



Full wwPDB EM Validation Report ⓘ

May 29, 2025 – 05:09 pm BST

PDB ID : 9H2H / pdb_00009h2h
EMDB ID : EMD-51803
Title : AcMNPV apical cap - composite map of the C2 plug
Authors : Effantin, G.; Kandiah, E.; Pelosse, M.
Deposited on : 2024-10-11
Resolution : 6.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

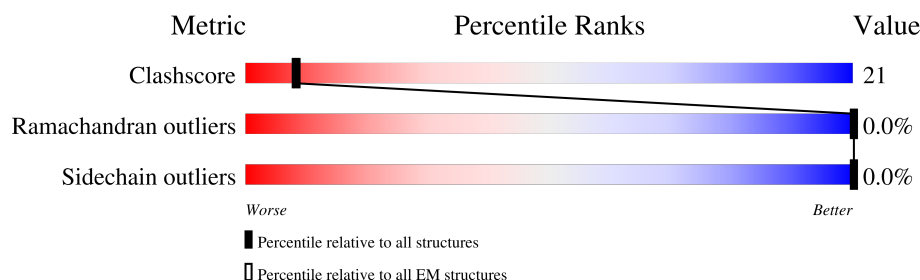
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.10 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 $\leq 5\%$. 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 | A | 365 | <div> <div>6%</div> <div>56%</div> <div>35%</div> <div>9%</div> </div> |
| 1 | B | 365 | <div> <div>5%</div> <div>54%</div> <div>39%</div> <div>8%</div> </div> |
| 1 | C | 365 | <div> <div>52%</div> <div>37%</div> <div>11%</div> </div> |
| 1 | D | 365 | <div> <div>50%</div> <div>39%</div> <div>11%</div> </div> |
| 2 | E | 58 | <div> <div>9%</div> <div>91%</div> </div> |
| 3 | F | 58 | <div> <div>100%</div> </div> |
| 4 | G | 290 | <div> <div>14%</div> <div>49%</div> <div>34%</div> <div>17%</div> </div> |
| 4 | H | 290 | <div> <div>14%</div> <div>39%</div> <div>16%</div> <div>45%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | K | 290 | |
| 4 | L | 290 | |
| 4 | O | 290 | |
| 4 | P | 290 | |
| 4 | S | 290 | |
| 4 | T | 290 | |
| 5 | I | 361 | |
| 5 | J | 361 | |
| 5 | M | 361 | |
| 5 | N | 361 | |
| 5 | Q | 361 | |
| 5 | R | 361 | |
| 5 | U | 361 | |
| 5 | V | 361 | |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 39098 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 Protein AC54.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 332 | Total | C | N | O | S | 0 | 0 |
| | | | 2717 | 1723 | 479 | 497 | 18 | | |
| 1 | B | 337 | Total | C | N | O | S | 0 | 0 |
| | | | 2757 | 1752 | 484 | 502 | 19 | | |
| 1 | C | 324 | Total | C | N | O | S | 0 | 0 |
| | | | 2660 | 1691 | 468 | 483 | 18 | | |
| 1 | D | 325 | Total | C | N | O | S | 0 | 0 |
| | | | 2666 | 1700 | 469 | 478 | 19 | | |

- Molecule 2 is a DNA chain called DNA (58-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2 | E | 58 | Total | C | N | O | P | 0 | 0 |
| | | | 1198 | 574 | 233 | 333 | 58 | | |

- Molecule 3 is a DNA chain called DNA (58-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3 | F | 58 | Total | C | N | O | P | 0 | 0 |
| | | | 1177 | 573 | 186 | 361 | 57 | | |

- Molecule 4 is a protein called Occlusion-derived virus envelope protein E27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | G | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1941 | 1247 | 312 | 373 | 9 | | |
| 4 | H | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1301 | 844 | 215 | 234 | 8 | | |
| 4 | K | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1850 | 1191 | 296 | 354 | 9 | | |
| 4 | L | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1061 | 692 | 172 | 190 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | O | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1926 | 1238 | 309 | 370 | 9 | | |
| 4 | P | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1302 | 847 | 212 | 235 | 8 | | |
| 4 | S | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1805 | 1164 | 284 | 349 | 8 | | |
| 4 | T | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1440 | 938 | 234 | 260 | 8 | | |

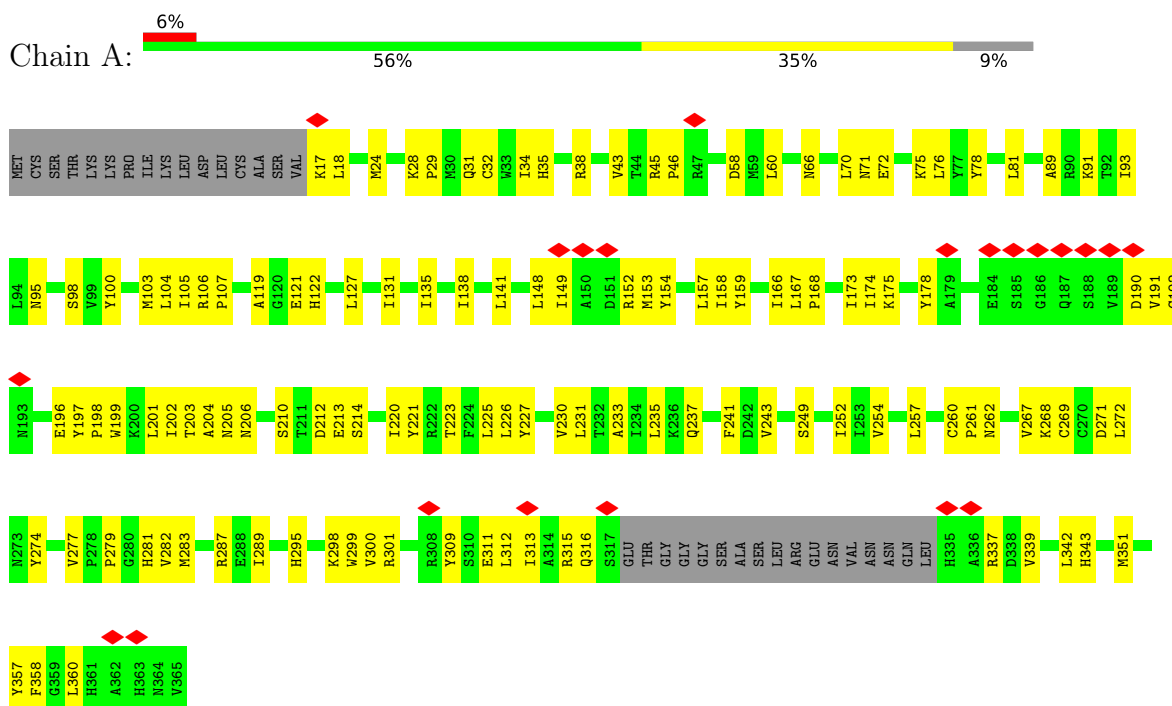
- Molecule 5 is a protein called Protein C42.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | I | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1760 | 1117 | 296 | 331 | 16 | | |
| 5 | J | 194 | Total | C | N | O | S | 0 | 0 |
| | | | 1622 | 1033 | 275 | 301 | 13 | | |
| 5 | M | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1760 | 1117 | 296 | 331 | 16 | | |
| 5 | N | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1517 | 966 | 257 | 282 | 12 | | |
| 5 | Q | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1760 | 1117 | 296 | 331 | 16 | | |
| 5 | R | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1488 | 943 | 253 | 279 | 13 | | |
| 5 | U | 213 | Total | C | N | O | S | 0 | 0 |
| | | | 1760 | 1117 | 296 | 331 | 16 | | |
| 5 | V | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1630 | 1036 | 276 | 306 | 12 | | |

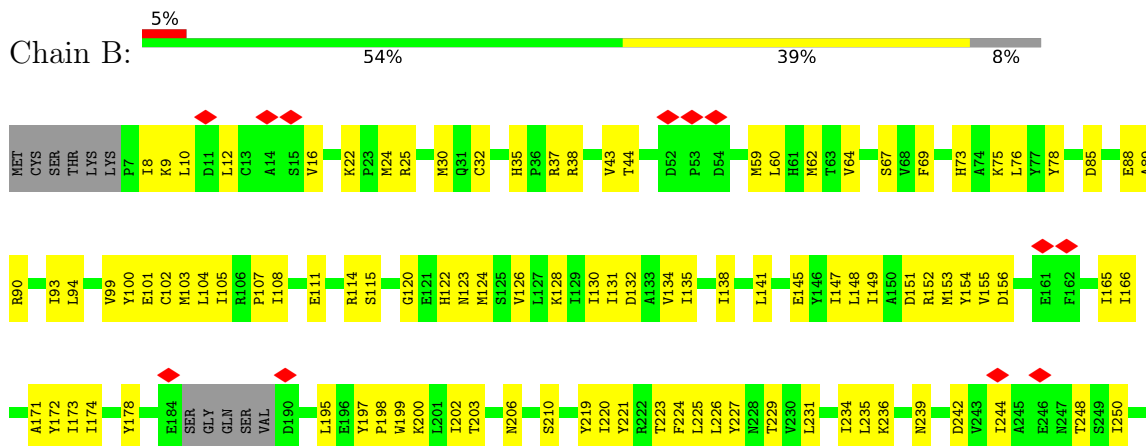
3 Residue-property plots

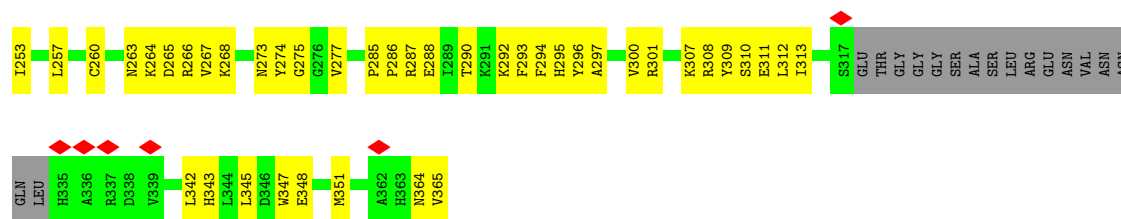
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Protein AC54



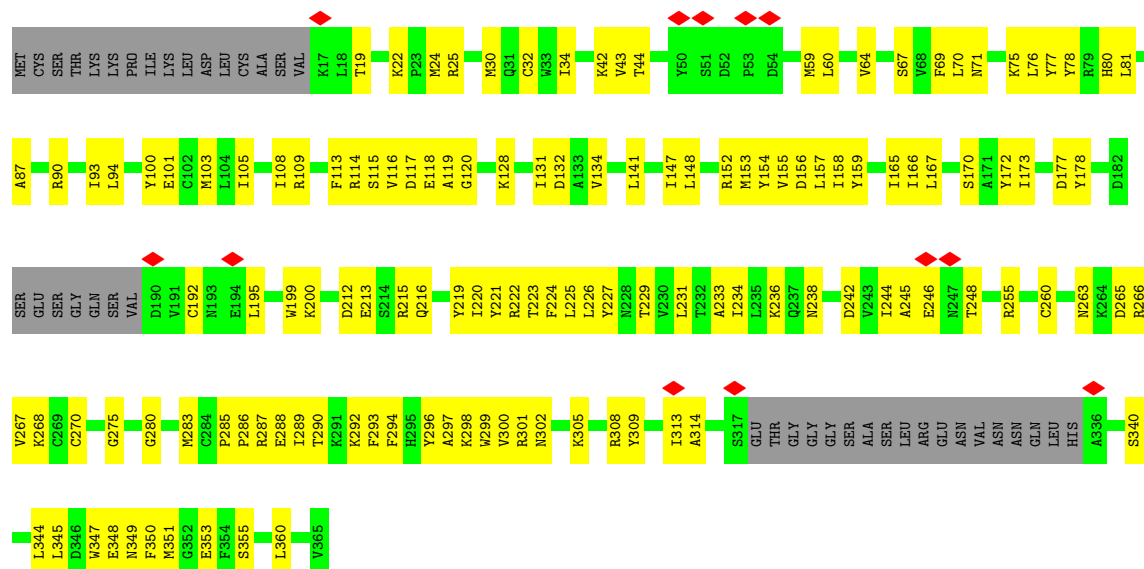
• Molecule 1: Protein AC54





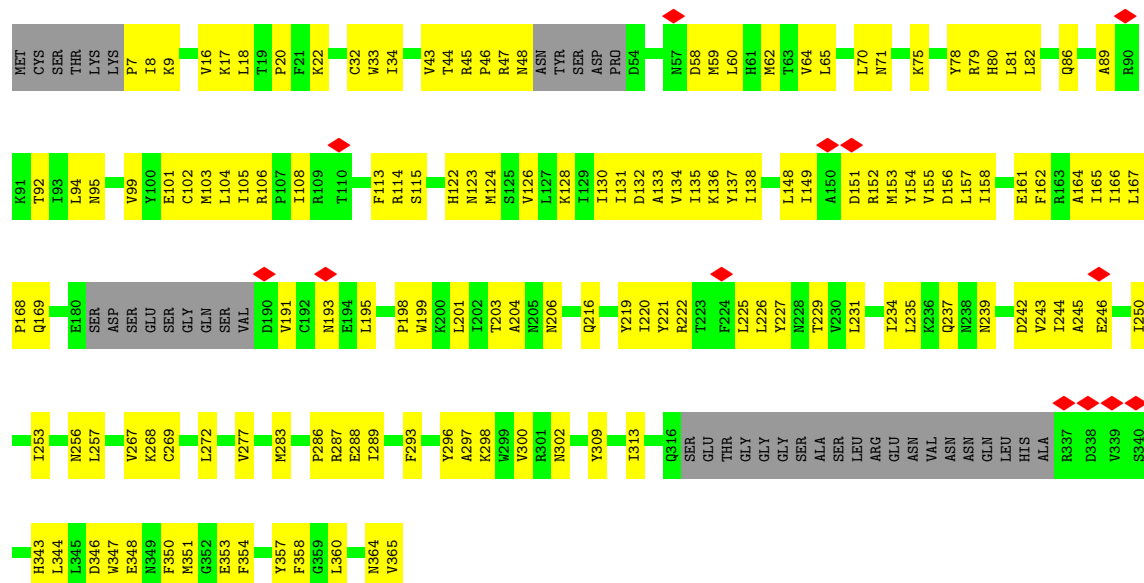
• Molecule 1: Protein AC54

Chain C: 52% 37% 11%

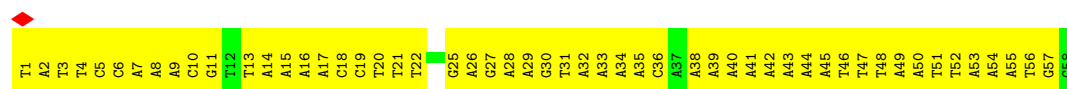
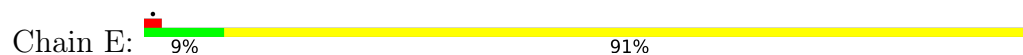


• Molecule 1: Protein AC54

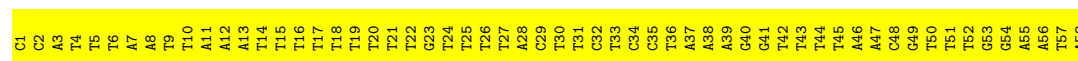
Chain D: 50% 39% 11%



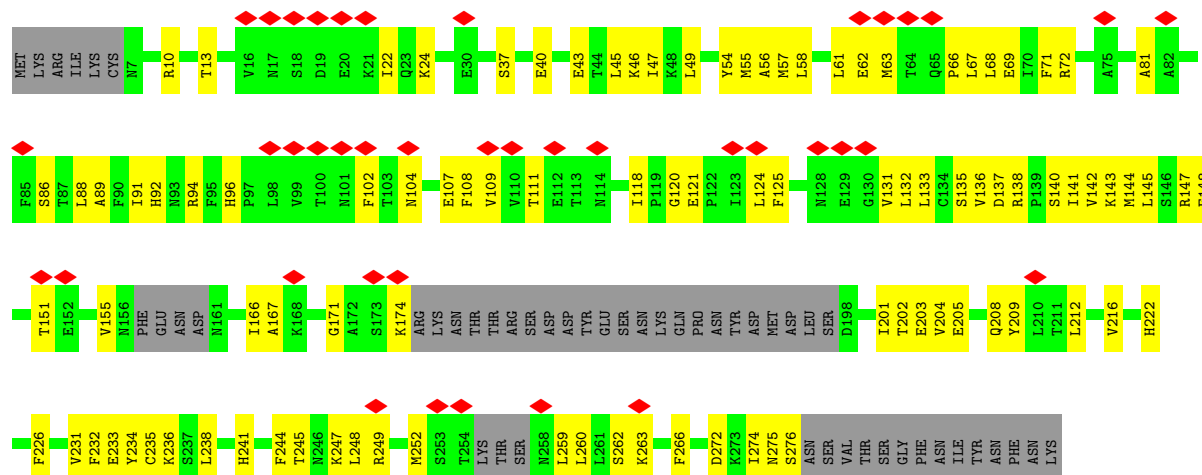
• Molecule 2: DNA (58-MER)



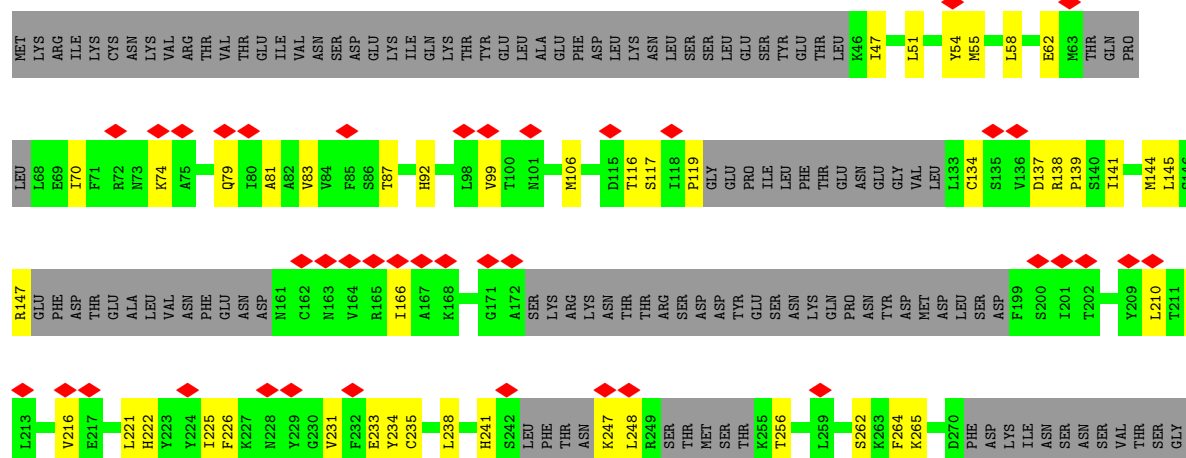
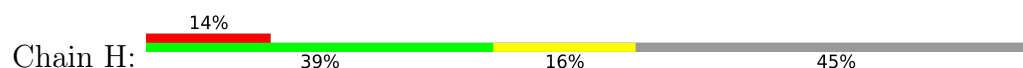
- Molecule 3: DNA (58-MER)



- Molecule 4: Occlusion-derived virus envelope protein E27



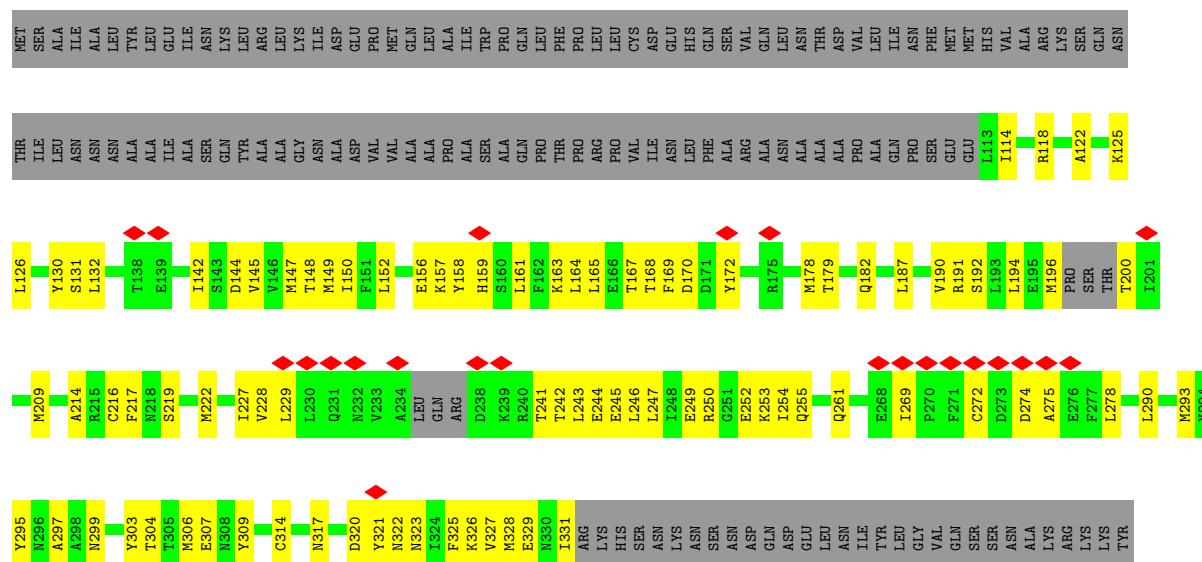
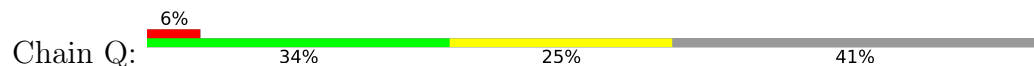
- Molecule 4: Occlusion-derived virus envelope protein E27



