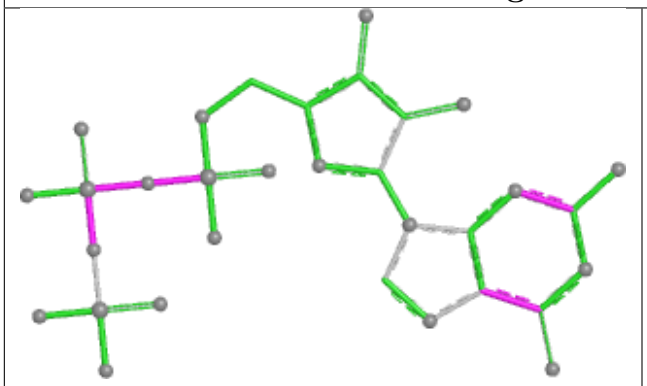

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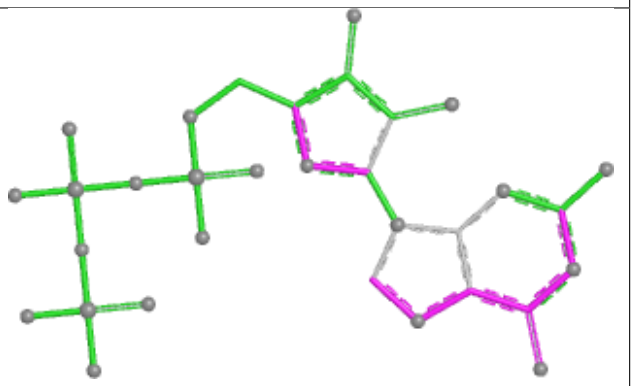

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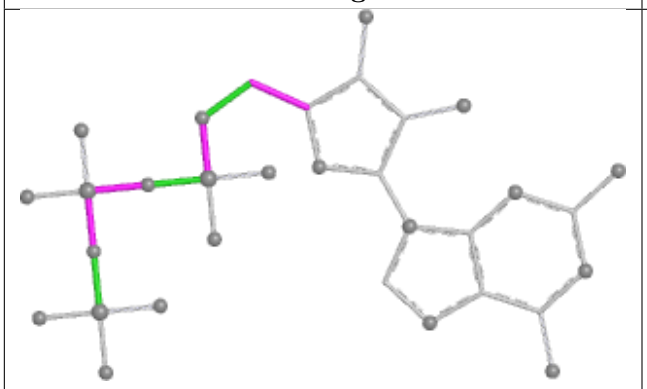

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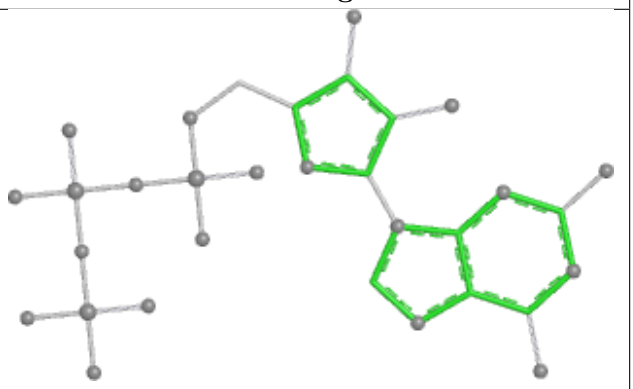

Rings

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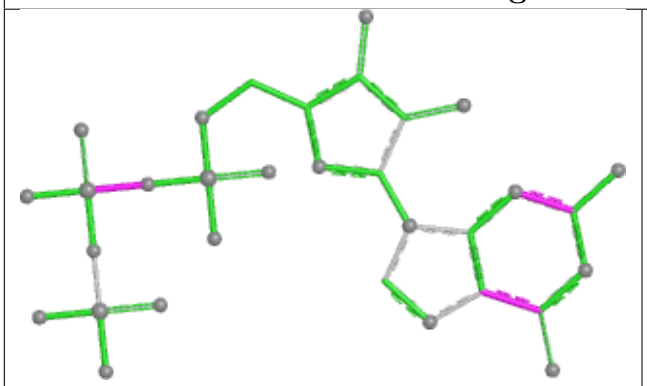

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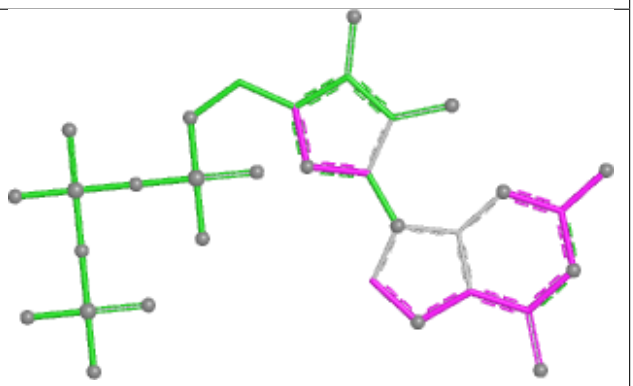

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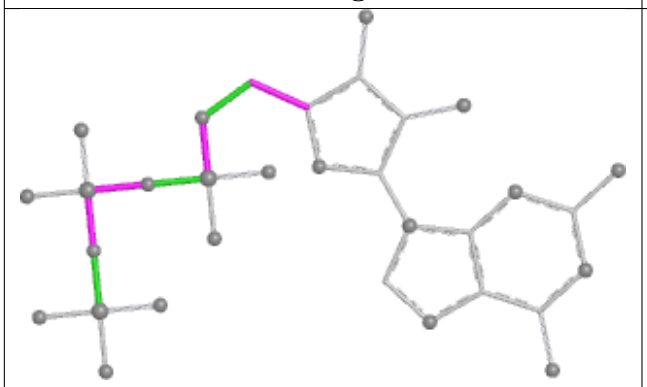

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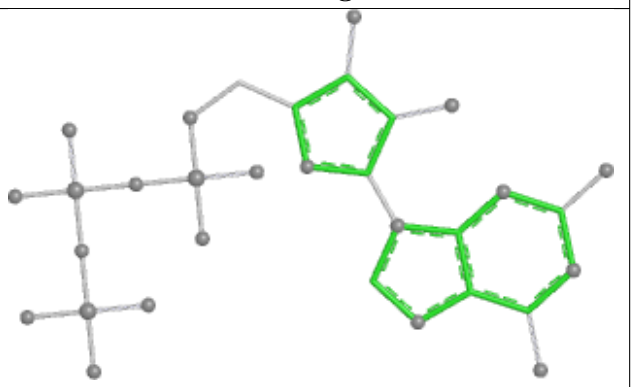

Rings

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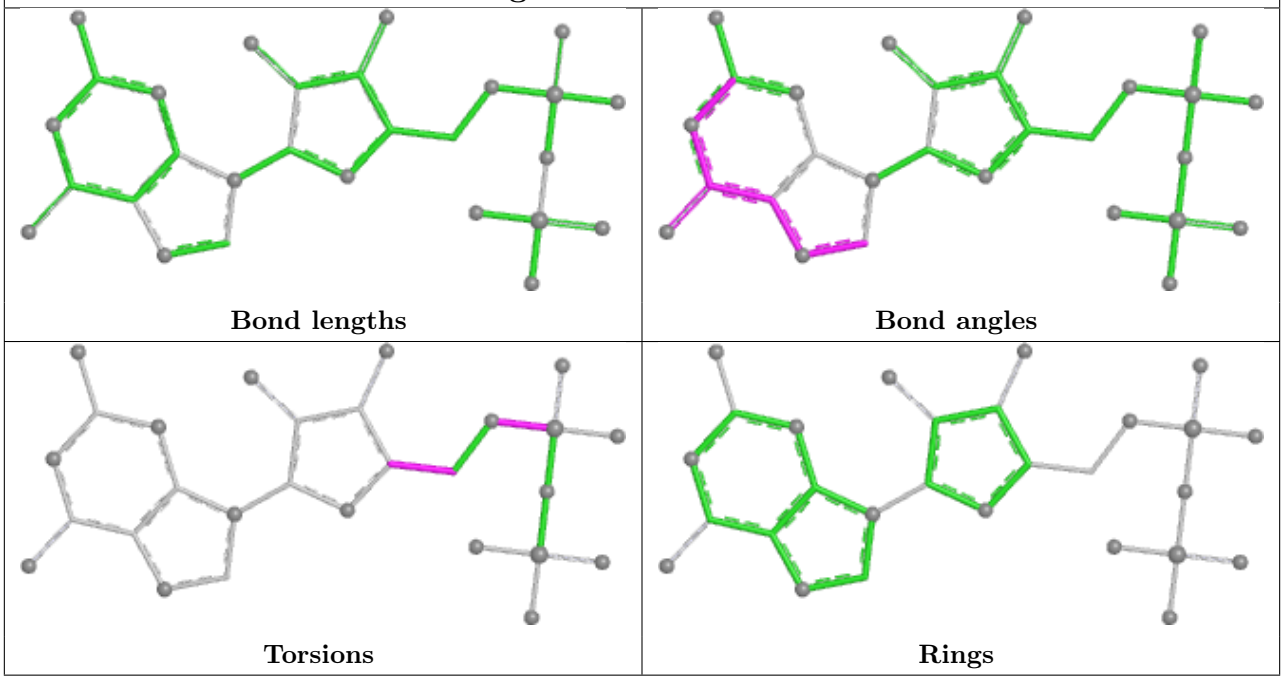


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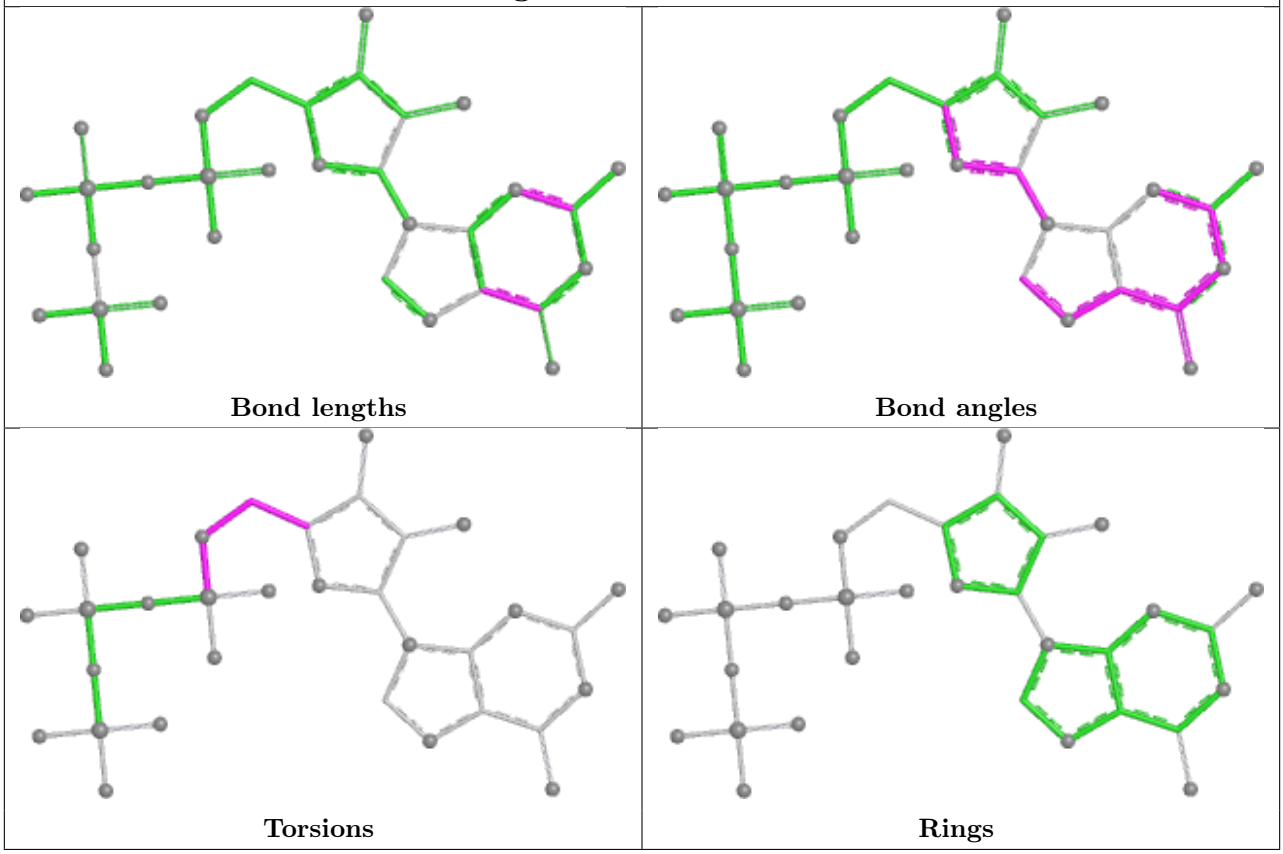

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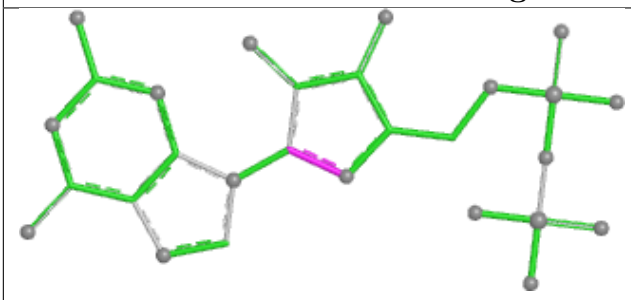

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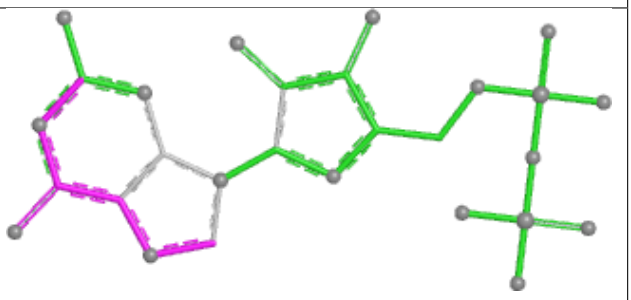

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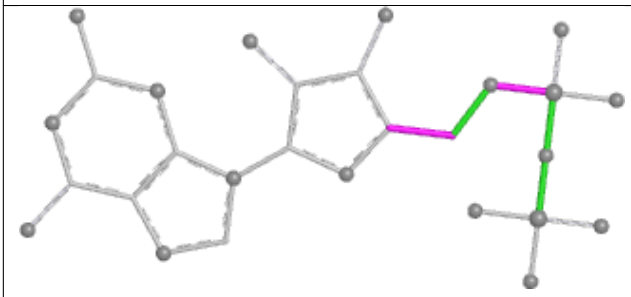

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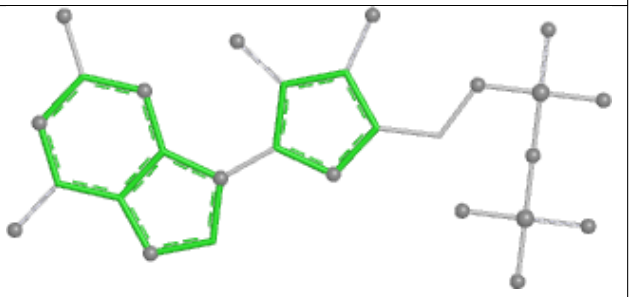

Rings

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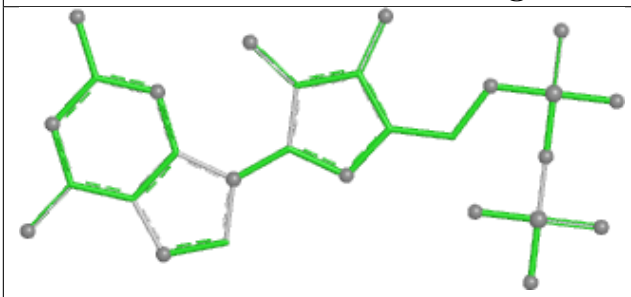

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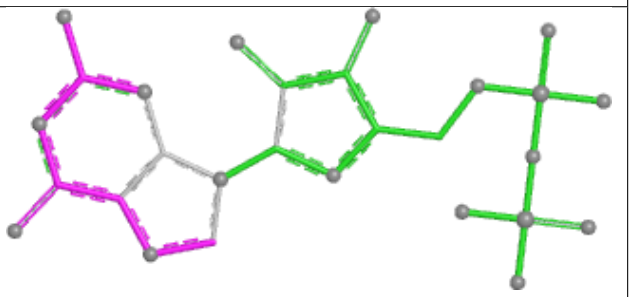

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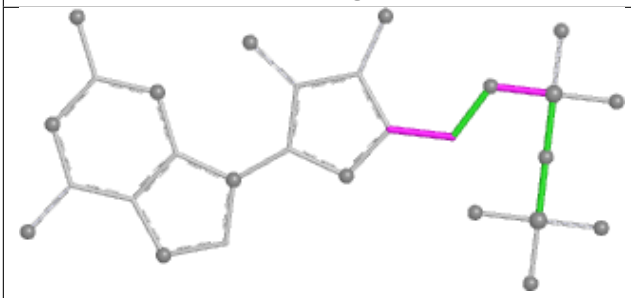

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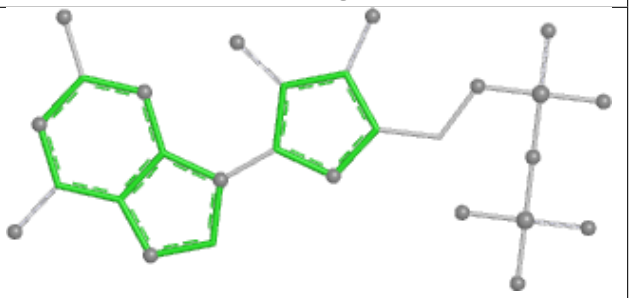

Rings

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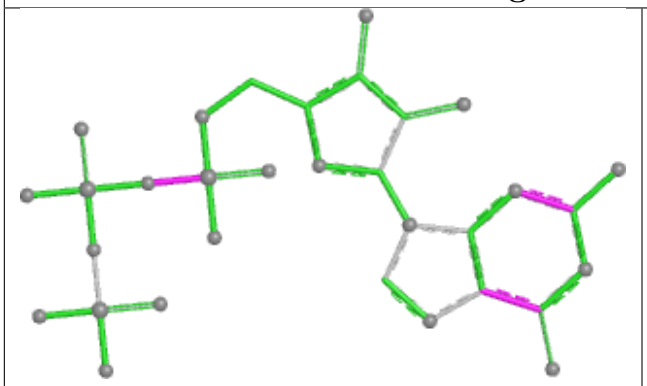

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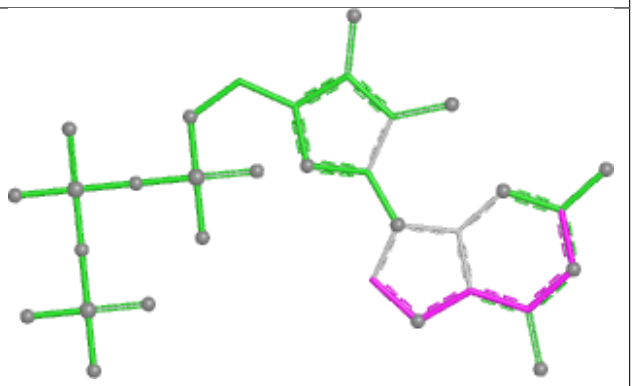

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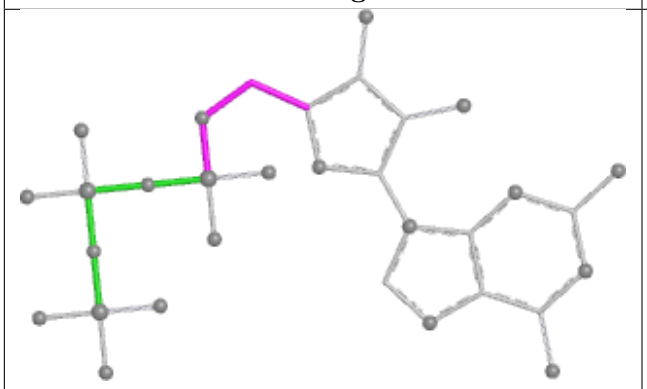

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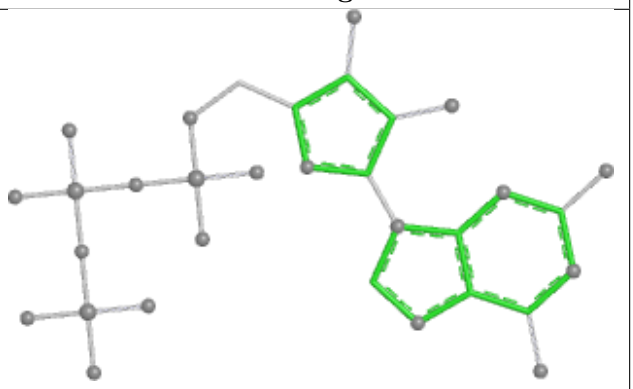

Rings

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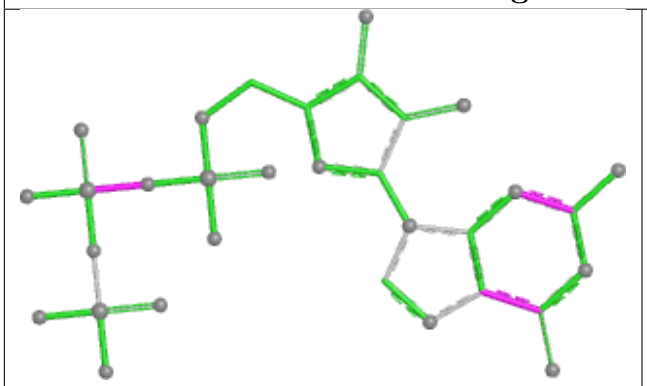

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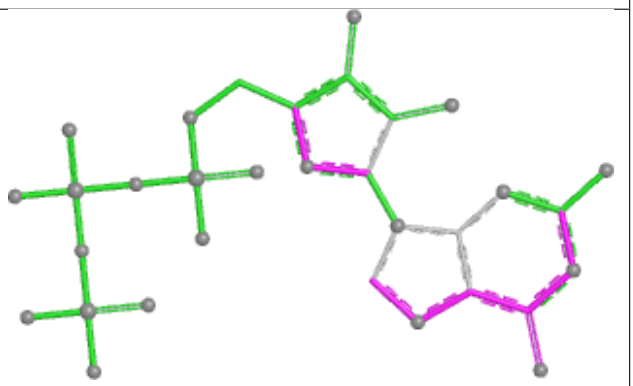

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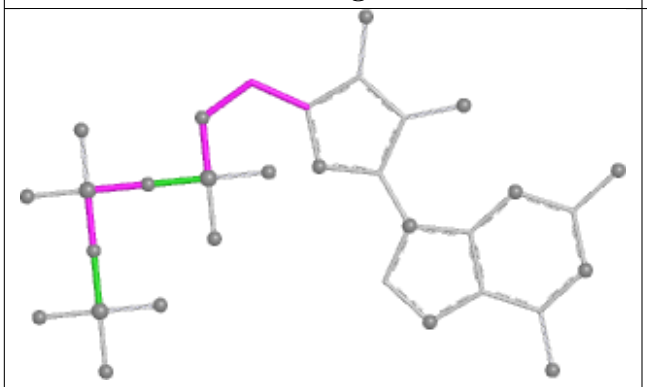

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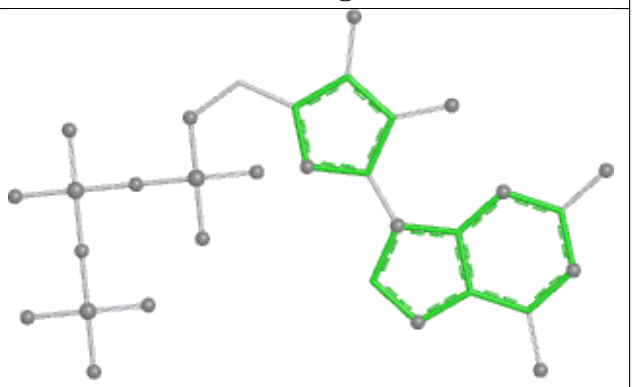

Rings

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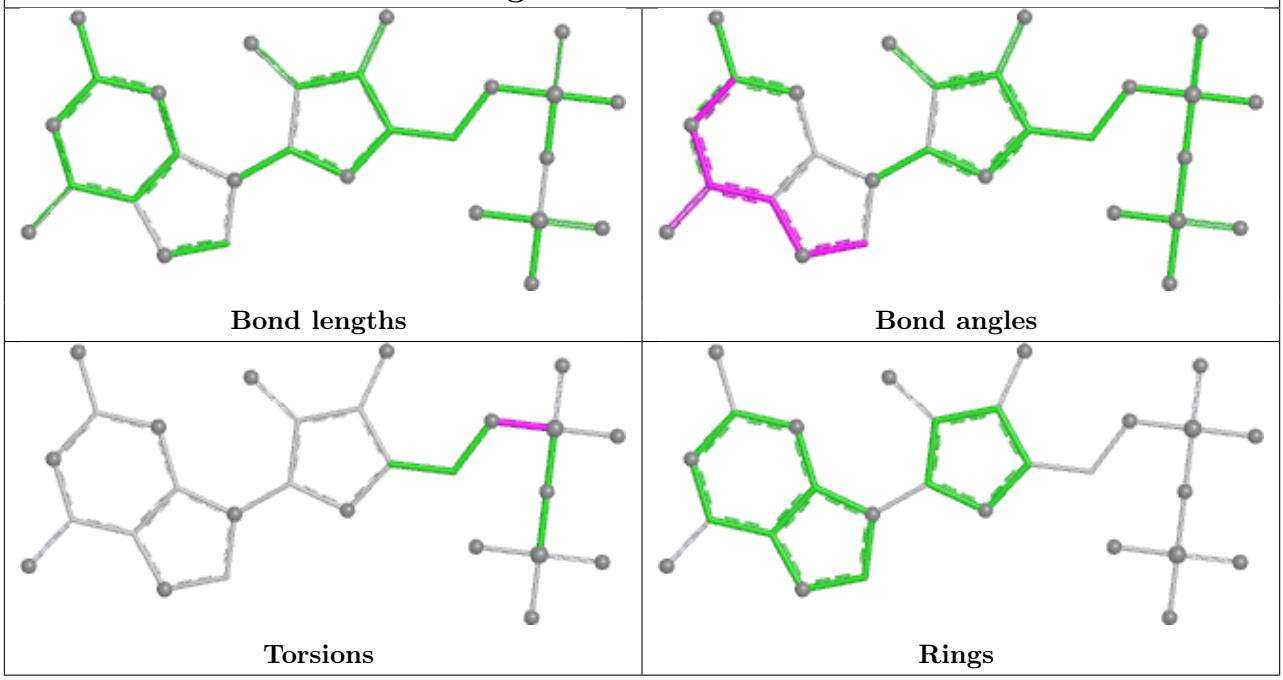


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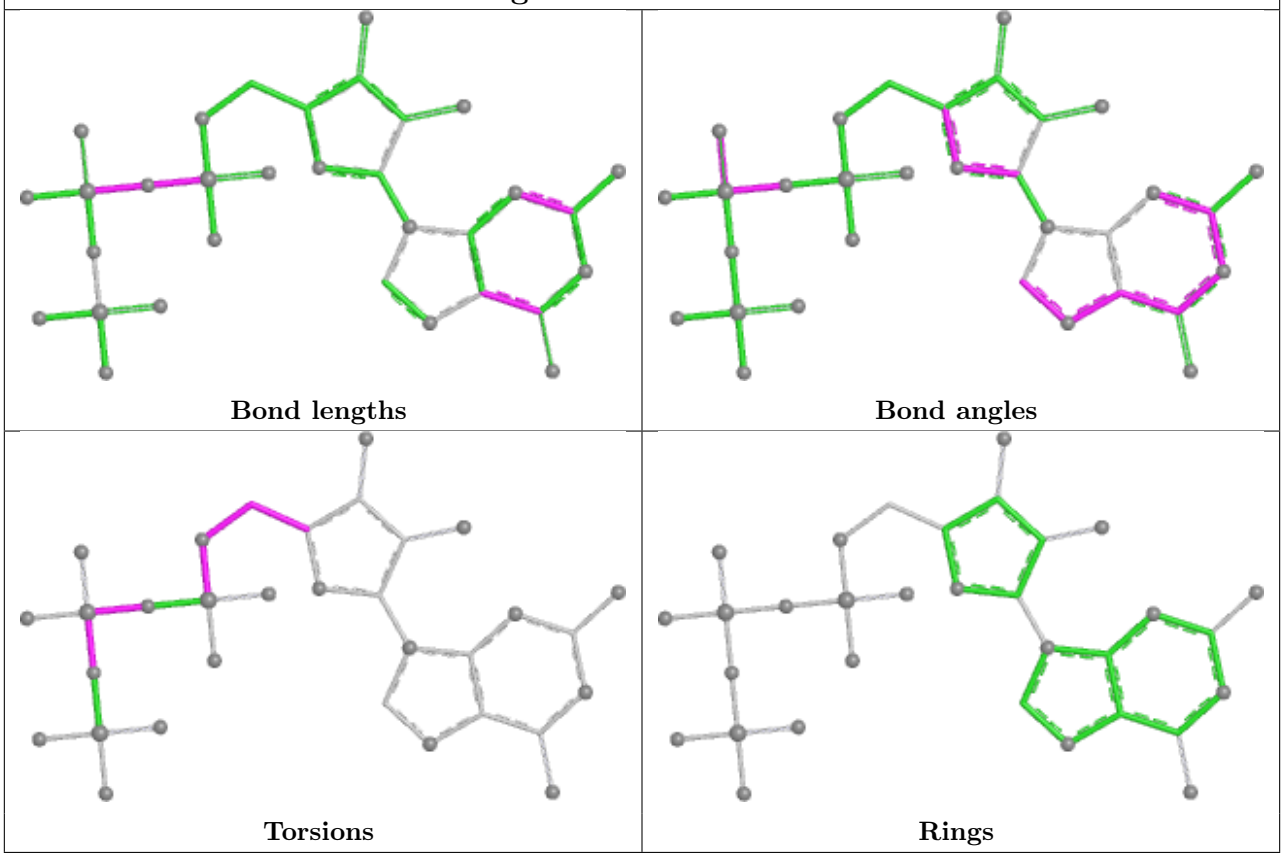

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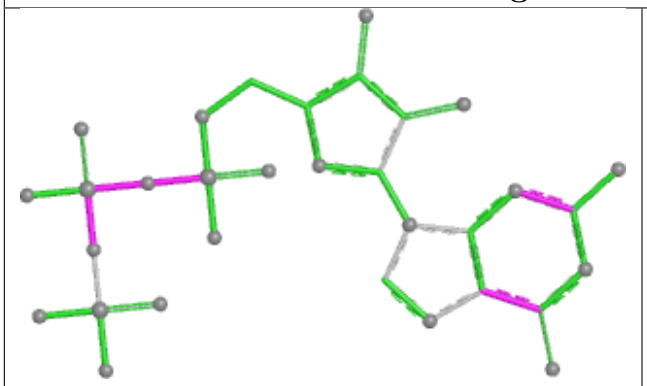

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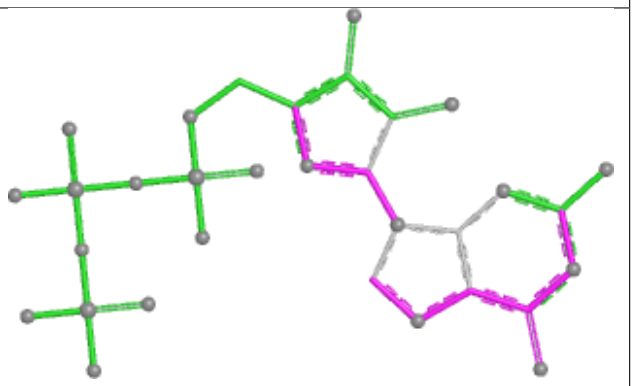

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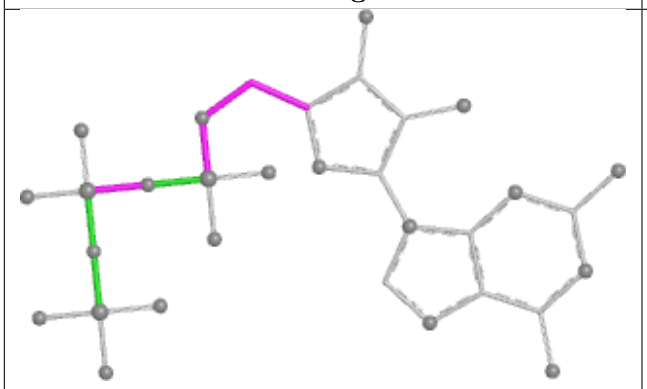

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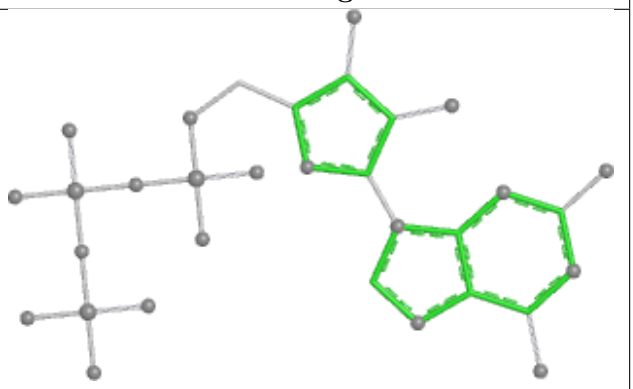

Rings

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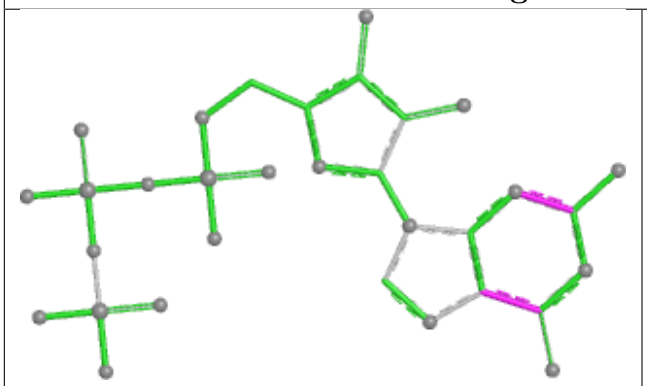

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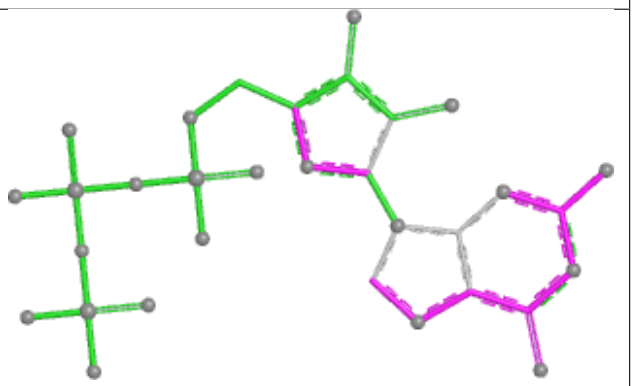

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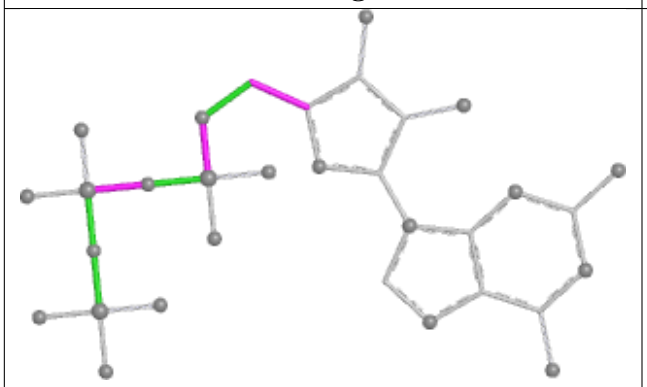

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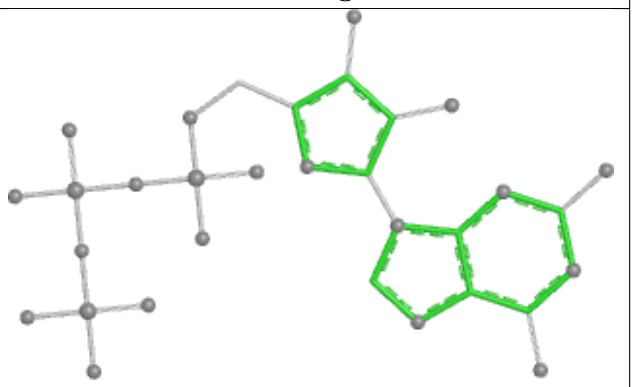

Rings

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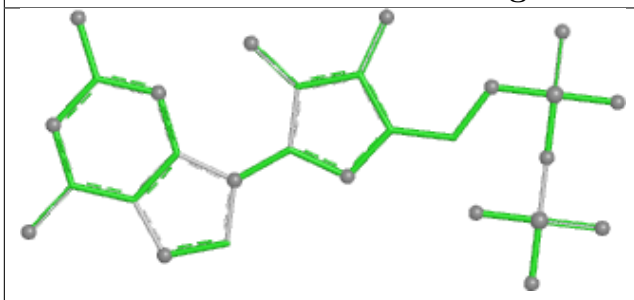

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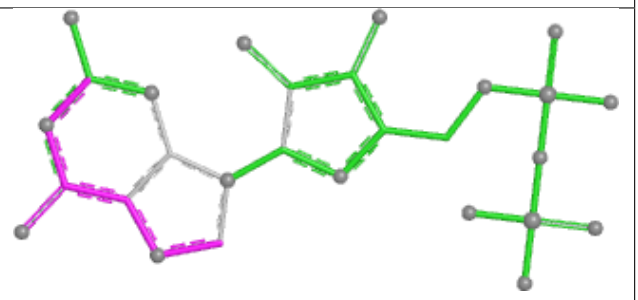

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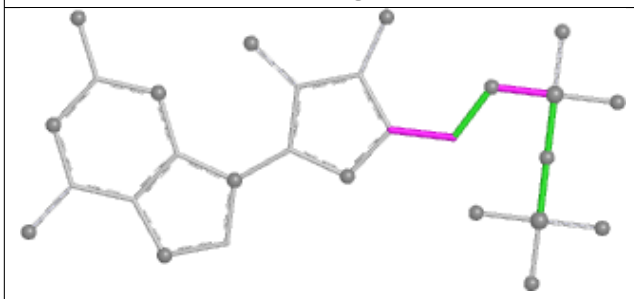
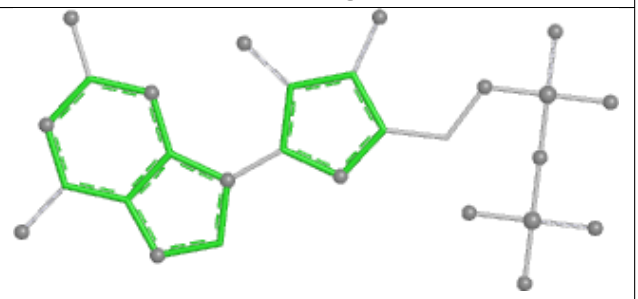


Torsions



Rings

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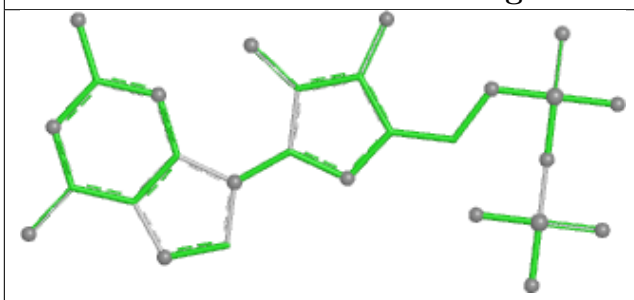

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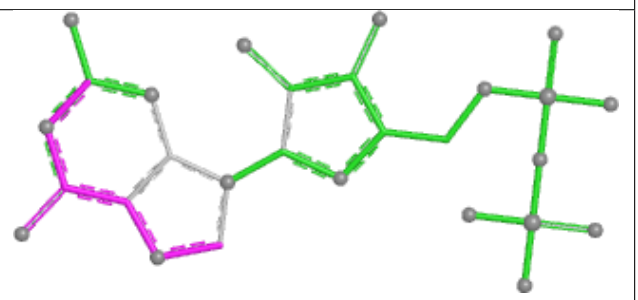

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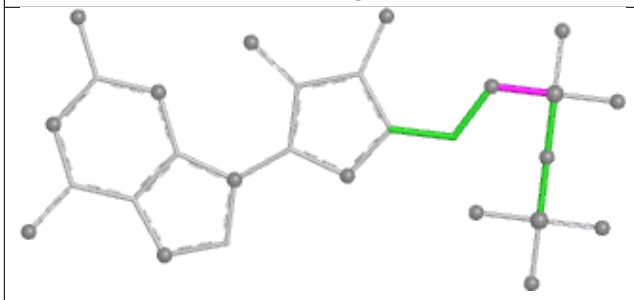

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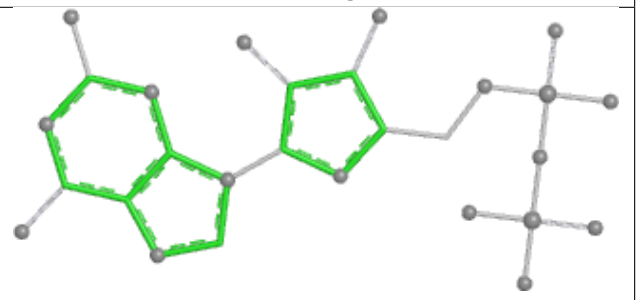

Rings

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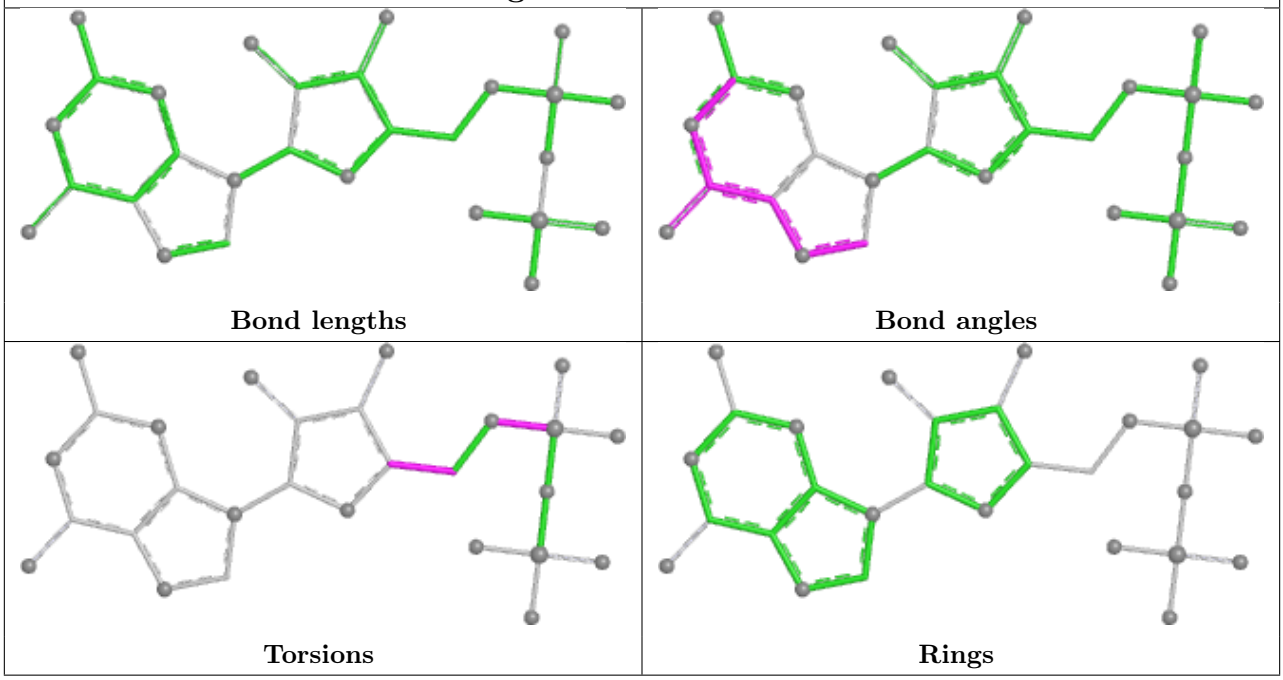


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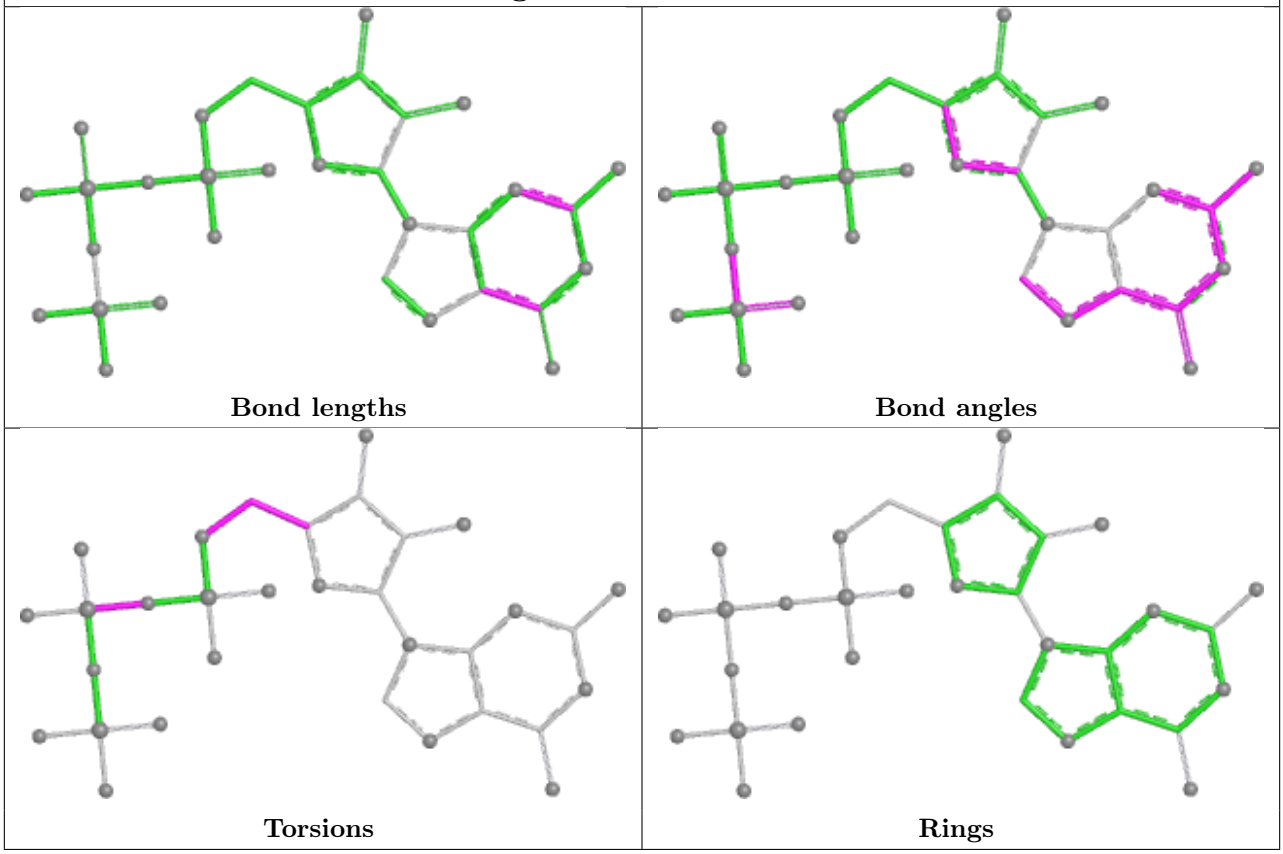

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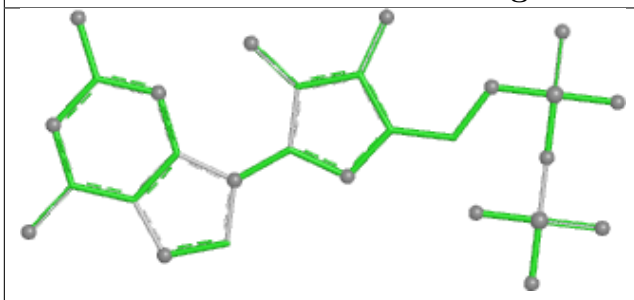

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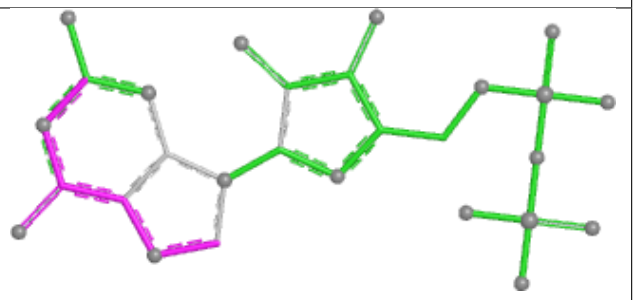

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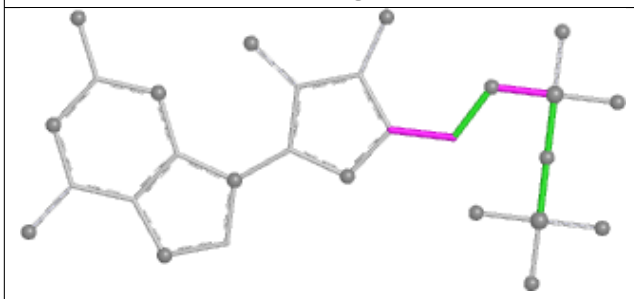

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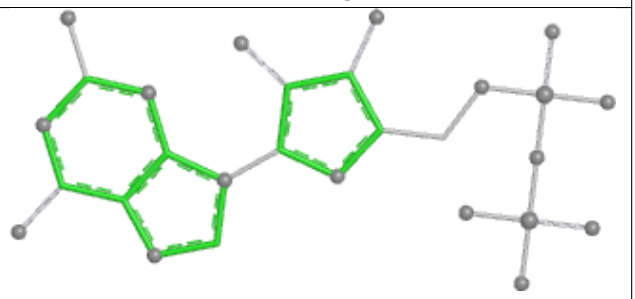

Rings

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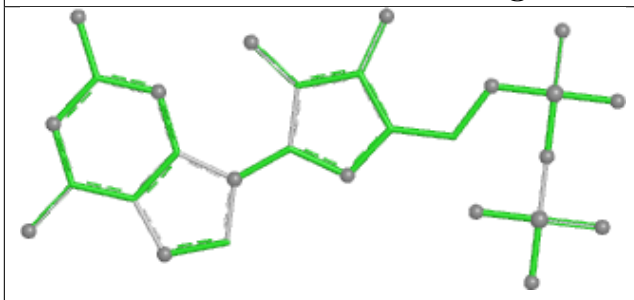

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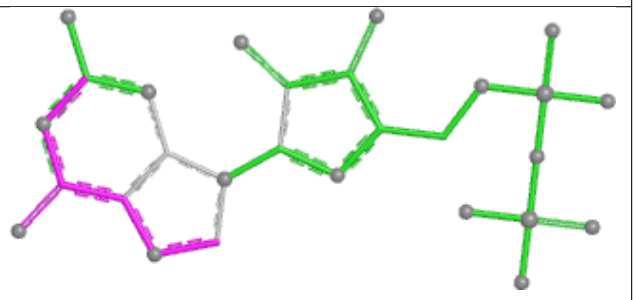

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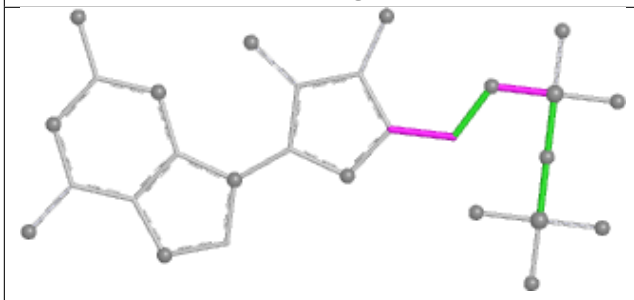

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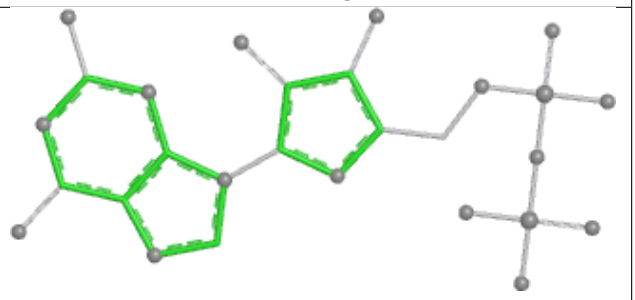

Rings

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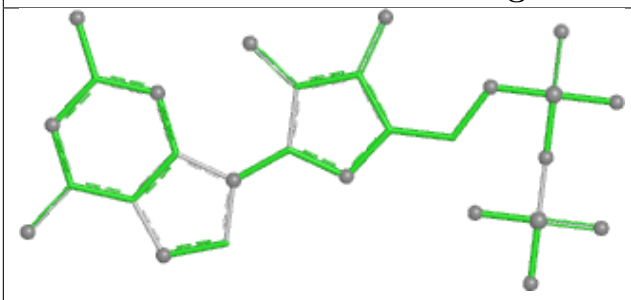