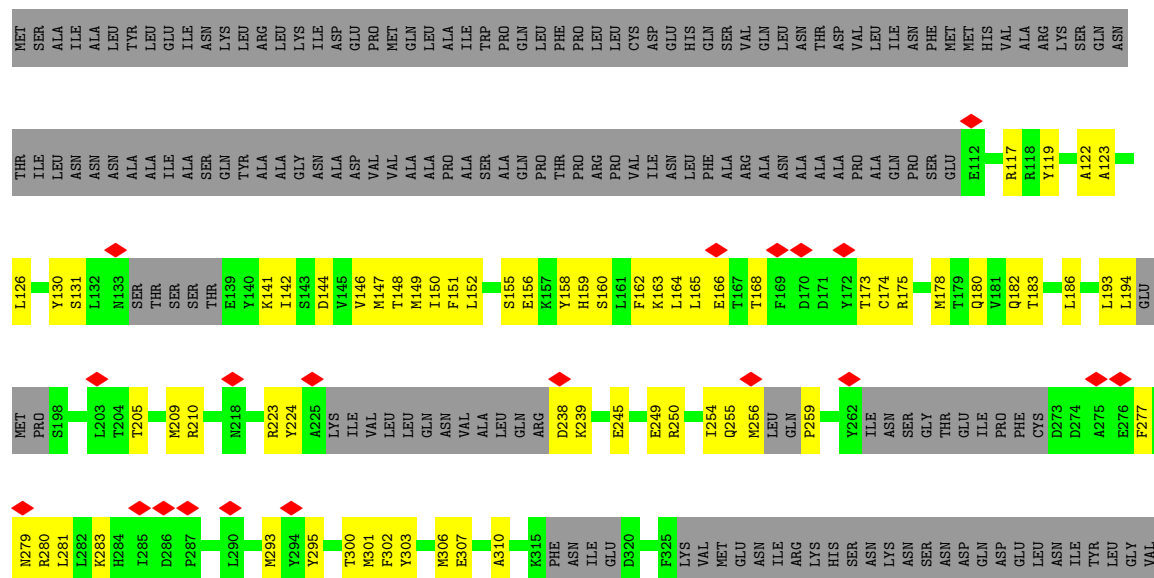
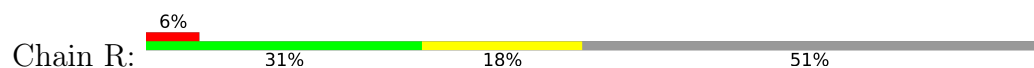
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| MET | SER | ALA | ALA | ILE | ALA | LEU | TYR | LEU | LEU | GLU | ILE | ASN | LYS | LEU | ARG | LEU | LYS | ILE | ASP | GLU | PRO | MET | GLN | LEU | ALA | ILE | TRP | PRO | GLN | LEU | PHE | PRO | LEU | LEU | CYS | ASP | GLU | GLU | HIS | GLN | SER | SER | VAL | VAL | LEU | ILE | ASN | ASN | PHE | MET | MET | HIS | VAL | ALA | ARG | LYS | SER | GLN | ASN |
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- Molecule 5: Protein C42



- Molecule 5: Protein C42



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• Molecule 5: Protein C42



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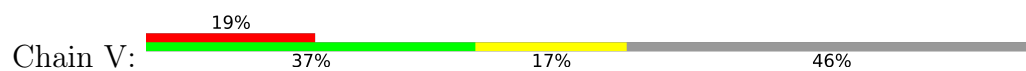
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• Molecule 5: Protein C42



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4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 12477 | 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 ($e^-/\text{\AA}^2$) | 30 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.027 | Depositor |
| Minimum map value | -0.007 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.0065 | Depositor |
| Map size (Å) | 405.0, 405.0, 405.0 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.35, 1.35, 1.35 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 | A | 0.15 | 0/2783 | 0.37 | 0/3772 |
| 1 | B | 0.16 | 0/2823 | 0.37 | 0/3825 |
| 1 | C | 0.16 | 0/2724 | 0.41 | 0/3691 |
| 1 | D | 0.17 | 0/2728 | 0.42 | 0/3693 |
| 2 | E | 0.19 | 0/1350 | 0.34 | 0/2081 |
| 3 | F | 0.19 | 0/1313 | 0.40 | 0/2025 |
| 4 | G | 0.14 | 0/1973 | 0.34 | 0/2664 |
| 4 | H | 0.13 | 0/1321 | 0.32 | 0/1774 |
| 4 | K | 0.16 | 0/1880 | 0.42 | 2/2538 (0.1%) |
| 4 | L | 0.11 | 0/1076 | 0.25 | 0/1439 |
| 4 | O | 0.15 | 0/1958 | 0.37 | 0/2645 |
| 4 | P | 0.13 | 0/1322 | 0.31 | 0/1778 |
| 4 | S | 0.17 | 0/1837 | 0.40 | 2/2484 (0.1%) |
| 4 | T | 0.12 | 0/1464 | 0.29 | 0/1972 |
| 5 | I | 0.14 | 0/1790 | 0.35 | 0/2415 |
| 5 | J | 0.16 | 0/1648 | 0.36 | 0/2219 |
| 5 | M | 0.16 | 0/1790 | 0.38 | 0/2415 |
| 5 | N | 0.14 | 0/1539 | 0.37 | 0/2065 |
| 5 | Q | 0.17 | 0/1790 | 0.40 | 0/2415 |
| 5 | R | 0.14 | 0/1511 | 0.36 | 0/2030 |
| 5 | U | 0.16 | 0/1790 | 0.35 | 0/2415 |
| 5 | V | 0.12 | 0/1656 | 0.30 | 0/2231 |
| All | All | 0.15 | 0/40066 | 0.37 | 4/54586 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | K | 233 | GLU | CA-C-N | -5.48 | 112.51 | 120.29 |
| 4 | K | 233 | GLU | C-N-CA | -5.48 | 112.51 | 120.29 |
| 4 | S | 69 | GLU | N-CA-C | -5.43 | 106.49 | 113.23 |
| 4 | S | 70 | ILE | N-CA-C | -5.34 | 104.20 | 111.89 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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 | A | 2717 | 0 | 2673 | 112 | 0 |
| 1 | B | 2757 | 0 | 2724 | 139 | 0 |
| 1 | C | 2660 | 0 | 2624 | 124 | 0 |
| 1 | D | 2666 | 0 | 2655 | 135 | 0 |
| 2 | E | 1198 | 0 | 654 | 113 | 0 |
| 3 | F | 1177 | 0 | 670 | 156 | 0 |
| 4 | G | 1941 | 0 | 1954 | 114 | 0 |
| 4 | H | 1301 | 0 | 1330 | 46 | 0 |
| 4 | K | 1850 | 0 | 1862 | 84 | 0 |
| 4 | L | 1061 | 0 | 1072 | 20 | 0 |
| 4 | O | 1926 | 0 | 1936 | 86 | 0 |
| 4 | P | 1302 | 0 | 1328 | 27 | 0 |
| 4 | S | 1805 | 0 | 1811 | 72 | 0 |
| 4 | T | 1440 | 0 | 1476 | 46 | 0 |
| 5 | I | 1760 | 0 | 1756 | 74 | 0 |
| 5 | J | 1622 | 0 | 1623 | 89 | 0 |
| 5 | M | 1760 | 0 | 1756 | 84 | 0 |
| 5 | N | 1517 | 0 | 1507 | 65 | 0 |
| 5 | Q | 1760 | 0 | 1756 | 89 | 0 |
| 5 | R | 1488 | 0 | 1469 | 74 | 0 |
| 5 | U | 1760 | 0 | 1756 | 92 | 0 |
| 5 | V | 1630 | 0 | 1628 | 65 | 0 |
| All | All | 39098 | 0 | 38020 | 1633 | 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 21.

All (1633) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 4:K:47:ILE:HD12 | 4:K:260:LEU:HD12 | 1.46 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:220:ILE:HD11 | 1:C:313:ILE:HG21 | 1.43 | 0.96 |
| 5:V:152:LEU:HD12 | 5:V:161:LEU:HD11 | 1.57 | 0.85 |
| 4:G:248:LEU:HD12 | 4:G:252:MET:HB2 | 1.59 | 0.85 |
| 4:O:54:TYR:OH | 4:O:87:THR:HG22 | 1.78 | 0.83 |
| 3:F:21:DT:H2'' | 3:F:22:DT:H71 | 1.60 | 0.82 |
| 1:A:269:CYS:HA | 1:A:272:LEU:HD23 | 1.62 | 0.80 |
| 1:B:348:GLU:HA | 1:B:351:MET:HE2 | 1.62 | 0.80 |
| 3:F:5:DT:H2' | 3:F:6:DT:C6 | 2.17 | 0.79 |
| 1:C:305:LYS:HD2 | 3:F:15:DT:H3' | 1.63 | 0.79 |
| 3:F:4:DT:H2' | 3:F:5:DT:C6 | 2.17 | 0.79 |
| 4:S:245:THR:OG1 | 5:U:327:VAL:HG22 | 1.82 | 0.79 |
| 5:R:160:SER:HB2 | 5:R:186:LEU:HD11 | 1.66 | 0.78 |
| 3:F:18:DT:H2'' | 3:F:19:DT:OP2 | 1.81 | 0.78 |
| 4:T:145:LEU:HD12 | 4:T:208:GLN:HG3 | 1.64 | 0.78 |
| 1:D:34:ILE:HG21 | 1:D:158:ILE:HD12 | 1.65 | 0.77 |
| 3:F:10:DT:H1' | 3:F:11:DA:O5' | 1.84 | 0.77 |
| 5:U:168:THR:HG22 | 5:U:210:ARG:HG3 | 1.67 | 0.77 |
| 4:S:226:PHE:CE1 | 4:S:231:VAL:HG22 | 2.20 | 0.77 |
| 1:B:126:VAL:O | 1:B:130:ILE:HD12 | 1.85 | 0.76 |
| 3:F:30:DT:H2'' | 3:F:31:DT:H72 | 1.67 | 0.76 |
| 5:M:171:ASP:O | 5:M:173:THR:HG23 | 1.86 | 0.76 |
| 1:A:32:CYS:HA | 1:A:43:VAL:HG12 | 1.68 | 0.76 |
| 5:Q:144:ASP:O | 5:Q:148:THR:HG23 | 1.85 | 0.76 |
| 1:C:156:ASP:HB3 | 1:C:167:LEU:HD12 | 1.66 | 0.76 |
| 4:S:144:MET:SD | 5:U:300:THR:HG22 | 2.26 | 0.76 |
| 3:F:21:DT:C2' | 3:F:22:DT:H71 | 2.15 | 0.76 |
| 5:M:228:VAL:HG22 | 5:N:223:ARG:O | 1.86 | 0.76 |
| 3:F:33:DT:H2' | 3:F:34:DC:C6 | 2.21 | 0.75 |
| 5:U:149:MET:HE1 | 5:V:150:ILE:HD11 | 1.68 | 0.75 |
| 3:F:20:DT:H1' | 3:F:21:DT:O5' | 1.86 | 0.75 |
| 2:E:50:DA:H1' | 2:E:51:DT:O5' | 1.86 | 0.75 |
| 4:H:70:ILE:HG21 | 4:H:79:GLN:OE1 | 1.86 | 0.75 |
| 4:G:57:MET:HE1 | 4:G:86:SER:HB2 | 1.69 | 0.75 |
| 4:K:132:LEU:HD21 | 4:K:226:PHE:CE2 | 2.21 | 0.74 |
| 2:E:6:DC:H2'' | 2:E:7:DA:OP2 | 1.85 | 0.74 |
| 1:D:43:VAL:HG23 | 1:D:59:MET:HE1 | 1.70 | 0.74 |
| 3:F:33:DT:H2'' | 3:F:34:DC:C5' | 2.18 | 0.74 |
| 1:A:72:GLU:OE2 | 1:B:93:ILE:HG23 | 1.88 | 0.74 |
| 1:C:32:CYS:HA | 1:C:43:VAL:HG12 | 1.68 | 0.73 |
| 3:F:19:DT:H2'' | 3:F:20:DT:OP2 | 1.85 | 0.73 |
| 1:C:308:ARG:CD | 3:F:15:DT:H5'' | 2.17 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:17:DT:H2'' | 3:F:18:DT:OP2 | 1.85 | 0.73 |
| 4:K:266:PHE:CE1 | 5:N:229:LEU:HD22 | 2.23 | 0.73 |
| 1:D:148:LEU:HB3 | 1:D:300:VAL:HG12 | 1.70 | 0.73 |
| 2:E:6:DC:H1' | 2:E:7:DA:O5' | 1.89 | 0.73 |
| 5:Q:164:LEU:O | 5:Q:168:THR:HG23 | 1.87 | 0.72 |
| 3:F:49:DG:H2' | 3:F:49:DG:OP2 | 1.89 | 0.72 |
| 4:H:87:THR:HG21 | 4:H:216:VAL:HG11 | 1.72 | 0.72 |
| 4:K:245:THR:OG1 | 5:M:327:VAL:HG22 | 1.89 | 0.72 |
| 1:B:147:ILE:HD11 | 1:B:171:ALA:HB1 | 1.70 | 0.72 |
| 5:J:126:LEU:HD22 | 5:J:148:THR:HG21 | 1.70 | 0.72 |
| 3:F:1:DC:H1' | 3:F:2:DC:O4' | 1.90 | 0.72 |
| 5:R:130:TYR:C | 5:R:209:MET:HE1 | 2.15 | 0.71 |
| 3:F:37:DA:H1' | 3:F:38:DA:H5' | 1.72 | 0.71 |
| 1:B:141:LEU:HD11 | 1:B:145:GLU:O | 1.91 | 0.71 |
| 3:F:45:DT:H1' | 3:F:46:DA:H5' | 1.72 | 0.71 |
| 5:N:290:LEU:HD11 | 5:N:294:TYR:CZ | 2.25 | 0.71 |
| 1:C:157:LEU:HB3 | 1:C:166:ILE:HD12 | 1.73 | 0.71 |
| 3:F:46:DA:H1' | 3:F:47:DA:O5' | 1.91 | 0.70 |
| 3:F:57:DT:H2'' | 3:F:58:DA:OP2 | 1.89 | 0.70 |
| 5:M:124:ARG:HE | 5:M:193:LEU:HD12 | 1.55 | 0.70 |
| 2:E:43:DA:H2'' | 2:E:44:DA:OP2 | 1.90 | 0.70 |
| 2:E:52:DT:H1' | 2:E:53:DA:O5' | 1.92 | 0.70 |
| 3:F:42:DT:H2'' | 3:F:43:DT:OP2 | 1.90 | 0.70 |
| 1:B:128:LYS:HA | 1:B:131:ILE:HG12 | 1.72 | 0.70 |
| 3:F:4:DT:H2' | 3:F:5:DT:H6 | 1.55 | 0.70 |
| 5:Q:172:TYR:CD2 | 5:Q:214:ALA:HB1 | 2.27 | 0.70 |
| 2:E:30:DG:H2'' | 2:E:31:DT:OP2 | 1.91 | 0.70 |
| 2:E:52:DT:H2'' | 2:E:53:DA:OP2 | 1.92 | 0.70 |
| 1:B:231:LEU:O | 1:B:235:LEU:HD23 | 1.92 | 0.70 |
| 1:C:220:ILE:CD1 | 1:C:313:ILE:HG21 | 2.18 | 0.70 |
| 3:F:17:DT:H1' | 3:F:18:DT:O5' | 1.92 | 0.69 |
| 3:F:41:DG:H1' | 3:F:42:DT:O5' | 1.92 | 0.69 |
| 5:V:164:LEU:O | 5:V:168:THR:HG23 | 1.91 | 0.69 |
| 5:R:144:ASP:O | 5:R:148:THR:HG23 | 1.92 | 0.69 |
| 5:M:163:LYS:O | 5:M:167:THR:HG23 | 1.91 | 0.69 |
| 4:K:231:VAL:HA | 4:K:234:TYR:CE1 | 2.28 | 0.69 |
| 4:O:54:TYR:CE2 | 4:O:58:LEU:HD11 | 2.28 | 0.69 |
| 5:R:152:LEU:CD2 | 5:R:165:LEU:HD12 | 2.23 | 0.69 |
| 5:I:323:ASN:O | 5:I:327:VAL:HG23 | 1.92 | 0.69 |
| 3:F:5:DT:H2' | 3:F:6:DT:H6 | 1.57 | 0.68 |
| 4:O:11:THR:HG22 | 4:P:268:ILE:HG23 | 1.73 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:O:45:LEU:O | 4:O:49:LEU:HD23 | 1.93 | 0.68 |
| 4:K:138:ARG:O | 4:K:142:VAL:HG23 | 1.93 | 0.68 |
| 5:Q:149:MET:HE1 | 5:R:150:ILE:HD11 | 1.76 | 0.68 |
| 1:A:119:ALA:HB1 | 1:A:159:TYR:OH | 1.93 | 0.68 |
| 2:E:27:DG:H2'' | 2:E:28:DA:C8 | 2.28 | 0.68 |
| 5:U:183:THR:HG23 | 5:U:203:LEU:HD11 | 1.75 | 0.68 |
| 4:G:67:LEU:HD12 | 4:G:212:LEU:HD11 | 1.75 | 0.68 |
| 5:I:127:ILE:HD13 | 5:I:193:LEU:HD22 | 1.76 | 0.68 |
| 3:F:35:DC:H1' | 3:F:36:DT:O5' | 1.94 | 0.67 |
| 5:Q:126:LEU:HD11 | 5:Q:130:TYR:CE2 | 2.29 | 0.67 |
| 4:T:45:LEU:HD23 | 4:T:48:LYS:HE2 | 1.74 | 0.67 |
| 1:D:113:PHE:HB3 | 1:D:158:ILE:HG12 | 1.76 | 0.67 |
| 2:E:10:DC:H1' | 2:E:11:DG:O5' | 1.94 | 0.67 |
| 3:F:44:DT:H2'' | 3:F:45:DT:OP2 | 1.95 | 0.67 |
| 4:K:145:LEU:HD22 | 4:K:208:GLN:CG | 2.25 | 0.67 |
| 4:O:83:VAL:O | 4:O:87:THR:HG23 | 1.95 | 0.67 |
| 3:F:14:DT:H2'' | 3:F:15:DT:H71 | 1.77 | 0.67 |
| 3:F:29:DC:H1' | 3:F:30:DT:O5' | 1.95 | 0.67 |
| 5:M:323:ASN:O | 5:M:327:VAL:HG23 | 1.94 | 0.67 |
| 3:F:29:DC:C2' | 3:F:30:DT:H71 | 2.25 | 0.67 |
| 3:F:37:DA:H1' | 3:F:38:DA:C5' | 2.24 | 0.67 |
| 5:M:142:ILE:HD12 | 5:N:216:CYS:O | 1.94 | 0.67 |
| 4:S:35:ASN:O | 4:S:39:LEU:HD23 | 1.95 | 0.67 |
| 4:S:241:HIS:O | 5:U:327:VAL:HG21 | 1.95 | 0.67 |
| 5:U:290:LEU:HA | 5:U:293:MET:HE2 | 1.75 | 0.67 |
| 4:S:61:LEU:HB2 | 4:S:63:MET:HE1 | 1.76 | 0.67 |
| 1:A:311:GLU:HB2 | 1:A:315:ARG:HE | 1.60 | 0.66 |
| 2:E:47:DT:H1' | 2:E:48:DT:O5' | 1.94 | 0.66 |
| 3:F:6:DT:H2'' | 3:F:7:DA:C8 | 2.29 | 0.66 |
| 5:Q:168:THR:HB | 5:Q:214:ALA:HB2 | 1.75 | 0.66 |
| 5:U:146:VAL:HG13 | 5:V:149:MET:HE3 | 1.74 | 0.66 |
| 4:G:245:THR:OG1 | 5:I:327:VAL:HG22 | 1.95 | 0.66 |
| 5:U:149:MET:HE3 | 5:V:146:VAL:HG13 | 1.76 | 0.66 |
| 4:T:87:THR:HB | 4:T:216:VAL:HG11 | 1.78 | 0.66 |
| 1:A:221:TYR:O | 1:A:225:LEU:HD23 | 1.95 | 0.66 |
| 2:E:51:DT:H2'' | 2:E:52:DT:OP2 | 1.94 | 0.66 |
| 5:U:144:ASP:O | 5:U:148:THR:HG23 | 1.95 | 0.66 |
| 1:C:154:TYR:HB2 | 1:C:229:THR:HG22 | 1.76 | 0.66 |
| 1:D:33:TRP:CE3 | 1:D:43:VAL:HG11 | 2.30 | 0.66 |
| 4:G:138:ARG:O | 4:G:142:VAL:HG23 | 1.96 | 0.66 |
| 5:I:144:ASP:O | 5:I:148:THR:HG23 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:K:47:ILE:HD12 | 4:K:260:LEU:CD1 | 2.23 | 0.66 |
| 3:F:25:DT:H2'' | 3:F:26:DT:H71 | 1.77 | 0.66 |
| 3:F:51:DT:H2'' | 3:F:52:DT:OP2 | 1.94 | 0.66 |
| 2:E:4:DT:H2' | 2:E:5:DC:C6 | 2.31 | 0.66 |
| 5:N:158:TYR:CE2 | 5:N:193:LEU:HD21 | 2.30 | 0.65 |
| 4:T:234:TYR:CE2 | 4:T:238:LEU:HD11 | 2.30 | 0.65 |
| 1:A:254:VAL:HG22 | 1:A:287:ARG:HH11 | 1.60 | 0.65 |
| 1:C:231:LEU:HD13 | 1:C:234:ILE:HD11 | 1.76 | 0.65 |
| 2:E:20:DT:H2'' | 2:E:21:DT:OP2 | 1.95 | 0.65 |
| 5:M:116:MET:HA | 5:M:116:MET:HE3 | 1.78 | 0.65 |
| 5:N:126:LEU:HD11 | 5:N:144:ASP:HB3 | 1.78 | 0.65 |
| 3:F:47:DA:H1' | 3:F:48:DC:O5' | 1.95 | 0.65 |
| 4:K:71:PHE:HB3 | 4:K:142:VAL:HG22 | 1.77 | 0.65 |
| 1:C:219:TYR:O | 1:C:223:THR:HG23 | 1.95 | 0.65 |
| 4:G:49:LEU:HD22 | 5:I:282:LEU:HD13 | 1.79 | 0.65 |
| 2:E:17:DA:H2'' | 2:E:18:DC:OP2 | 1.96 | 0.65 |
| 3:F:33:DT:H2'' | 3:F:34:DC:H5' | 1.77 | 0.65 |
| 3:F:29:DC:H2'' | 3:F:30:DT:OP2 | 1.97 | 0.65 |
| 4:G:241:HIS:O | 5:I:327:VAL:HG21 | 1.96 | 0.65 |
| 4:O:125:PHE:HB3 | 4:O:132:LEU:HD22 | 1.78 | 0.65 |
| 1:A:316:GLN:OE1 | 1:A:337:ARG:HA | 1.97 | 0.65 |
| 3:F:21:DT:H2'' | 3:F:22:DT:OP2 | 1.95 | 0.65 |
| 4:O:266:PHE:CD2 | 5:Q:328:MET:HE2 | 2.32 | 0.65 |
| 1:B:248:THR:CG2 | 1:B:253:ILE:HD11 | 2.27 | 0.64 |
| 1:D:124:MET:HE3 | 5:N:139:GLU:HB2 | 1.79 | 0.64 |
| 3:F:25:DT:H2'' | 3:F:26:DT:OP2 | 1.98 | 0.64 |
| 4:H:106:MET:HE1 | 4:H:134:CYS:HB2 | 1.79 | 0.64 |
| 4:H:226:PHE:CE2 | 4:H:231:VAL:HG22 | 2.32 | 0.64 |
| 1:B:60:LEU:HA | 1:B:103:MET:O | 1.98 | 0.64 |
| 2:E:15:DA:H1' | 2:E:16:DA:H5' | 1.80 | 0.64 |
| 4:K:54:TYR:CE2 | 4:K:58:LEU:HD21 | 2.33 | 0.64 |
| 4:S:61:LEU:HD11 | 4:S:86:SER:CB | 2.28 | 0.64 |
| 2:E:6:DC:H2' | 2:E:6:DC:OP2 | 1.97 | 0.64 |
| 3:F:45:DT:H1' | 3:F:46:DA:C5' | 2.27 | 0.64 |
| 1:B:219:TYR:CE1 | 1:B:365:VAL:HG13 | 2.32 | 0.64 |
| 4:S:78:ARG:HA | 5:U:261:GLN:NE2 | 2.13 | 0.64 |
| 3:F:30:DT:H2'' | 3:F:31:DT:C7 | 2.27 | 0.64 |
| 5:Q:169:PHE:CE2 | 5:R:147:MET:HE3 | 2.33 | 0.64 |
| 4:T:67:LEU:HD13 | 4:T:209:TYR:CZ | 2.31 | 0.64 |
| 2:E:20:DT:H1' | 2:E:21:DT:O5' | 1.97 | 0.64 |
| 4:O:47:ILE:O | 4:O:51:LEU:HD23 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:GLU:HB3 | 1:A:311:GLU:OE1 | 1.97 | 0.64 |
| 5:I:182:GLN:O | 5:I:186:LEU:HD23 | 1.98 | 0.63 |
| 5:Q:149:MET:HE3 | 5:R:146:VAL:HG13 | 1.79 | 0.63 |
| 3:F:8:DA:H1' | 3:F:9:DT:C5' | 2.28 | 0.63 |
| 5:M:307:GLU:O | 5:M:311:VAL:HG22 | 1.97 | 0.63 |
| 1:B:345:LEU:HD23 | 1:B:348:GLU:OE1 | 1.98 | 0.63 |
| 4:G:71:PHE:HE2 | 4:G:212:LEU:HD21 | 1.64 | 0.63 |
| 4:G:91:ILE:HD12 | 4:G:216:VAL:HG12 | 1.80 | 0.63 |
| 2:E:16:DA:H2'' | 2:E:17:DA:OP2 | 1.97 | 0.63 |
| 5:U:164:LEU:O | 5:U:168:THR:HG23 | 1.98 | 0.63 |
| 3:F:34:DC:H2'' | 3:F:35:DC:C6 | 2.34 | 0.63 |
| 4:K:54:TYR:O | 4:K:58:LEU:HD23 | 1.99 | 0.63 |
| 5:I:216:CYS:O | 5:J:142:ILE:HD11 | 1.98 | 0.63 |
| 5:N:175:ARG:HD3 | 5:N:203:LEU:HD21 | 1.80 | 0.63 |
| 1:A:157:LEU:HB3 | 1:A:166:ILE:HD12 | 1.80 | 0.63 |
| 1:B:257:LEU:HD11 | 1:B:268:LYS:O | 1.99 | 0.63 |
| 4:G:232:PHE:CD2 | 4:K:33:LEU:HD21 | 2.34 | 0.63 |
| 1:A:135:ILE:HG22 | 1:A:226:LEU:HD13 | 1.80 | 0.63 |
| 4:S:147:ARG:HD2 | 5:U:300:THR:HG23 | 1.81 | 0.63 |
| 1:C:24:MET:HB3 | 1:D:203:THR:HG21 | 1.80 | 0.62 |
| 1:C:227:TYR:O | 1:C:231:LEU:HD23 | 1.99 | 0.62 |
| 5:U:161:LEU:HD11 | 5:U:189:ALA:HB3 | 1.80 | 0.62 |
| 2:E:33:DA:H2'' | 2:E:34:DA:OP2 | 2.00 | 0.62 |
| 4:G:109:VAL:HG23 | 5:I:257:LEU:HD22 | 1.81 | 0.62 |
| 5:N:128:HIS:NE2 | 5:N:132:LEU:HD11 | 2.14 | 0.62 |
| 2:E:39:DA:H1' | 2:E:40:DA:O5' | 1.99 | 0.62 |
| 3:F:25:DT:H1' | 3:F:26:DT:O5' | 2.00 | 0.62 |
| 4:P:234:TYR:CZ | 4:P:238:LEU:HD11 | 2.34 | 0.62 |
| 5:I:168:THR:HG22 | 5:I:210:ARG:HG3 | 1.82 | 0.62 |
| 4:G:67:LEU:HD11 | 4:G:208:GLN:HB3 | 1.81 | 0.62 |
| 5:M:183:THR:O | 5:M:187:LEU:HD23 | 1.99 | 0.62 |
| 1:C:227:TYR:CZ | 1:C:231:LEU:HD21 | 2.35 | 0.62 |
| 2:E:56:DT:H1' | 2:E:57:DG:O5' | 1.99 | 0.62 |
| 2:E:5:DC:H2'' | 2:E:6:DC:OP2 | 1.99 | 0.62 |
| 4:G:111:THR:HG22 | 5:I:254:ILE:CD1 | 2.30 | 0.62 |
| 1:C:113:PHE:HB3 | 1:C:158:ILE:HG22 | 1.81 | 0.62 |
| 2:E:7:DA:H1' | 2:E:8:DA:O5' | 2.00 | 0.62 |
| 4:T:91:ILE:HD13 | 4:T:217:GLU:HA | 1.82 | 0.62 |
| 5:Q:191:ARG:HH12 | 5:Q:194:LEU:HD22 | 1.65 | 0.62 |
| 1:A:24:MET:CE | 1:B:203:THR:HG21 | 2.29 | 0.61 |
| 1:A:227:TYR:CZ | 1:A:231:LEU:HD11 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:8:DA:H1' | 3:F:9:DT:O5' | 1.99 | 0.61 |
| 4:K:231:VAL:HA | 4:K:234:TYR:CD1 | 2.34 | 0.61 |
| 5:U:158:TYR:CD1 | 5:U:189:ALA:HB1 | 2.35 | 0.61 |
| 1:C:267:VAL:HG12 | 1:C:287:ARG:HG2 | 1.82 | 0.61 |
| 2:E:44:DA:H2'' | 2:E:45:DA:OP2 | 2.01 | 0.61 |
| 5:I:142:ILE:HD12 | 5:J:216:CYS:O | 2.00 | 0.61 |
| 4:K:144:MET:CE | 5:M:304:THR:HG21 | 2.30 | 0.61 |
| 3:F:51:DT:C6 | 3:F:52:DT:H72 | 2.35 | 0.61 |
| 5:Q:228:VAL:HG22 | 5:R:223:ARG:O | 2.00 | 0.61 |
| 5:U:158:TYR:HD1 | 5:U:189:ALA:HB1 | 1.64 | 0.61 |
| 1:A:148:LEU:HB2 | 1:A:300:VAL:HG12 | 1.82 | 0.61 |
| 1:B:105:ILE:HG22 | 1:B:107:PRO:HD3 | 1.81 | 0.61 |
| 1:C:308:ARG:HD3 | 3:F:15:DT:H5'' | 1.81 | 0.61 |
| 2:E:42:DA:H2'' | 2:E:43:DA:OP2 | 2.01 | 0.61 |
| 1:B:147:ILE:HD12 | 1:B:172:TYR:O | 2.01 | 0.61 |
| 2:E:35:DA:H1' | 2:E:36:DC:C5' | 2.31 | 0.61 |
| 1:B:147:ILE:HD13 | 1:B:173:ILE:HD13 | 1.83 | 0.61 |
| 1:D:32:CYS:HA | 1:D:43:VAL:HG12 | 1.83 | 0.61 |
| 4:G:45:LEU:O | 4:G:49:LEU:HD23 | 2.01 | 0.61 |
| 1:A:153:MET:HE3 | 1:A:241:PHE:O | 2.01 | 0.60 |
| 5:I:122:ALA:C | 5:I:148:THR:HG22 | 2.26 | 0.60 |
| 4:K:144:MET:HE2 | 5:M:304:THR:HG21 | 1.83 | 0.60 |
| 1:A:149:ILE:HG22 | 1:A:221:TYR:OH | 2.01 | 0.60 |
| 1:C:255:ARG:HH22 | 3:F:6:DT:H3' | 1.65 | 0.60 |
| 4:G:226:PHE:CE2 | 4:G:231:VAL:HG22 | 2.35 | 0.60 |
| 4:O:226:PHE:CE2 | 4:O:231:VAL:HG22 | 2.36 | 0.60 |
| 5:U:146:VAL:HG11 | 5:V:169:PHE:CZ | 2.37 | 0.60 |
| 1:B:138:ILE:HD13 | 1:B:226:LEU:HD21 | 1.81 | 0.60 |
| 1:B:342:LEU:HD11 | 5:J:191:ARG:HB2 | 1.83 | 0.60 |
| 4:H:92:HIS:NE2 | 4:H:99:VAL:HG12 | 2.16 | 0.60 |
| 5:N:149:MET:HE3 | 5:N:149:MET:O | 2.01 | 0.60 |
| 4:O:47:ILE:HG22 | 4:O:260:LEU:CD1 | 2.31 | 0.60 |
| 1:C:114:ARG:NH1 | 1:C:119:ALA:HA | 2.17 | 0.60 |
| 1:C:244:ILE:O | 1:C:244:ILE:HG22 | 2.01 | 0.60 |
| 4:O:9:VAL:HG21 | 4:O:28:LEU:HD21 | 1.82 | 0.60 |
| 3:F:13:DA:C2' | 3:F:14:DT:H71 | 2.31 | 0.60 |
| 4:H:79:GLN:NE2 | 4:H:83:VAL:HG21 | 2.16 | 0.60 |
| 4:T:256:THR:HG23 | 4:T:259:LEU:HD12 | 1.84 | 0.60 |
| 4:G:171:GLY:HA2 | 4:S:231:VAL:HG21 | 1.82 | 0.60 |