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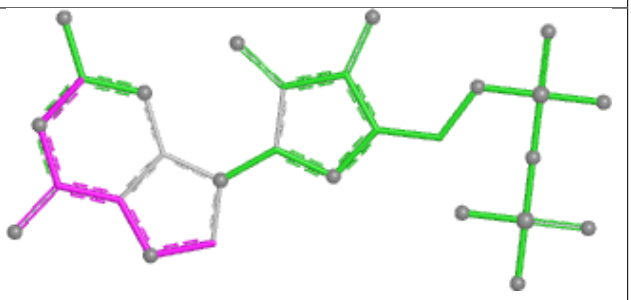

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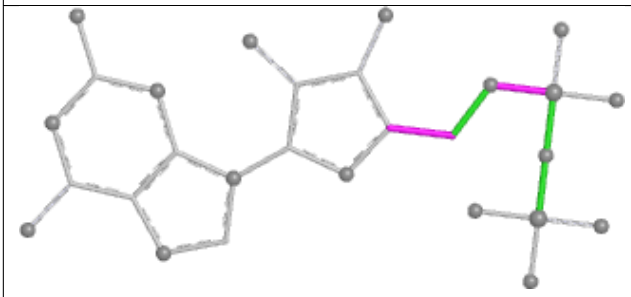

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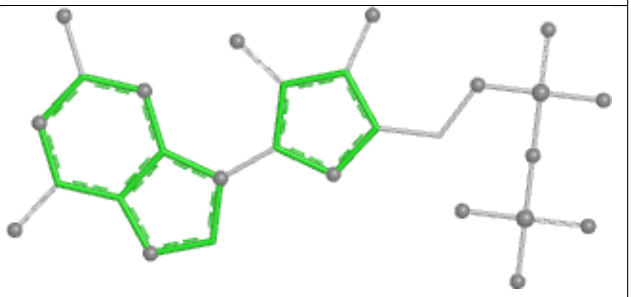

Rings

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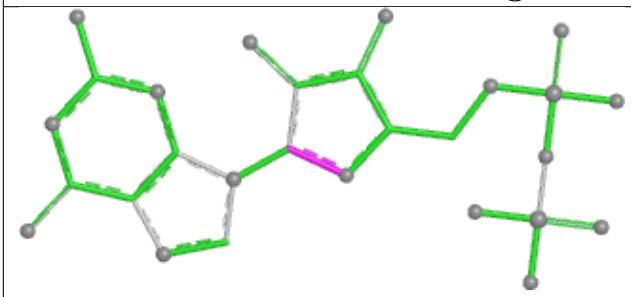

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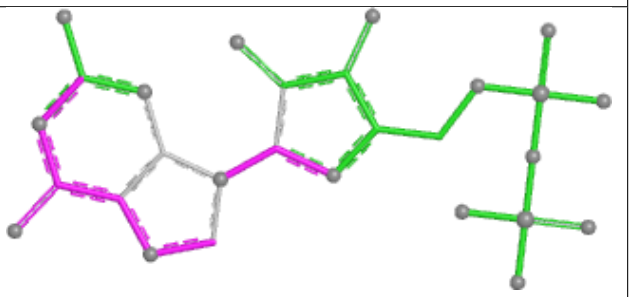

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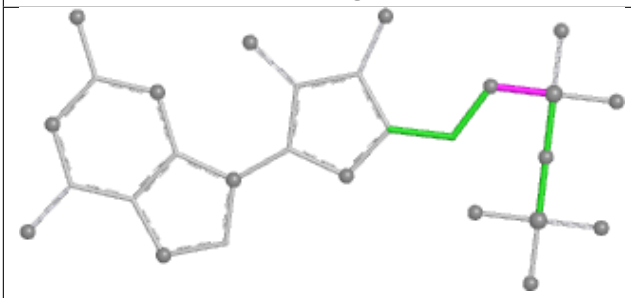

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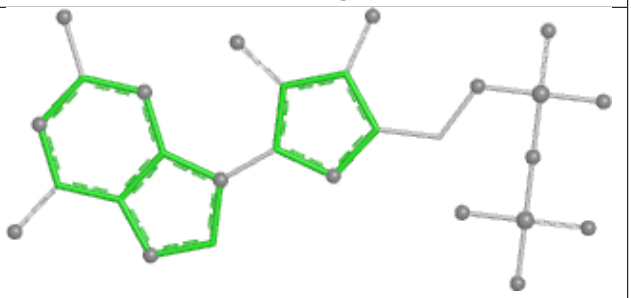

Rings

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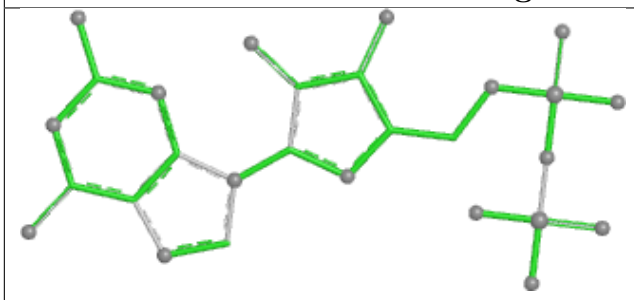

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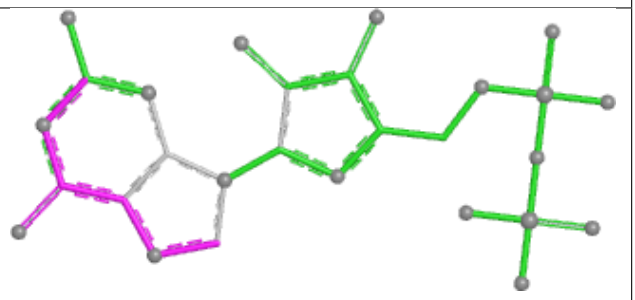

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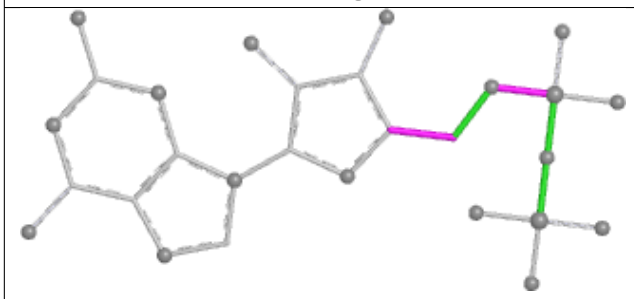

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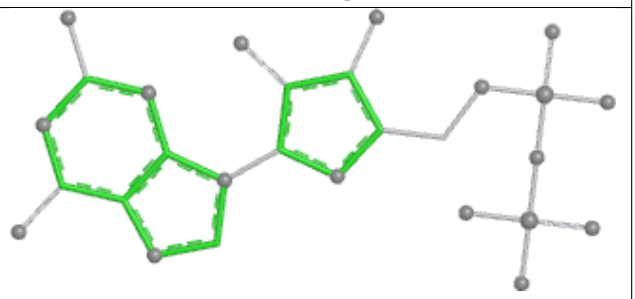

Rings

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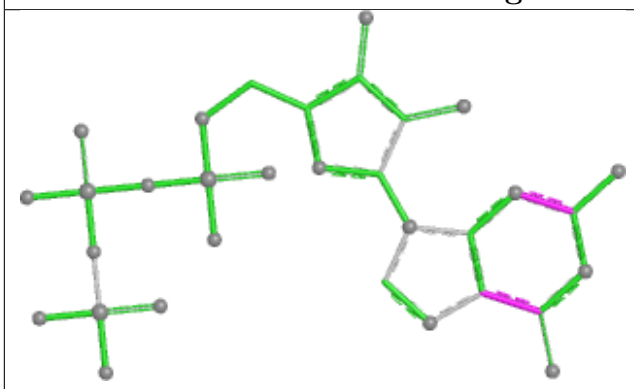

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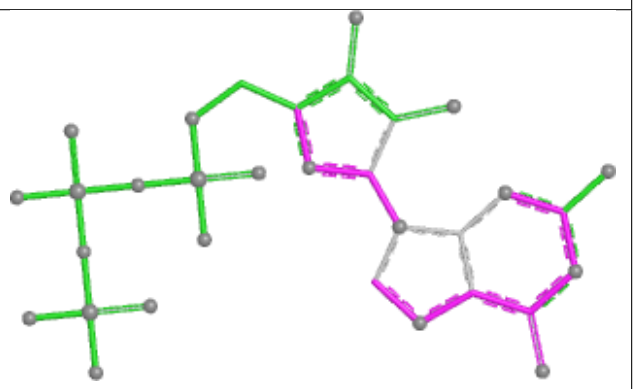

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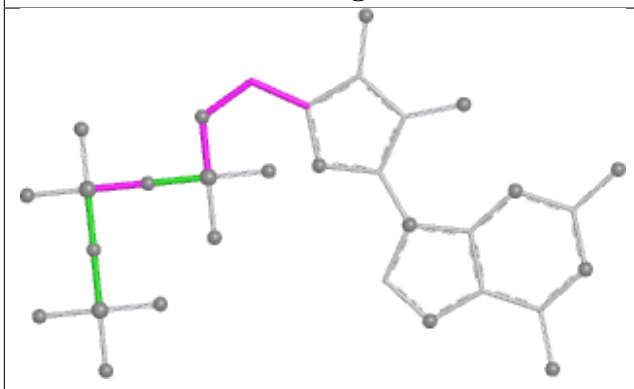

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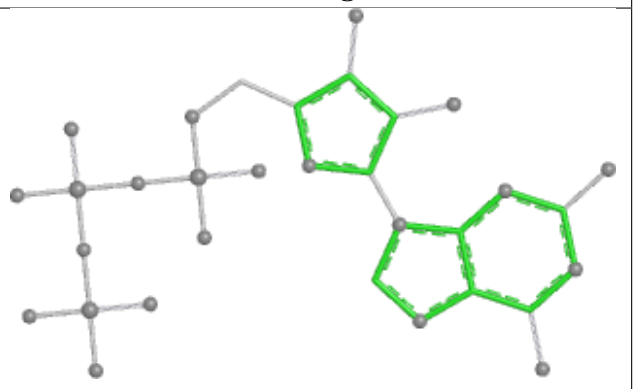

Rings

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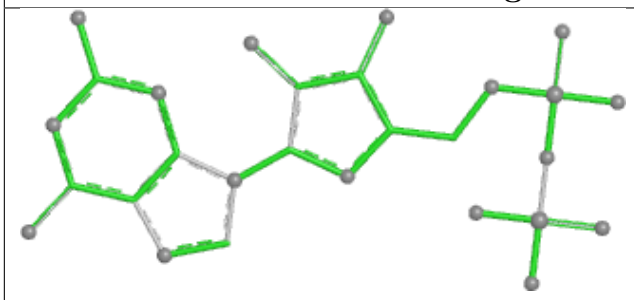

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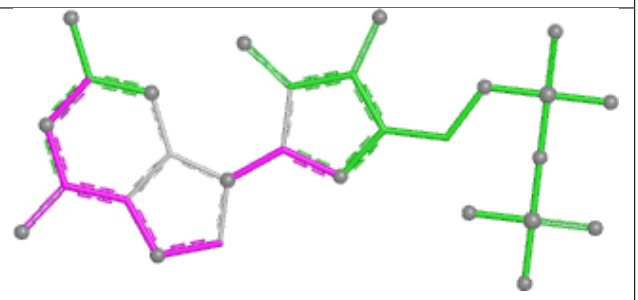

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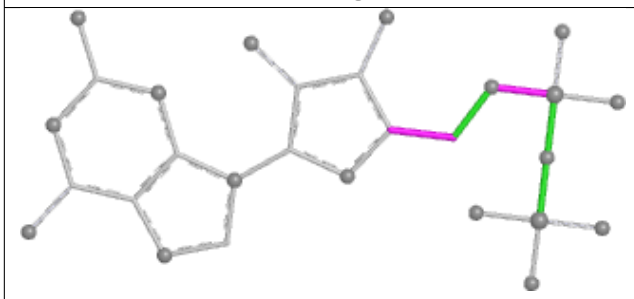

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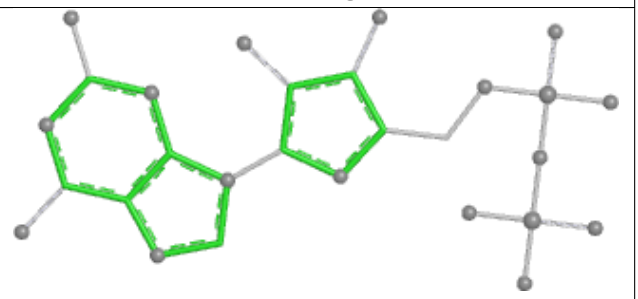

Rings

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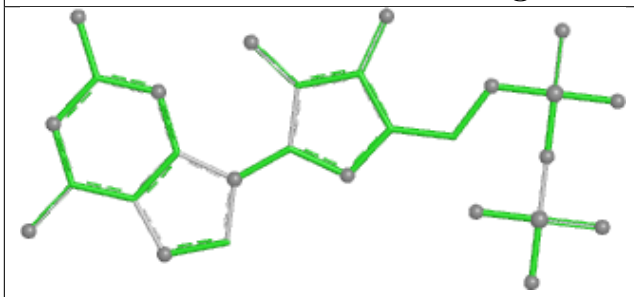

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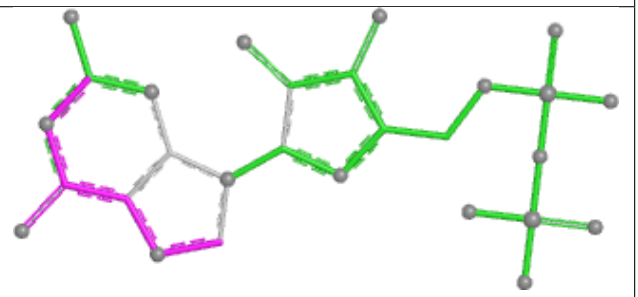

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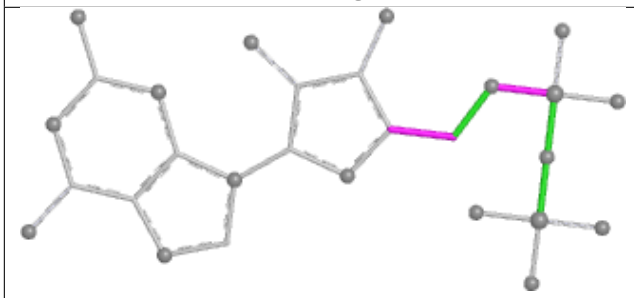

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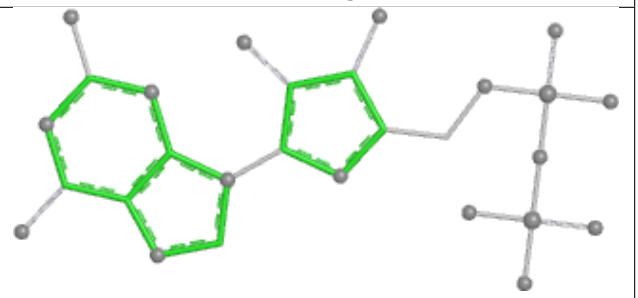

Rings

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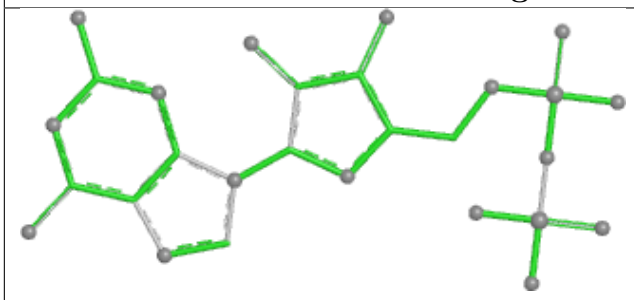

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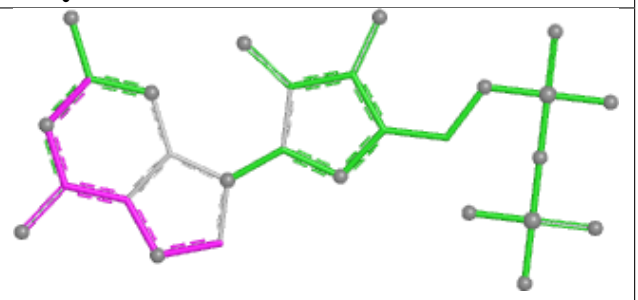

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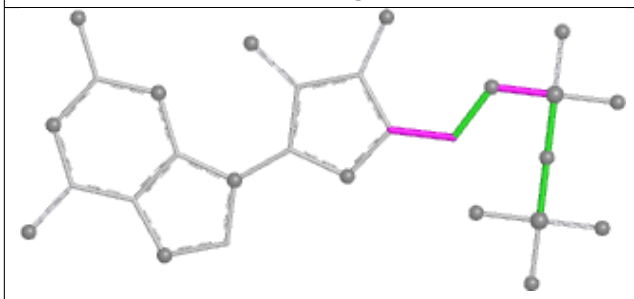

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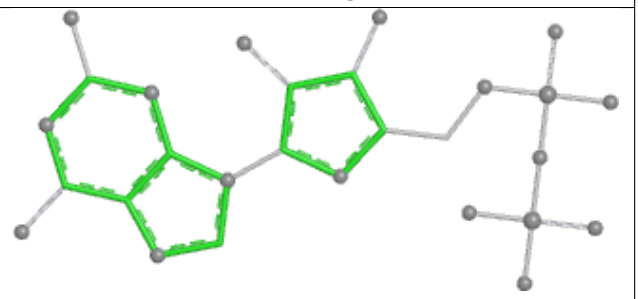

Rings

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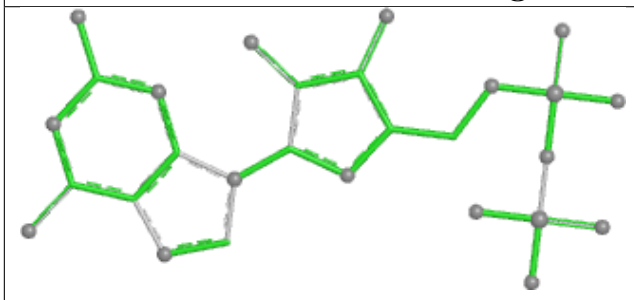

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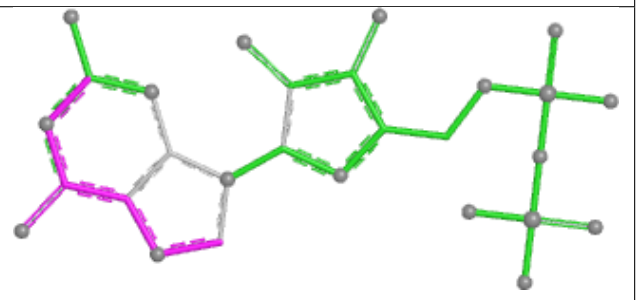

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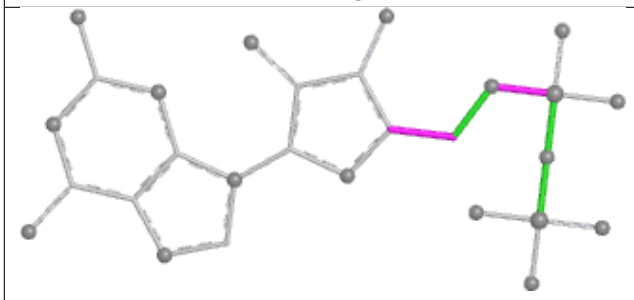

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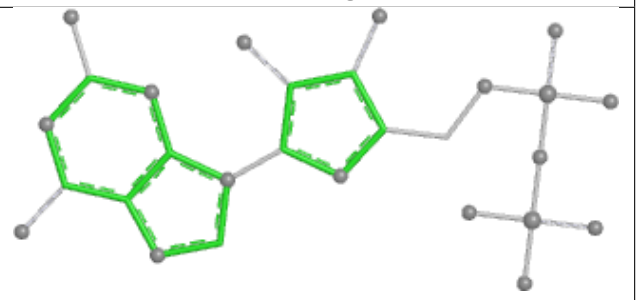

Rings

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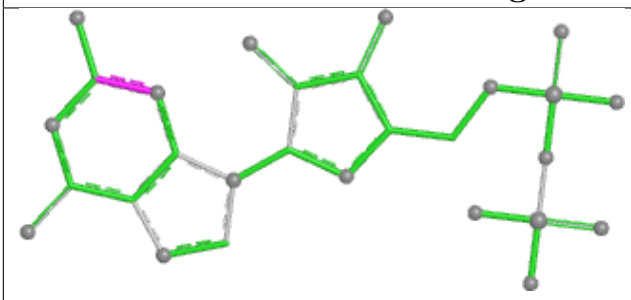

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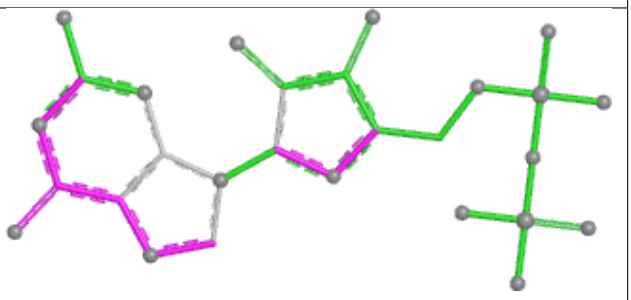

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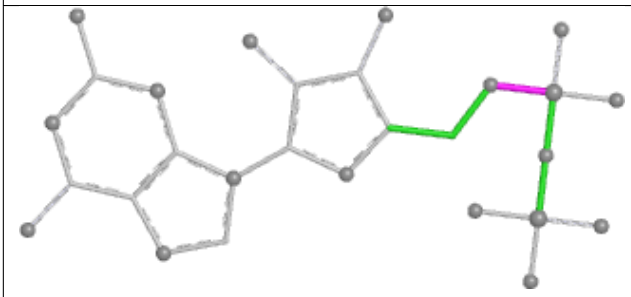

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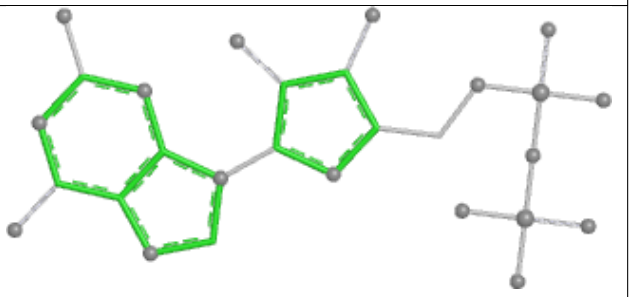

Rings

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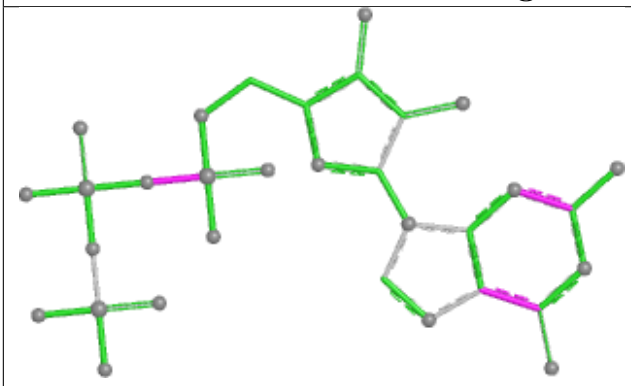

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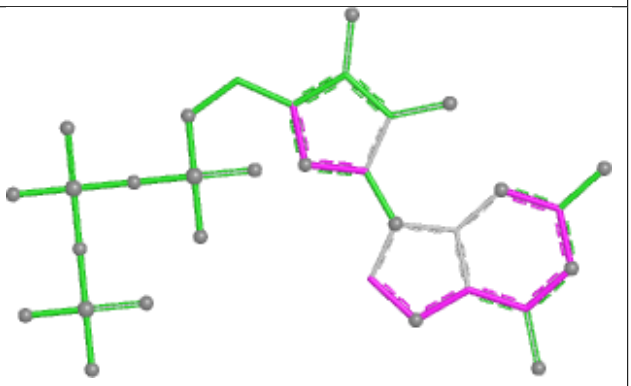

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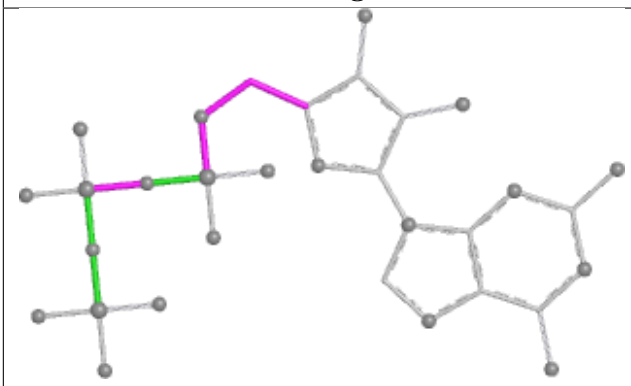
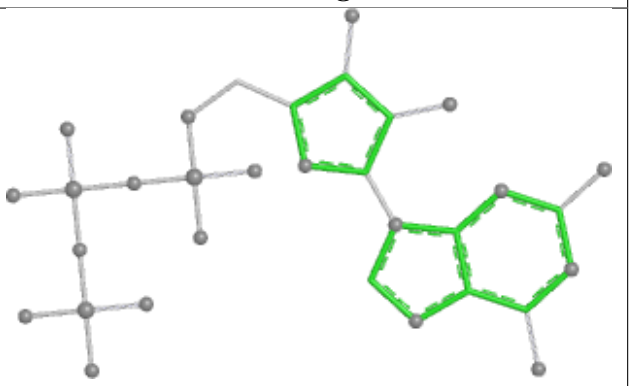
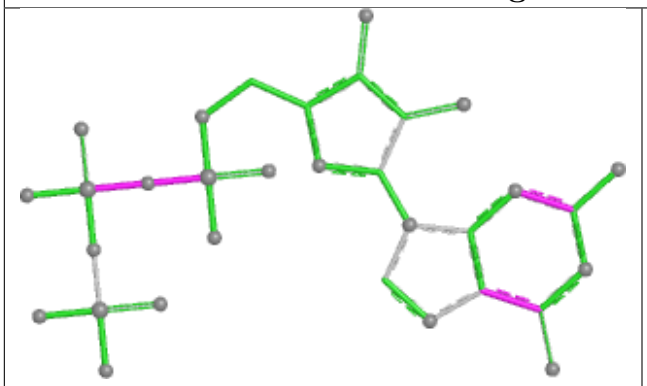


Torsions



Rings

## Ligand GTP DG 501



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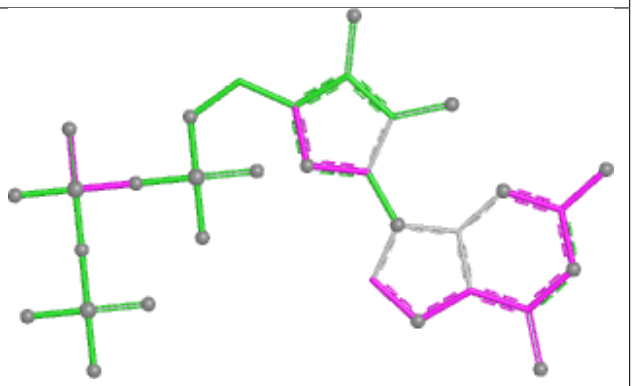

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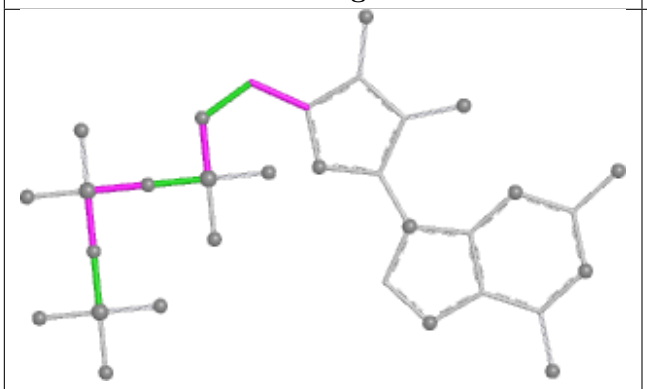

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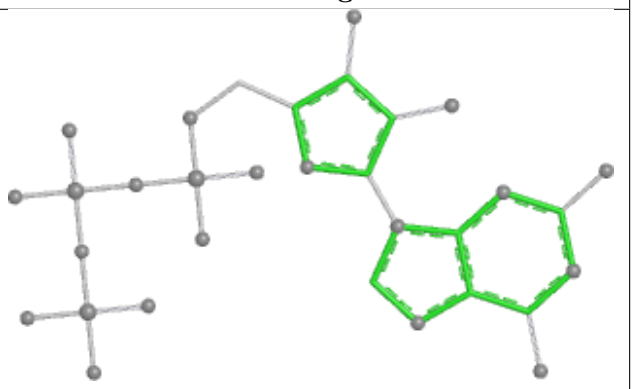
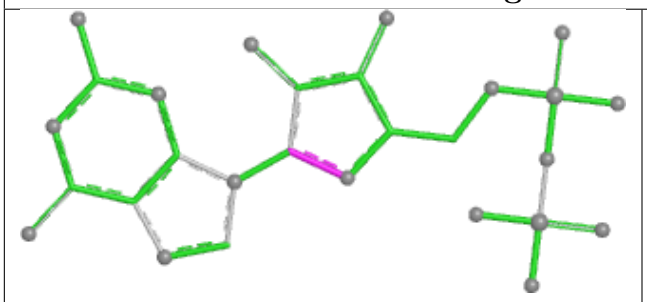


Rings

## Ligand GDP GM 501



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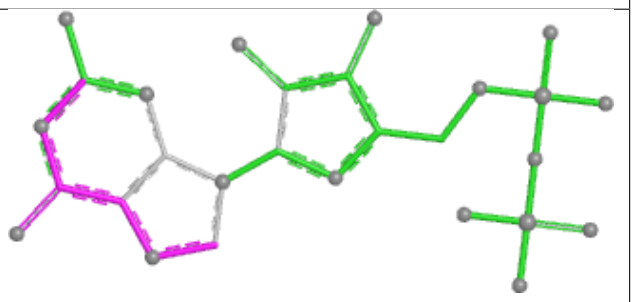

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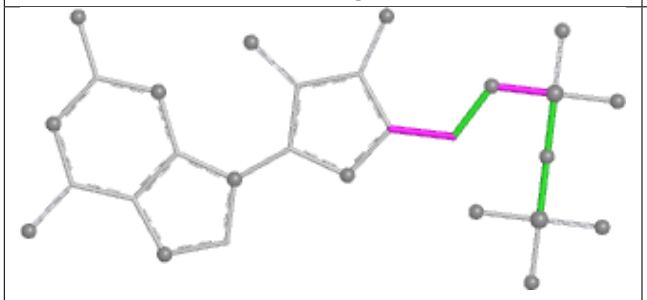

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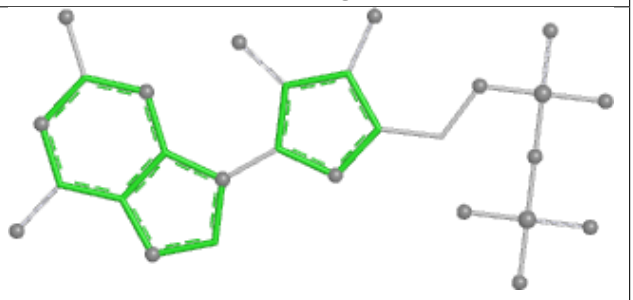
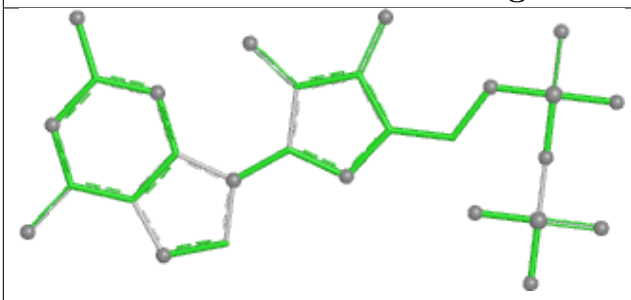


Rings

## Ligand GDP RB 501



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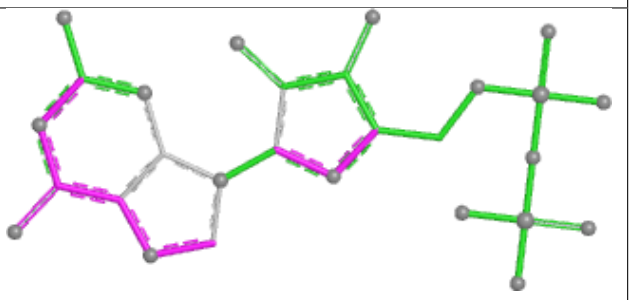

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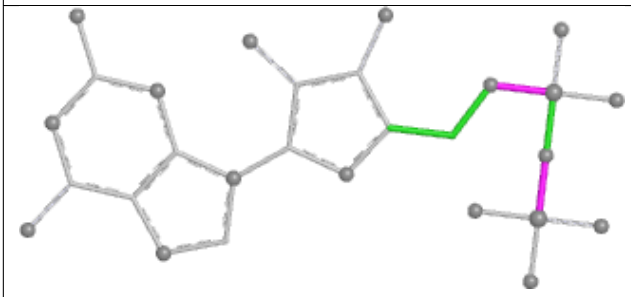

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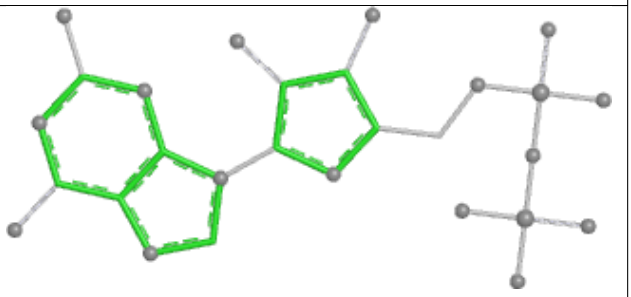
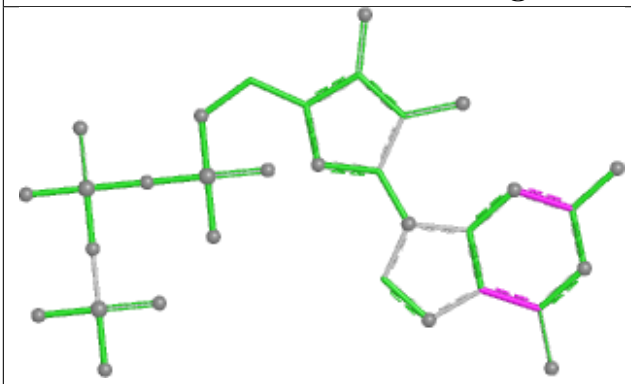


Rings

## Ligand GTP PN 501



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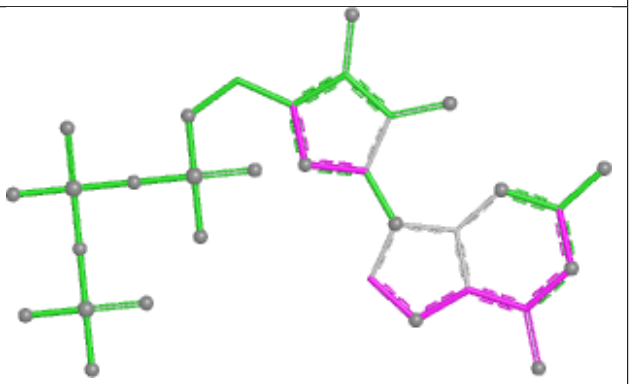

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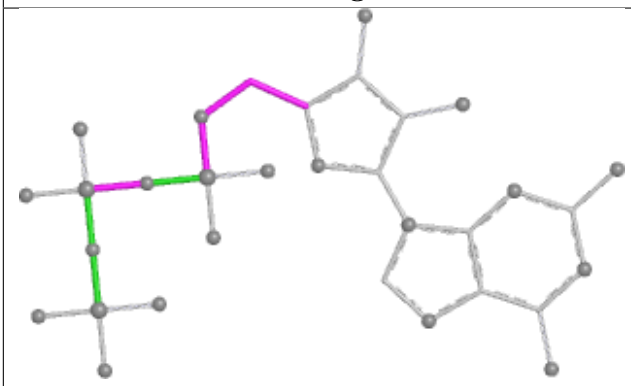

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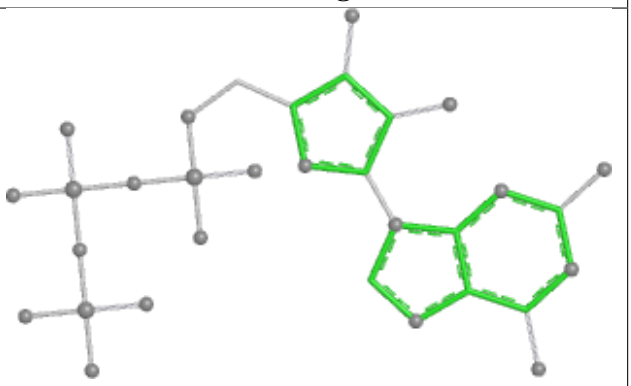
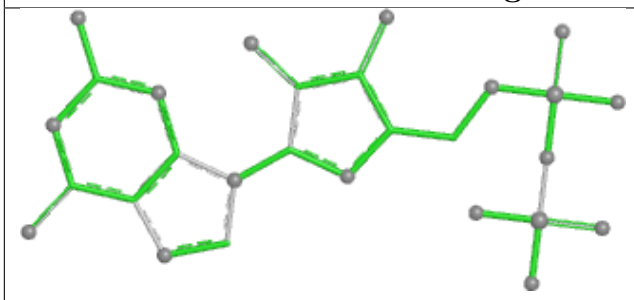


Rings

## Ligand GDP WB 501



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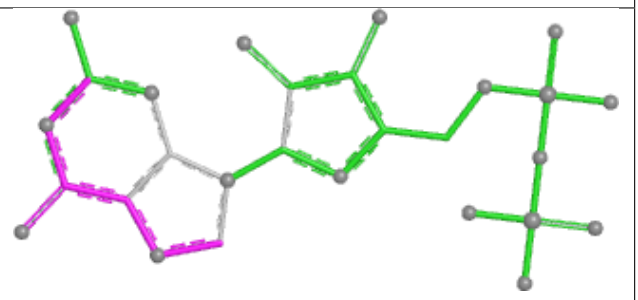

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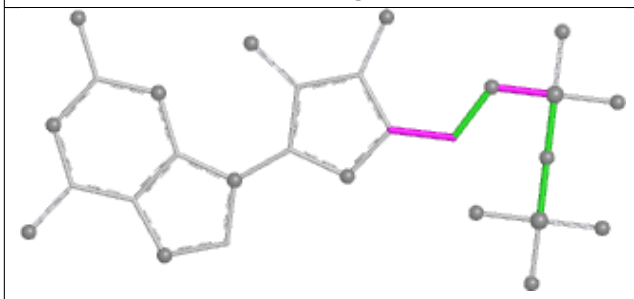

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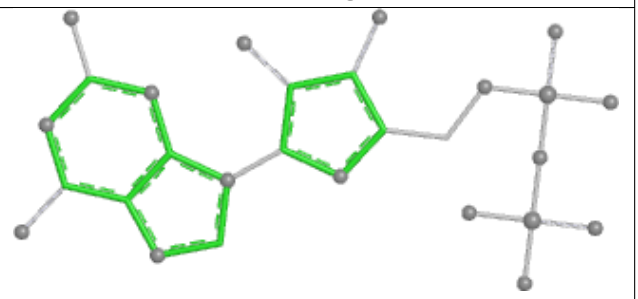

Rings

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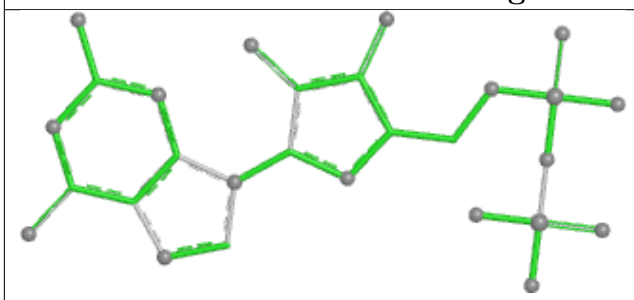

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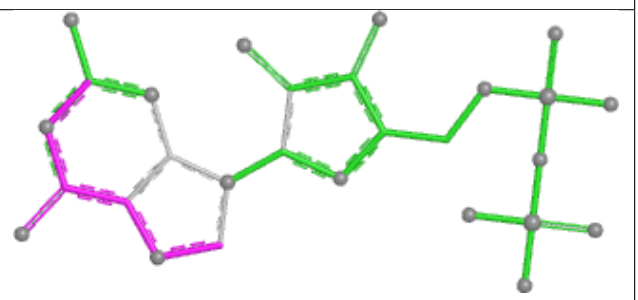

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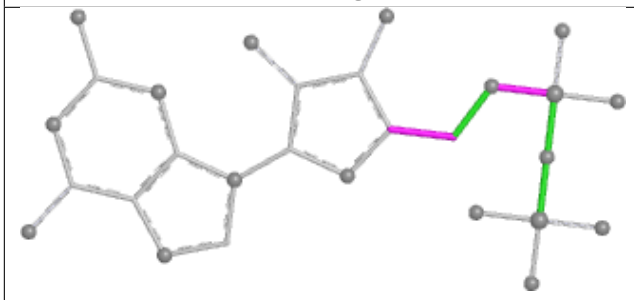

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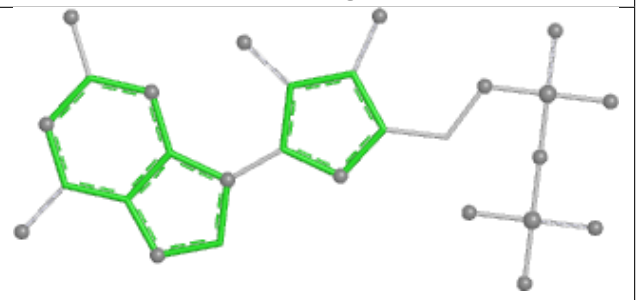
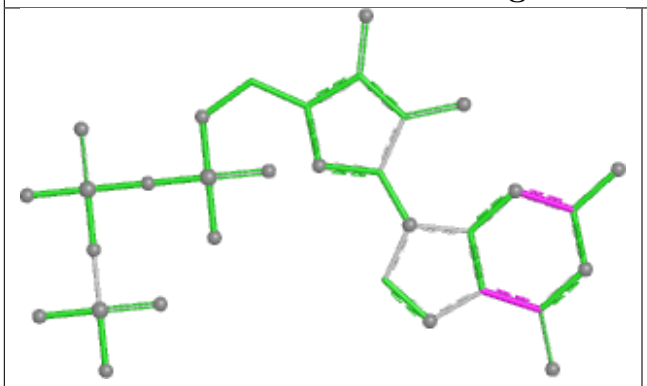


Rings

## Ligand GTP NG 501



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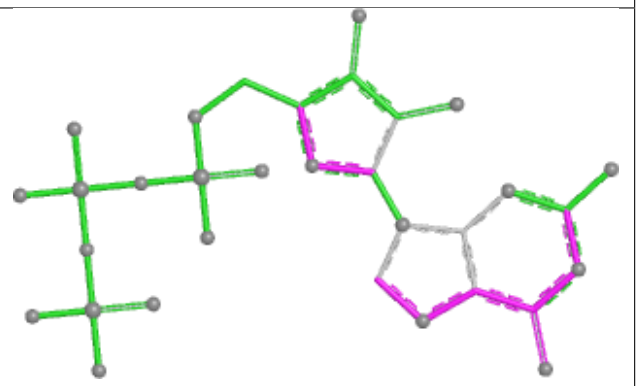

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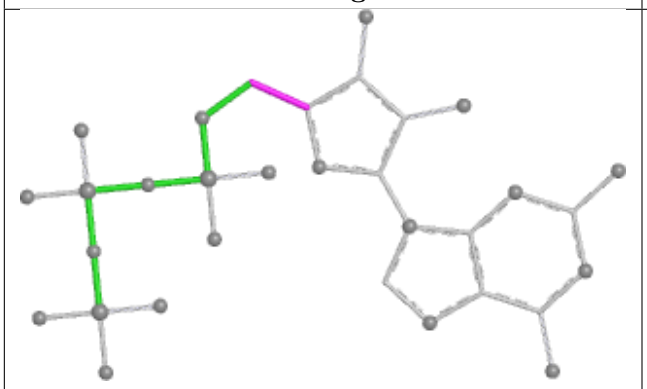

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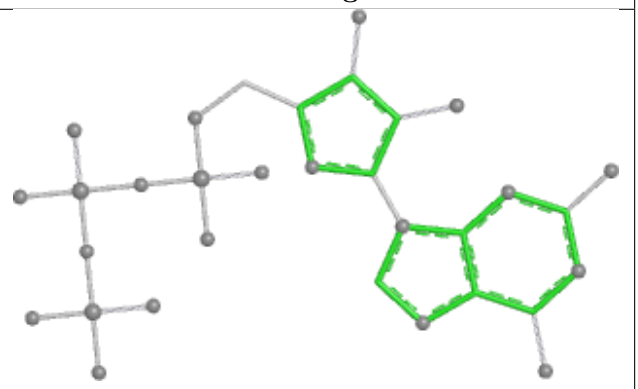

Rings

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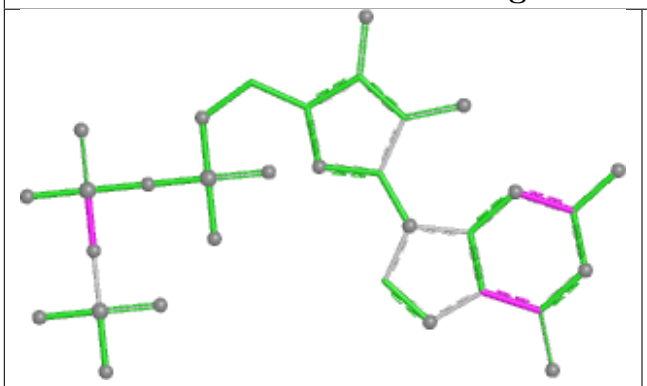

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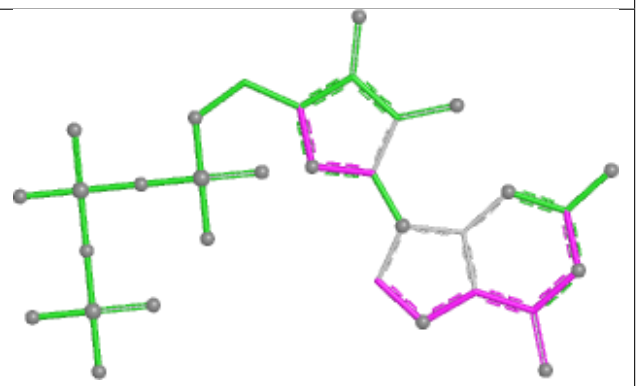

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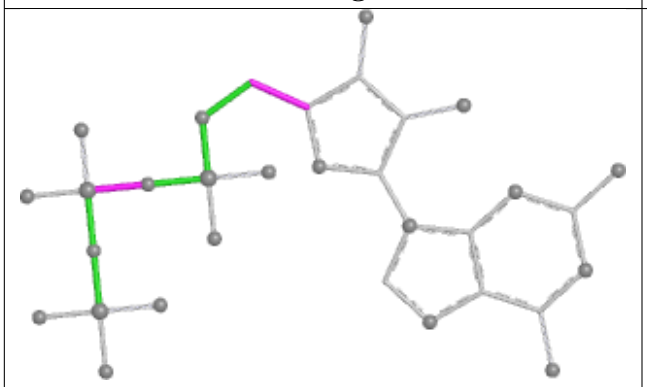

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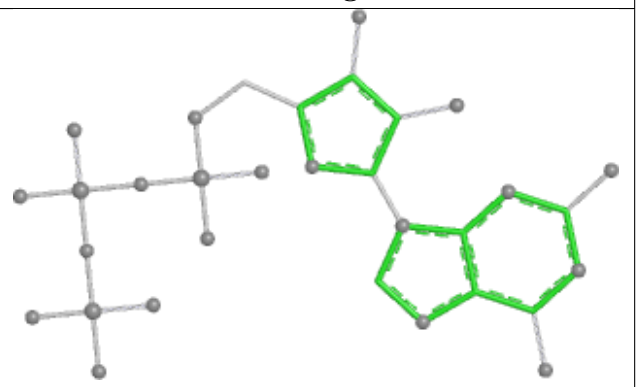

Rings

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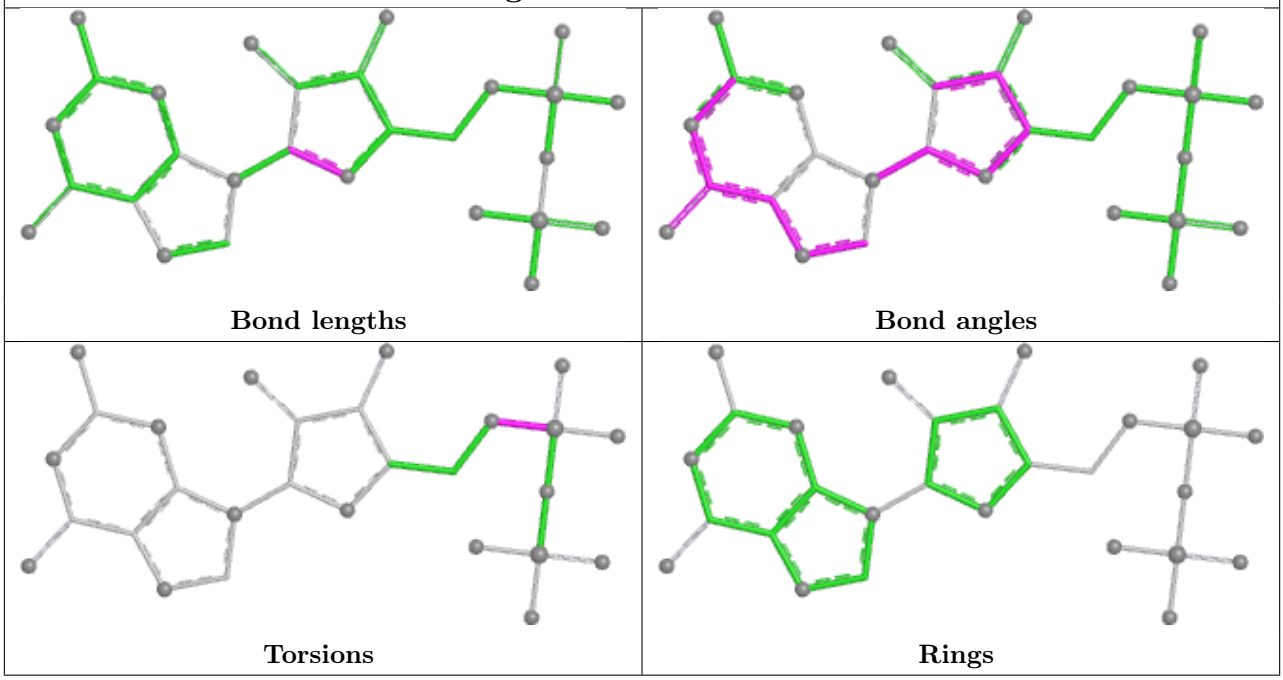


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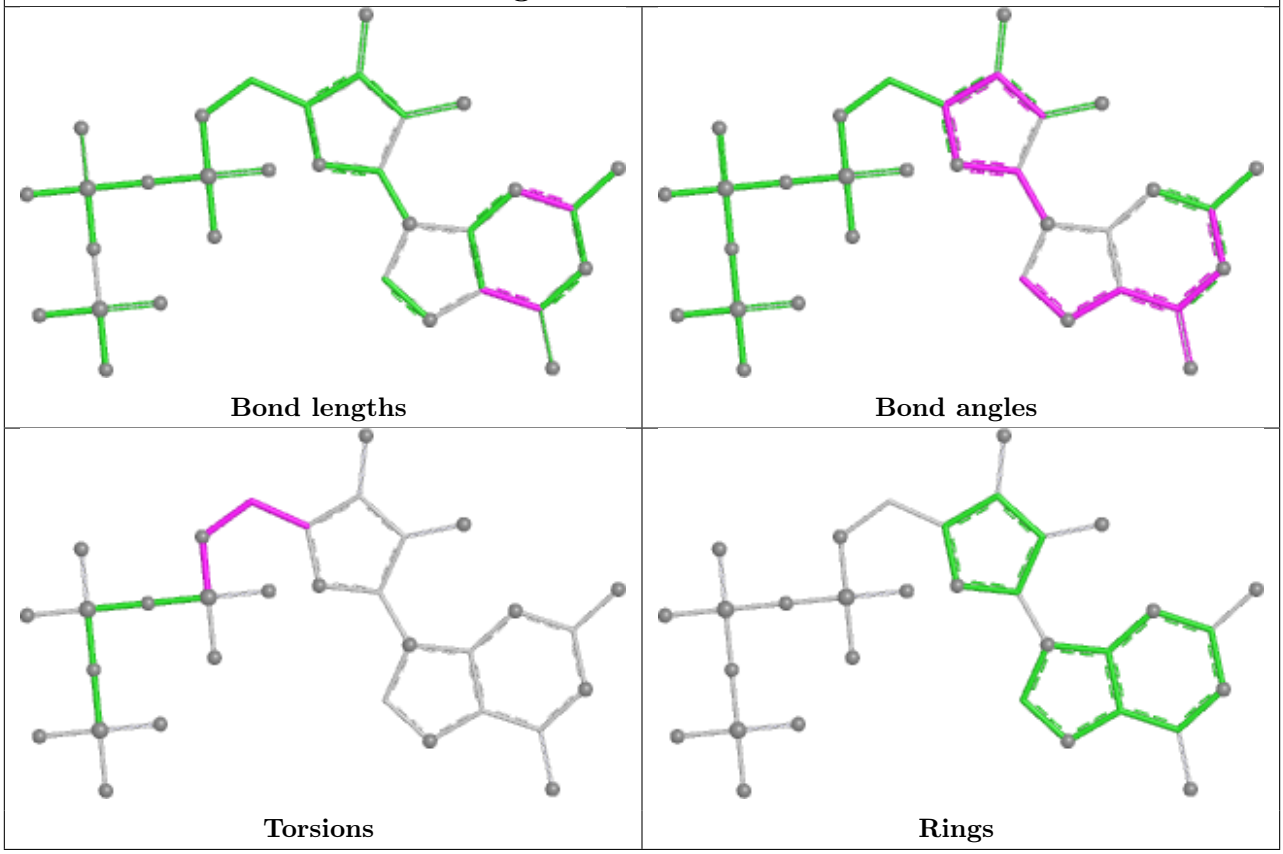