| 5:Q:272:CYS:O | 5:Q:278:LEU:HD11 | 2.02 | 0.60 |
| 5:U:290:LEU:HG | 5:U:294:TYR:HE2 | 1.67 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:R:119:TYR:HB3 | 5:R:151:PHE:HB2 | 1.84 | 0.60 |
| 1:C:308:ARG:NE | 3:F:15:DT:H5'' | 2.17 | 0.60 |
| 1:D:155:VAL:HG12 | 1:D:229:THR:HG21 | 1.83 | 0.60 |
| 5:I:146:VAL:HG22 | 5:J:149:MET:SD | 2.42 | 0.60 |
| 5:V:148:THR:O | 5:V:152:LEU:HD23 | 2.01 | 0.60 |
| 1:B:267:VAL:HG22 | 1:B:287:ARG:HG2 | 1.83 | 0.59 |
| 3:F:9:DT:H2'' | 3:F:10:DT:H71 | 1.85 | 0.59 |
| 3:F:51:DT:OP2 | 3:F:51:DT:H6 | 1.85 | 0.59 |
| 1:C:153:MET:HE1 | 1:C:294:PHE:CD2 | 2.38 | 0.59 |
| 4:L:118:ILE:HD12 | 5:N:247:LEU:HD13 | 1.84 | 0.59 |
| 1:B:108:ILE:HG12 | 1:B:111:GLU:HB2 | 1.83 | 0.59 |
| 3:F:13:DA:H1' | 3:F:14:DT:O5' | 2.02 | 0.59 |
| 4:S:274:ILE:HD11 | 5:U:227:ILE:HG22 | 1.84 | 0.59 |
| 3:F:14:DT:H1' | 3:F:15:DT:O5' | 2.01 | 0.59 |
| 4:H:226:PHE:CZ | 4:H:231:VAL:HG22 | 2.37 | 0.59 |
| 5:I:181:VAL:O | 5:I:184:ASP:OD1 | 2.21 | 0.59 |
| 1:B:32:CYS:HA | 1:B:43:VAL:HG12 | 1.85 | 0.59 |
| 4:K:125:PHE:HB3 | 4:K:132:LEU:HD22 | 1.85 | 0.59 |
| 2:E:34:DA:H1' | 2:E:35:DA:H5' | 1.84 | 0.59 |
| 5:J:263:ILE:O | 5:J:263:ILE:HG22 | 2.02 | 0.59 |
| 3:F:36:DT:H1' | 3:F:37:DA:O5' | 2.03 | 0.59 |
| 4:H:87:THR:CG2 | 4:H:216:VAL:HG11 | 2.32 | 0.59 |
| 1:A:34:ILE:HG13 | 1:A:43:VAL:HG11 | 1.85 | 0.59 |
| 2:E:41:DA:H1' | 2:E:42:DA:O5' | 2.01 | 0.59 |
| 1:C:155:VAL:CG2 | 1:C:166:ILE:HD11 | 2.33 | 0.59 |
| 3:F:52:DT:H2'' | 3:F:53:DG:OP2 | 2.02 | 0.59 |
| 5:U:222:MET:HE1 | 5:U:226:LYS:HE3 | 1.85 | 0.59 |
| 1:A:153:MET:HE3 | 1:A:241:PHE:C | 2.27 | 0.58 |
| 4:G:111:THR:HG22 | 5:I:254:ILE:HD11 | 1.85 | 0.58 |
| 4:O:58:LEU:C | 4:O:63:MET:HE1 | 2.28 | 0.58 |
| 5:Q:246:LEU:HD12 | 5:Q:249:GLU:OE2 | 2.03 | 0.58 |
| 1:A:121:GLU:HB3 | 1:A:127:LEU:HD21 | 1.84 | 0.58 |
| 4:K:207:THR:OG1 | 5:M:293:MET:HG3 | 2.03 | 0.58 |
| 4:L:72:ARG:HH12 | 4:L:142:VAL:HG13 | 1.67 | 0.58 |
| 3:F:50:DT:H2'' | 3:F:51:DT:OP2 | 2.02 | 0.58 |
| 4:H:234:TYR:CE2 | 4:H:238:LEU:HD11 | 2.39 | 0.58 |
| 2:E:21:DT:H2'' | 2:E:22:DT:OP2 | 2.03 | 0.58 |
| 4:G:226:PHE:CZ | 4:G:231:VAL:HG22 | 2.39 | 0.58 |
| 4:G:235:CYS:HA | 4:G:238:LEU:HD12 | 1.84 | 0.58 |
| 4:G:166:ILE:HD11 | 5:U:244:GLU:HB2 | 1.83 | 0.58 |
| 1:C:221:TYR:CE2 | 1:C:225:LEU:HD11 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:246:LEU:HD12 | 5:M:249:GLU:OE2 | 2.03 | 0.58 |
| 5:Q:323:ASN:O | 5:Q:327:VAL:HG23 | 2.04 | 0.58 |
| 4:S:61:LEU:HD21 | 4:S:86:SER:OG | 2.03 | 0.58 |
| 1:D:221:TYR:HA | 1:D:293:PHE:CE1 | 2.39 | 0.58 |
| 3:F:16:DT:H1' | 3:F:17:DT:O5' | 2.04 | 0.58 |
| 1:C:212:ASP:O | 1:C:216:GLN:OE1 | 2.21 | 0.58 |
| 1:D:220:ILE:HG23 | 1:D:347:TRP:NE1 | 2.19 | 0.58 |
| 5:U:122:ALA:C | 5:U:148:THR:HG22 | 2.29 | 0.58 |
| 4:S:226:PHE:HE1 | 4:S:231:VAL:HG22 | 1.65 | 0.58 |
| 1:A:283:MET:HE2 | 1:A:283:MET:HA | 1.86 | 0.57 |
| 1:C:223:THR:HG21 | 1:C:347:TRP:HZ2 | 1.69 | 0.57 |
| 4:G:266:PHE:HD1 | 5:I:328:MET:HE2 | 1.68 | 0.57 |
| 5:N:122:ALA:O | 5:N:126:LEU:HD13 | 2.04 | 0.57 |
| 5:U:152:LEU:HG | 5:U:165:LEU:HD11 | 1.84 | 0.57 |
| 1:B:286:PRO:O | 1:B:290:THR:HG23 | 2.04 | 0.57 |
| 3:F:29:DC:H2' | 3:F:30:DT:H71 | 1.86 | 0.57 |
| 1:B:148:LEU:HD13 | 1:B:300:VAL:HG12 | 1.86 | 0.57 |
| 4:L:57:MET:HE1 | 4:L:90:PHE:CB | 2.33 | 0.57 |
| 1:B:307:LYS:CE | 2:E:18:DC:H5'' | 2.34 | 0.57 |
| 3:F:35:DC:H2'' | 3:F:36:DT:H71 | 1.84 | 0.57 |
| 5:Q:149:MET:HE3 | 5:R:146:VAL:CG1 | 2.35 | 0.57 |
| 1:D:138:ILE:HD12 | 1:D:222:ARG:HB3 | 1.86 | 0.57 |
| 2:E:25:DG:H1' | 2:E:26:DA:C5' | 2.34 | 0.57 |
| 3:F:20:DT:OP2 | 3:F:20:DT:H2' | 2.05 | 0.57 |
| 3:F:28:DA:H2'' | 3:F:29:DC:OP2 | 2.05 | 0.57 |
| 4:G:92:HIS:HB3 | 4:G:102:PHE:HZ | 1.70 | 0.57 |
| 4:G:171:GLY:N | 4:S:231:VAL:HG11 | 2.19 | 0.57 |
| 1:B:155:VAL:HG21 | 1:B:166:ILE:HD11 | 1.85 | 0.57 |
| 1:B:307:LYS:HE3 | 2:E:18:DC:H5'' | 1.85 | 0.57 |
| 4:K:36:LEU:O | 4:K:40:GLU:OE1 | 2.21 | 0.57 |
| 4:T:235:CYS:O | 4:T:239:THR:HG23 | 2.05 | 0.57 |
| 4:H:144:MET:SD | 5:J:304:THR:OG1 | 2.61 | 0.57 |
| 4:S:68:LEU:HA | 4:S:145:LEU:HD23 | 1.87 | 0.57 |
| 5:V:127:ILE:HD11 | 5:V:152:LEU:HD21 | 1.87 | 0.57 |
| 1:D:75:LYS:HZ3 | 1:D:79:ARG:HB2 | 1.68 | 0.57 |
| 1:D:225:LEU:O | 1:D:229:THR:HG23 | 2.05 | 0.57 |
| 4:K:161:ASN:HB3 | 4:K:164:VAL:HG12 | 1.87 | 0.57 |
| 1:B:308:ARG:NH2 | 2:E:18:DC:H2' | 2.20 | 0.57 |
| 4:O:56:ALA:O | 4:O:60:THR:HG23 | 2.04 | 0.57 |
| 5:Q:152:LEU:HD23 | 5:Q:165:LEU:HD13 | 1.87 | 0.57 |
| 1:A:34:ILE:HG22 | 1:A:35:HIS:CE1 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:22:ILE:HG21 | 5:J:295:TYR:CE1 | 2.40 | 0.57 |
| 5:R:178:MET:HE2 | 5:R:183:THR:HA | 1.87 | 0.57 |
| 2:E:50:DA:H1' | 2:E:51:DT:C5' | 2.35 | 0.56 |
| 3:F:13:DA:H2'' | 3:F:14:DT:H71 | 1.87 | 0.56 |
| 3:F:56:DA:H2'' | 3:F:57:DT:OP2 | 2.04 | 0.56 |
| 5:R:245:GLU:O | 5:R:249:GLU:OE1 | 2.23 | 0.56 |
| 1:A:254:VAL:HG22 | 1:A:287:ARG:NH1 | 2.20 | 0.56 |
| 1:B:250:ILE:HA | 1:B:253:ILE:HD12 | 1.87 | 0.56 |
| 4:K:63:MET:SD | 4:K:63:MET:O | 2.63 | 0.56 |
| 1:A:282:VAL:HG21 | 1:A:357:TYR:CE1 | 2.40 | 0.56 |
| 2:E:35:DA:H1' | 2:E:36:DC:H5' | 1.88 | 0.56 |
| 3:F:9:DT:C2' | 3:F:10:DT:H71 | 2.36 | 0.56 |
| 3:F:35:DC:C2' | 3:F:36:DT:H71 | 2.35 | 0.56 |
| 5:I:146:VAL:HG11 | 5:J:169:PHE:HZ | 1.69 | 0.56 |
| 5:U:160:SER:O | 5:U:164:LEU:HD23 | 2.05 | 0.56 |
| 5:I:146:VAL:HG11 | 5:J:169:PHE:CZ | 2.40 | 0.56 |
| 4:O:36:LEU:O | 4:O:40:GLU:OE1 | 2.23 | 0.56 |
| 1:A:105:ILE:HG22 | 1:A:107:PRO:HD3 | 1.88 | 0.56 |
| 1:B:101:GLU:HG3 | 1:B:103:MET:HE3 | 1.88 | 0.56 |
| 3:F:19:DT:H1' | 3:F:20:DT:O5' | 2.06 | 0.56 |
| 3:F:30:DT:OP2 | 3:F:30:DT:H2' | 2.06 | 0.56 |
| 5:J:241:THR:HG23 | 5:J:313:ASN:HD22 | 1.70 | 0.56 |
| 5:N:153:LEU:HA | 5:N:162:PHE:CZ | 2.40 | 0.56 |
| 5:R:178:MET:HE1 | 5:R:186:LEU:HG | 1.86 | 0.56 |
| 1:D:44:THR:HG23 | 1:D:44:THR:O | 2.05 | 0.56 |
| 2:E:25:DG:H1' | 2:E:26:DA:O5' | 2.06 | 0.56 |
| 2:E:13:DT:H2'' | 2:E:14:DA:H8 | 1.70 | 0.56 |
| 2:E:54:DA:H2'' | 2:E:55:DA:C8 | 2.39 | 0.56 |
| 4:K:145:LEU:HD22 | 4:K:208:GLN:HG3 | 1.87 | 0.56 |
| 5:U:153:LEU:HD23 | 5:V:153:LEU:HD23 | 1.88 | 0.56 |
| 1:A:135:ILE:HG22 | 1:A:226:LEU:CD1 | 2.35 | 0.56 |
| 5:N:159:HIS:HD2 | 5:N:162:PHE:CE2 | 2.24 | 0.56 |
| 4:T:54:TYR:CE1 | 4:T:87:THR:HG23 | 2.40 | 0.56 |
| 1:B:174:ILE:HG23 | 1:B:174:ILE:O | 2.06 | 0.56 |
| 2:E:15:DA:H1' | 2:E:16:DA:C5' | 2.36 | 0.56 |
| 4:G:234:TYR:CE2 | 4:G:238:LEU:HD11 | 2.40 | 0.56 |
| 4:L:71:PHE:CE1 | 4:L:141:ILE:HG21 | 2.41 | 0.56 |
| 5:M:228:VAL:C | 5:M:229:LEU:HD22 | 2.31 | 0.56 |
| 5:I:126:LEU:HD11 | 5:I:130:TYR:CZ | 2.41 | 0.56 |
| 5:M:254:ILE:HD13 | 5:M:257:LEU:HD12 | 1.88 | 0.56 |
| 5:N:175:ARG:CD | 5:N:203:LEU:HD21 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:R:131:SER:N | 5:R:209:MET:HE1 | 2.21 | 0.56 |
| 1:A:91:LYS:HZ3 | 1:B:199:TRP:CD1 | 2.24 | 0.55 |
| 2:E:6:DC:H1' | 2:E:7:DA:C5' | 2.36 | 0.55 |
| 5:I:175:ARG:HD2 | 5:I:175:ARG:O | 2.06 | 0.55 |
| 5:J:122:ALA:C | 5:J:148:THR:HG22 | 2.31 | 0.55 |
| 3:F:19:DT:C6 | 3:F:20:DT:H72 | 2.41 | 0.55 |
| 4:K:204:VAL:O | 4:K:208:GLN:OE1 | 2.25 | 0.55 |
| 1:D:8:ILE:HD12 | 1:D:18:LEU:O | 2.05 | 0.55 |
| 4:P:85:PHE:HZ | 4:P:104:ASN:HA | 1.70 | 0.55 |
| 5:R:122:ALA:C | 5:R:148:THR:HG22 | 2.31 | 0.55 |
| 1:C:34:ILE:HG22 | 1:C:115:SER:HB2 | 1.87 | 0.55 |
| 1:C:349:ASN:O | 1:C:353:GLU:OE1 | 2.24 | 0.55 |
| 1:D:103:MET:HE3 | 1:D:168:PRO:HD3 | 1.87 | 0.55 |
| 2:E:55:DA:H2'' | 2:E:56:DT:OP2 | 2.07 | 0.55 |
| 5:N:113:LEU:HD23 | 5:N:113:LEU:H | 1.72 | 0.55 |
| 4:T:103:THR:HG22 | 4:T:106:MET:SD | 2.47 | 0.55 |
| 1:D:364:ASN:OD1 | 1:D:365:VAL:HG23 | 2.07 | 0.55 |
| 2:E:20:DT:OP1 | 2:E:20:DT:H3' | 2.06 | 0.55 |
| 3:F:9:DT:H1' | 3:F:10:DT:O5' | 2.07 | 0.55 |
| 4:K:249:ARG:NH2 | 5:M:331:ILE:HG22 | 2.22 | 0.55 |
| 4:O:47:ILE:HG22 | 4:O:260:LEU:HD12 | 1.88 | 0.55 |
| 4:P:109:VAL:CG1 | 4:P:133:LEU:HD11 | 2.37 | 0.55 |
| 4:S:47:ILE:O | 4:S:51:LEU:HD23 | 2.07 | 0.55 |
| 1:B:267:VAL:HG23 | 1:B:285:PRO:O | 2.07 | 0.55 |
| 5:J:144:ASP:O | 5:J:148:THR:HG23 | 2.07 | 0.55 |
| 5:U:298:ALA:HB1 | 5:V:227:ILE:HG21 | 1.88 | 0.55 |
| 1:A:119:ALA:HB3 | 1:A:233:ALA:O | 2.07 | 0.55 |
| 1:C:225:LEU:O | 1:C:229:THR:HG23 | 2.07 | 0.55 |
| 5:J:203:LEU:HA | 5:J:206:VAL:HG22 | 1.89 | 0.55 |
| 4:O:44:THR:HG22 | 5:Q:290:LEU:CD1 | 2.36 | 0.55 |
| 2:E:35:DA:H1' | 2:E:36:DC:O5' | 2.07 | 0.55 |
| 3:F:53:DG:H2'' | 3:F:54:DG:OP2 | 2.07 | 0.55 |
| 3:F:54:DG:H2'' | 3:F:55:DA:OP2 | 2.05 | 0.55 |
| 2:E:16:DA:H1' | 2:E:17:DA:O5' | 2.07 | 0.55 |
| 5:Q:325:PHE:O | 5:Q:329:GLU:OE1 | 2.25 | 0.55 |
| 1:B:60:LEU:HD13 | 1:B:104:LEU:HA | 1.90 | 0.54 |
| 1:D:203:THR:HG22 | 1:D:204:ALA:H | 1.71 | 0.54 |
| 4:G:141:ILE:HD11 | 4:G:212:LEU:HD23 | 1.89 | 0.54 |
| 4:K:44:THR:HG23 | 5:M:290:LEU:HD13 | 1.90 | 0.54 |
| 4:O:165:ARG:O | 4:O:169:THR:HG23 | 2.07 | 0.54 |
| 1:C:299:TRP:CD2 | 1:C:309:TYR:HB2 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:71:PHE:CE2 | 4:G:212:LEU:HD21 | 2.43 | 0.54 |
| 4:L:68:LEU:HD12 | 4:L:71:PHE:HB2 | 1.89 | 0.54 |
| 4:T:114:ASN:HD22 | 5:V:311:VAL:HG11 | 1.72 | 0.54 |
| 4:T:214:LEU:HD23 | 4:T:217:GLU:OE2 | 2.08 | 0.54 |
| 1:A:72:GLU:OE1 | 1:B:24:MET:HG3 | 2.08 | 0.54 |
| 2:E:43:DA:H1' | 2:E:44:DA:O5' | 2.08 | 0.54 |
| 5:U:149:MET:HE1 | 5:V:150:ILE:CD1 | 2.37 | 0.54 |
| 3:F:23:DG:H2'' | 3:F:24:DT:OP2 | 2.08 | 0.54 |
| 4:K:91:ILE:HD13 | 4:K:217:GLU:HA | 1.90 | 0.54 |
| 4:O:259:LEU:HD22 | 5:Q:331:ILE:HD11 | 1.88 | 0.54 |
| 4:S:47:ILE:HG21 | 5:U:294:TYR:OH | 2.07 | 0.54 |
| 3:F:16:DT:C2' | 3:F:17:DT:H72 | 2.37 | 0.54 |
| 3:F:33:DT:H2' | 3:F:34:DC:H6 | 1.70 | 0.54 |
| 4:G:54:TYR:CZ | 4:G:58:LEU:HD11 | 2.43 | 0.54 |
| 4:O:98:LEU:HG | 4:O:99:VAL:HG23 | 1.88 | 0.54 |
| 4:O:235:CYS:HA | 4:O:238:LEU:HD12 | 1.89 | 0.54 |
| 5:Q:142:ILE:HA | 5:Q:145:VAL:HG22 | 1.88 | 0.54 |
| 3:F:32:DC:H2'' | 3:F:33:DT:OP2 | 2.07 | 0.54 |
| 4:O:125:PHE:CE1 | 4:O:134:CYS:HB3 | 2.43 | 0.54 |
| 4:S:80:ILE:O | 4:S:84:VAL:HG23 | 2.08 | 0.54 |
| 5:V:158:TYR:CE1 | 5:V:189:ALA:HB1 | 2.42 | 0.54 |
| 1:A:46:PRO:HG3 | 1:A:60:LEU:HD11 | 1.90 | 0.54 |
| 1:C:25:ARG:O | 1:D:203:THR:HG23 | 2.07 | 0.54 |
| 2:E:14:DA:H2'' | 2:E:15:DA:O5' | 2.08 | 0.54 |
| 3:F:23:DG:C2' | 3:F:24:DT:H71 | 2.37 | 0.54 |
| 4:G:88:LEU:HD12 | 4:G:102:PHE:HE2 | 1.71 | 0.54 |
| 4:O:32:ASP:O | 4:O:36:LEU:HD23 | 2.08 | 0.54 |
| 4:O:70:ILE:HG23 | 4:O:79:GLN:OE1 | 2.07 | 0.54 |
| 1:A:122:HIS:CE1 | 1:A:277:VAL:HG13 | 2.43 | 0.54 |
| 2:E:42:DA:H1' | 2:E:43:DA:O5' | 2.08 | 0.54 |
| 3:F:8:DA:H1' | 3:F:9:DT:H5' | 1.90 | 0.54 |
| 5:J:164:LEU:O | 5:J:168:THR:HG23 | 2.08 | 0.54 |
| 4:K:222:HIS:CE1 | 4:K:238:LEU:HD23 | 2.43 | 0.54 |
| 1:D:343:HIS:O | 1:D:346:ASP:OD1 | 2.26 | 0.54 |
| 5:I:153:LEU:HD23 | 5:J:153:LEU:HD23 | 1.90 | 0.54 |
| 5:J:119:TYR:HB3 | 5:J:151:PHE:HB2 | 1.90 | 0.54 |
| 1:C:114:ARG:NH1 | 1:C:115:SER:O | 2.41 | 0.53 |
| 3:F:18:DT:C6 | 3:F:19:DT:H72 | 2.43 | 0.53 |
| 4:L:55:MET:HB2 | 5:N:281:LEU:HD13 | 1.89 | 0.53 |
| 4:O:13:THR:HG23 | 4:P:266:PHE:HD2 | 1.71 | 0.53 |
| 1:B:155:VAL:HG12 | 1:B:229:THR:HG21 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:255:ARG:NH2 | 3:F:6:DT:H3' | 2.22 | 0.53 |
| 1:D:94:LEU:HD23 | 1:D:94:LEU:H | 1.73 | 0.53 |
| 1:D:135:ILE:HD12 | 1:D:138:ILE:HD11 | 1.90 | 0.53 |
| 3:F:23:DG:H2'' | 3:F:24:DT:H71 | 1.89 | 0.53 |
| 3:F:30:DT:C2' | 3:F:31:DT:H72 | 2.36 | 0.53 |
| 3:F:48:DC:H2'' | 3:F:49:DG:OP2 | 2.07 | 0.53 |
| 4:G:54:TYR:CE2 | 4:G:58:LEU:HD11 | 2.43 | 0.53 |
| 4:K:237:SER:HB3 | 4:K:243:LEU:HD22 | 1.89 | 0.53 |
| 5:M:290:LEU:HA | 5:M:293:MET:HE2 | 1.90 | 0.53 |
| 4:G:67:LEU:HD13 | 4:G:209:TYR:CE1 | 2.42 | 0.53 |
| 1:B:308:ARG:CZ | 2:E:18:DC:H2' | 2.39 | 0.53 |
| 4:L:68:LEU:HD13 | 4:L:145:LEU:HB2 | 1.90 | 0.53 |
| 4:O:11:THR:HG21 | 5:R:302:PHE:CE2 | 2.43 | 0.53 |
| 5:U:302:PHE:HE1 | 5:U:318:ILE:HD13 | 1.73 | 0.53 |
| 5:I:298:ALA:HB1 | 5:J:227:ILE:HG21 | 1.90 | 0.53 |
| 5:Q:187:LEU:HA | 5:Q:190:VAL:HG22 | 1.91 | 0.53 |
| 1:D:203:THR:HG22 | 1:D:204:ALA:N | 2.24 | 0.53 |
| 5:N:158:TYR:CE1 | 5:N:189:ALA:HB1 | 2.43 | 0.53 |
| 4:T:222:HIS:HB3 | 4:T:234:TYR:CE1 | 2.44 | 0.53 |
| 1:A:196:GLU:OE1 | 1:A:198:PRO:HD2 | 2.08 | 0.53 |
| 1:A:202:ILE:HD12 | 1:B:44:THR:HG21 | 1.91 | 0.53 |
| 1:B:250:ILE:HD13 | 1:B:294:PHE:CE2 | 2.44 | 0.53 |
| 1:D:157:LEU:HD21 | 1:D:164:ALA:HB1 | 1.90 | 0.53 |
| 2:E:48:DT:H1' | 2:E:49:DA:C5' | 2.38 | 0.53 |
| 5:U:142:ILE:O | 5:U:146:VAL:HG23 | 2.09 | 0.53 |
| 5:V:158:TYR:CD1 | 5:V:189:ALA:HB1 | 2.44 | 0.53 |
| 1:C:345:LEU:HA | 1:C:348:GLU:HG3 | 1.91 | 0.53 |
| 3:F:37:DA:H2'' | 3:F:38:DA:OP2 | 2.09 | 0.53 |
| 5:J:158:TYR:CE1 | 5:J:189:ALA:HB1 | 2.44 | 0.53 |
| 4:K:22:ILE:HG22 | 5:N:295:TYR:CZ | 2.44 | 0.53 |
| 4:K:144:MET:O | 5:M:300:THR:HG21 | 2.08 | 0.53 |
| 5:M:217:PHE:CE1 | 5:N:143:SER:HB2 | 2.44 | 0.53 |
| 4:S:91:ILE:HD12 | 4:S:216:VAL:HG12 | 1.91 | 0.53 |
| 2:E:25:DG:H1' | 2:E:26:DA:H5' | 1.91 | 0.53 |
| 4:G:174:LYS:HE3 | 5:U:252:GLU:HA | 1.90 | 0.53 |
| 5:J:168:THR:HB | 5:J:214:ALA:HB2 | 1.90 | 0.53 |
| 1:A:72:GLU:OE2 | 1:B:93:ILE:HA | 2.09 | 0.53 |
| 4:G:108:PHE:CZ | 5:I:263:ILE:HD12 | 2.44 | 0.53 |
| 4:G:234:TYR:CZ | 4:G:238:LEU:HD11 | 2.44 | 0.53 |
| 4:H:62:GLU:O | 4:H:62:GLU:CD | 2.52 | 0.53 |
| 5:N:123:ALA:O | 5:N:127:ILE:HG12 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:81:LEU:HD21 | 1:C:141:LEU:HD23 | 1.91 | 0.52 |
| 1:D:78:TYR:OH | 1:D:101:GLU:HG2 | 2.09 | 0.52 |
| 2:E:16:DA:H1' | 2:E:17:DA:C5' | 2.39 | 0.52 |
| 5:N:160:SER:O | 5:N:164:LEU:HD13 | 2.09 | 0.52 |
| 4:O:214:LEU:HD21 | 5:Q:297:ALA:HB1 | 1.90 | 0.52 |
| 5:Q:132:LEU:HD12 | 5:Q:303:TYR:CG | 2.44 | 0.52 |
| 1:D:124:MET:HB2 | 1:D:358:PHE:HE1 | 1.75 | 0.52 |
| 1:D:243:VAL:HG12 | 1:D:245:ALA:H | 1.73 | 0.52 |
| 2:E:13:DT:H2'' | 2:E:14:DA:C8 | 2.44 | 0.52 |
| 4:G:63:MET:O | 4:G:63:MET:SD | 2.67 | 0.52 |
| 4:L:74:LYS:O | 4:L:77:THR:HG23 | 2.09 | 0.52 |
| 1:D:148:LEU:HD13 | 1:D:300:VAL:HA | 1.91 | 0.52 |
| 5:Q:152:LEU:HD11 | 5:Q:161:LEU:HB2 | 1.90 | 0.52 |
| 1:B:102:CYS:O | 1:B:103:MET:HE2 | 2.09 | 0.52 |
| 1:B:277:VAL:HG11 | 5:N:198:SER:OG | 2.09 | 0.52 |
| 1:C:155:VAL:HG21 | 1:C:166:ILE:HD11 | 1.91 | 0.52 |
| 1:D:267:VAL:HG22 | 1:D:287:ARG:HG2 | 1.91 | 0.52 |
| 2:E:51:DT:H1' | 2:E:52:DT:H5' | 1.91 | 0.52 |
| 4:O:268:ILE:HB | 4:O:271:PHE:CE1 | 2.44 | 0.52 |
| 4:K:147:ARG:HD2 | 5:M:300:THR:HG23 | 1.90 | 0.52 |
| 4:O:9:VAL:CG2 | 4:O:28:LEU:HD21 | 2.39 | 0.52 |
| 5:R:163:LYS:HA | 5:R:166:GLU:HG2 | 1.89 | 0.52 |
| 5:J:254:ILE:HD13 | 5:J:257:LEU:HD11 | 1.91 | 0.52 |
| 4:K:47:ILE:HG23 | 4:K:260:LEU:CD1 | 2.39 | 0.52 |
| 4:K:232:PHE:HE2 | 4:O:33:LEU:HD13 | 1.75 | 0.52 |
| 4:O:213:LEU:O | 4:O:217:GLU:HG2 | 2.09 | 0.52 |
| 4:P:87:THR:CG2 | 4:P:216:VAL:HG11 | 2.40 | 0.52 |
| 4:T:80:ILE:CG2 | 4:T:136:VAL:HG11 | 2.40 | 0.52 |
| 3:F:4:DT:H2' | 3:F:5:DT:O4' | 2.09 | 0.52 |
| 4:H:51:LEU:HD22 | 5:J:285:ILE:HD13 | 1.91 | 0.52 |
| 5:J:173:THR:C | 5:U:174:CYS:HB2 | 2.35 | 0.52 |
| 5:M:116:MET:HE1 | 5:M:154:ARG:HG2 | 1.92 | 0.52 |
| 5:N:119:TYR:CD2 | 5:N:147:MET:SD | 3.02 | 0.52 |
| 5:N:203:LEU:C | 5:N:203:LEU:HD23 | 2.35 | 0.52 |
| 5:Q:275:ALA:HA | 5:Q:278:LEU:HD12 | 1.91 | 0.52 |
| 5:R:164:LEU:O | 5:R:168:THR:HG23 | 2.10 | 0.52 |
| 1:D:8:ILE:HD11 | 1:D:20:PRO:HB3 | 1.91 | 0.52 |
| 2:E:31:DT:H2'' | 2:E:32:DA:OP2 | 2.09 | 0.52 |
| 4:G:81:ALA:HB2 | 5:I:261:GLN:HG3 | 1.91 | 0.52 |
| 5:J:146:VAL:HG13 | 5:J:149:MET:HE2 | 1.92 | 0.52 |
| 4:K:49:LEU:HD23 | 5:M:282:LEU:HD22 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:K:235:CYS:HA | 4:K:238:LEU:HD12 | 1.90 | 0.52 |
| 1:C:30:MET:HE2 | 1:C:64:VAL:HG23 | 1.92 | 0.52 |
| 1:C:263:ASN:OD1 | 1:C:265:ASP:OD1 | 2.27 | 0.52 |
| 1:D:105:ILE:HG12 | 1:D:165:ILE:HD13 | 1.92 | 0.52 |
| 2:E:31:DT:H1' | 2:E:32:DA:H5' | 1.92 | 0.52 |
| 4:H:54:TYR:HH | 4:H:87:THR:HG1 | 1.58 | 0.52 |
| 1:D:227:TYR:O | 1:D:231:LEU:HG | 2.10 | 0.52 |
| 2:E:4:DT:H2'' | 2:E:5:DC:O4' | 2.10 | 0.52 |
| 2:E:32:DA:H2'' | 2:E:33:DA:C8 | 2.45 | 0.52 |
| 4:O:56:ALA:HB1 | 5:Q:272:CYS:HB3 | 1.92 | 0.52 |
| 5:Q:243:LEU:HD12 | 5:Q:246:LEU:HD23 | 1.91 | 0.52 |
| 4:S:67:LEU:HD11 | 4:S:208:GLN:HB3 | 1.91 | 0.52 |
| 4:S:235:CYS:HA | 4:S:238:LEU:HD12 | 1.91 | 0.52 |
| 1:A:35:HIS:CD2 | 1:A:38:ARG:NH2 | 2.77 | 0.51 |
| 1:B:236:LYS:HD3 | 1:B:275:GLY:HA2 | 1.92 | 0.51 |
| 1:C:71:ASN:O | 1:D:94:LEU:HD21 | 2.10 | 0.51 |
| 4:O:118:ILE:CD1 | 5:Q:247:LEU:HD23 | 2.40 | 0.51 |
| 5:Q:250:ARG:O | 5:Q:254:ILE:HG12 | 2.10 | 0.51 |
| 2:E:16:DA:H1' | 2:E:17:DA:H5' | 1.92 | 0.51 |
| 4:O:77:THR:HG22 | 4:O:110:VAL:HG21 | 1.91 | 0.51 |
| 4:O:119:PRO:HD2 | 5:Q:246:LEU:HD21 | 1.92 | 0.51 |
| 5:Q:152:LEU:HD12 | 5:Q:158:TYR:HB3 | 1.91 | 0.51 |
| 1:D:114:ARG:HD2 | 1:D:115:SER:O | 2.10 | 0.51 |
| 4:G:262:SER:HA | 5:I:328:MET:SD | 2.50 | 0.51 |
| 5:I:158:TYR:CD2 | 5:I:193:LEU:HD12 | 2.45 | 0.51 |
| 1:D:82:LEU:O | 1:D:82:LEU:HD12 | 2.11 | 0.51 |
| 2:E:49:DA:H2'' | 2:E:50:DA:OP2 | 2.10 | 0.51 |
| 4:H:265:LYS:HE3 | 5:J:327:VAL:HB | 1.91 | 0.51 |
| 4:K:252:MET:HE1 | 5:M:331:ILE:HB | 1.93 | 0.51 |
| 3:F:40:DG:H1' | 3:F:41:DG:O5' | 2.10 | 0.51 |
| 4:K:241:HIS:O | 5:M:327:VAL:HG21 | 2.10 | 0.51 |
| 5:M:164:LEU:O | 5:M:168:THR:HG23 | 2.10 | 0.51 |
| 1:D:130:ILE:CD1 | 1:D:164:ALA:HB2 | 2.41 | 0.51 |
| 1:D:293:PHE:HD1 | 1:D:313:ILE:HD11 | 1.75 | 0.51 |
| 1:D:297:ALA:O | 1:D:300:VAL:HG13 | 2.10 | 0.51 |
| 3:F:29:DC:H2'' | 3:F:30:DT:H71 | 1.92 | 0.51 |
| 5:R:277:PHE:CE1 | 5:R:281:LEU:HD11 | 2.46 | 0.51 |
| 4:S:68:LEU:HD12 | 4:S:69:GLU:N | 2.26 | 0.51 |
| 4:T:93:ASN:OD1 | 4:T:100:THR:HA | 2.10 | 0.51 |
| 1:A:260:CYS:SG | 1:A:281:HIS:CE1 | 3.04 | 0.51 |
| 4:P:138:ARG:O | 4:P:141:ILE:HG22 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:Q:216:CYS:O | 5:R:142:ILE:HD11 | 2.10 | 0.51 |
| 4:S:144:MET:CE | 4:S:211:THR:HG23 | 2.41 | 0.51 |
| 1:B:221:TYR:CD1 | 1:B:293:PHE:CE1 | 2.99 | 0.51 |
| 1:B:231:LEU:C | 1:B:235:LEU:HD23 | 2.35 | 0.51 |
| 1:D:59:MET:O | 1:D:104:LEU:HD12 | 2.10 | 0.51 |
| 2:E:38:DA:H2'' | 2:E:39:DA:C8 | 2.45 | 0.51 |
| 4:G:67:LEU:HD22 | 4:G:209:TYR:CZ | 2.46 | 0.51 |
| 5:I:159:HIS:HB3 | 5:I:163:LYS:HZ3 | 1.75 | 0.51 |
| 4:O:270:ASP:O | 4:O:274:ILE:HG12 | 2.11 | 0.51 |
| 4:O:274:ILE:HD11 | 5:Q:227:ILE:HB | 1.92 | 0.51 |
| 2:E:8:DA:H2'' | 2:E:9:DA:OP2 | 2.11 | 0.51 |
| 4:H:247:LYS:HD2 | 5:J:327:VAL:HG22 | 1.92 | 0.51 |
| 4:P:133:LEU:HD13 | 5:R:259:PRO:HG3 | 1.92 | 0.51 |
| 1:D:153:MET:HE1 | 1:D:297:ALA:HB3 | 1.92 | 0.51 |
| 3:F:43:DT:H2'' | 3:F:44:DT:OP2 | 2.09 | 0.51 |
| 5:J:241:THR:HB | 5:J:245:GLU:OE2 | 2.11 | 0.51 |
| 1:B:124:MET:HE2 | 5:N:194:LEU:HB2 | 1.92 | 0.50 |
| 3:F:41:DG:H2'' | 3:F:42:DT:H71 | 1.93 | 0.50 |
| 4:K:133:LEU:HD13 | 5:M:259:PRO:HB3 | 1.93 | 0.50 |
| 1:B:197:TYR:HB2 | 1:B:198:PRO:HD3 | 1.93 | 0.50 |
| 3:F:25:DT:C2' | 3:F:26:DT:H71 | 2.41 | 0.50 |
| 3:F:56:DA:H2'' | 3:F:57:DT:H71 | 1.93 | 0.50 |
| 4:G:201:ILE:O | 5:I:284:HIS:NE2 | 2.43 | 0.50 |
| 4:S:91:ILE:HD13 | 4:S:217:GLU:HA | 1.93 | 0.50 |
| 1:B:297:ALA:O | 1:B:300:VAL:HG13 | 2.12 | 0.50 |
| 1:C:267:VAL:HG13 | 1:C:285:PRO:O | 2.11 | 0.50 |
| 5:J:122:ALA:O | 5:J:126:LEU:HD13 | 2.11 | 0.50 |
| 5:J:175:ARG:O | 5:J:175:ARG:HG2 | 2.11 | 0.50 |
| 1:A:198:PRO:O | 1:A:201:LEU:HB3 | 2.12 | 0.50 |
| 1:D:220:ILE:HG23 | 1:D:347:TRP:HE1 | 1.76 | 0.50 |
| 5:N:247:LEU:HB3 | 4:P:166:ILE:HD11 | 1.94 | 0.50 |
| 4:O:241:HIS:O | 5:Q:327:VAL:HG21 | 2.11 | 0.50 |
| 4:S:69:GLU:HA | 4:S:72:ARG:HB3 | 1.92 | 0.50 |
| 4:T:261:LEU:HD11 | 5:V:325:PHE:CD1 | 2.45 | 0.50 |
| 4:T:268:ILE:HD13 | 5:V:302:PHE:CE1 | 2.46 | 0.50 |
| 1:B:288:GLU:OE1 | 1:B:343:HIS:CD2 | 2.65 | 0.50 |
| 1:C:220:ILE:HG22 | 1:C:347:TRP:CZ2 | 2.47 | 0.50 |
| 4:G:67:LEU:HD13 | 4:G:209:TYR:CD1 | 2.46 | 0.50 |
| 4:O:140:SER:O | 4:O:144:MET:HG3 | 2.11 | 0.50 |
| 5:V:147:MET:HE2 | 5:V:147:MET:HA | 1.94 | 0.50 |
| 1:D:149:ILE:O | 1:D:300:VAL:HG11 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:153:MET:HE2 | 1:D:244:ILE:HG22 | 1.93 | 0.50 |
| 3:F:44:DT:H1' | 3:F:45:DT:O5' | 2.11 | 0.50 |
| 5:I:164:LEU:O | 5:I:168:THR:HG23 | 2.12 | 0.50 |
| 4:K:57:MET:SD | 4:K:58:LEU:HD22 | 2.51 | 0.50 |
| 1:B:267:VAL:HG22 | 1:B:287:ARG:CG | 2.42 | 0.50 |
| 1:C:103:MET:HG3 | 1:C:105:ILE:HD11 | 1.94 | 0.50 |
| 1:C:212:ASP:HA | 1:C:215:ARG:HD2 | 1.93 | 0.50 |
| 1:D:191:VAL:HG23 | 1:D:193:ASN:OD1 | 2.11 | 0.50 |
| 2:E:14:DA:H2'' | 2:E:15:DA:C5' | 2.42 | 0.50 |
| 4:H:212:LEU:O | 4:H:216:VAL:HG23 | 2.12 | 0.50 |
| 4:K:268:ILE:HD13 | 5:M:318:ILE:HD11 | 1.92 | 0.50 |
| 1:A:257:LEU:HD23 | 1:A:267:VAL:CG2 | 2.42 | 0.50 |
| 1:A:267:VAL:HG13 | 1:A:269:CYS:SG | 2.52 | 0.50 |
| 1:D:86:GLN:HE21 | 1:D:165:ILE:HA | 1.76 | 0.50 |
| 3:F:43:DT:H1' | 3:F:44:DT:O5' | 2.12 | 0.50 |
| 4:H:51:LEU:HD23 | 4:H:51:LEU:C | 2.37 | 0.50 |
| 5:R:164:LEU:HD21 | 5:R:210:ARG:HG3 | 1.94 | 0.50 |
| 5:V:278:LEU:HD23 | 5:V:278:LEU:C | 2.37 | 0.50 |
| 1:A:197:TYR:HB3 | 1:A:198:PRO:HD3 | 1.93 | 0.50 |
| 1:C:70:LEU:HD13 | 1:C:76:LEU:N | 2.27 | 0.50 |
| 1:C:116:VAL:HA | 1:C:159:TYR:HE1 | 1.76 | 0.50 |
| 1:D:60:LEU:HD12 | 1:D:103:MET:O | 2.12 | 0.50 |
| 3:F:52:DT:H1' | 3:F:53:DG:C8 | 2.47 | 0.50 |
| 4:G:202:THR:HG23 | 4:G:204:VAL:H | 1.76 | 0.50 |
| 4:G:266:PHE:CD1 | 5:I:328:MET:HE2 | 2.47 | 0.50 |
| 5:N:158:TYR:HE1 | 5:N:189:ALA:HB1 | 1.76 | 0.50 |
| 4:S:144:MET:SD | 5:U:304:THR:OG1 | 2.68 | 0.50 |
| 1:A:342:LEU:HD12 | 1:A:343:HIS:N | 2.27 | 0.49 |
| 1:D:7:PRO:N | 1:D:17:LYS:HZ3 | 2.10 | 0.49 |
| 2:E:48:DT:H1' | 2:E:49:DA:O5' | 2.12 | 0.49 |
| 5:M:129:HIS:HB2 | 5:M:140:TYR:OH | 2.11 | 0.49 |
| 5:U:172:TYR:CG | 5:U:214:ALA:HB1 | 2.46 | 0.49 |
| 1:A:223:THR:HB | 1:A:351:MET:SD | 2.52 | 0.49 |
| 1:A:274:TYR:CD2 | 1:A:279:PRO:HD2 | 2.48 | 0.49 |
| 1:A:295:HIS:HB3 | 1:A:312:LEU:HD11 | 1.93 | 0.49 |
| 1:D:193:ASN:OD1 | 1:D:193:ASN:O | 2.31 | 0.49 |
| 4:G:109:VAL:HG13 | 4:G:135:SER:HA | 1.93 | 0.49 |
| 4:O:151:THR:HG22 | 4:O:151:THR:O | 2.11 | 0.49 |
| 1:C:78:TYR:OH | 1:C:101:GLU:HG2 | 2.11 | 0.49 |
| 1:C:227:TYR:CE1 | 1:C:231:LEU:HD21 | 2.48 | 0.49 |
| 5:M:208:ILE:HG12 | 5:M:230:LEU:HD21 | 1.92 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:O:245:THR:OG1 | 5:Q:327:VAL:HG13 | 2.13 | 0.49 |
| 4:T:240:ASP:HA | 5:V:320:ASP:OD1 | 2.12 | 0.49 |
| 1:D:89:ALA:HB3 | 1:D:104:LEU:HB3 | 1.94 | 0.49 |
| 1:D:253:ILE:O | 1:D:256:ASN:OD1 | 2.31 | 0.49 |
| 2:E:45:DA:H1' | 2:E:46:DT:O5' | 2.12 | 0.49 |
| 3:F:11:DA:H1' | 3:F:12:DA:O5' | 2.12 | 0.49 |
| 3:F:25:DT:H1' | 3:F:26:DT:C5' | 2.42 | 0.49 |
| 4:G:222:HIS:ND1 | 4:G:238:LEU:HD23 | 2.27 | 0.49 |
| 5:J:146:VAL:HA | 5:J:149:MET:HE2 | 1.94 | 0.49 |
| 5:J:152:LEU:HG | 5:J:162:PHE:CD1 | 2.47 | 0.49 |
| 4:O:44:THR:HG22 | 5:Q:290:LEU:HD13 | 1.94 | 0.49 |
| 4:T:55:MET:HG3 | 5:V:281:LEU:HD13 | 1.94 | 0.49 |
| 5:V:302:PHE:CE1 | 5:V:306:MET:HE3 | 2.48 | 0.49 |
| 1:B:138:ILE:CD1 | 1:B:226:LEU:HD21 | 2.40 | 0.49 |
| 1:D:47:ARG:HD2 | 4:G:272:ASP:O | 2.13 | 0.49 |
| 5:J:123:ALA:N | 5:J:148:THR:HG22 | 2.27 | 0.49 |
| 5:Q:156:GLU:O | 5:Q:159:HIS:CD2 | 2.66 | 0.49 |
| 4:S:234:TYR:CE2 | 4:S:238:LEU:HD11 | 2.47 | 0.49 |
| 1:B:103:MET:HB3 | 1:B:105:ILE:HD11 | 1.94 | 0.49 |
| 1:D:358:PHE:HB2 | 1:D:360:LEU:HD23 | 1.95 | 0.49 |
| 2:E:30:DG:H3' | 2:E:30:DG:OP1 | 2.12 | 0.49 |
| 3:F:30:DT:H2' | 3:F:30:DT:P | 2.52 | 0.49 |
| 5:I:149:MET:SD | 5:J:149:MET:HE3 | 2.52 | 0.49 |
| 4:K:61:LEU:HD21 | 5:M:270:PRO:HG3 | 1.95 | 0.49 |
| 4:K:95:PHE:CZ | 4:K:217:GLU:OE2 | 2.65 | 0.49 |
| 4:S:9:VAL:HG13 | 4:T:270:ASP:HA | 1.93 | 0.49 |
| 4:T:222:HIS:HB3 | 4:T:234:TYR:HE1 | 1.78 | 0.49 |
| 5:V:168:THR:HG21 | 5:V:210:ARG:CG | 2.42 | 0.49 |
| 1:A:227:TYR:CE2 | 1:A:231:LEU:HD11 | 2.47 | 0.49 |
| 1:B:223:THR:HG21 | 1:B:351:MET:HG2 | 1.95 | 0.49 |
| 1:C:236:LYS:HZ2 | 1:C:275:GLY:HA2 | 1.77 | 0.49 |
| 1:B:290:THR:O | 1:B:294:PHE:CD2 | 2.65 | 0.49 |
| 2:E:48:DT:H1' | 2:E:49:DA:H5' | 1.94 | 0.49 |
| 3:F:9:DT:H1' | 3:F:10:DT:C5' | 2.43 | 0.49 |
| 4:K:211:THR:HG23 | 5:M:301:MET:HE3 | 1.94 | 0.49 |
| 4:L:138:ARG:NH1 | 4:L:142:VAL:HG21 | 2.27 | 0.49 |
| 5:M:128:HIS:HB3 | 5:M:134:SER:HB2 | 1.94 | 0.49 |
| 4:O:13:THR:HG21 | 5:R:295:TYR:HA | 1.94 | 0.49 |
| 5:R:303:TYR:O | 5:R:307:GLU:HG3 | 2.12 | 0.49 |
| 4:T:226:PHE:HB2 | 4:T:234:TYR:CD1 | 2.46 | 0.49 |
| 2:E:17:DA:H1' | 2:E:18:DC:H5' | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:226:PHE:HB2 | 4:H:234:TYR:CD1 | 2.47 | 0.49 |
| 5:N:164:LEU:O | 5:N:168:THR:HG23 | 2.13 | 0.49 |
| 5:J:159:HIS:CD2 | 5:J:162:PHE:CE2 | 3.00 | 0.49 |
| 4:S:49:LEU:HD23 | 5:U:282:LEU:HD22 | 1.95 | 0.49 |
| 1:C:347:TRP:CZ2 | 1:C:351:MET:HG3 | 2.48 | 0.48 |
| 2:E:5:DC:H2'' | 2:E:6:DC:C6 | 2.48 | 0.48 |
| 3:F:43:DT:H1' | 3:F:44:DT:C5' | 2.43 | 0.48 |
| 4:G:121:GLU:HB2 | 4:G:124:LEU:HD21 | 1.95 | 0.48 |
| 5:R:280:ARG:HA | 5:R:283:LYS:HE2 | 1.95 | 0.48 |
| 1:B:347:TRP:CD1 | 1:B:351:MET:HE1 | 2.48 | 0.48 |
| 1:C:340:SER:O | 1:C:344:LEU:HG | 2.13 | 0.48 |
| 1:D:59:MET:HE3 | 1:D:60:LEU:O | 2.12 | 0.48 |
| 2:E:6:DC:H2' | 2:E:6:DC:P | 2.53 | 0.48 |
| 3:F:45:DT:H1' | 3:F:46:DA:O5' | 2.13 | 0.48 |
| 5:U:169:PHE:CE2 | 5:V:147:MET:HE3 | 2.48 | 0.48 |
| 1:A:213:GLU:OE2 | 1:A:315:ARG:HA | 2.12 | 0.48 |
| 1:D:92:THR:HG22 | 1:D:101:GLU:OE1 | 2.14 | 0.48 |
| 1:D:94:LEU:HD23 | 1:D:94:LEU:N | 2.27 | 0.48 |
| 4:G:68:LEU:HD13 | 4:G:145:LEU:HB3 | 1.96 | 0.48 |
| 5:M:158:TYR:CE2 | 5:M:193:LEU:HD13 | 2.48 | 0.48 |
| 1:C:298:LYS:HG3 | 1:C:301:ARG:NH1 | 2.29 | 0.48 |
| 2:E:19:DC:H1' | 2:E:20:DT:O5' | 2.12 | 0.48 |
| 4:K:102:PHE:CG | 4:K:103:THR:N | 2.81 | 0.48 |
| 4:K:229:TYR:HB3 | 4:K:233:GLU:HG3 | 1.94 | 0.48 |
| 5:Q:157:LYS:NZ | 5:Q:192:SER:OG | 2.46 | 0.48 |
| 5:Q:219:SER:HB2 | 5:Q:222:MET:HE1 | 1.96 | 0.48 |
| 4:S:210:LEU:HD22 | 5:U:297:ALA:HB3 | 1.96 | 0.48 |
| 1:B:149:ILE:HD11 | 1:B:151:ASP:HB3 | 1.96 | 0.48 |
| 1:D:235:LEU:HD12 | 1:D:239:ASN:HB2 | 1.95 | 0.48 |
| 5:N:243:LEU:HD13 | 5:N:314:CYS:SG | 2.54 | 0.48 |
| 5:R:152:LEU:HD23 | 5:R:165:LEU:HD12 | 1.93 | 0.48 |
| 4:S:67:LEU:HA | 4:S:70:ILE:HB | 1.93 | 0.48 |
| 1:A:158:ILE:HG23 | 1:A:167:LEU:HD11 | 1.94 | 0.48 |
| 1:C:195:LEU:HB2 | 1:C:200:LYS:HB3 | 1.96 | 0.48 |
| 4:O:119:PRO:CD | 5:Q:246:LEU:HD21 | 2.44 | 0.48 |
| 5:R:178:MET:HE2 | 5:R:182:GLN:C | 2.39 | 0.48 |
| 1:B:135:ILE:HD12 | 1:B:138:ILE:HD11 | 1.95 | 0.48 |
| 1:D:32:CYS:HA | 1:D:43:VAL:CG1 | 2.44 | 0.48 |