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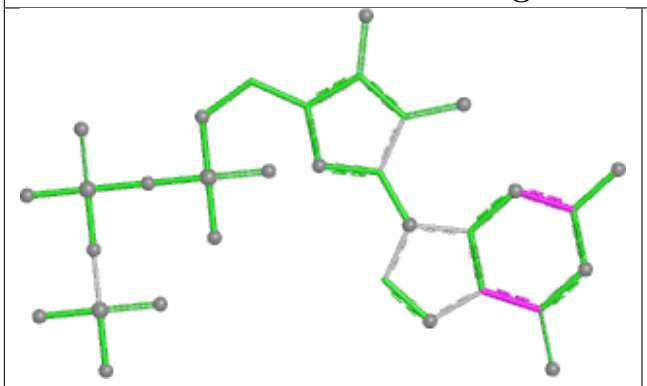

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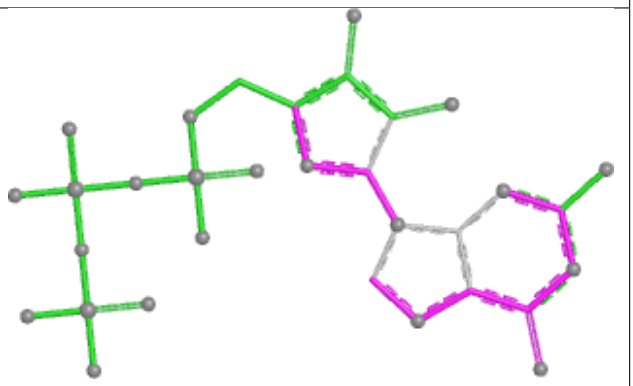

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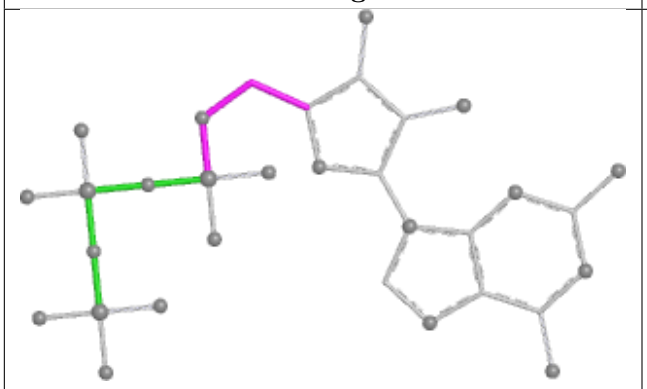

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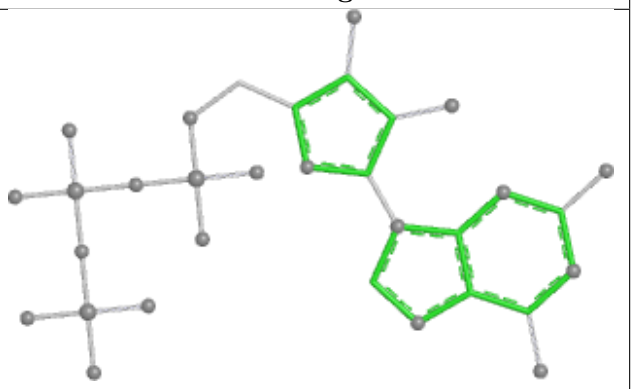
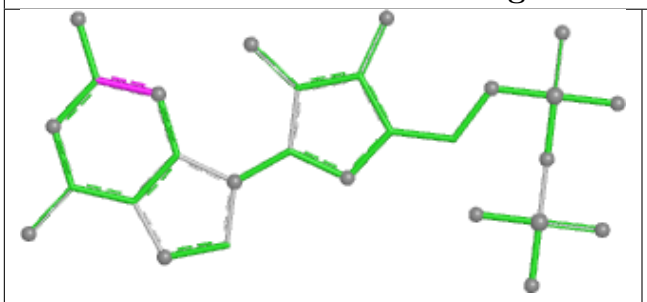


Rings

## Ligand GDP RN 502



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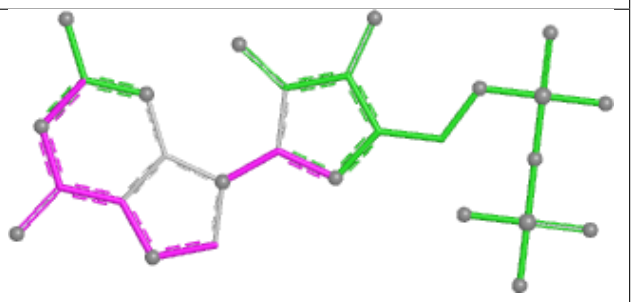

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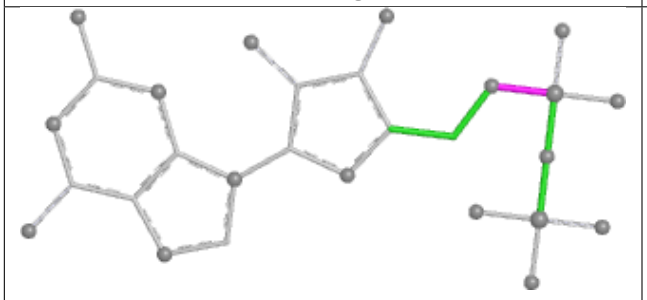

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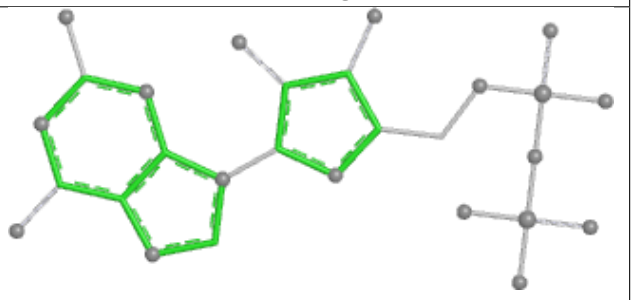
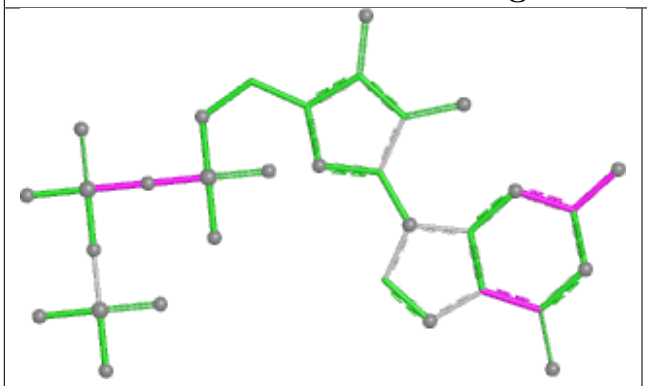


Rings

## Ligand GTP KO 501



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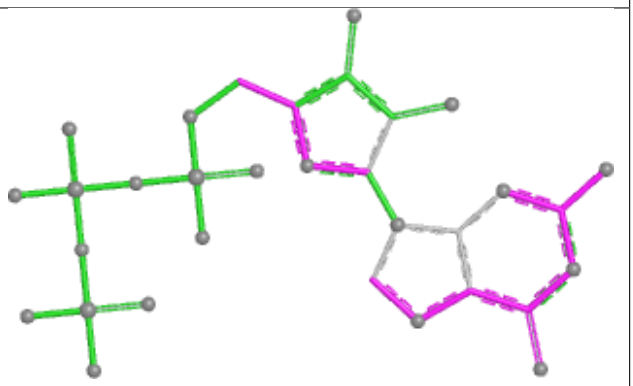

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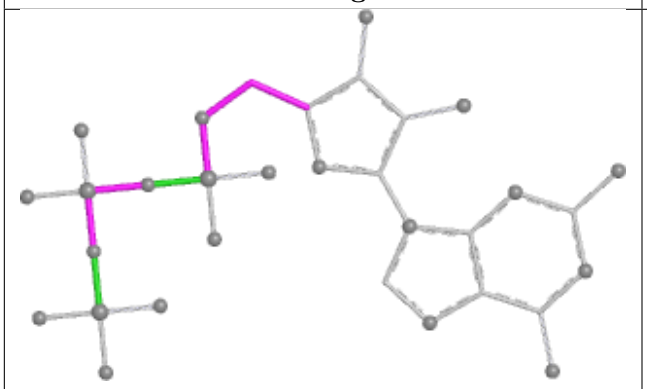

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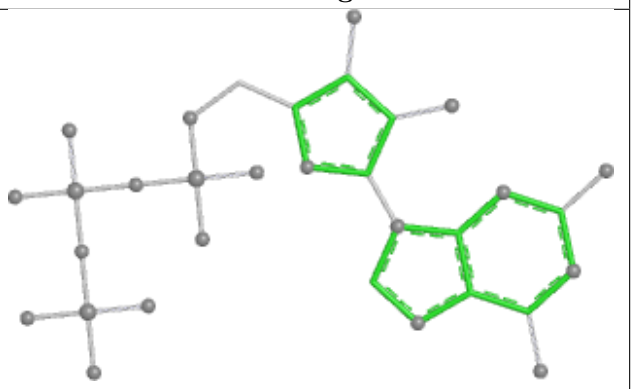

Rings

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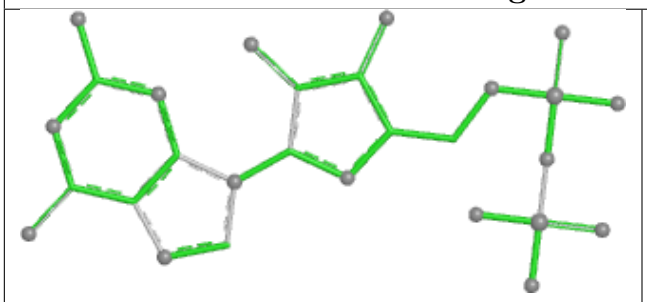

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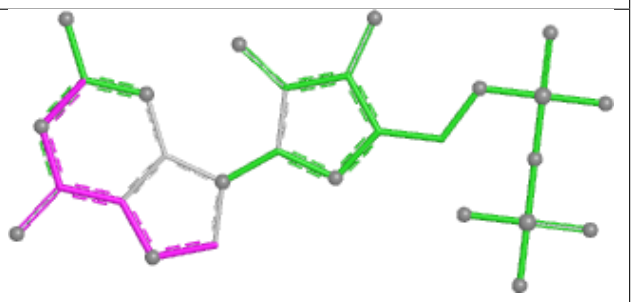

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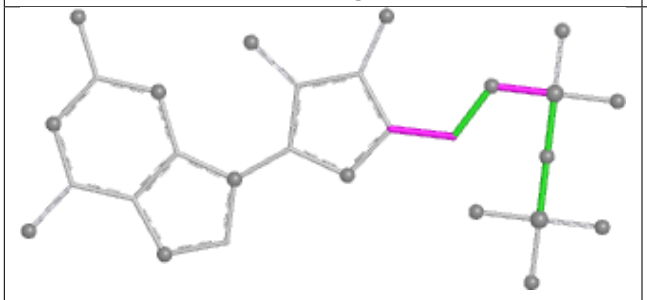

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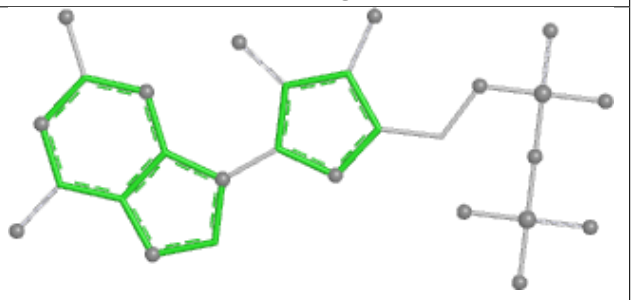
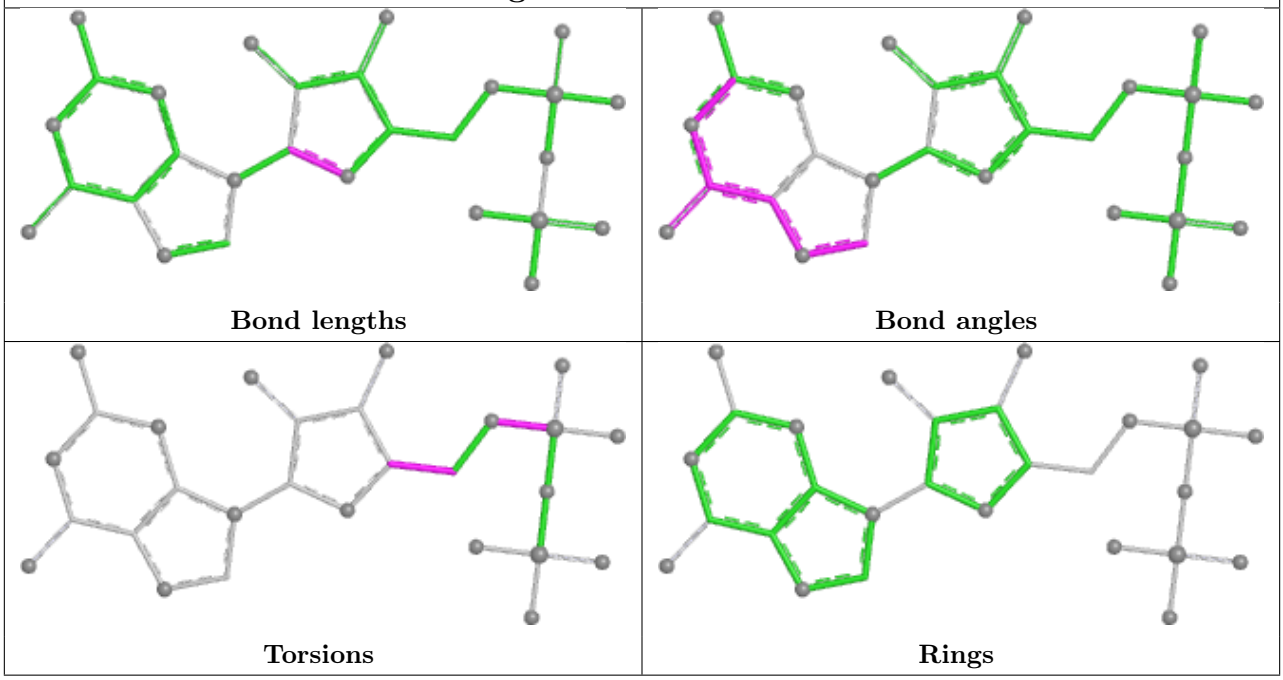
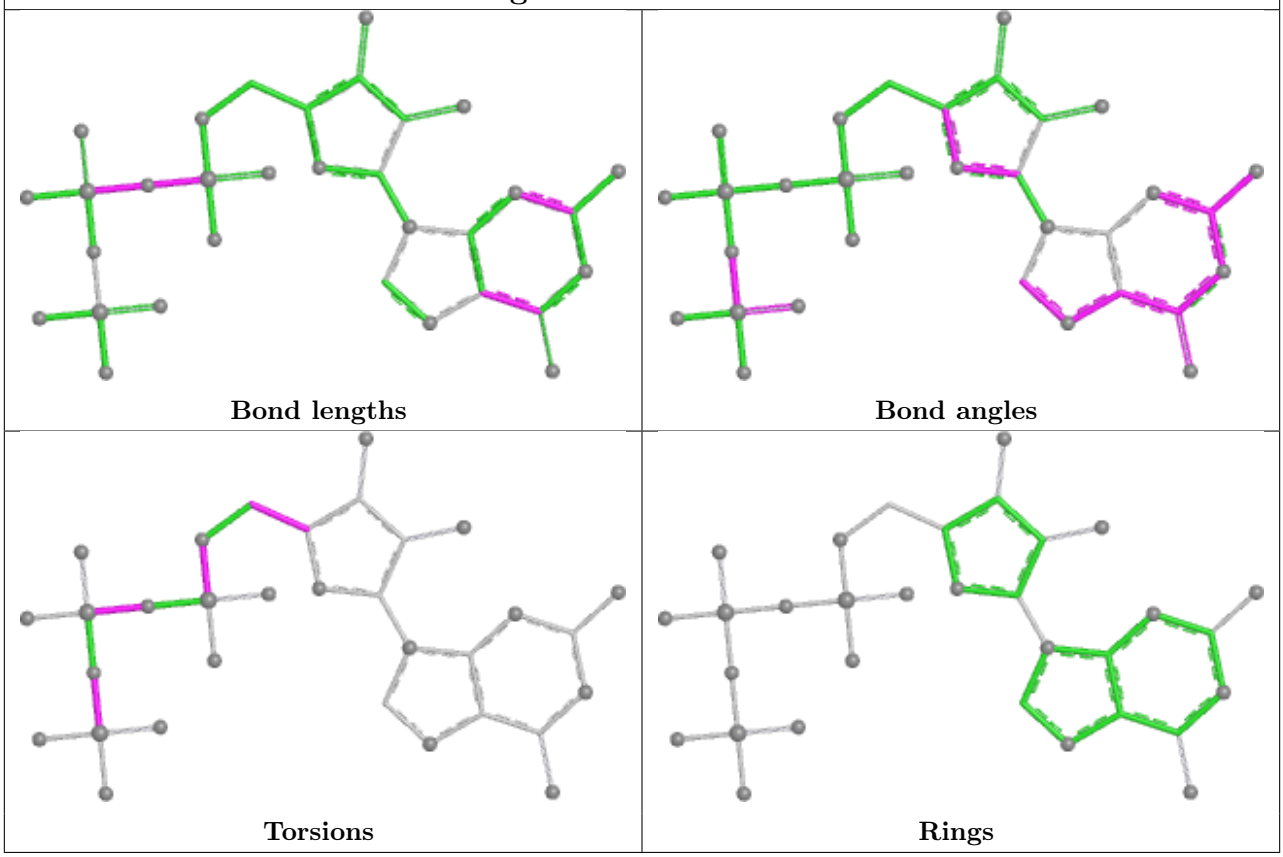


Rings

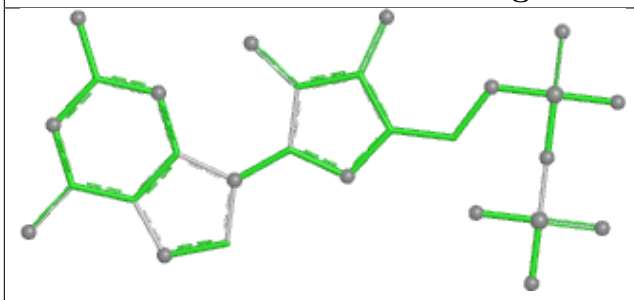
## Ligand GDP CN 501



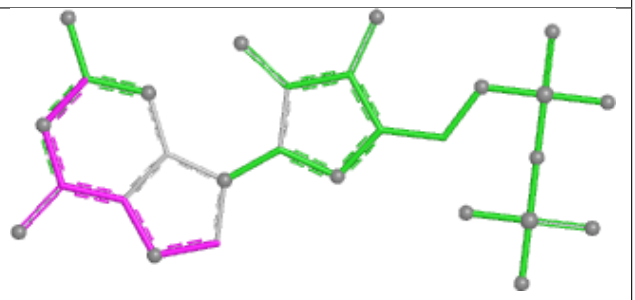

## Ligand GTP DA 501



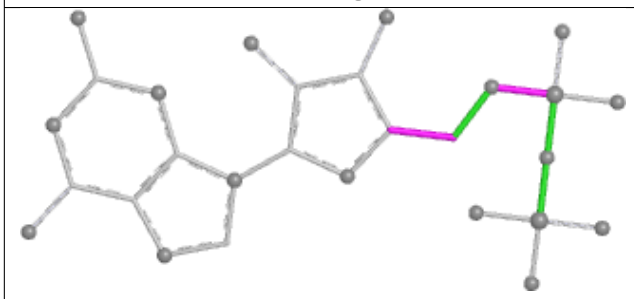
## Ligand GDP JN 501



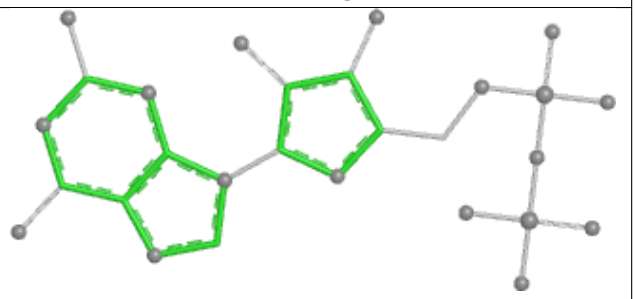
Bond lengths



Bond angles

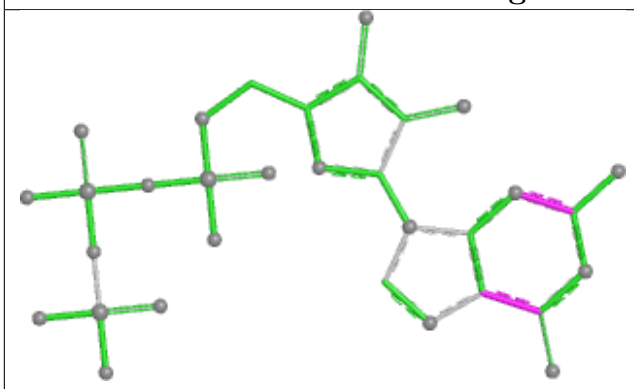


Torsions



Rings

## Ligand GTP GH 501



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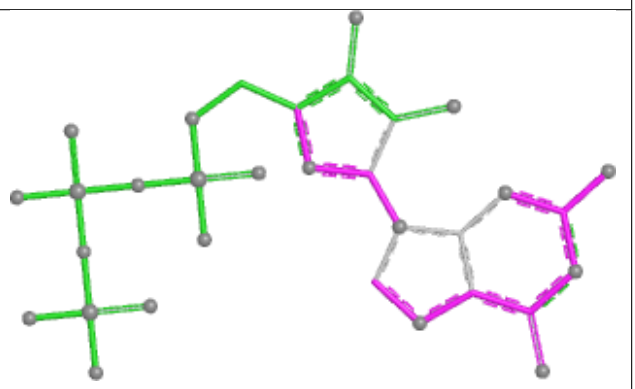

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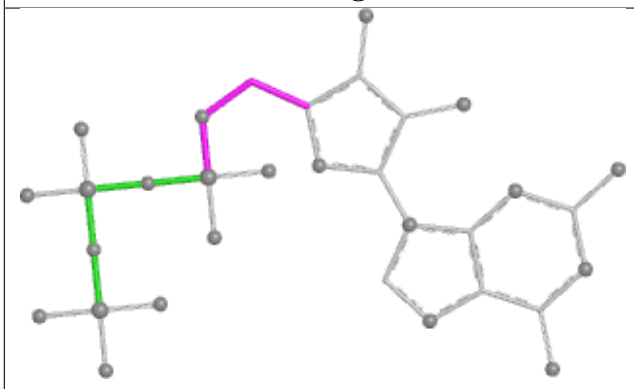

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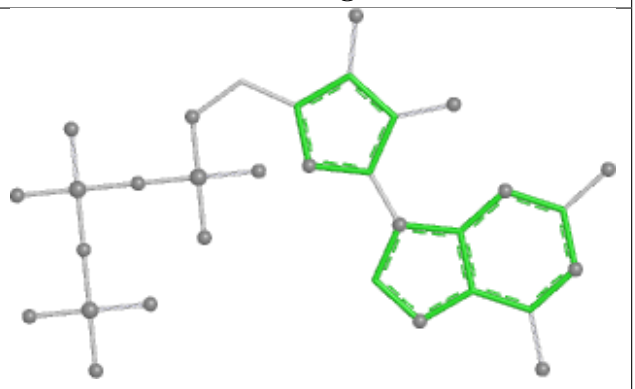

Rings

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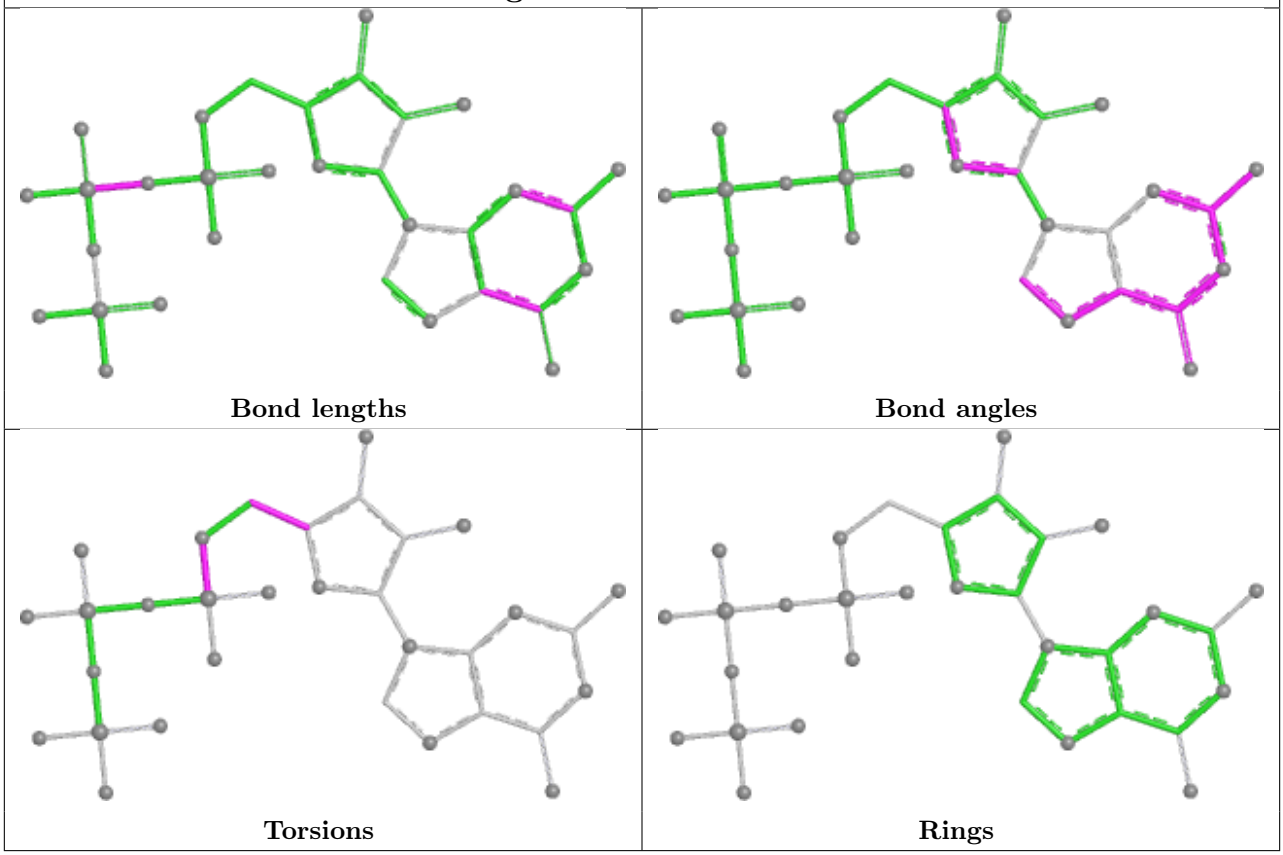


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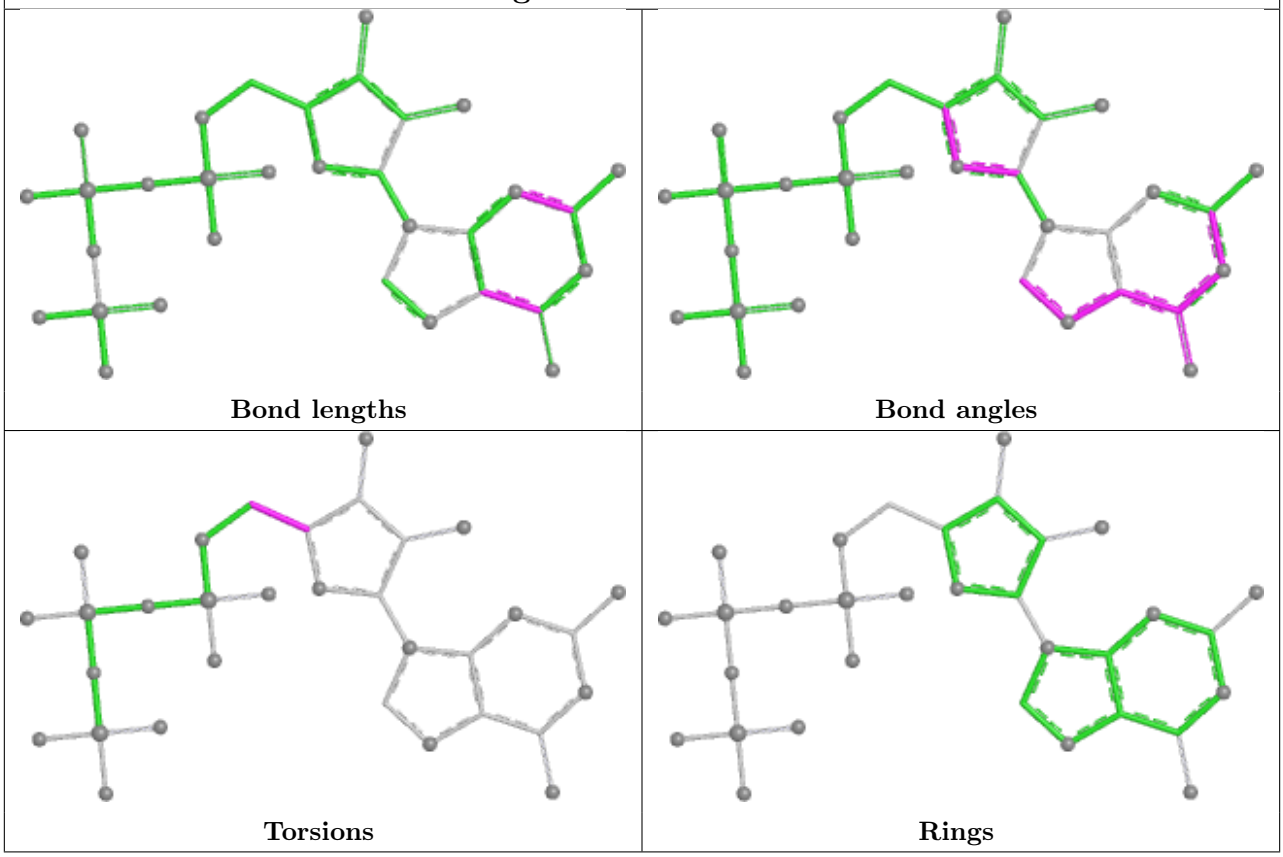

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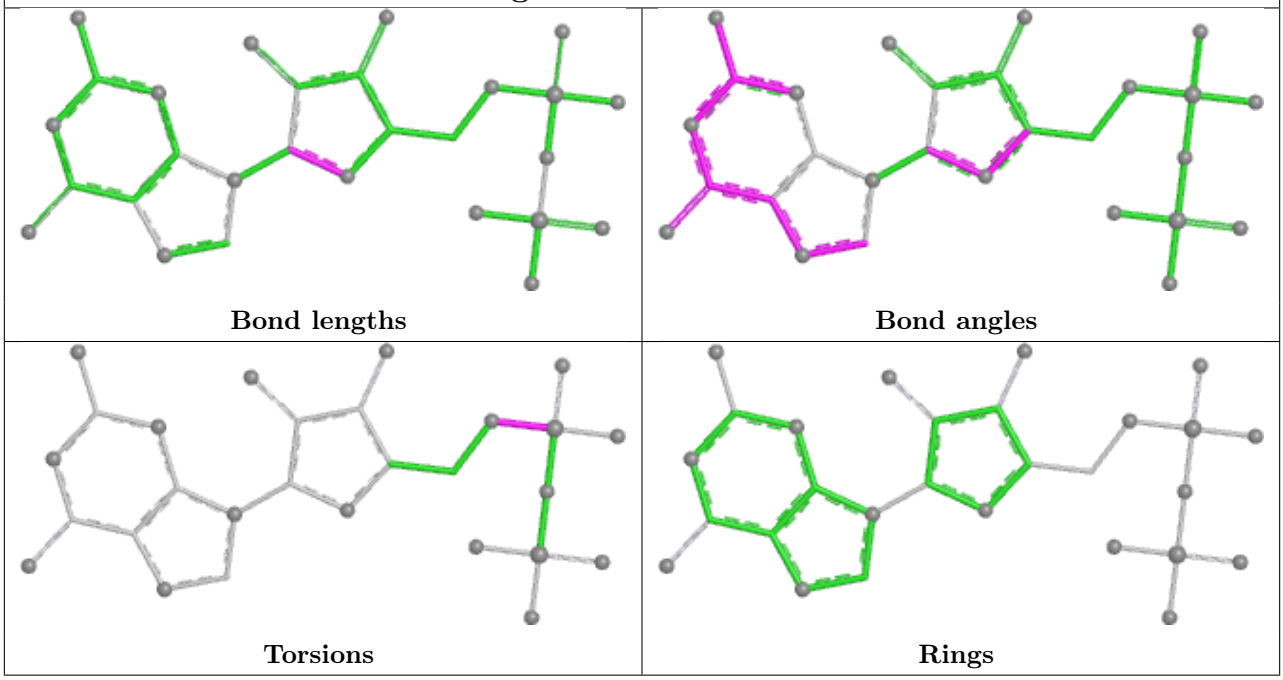


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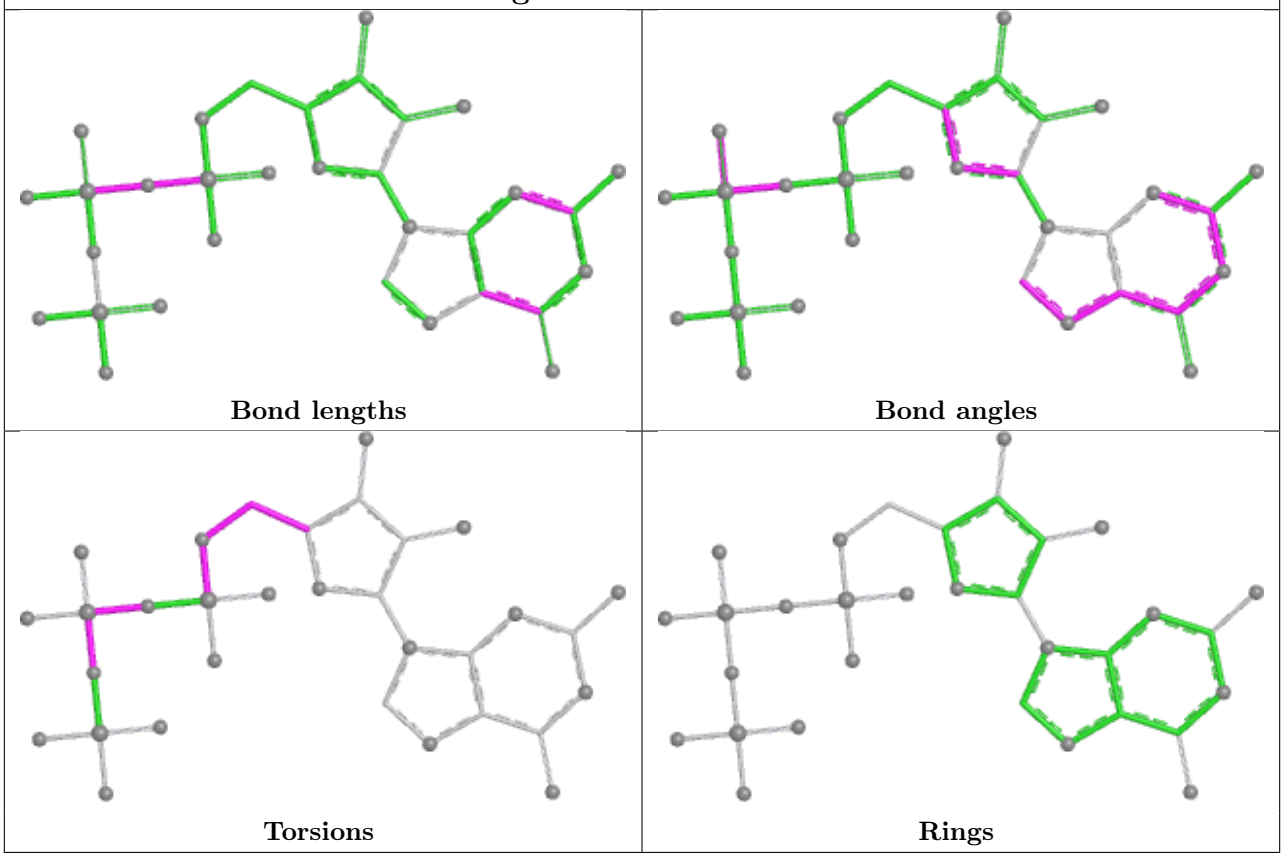
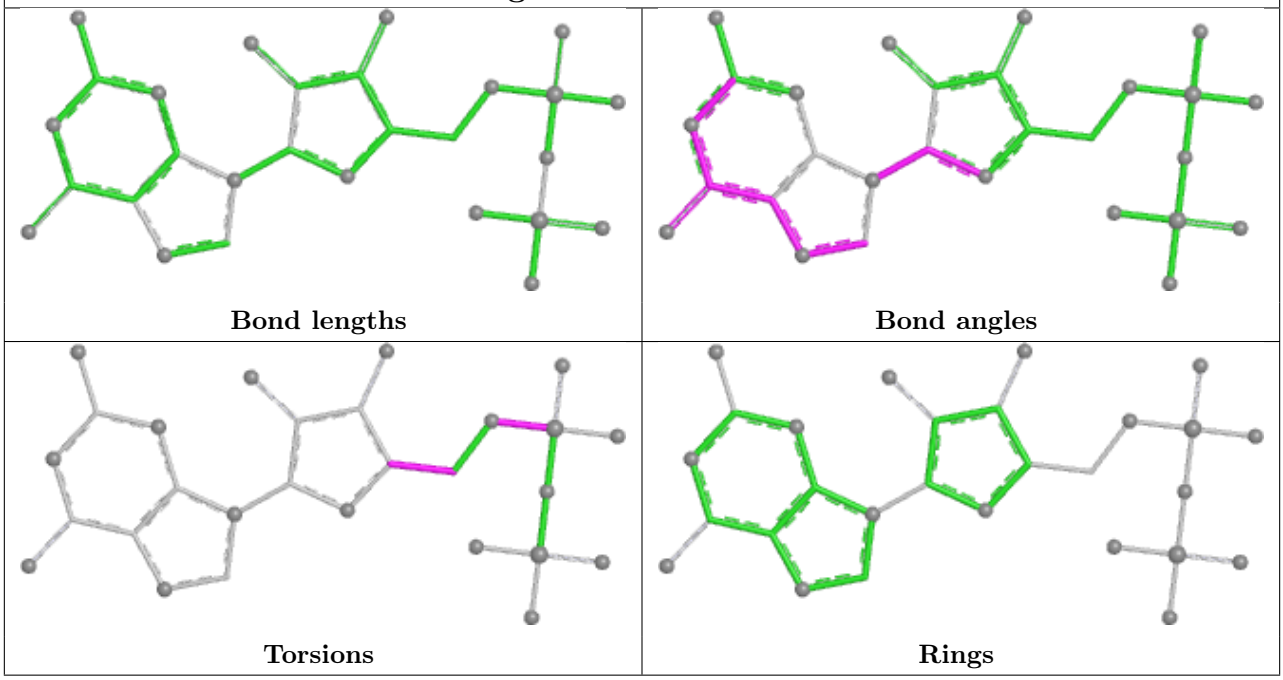


## Ligand GDP UO 502

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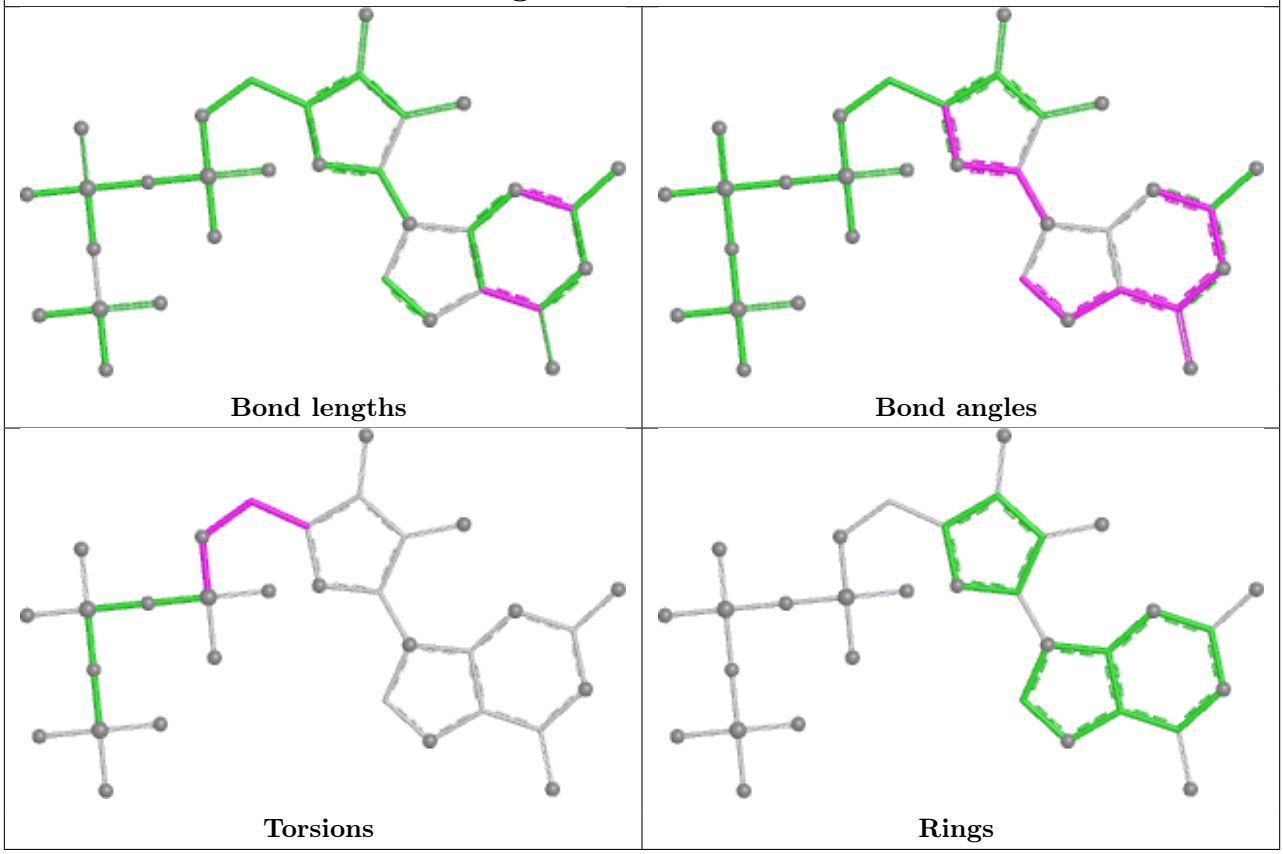

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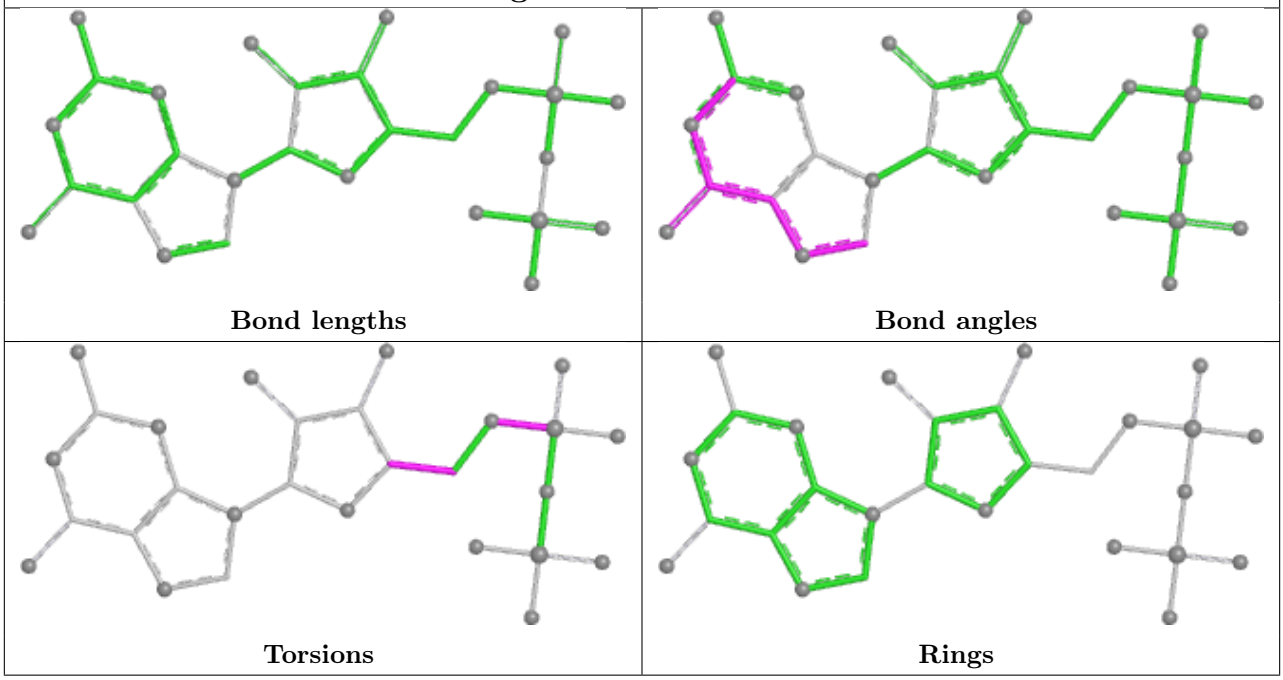


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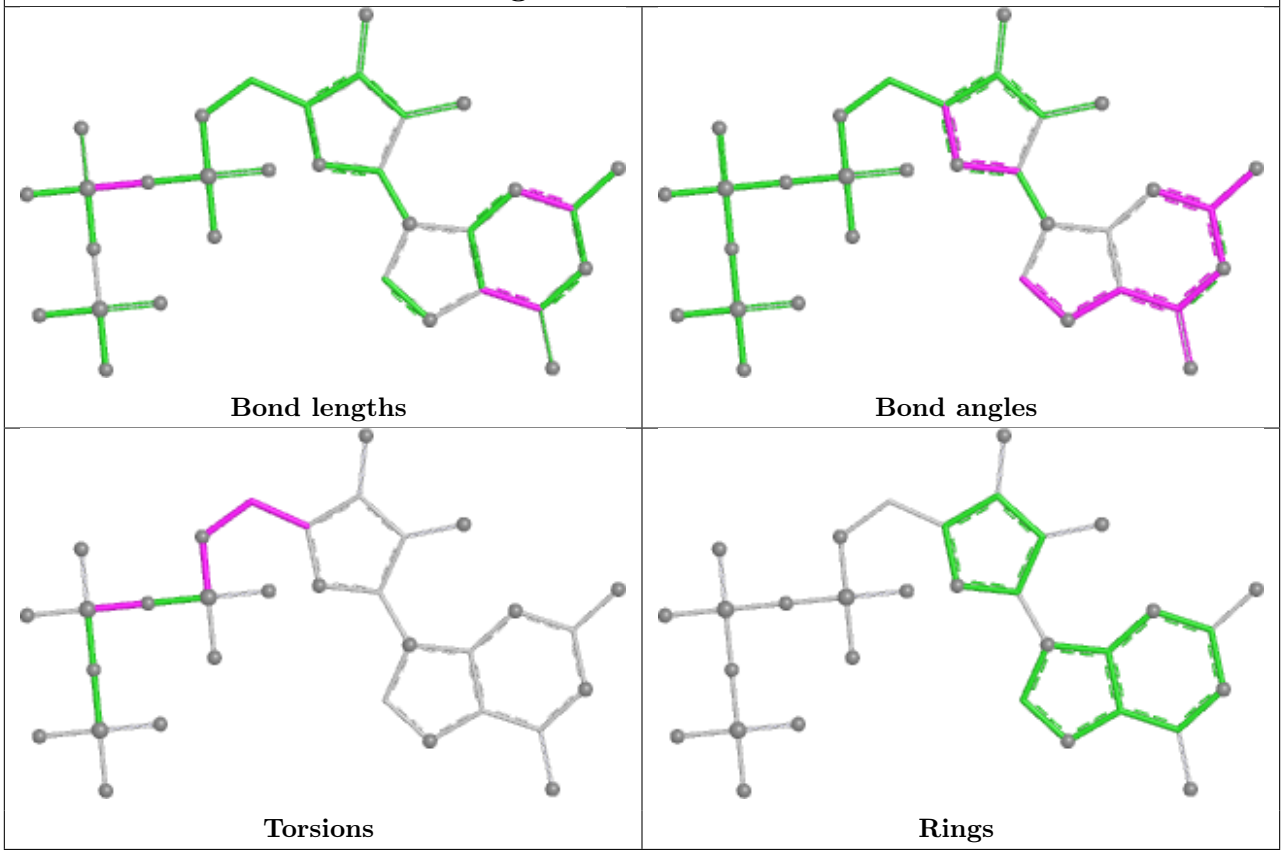

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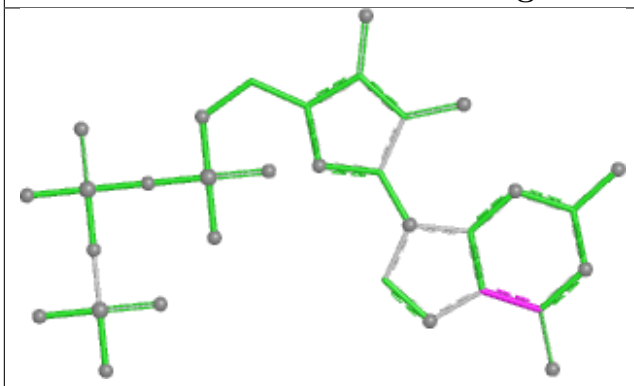
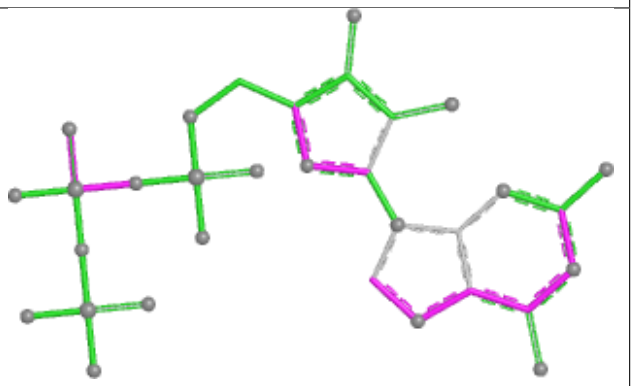
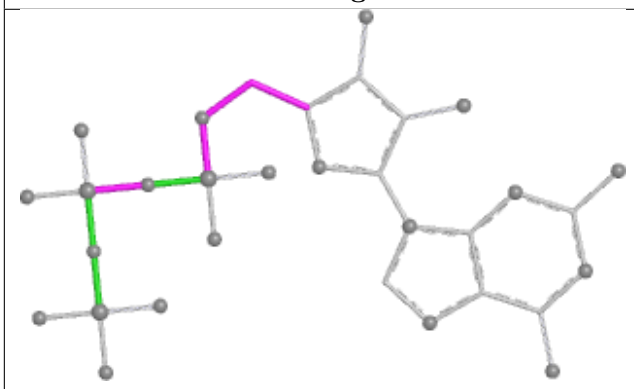


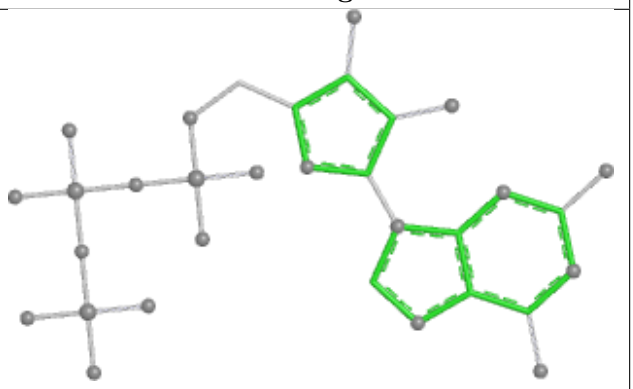
Bond lengths



Bond angles

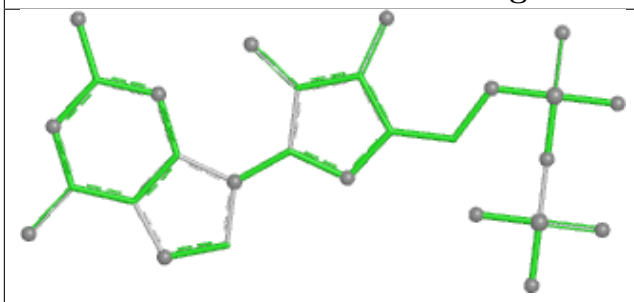


Torsions



Rings

## Ligand GDP VP 502



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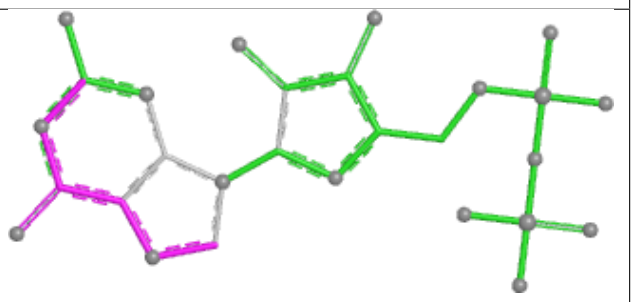

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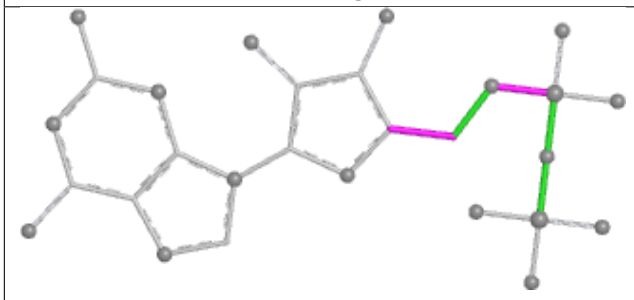

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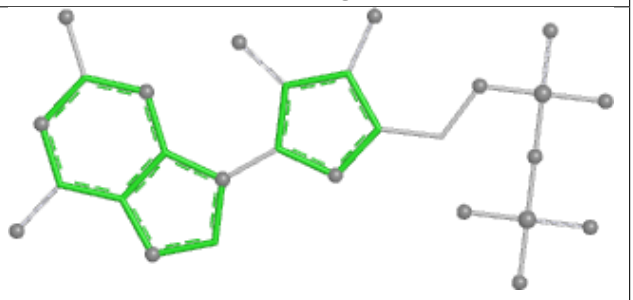
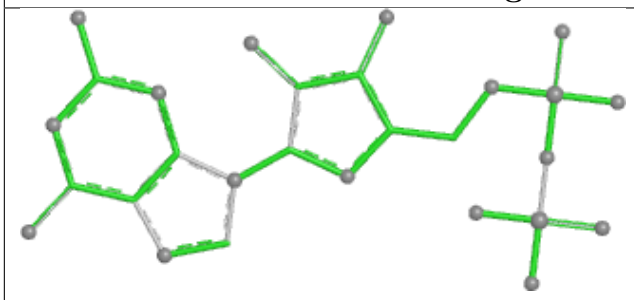


Rings

## Ligand GDP MO 501



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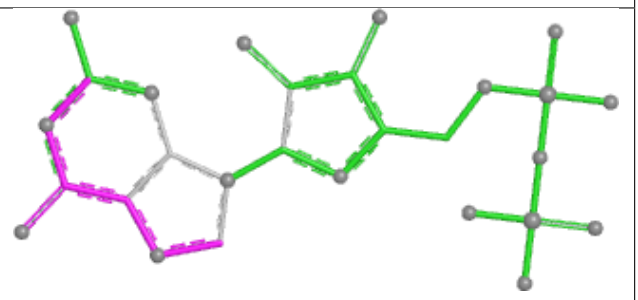

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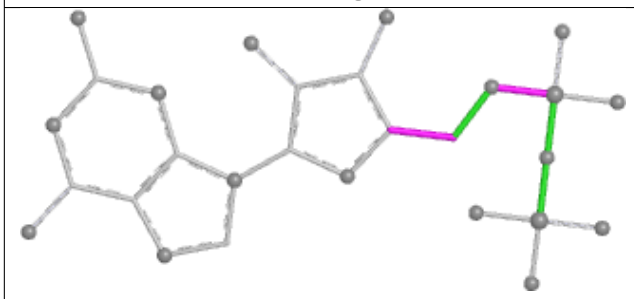

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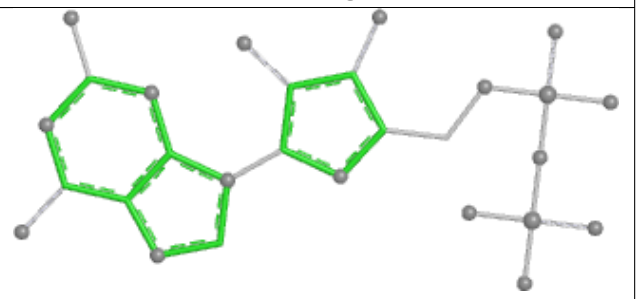

Rings

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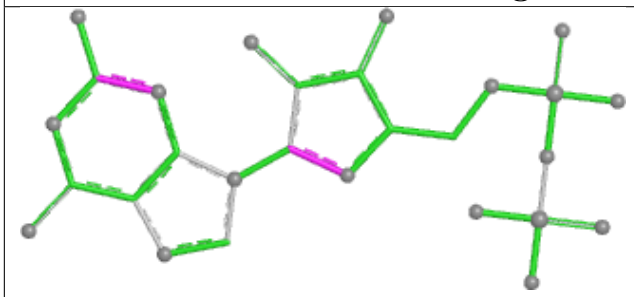

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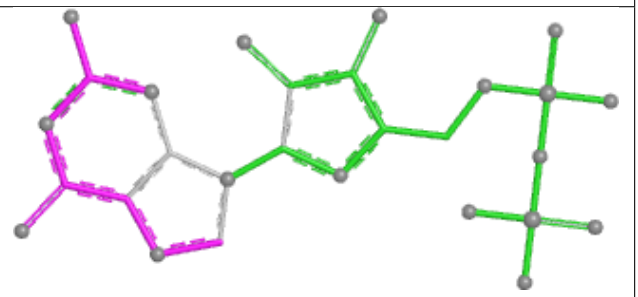

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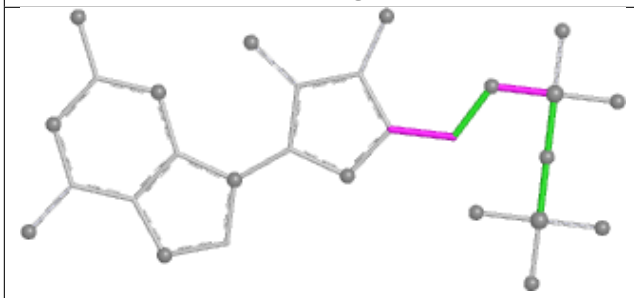

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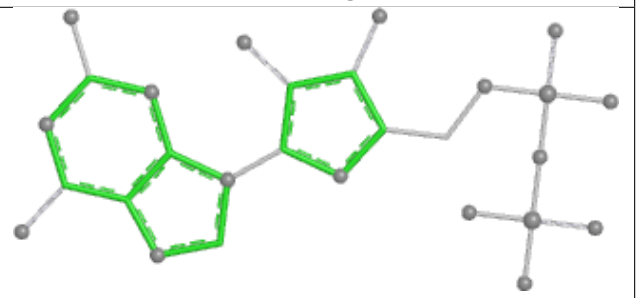

Rings

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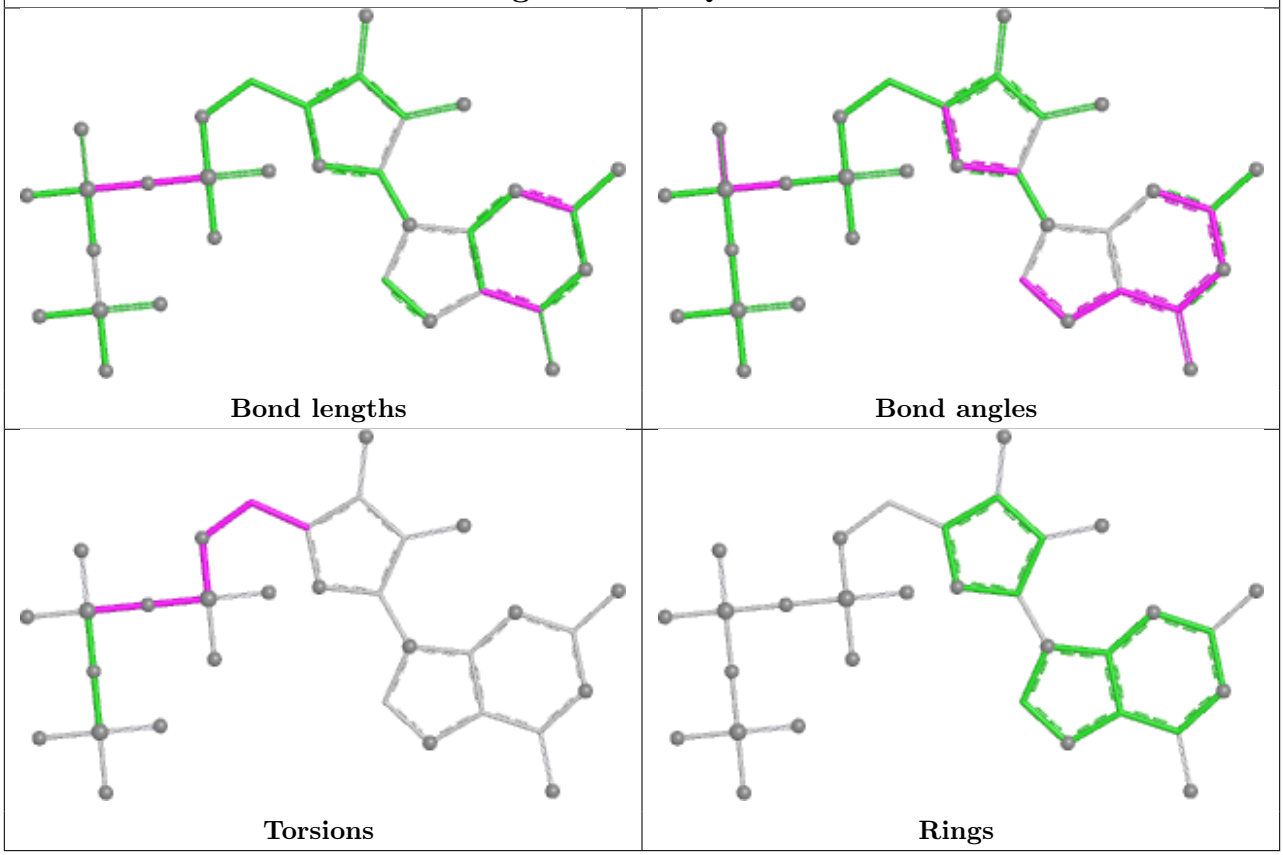


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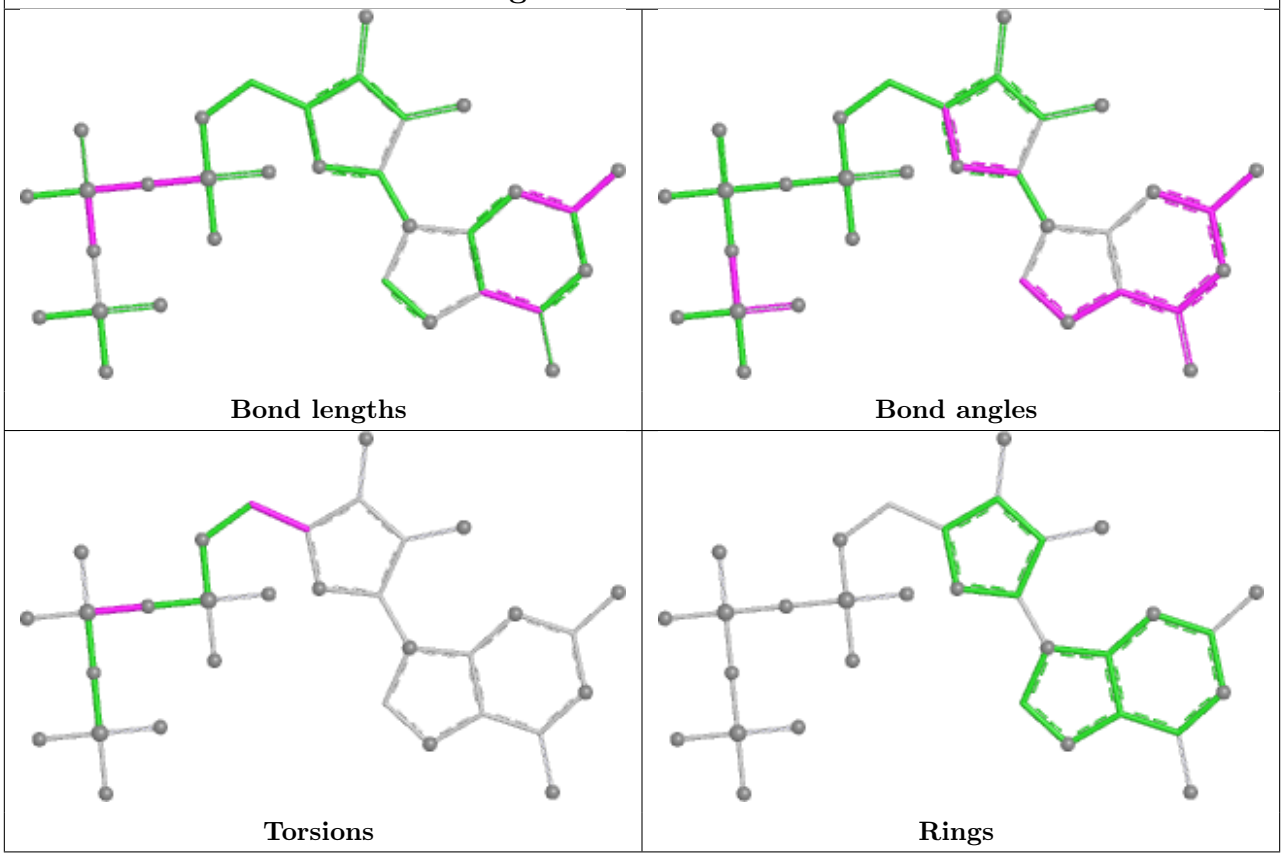

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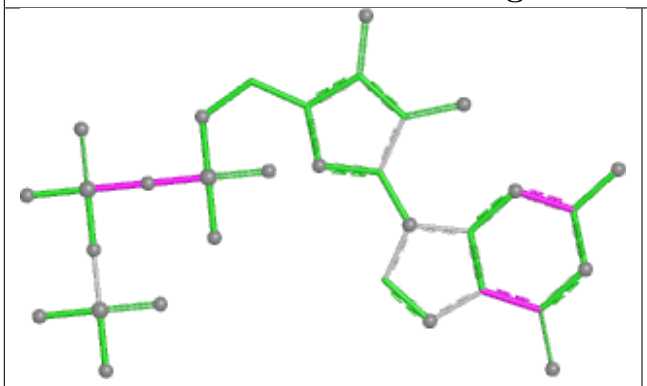
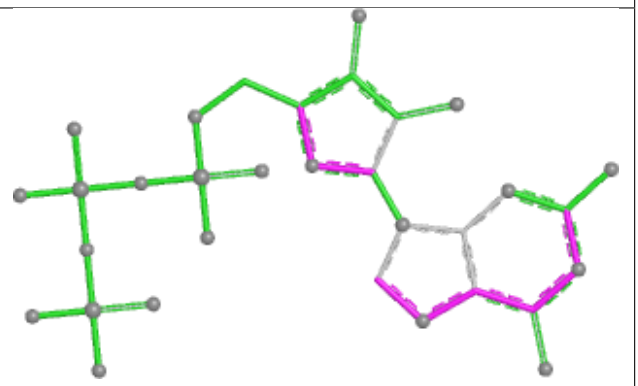
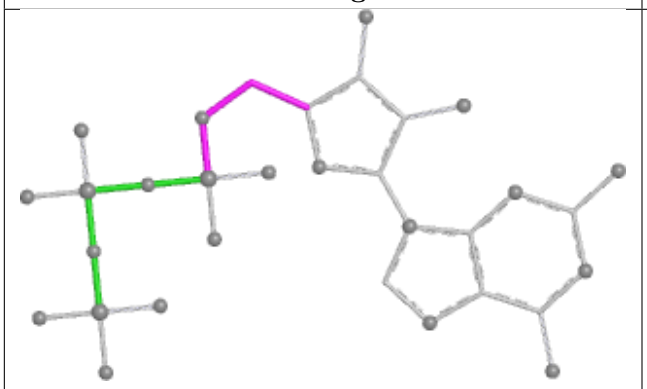


Bond lengths



Bond angles



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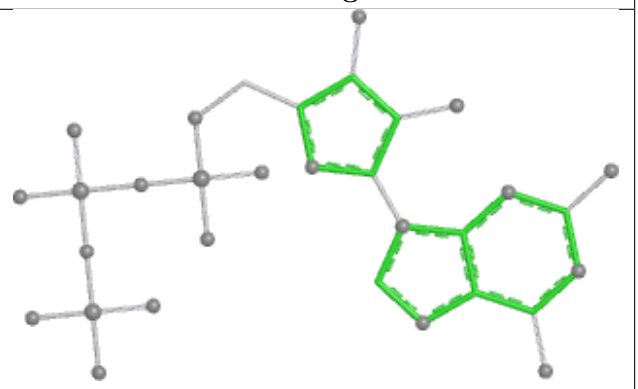

Rings

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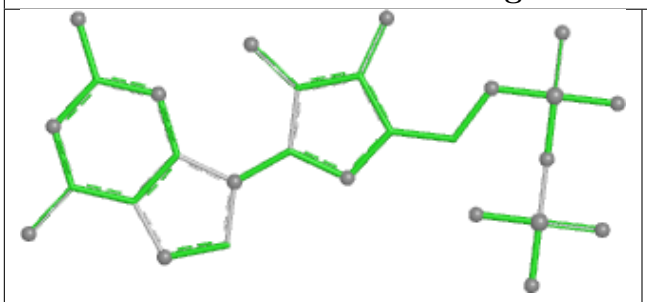

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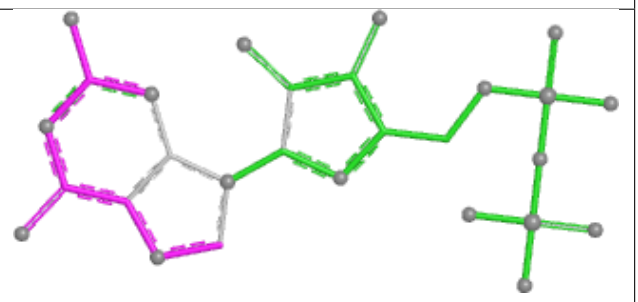

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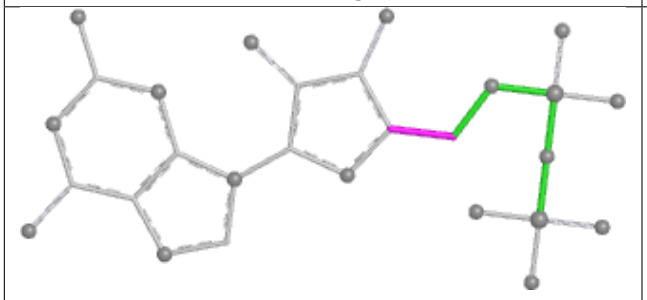

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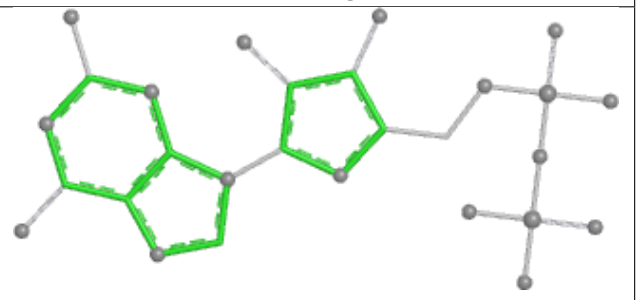
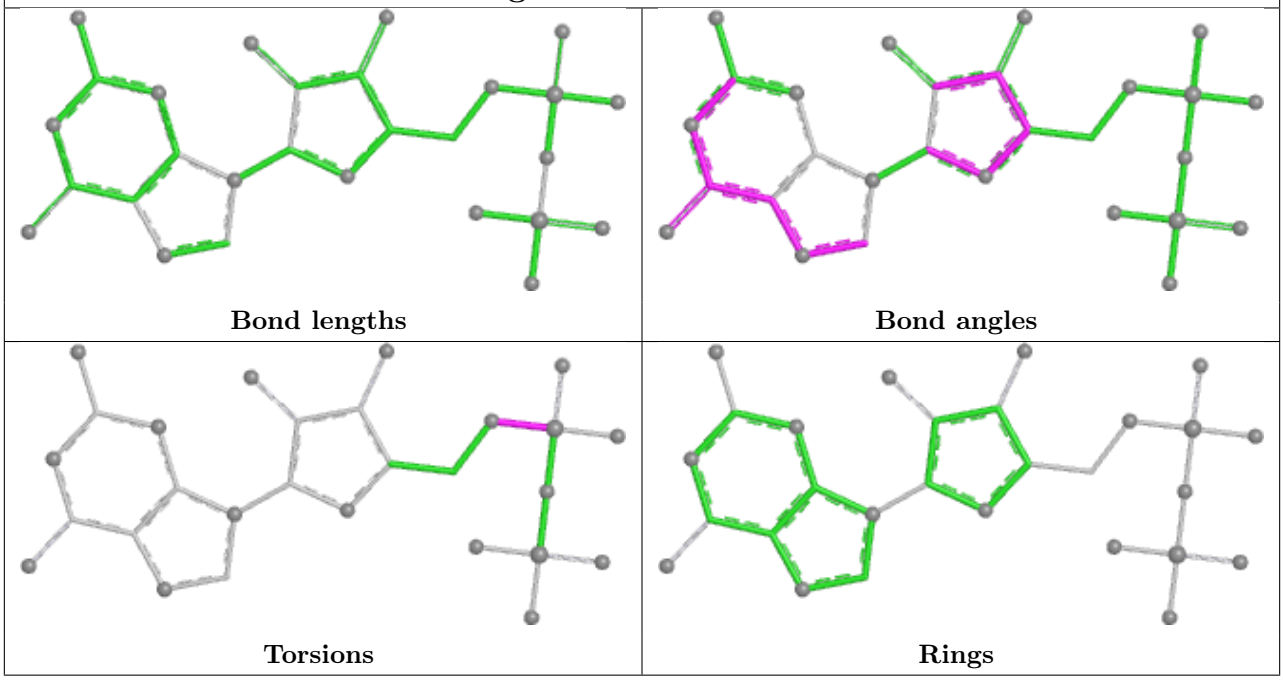
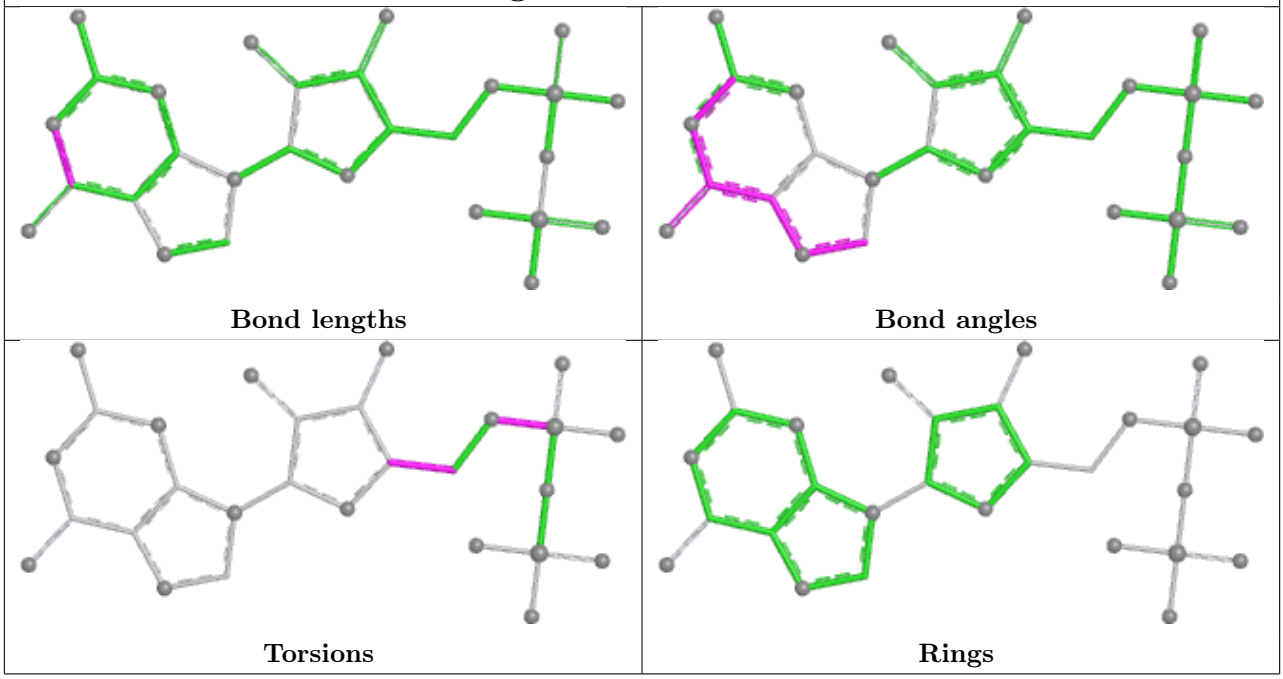


Rings

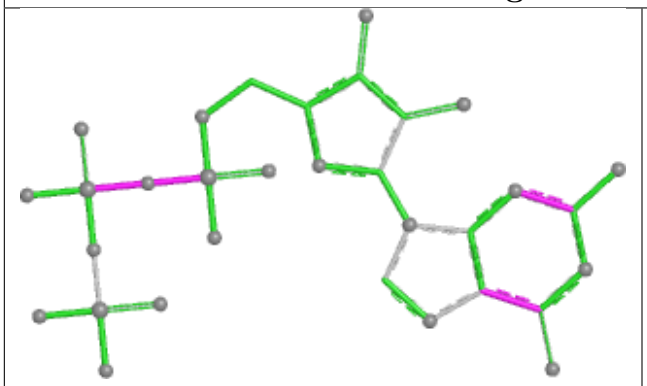
## Ligand GDP SM 502




## Ligand GDP TN 502



## Ligand GTP MD 501



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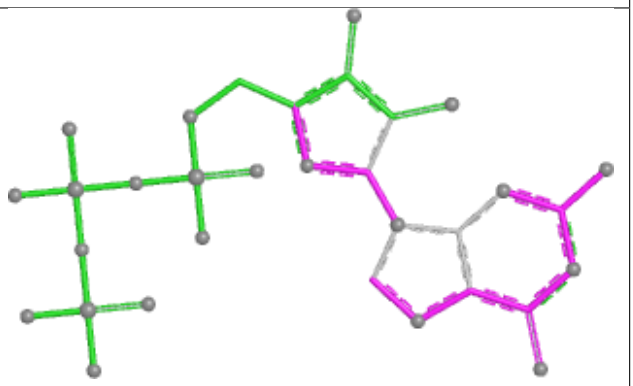
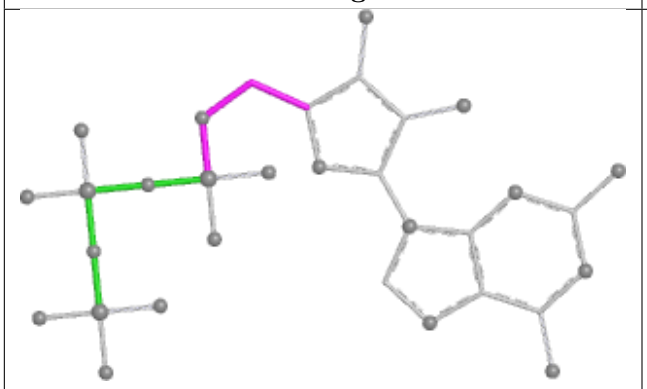


Bond angles



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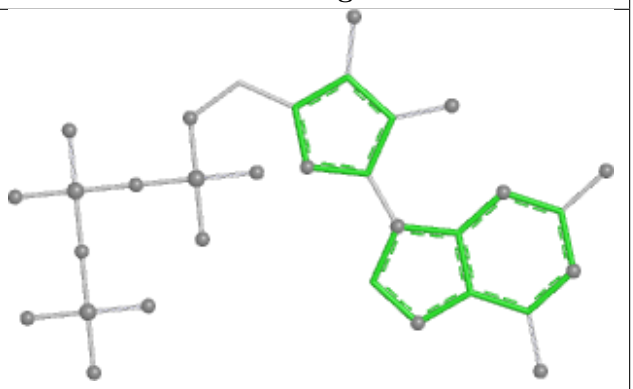
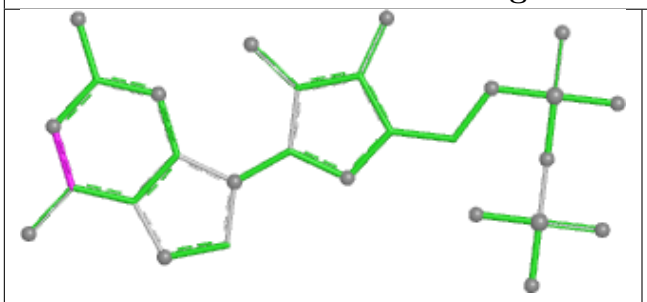


Rings

## Ligand GDP AP 501



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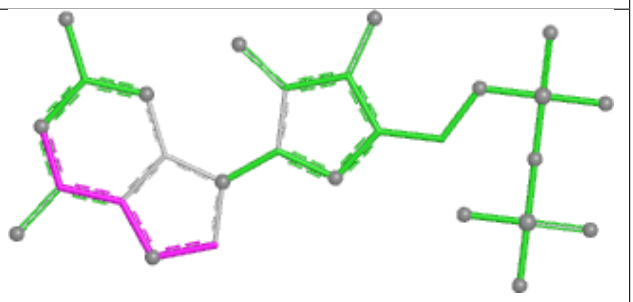
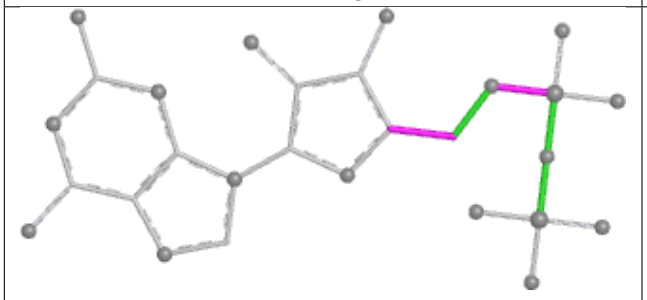


Bond angles



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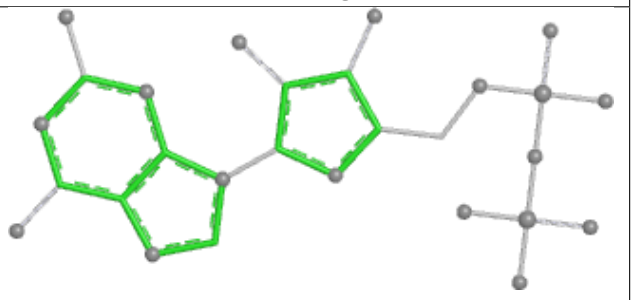
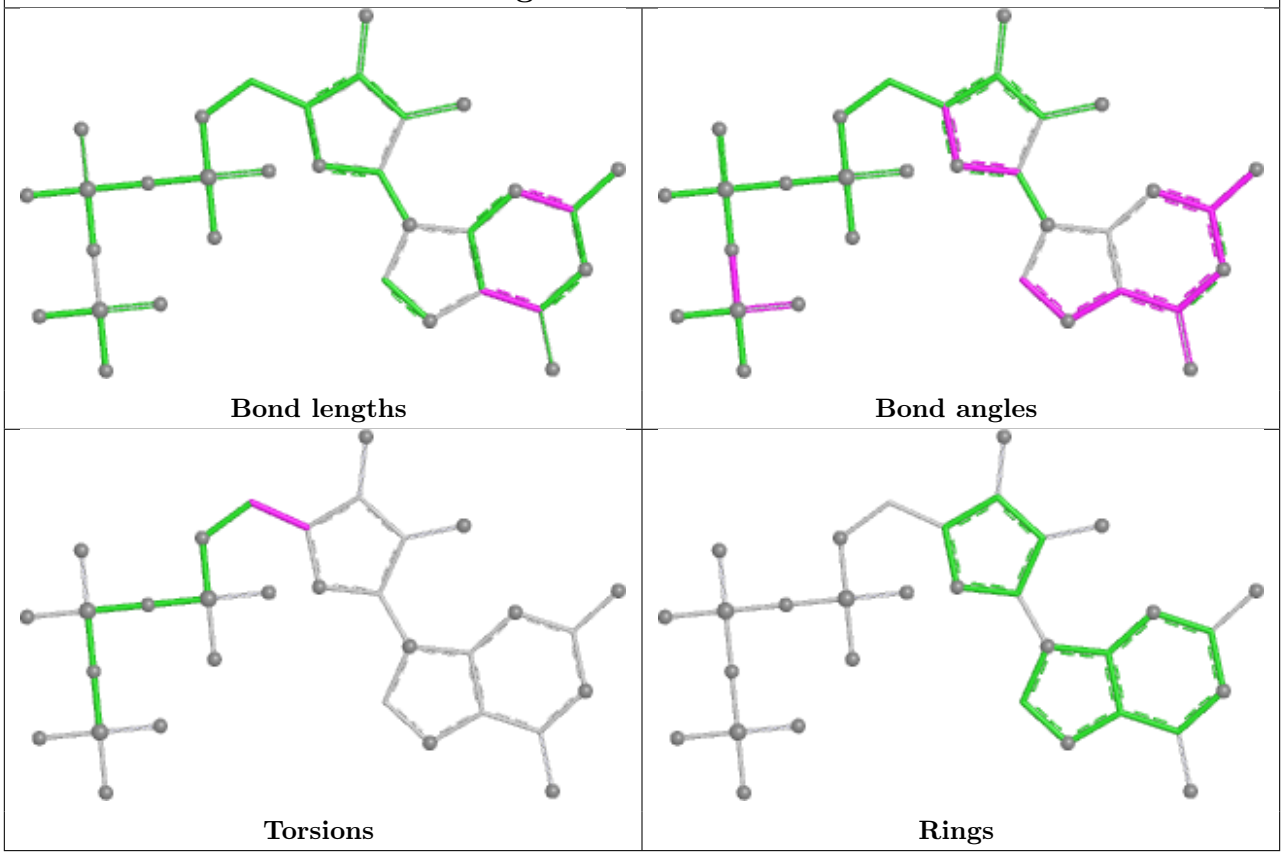
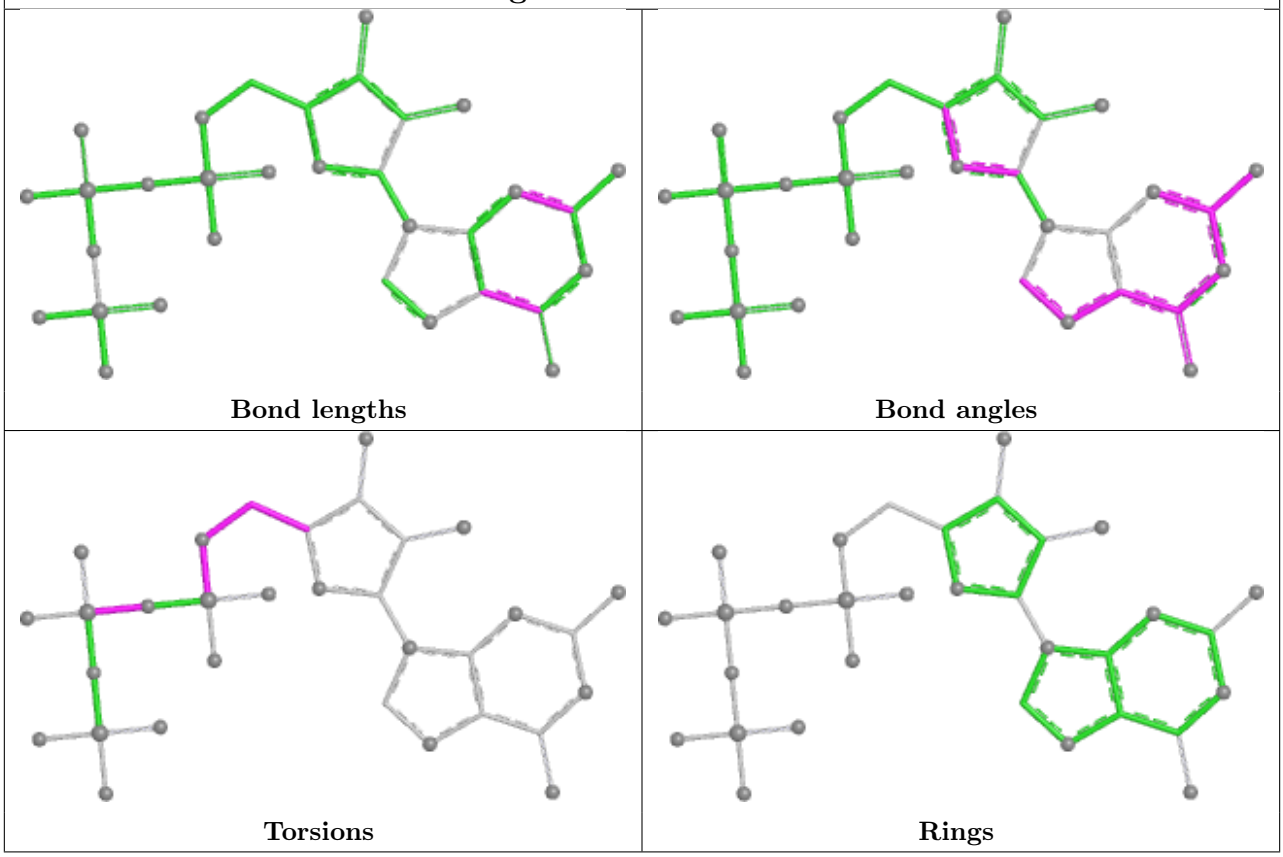


Rings

## Ligand GTP JF 501




## Ligand GTP UO 501



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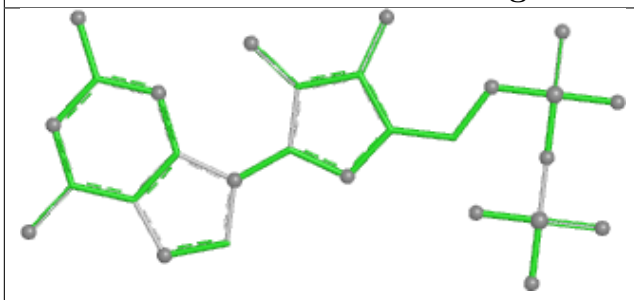
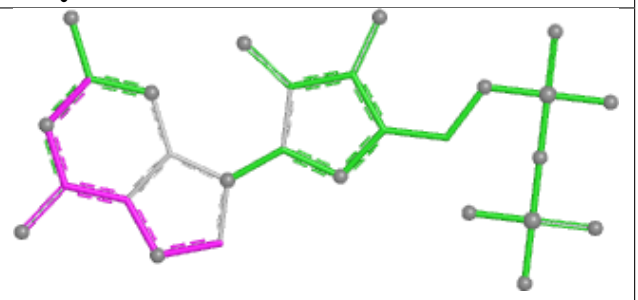
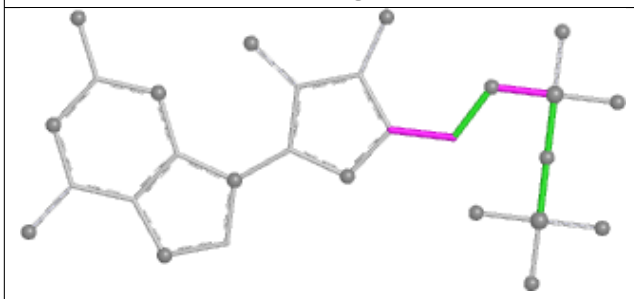


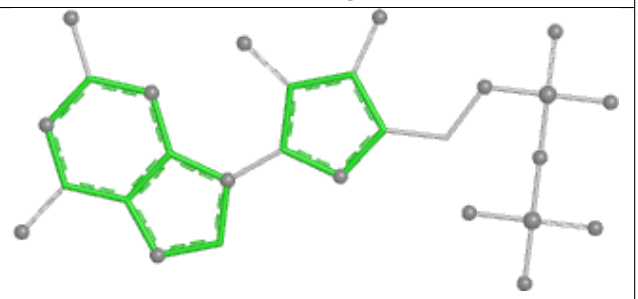
Bond lengths



Bond angles



Torsions



Rings

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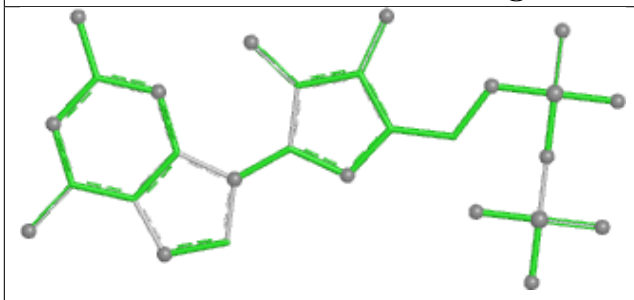

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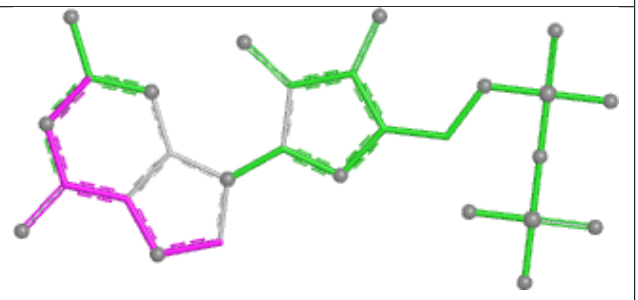

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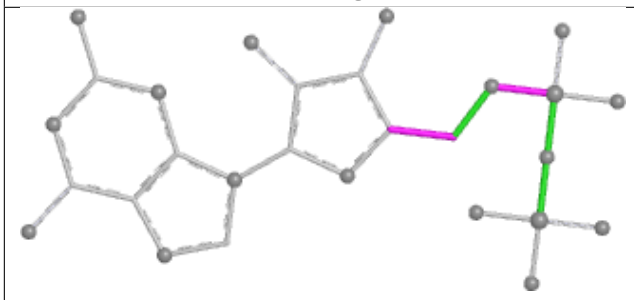

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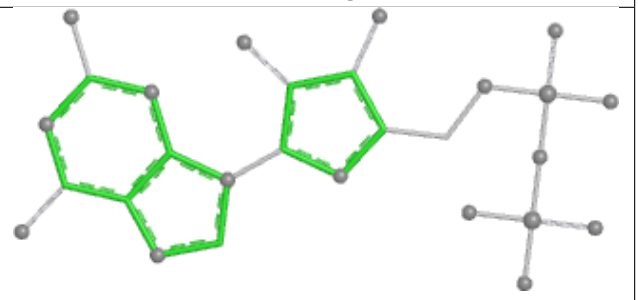

Rings

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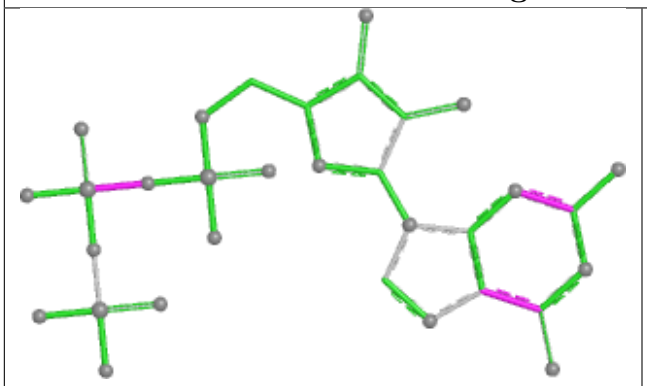

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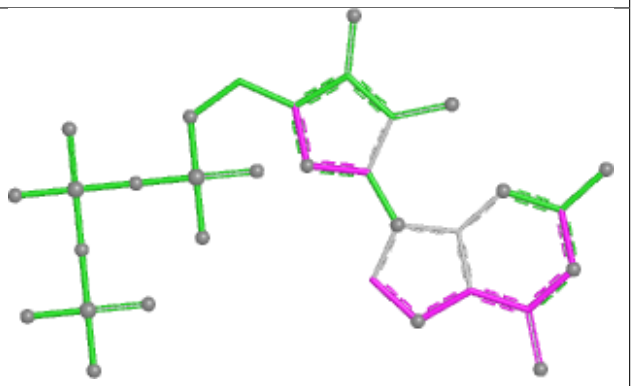

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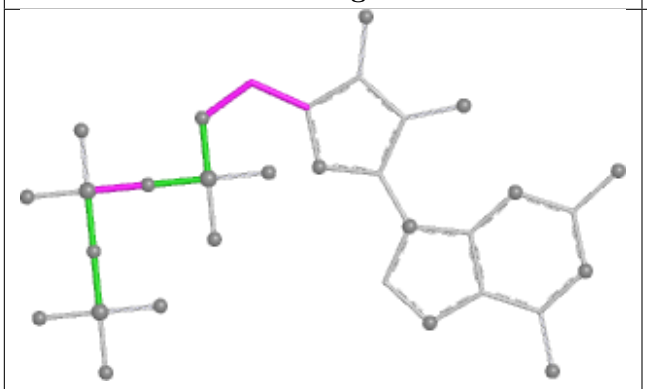

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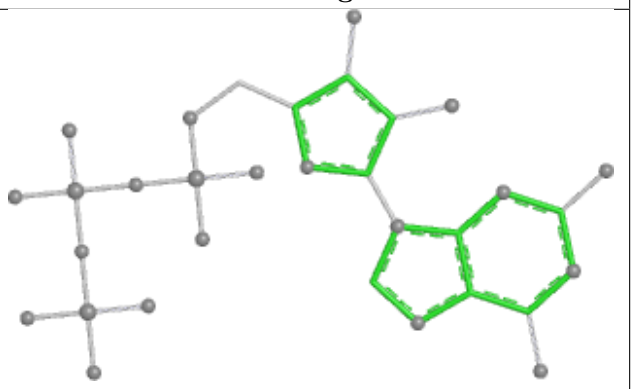

Rings

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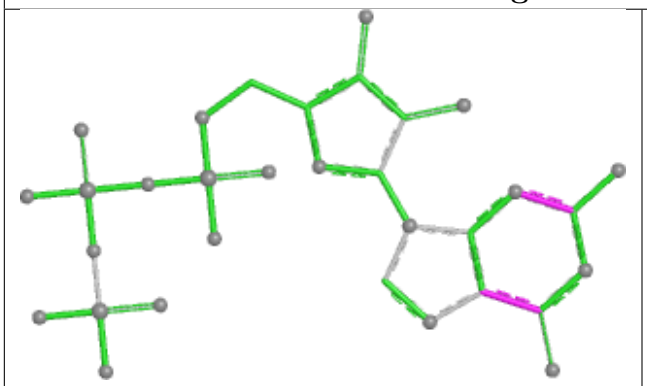

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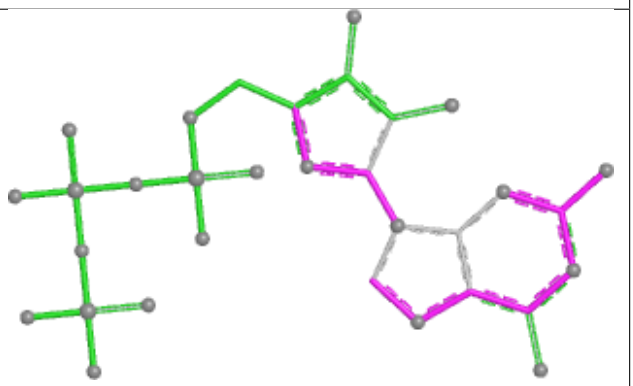

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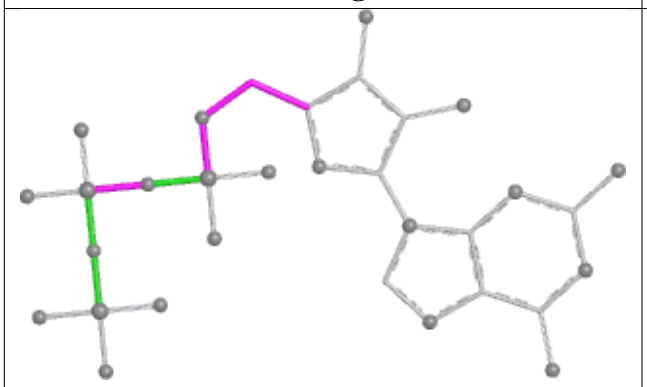

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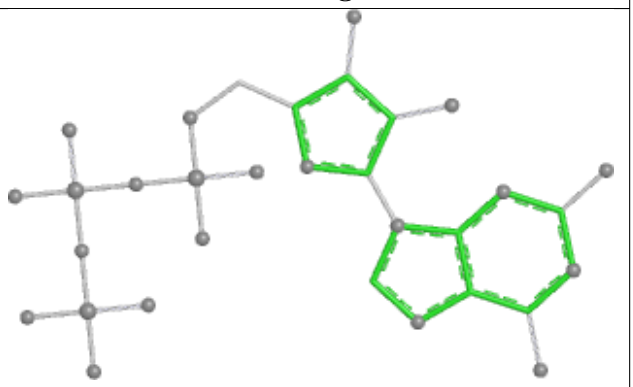

Rings

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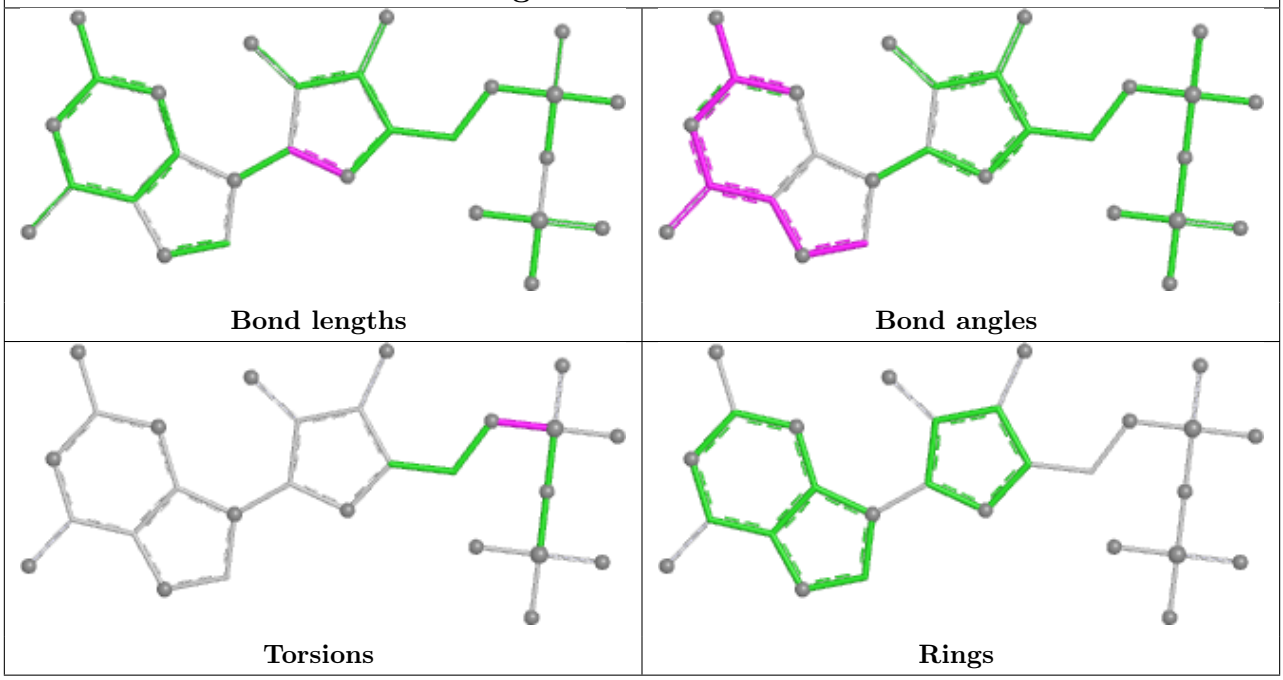