| 3:F:26:DT:C2' | 3:F:27:DT:H71 | 2.44 | 0.48 |
| 4:O:252:MET:HE2 | 5:Q:331:ILE:HB | 1.95 | 0.48 |
| 4:P:71:PHE:HD1 | 4:P:80:ILE:HD12 | 1.76 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:U:298:ALA:HA | 5:U:301:MET:HE2 | 1.94 | 0.48 |
| 1:A:81:LEU:HD11 | 1:A:141:LEU:HD21 | 1.95 | 0.48 |
| 2:E:1:DT:H73 | 2:E:1:DT:OP1 | 2.14 | 0.48 |
| 4:K:226:PHE:CD2 | 4:K:234:TYR:CD1 | 3.01 | 0.48 |
| 4:P:144:MET:SD | 5:R:301:MET:HE1 | 2.53 | 0.48 |
| 1:C:22:LYS:HD2 | 1:D:206:ASN:ND2 | 2.28 | 0.48 |
| 1:D:250:ILE:HA | 1:D:253:ILE:HD12 | 1.96 | 0.48 |
| 4:G:94:ARG:HE | 4:G:260:LEU:HD22 | 1.78 | 0.48 |
| 4:G:151:THR:HG22 | 5:I:293:MET:HE1 | 1.96 | 0.48 |
| 4:H:231:VAL:O | 4:H:234:TYR:HB3 | 2.14 | 0.48 |
| 5:I:153:LEU:HD23 | 5:J:153:LEU:CD2 | 2.43 | 0.48 |
| 5:M:171:ASP:OD1 | 5:R:174:CYS:HA | 2.13 | 0.48 |
| 5:Q:196:MET:HE1 | 5:Q:200:THR:OG1 | 2.14 | 0.48 |
| 5:U:249:GLU:HA | 5:U:252:GLU:HG2 | 1.96 | 0.48 |
| 5:U:290:LEU:HG | 5:U:294:TYR:CE2 | 2.48 | 0.48 |
| 1:B:155:VAL:CG2 | 1:B:166:ILE:HD11 | 2.42 | 0.48 |
| 1:B:239:ASN:O | 1:B:242:ASP:OD1 | 2.32 | 0.48 |
| 1:C:25:ARG:HG3 | 1:D:206:ASN:OD1 | 2.14 | 0.48 |
| 1:D:65:LEU:O | 1:D:99:VAL:HG22 | 2.14 | 0.48 |
| 1:D:350:PHE:O | 1:D:353:GLU:HG2 | 2.14 | 0.48 |
| 3:F:37:DA:H1' | 3:F:38:DA:O5' | 2.14 | 0.48 |
| 5:I:277:PHE:CE1 | 5:I:281:LEU:HD11 | 2.49 | 0.48 |
| 4:P:92:HIS:NE2 | 4:P:99:VAL:HG12 | 2.29 | 0.48 |
| 4:S:229:TYR:HB3 | 4:S:233:GLU:HG3 | 1.96 | 0.48 |
| 1:C:155:VAL:HG12 | 1:C:229:THR:HG21 | 1.96 | 0.47 |
| 1:D:105:ILE:HG22 | 1:D:106:ARG:N | 2.29 | 0.47 |
| 4:H:210:LEU:HD21 | 5:J:294:TYR:HA | 1.95 | 0.47 |
| 4:K:65:GLN:HG3 | 4:K:69:GLU:OE1 | 2.14 | 0.47 |
| 5:Q:290:LEU:O | 5:Q:293:MET:HB2 | 2.13 | 0.47 |
| 4:G:24:LYS:HZ2 | 5:J:295:TYR:HE1 | 1.59 | 0.47 |
| 4:H:241:HIS:HD1 | 5:J:320:ASP:CG | 2.22 | 0.47 |
| 5:J:255:GLN:HG3 | 4:L:169:THR:HG22 | 1.96 | 0.47 |
| 4:O:16:VAL:HG22 | 4:P:265:LYS:NZ | 2.29 | 0.47 |
| 5:R:255:GLN:C | 5:R:256:MET:HE2 | 2.39 | 0.47 |
| 5:U:281:LEU:O | 5:U:285:ILE:HG12 | 2.14 | 0.47 |
| 5:V:168:THR:HB | 5:V:214:ALA:HB2 | 1.96 | 0.47 |
| 4:G:92:HIS:HB3 | 4:G:102:PHE:CZ | 2.49 | 0.47 |
| 4:S:264:PHE:HE2 | 5:U:294:TYR:CE2 | 2.33 | 0.47 |
| 1:D:161:GLU:N | 1:D:161:GLU:OE1 | 2.46 | 0.47 |
| 2:E:17:DA:H1' | 2:E:18:DC:C5' | 2.44 | 0.47 |
| 4:G:55:MET:SD | 4:G:209:TYR:CZ | 3.07 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:125:LYS:HG3 | 5:J:126:LEU:HD12 | 1.96 | 0.47 |
| 5:J:143:SER:O | 5:J:147:MET:HG2 | 2.15 | 0.47 |
| 5:U:119:TYR:HB3 | 5:U:151:PHE:HB2 | 1.96 | 0.47 |
| 5:U:131:SER:N | 5:U:209:MET:HE1 | 2.29 | 0.47 |
| 1:D:234:ILE:O | 1:D:234:ILE:HG13 | 2.14 | 0.47 |
| 5:I:146:VAL:HG13 | 5:J:149:MET:SD | 2.54 | 0.47 |
| 5:J:246:LEU:HD21 | 5:J:312:SER:HB2 | 1.95 | 0.47 |
| 4:O:274:ILE:CD1 | 5:Q:227:ILE:HB | 2.44 | 0.47 |
| 4:P:132:LEU:HD13 | 4:P:223:TYR:CE1 | 2.49 | 0.47 |
| 5:Q:118:ARG:HG2 | 5:Q:147:MET:CE | 2.43 | 0.47 |
| 5:R:147:MET:HE2 | 5:R:147:MET:HA | 1.97 | 0.47 |
| 4:S:108:PHE:CE1 | 5:U:263:ILE:HD12 | 2.50 | 0.47 |
| 5:U:135:THR:HG22 | 5:U:303:TYR:CD2 | 2.50 | 0.47 |
| 1:A:28:LYS:N | 1:A:29:PRO:CD | 2.77 | 0.47 |
| 1:B:22:LYS:HD3 | 1:B:24:MET:O | 2.15 | 0.47 |
| 1:C:93:ILE:HD12 | 1:C:100:TYR:O | 2.15 | 0.47 |
| 1:C:178:TYR:CD1 | 1:C:215:ARG:NH2 | 2.83 | 0.47 |
| 4:G:88:LEU:HD12 | 4:G:102:PHE:CE2 | 2.50 | 0.47 |
| 4:H:221:LEU:O | 4:H:225:ILE:HG12 | 2.15 | 0.47 |
| 5:I:119:TYR:HA | 5:I:147:MET:HG3 | 1.96 | 0.47 |
| 5:M:161:LEU:HD21 | 5:M:190:VAL:HG12 | 1.96 | 0.47 |
| 1:A:89:ALA:HB3 | 1:A:104:LEU:HB3 | 1.95 | 0.47 |
| 1:B:124:MET:N | 1:B:124:MET:SD | 2.88 | 0.47 |
| 1:C:131:ILE:HD12 | 1:C:360:LEU:HD11 | 1.97 | 0.47 |
| 1:C:345:LEU:O | 1:C:348:GLU:HG3 | 2.15 | 0.47 |
| 1:D:126:VAL:O | 1:D:130:ILE:HG12 | 2.14 | 0.47 |
| 1:D:131:ILE:HA | 1:D:134:VAL:HG22 | 1.96 | 0.47 |
| 2:E:14:DA:H2'' | 2:E:15:DA:H5' | 1.96 | 0.47 |
| 2:E:47:DT:H1' | 2:E:48:DT:C5' | 2.45 | 0.47 |
| 2:E:51:DT:H1' | 2:E:52:DT:C5' | 2.45 | 0.47 |
| 3:F:30:DT:H1' | 3:F:31:DT:C6 | 2.49 | 0.47 |
| 4:G:81:ALA:HB1 | 4:G:108:PHE:CD1 | 2.49 | 0.47 |
| 5:I:113:LEU:N | 5:J:163:LYS:HZ1 | 2.13 | 0.47 |
| 5:J:172:TYR:CD2 | 5:U:174:CYS:HB3 | 2.50 | 0.47 |
| 5:M:217:PHE:O | 5:N:143:SER:HB3 | 2.15 | 0.47 |
| 5:Q:229:LEU:HD11 | 5:Q:306:MET:HB2 | 1.95 | 0.47 |
| 4:S:138:ARG:O | 4:S:142:VAL:HG23 | 2.15 | 0.47 |
| 1:A:71:ASN:O | 1:B:94:LEU:HD23 | 2.15 | 0.47 |
| 1:A:227:TYR:OH | 1:A:283:MET:O | 2.33 | 0.47 |
| 1:D:128:LYS:O | 1:D:131:ILE:HG22 | 2.15 | 0.47 |
| 2:E:33:DA:OP2 | 2:E:33:DA:H8 | 1.98 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:30:DT:H2'' | 3:F:31:DT:OP2 | 2.15 | 0.47 |
| 4:G:111:THR:OG1 | 4:G:137:ASP:HA | 2.15 | 0.47 |
| 4:K:45:LEU:O | 4:K:49:LEU:HG | 2.15 | 0.47 |
| 4:L:118:ILE:HG23 | 5:N:247:LEU:HD11 | 1.97 | 0.47 |
| 4:S:49:LEU:CD2 | 5:U:282:LEU:HD22 | 2.45 | 0.47 |
| 4:T:72:ARG:HH21 | 4:T:142:VAL:HG11 | 1.80 | 0.47 |
| 5:V:164:LEU:HD21 | 5:V:210:ARG:HD2 | 1.96 | 0.47 |
| 1:A:260:CYS:SG | 1:A:261:PRO:HD2 | 2.55 | 0.47 |
| 4:G:125:PHE:HD2 | 4:G:132:LEU:HD22 | 1.79 | 0.47 |
| 5:J:116:MET:HE3 | 5:J:151:PHE:CE1 | 2.50 | 0.47 |
| 5:Q:228:VAL:HG23 | 5:R:224:TYR:CD2 | 2.50 | 0.47 |
| 4:S:111:THR:HG1 | 4:S:137:ASP:HA | 1.80 | 0.47 |
| 4:T:256:THR:O | 4:T:256:THR:HG22 | 2.14 | 0.47 |
| 5:U:244:GLU:HG2 | 5:U:245:GLU:N | 2.30 | 0.47 |
| 1:D:79:ARG:HA | 1:D:82:LEU:HD23 | 1.97 | 0.47 |
| 3:F:12:DA:H1' | 3:F:13:DA:C8 | 2.49 | 0.47 |
| 3:F:23:DG:H1' | 3:F:24:DT:O5' | 2.15 | 0.47 |
| 4:G:72:ARG:HD3 | 4:G:142:VAL:HG13 | 1.97 | 0.47 |
| 4:G:249:ARG:HA | 5:I:331:ILE:HG22 | 1.97 | 0.47 |
| 5:J:173:THR:O | 5:U:174:CYS:HB2 | 2.15 | 0.47 |
| 1:D:237:GLN:HE21 | 1:D:272:LEU:HD12 | 1.81 | 0.46 |
| 3:F:54:DG:H1' | 3:F:55:DA:H5' | 1.97 | 0.46 |
| 3:F:56:DA:C2' | 3:F:57:DT:H71 | 2.45 | 0.46 |
| 4:G:61:LEU:HD11 | 4:G:86:SER:CB | 2.44 | 0.46 |
| 4:K:71:PHE:CE2 | 4:K:141:ILE:HG22 | 2.50 | 0.46 |
| 5:N:142:ILE:HA | 5:N:145:VAL:HG12 | 1.97 | 0.46 |
| 5:N:209:MET:HE2 | 5:N:213:PHE:CZ | 2.49 | 0.46 |
| 4:O:222:HIS:ND1 | 4:O:238:LEU:HD23 | 2.30 | 0.46 |
| 1:A:138:ILE:HD11 | 1:A:226:LEU:HD11 | 1.97 | 0.46 |
| 1:C:155:VAL:HG22 | 1:C:166:ILE:HD11 | 1.96 | 0.46 |
| 1:C:221:TYR:CD1 | 1:C:296:TYR:HD2 | 2.34 | 0.46 |
| 1:D:60:LEU:HA | 1:D:103:MET:O | 2.15 | 0.46 |
| 1:D:289:ILE:HB | 1:D:343:HIS:CD2 | 2.50 | 0.46 |
| 2:E:14:DA:H2'' | 2:E:15:DA:C8 | 2.51 | 0.46 |
| 3:F:36:DT:OP1 | 3:F:36:DT:H3' | 2.16 | 0.46 |
| 4:G:56:ALA:HB1 | 5:I:272:CYS:HB3 | 1.97 | 0.46 |
| 4:G:274:ILE:HD11 | 5:I:227:ILE:HB | 1.96 | 0.46 |
| 5:I:140:TYR:O | 5:J:221:ILE:HG12 | 2.15 | 0.46 |
| 5:M:175:ARG:O | 5:M:176:PRO:C | 2.58 | 0.46 |
| 4:O:268:ILE:HB | 4:O:271:PHE:CZ | 2.50 | 0.46 |
| 1:A:249:SER:O | 1:A:252:ILE:HG22 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:108:ILE:HG22 | 1:C:109:ARG:N | 2.31 | 0.46 |
| 1:C:224:PHE:CZ | 1:C:347:TRP:HD1 | 2.33 | 0.46 |
| 1:D:32:CYS:SG | 1:D:34:ILE:HB | 2.55 | 0.46 |
| 1:D:60:LEU:HD11 | 1:D:102:CYS:HB3 | 1.96 | 0.46 |
| 1:D:123:ASN:CG | 1:D:126:VAL:HG23 | 2.41 | 0.46 |
| 1:D:154:TYR:HB2 | 1:D:229:THR:HG22 | 1.97 | 0.46 |
| 2:E:51:DT:H3' | 2:E:51:DT:OP1 | 2.16 | 0.46 |
| 4:H:264:PHE:C | 4:H:265:LYS:HD2 | 2.40 | 0.46 |
| 5:J:114:ILE:HD11 | 5:J:154:ARG:HE | 1.78 | 0.46 |
| 5:J:123:ALA:O | 5:J:127:ILE:HG12 | 2.16 | 0.46 |
| 5:M:299:ASN:ND2 | 5:N:227:ILE:H | 2.12 | 0.46 |
| 4:P:163:ASN:O | 4:P:166:ILE:HG22 | 2.16 | 0.46 |
| 5:Q:249:GLU:HA | 5:Q:252:GLU:HG2 | 1.98 | 0.46 |
| 5:R:123:ALA:N | 5:R:148:THR:HG22 | 2.30 | 0.46 |
| 1:A:72:GLU:OE1 | 1:B:94:LEU:O | 2.32 | 0.46 |
| 1:A:262:ASN:HB2 | 1:A:281:HIS:CE1 | 2.50 | 0.46 |
| 1:B:85:ASP:CG | 1:B:90:ARG:HE | 2.23 | 0.46 |
| 1:B:236:LYS:HE3 | 1:B:273:ASN:OD1 | 2.15 | 0.46 |
| 2:E:28:DA:H2'' | 2:E:29:DA:N7 | 2.31 | 0.46 |
| 3:F:34:DC:H2'' | 3:F:35:DC:C5 | 2.50 | 0.46 |
| 4:G:111:THR:HG22 | 5:I:254:ILE:HD12 | 1.98 | 0.46 |
| 4:L:234:TYR:CZ | 4:L:238:LEU:HD11 | 2.50 | 0.46 |
| 5:M:164:LEU:HD11 | 5:M:186:LEU:HD22 | 1.97 | 0.46 |
| 5:R:301:MET:N | 5:R:301:MET:HE2 | 2.30 | 0.46 |
| 4:S:144:MET:HE2 | 4:S:211:THR:HG23 | 1.95 | 0.46 |
| 4:T:68:LEU:HB2 | 4:T:208:GLN:NE2 | 2.30 | 0.46 |
| 5:U:302:PHE:CE2 | 5:U:306:MET:CE | 2.99 | 0.46 |
| 1:A:24:MET:N | 1:B:206:ASN:HB2 | 2.31 | 0.46 |
| 1:A:131:ILE:HG22 | 1:A:230:VAL:HG12 | 1.96 | 0.46 |
| 1:D:231:LEU:O | 1:D:235:LEU:HG | 2.15 | 0.46 |
| 2:E:31:DT:H1' | 2:E:32:DA:C5' | 2.45 | 0.46 |
| 5:J:303:TYR:O | 5:J:307:GLU:HG3 | 2.16 | 0.46 |
| 5:M:194:LEU:HD13 | 5:M:201:ILE:HD11 | 1.96 | 0.46 |
| 5:R:159:HIS:O | 5:R:162:PHE:HB3 | 2.16 | 0.46 |
| 5:R:205:THR:O | 5:R:209:MET:HG2 | 2.15 | 0.46 |
| 4:S:248:LEU:HD12 | 4:S:252:MET:HB2 | 1.97 | 0.46 |
| 1:A:148:LEU:HD12 | 1:A:148:LEU:O | 2.15 | 0.46 |
| 1:B:122:HIS:O | 1:B:122:HIS:CG | 2.69 | 0.46 |
| 4:G:141:ILE:HD11 | 4:G:212:LEU:CD2 | 2.45 | 0.46 |
| 4:H:47:ILE:HG21 | 5:J:294:TYR:OH | 2.16 | 0.46 |
| 4:H:210:LEU:HD23 | 5:J:293:MET:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:K:68:LEU:HD11 | 4:K:145:LEU:HB3 | 1.97 | 0.46 |
| 5:R:168:THR:HG22 | 5:R:210:ARG:CZ | 2.45 | 0.46 |
| 1:D:123:ASN:ND2 | 1:D:126:VAL:HG23 | 2.30 | 0.46 |
| 2:E:55:DA:C2 | 2:E:56:DT:C2 | 3.04 | 0.46 |
| 5:I:242:THR:HG22 | 5:I:315:LYS:HZ3 | 1.81 | 0.46 |
| 5:N:243:LEU:O | 5:N:247:LEU:HD23 | 2.16 | 0.46 |
| 1:B:220:ILE:HB | 1:B:313:ILE:HG21 | 1.98 | 0.46 |
| 1:B:307:LYS:NZ | 2:E:18:DC:H3' | 2.30 | 0.46 |
| 3:F:9:DT:OP1 | 3:F:9:DT:H3' | 2.16 | 0.46 |
| 4:K:92:HIS:NE2 | 4:K:99:VAL:HG11 | 2.30 | 0.46 |
| 5:N:159:HIS:HB3 | 5:N:163:LYS:NZ | 2.31 | 0.46 |
| 5:Q:327:VAL:O | 5:Q:331:ILE:HG12 | 2.16 | 0.46 |
| 5:R:300:THR:C | 5:R:301:MET:HE2 | 2.40 | 0.46 |
| 5:R:301:MET:HE2 | 5:R:301:MET:HA | 1.98 | 0.46 |
| 1:A:153:MET:HE2 | 1:A:243:VAL:O | 2.16 | 0.46 |
| 1:C:152:ARG:HD3 | 1:C:242:ASP:OD2 | 2.16 | 0.46 |
| 5:J:202:ASP:OD1 | 5:J:205:THR:HG23 | 2.16 | 0.46 |
| 5:M:220:PRO:HA | 5:N:141:LYS:HA | 1.97 | 0.46 |
| 5:N:158:TYR:CE1 | 5:N:193:LEU:HD11 | 2.51 | 0.46 |
| 5:R:178:MET:HE1 | 5:R:186:LEU:CG | 2.46 | 0.46 |
| 4:T:54:TYR:CZ | 4:T:58:LEU:HD11 | 2.51 | 0.46 |
| 5:U:307:GLU:O | 5:U:311:VAL:HG12 | 2.15 | 0.46 |
| 1:A:24:MET:HE2 | 1:B:203:THR:OG1 | 2.15 | 0.46 |
| 1:A:131:ILE:CG2 | 1:A:230:VAL:HG12 | 2.46 | 0.46 |
| 1:D:124:MET:HB2 | 1:D:358:PHE:CE1 | 2.51 | 0.46 |
| 2:E:54:DA:H2'' | 2:E:55:DA:H8 | 1.81 | 0.46 |
| 4:G:10:ARG:HA | 4:G:24:LYS:O | 2.16 | 0.46 |
| 4:G:61:LEU:O | 4:G:62:GLU:HG3 | 2.15 | 0.46 |
| 4:L:141:ILE:O | 4:L:145:LEU:HD23 | 2.16 | 0.46 |
| 5:M:114:ILE:HD13 | 5:M:150:ILE:HG22 | 1.98 | 0.46 |
| 4:P:222:HIS:HB3 | 4:P:234:TYR:HE1 | 1.81 | 0.46 |
| 4:S:222:HIS:CE1 | 4:S:238:LEU:HD23 | 2.51 | 0.46 |
| 1:C:114:ARG:C | 1:C:158:ILE:HG23 | 2.41 | 0.45 |
| 1:C:227:TYR:OH | 1:C:285:PRO:HD3 | 2.16 | 0.45 |
| 1:C:266:ARG:HA | 1:C:286:PRO:HA | 1.98 | 0.45 |
| 3:F:9:DT:H1' | 3:F:10:DT:H5' | 1.99 | 0.45 |
| 3:F:14:DT:C2' | 3:F:15:DT:H71 | 2.44 | 0.45 |
| 5:V:166:GLU:OE2 | 5:V:167:THR:HG23 | 2.16 | 0.45 |
| 1:C:355:SER:HB3 | 1:C:360:LEU:HB2 | 1.98 | 0.45 |
| 3:F:14:DT:OP1 | 3:F:14:DT:H3' | 2.16 | 0.45 |
| 4:G:13:THR:HG21 | 5:J:295:TYR:HA | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:G:120:GLY:HA2 | 5:I:305:THR:HG23 | 1.99 | 0.45 |
| 5:N:116:MET:HA | 5:N:119:TYR:CD1 | 2.51 | 0.45 |
| 1:B:141:LEU:HD11 | 1:B:145:GLU:C | 2.42 | 0.45 |
| 1:C:76:LEU:CD2 | 1:C:78:TYR:HE1 | 2.29 | 0.45 |
| 1:D:101:GLU:HG3 | 1:D:103:MET:SD | 2.56 | 0.45 |
| 2:E:45:DA:C8 | 2:E:46:DT:H72 | 2.51 | 0.45 |
| 5:R:193:LEU:C | 5:R:194:LEU:HD22 | 2.41 | 0.45 |
| 1:A:269:CYS:HB2 | 1:A:283:MET:O | 2.16 | 0.45 |
| 1:B:62:MET:SD | 1:B:100:TYR:HB3 | 2.57 | 0.45 |
| 1:B:234:ILE:HG13 | 1:B:274:TYR:HD1 | 1.82 | 0.45 |
| 1:C:128:LYS:HA | 1:C:131:ILE:HG12 | 1.98 | 0.45 |
| 1:C:134:VAL:HG11 | 1:C:226:LEU:CD1 | 2.47 | 0.45 |
| 1:C:153:MET:N | 1:C:242:ASP:OD1 | 2.49 | 0.45 |
| 1:C:224:PHE:HZ | 1:C:289:ILE:HD12 | 1.81 | 0.45 |
| 4:H:116:THR:HA | 5:J:254:ILE:HD11 | 1.98 | 0.45 |
| 5:I:119:TYR:HB3 | 5:I:151:PHE:HB2 | 1.97 | 0.45 |
| 5:I:148:THR:O | 5:I:152:LEU:HD23 | 2.17 | 0.45 |
| 5:I:149:MET:HE3 | 5:J:146:VAL:HG13 | 1.99 | 0.45 |
| 5:J:175:ARG:NH2 | 5:U:170:ASP:HB3 | 2.32 | 0.45 |
| 5:M:207:ASP:OD2 | 5:M:233:VAL:HG12 | 2.17 | 0.45 |
| 5:M:295:TYR:CD1 | 5:M:299:ASN:OD1 | 2.69 | 0.45 |
| 4:P:55:MET:HB3 | 5:R:281:LEU:HD13 | 1.98 | 0.45 |
| 1:A:205:ASN:HA | 1:B:24:MET:SD | 2.56 | 0.45 |
| 1:A:212:ASP:OD1 | 1:A:213:GLU:N | 2.48 | 0.45 |
| 1:B:124:MET:SD | 5:N:192:SER:HA | 2.57 | 0.45 |
| 1:D:8:ILE:O | 1:D:9:LYS:HE2 | 2.17 | 0.45 |
| 1:D:80:HIS:O | 1:D:81:LEU:HD23 | 2.16 | 0.45 |
| 3:F:57:DT:H1' | 3:F:58:DA:C8 | 2.51 | 0.45 |
| 4:G:205:GLU:O | 4:G:209:TYR:CD2 | 2.70 | 0.45 |
| 4:H:117:SER:HG | 4:H:137:ASP:CG | 2.25 | 0.45 |
| 4:H:225:ILE:HG23 | 4:H:233:GLU:OE1 | 2.17 | 0.45 |
| 4:K:80:ILE:O | 4:K:84:VAL:HG23 | 2.16 | 0.45 |
| 4:O:56:ALA:HB1 | 5:Q:272:CYS:CB | 2.46 | 0.45 |
| 5:Q:114:ILE:CG2 | 5:R:166:GLU:OE1 | 2.65 | 0.45 |
| 5:R:164:LEU:C | 5:R:164:LEU:HD23 | 2.41 | 0.45 |
| 1:A:70:LEU:HD13 | 1:A:76:LEU:N | 2.32 | 0.45 |
| 1:B:178:TYR:N | 1:B:210:SER:HB3 | 2.32 | 0.45 |
| 4:G:136:VAL:O | 4:G:136:VAL:HG23 | 2.16 | 0.45 |