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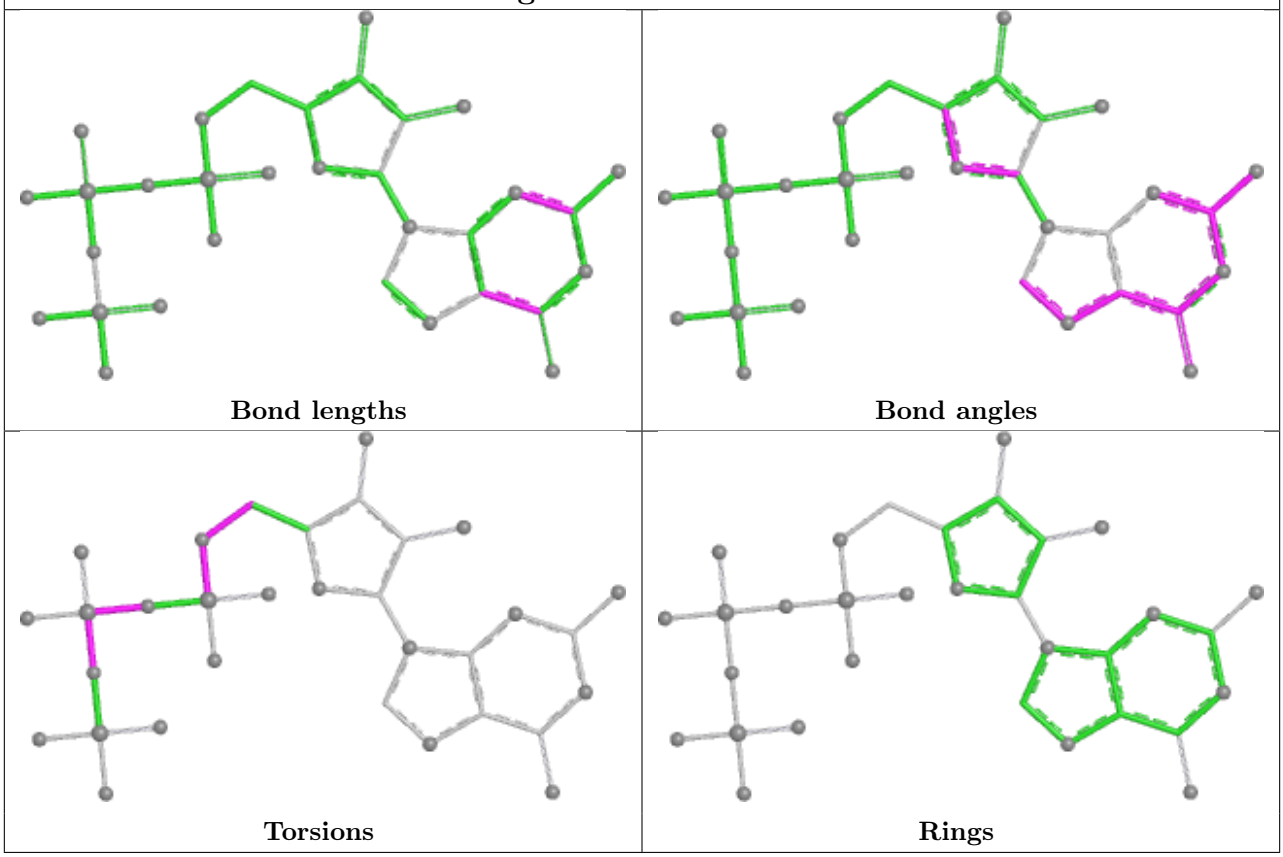

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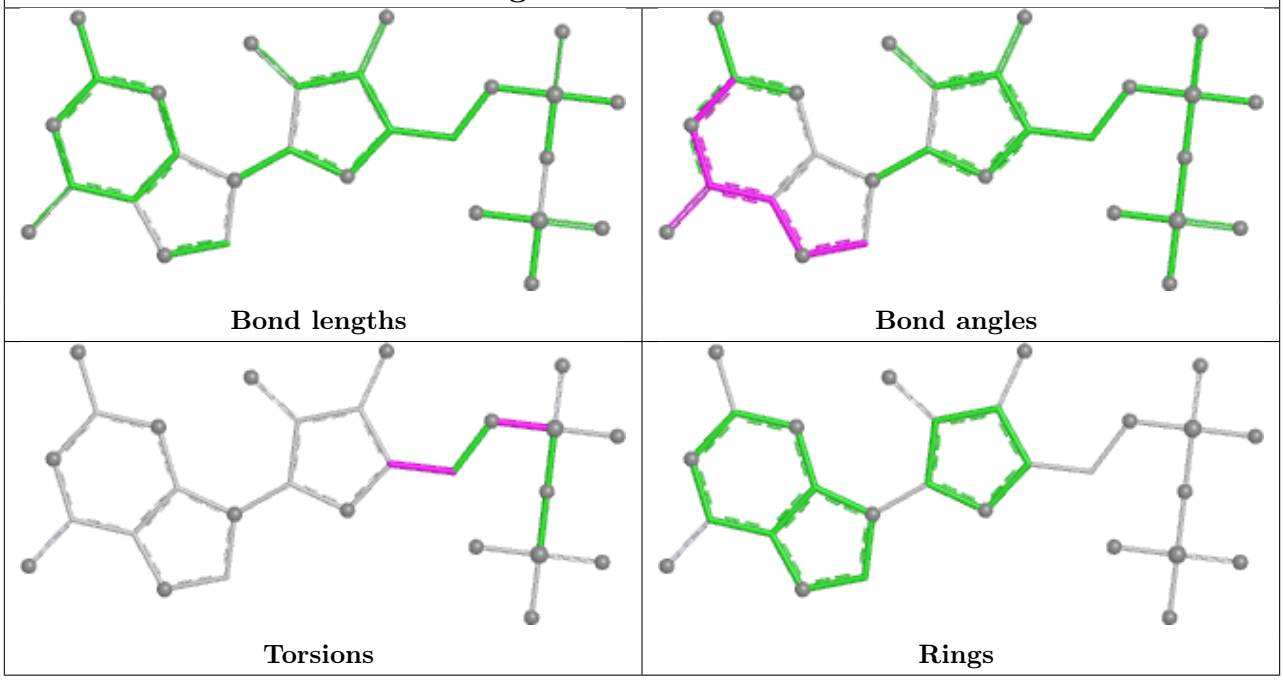


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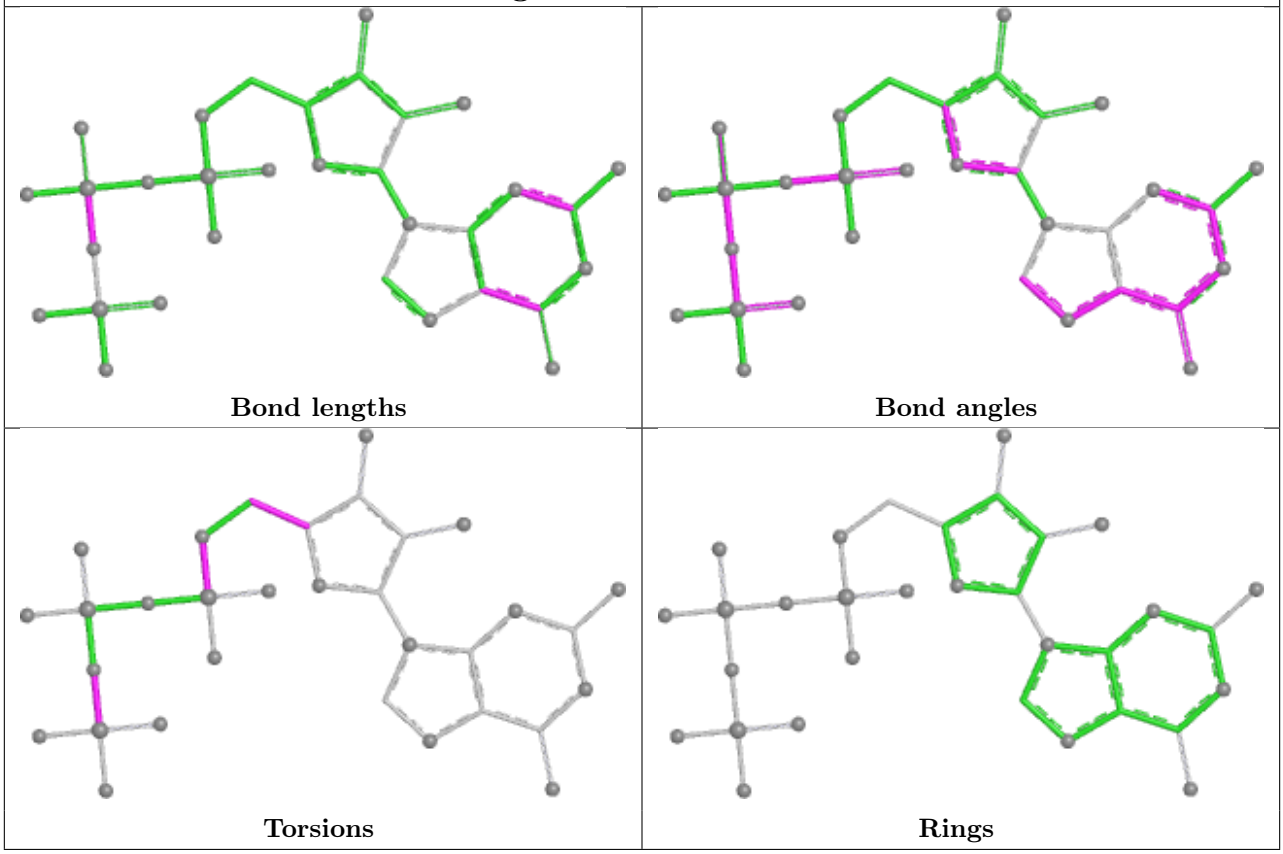

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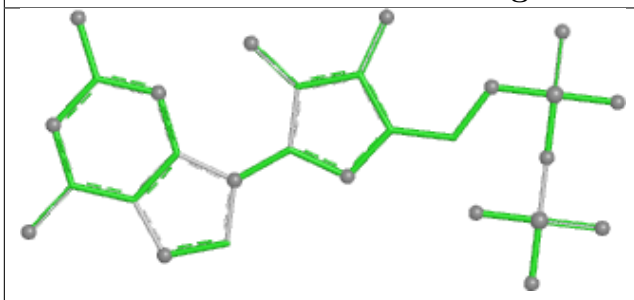

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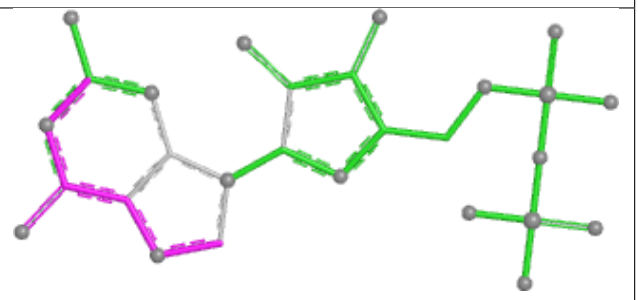
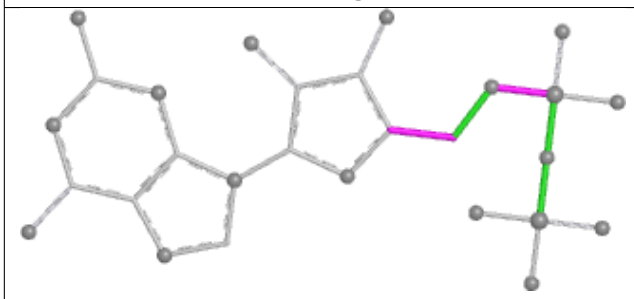
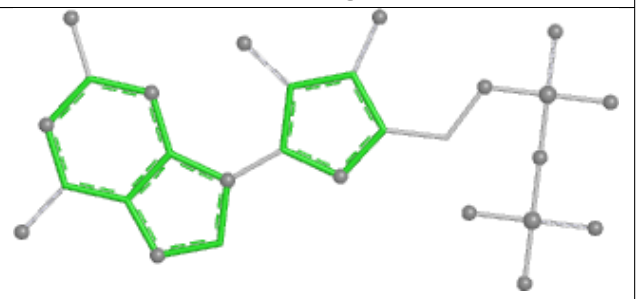


Bond angles

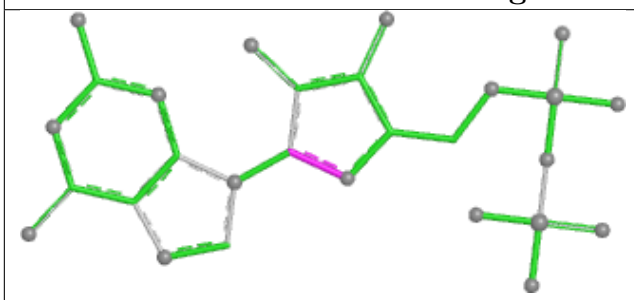


Torsions



Rings

## Ligand GDP CO 501



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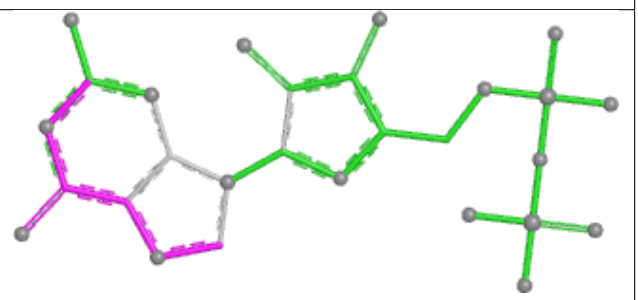

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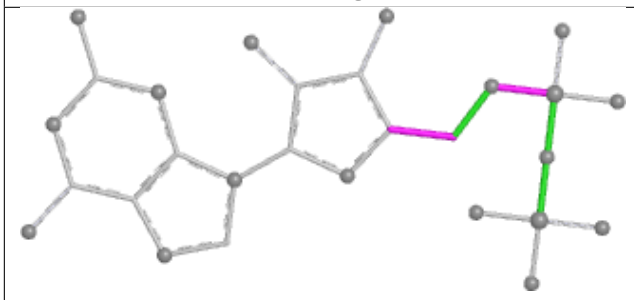

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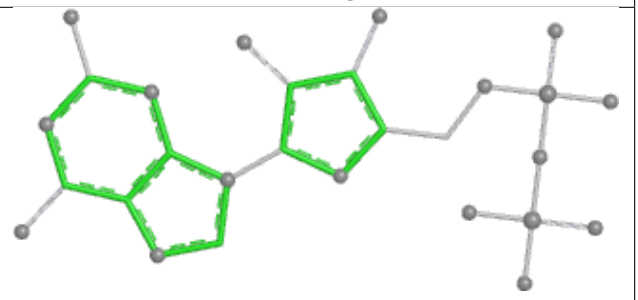

Rings

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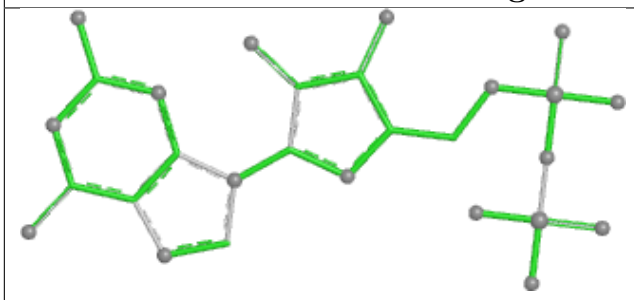

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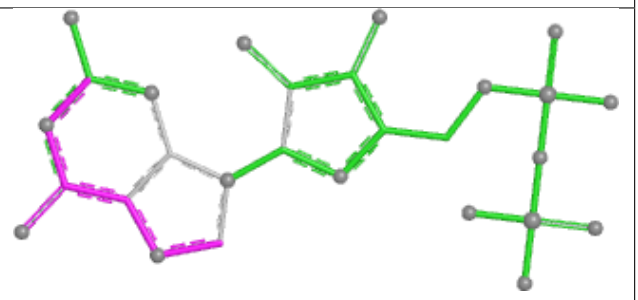

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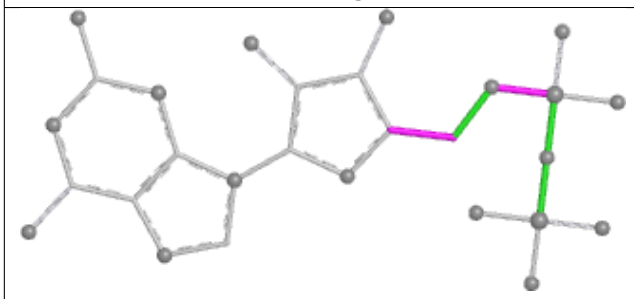

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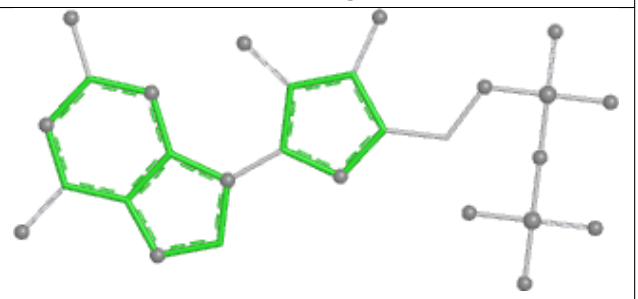

Rings

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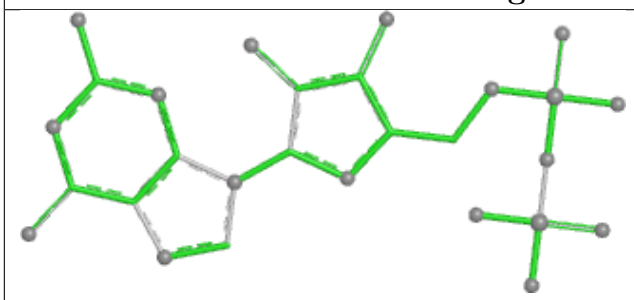

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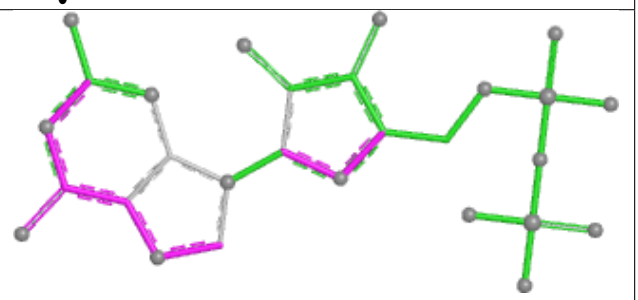

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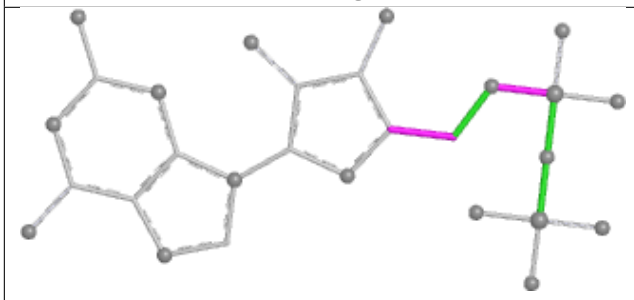

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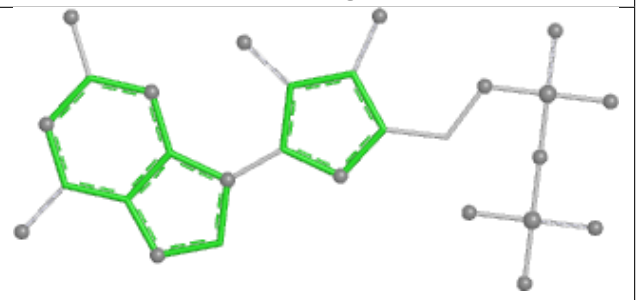

Rings

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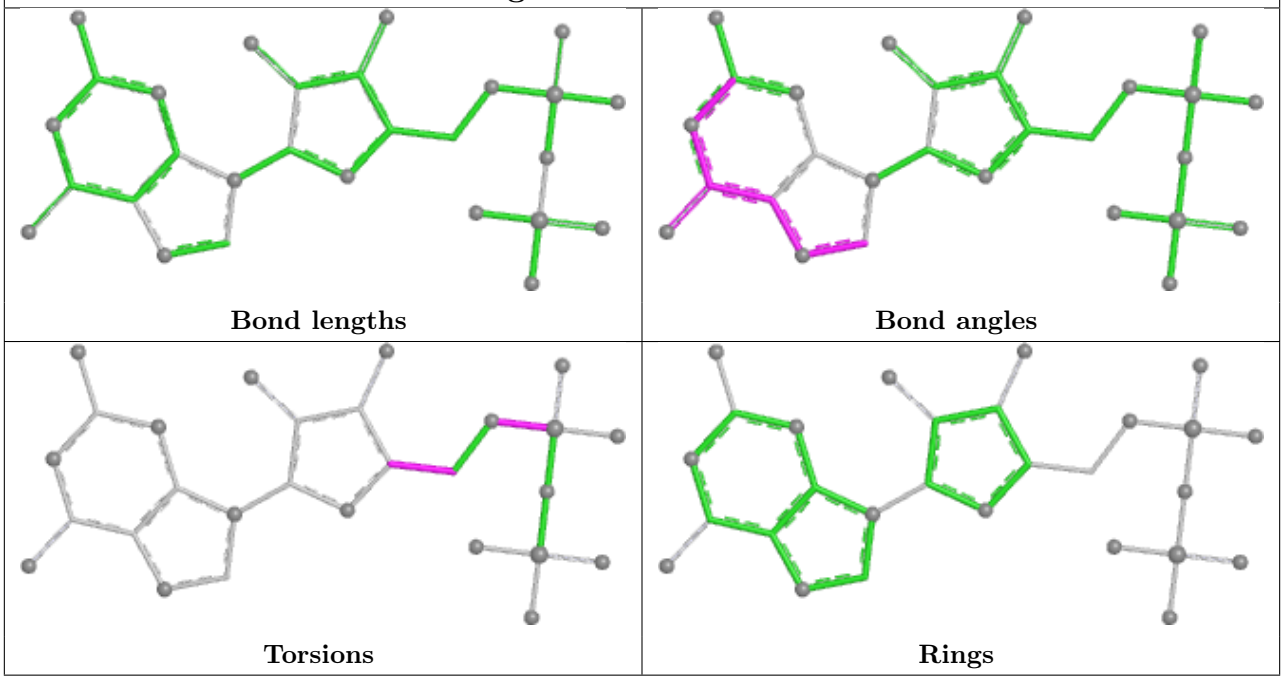


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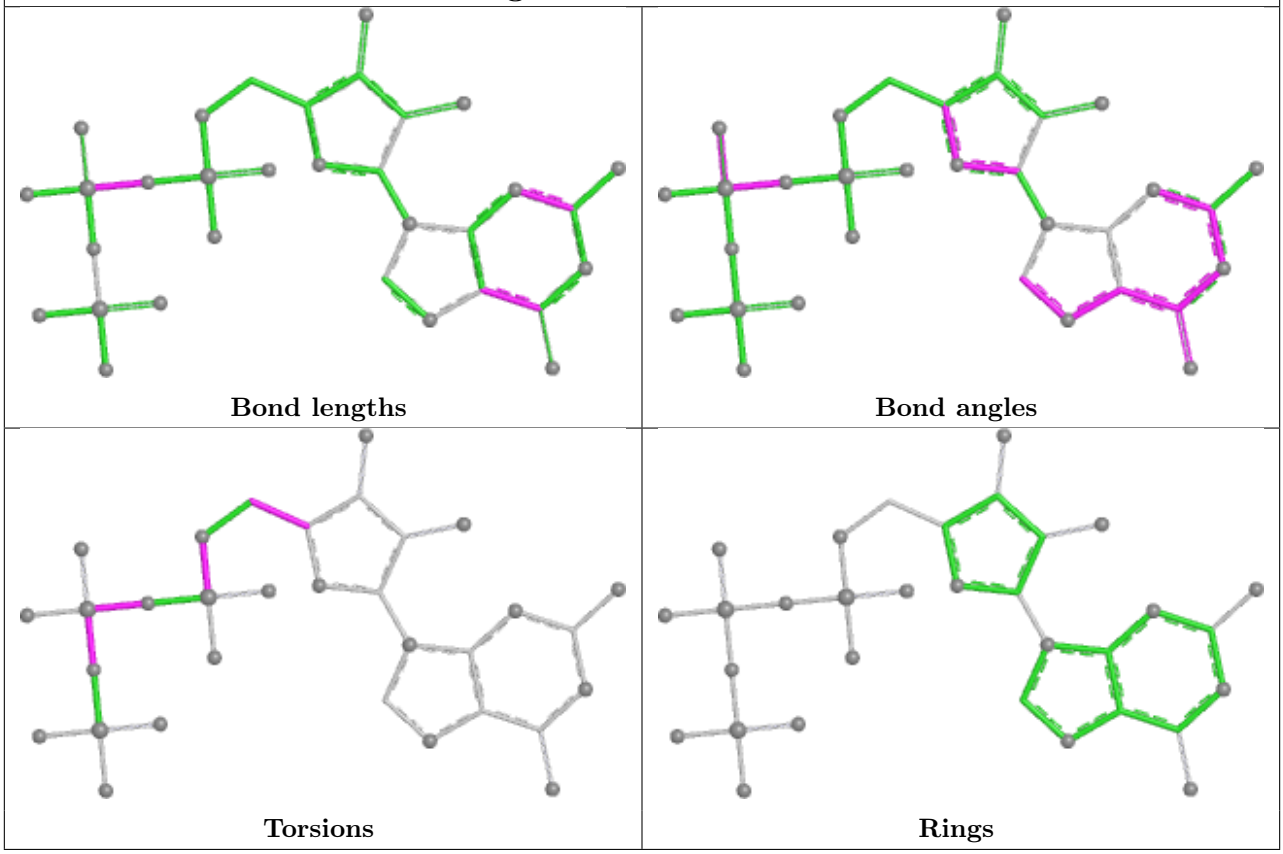

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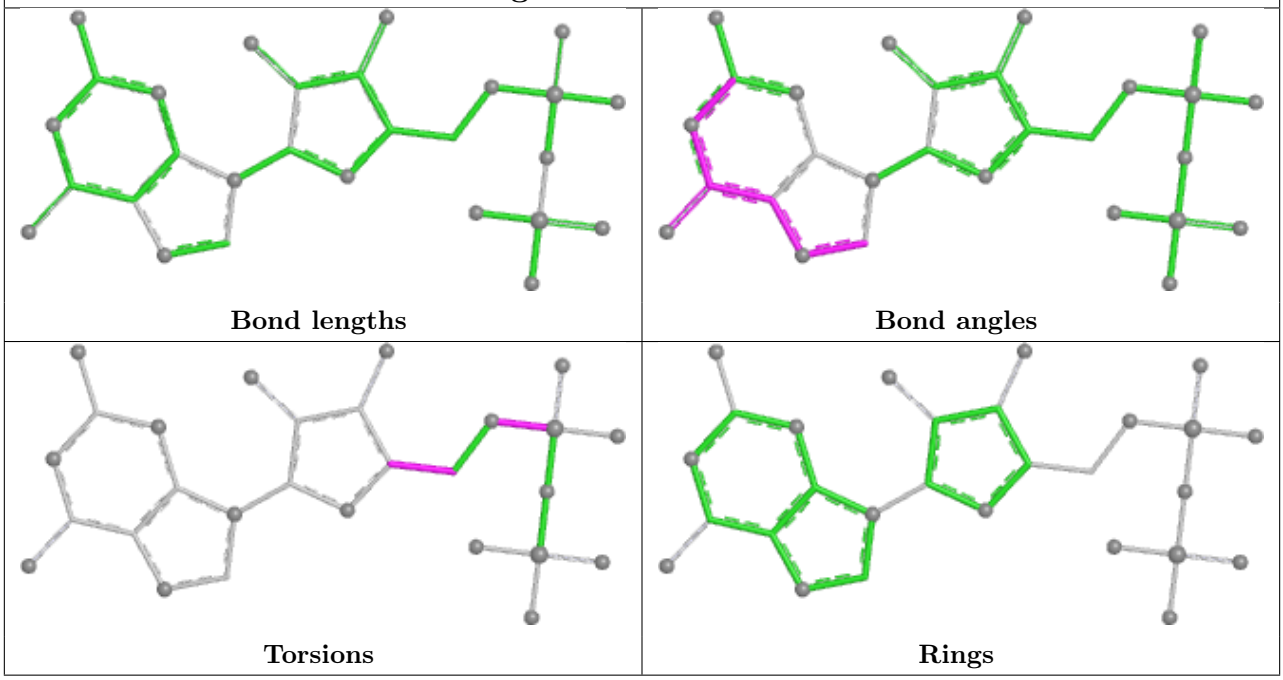


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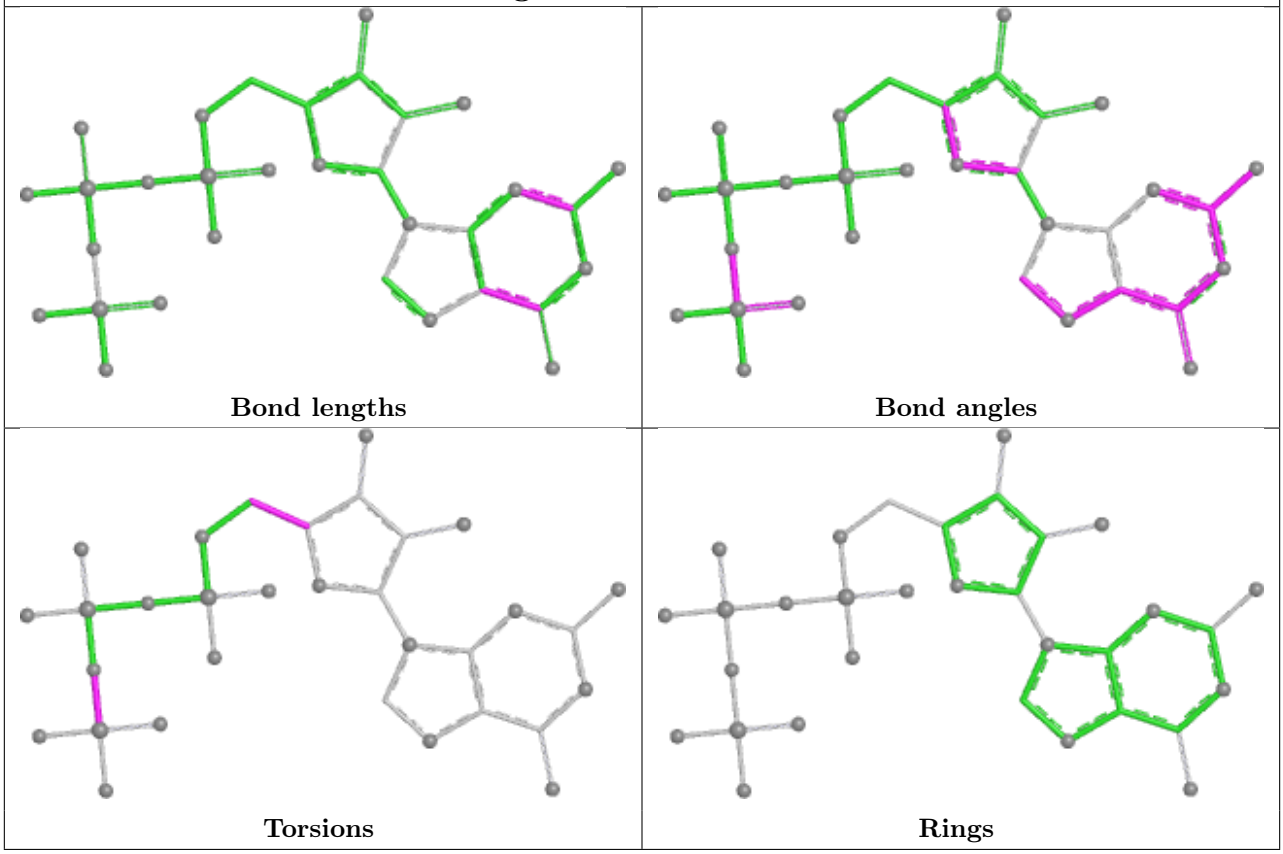

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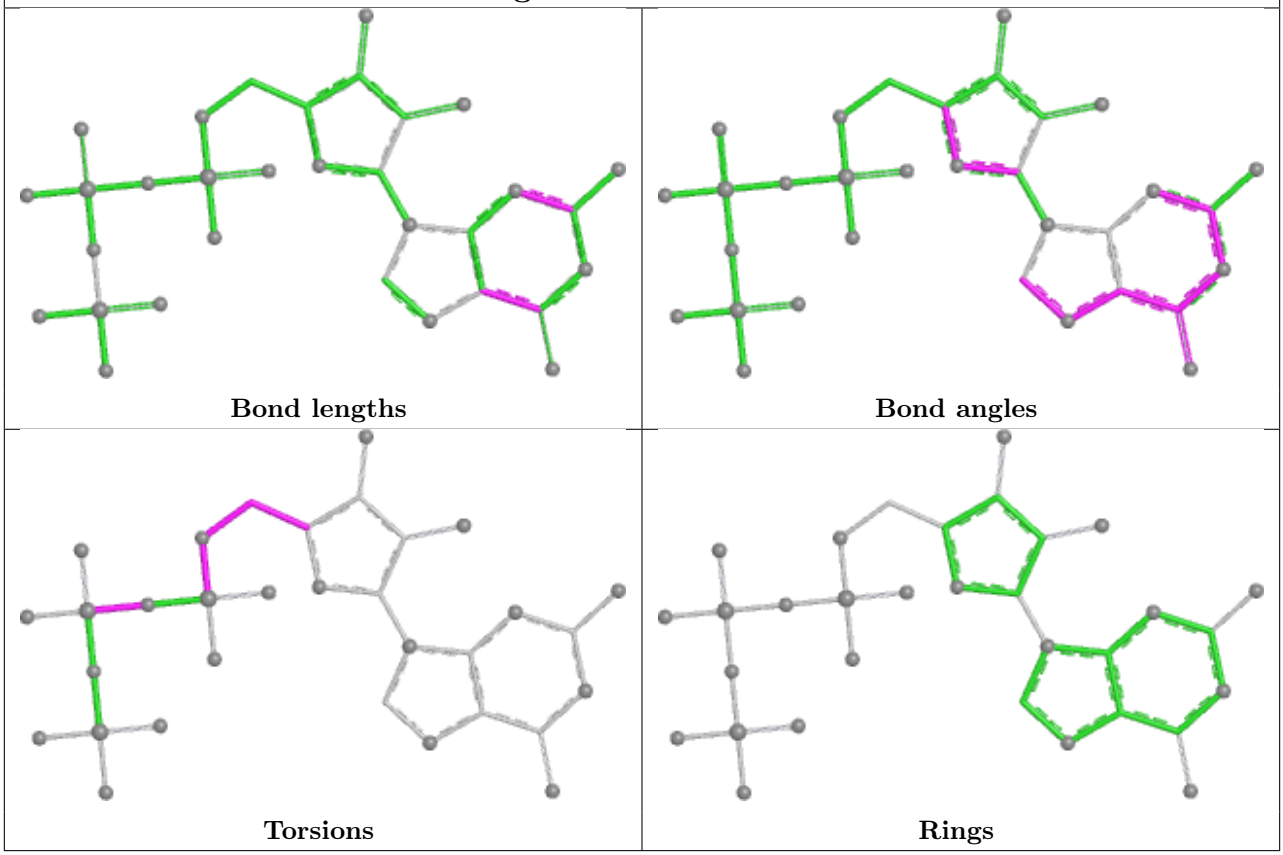


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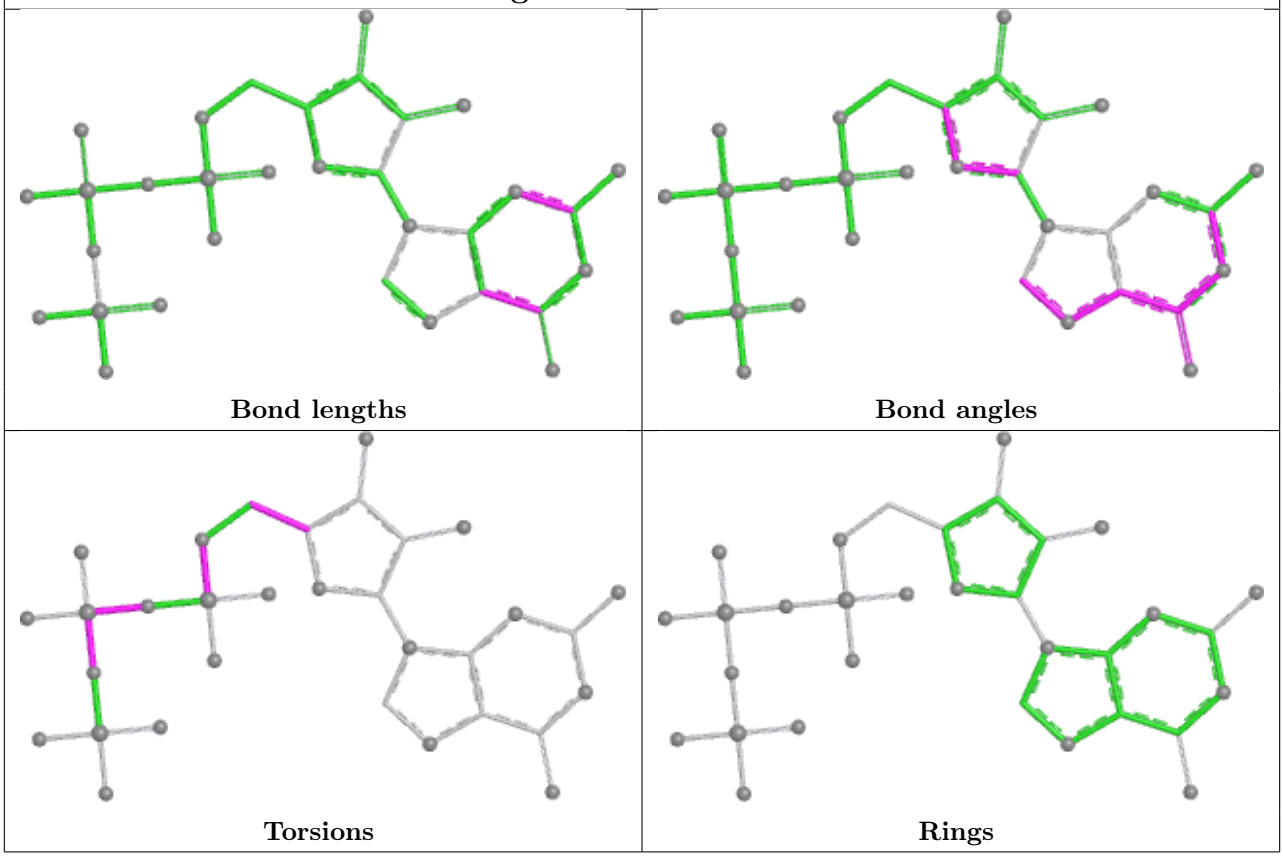

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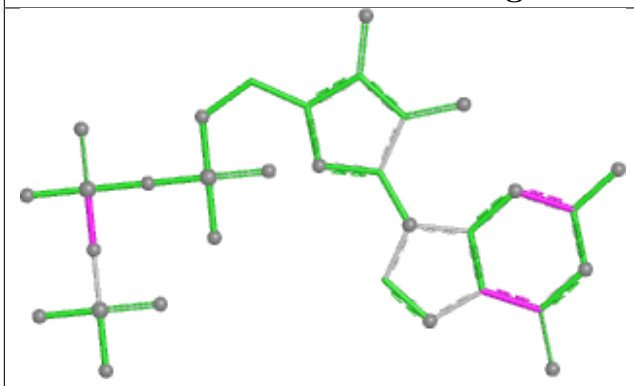
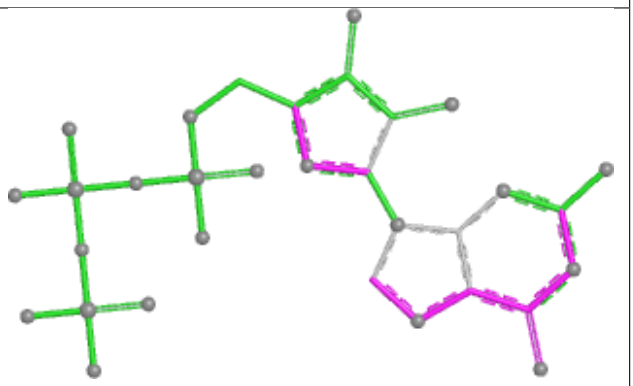
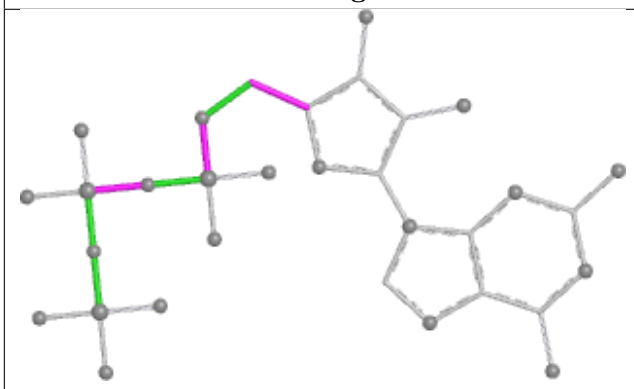


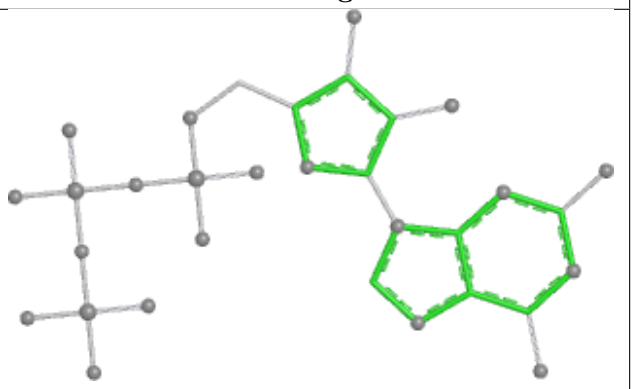
Bond lengths



Bond angles

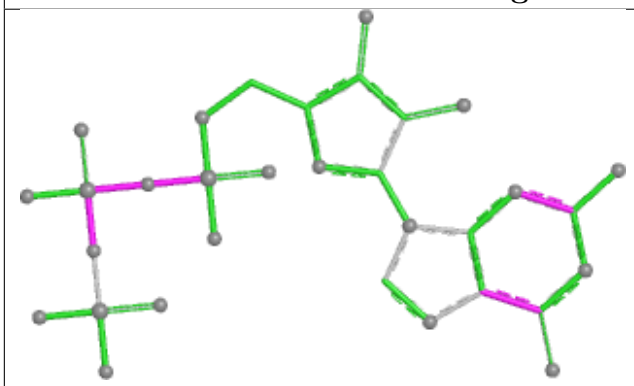


Torsions



Rings

## Ligand GTP UE 501



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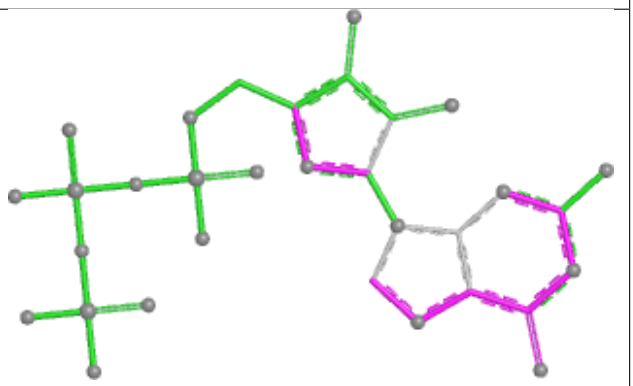

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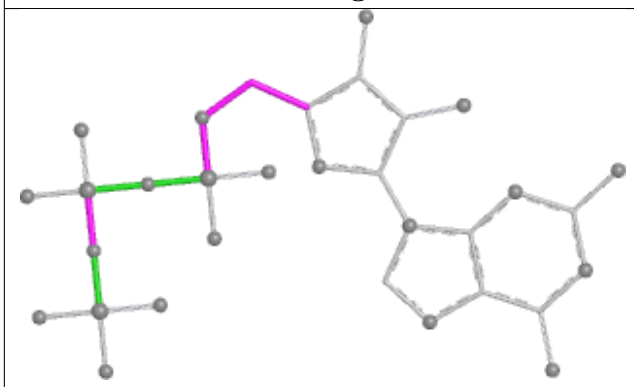

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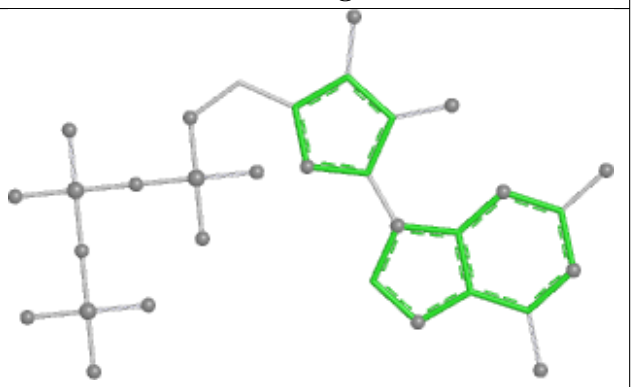

Rings

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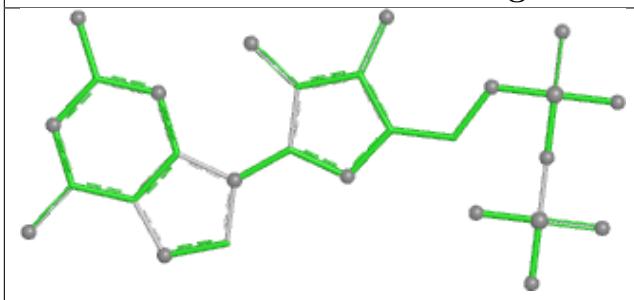

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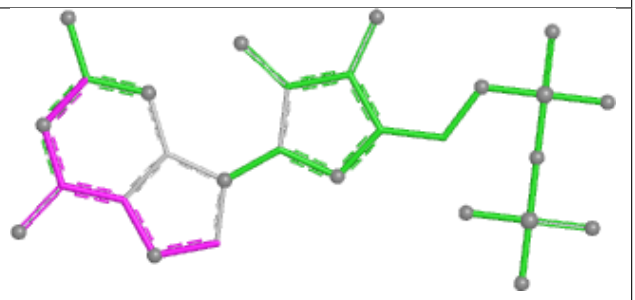

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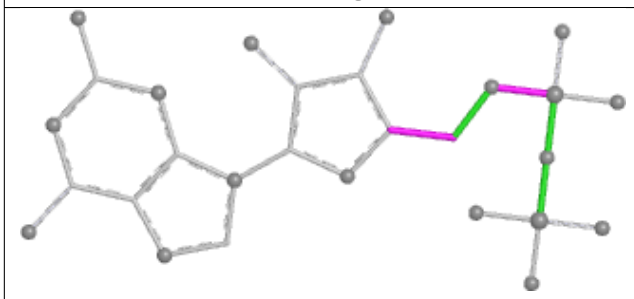
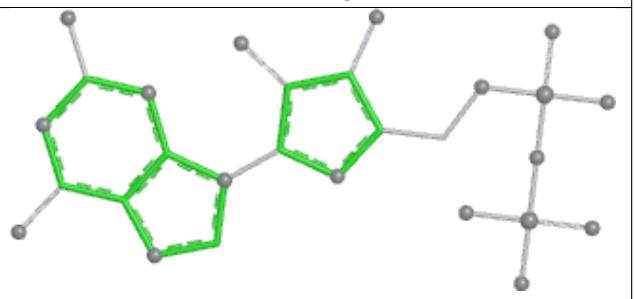


Torsions



Rings

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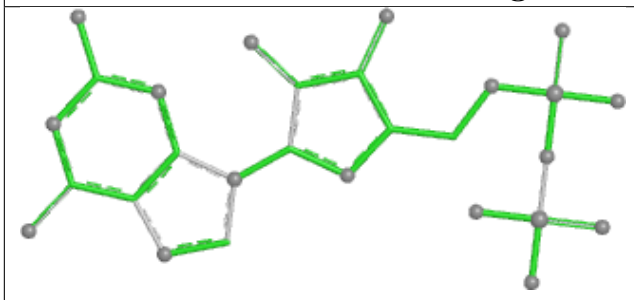

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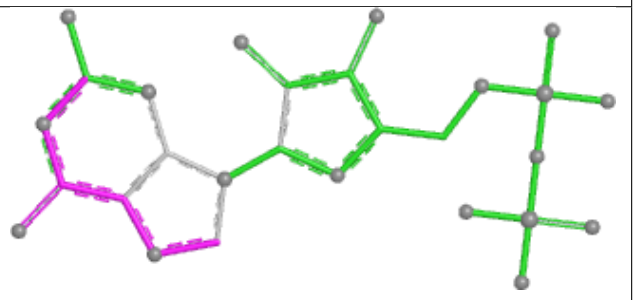

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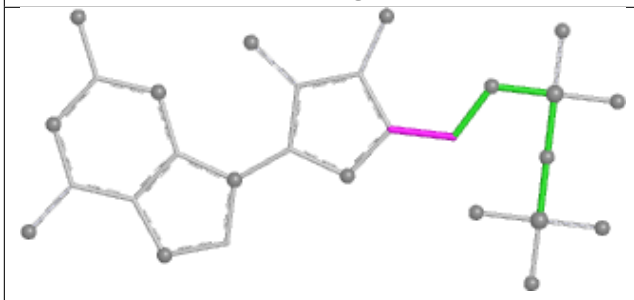

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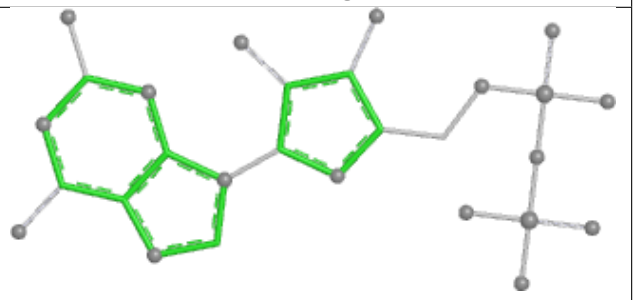

Rings

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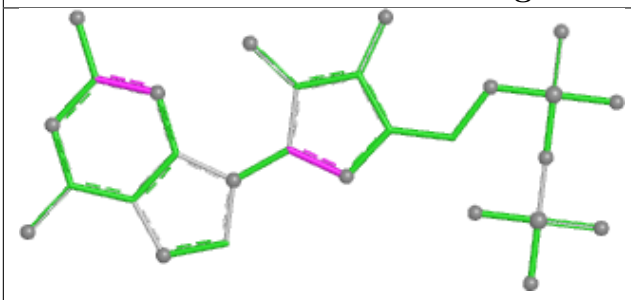

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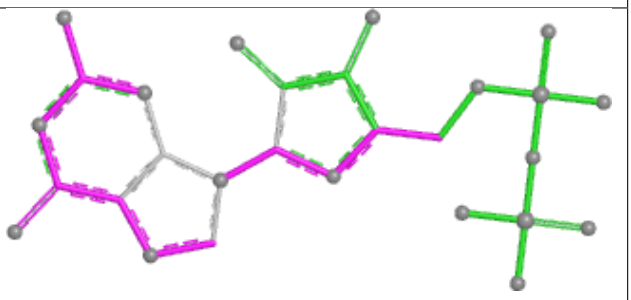

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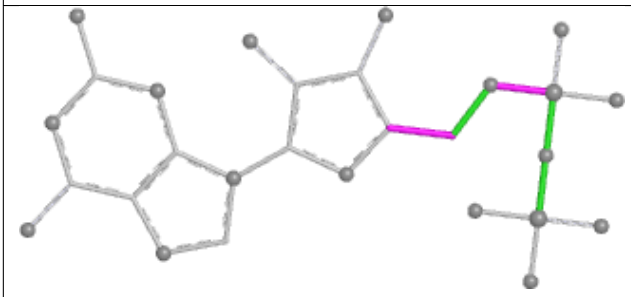

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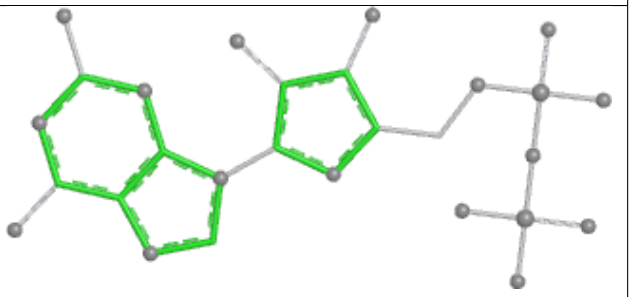
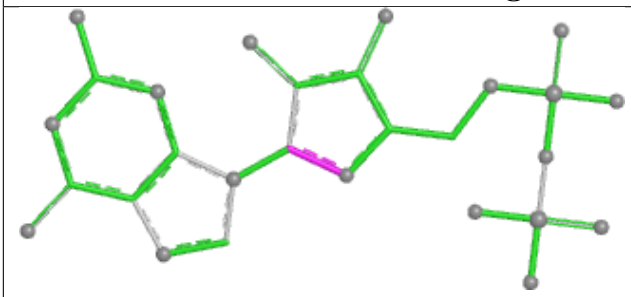


Rings

## Ligand GDP MP 501



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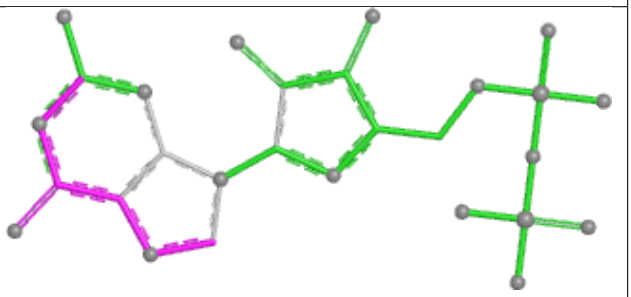

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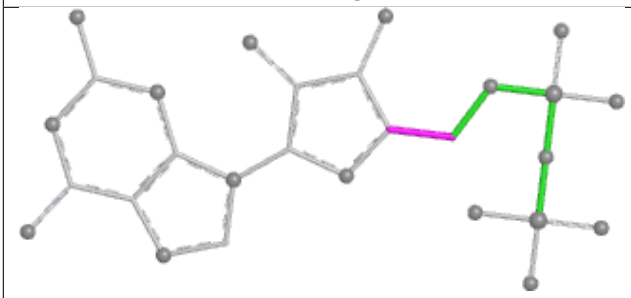

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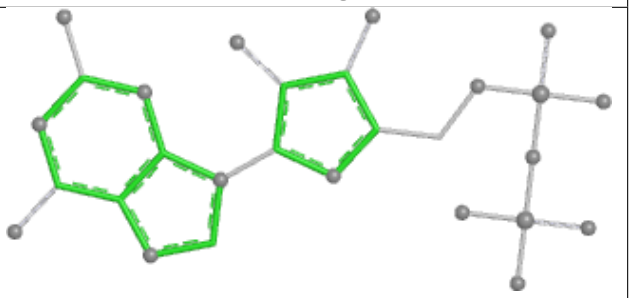

Rings

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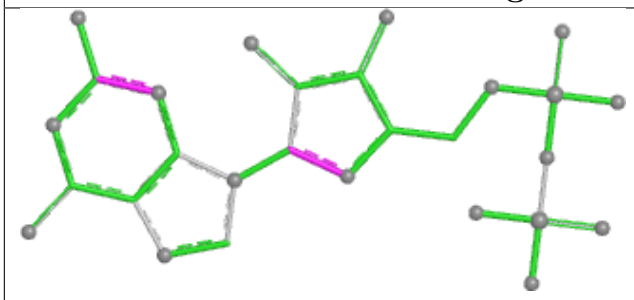

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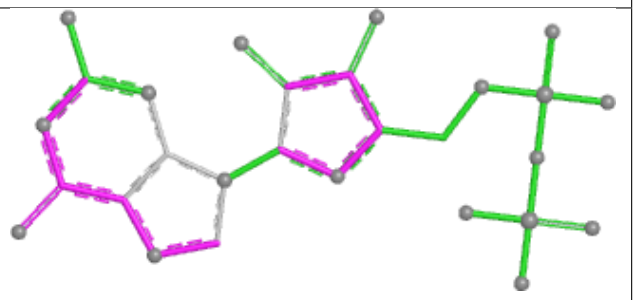

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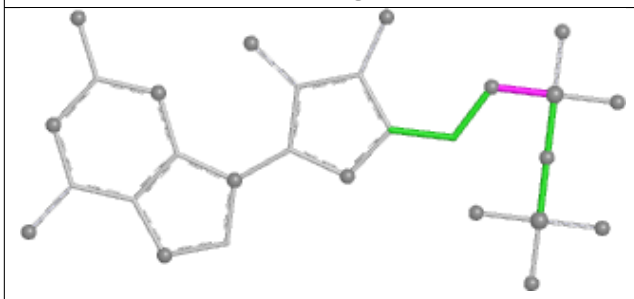

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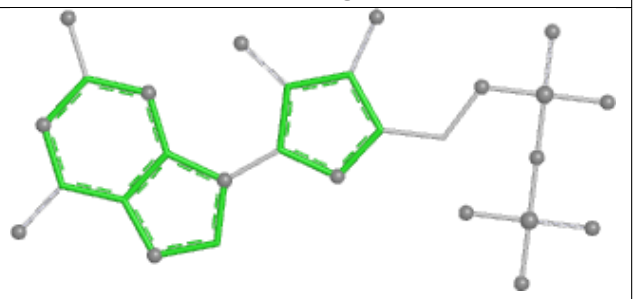

Rings

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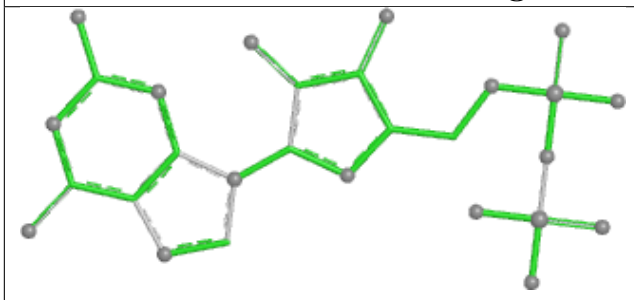

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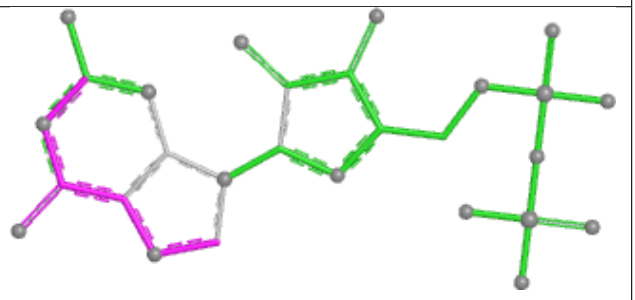

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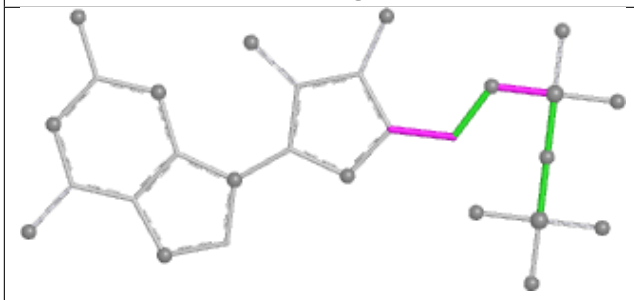

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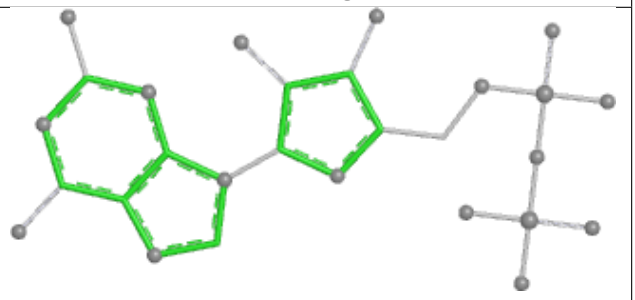

Rings

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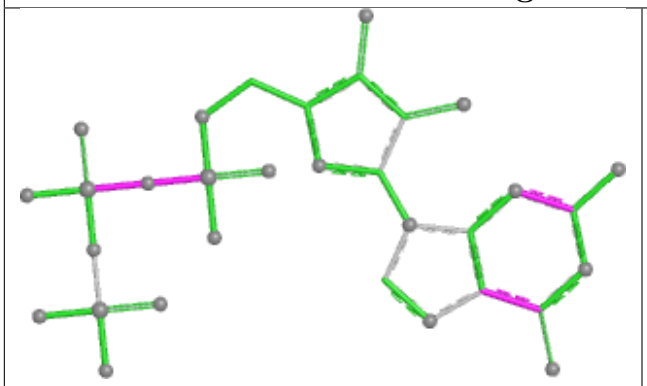

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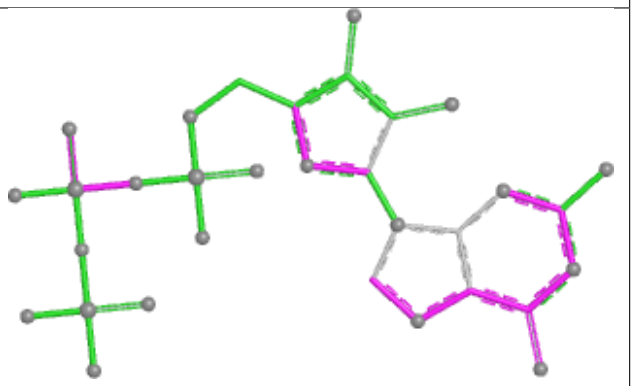

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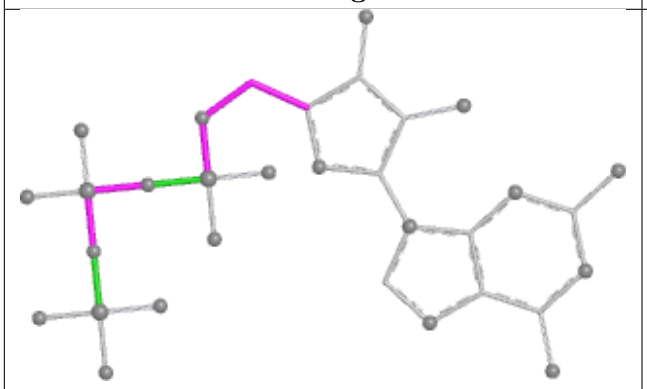

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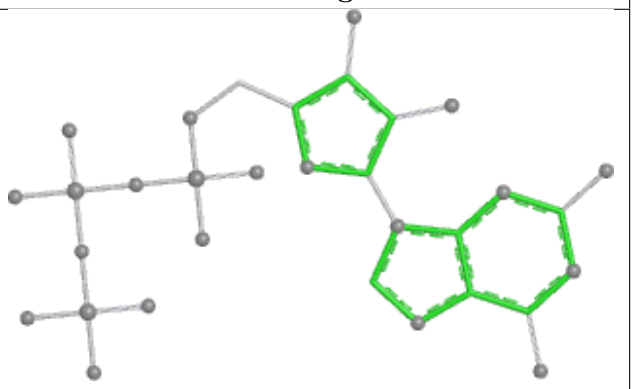

Rings

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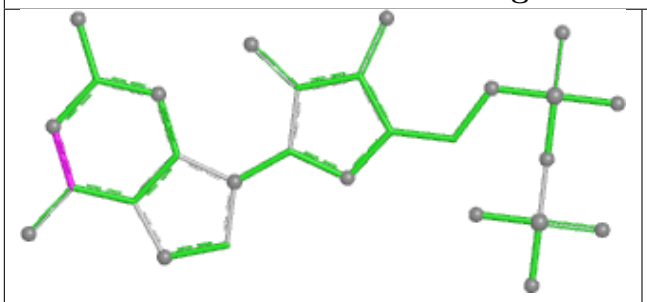

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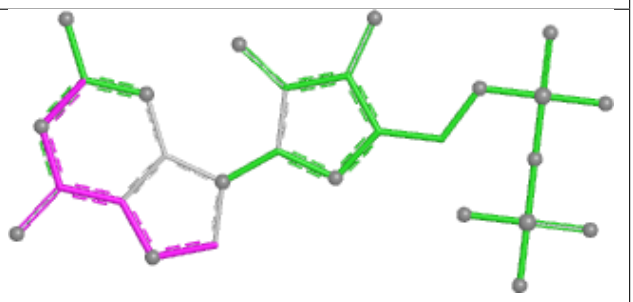

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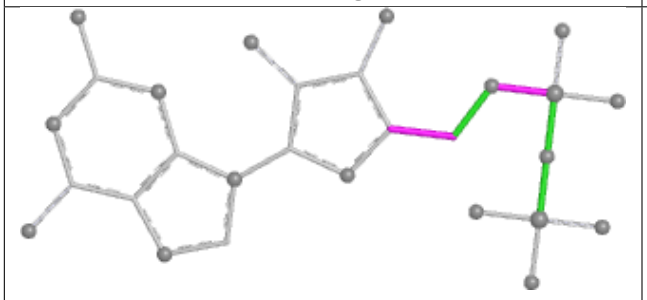

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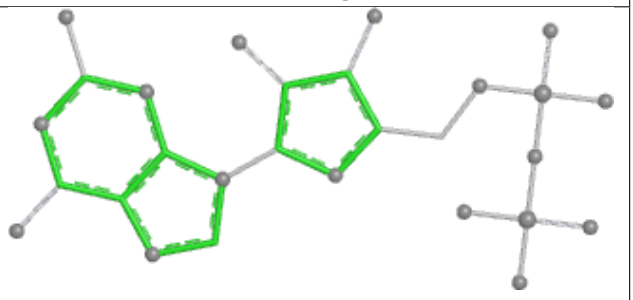

Rings

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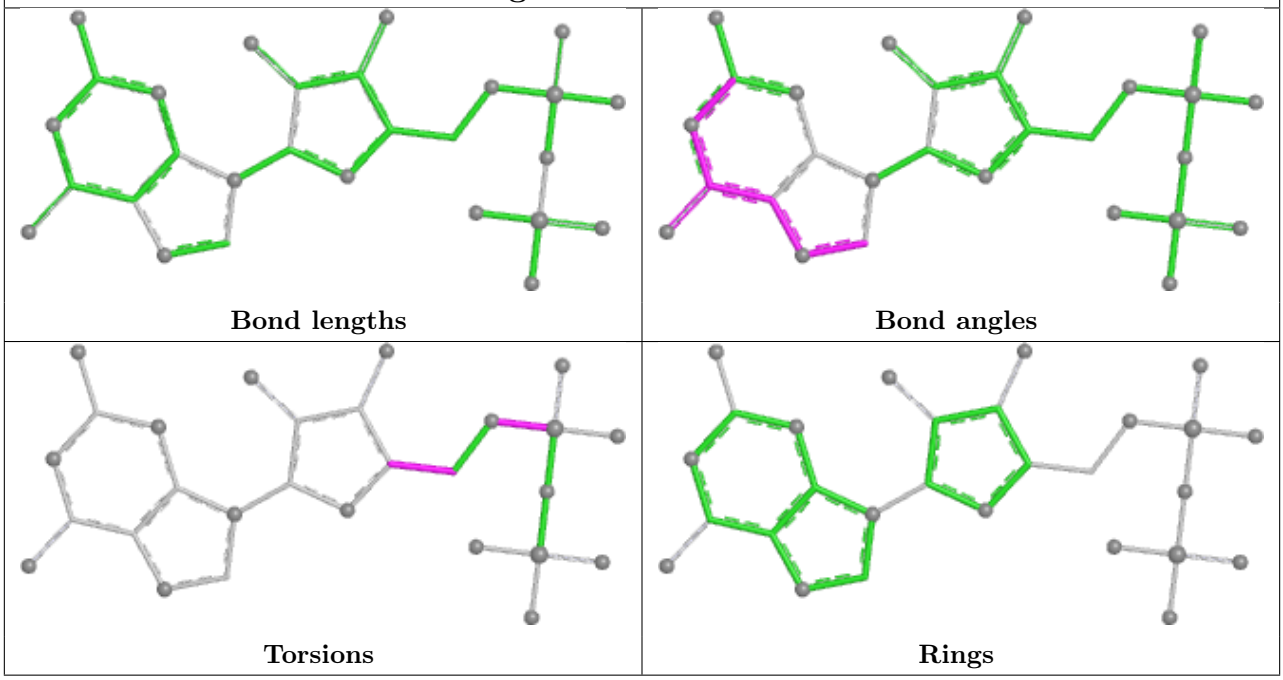


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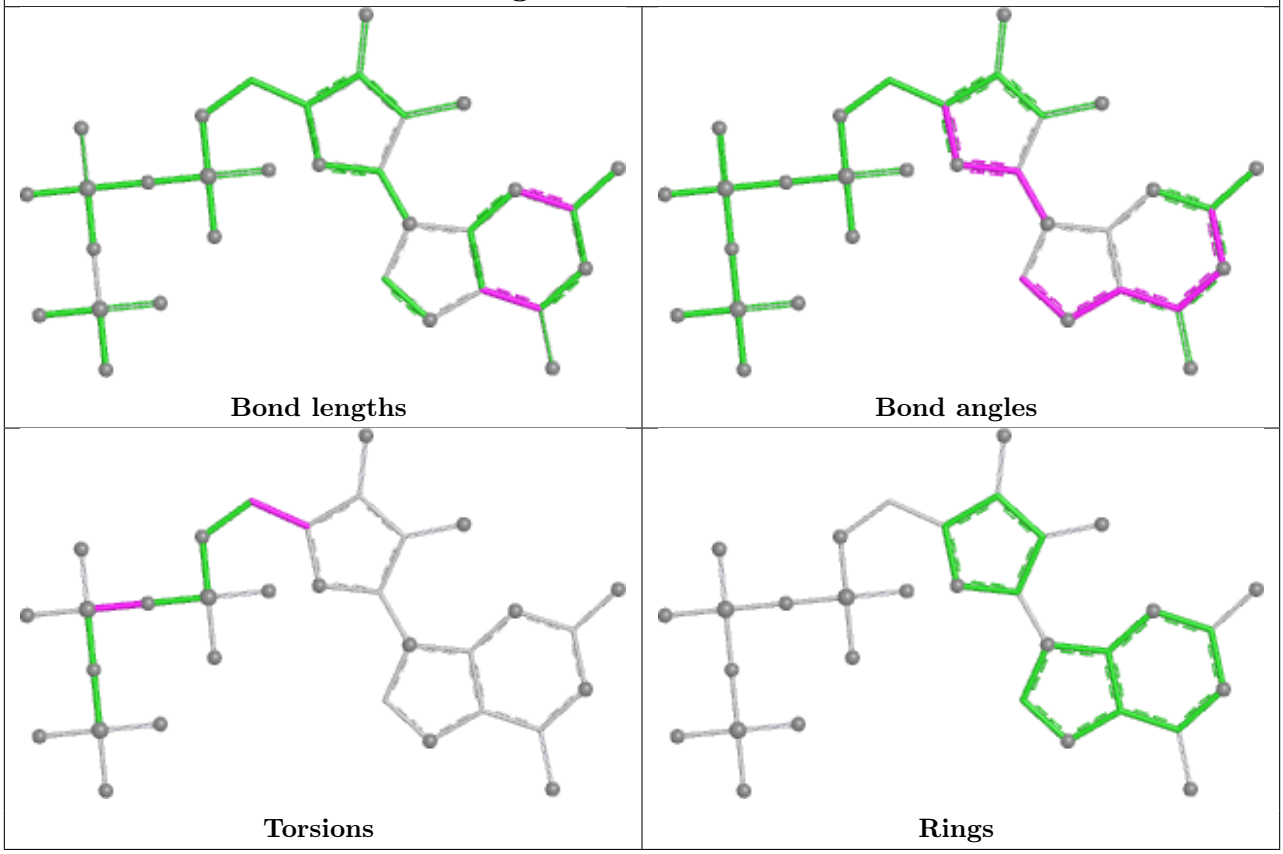

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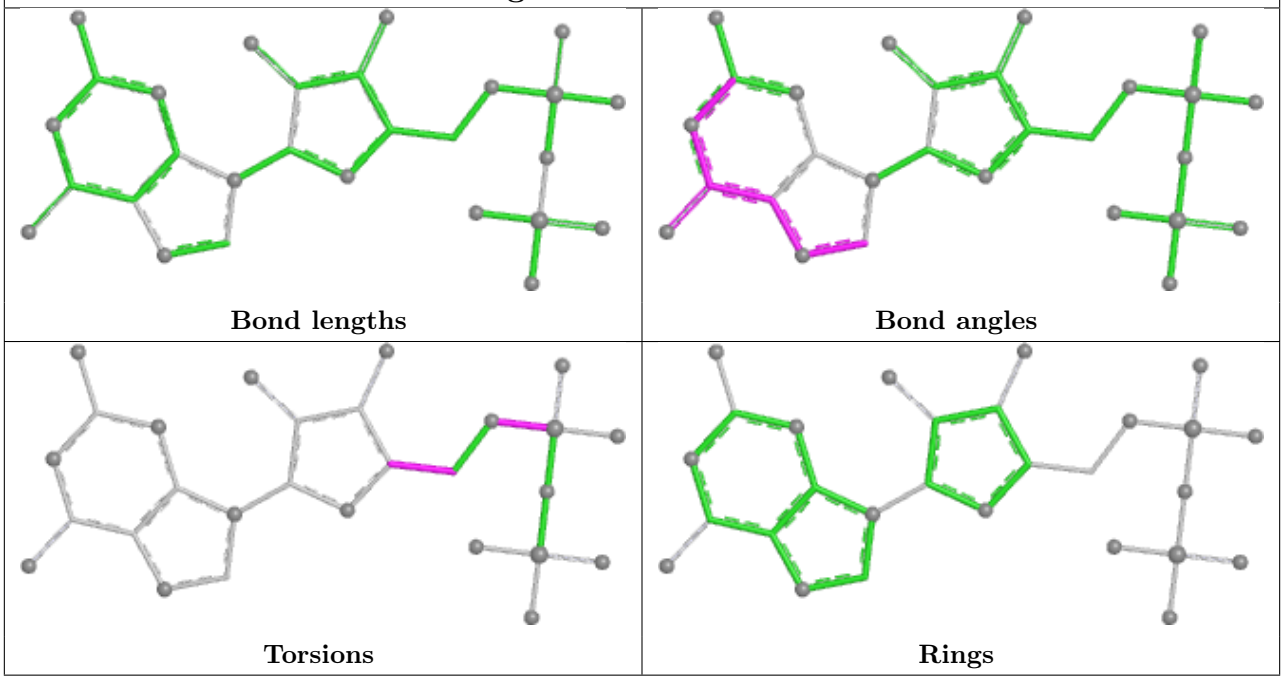


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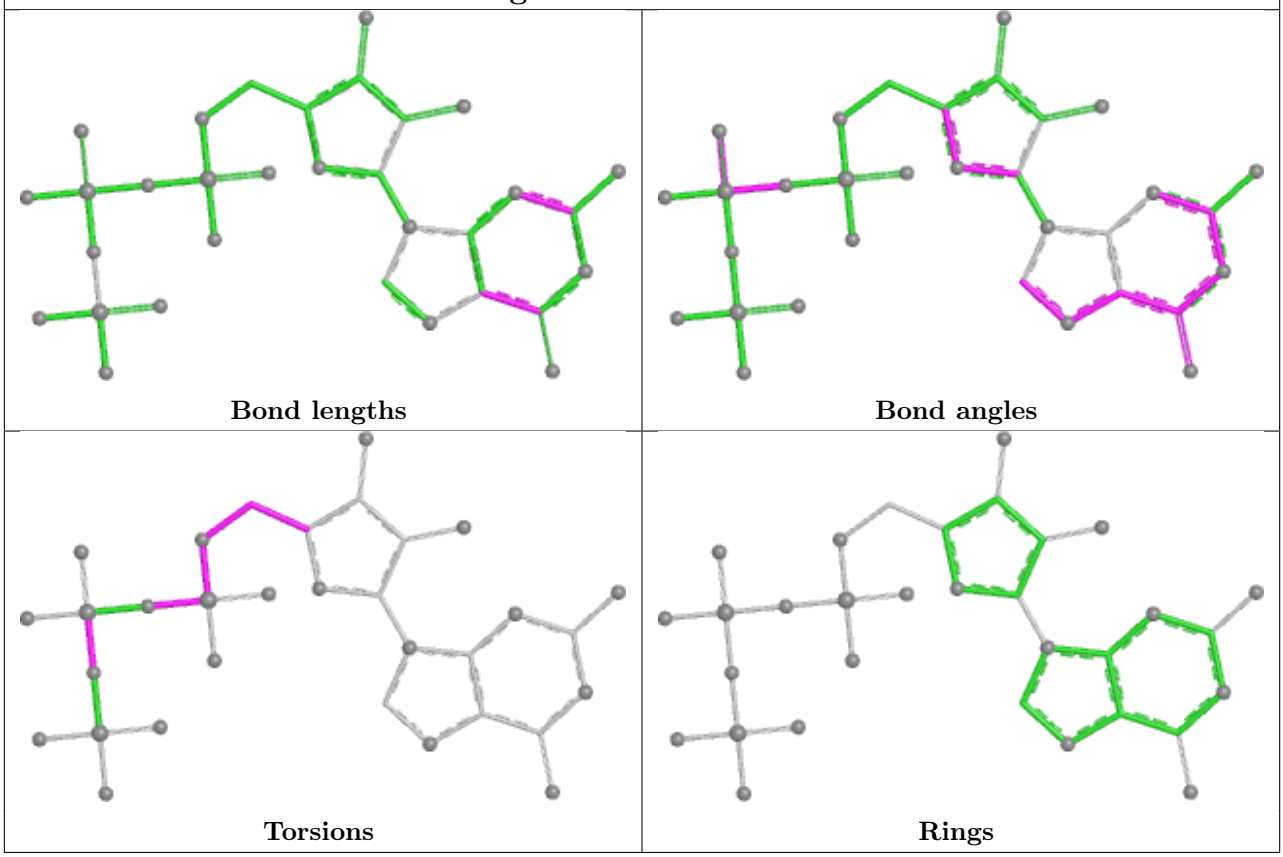

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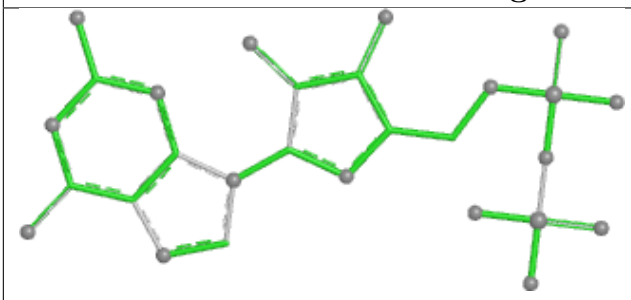

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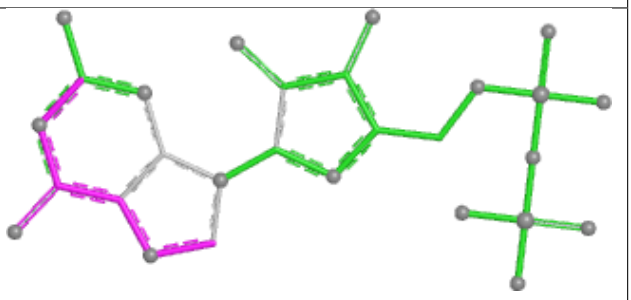

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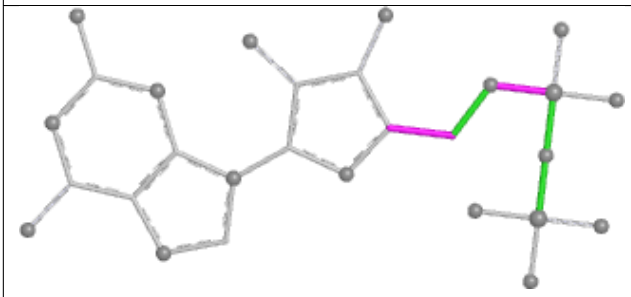

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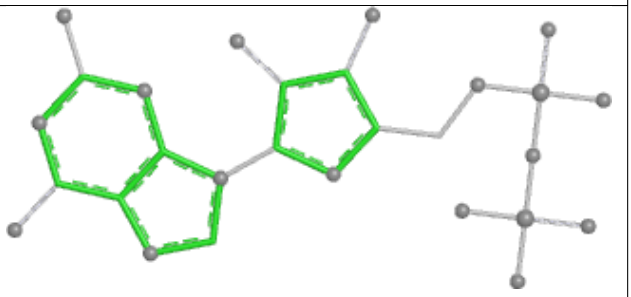
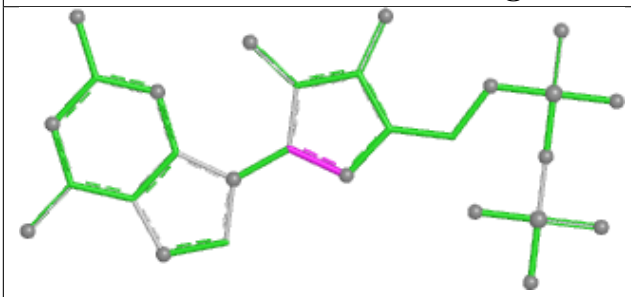


Rings

## Ligand GDP MB 501



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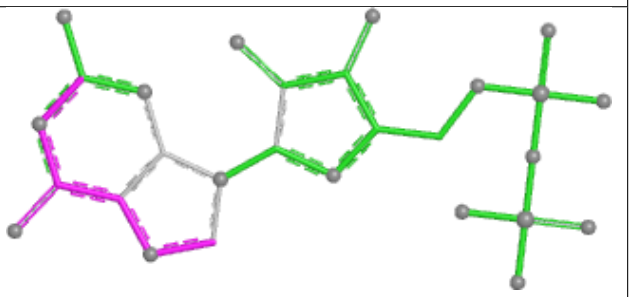

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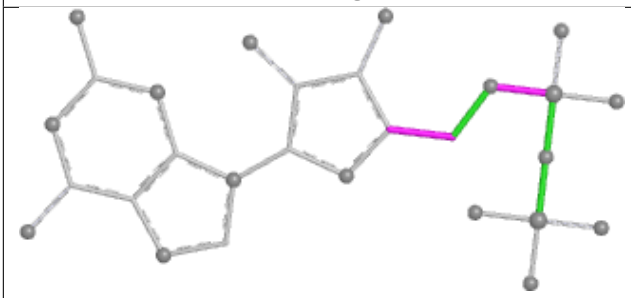

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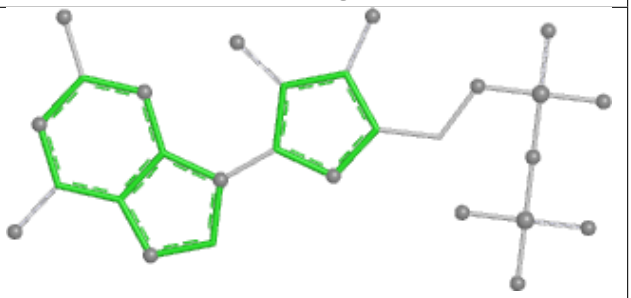

Rings

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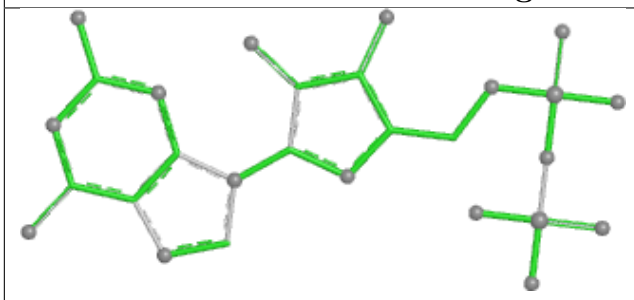

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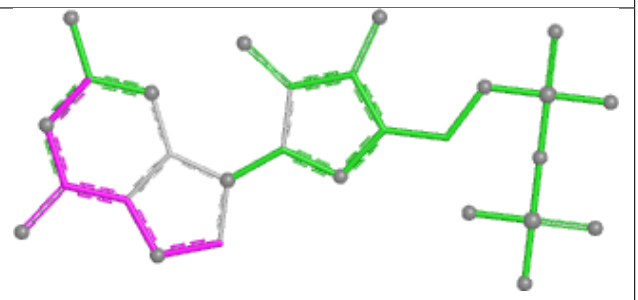

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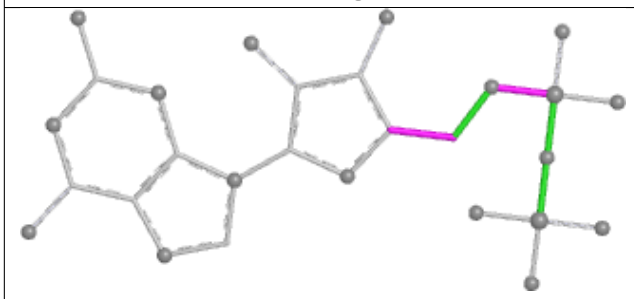

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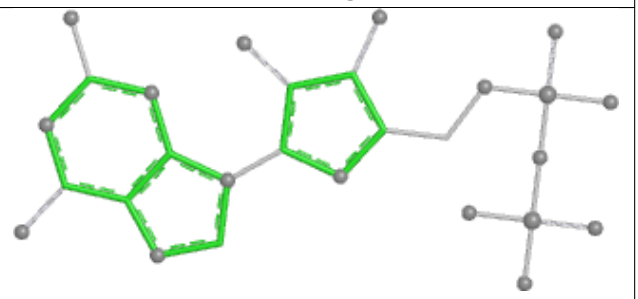

Rings

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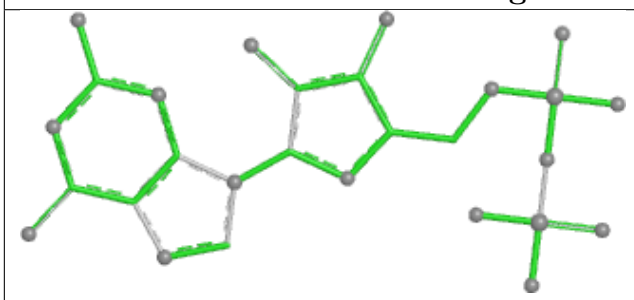

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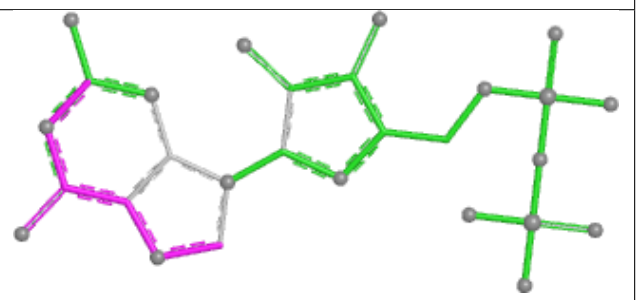

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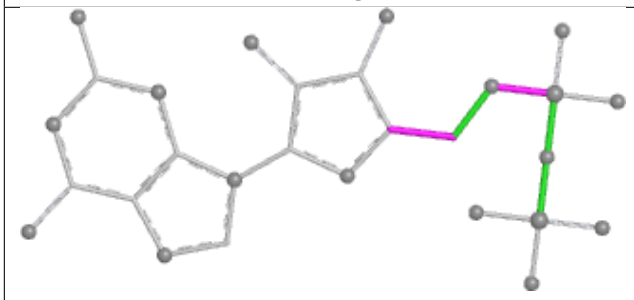

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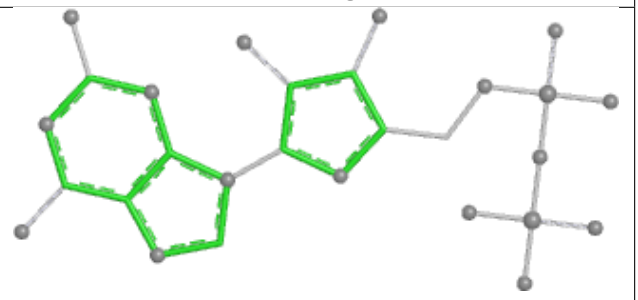

Rings

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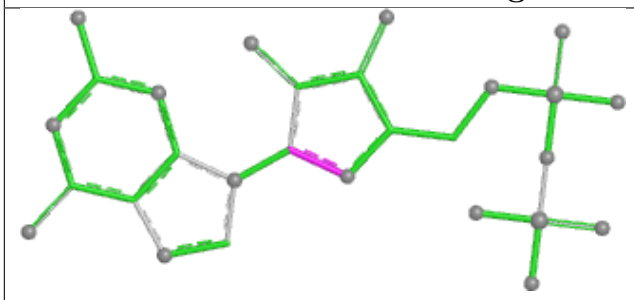

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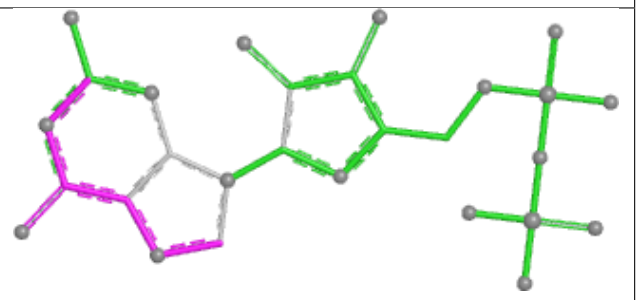
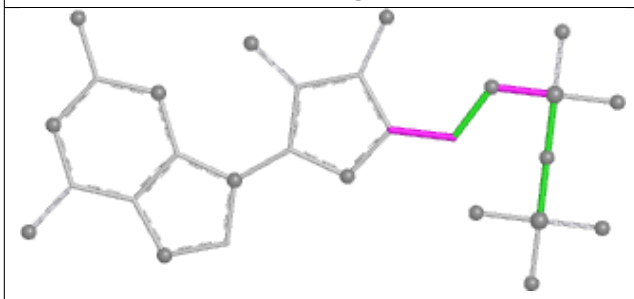


Bond angles



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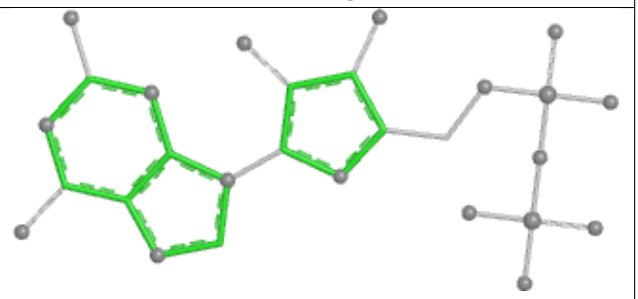
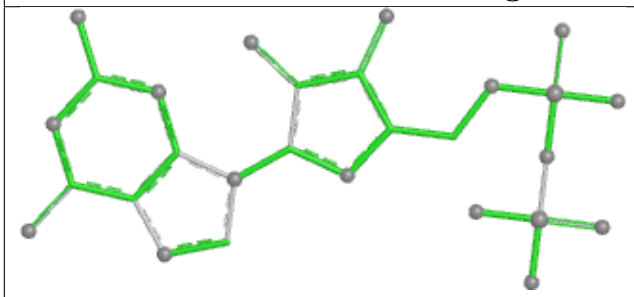
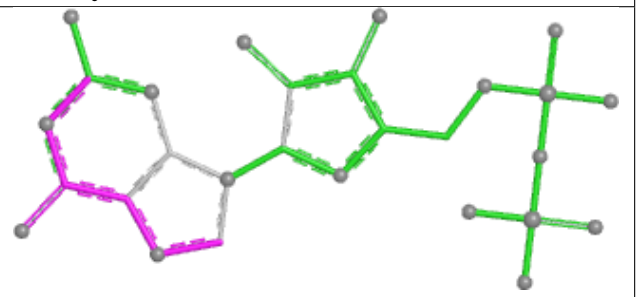


Rings

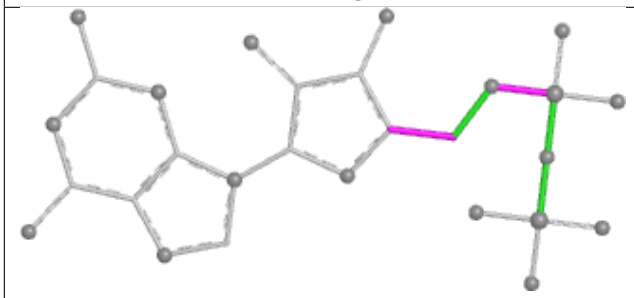
## Ligand GDP WQ 501



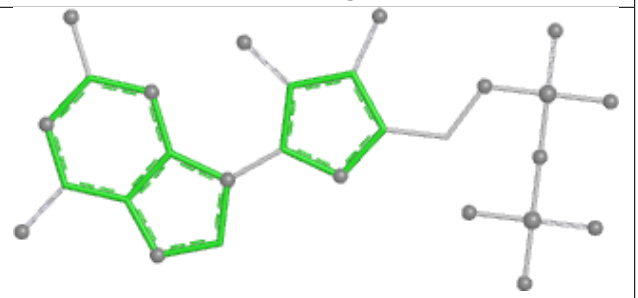
Bond lengths



Bond angles

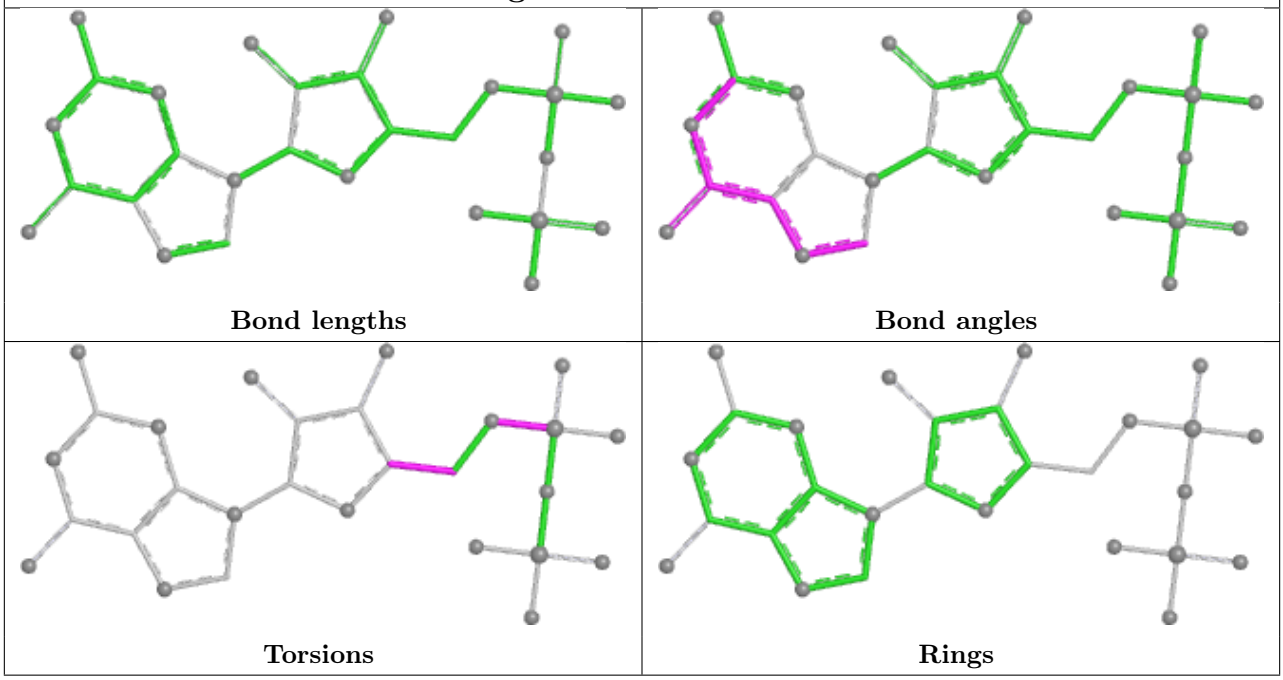


Torsions



Rings

## Ligand GDP NO 502

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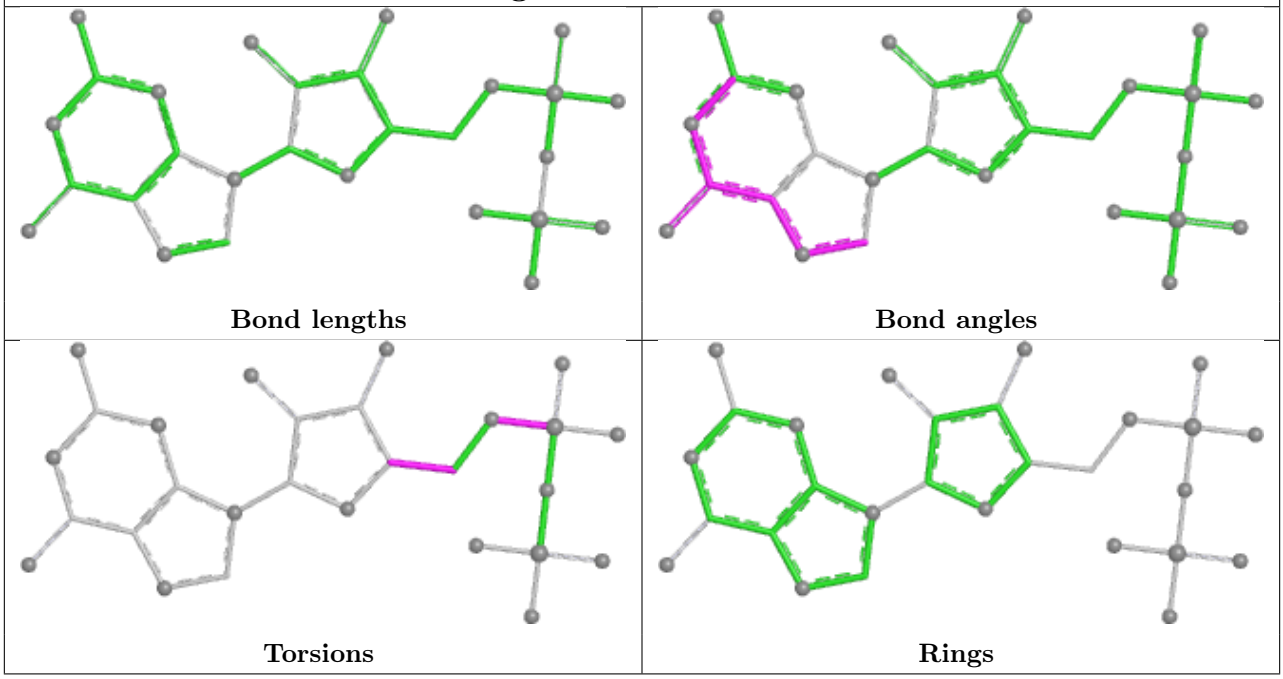
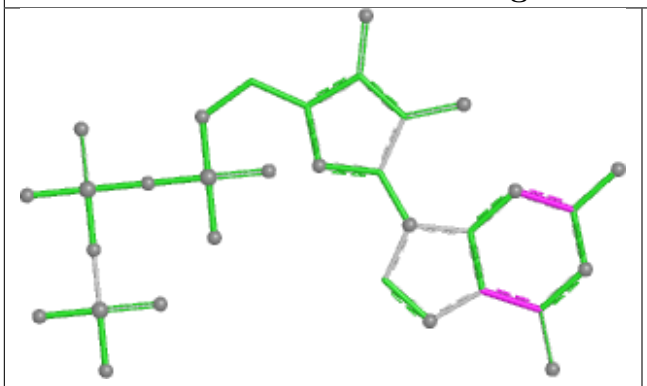


## Ligand GTP BA 501



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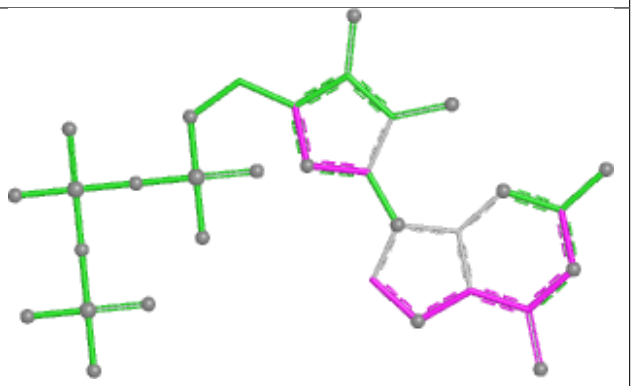
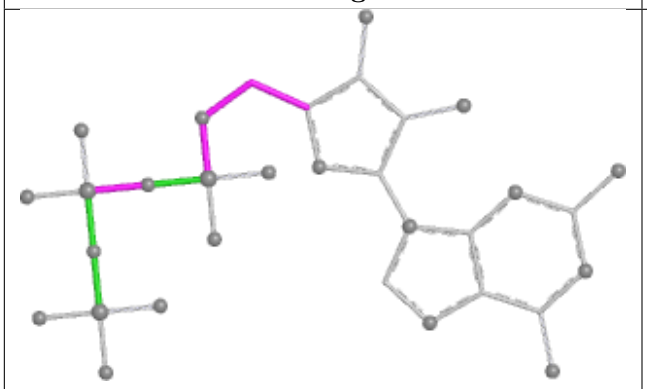


Bond angles



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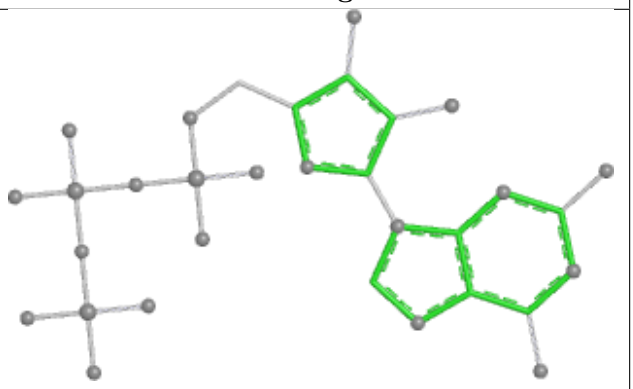

Rings

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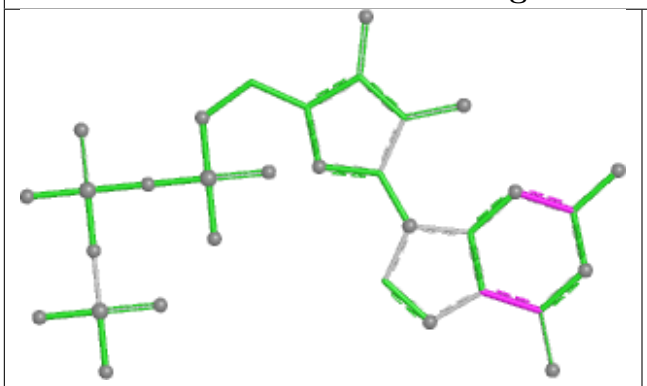

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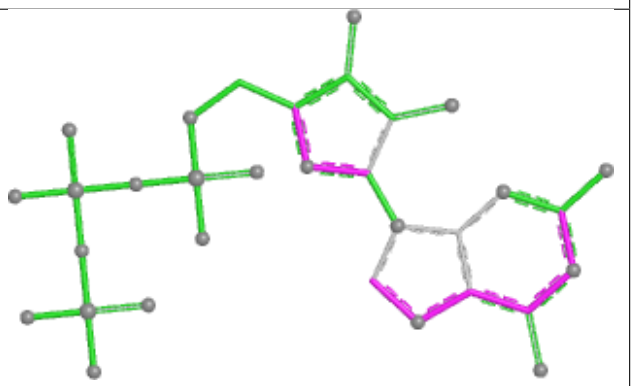
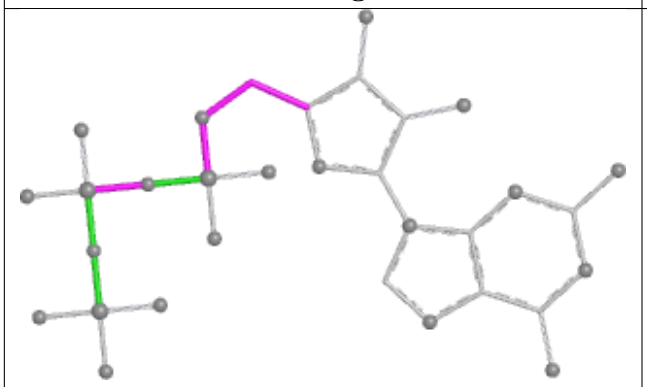