| 5:V:168:THR:HG21 | 5:V:210:ARG:HG2 | 1.97 | 0.45 |
| 5:V:306:MET:HE1 | 5:V:316:PHE:CG | 2.52 | 0.45 |
| 1:A:235:LEU:HD23 | 1:A:274:TYR:CD1 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:267:VAL:HG12 | 1:D:268:LYS:N | 2.31 | 0.45 |
| 2:E:38:DA:H1' | 2:E:39:DA:O5' | 2.16 | 0.45 |
| 3:F:48:DC:H1' | 3:F:49:DG:C8 | 2.51 | 0.45 |
| 4:H:138:ARG:HB3 | 4:H:139:PRO:HD3 | 1.98 | 0.45 |
| 5:M:291:SER:O | 5:N:229:LEU:HD11 | 2.16 | 0.45 |
| 5:N:301:MET:HG3 | 5:N:321:TYR:OH | 2.16 | 0.45 |
| 5:R:300:THR:HG22 | 5:R:301:MET:CE | 2.46 | 0.45 |
| 1:A:227:TYR:O | 1:A:230:VAL:HG22 | 2.16 | 0.45 |
| 4:K:72:ARG:HH22 | 4:K:142:VAL:HG21 | 1.82 | 0.45 |
| 5:M:207:ASP:OD2 | 5:M:233:VAL:HA | 2.17 | 0.45 |
| 4:O:43:GLU:HA | 4:O:46:LYS:HG2 | 1.99 | 0.45 |
| 4:O:77:THR:CG2 | 4:O:110:VAL:HG21 | 2.47 | 0.45 |
| 4:O:105:LYS:HG3 | 4:O:131:VAL:HG11 | 1.98 | 0.45 |
| 1:B:30:MET:HE2 | 1:B:64:VAL:HG23 | 1.98 | 0.45 |
| 1:B:101:GLU:OE2 | 1:B:103:MET:CE | 2.65 | 0.45 |
| 1:C:246:GLU:OE2 | 1:D:16:VAL:HG22 | 2.17 | 0.45 |
| 1:C:299:TRP:CH2 | 1:C:302:ASN:O | 2.70 | 0.45 |
| 4:G:252:MET:HE2 | 4:G:259:LEU:HG | 1.98 | 0.45 |
| 4:H:141:ILE:O | 4:H:145:LEU:HD23 | 2.16 | 0.45 |
| 4:K:70:ILE:O | 4:K:80:ILE:HD11 | 2.16 | 0.45 |
| 4:K:123:ILE:HD11 | 4:K:141:ILE:HD11 | 1.99 | 0.45 |
| 5:M:131:SER:N | 5:M:209:MET:HE1 | 2.31 | 0.45 |
| 4:O:81:ALA:HB1 | 4:O:108:PHE:CD2 | 2.52 | 0.45 |
| 4:P:132:LEU:HD13 | 4:P:223:TYR:HE1 | 1.81 | 0.45 |
| 1:B:59:MET:C | 1:B:60:LEU:HD22 | 2.42 | 0.45 |
| 1:B:93:ILE:HG22 | 1:B:100:TYR:HD2 | 1.81 | 0.45 |
| 1:D:48:ASN:C | 4:G:275:ASN:HB3 | 2.42 | 0.45 |
| 1:D:122:HIS:HE1 | 1:D:277:VAL:HG22 | 1.82 | 0.45 |
| 1:D:132:ASP:HA | 1:D:135:ILE:HG22 | 1.99 | 0.45 |
| 3:F:18:DT:H6 | 3:F:18:DT:H2' | 1.61 | 0.45 |
| 5:I:216:CYS:HB2 | 5:J:222:MET:HE2 | 1.98 | 0.45 |
| 4:K:12:VAL:HG22 | 4:K:23:GLN:HG3 | 1.99 | 0.45 |
| 4:K:24:LYS:HB2 | 5:N:295:TYR:OH | 2.17 | 0.45 |
| 5:M:219:SER:O | 5:N:142:ILE:HG12 | 2.17 | 0.45 |
| 4:O:31:PHE:O | 5:R:310:ALA:HB1 | 2.17 | 0.45 |
| 4:P:138:ARG:HB3 | 4:P:139:PRO:HD3 | 1.98 | 0.45 |
| 5:Q:156:GLU:HA | 5:Q:159:HIS:NE2 | 2.32 | 0.45 |
| 5:U:243:LEU:HD12 | 5:U:244:GLU:N | 2.32 | 0.45 |
| 1:B:260:CYS:HB2 | 1:B:267:VAL:O | 2.17 | 0.44 |
| 4:H:54:TYR:CE2 | 4:H:58:LEU:HD11 | 2.52 | 0.44 |
| 4:H:166:ILE:HD13 | 5:V:248:ILE:HG13 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:I:171:ASP:O | 5:I:172:TYR:CG | 2.69 | 0.44 |
| 4:K:47:ILE:HG23 | 4:K:260:LEU:HD11 | 1.98 | 0.44 |
| 5:M:194:LEU:HD13 | 5:M:201:ILE:CD1 | 2.47 | 0.44 |
| 4:O:87:THR:O | 4:O:91:ILE:HG12 | 2.17 | 0.44 |
| 5:Q:178:MET:HB2 | 5:Q:182:GLN:OE1 | 2.17 | 0.44 |
| 5:R:250:ARG:O | 5:R:254:ILE:HG13 | 2.17 | 0.44 |
| 4:T:222:HIS:CE1 | 4:T:238:LEU:HD23 | 2.52 | 0.44 |
| 5:U:146:VAL:HG11 | 5:V:169:PHE:HZ | 1.78 | 0.44 |
| 1:A:235:LEU:HD22 | 1:A:237:GLN:HG3 | 1.98 | 0.44 |
| 1:A:267:VAL:HG23 | 1:A:287:ARG:HH22 | 1.82 | 0.44 |
| 4:G:43:GLU:O | 4:G:47:ILE:HG12 | 2.17 | 0.44 |
| 4:G:144:MET:HE1 | 5:I:301:MET:HG2 | 2.00 | 0.44 |
| 4:G:148:GLU:O | 5:I:133:ASN:O | 2.36 | 0.44 |
| 4:H:55:MET:CG | 5:J:281:LEU:HD13 | 2.48 | 0.44 |
| 4:K:27:GLU:HB3 | 4:K:30:GLU:OE1 | 2.17 | 0.44 |
| 4:S:133:LEU:CD1 | 5:U:259:PRO:HB3 | 2.47 | 0.44 |
| 5:V:202:ASP:O | 5:V:206:VAL:HG23 | 2.17 | 0.44 |
| 1:C:154:TYR:HD1 | 1:C:242:ASP:OD1 | 2.00 | 0.44 |
| 1:C:213:GLU:CG | 1:C:314:ALA:HB3 | 2.47 | 0.44 |
| 1:D:130:ILE:HD13 | 1:D:164:ALA:HB2 | 1.99 | 0.44 |
| 1:D:151:ASP:OD1 | 1:D:152:ARG:N | 2.50 | 0.44 |
| 1:D:257:LEU:HD11 | 1:D:268:LYS:O | 2.17 | 0.44 |
| 4:K:202:THR:OG1 | 4:K:205:GLU:HG3 | 2.18 | 0.44 |
| 5:M:132:LEU:HD11 | 5:M:303:TYR:CD1 | 2.52 | 0.44 |
| 5:Q:295:TYR:CE1 | 5:Q:299:ASN:OD1 | 2.70 | 0.44 |
| 5:R:155:SER:OG | 5:R:158:TYR:HB2 | 2.18 | 0.44 |
| 1:B:131:ILE:O | 1:B:135:ILE:HG22 | 2.17 | 0.44 |
| 1:C:59:MET:C | 1:C:60:LEU:HD22 | 2.42 | 0.44 |
| 1:C:75:LYS:NZ | 1:C:80:HIS:HB2 | 2.33 | 0.44 |
| 1:C:117:ASP:O | 1:C:118:GLU:HB2 | 2.16 | 0.44 |
| 1:C:177:ASP:HB2 | 1:C:192:CYS:SG | 2.58 | 0.44 |
| 1:C:245:ALA:HB3 | 1:C:248:THR:OG1 | 2.18 | 0.44 |
| 1:D:216:GLN:HA | 1:D:219:TYR:HD2 | 1.82 | 0.44 |
| 3:F:24:DT:H1' | 3:F:25:DT:O5' | 2.17 | 0.44 |
| 4:G:107:GLU:OE2 | 4:G:131:VAL:HG11 | 2.17 | 0.44 |
| 4:L:226:PHE:CE2 | 4:L:231:VAL:HG22 | 2.52 | 0.44 |
| 5:N:158:TYR:CZ | 5:N:193:LEU:HD21 | 2.53 | 0.44 |
| 4:O:44:THR:HG22 | 5:Q:290:LEU:HD11 | 1.99 | 0.44 |
| 5:R:193:LEU:O | 5:R:194:LEU:HD22 | 2.18 | 0.44 |
| 5:R:303:TYR:HA | 5:R:306:MET:HE3 | 1.99 | 0.44 |
| 5:V:163:LYS:HA | 5:V:166:GLU:HG3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:V:187:LEU:O | 5:V:201:ILE:HD11 | 2.18 | 0.44 |
| 5:V:277:PHE:CE1 | 5:V:281:LEU:HD11 | 2.52 | 0.44 |
| 1:A:46:PRO:HG2 | 1:A:58:ASP:HB2 | 1.99 | 0.44 |
| 1:B:22:LYS:HD2 | 1:B:22:LYS:O | 2.18 | 0.44 |
| 1:B:195:LEU:HB2 | 1:B:200:LYS:HG2 | 2.00 | 0.44 |
| 1:B:197:TYR:HB2 | 1:B:198:PRO:CD | 2.47 | 0.44 |
| 1:B:286:PRO:HB3 | 1:B:343:HIS:CE1 | 2.52 | 0.44 |
| 2:E:18:DC:H2'' | 2:E:19:DC:C5 | 2.53 | 0.44 |
| 2:E:44:DA:O5' | 2:E:44:DA:H2' | 2.18 | 0.44 |
| 3:F:44:DT:H1' | 3:F:45:DT:C5' | 2.47 | 0.44 |
| 5:J:152:LEU:O | 5:J:162:PHE:CE1 | 2.69 | 0.44 |
| 5:J:193:LEU:C | 5:J:194:LEU:HD22 | 2.42 | 0.44 |
| 4:K:201:ILE:HB | 5:M:284:HIS:CD2 | 2.52 | 0.44 |
| 5:Q:122:ALA:HB2 | 5:Q:147:MET:HE2 | 2.00 | 0.44 |
| 5:Q:163:LYS:HA | 5:Q:163:LYS:HE2 | 1.99 | 0.44 |
| 5:V:152:LEU:CD1 | 5:V:161:LEU:HD11 | 2.36 | 0.44 |
| 1:B:67:SER:HA | 1:B:99:VAL:HG21 | 2.00 | 0.44 |
| 1:B:76:LEU:CD2 | 1:B:78:TYR:HE2 | 2.31 | 0.44 |
| 1:C:77:TYR:HB3 | 1:C:173:ILE:HD11 | 2.00 | 0.44 |
| 2:E:56:DT:O2 | 2:E:57:DG:O4' | 2.36 | 0.44 |
| 5:I:179:THR:HG23 | 5:I:182:GLN:H | 1.82 | 0.44 |
| 5:M:114:ILE:HG21 | 5:M:150:ILE:HG21 | 1.98 | 0.44 |
| 5:N:159:HIS:O | 5:N:162:PHE:HB2 | 2.17 | 0.44 |
| 4:O:16:VAL:HG22 | 4:P:265:LYS:CE | 2.47 | 0.44 |
| 4:S:58:LEU:O | 4:S:63:MET:HE1 | 2.18 | 0.44 |
| 4:S:118:ILE:HD12 | 4:S:119:PRO:HD2 | 2.00 | 0.44 |
| 5:U:145:VAL:O | 5:U:149:MET:HG3 | 2.18 | 0.44 |
| 1:C:286:PRO:O | 1:C:290:THR:HG23 | 2.18 | 0.44 |
| 1:D:64:VAL:C | 1:D:65:LEU:HD12 | 2.42 | 0.44 |
| 3:F:33:DT:H2'' | 3:F:34:DC:O4' | 2.18 | 0.44 |
| 4:G:247:LYS:C | 4:G:248:LEU:HD22 | 2.43 | 0.44 |
| 4:K:211:THR:CG2 | 5:M:301:MET:HE3 | 2.47 | 0.44 |
| 5:N:128:HIS:CD2 | 5:N:132:LEU:HD11 | 2.52 | 0.44 |
| 5:R:126:LEU:HD11 | 5:R:130:TYR:CZ | 2.53 | 0.44 |
| 4:S:144:MET:HE1 | 5:U:301:MET:N | 2.32 | 0.44 |
| 5:U:280:ARG:HE | 5:U:281:LEU:HD22 | 1.82 | 0.44 |
| 5:V:166:GLU:HA | 5:V:169:PHE:CD1 | 2.53 | 0.44 |
| 2:E:14:DA:C2' | 2:E:15:DA:C8 | 3.00 | 0.44 |
| 3:F:36:DT:H1' | 3:F:37:DA:C8 | 2.53 | 0.44 |
| 4:G:232:PHE:CE2 | 4:K:164:VAL:HA | 2.53 | 0.44 |
| 5:I:286:ASP:N | 5:I:287:PRO:HD2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:159:HIS:HA | 5:J:162:PHE:CG | 2.53 | 0.44 |
| 5:M:166:GLU:O | 5:M:169:PHE:HB2 | 2.18 | 0.44 |
| 4:O:245:THR:OG1 | 5:Q:327:VAL:HG22 | 2.17 | 0.44 |
| 5:R:279:ASN:HB3 | 5:R:283:LYS:NZ | 2.33 | 0.44 |
| 4:T:55:MET:HE1 | 5:V:285:ILE:HG21 | 2.00 | 0.44 |
| 5:V:321:TYR:HA | 5:V:324:ILE:HD12 | 2.00 | 0.44 |
| 1:C:119:ALA:HB3 | 1:C:233:ALA:O | 2.17 | 0.44 |
| 3:F:21:DT:H1' | 3:F:22:DT:H5' | 2.00 | 0.44 |
| 4:G:212:LEU:O | 4:G:216:VAL:HG23 | 2.17 | 0.44 |
| 5:J:246:LEU:HG | 5:J:250:ARG:HE | 1.83 | 0.44 |
| 4:L:138:ARG:HH12 | 4:L:142:VAL:HG21 | 1.83 | 0.44 |
| 5:N:158:TYR:CD1 | 5:N:193:LEU:HD11 | 2.53 | 0.44 |
| 4:O:249:ARG:NE | 4:O:249:ARG:HA | 2.32 | 0.44 |
| 5:Q:165:LEU:HD23 | 5:Q:169:PHE:HE1 | 1.83 | 0.44 |
| 5:Q:167:THR:O | 5:Q:170:ASP:OD1 | 2.36 | 0.44 |
| 5:Q:241:THR:HG22 | 5:Q:242:THR:O | 2.18 | 0.44 |
| 5:R:302:PHE:CD2 | 5:R:306:MET:HE2 | 2.53 | 0.44 |
| 1:A:339:VAL:O | 1:A:342:LEU:HG | 2.18 | 0.43 |
| 1:A:342:LEU:HD12 | 1:A:342:LEU:C | 2.43 | 0.43 |
| 1:B:120:GLY:HA2 | 1:B:234:ILE:C | 2.42 | 0.43 |
| 1:C:221:TYR:CD1 | 1:C:293:PHE:CE1 | 3.05 | 0.43 |
| 1:D:221:TYR:HA | 1:D:293:PHE:HE1 | 1.80 | 0.43 |
| 3:F:32:DC:P | 3:F:32:DC:H2' | 2.58 | 0.43 |
| 4:G:144:MET:HE1 | 5:I:301:MET:CG | 2.48 | 0.43 |
| 4:G:174:LYS:HE3 | 5:U:252:GLU:OE1 | 2.18 | 0.43 |
| 5:J:152:LEU:O | 5:J:162:PHE:HE1 | 2.01 | 0.43 |
| 4:S:89:ALA:HB1 | 5:U:269:ILE:CD1 | 2.48 | 0.43 |
| 1:B:266:ARG:HA | 1:B:286:PRO:HA | 2.00 | 0.43 |
| 1:D:153:MET:HB2 | 1:D:242:ASP:HA | 2.00 | 0.43 |
| 2:E:32:DA:H2'' | 2:E:33:DA:H8 | 1.83 | 0.43 |
| 3:F:44:DT:H3' | 3:F:44:DT:OP1 | 2.18 | 0.43 |
| 4:G:89:ALA:HA | 4:G:102:PHE:CZ | 2.52 | 0.43 |
| 5:J:120:ARG:HG2 | 5:J:151:PHE:CE1 | 2.53 | 0.43 |
| 5:M:286:ASP:N | 5:M:287:PRO:HD2 | 2.33 | 0.43 |
| 5:R:152:LEU:HD11 | 5:R:158:TYR:O | 2.18 | 0.43 |
| 4:S:270:ASP:O | 4:S:274:ILE:HG12 | 2.19 | 0.43 |
| 5:V:243:LEU:HD22 | 5:V:314:CYS:SG | 2.58 | 0.43 |
| 1:D:46:PRO:HG3 | 1:D:60:LEU:HB3 | 1.99 | 0.43 |
| 1:D:46:PRO:HD3 | 1:D:60:LEU:N | 2.33 | 0.43 |
| 1:D:80:HIS:O | 1:D:80:HIS:ND1 | 2.45 | 0.43 |
| 2:E:33:DA:H2'' | 2:E:34:DA:C8 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:46:DT:H1' | 2:E:47:DT:O5' | 2.18 | 0.43 |
| 3:F:50:DT:H2'' | 3:F:51:DT:C6 | 2.54 | 0.43 |
| 4:G:67:LEU:HD12 | 4:G:212:LEU:CD1 | 2.48 | 0.43 |
| 4:L:54:TYR:CD1 | 4:L:213:LEU:HD21 | 2.52 | 0.43 |
| 5:M:149:MET:HE2 | 5:N:150:ILE:HG13 | 2.00 | 0.43 |
| 5:M:298:ALA:HB1 | 5:N:227:ILE:HG21 | 2.00 | 0.43 |
| 5:R:238:ASP:CG | 5:R:239:LYS:H | 2.26 | 0.43 |
| 1:A:17:LYS:C | 1:A:18:LEU:HD22 | 2.43 | 0.43 |
| 1:B:154:TYR:CE2 | 1:B:156:ASP:OD1 | 2.71 | 0.43 |
| 2:E:55:DA:C8 | 2:E:56:DT:H72 | 2.53 | 0.43 |
| 3:F:50:DT:P | 3:F:50:DT:H2' | 2.58 | 0.43 |
| 4:G:233:GLU:OE2 | 4:K:30:GLU:HG3 | 2.18 | 0.43 |
| 5:J:131:SER:HA | 5:J:209:MET:CE | 2.48 | 0.43 |
| 4:K:243:LEU:O | 4:K:246:ASN:OD1 | 2.36 | 0.43 |
| 4:L:210:LEU:HD11 | 5:N:297:ALA:HB2 | 2.00 | 0.43 |
| 5:M:196:MET:HE1 | 5:M:200:THR:HG23 | 1.99 | 0.43 |
| 4:O:211:THR:O | 4:O:214:LEU:HG | 2.19 | 0.43 |
| 5:R:164:LEU:HD21 | 5:R:210:ARG:CD | 2.49 | 0.43 |
| 1:A:28:LYS:HG3 | 1:A:29:PRO:HD3 | 2.01 | 0.43 |
| 1:A:89:ALA:HB3 | 1:A:104:LEU:CB | 2.49 | 0.43 |
| 1:C:227:TYR:OH | 1:C:283:MET:O | 2.37 | 0.43 |
| 1:D:45:ARG:HE | 4:G:276:SER:HB2 | 1.83 | 0.43 |
| 1:D:154:TYR:HA | 1:D:225:LEU:HG | 2.01 | 0.43 |
| 1:D:195:LEU:HD12 | 1:D:199:TRP:HB3 | 2.00 | 0.43 |
| 4:H:222:HIS:HB3 | 4:H:234:TYR:CE1 | 2.54 | 0.43 |
| 4:H:248:LEU:HA | 4:H:256:THR:HB | 2.00 | 0.43 |
| 4:H:262:SER:HA | 5:J:327:VAL:HG21 | 2.00 | 0.43 |
| 4:K:49:LEU:CD2 | 5:M:282:LEU:HD22 | 2.49 | 0.43 |
| 4:K:132:LEU:HD21 | 4:K:226:PHE:CZ | 2.53 | 0.43 |
| 5:M:142:ILE:HD11 | 5:M:221:ILE:HG13 | 2.00 | 0.43 |
| 5:N:202:ASP:OD1 | 5:N:205:THR:HG23 | 2.18 | 0.43 |
| 4:P:264:PHE:C | 4:P:265:LYS:HD3 | 2.44 | 0.43 |
| 5:U:302:PHE:HD1 | 5:U:321:TYR:CE2 | 2.37 | 0.43 |
| 5:V:161:LEU:C | 5:V:161:LEU:HD12 | 2.44 | 0.43 |
| 5:V:301:MET:HE2 | 5:V:301:MET:N | 2.33 | 0.43 |
| 1:A:191:VAL:HG22 | 1:A:192:CYS:N | 2.34 | 0.43 |
| 1:C:147:ILE:HD12 | 1:C:173:ILE:HD13 | 2.01 | 0.43 |
| 1:C:152:ARG:HA | 1:C:152:ARG:HE | 1.81 | 0.43 |
| 1:C:297:ALA:O | 1:C:300:VAL:HG12 | 2.18 | 0.43 |
| 2:E:28:DA:P | 2:E:28:DA:H2' | 2.57 | 0.43 |
| 3:F:16:DT:H2'' | 3:F:17:DT:C7 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:48:DC:C2' | 3:F:49:DG:OP2 | 2.67 | 0.43 |
| 4:H:81:ALA:HB3 | 5:J:263:ILE:HD12 | 2.01 | 0.43 |
| 4:K:12:VAL:HG22 | 4:K:23:GLN:CG | 2.48 | 0.43 |
| 4:L:54:TYR:CE1 | 4:L:213:LEU:HD21 | 2.53 | 0.43 |
| 4:O:126:THR:O | 4:O:133:LEU:HG | 2.19 | 0.43 |
| 5:R:277:PHE:HE1 | 5:R:281:LEU:HD11 | 1.83 | 0.43 |
| 4:S:207:THR:OG1 | 5:U:293:MET:HG3 | 2.18 | 0.43 |
| 4:T:87:THR:HG22 | 4:T:91:ILE:HD11 | 1.99 | 0.43 |
| 1:A:66:ASN:HD22 | 1:B:8:ILE:HG21 | 1.84 | 0.43 |
| 1:A:214:SER:HB3 | 1:A:311:GLU:OE2 | 2.19 | 0.43 |
| 1:A:358:PHE:HB2 | 1:A:360:LEU:HD23 | 2.01 | 0.43 |
| 1:B:151:ASP:O | 1:B:152:ARG:HG3 | 2.18 | 0.43 |
| 1:C:94:LEU:HG | 1:C:94:LEU:O | 2.18 | 0.43 |
| 1:D:286:PRO:HB2 | 1:D:289:ILE:HG22 | 1.98 | 0.43 |
| 2:E:2:DA:H2' | 2:E:3:DT:H71 | 2.00 | 0.43 |
| 2:E:6:DC:H1' | 2:E:7:DA:H5' | 2.00 | 0.43 |
| 4:G:94:ARG:HE | 4:G:260:LEU:CD2 | 2.32 | 0.43 |
| 4:G:140:SER:O | 4:G:143:LYS:HG2 | 2.19 | 0.43 |
| 5:J:126:LEU:O | 5:J:130:TYR:HD1 | 2.01 | 0.43 |
| 4:K:104:ASN:O | 5:M:265:SER:N | 2.52 | 0.43 |
| 5:N:298:ALA:HA | 5:N:301:MET:HE2 | 2.00 | 0.43 |
| 4:O:108:PHE:CD2 | 4:O:134:CYS:SG | 3.12 | 0.43 |
| 4:S:225:ILE:HD12 | 4:S:247:LYS:HG3 | 2.00 | 0.43 |
| 4:T:114:ASN:ND2 | 5:V:311:VAL:HG11 | 2.34 | 0.43 |
| 1:A:203:THR:HG22 | 1:A:204:ALA:N | 2.34 | 0.43 |
| 1:A:220:ILE:HD12 | 1:A:313:ILE:HG21 | 2.00 | 0.43 |
| 1:D:298:LYS:HE3 | 1:D:309:TYR:OH | 2.19 | 0.43 |
| 4:H:55:MET:HG2 | 5:J:281:LEU:HD22 | 2.01 | 0.43 |
| 5:J:124:ARG:HG3 | 5:J:193:LEU:HD12 | 2.00 | 0.43 |
| 4:P:145:LEU:CD1 | 4:P:208:GLN:HB3 | 2.48 | 0.43 |
| 4:S:108:PHE:HE1 | 5:U:263:ILE:HD12 | 1.83 | 0.43 |
| 1:A:72:GLU:OE2 | 1:B:93:ILE:CG2 | 2.62 | 0.43 |
| 1:A:173:ILE:HG22 | 1:A:174:ILE:N | 2.34 | 0.43 |
| 1:A:262:ASN:HB2 | 1:A:281:HIS:ND1 | 2.33 | 0.43 |
| 5:J:117:ARG:CG | 5:J:118:ARG:N | 2.82 | 0.43 |
| 4:K:205:GLU:HA | 4:K:208:GLN:OE1 | 2.19 | 0.43 |
| 4:K:252:MET:C | 4:K:252:MET:SD | 3.02 | 0.43 |
| 5:M:295:TYR:CE1 | 5:M:299:ASN:OD1 | 2.72 | 0.43 |
| 4:O:119:PRO:CG | 5:Q:246:LEU:HD21 | 2.49 | 0.43 |