Bond angles



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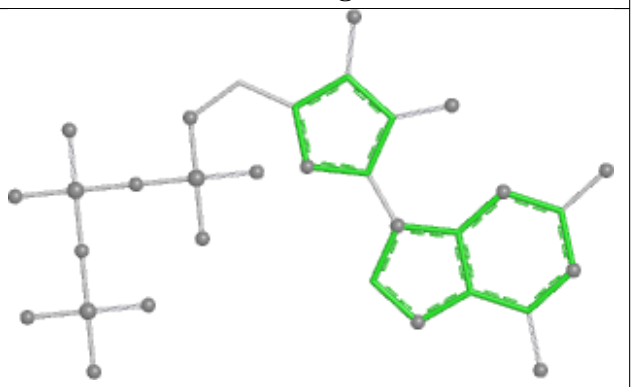
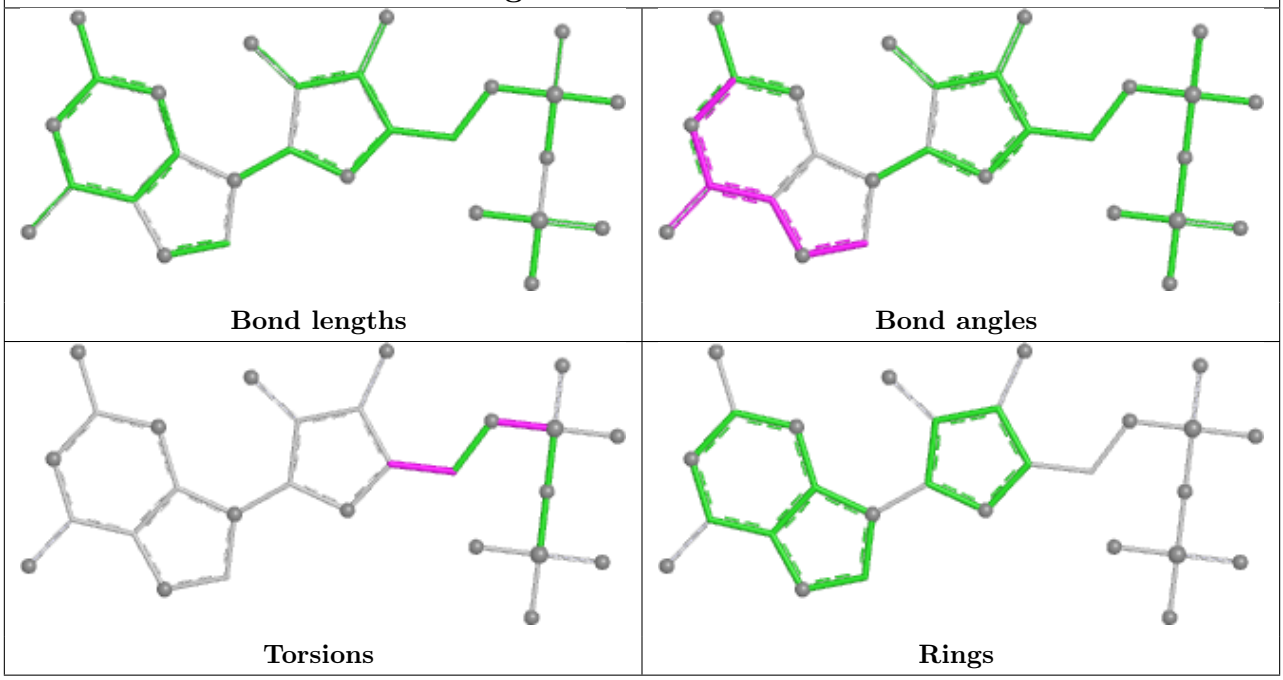
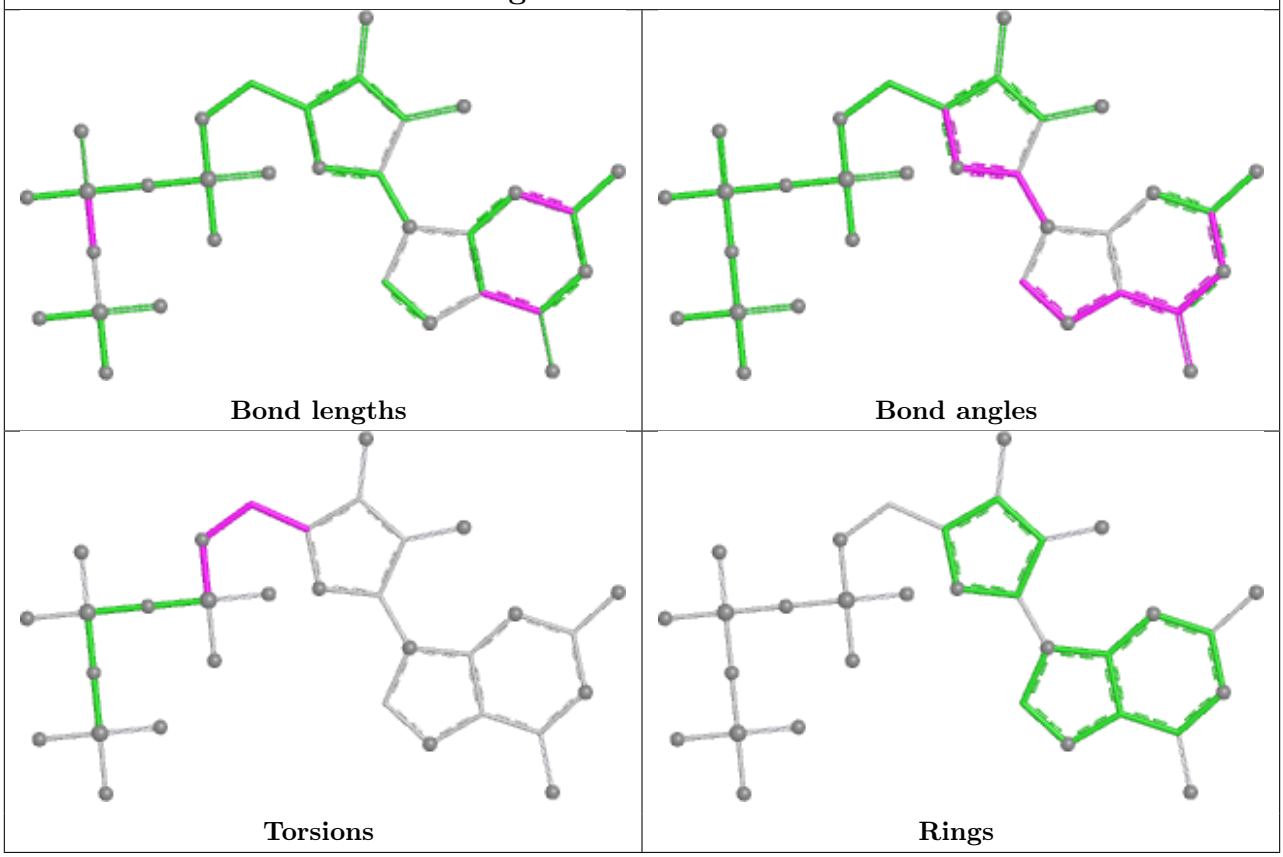


Rings

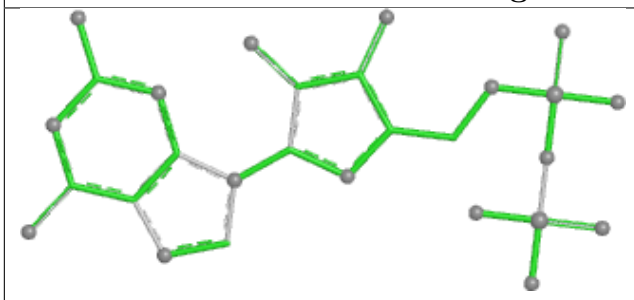
## Ligand GDP OM 502



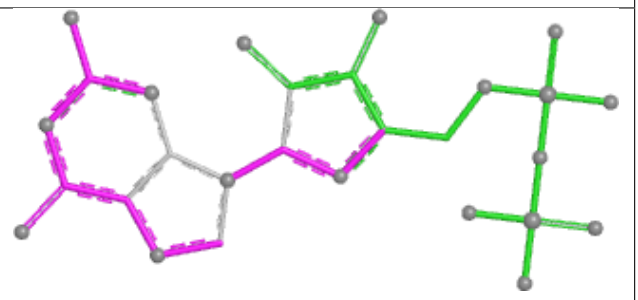

## Ligand GTP HH 501



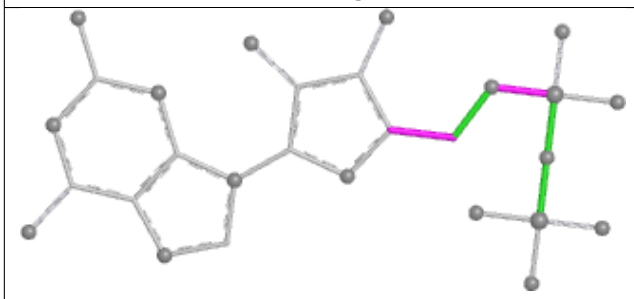
## Ligand GDP TB 501



Bond lengths



Bond angles



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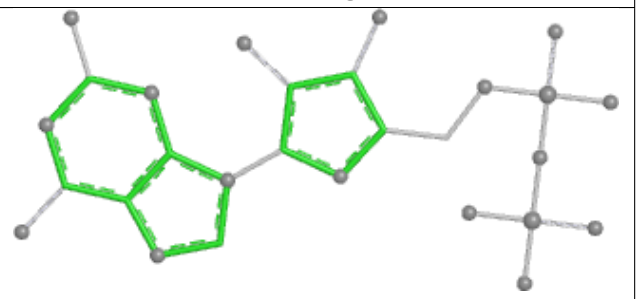
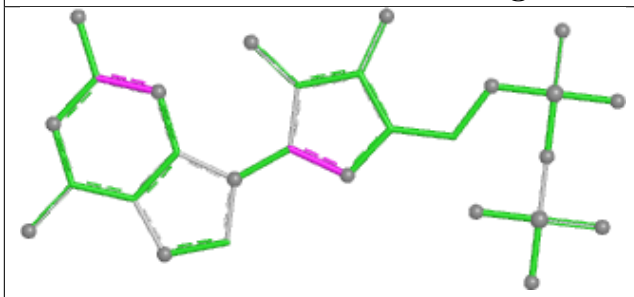


Rings

## Ligand GDP RP 502



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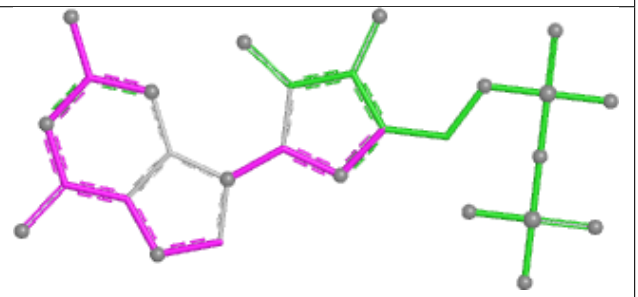

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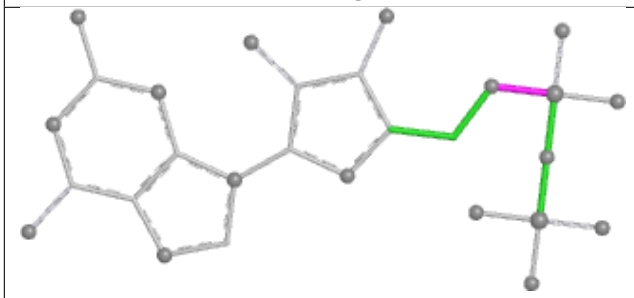

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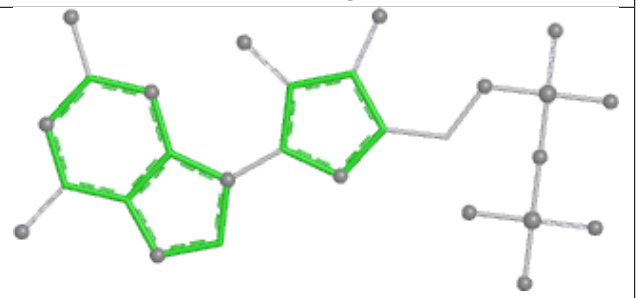
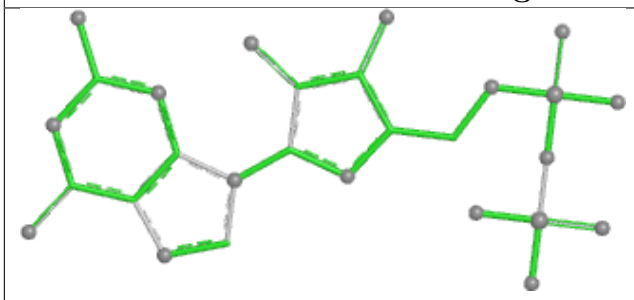


Rings

## Ligand GDP JB 501



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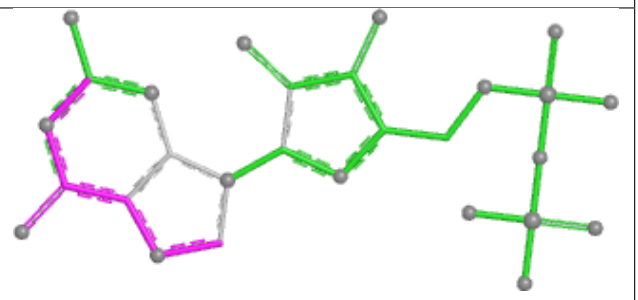

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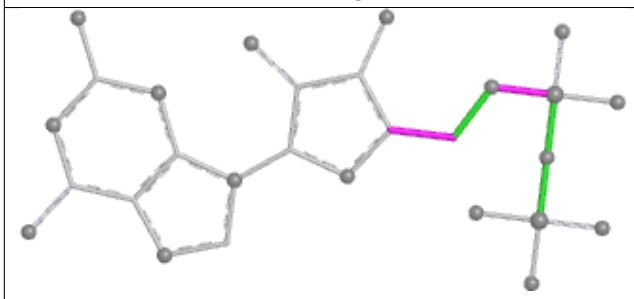

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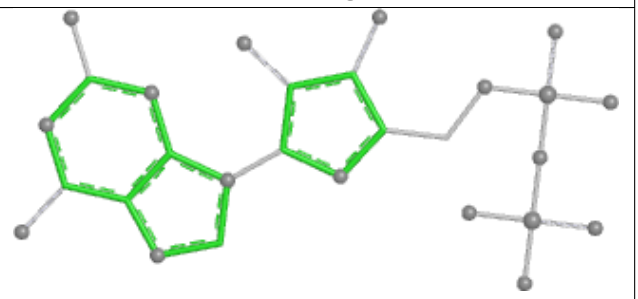
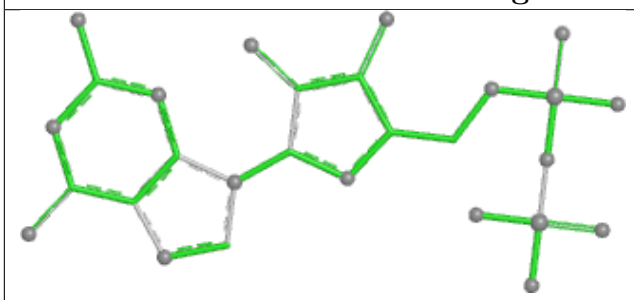


Rings

## Ligand GDP IM 501



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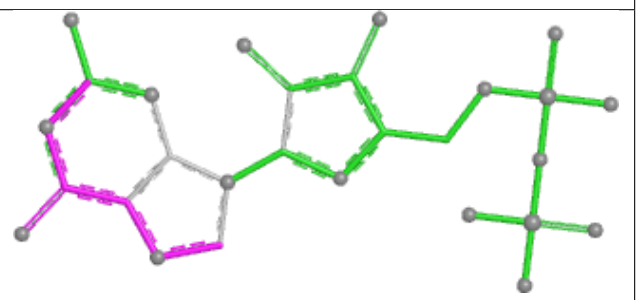

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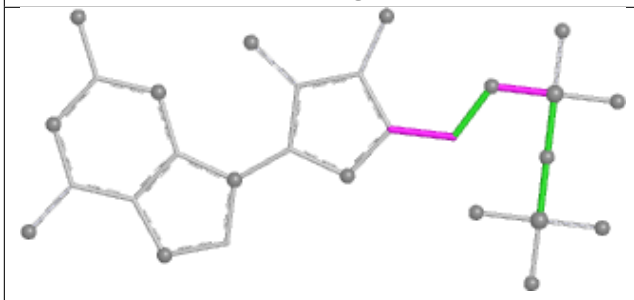

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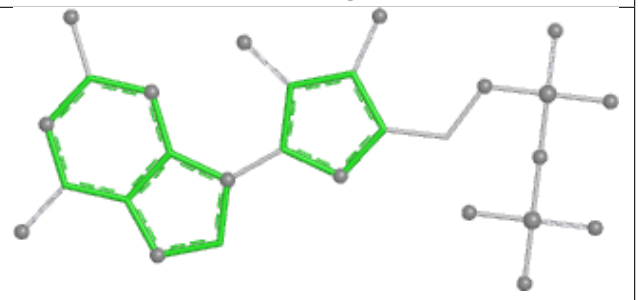
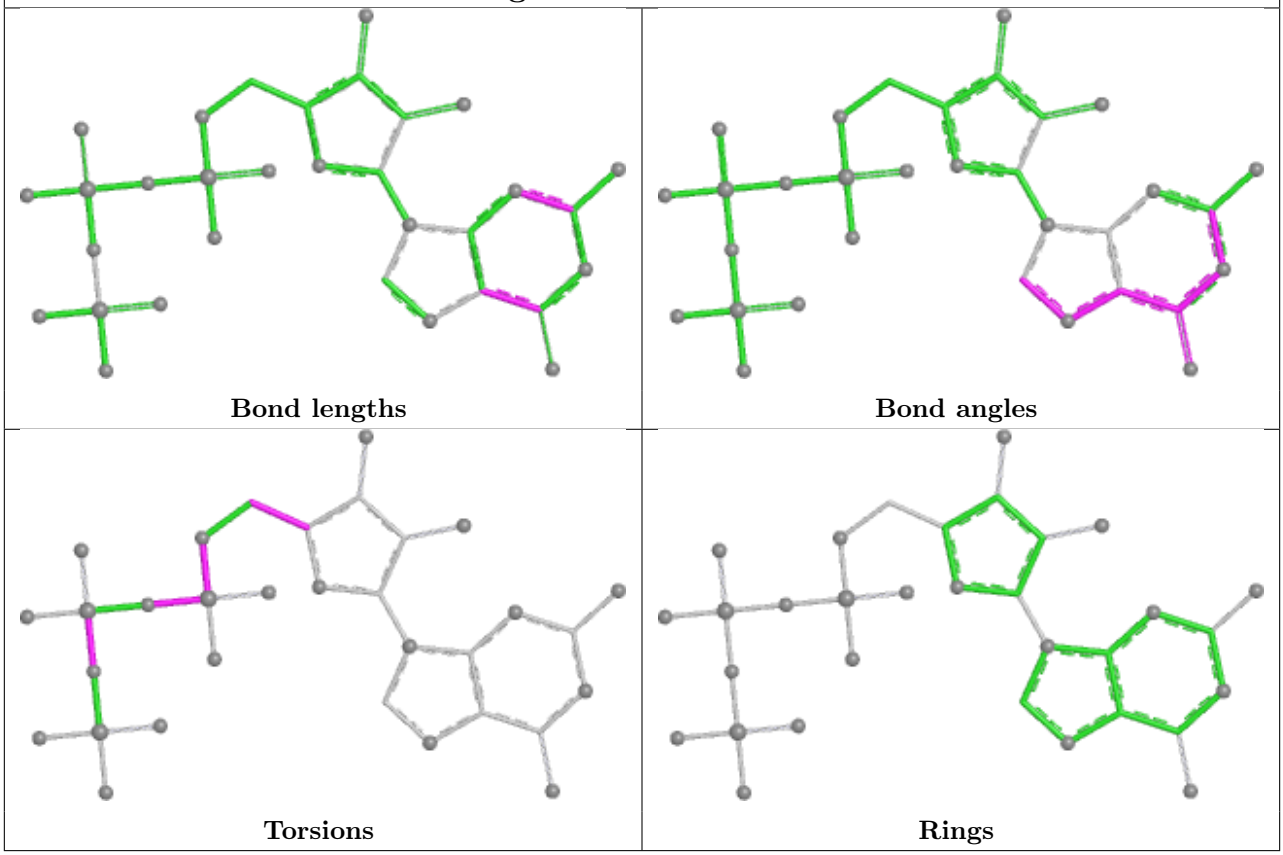
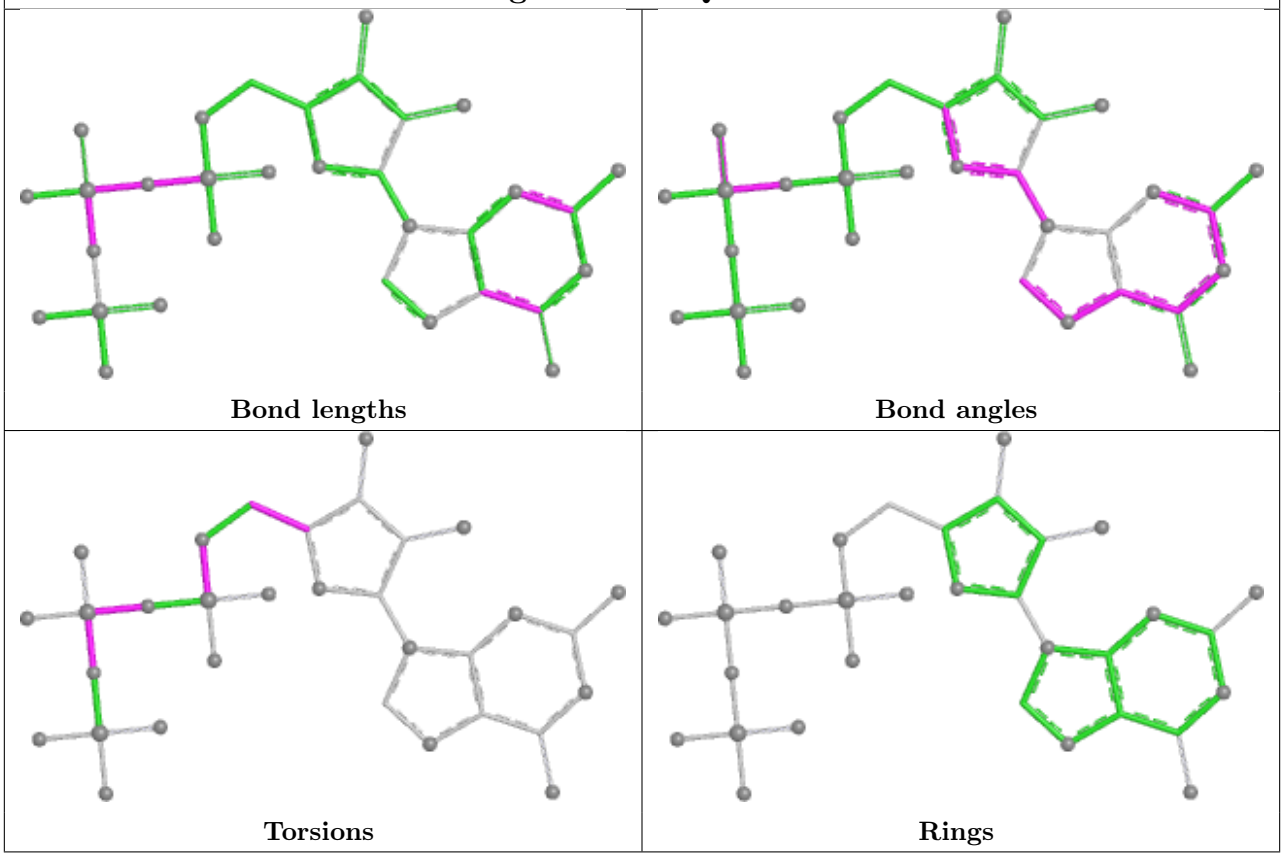


Rings

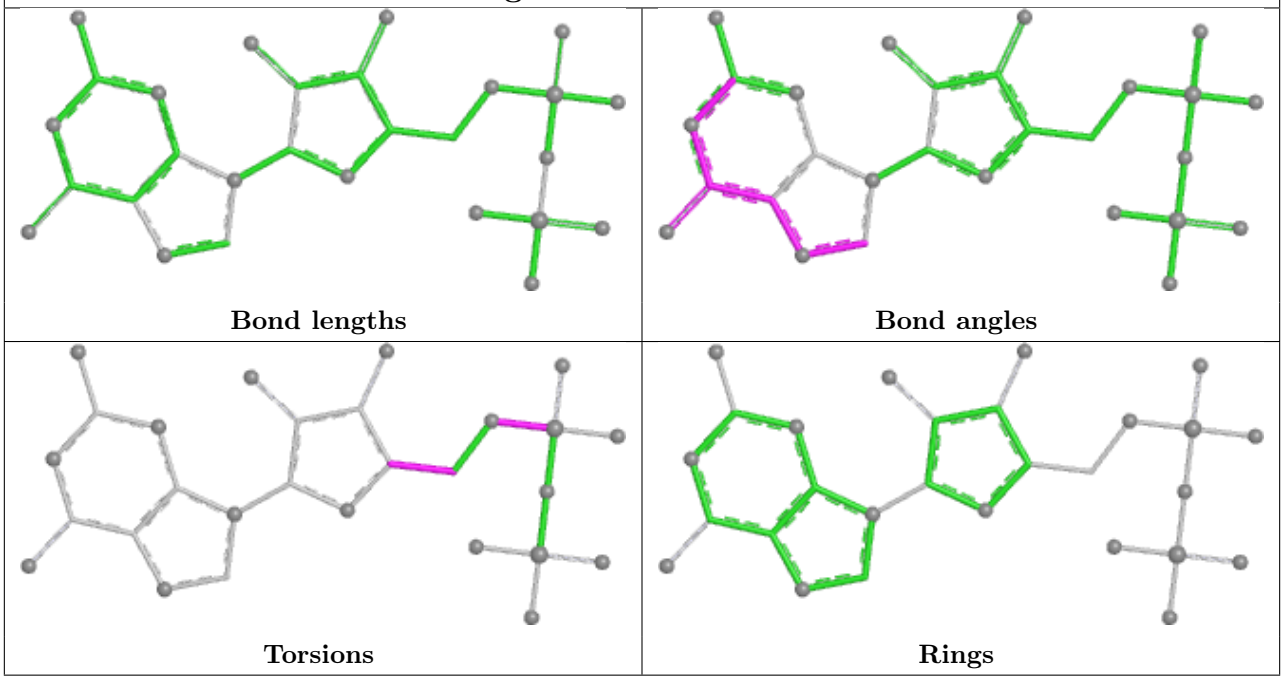
## Ligand GTP NN 501



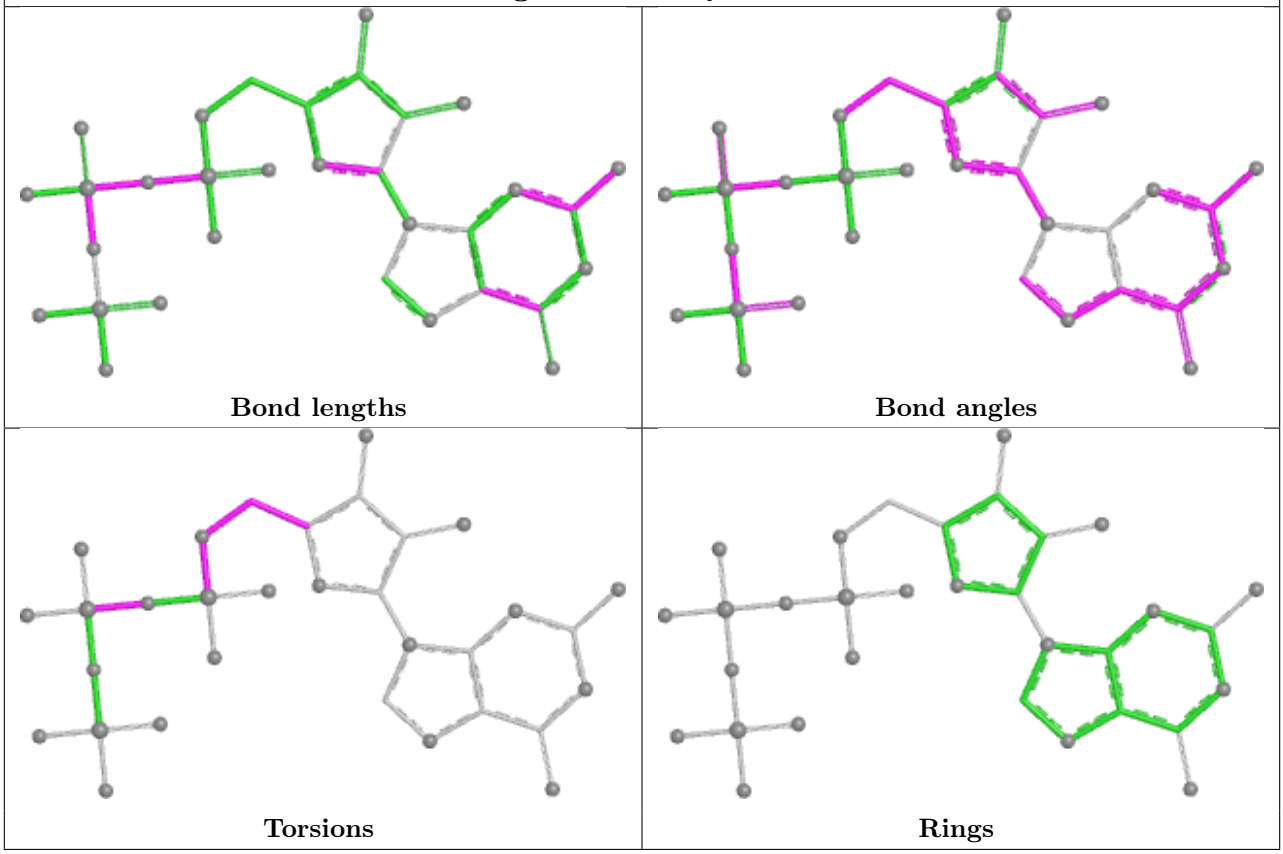

## Ligand GTP QN 501



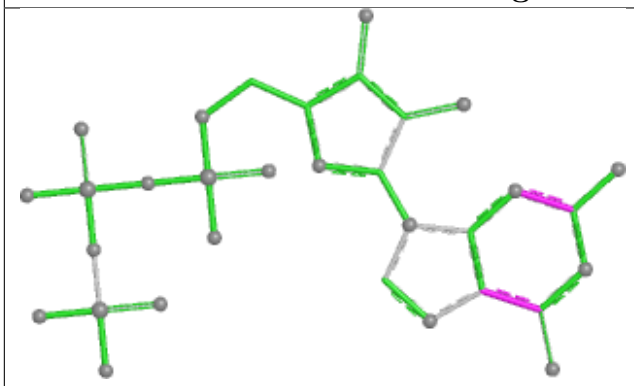
## Ligand GDP WP 501



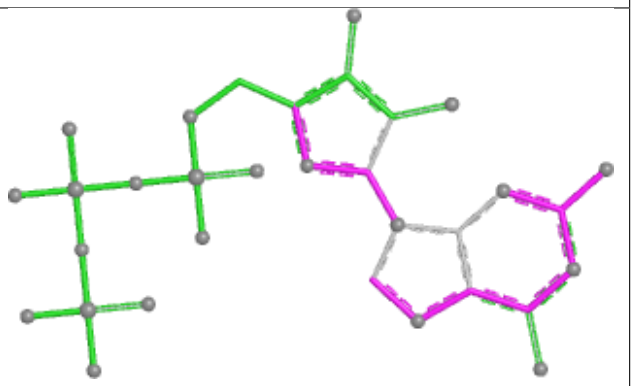

## Ligand GTP QL 501



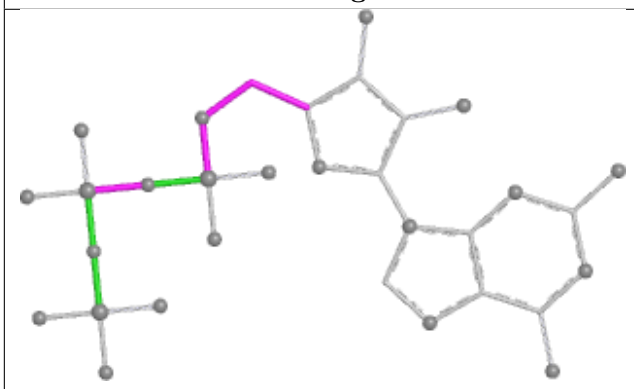
## Ligand GTP RF 501



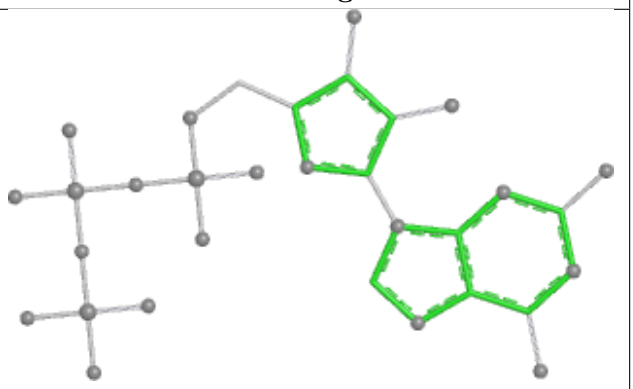
Bond lengths



Bond angles

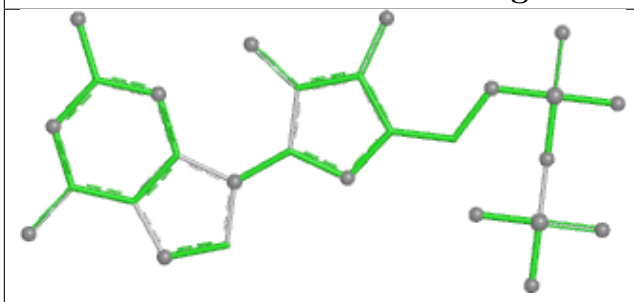


Torsions



Rings

## Ligand GDP PP 501



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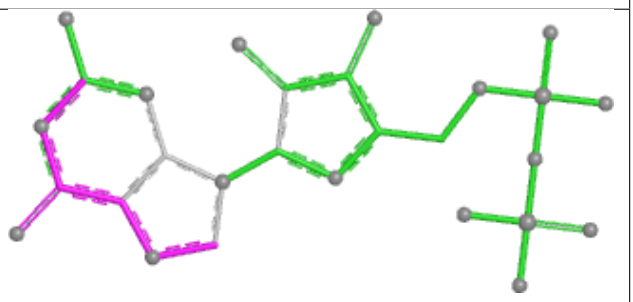
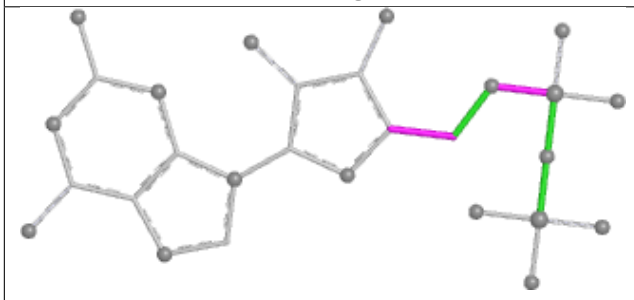
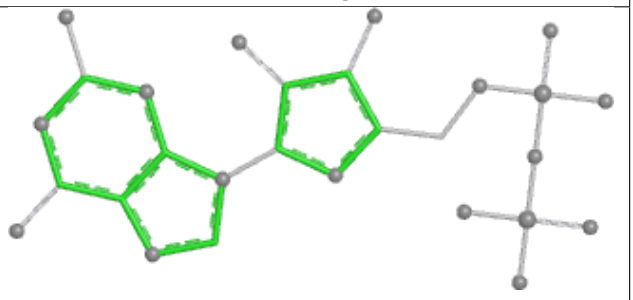


Bond angles

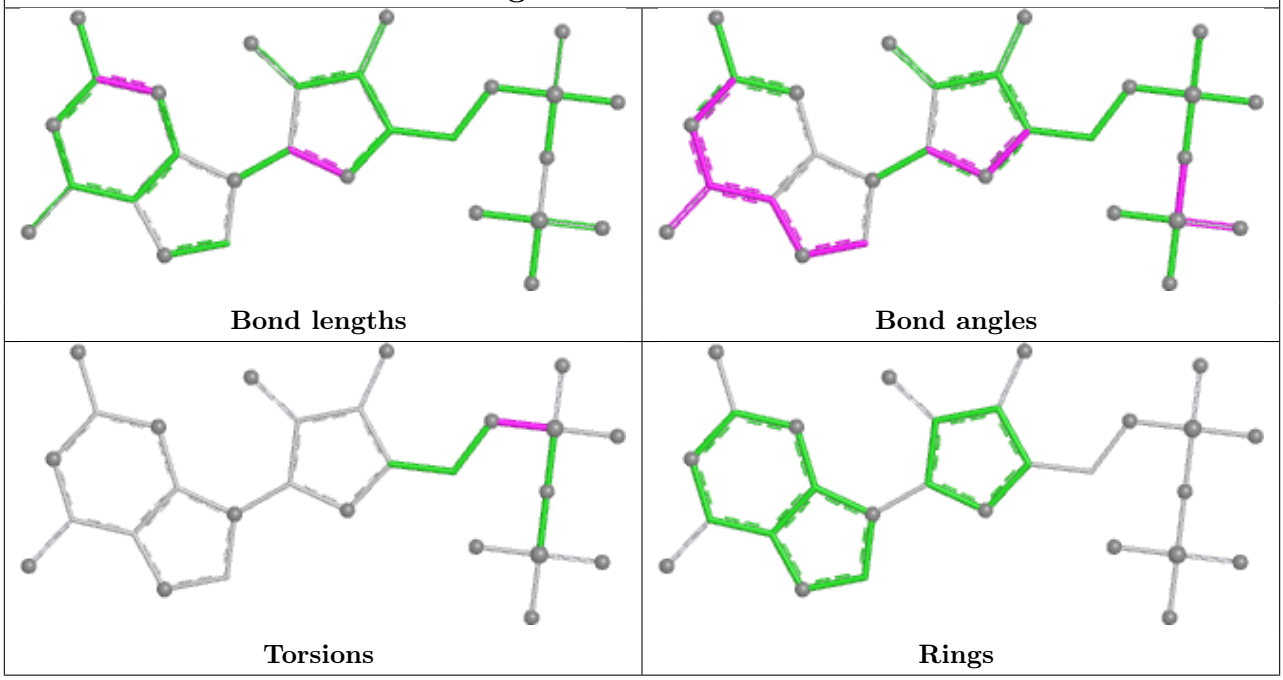


Torsions

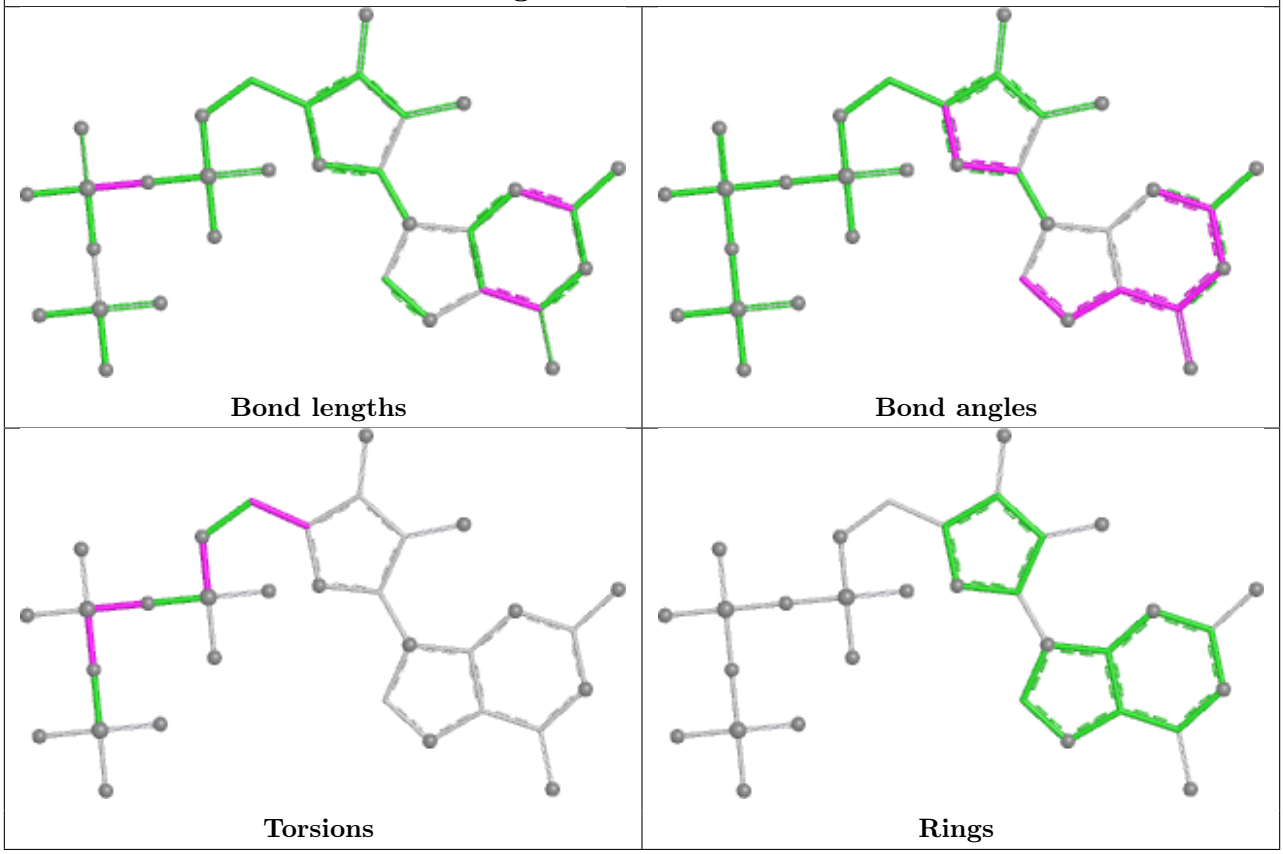


Rings

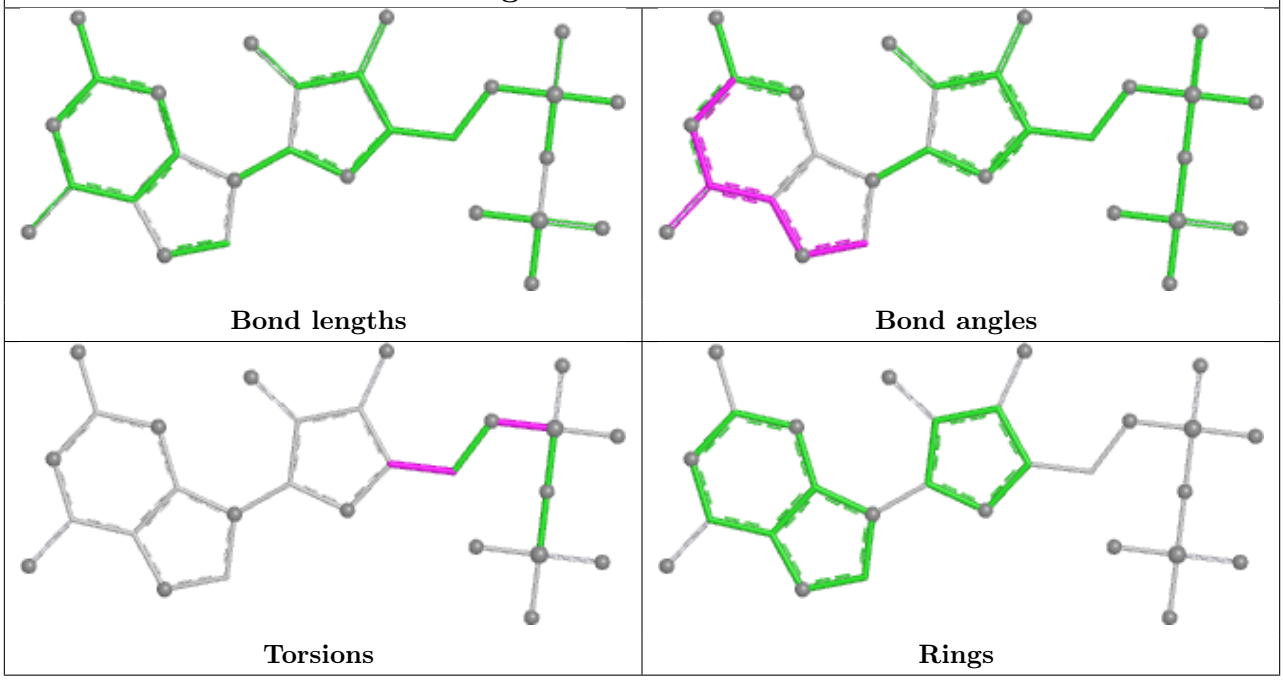
## Ligand GDP KO 502



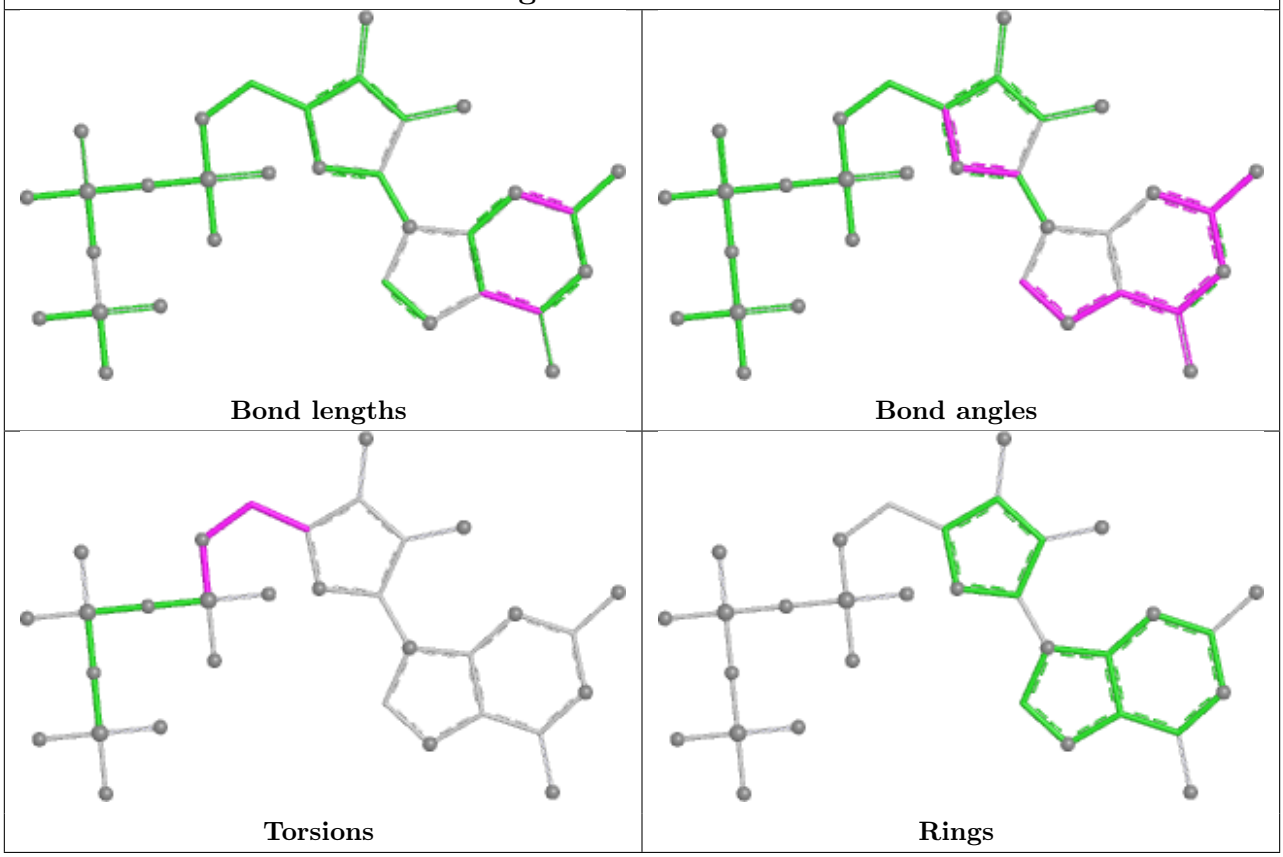

## Ligand GTP LO 501



**Ligand GDP MM 502**




**Ligand GTP FI 501**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

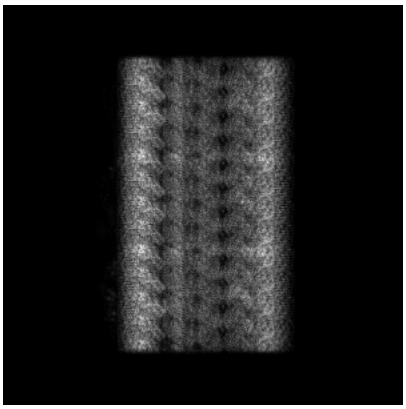
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-45802. These allow visual inspection of the internal detail of the map and identification of artifacts.

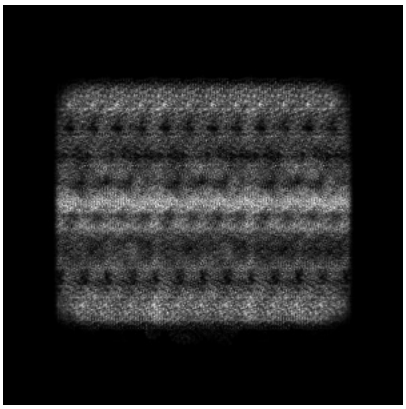
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

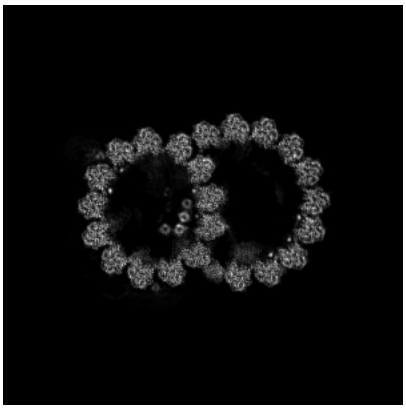
### 6.1.1 Primary map



X

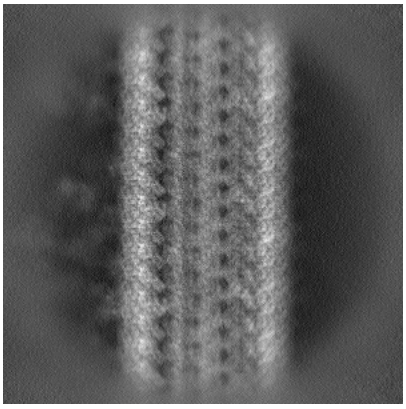


Y

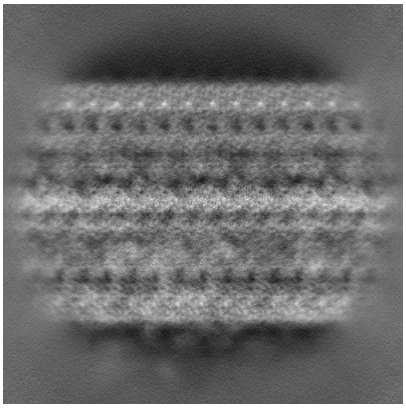


Z

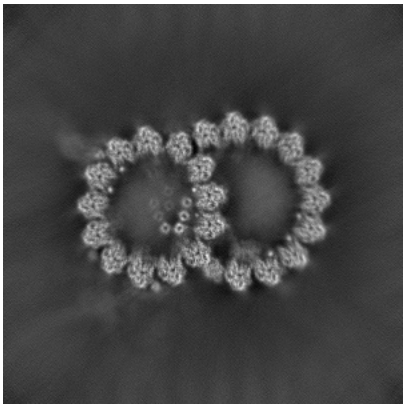
### 6.1.2 Raw map



X



Y

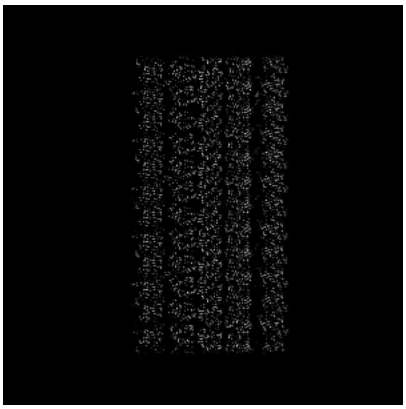


Z

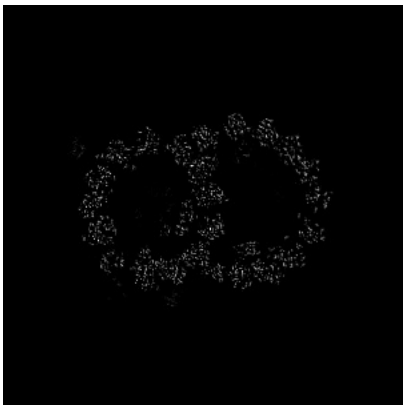
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

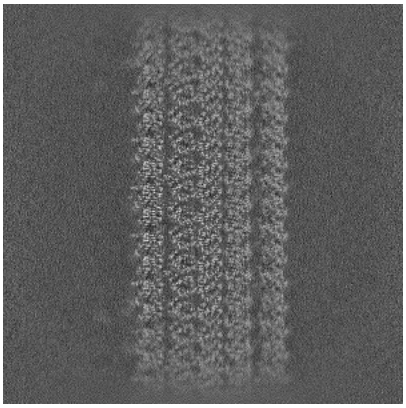
### 6.2.1 Primary map

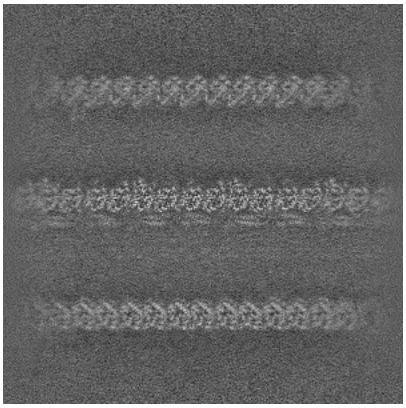

X Index: 256

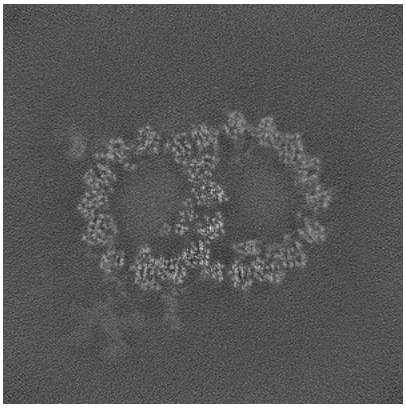
Y Index: 256


Z Index: 256

### 6.2.2 Raw map


X Index: 256

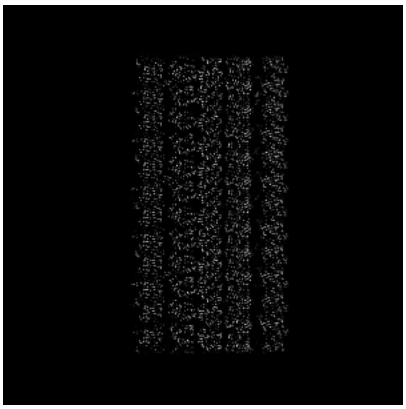

Y Index: 256


Z Index: 256

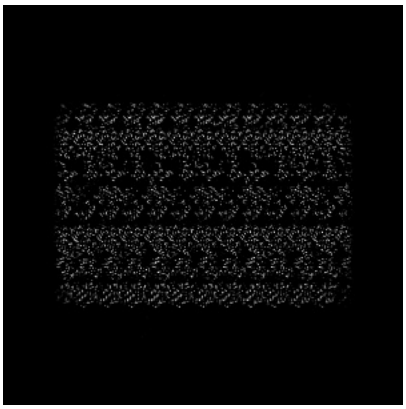
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

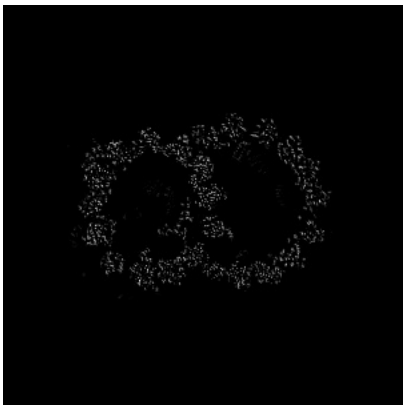
### 6.3.1 Primary map



X Index: 256

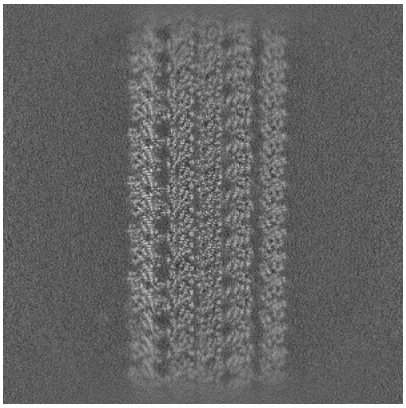


Y Index: 177

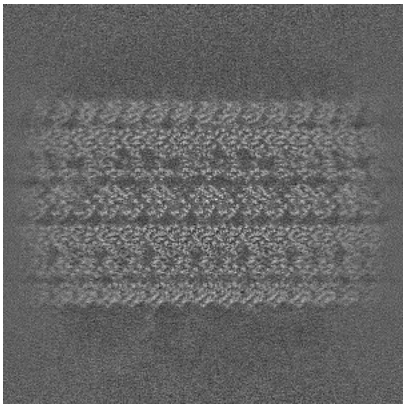


Z Index: 197

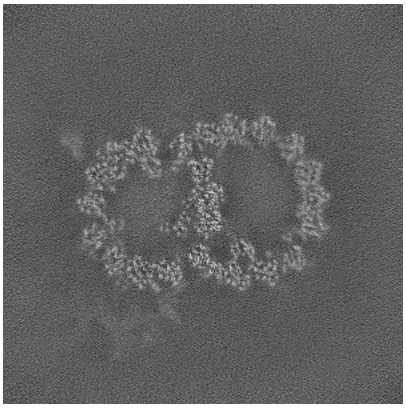
### 6.3.2 Raw map



X Index: 261



Y Index: 177

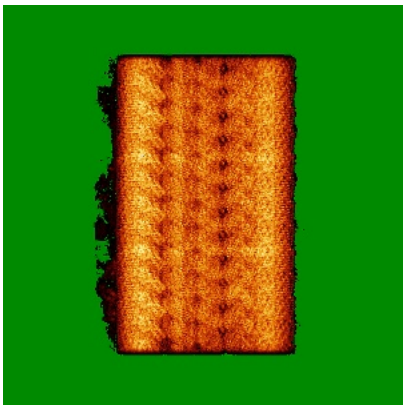


Z Index: 266

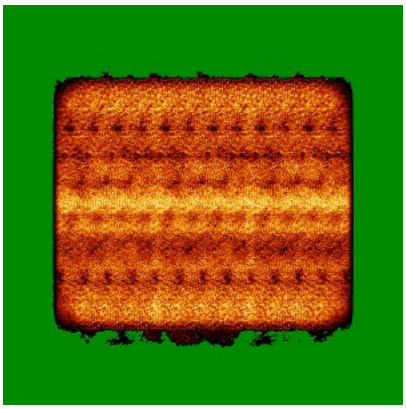
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

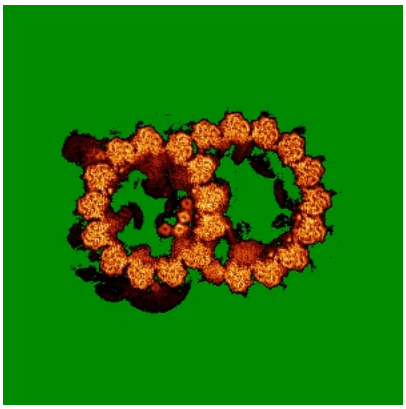
### 6.4.1 Primary map



X

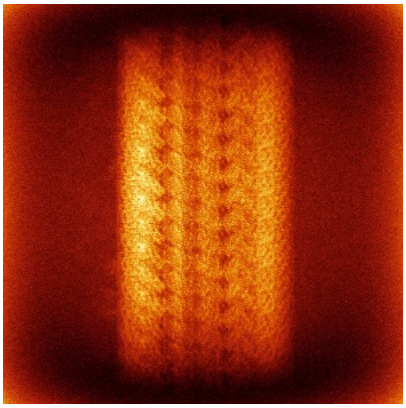


Y

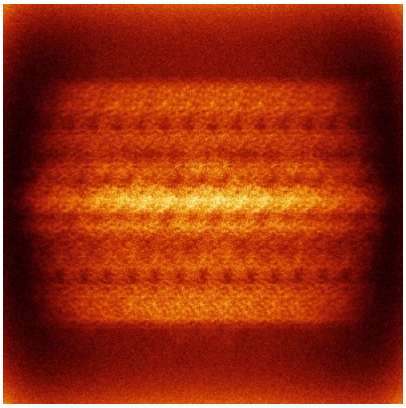


Z

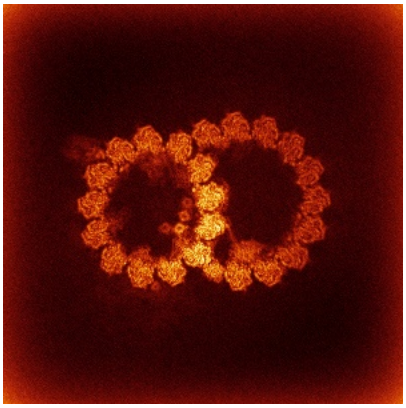
### 6.4.2 Raw map



X



Y

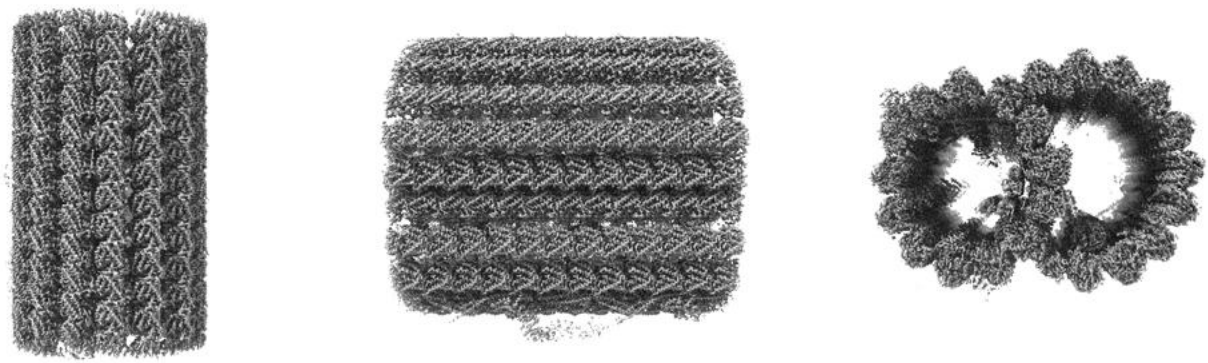


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

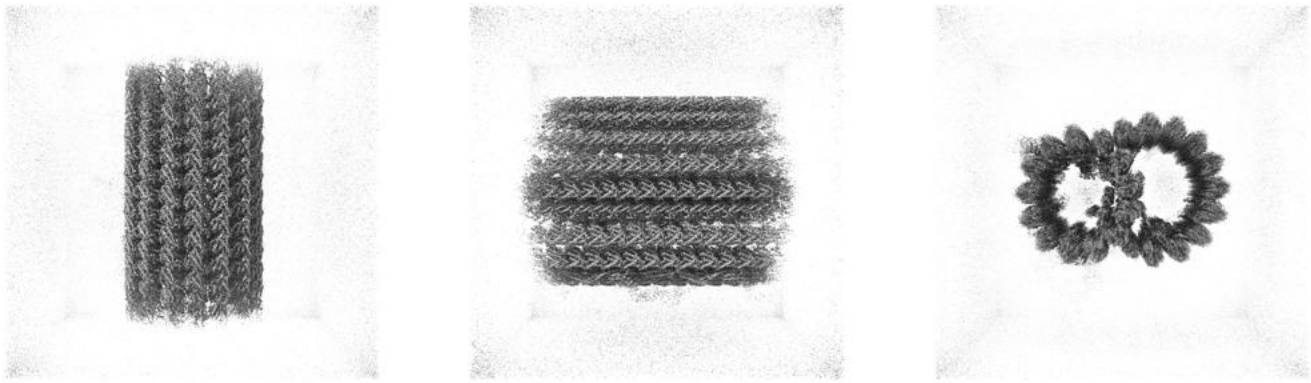
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

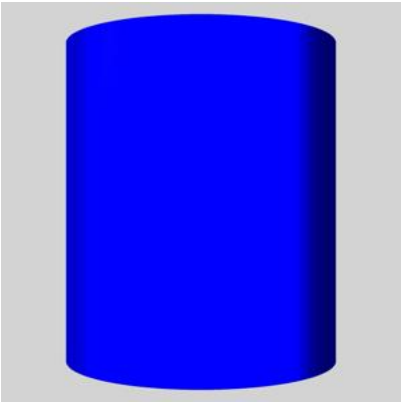
## 6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

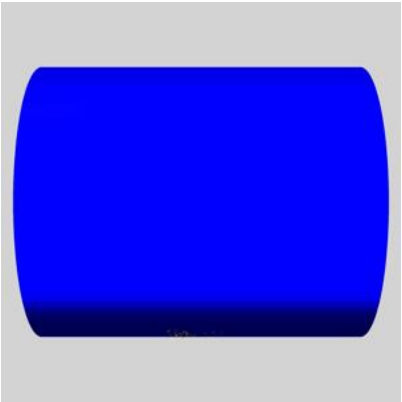
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

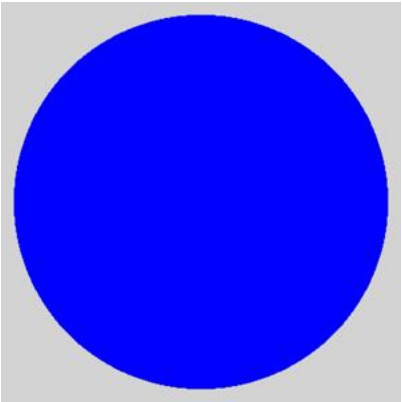
### 6.6.1 emd_45802_msk_1.map (i)



X



Y

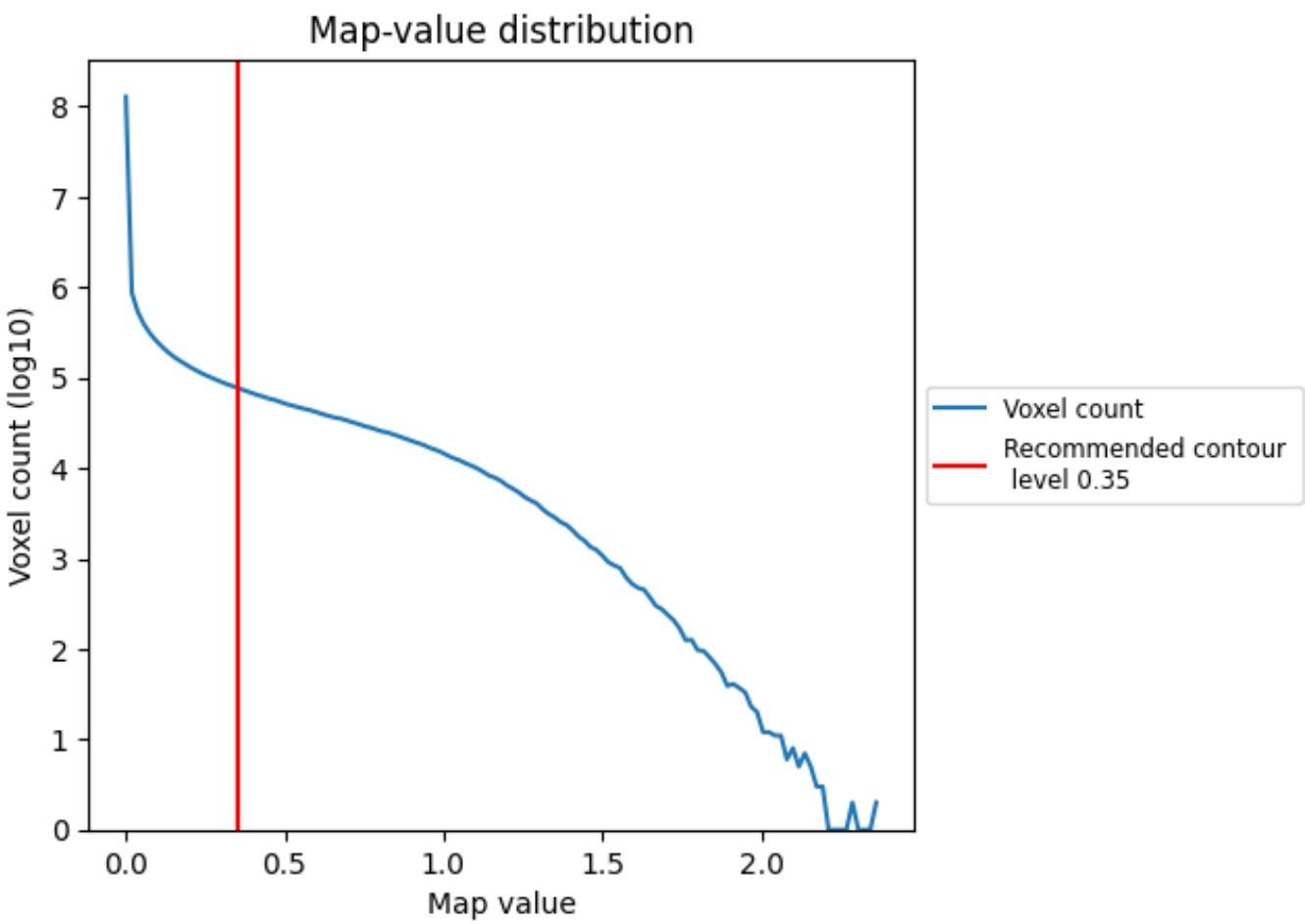


Z

# 7 Map analysis (i)

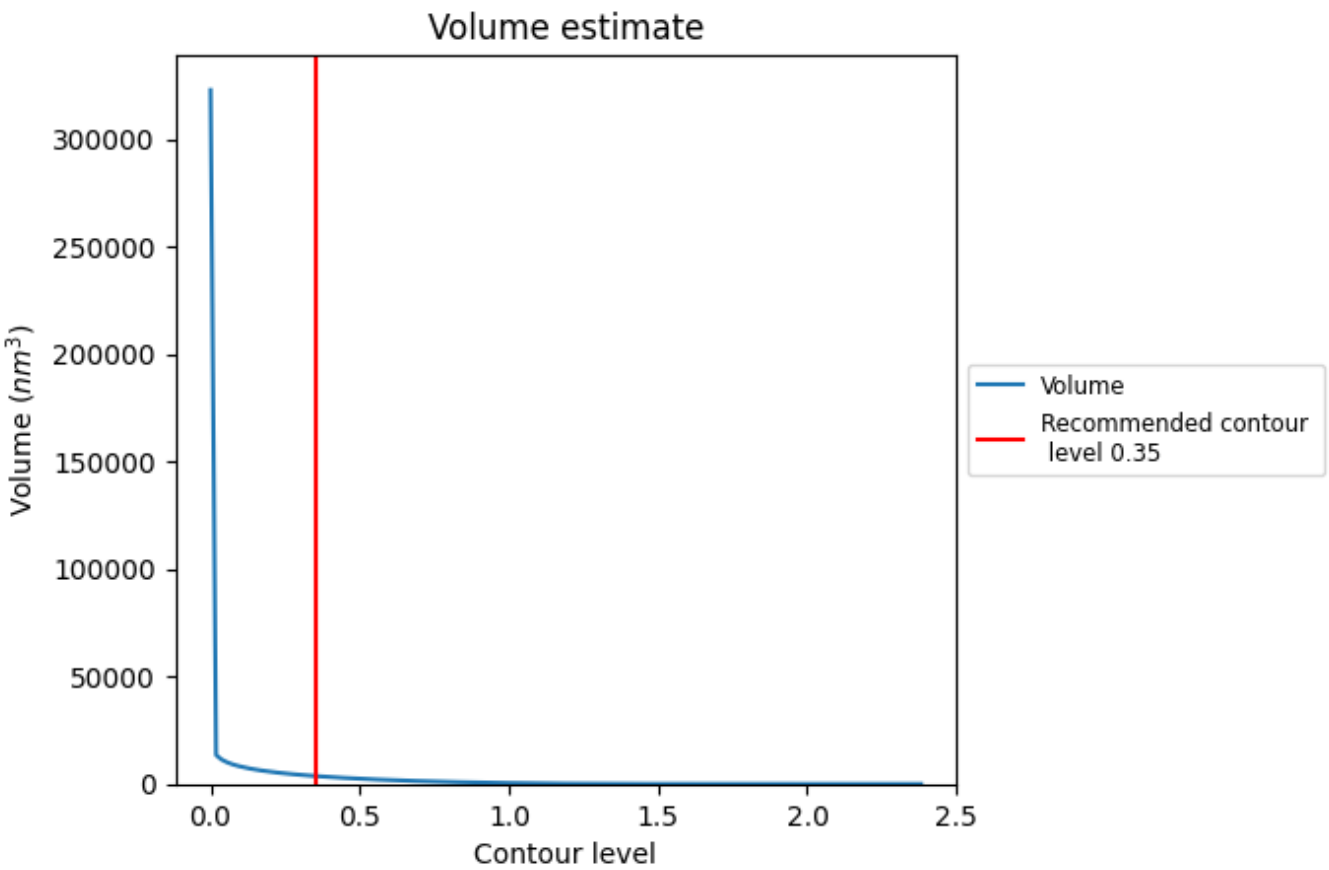
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

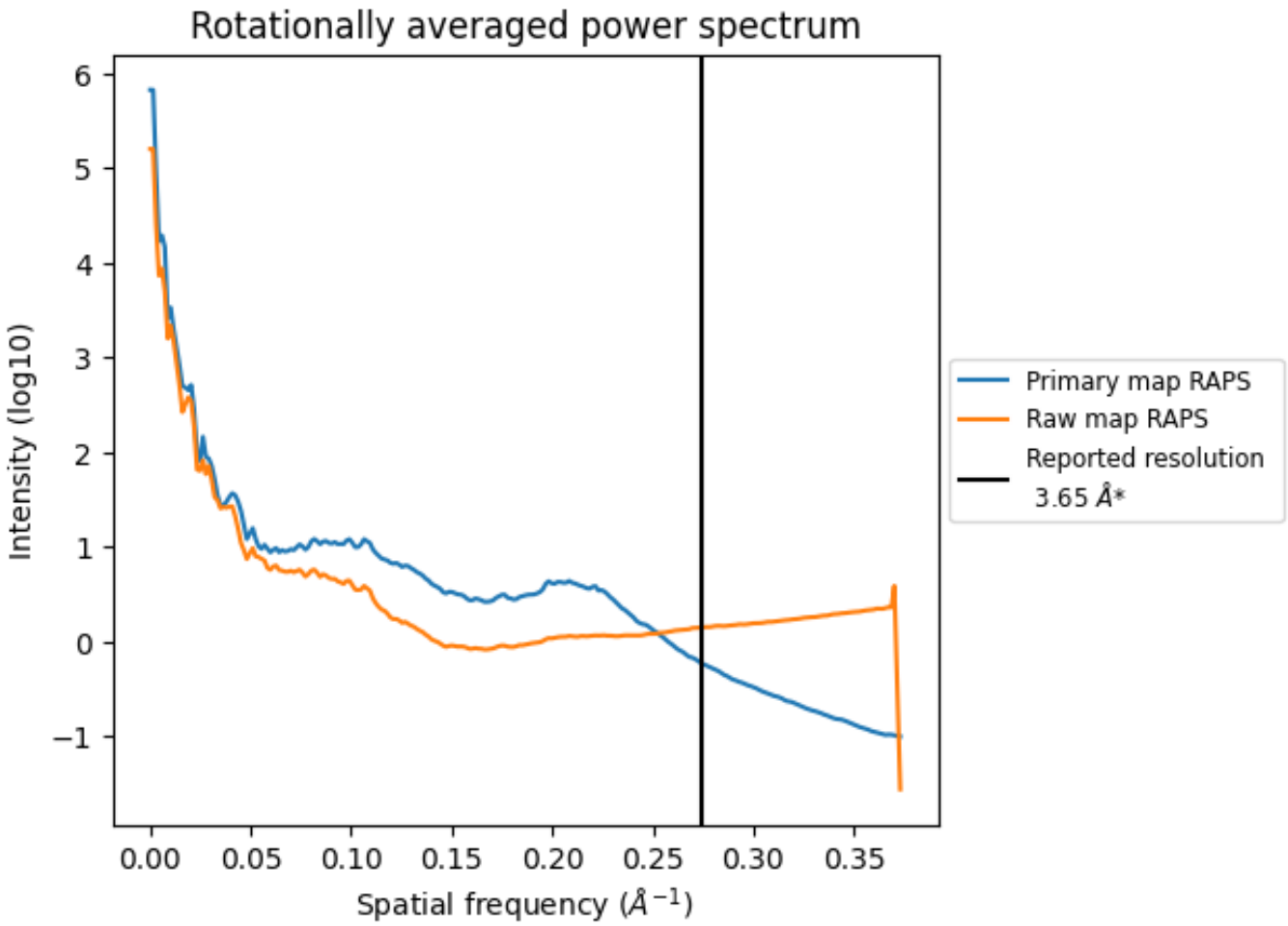
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 3691 $nm^3$; this corresponds to an approximate mass of 3334 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

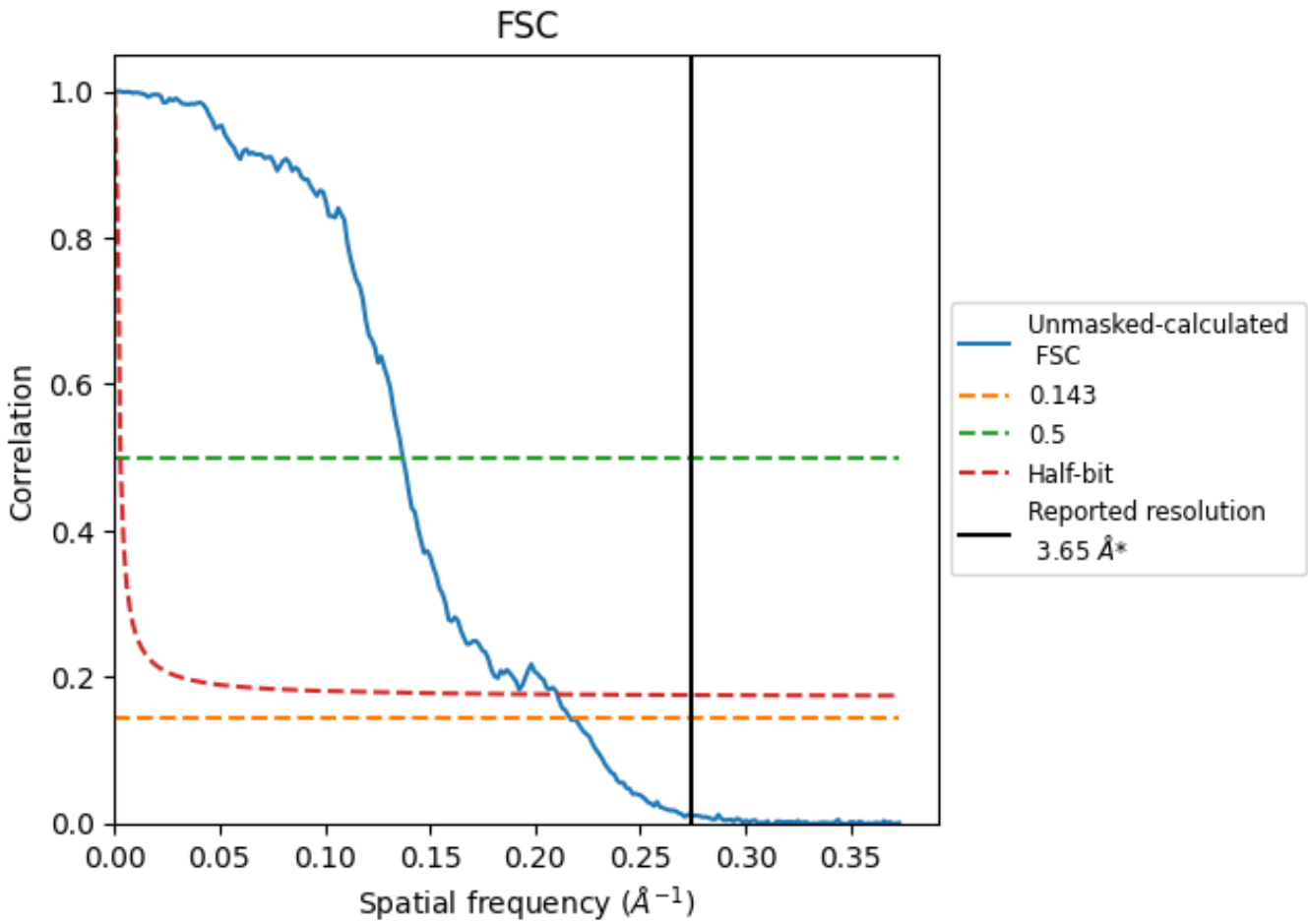



*Reported resolution corresponds to spatial frequency of 0.274 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.274 Å$^{-1}$

## 8.2 Resolution estimates (i)

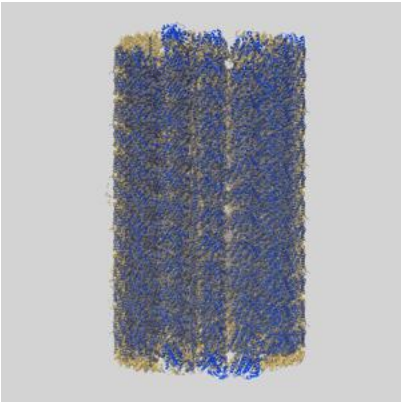
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.65 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 4.62 | 7.30 | 4.75 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.62 differs from the reported value 3.65 by more than 10 %

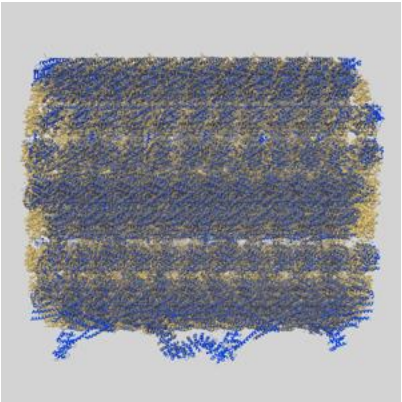
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-45802 and PDB model 9CPC. Per-residue inclusion information can be found in section 3 on page 56.

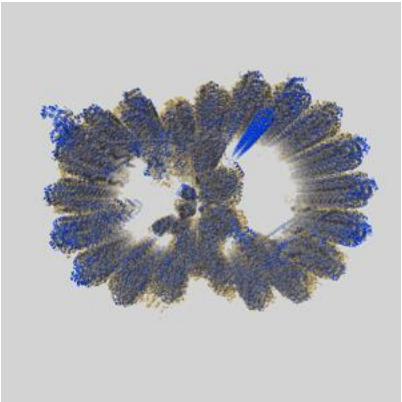
## 9.1 Map-model overlay (i)



X



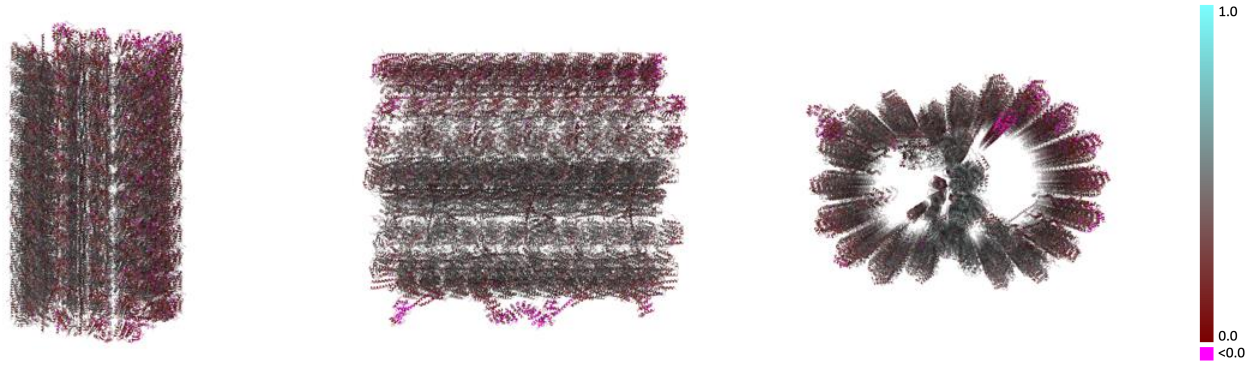
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

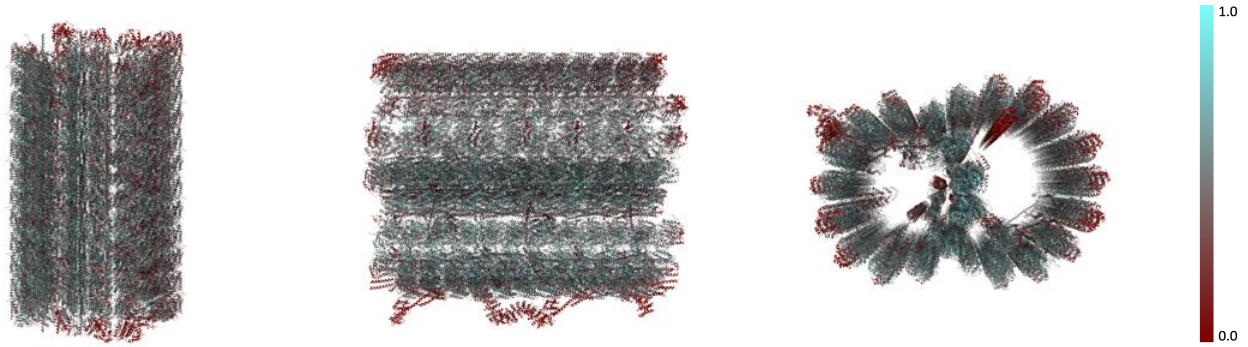
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

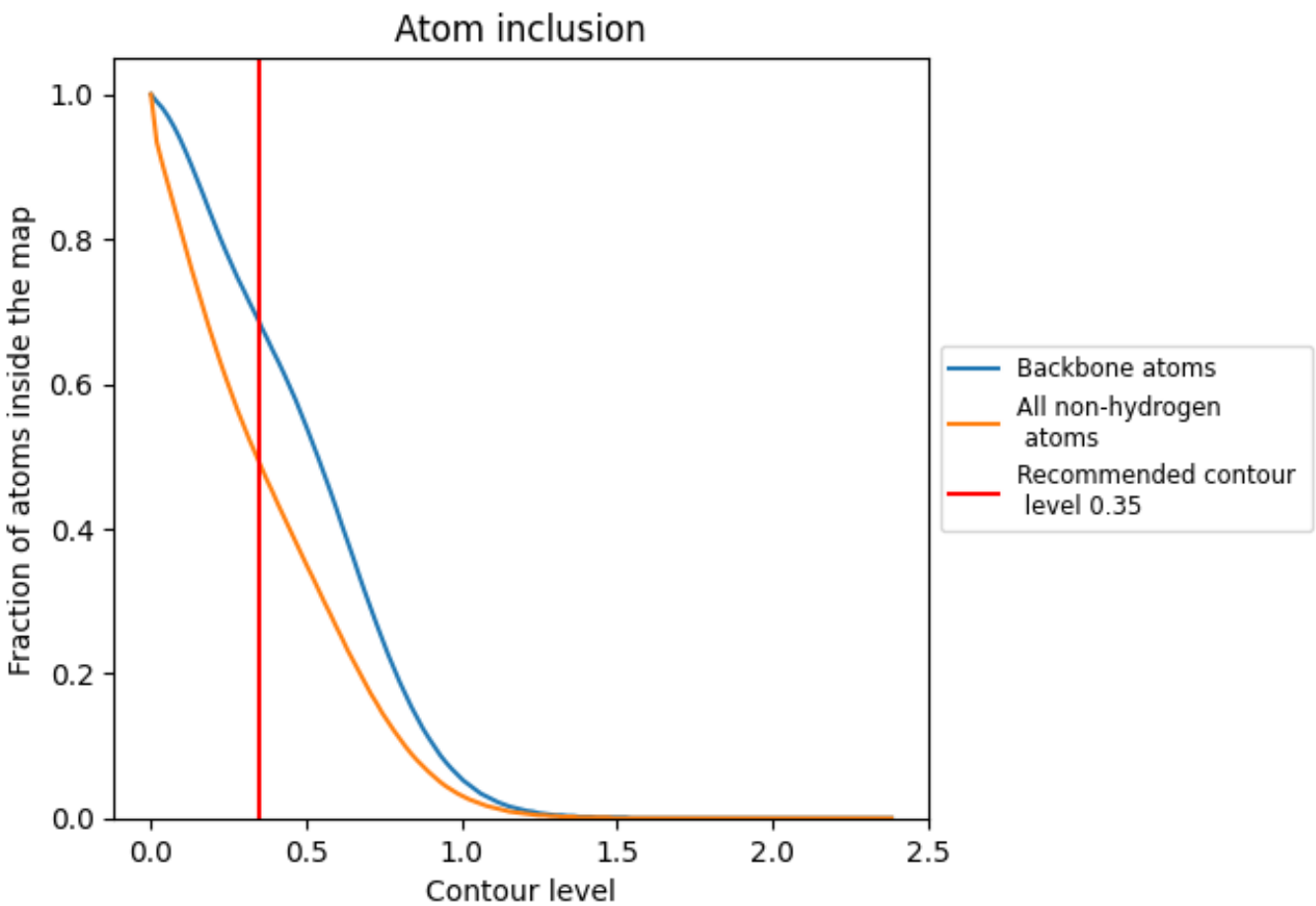
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

## 9.4 Atom inclusion (i)




At the recommended contour level, 68% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4900 | 0.3780 |
| 1A | 0.0730 | 0.0860 |
| 1B | 0.0630 | 0.1520 |
| 1C | 0.2910 | 0.2880 |
| 1D | 0.3500 | 0.2990 |
| 1F | 0.0070 | 0.0710 |
| 1G | 0.0000 | -0.0110 |
| 1H | 0.3100 | 0.3130 |
| 1I | 0.1710 | 0.2420 |
| 1J | 0.2620 | 0.2890 |
| 1L | 0.2220 | 0.2360 |
| 1M | 0.2940 | 0.2650 |
| 1N | 0.1930 | 0.2080 |
| 1P | 0.1300 | 0.3070 |
| 1Q | 0.0110 | 0.1820 |
| 1S | 0.5180 | 0.4400 |
| 1T | 0.5280 | 0.4460 |
| 1U | 0.5340 | 0.4410 |
| 1W | 0.3090 | 0.2320 |
| 1X | 0.2830 | 0.2480 |
| 1Y | 0.2890 | 0.2670 |
| 1Z | 0.2870 | 0.2150 |
| 2B | 0.3750 | 0.2300 |
| 2C | 0.4330 | 0.2440 |
| 2E | 0.4630 | 0.3970 |
| 2F | 0.4240 | 0.3860 |
| 2G | 0.4500 | 0.3830 |
| 2I | 0.4350 | 0.3860 |
| 2J | 0.4120 | 0.3660 |
| 2K | 0.4110 | 0.3890 |
| 2M | 0.4280 | 0.4350 |
| 2N | 0.5240 | 0.4490 |
| 2O | 0.5070 | 0.4500 |
| 2P | 0.5450 | 0.4500 |
| 2Q | 0.5370 | 0.4550 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| 2R | 0.1760 | 0.3480 |
| 2T | 0.5600 | 0.4740 |
| 2U | 0.5580 | 0.4550 |
| 2V | 0.5540 | 0.4770 |
| 2W | 0.5730 | 0.4740 |
| 2X | 0.5600 | 0.4710 |
| 3A | 0.5670 | 0.4520 |
| 3B | 0.5620 | 0.4420 |
| 3C | 0.5640 | 0.4650 |
| 3E | 0.5440 | 0.4600 |
| 3F | 0.5360 | 0.4560 |
| 3G | 0.4730 | 0.4520 |
| 3H | 0.5210 | 0.4400 |
| 3J | 0.5240 | 0.4470 |
| 3K | 0.5000 | 0.4260 |
| 3L | 0.5370 | 0.4390 |
| 3M | 0.4660 | 0.4220 |
| 3O | 0.3050 | 0.3780 |
| 3P | 0.3370 | 0.3810 |
| 3Q | 0.3360 | 0.3640 |
| 3R | 0.2840 | 0.3220 |
| 3T | 0.2770 | 0.3520 |
| 3U | 0.2980 | 0.3680 |
| 3V | 0.1410 | 0.2510 |
| 3W | 0.2030 | 0.3110 |
| 3Y | 0.5140 | 0.4460 |
| 3Z | 0.4790 | 0.4300 |
| 4A | 0.1910 | 0.3050 |
| 4B | 0.2790 | 0.3260 |
| 4D | 0.4750 | 0.4210 |
| 4E | 0.4810 | 0.3980 |
| 4F | 0.4660 | 0.3800 |
| 4H | 0.3990 | 0.3710 |
| 4I | 0.4030 | 0.3690 |
| 4J | 0.4010 | 0.3520 |
| 4K | 0.0980 | 0.2030 |
| 4M | 0.3630 | 0.3850 |
| 4N | 0.3990 | 0.3680 |
| 4O | 0.2340 | 0.2680 |
| 4P | 0.1590 | 0.2620 |
| 4Q | 0.1800 | 0.3250 |
| 4R | 0.2890 | 0.3370 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| 4T | 0.3790 | 0.3560 |
| 4V | 0.4440 | 0.3870 |
| 4W | 0.3460 | 0.3280 |
| 4Y | 0.4880 | 0.4110 |
| 4Z | 0.5130 | 0.4140 |
| 5B | 0.3820 | 0.3630 |
| 5D | 0.4460 | 0.3890 |
| 5E | 0.3090 | 0.2930 |
| 5G | 0.0790 | 0.2220 |
| 5I | 0.4110 | 0.3740 |
| 5J | 0.2560 | 0.2900 |
| 5L | 0.4270 | 0.3700 |
| 5N | 0.3500 | 0.2920 |
| 5O | 0.3890 | 0.2990 |
| 5Q | 0.3820 | 0.3020 |
| 5R | 0.4030 | 0.3080 |
| 5T | 0.0660 | 0.2300 |
| 5U | 0.0470 | 0.1580 |
| 5W | 0.3770 | 0.3360 |
| 5X | 0.3650 | 0.3300 |
| 5Y | 0.3720 | 0.3050 |
| 5Z | 0.3570 | 0.3570 |
| 6A | 0.4110 | 0.3070 |
| 6C | 0.3790 | 0.3170 |
| 6D | 0.4490 | 0.3790 |
| 6F | 0.0740 | 0.1900 |
| 6G | 0.0470 | 0.1490 |
| 6H | 0.0320 | 0.1080 |
| 6I | 0.0790 | 0.1960 |
| 6J | 0.0220 | 0.1330 |
| 6K | 0.0560 | 0.1620 |
| 6L | 0.0110 | 0.0900 |
| AA | 0.5760 | 0.4780 |
| AB | 0.5620 | 0.4740 |
| AE | 0.5820 | 0.4890 |
| AF | 0.6020 | 0.4800 |
| AG | 0.5920 | 0.4820 |
| AH | 0.5860 | 0.4820 |
| AL | 0.5960 | 0.4760 |
| AM | 0.5910 | 0.4810 |
| AN | 0.5810 | 0.4770 |
| AO | 0.5960 | 0.4970 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| AP | 0.5780 | 0.4730 |
| BA | 0.5610 | 0.4460 |
| BB | 0.5600 | 0.4630 |
| BE | 0.5560 | 0.4510 |
| BF | 0.5780 | 0.4310 |
| BG | 0.5810 | 0.4390 |
| BH | 0.5670 | 0.4600 |
| BI | 0.4730 | 0.4150 |
| BL | 0.5320 | 0.4160 |
| BM | 0.5540 | 0.4490 |
| BN | 0.5470 | 0.4280 |
| BO | 0.5570 | 0.4580 |
| BP | 0.5680 | 0.4520 |
| CA | 0.5370 | 0.4330 |
| CB | 0.5300 | 0.4050 |
| CE | 0.5200 | 0.3900 |
| CF | 0.5390 | 0.4010 |
| CG | 0.5490 | 0.4120 |
| CH | 0.5480 | 0.4430 |
| CI | 0.4540 | 0.3620 |
| CL | 0.5000 | 0.3930 |
| CM | 0.5430 | 0.4340 |
| CN | 0.5610 | 0.4310 |
| CO | 0.5520 | 0.4350 |
| CP | 0.5510 | 0.4240 |
| DA | 0.5230 | 0.3970 |
| DB | 0.5370 | 0.3940 |
| DE | 0.4890 | 0.3530 |
| DF | 0.5150 | 0.3800 |
| DG | 0.5060 | 0.3590 |
| DH | 0.5150 | 0.3880 |
| DI | 0.4360 | 0.3410 |
| DL | 0.3490 | 0.2960 |
| DM | 0.5160 | 0.3820 |
| DN | 0.5440 | 0.3920 |
| DO | 0.5140 | 0.3600 |
| DP | 0.5280 | 0.3800 |
| EA | 0.5410 | 0.3700 |
| EB | 0.5520 | 0.3760 |
| EE | 0.4810 | 0.3210 |
| EF | 0.5380 | 0.3670 |
| EG | 0.5540 | 0.3800 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| EH | 0.5610 | 0.4080 |
| EI | 0.4740 | 0.3570 |
| EL | 0.2490 | 0.2560 |
| EM | 0.5500 | 0.4020 |
| EN | 0.5480 | 0.3600 |
| EO | 0.5570 | 0.3730 |
| EP | 0.5400 | 0.3920 |
| FA | 0.5460 | 0.4140 |
| FB | 0.5470 | 0.4050 |
| FE | 0.4320 | 0.3320 |
| FF | 0.5290 | 0.3890 |
| FG | 0.5360 | 0.4010 |
| FH | 0.5220 | 0.3970 |
| FI | 0.4700 | 0.3560 |
| FM | 0.5210 | 0.3820 |
| FN | 0.5380 | 0.3840 |
| FO | 0.5550 | 0.3950 |
| FP | 0.5060 | 0.3800 |
| GA | 0.5330 | 0.3940 |
| GB | 0.5620 | 0.4110 |
| GE | 0.4500 | 0.3690 |
| GF | 0.5340 | 0.4070 |
| GG | 0.5520 | 0.4180 |
| GH | 0.5540 | 0.4280 |
| GI | 0.5260 | 0.4040 |
| GM | 0.5310 | 0.3920 |
| GN | 0.5660 | 0.4160 |
| GO | 0.5680 | 0.3990 |
| GP | 0.5380 | 0.3990 |
| HA | 0.5620 | 0.4040 |
| HB | 0.5640 | 0.4220 |
| HE | 0.4660 | 0.3820 |
| HF | 0.5480 | 0.4160 |
| HG | 0.5630 | 0.4280 |
| HH | 0.5550 | 0.4200 |
| HI | 0.5330 | 0.3960 |
| HM | 0.5470 | 0.4050 |
| HN | 0.5620 | 0.4280 |
| HO | 0.5650 | 0.4160 |
| HP | 0.5470 | 0.4160 |
| HQ | 0.4410 | 0.3480 |
| IA | 0.5510 | 0.4050 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| IB | 0.5530 | 0.4180 |
| IE | 0.4250 | 0.3490 |
| IF | 0.5270 | 0.4150 |
| IG | 0.5460 | 0.4180 |
| IH | 0.5630 | 0.4260 |
| II | 0.5410 | 0.4160 |
| IM | 0.5310 | 0.4080 |
| IN | 0.5330 | 0.4130 |
| IO | 0.5530 | 0.4190 |
| IP | 0.5590 | 0.4380 |
| IQ | 0.5160 | 0.4010 |
| JA | 0.5480 | 0.4040 |
| JB | 0.5690 | 0.4090 |
| JD | 0.5190 | 0.3820 |
| JE | 0.5330 | 0.4000 |
| JF | 0.5510 | 0.4120 |
| JG | 0.5510 | 0.4200 |
| JH | 0.5480 | 0.4070 |
| JL | 0.5400 | 0.4000 |
| JM | 0.5780 | 0.4280 |
| JN | 0.5410 | 0.4020 |
| JO | 0.5660 | 0.4230 |
| KA | 0.5840 | 0.4490 |
| KB | 0.6030 | 0.4490 |
| KD | 0.5780 | 0.4260 |
| KE | 0.5840 | 0.4430 |
| KF | 0.5750 | 0.4410 |
| KG | 0.5810 | 0.4420 |
| KH | 0.5810 | 0.4430 |
| KL | 0.5980 | 0.4610 |
| KM | 0.5950 | 0.4330 |
| KN | 0.5780 | 0.4450 |
| KO | 0.5810 | 0.4370 |
| KP | 0.5080 | 0.4090 |
| LA | 0.5960 | 0.4730 |
| LB | 0.6310 | 0.4820 |
| LD | 0.6100 | 0.4730 |
| LE | 0.5960 | 0.4710 |
| LF | 0.6190 | 0.5070 |
| LG | 0.6170 | 0.5000 |
| LH | 0.6040 | 0.4730 |
| LL | 0.6070 | 0.4780 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| LM | 0.6080 | 0.4750 |
| LN | 0.6110 | 0.4880 |
| LO | 0.6180 | 0.4830 |
| LP | 0.5880 | 0.4670 |
| MA | 0.6150 | 0.5070 |
| MB | 0.6100 | 0.4820 |
| MD | 0.5980 | 0.4810 |
| ME | 0.6050 | 0.4790 |
| MF | 0.6350 | 0.5100 |
| MG | 0.6300 | 0.5130 |
| MH | 0.6150 | 0.5060 |
| ML | 0.6240 | 0.4920 |
| MM | 0.6040 | 0.4750 |
| MN | 0.6130 | 0.4920 |
| MO | 0.6250 | 0.5070 |
| MP | 0.6050 | 0.4720 |
| NA | 0.5090 | 0.3890 |
| NB | 0.5210 | 0.3810 |
| ND | 0.4920 | 0.3850 |
| NE | 0.4920 | 0.3830 |
| NF | 0.5050 | 0.3840 |
| NG | 0.5000 | 0.3810 |
| NH | 0.4870 | 0.3700 |
| NL | 0.4920 | 0.3800 |
| NM | 0.5140 | 0.3850 |
| NN | 0.4920 | 0.3810 |
| NO | 0.4950 | 0.3800 |
| NP | 0.4230 | 0.3260 |
| OA | 0.5140 | 0.3740 |
| OB | 0.5190 | 0.3580 |
| OD | 0.4180 | 0.3120 |
| OE | 0.5060 | 0.3710 |
| OF | 0.5010 | 0.3540 |
| OG | 0.5050 | 0.3600 |
| OH | 0.5040 | 0.3830 |
| OL | 0.4930 | 0.3560 |
| OM | 0.5100 | 0.3580 |
| ON | 0.5130 | 0.3730 |
| OO | 0.5040 | 0.3670 |
| OP | 0.4400 | 0.3000 |
| PA | 0.4710 | 0.3240 |
| PB | 0.4550 | 0.3050 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| PD | 0.2750 | 0.1850 |
| PE | 0.4470 | 0.2930 |
| PF | 0.4570 | 0.2930 |
| PG | 0.4600 | 0.2910 |
| PH | 0.4440 | 0.2930 |
| PL | 0.4270 | 0.2790 |
| PM | 0.4440 | 0.2990 |
| PN | 0.4790 | 0.3150 |
| PO | 0.4370 | 0.2890 |
| PP | 0.3980 | 0.2380 |
| QA | 0.4210 | 0.2830 |
| QB | 0.4740 | 0.3250 |
| QE | 0.3910 | 0.2390 |
| QF | 0.4510 | 0.2710 |
| QG | 0.4450 | 0.2660 |
| QH | 0.4010 | 0.2650 |
| QL | 0.3510 | 0.2060 |
| QM | 0.4210 | 0.2700 |
| QN | 0.4300 | 0.2770 |
| QO | 0.4100 | 0.2730 |
| QP | 0.4150 | 0.2620 |
| RA | 0.4340 | 0.3000 |
| RB | 0.4440 | 0.2870 |
| RE | 0.3900 | 0.2440 |
| RF | 0.4510 | 0.2740 |
| RG | 0.4580 | 0.2840 |
| RH | 0.4230 | 0.2820 |
| RI | 0.1670 | 0.1800 |
| RL | 0.3030 | 0.2020 |
| RM | 0.4270 | 0.2730 |
| RN | 0.4430 | 0.2920 |
| RO | 0.4390 | 0.3000 |
| RP | 0.3860 | 0.2420 |
| SA | 0.4680 | 0.3240 |
| SB | 0.4620 | 0.3120 |
| SE | 0.4080 | 0.2640 |
| SF | 0.4500 | 0.2920 |
| SG | 0.4690 | 0.3070 |
| SH | 0.4600 | 0.3160 |
| SI | 0.2480 | 0.2280 |
| SL | 0.2910 | 0.2130 |
| SM | 0.4470 | 0.2910 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| SN | 0.4660 | 0.2990 |
| SO | 0.5010 | 0.3430 |
| SP | 0.4280 | 0.2870 |
| TA | 0.4800 | 0.3310 |
| TB | 0.4860 | 0.3400 |
| TE | 0.4050 | 0.2780 |
| TF | 0.4680 | 0.3230 |
| TG | 0.4760 | 0.3270 |
| TH | 0.5110 | 0.3640 |
| TI | 0.3740 | 0.3020 |
| TL | 0.2390 | 0.2220 |
| TM | 0.4740 | 0.3270 |
| TN | 0.5090 | 0.3290 |
| TO | 0.5200 | 0.3530 |
| TP | 0.4860 | 0.3390 |
| UA | 0.4940 | 0.3600 |
| UB | 0.5000 | 0.3570 |
| UE | 0.4290 | 0.3000 |
| UF | 0.4930 | 0.3790 |
| UG | 0.4750 | 0.3500 |
| UH | 0.5060 | 0.3800 |
| UI | 0.4810 | 0.3670 |
| UM | 0.4780 | 0.3390 |
| UN | 0.4950 | 0.3340 |
| UO | 0.5300 | 0.3640 |
| UP | 0.5190 | 0.3870 |
| VA | 0.5230 | 0.4090 |
| VB | 0.5440 | 0.4240 |
| VF | 0.5070 | 0.4030 |
| VG | 0.5510 | 0.4280 |
| VH | 0.5380 | 0.4200 |
| VI | 0.5300 | 0.4260 |
| VJ | 0.5150 | 0.4000 |
| VN | 0.5460 | 0.4230 |
| VO | 0.5430 | 0.4090 |
| VP | 0.5310 | 0.3970 |
| VQ | 0.5380 | 0.4150 |
| WA | 0.5270 | 0.4180 |
| WB | 0.5580 | 0.4260 |
| WE | 0.5240 | 0.4130 |
| WF | 0.5610 | 0.4330 |
| WG | 0.5570 | 0.4360 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| WH | 0.5430 | 0.4290 |
| WI | 0.5440 | 0.4330 |
| WM | 0.5670 | 0.4560 |
| WN | 0.5700 | 0.4460 |
| WO | 0.5420 | 0.4090 |
| WP | 0.5590 | 0.4400 |
| WQ | 0.4940 | 0.3860 |