| 4:O:270:ASP:O | 4:O:271:PHE:C | 2.62 | 0.43 |
| 4:S:111:THR:OG1 | 4:S:137:ASP:HA | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:T:147:ARG:CB | 5:V:300:THR:HG23 | 2.48 | 0.43 |
| 5:U:142:ILE:HA | 5:U:145:VAL:HG22 | 2.00 | 0.43 |
| 1:A:206:ASN:HA | 1:B:25:ARG:NH1 | 2.34 | 0.43 |
| 1:C:154:TYR:CD1 | 1:C:242:ASP:OD1 | 2.72 | 0.43 |
| 1:D:296:TYR:CE2 | 1:D:309:TYR:O | 2.72 | 0.43 |
| 2:E:53:DA:H2'' | 2:E:54:DA:OP2 | 2.18 | 0.43 |
| 3:F:30:DT:H2'' | 3:F:31:DT:C5 | 2.54 | 0.43 |
| 3:F:50:DT:H2'' | 3:F:51:DT:H71 | 2.01 | 0.43 |
| 5:J:146:VAL:O | 5:J:149:MET:HG2 | 2.19 | 0.43 |
| 4:O:54:TYR:HH | 4:O:87:THR:HG22 | 1.82 | 0.43 |
| 4:O:147:ARG:CZ | 5:Q:132:LEU:O | 2.67 | 0.43 |
| 4:O:225:ILE:HD12 | 4:O:247:LYS:HG3 | 2.00 | 0.43 |
| 5:R:175:ARG:NH2 | 5:R:178:MET:SD | 2.92 | 0.43 |
| 4:T:214:LEU:HA | 4:T:217:GLU:HG2 | 2.00 | 0.43 |
| 1:B:73:HIS:CB | 1:B:75:LYS:HE2 | 2.49 | 0.42 |
| 1:B:123:ASN:ND2 | 1:B:126:VAL:HG23 | 2.33 | 0.42 |
| 1:D:239:ASN:ND2 | 1:D:242:ASP:OD1 | 2.51 | 0.42 |
| 1:D:351:MET:HE3 | 1:D:365:VAL:HG21 | 2.00 | 0.42 |
| 2:E:20:DT:C2 | 3:F:40:DG:N2 | 2.87 | 0.42 |
| 2:E:31:DT:H6 | 2:E:31:DT:H2' | 1.71 | 0.42 |
| 4:K:147:ARG:CD | 5:M:300:THR:HG23 | 2.49 | 0.42 |
| 5:M:173:THR:OG1 | 5:R:173:THR:N | 2.52 | 0.42 |
| 4:O:78:ARG:HA | 5:Q:261:GLN:HG2 | 2.01 | 0.42 |
| 4:O:91:ILE:HG21 | 4:O:220:TYR:CG | 2.54 | 0.42 |
| 5:R:178:MET:CE | 5:R:186:LEU:HD23 | 2.49 | 0.42 |
| 5:V:123:ALA:HA | 5:V:148:THR:HG23 | 2.00 | 0.42 |
| 1:A:24:MET:HE2 | 1:B:203:THR:HG21 | 2.01 | 0.42 |
| 1:C:43:VAL:HG22 | 1:C:44:THR:N | 2.34 | 0.42 |
| 1:C:199:TRP:NE1 | 1:D:102:CYS:HB2 | 2.34 | 0.42 |
| 3:F:57:DT:H1' | 3:F:58:DA:O5' | 2.19 | 0.42 |
| 4:G:133:LEU:N | 4:G:133:LEU:HD12 | 2.34 | 0.42 |
| 4:G:155:VAL:CG1 | 5:J:229:LEU:HD12 | 2.49 | 0.42 |
| 4:H:119:PRO:O | 5:J:305:THR:HG23 | 2.19 | 0.42 |
| 4:K:109:VAL:N | 4:K:133:LEU:HD11 | 2.34 | 0.42 |
| 5:N:123:ALA:HA | 5:N:148:THR:OG1 | 2.19 | 0.42 |
| 4:O:26:TYR:CD2 | 5:R:306:MET:HE1 | 2.54 | 0.42 |
| 4:O:89:ALA:O | 5:Q:269:ILE:HD11 | 2.19 | 0.42 |
| 5:Q:126:LEU:CD2 | 5:Q:148:THR:HG21 | 2.49 | 0.42 |
| 5:Q:172:TYR:CG | 5:Q:214:ALA:HB1 | 2.54 | 0.42 |
| 5:R:164:LEU:HD21 | 5:R:210:ARG:CG | 2.49 | 0.42 |
| 4:S:144:MET:HE2 | 5:U:301:MET:SD | 2.59 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:U:318:ILE:HD12 | 5:U:321:TYR:HB3 | 2.00 | 0.42 |
| 5:V:119:TYR:HB3 | 5:V:151:PHE:HB2 | 2.00 | 0.42 |
| 5:V:163:LYS:HA | 5:V:166:GLU:CG | 2.49 | 0.42 |
| 1:A:295:HIS:HB2 | 1:A:312:LEU:HD21 | 2.01 | 0.42 |
| 1:C:260:CYS:HB2 | 1:C:267:VAL:O | 2.19 | 0.42 |
| 1:D:269:CYS:HA | 1:D:272:LEU:HD23 | 2.01 | 0.42 |
| 3:F:58:DA:O5' | 3:F:58:DA:H8 | 2.02 | 0.42 |
| 5:N:298:ALA:O | 5:N:301:MET:HG2 | 2.19 | 0.42 |
| 5:Q:249:GLU:O | 5:Q:253:LYS:HG2 | 2.19 | 0.42 |
| 5:R:301:MET:HE2 | 5:R:301:MET:CA | 2.49 | 0.42 |
| 4:S:54:TYR:CE1 | 4:S:213:LEU:HD21 | 2.54 | 0.42 |
| 1:A:301:ARG:HH11 | 1:B:16:VAL:HG13 | 1.85 | 0.42 |
| 1:B:290:THR:O | 1:B:294:PHE:HD2 | 2.02 | 0.42 |
| 1:C:288:GLU:O | 1:C:292:LYS:HG2 | 2.20 | 0.42 |
| 4:G:62:GLU:OE1 | 4:G:62:GLU:O | 2.37 | 0.42 |
| 4:G:202:THR:HG22 | 4:G:205:GLU:CD | 2.44 | 0.42 |
| 5:I:161:LEU:HD12 | 5:I:186:LEU:HD13 | 2.01 | 0.42 |
| 5:M:229:LEU:HB3 | 5:M:306:MET:HE2 | 2.01 | 0.42 |
| 4:O:270:ASP:C | 4:O:274:ILE:HG12 | 2.44 | 0.42 |
| 5:Q:217:PHE:C | 5:R:141:LYS:HZ2 | 2.27 | 0.42 |
| 5:Q:272:CYS:SG | 5:Q:274:ASP:OD1 | 2.74 | 0.42 |
| 4:S:233:GLU:HA | 4:S:236:LYS:HG2 | 2.01 | 0.42 |
| 1:B:105:ILE:HG12 | 1:B:165:ILE:HD13 | 2.00 | 0.42 |
| 1:C:94:LEU:HD23 | 1:C:94:LEU:H | 1.83 | 0.42 |
| 1:D:344:LEU:O | 1:D:348:GLU:HG2 | 2.19 | 0.42 |
| 1:D:354:PHE:O | 1:D:357:TYR:HB3 | 2.20 | 0.42 |
| 2:E:1:DT:H2'' | 2:E:2:DA:O5' | 2.20 | 0.42 |
| 4:H:74:LYS:NZ | 4:H:138:ARG:NH2 | 2.67 | 0.42 |
| 5:M:123:ALA:HA | 5:M:148:THR:HG23 | 2.01 | 0.42 |
| 5:M:239:LYS:C | 5:M:313:ASN:ND2 | 2.78 | 0.42 |
| 4:S:92:HIS:HE2 | 4:S:99:VAL:HG21 | 1.84 | 0.42 |
| 4:S:201:ILE:HG22 | 4:S:202:THR:N | 2.35 | 0.42 |
| 4:T:67:LEU:HD11 | 4:T:212:LEU:CD2 | 2.49 | 0.42 |
| 5:V:161:LEU:HD12 | 5:V:162:PHE:N | 2.33 | 0.42 |
| 5:V:213:PHE:HB3 | 5:V:217:PHE:CZ | 2.54 | 0.42 |
| 1:A:58:ASP:OD1 | 1:A:106:ARG:HB2 | 2.19 | 0.42 |
| 1:B:69:PHE:O | 1:B:76:LEU:HD12 | 2.20 | 0.42 |
| 1:B:153:MET:HG3 | 1:B:242:ASP:O | 2.19 | 0.42 |
| 1:C:69:PHE:CE1 | 1:C:170:SER:C | 2.98 | 0.42 |
| 1:C:238:ASN:OD1 | 1:C:238:ASN:O | 2.37 | 0.42 |
| 1:D:45:ARG:HG3 | 1:D:58:ASP:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:108:ILE:HD11 | 1:D:162:PHE:CE2 | 2.53 | 0.42 |
| 3:F:34:DC:H2'' | 3:F:35:DC:H6 | 1.81 | 0.42 |
| 4:G:167:ALA:CB | 4:S:232:PHE:HD1 | 2.31 | 0.42 |
| 5:I:250:ARG:O | 5:I:254:ILE:HG12 | 2.20 | 0.42 |
| 5:N:117:ARG:HA | 5:N:120:ARG:HG2 | 2.00 | 0.42 |
| 5:R:156:GLU:HA | 5:R:159:HIS:CG | 2.54 | 0.42 |
| 4:S:125:PHE:HA | 4:S:133:LEU:O | 2.20 | 0.42 |
| 1:A:71:ASN:ND2 | 1:A:75:LYS:HE3 | 2.35 | 0.42 |
| 1:A:257:LEU:HD23 | 1:A:267:VAL:HG22 | 2.01 | 0.42 |
| 1:B:88:GLU:HB3 | 1:B:104:LEU:HG | 2.02 | 0.42 |
| 1:C:19:THR:OG1 | 1:D:302:ASN:HA | 2.20 | 0.42 |
| 1:C:30:MET:CE | 1:C:64:VAL:HG23 | 2.50 | 0.42 |
| 1:C:147:ILE:HD12 | 1:C:173:ILE:CD1 | 2.50 | 0.42 |
| 2:E:27:DG:H2'' | 2:E:28:DA:H8 | 1.78 | 0.42 |
| 2:E:34:DA:C8 | 2:E:34:DA:O5' | 2.73 | 0.42 |
| 4:K:140:SER:O | 4:K:144:MET:HG2 | 2.20 | 0.42 |
| 5:Q:131:SER:CA | 5:Q:209:MET:HE1 | 2.50 | 0.42 |
| 5:Q:304:THR:HA | 5:Q:307:GLU:HG2 | 2.01 | 0.42 |
| 5:V:129:HIS:CE1 | 5:V:137:SER:CB | 3.02 | 0.42 |
| 5:V:190:VAL:HB | 5:V:201:ILE:CD1 | 2.49 | 0.42 |
| 1:A:45:ARG:H | 1:A:45:ARG:HD3 | 1.85 | 0.42 |
| 1:A:93:ILE:HG23 | 1:A:100:TYR:HB2 | 2.01 | 0.42 |
| 1:C:213:GLU:HG2 | 1:C:314:ALA:HB3 | 2.01 | 0.42 |
| 1:D:62:MET:HA | 1:D:101:GLU:O | 2.19 | 0.42 |
| 1:D:104:LEU:C | 1:D:105:ILE:HD12 | 2.45 | 0.42 |
| 2:E:1:DT:H1' | 2:E:2:DA:O4' | 2.20 | 0.42 |
| 3:F:43:DT:H1' | 3:F:44:DT:H5' | 2.02 | 0.42 |
| 4:H:144:MET:CE | 4:H:147:ARG:HE | 2.32 | 0.42 |
| 4:H:210:LEU:HD21 | 5:J:294:TYR:HD1 | 1.84 | 0.42 |
| 5:M:171:ASP:C | 5:M:172:TYR:CD2 | 2.98 | 0.42 |
| 4:S:51:LEU:O | 4:S:55:MET:SD | 2.78 | 0.42 |
| 4:T:213:LEU:HD23 | 4:T:260:LEU:HD11 | 2.02 | 0.42 |
| 5:V:306:MET:HE1 | 5:V:316:PHE:CD1 | 2.55 | 0.42 |
| 5:V:317:ASN:CG | 5:V:320:ASP:HB3 | 2.44 | 0.42 |
| 1:A:149:ILE:HG21 | 1:A:152:ARG:O | 2.20 | 0.42 |
| 1:C:147:ILE:C | 1:C:148:LEU:HD12 | 2.44 | 0.42 |
| 2:E:27:DG:N2 | 3:F:33:DT:O2 | 2.53 | 0.42 |
| 2:E:34:DA:H2'' | 2:E:35:DA:O5' | 2.20 | 0.42 |
| 3:F:11:DA:O5' | 3:F:11:DA:C8 | 2.72 | 0.42 |
| 4:G:43:GLU:O | 4:G:46:LYS:HG2 | 2.20 | 0.42 |
| 5:I:249:GLU:OE2 | 5:I:253:LYS:HG3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:I:297:ALA:O | 5:I:300:THR:HG22 | 2.20 | 0.42 |
| 5:M:127:ILE:HD11 | 5:M:194:LEU:HA | 2.01 | 0.42 |
| 5:M:233:VAL:CG2 | 5:M:310:ALA:HB1 | 2.49 | 0.42 |
| 4:O:137:ASP:OD2 | 4:O:140:SER:HB3 | 2.20 | 0.42 |
| 4:P:226:PHE:HB2 | 4:P:234:TYR:CD1 | 2.55 | 0.42 |
| 5:Q:245:GLU:O | 5:Q:249:GLU:HG3 | 2.19 | 0.42 |
| 4:T:138:ARG:NH1 | 4:T:142:VAL:HG21 | 2.35 | 0.42 |
| 5:U:246:LEU:HD11 | 5:U:250:ARG:NH1 | 2.35 | 0.42 |
| 5:U:302:PHE:CD1 | 5:V:227:ILE:HD11 | 2.55 | 0.42 |
| 1:A:78:TYR:CZ | 1:A:168:PRO:HA | 2.54 | 0.42 |
| 1:B:8:ILE:C | 1:B:9:LYS:HD3 | 2.45 | 0.42 |
| 1:B:195:LEU:HB3 | 1:B:199:TRP:HB2 | 2.02 | 0.42 |
| 1:C:30:MET:HA | 1:C:42:LYS:HG3 | 2.02 | 0.42 |
| 1:C:219:TYR:O | 1:C:222:ARG:HG2 | 2.20 | 0.42 |
| 1:D:283:MET:HE1 | 1:D:354:PHE:CE2 | 2.54 | 0.42 |
| 4:G:118:ILE:CD1 | 5:I:247:LEU:HD23 | 2.50 | 0.42 |
| 4:G:138:ARG:NH1 | 4:G:142:VAL:HG21 | 2.35 | 0.42 |
| 5:J:130:TYR:HB3 | 5:J:209:MET:SD | 2.60 | 0.42 |
| 4:K:61:LEU:C | 4:K:62:GLU:HG3 | 2.45 | 0.42 |
| 4:K:98:LEU:HG | 4:K:99:VAL:HG23 | 2.02 | 0.42 |
| 5:N:123:ALA:HA | 5:N:148:THR:HG23 | 2.02 | 0.42 |
| 4:O:151:THR:O | 4:O:151:THR:CG2 | 2.68 | 0.42 |
| 4:S:145:LEU:HD11 | 4:S:208:GLN:CB | 2.50 | 0.42 |
| 4:S:226:PHE:HB2 | 4:S:234:TYR:CD1 | 2.55 | 0.42 |
| 1:A:152:ARG:HD3 | 1:A:154:TYR:CE1 | 2.55 | 0.41 |
| 1:A:271:ASP:OD1 | 1:A:272:LEU:HD22 | 2.20 | 0.41 |
| 1:B:153:MET:SD | 1:B:294:PHE:CE1 | 3.13 | 0.41 |
| 1:C:69:PHE:CE1 | 1:C:172:TYR:CD1 | 3.08 | 0.41 |
| 1:D:288:GLU:HG2 | 1:D:343:HIS:NE2 | 2.35 | 0.41 |
| 1:D:293:PHE:CD1 | 1:D:313:ILE:HD11 | 2.55 | 0.41 |
| 2:E:17:DA:H1' | 2:E:18:DC:C6 | 2.55 | 0.41 |
| 3:F:53:DG:H2'' | 3:F:54:DG:C8 | 2.55 | 0.41 |
| 4:G:201:ILE:C | 5:I:284:HIS:HE2 | 2.27 | 0.41 |
| 4:G:263:LYS:HE3 | 5:I:290:LEU:HD11 | 2.02 | 0.41 |
| 4:K:32:ASP:O | 4:K:36:LEU:HD23 | 2.20 | 0.41 |
| 5:N:246:LEU:HD22 | 5:N:312:SER:HB2 | 2.02 | 0.41 |
| 4:P:207:THR:OG1 | 5:R:293:MET:HE3 | 2.20 | 0.41 |
| 1:C:94:LEU:HD11 | 1:D:70:LEU:HD23 | 2.01 | 0.41 |
| 3:F:53:DG:H2'' | 3:F:54:DG:H8 | 1.85 | 0.41 |
| 4:H:166:ILE:HD13 | 5:V:248:ILE:CG1 | 2.50 | 0.41 |
| 5:N:153:LEU:HD23 | 5:N:153:LEU:C | 2.45 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:Q:317:ASN:ND2 | 5:Q:320:ASP:HB2 | 2.35 | 0.41 |
| 5:Q:322:ASN:O | 5:Q:326:LYS:HG2 | 2.20 | 0.41 |
| 5:U:297:ALA:O | 5:U:301:MET:SD | 2.78 | 0.41 |
| 1:A:190:ASP:OD1 | 1:A:190:ASP:O | 2.38 | 0.41 |
| 1:B:292:LYS:HG2 | 1:B:312:LEU:HD23 | 2.01 | 0.41 |
| 1:C:67:SER:HA | 1:C:70:LEU:HD23 | 2.01 | 0.41 |
| 1:D:65:LEU:HB2 | 1:D:99:VAL:HG23 | 2.01 | 0.41 |
| 1:D:137:TYR:CD1 | 1:D:137:TYR:C | 2.97 | 0.41 |
| 3:F:25:DT:H1' | 3:F:26:DT:H5' | 2.03 | 0.41 |
| 3:F:53:DG:H1' | 3:F:54:DG:O5' | 2.19 | 0.41 |
| 5:I:126:LEU:CD2 | 5:I:148:THR:HG21 | 2.51 | 0.41 |
| 5:J:130:TYR:O | 5:J:209:MET:HE1 | 2.20 | 0.41 |
| 5:J:205:THR:O | 5:J:209:MET:HG2 | 2.19 | 0.41 |
| 5:M:245:GLU:O | 5:M:249:GLU:HG3 | 2.20 | 0.41 |
| 5:M:249:GLU:HB2 | 5:M:253:LYS:NZ | 2.35 | 0.41 |
| 5:M:311:VAL:C | 5:M:313:ASN:N | 2.78 | 0.41 |
| 5:Q:179:THR:HG23 | 5:Q:182:GLN:H | 1.85 | 0.41 |
| 5:Q:196:MET:HE1 | 5:Q:200:THR:HA | 2.02 | 0.41 |
| 4:S:56:ALA:CB | 5:U:278:LEU:HD23 | 2.50 | 0.41 |
| 4:S:233:GLU:CD | 4:S:236:LYS:HZ3 | 2.28 | 0.41 |
| 4:S:248:LEU:HD12 | 4:S:252:MET:CB | 2.51 | 0.41 |
| 4:T:111:THR:HG22 | 5:V:257:LEU:CD1 | 2.50 | 0.41 |
| 5:U:132:LEU:HD11 | 5:U:303:TYR:CD1 | 2.55 | 0.41 |
| 1:B:10:LEU:HD12 | 1:B:12:LEU:HD13 | 2.01 | 0.41 |
| 1:B:131:ILE:HA | 1:B:134:VAL:HG12 | 2.01 | 0.41 |
| 1:B:257:LEU:O | 1:B:268:LYS:HB3 | 2.20 | 0.41 |
| 1:B:296:TYR:CD1 | 1:B:309:TYR:O | 2.73 | 0.41 |
| 1:C:220:ILE:HD11 | 1:C:313:ILE:CG2 | 2.32 | 0.41 |
| 1:D:138:ILE:HD11 | 1:D:226:LEU:HD11 | 2.01 | 0.41 |
| 1:D:156:ASP:H | 1:D:169:GLN:NE2 | 2.18 | 0.41 |
| 1:D:246:GLU:OE1 | 1:D:246:GLU:N | 2.52 | 0.41 |
| 3:F:30:DT:H2' | 3:F:30:DT:H6 | 1.70 | 0.41 |
| 4:K:232:PHE:CE2 | 4:O:33:LEU:HD13 | 2.54 | 0.41 |
| 5:N:116:MET:SD | 5:R:180:GLN:CD | 3.04 | 0.41 |
| 4:P:110:VAL:HG12 | 4:P:112:GLU:OE2 | 2.20 | 0.41 |
| 5:Q:132:LEU:HD12 | 5:Q:303:TYR:CD2 | 2.55 | 0.41 |
| 4:S:34:LYS:HE3 | 5:V:307:GLU:OE2 | 2.19 | 0.41 |
| 5:U:219:SER:O | 5:V:142:ILE:HD12 | 2.20 | 0.41 |
| 1:A:257:LEU:CD2 | 1:A:267:VAL:HG22 | 2.51 | 0.41 |
| 1:A:289:ILE:HD11 | 1:A:343:HIS:O | 2.20 | 0.41 |
| 1:D:46:PRO:HG3 | 1:D:60:LEU:CB | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:133:ALA:O | 1:D:136:LYS:HG3 | 2.20 | 0.41 |
| 3:F:44:DT:H6 | 3:F:44:DT:H2' | 1.70 | 0.41 |
| 4:G:88:LEU:CD1 | 4:G:102:PHE:HE2 | 2.33 | 0.41 |
| 4:G:92:HIS:O | 4:G:96:HIS:N | 2.53 | 0.41 |
| 4:G:104:ASN:O | 5:I:265:SER:N | 2.54 | 0.41 |
| 4:G:201:ILE:HB | 5:I:284:HIS:NE2 | 2.35 | 0.41 |
| 4:K:82:ALA:HA | 5:M:263:ILE:HD11 | 2.02 | 0.41 |
| 5:M:152:LEU:O | 5:M:159:HIS:HD2 | 2.02 | 0.41 |
| 5:M:233:VAL:HG22 | 5:M:310:ALA:HB1 | 2.02 | 0.41 |
| 5:Q:150:ILE:HD11 | 5:R:149:MET:HE1 | 2.02 | 0.41 |
| 5:Q:228:VAL:HG23 | 5:R:224:TYR:CE2 | 2.56 | 0.41 |
| 5:Q:244:GLU:HG2 | 5:Q:245:GLU:N | 2.36 | 0.41 |
| 1:B:89:ALA:HB3 | 1:B:104:LEU:HB3 | 2.01 | 0.41 |
| 1:B:244:ILE:O | 1:B:301:ARG:NH2 | 2.54 | 0.41 |
| 1:B:295:HIS:HB2 | 1:B:312:LEU:HD21 | 2.02 | 0.41 |
| 1:C:71:ASN:ND2 | 1:C:75:LYS:HE3 | 2.36 | 0.41 |
| 1:C:166:ILE:HD12 | 1:C:166:ILE:HA | 1.96 | 0.41 |
| 3:F:14:DT:H1' | 3:F:15:DT:C5' | 2.50 | 0.41 |
| 3:F:26:DT:H2'' | 3:F:27:DT:H71 | 2.02 | 0.41 |
| 4:G:137:ASP:OD2 | 4:G:140:SER:HB2 | 2.21 | 0.41 |
| 5:I:146:VAL:HG12 | 5:I:150:ILE:HD12 | 2.02 | 0.41 |
| 4:O:151:THR:HG23 | 4:O:203:GLU:HG2 | 2.02 | 0.41 |
| 4:O:234:TYR:CE2 | 4:O:238:LEU:HD11 | 2.55 | 0.41 |
| 4:S:203:GLU:HG3 | 5:U:293:MET:SD | 2.61 | 0.41 |
| 4:T:48:LYS:HG3 | 5:V:282:LEU:HD11 | 2.02 | 0.41 |
| 4:T:231:VAL:O | 4:T:234:TYR:HB3 | 2.21 | 0.41 |
| 5:U:151:PHE:CE2 | 5:U:193:LEU:HD13 | 2.56 | 0.41 |
| 5:U:171:ASP:O | 5:U:172:TYR:CD2 | 2.74 | 0.41 |
| 1:B:10:LEU:HD23 | 1:B:10:LEU:H | 1.86 | 0.41 |
| 1:B:225:LEU:O | 1:B:229:THR:HG23 | 2.20 | 0.41 |
| 1:C:32:CYS:HA | 1:C:43:VAL:H | 1.86 | 0.41 |
| 1:D:71:ASN:ND2 | 1:D:75:LYS:HB3 | 2.34 | 0.41 |
| 2:E:15:DA:H1' | 2:E:16:DA:O5' | 2.20 | 0.41 |
| 3:F:17:DT:C1' | 3:F:18:DT:O5' | 2.67 | 0.41 |
| 4:H:235:CYS:HA | 4:H:238:LEU:HD12 | 2.02 | 0.41 |
| 5:I:277:PHE:HE1 | 5:I:281:LEU:HD11 | 1.85 | 0.41 |
| 4:O:102:PHE:CG | 4:O:103:THR:N | 2.89 | 0.41 |
| 4:O:151:THR:HG23 | 4:O:203:GLU:CG | 2.50 | 0.41 |
| 4:P:109:VAL:HB | 4:P:133:LEU:HD11 | 2.03 | 0.41 |
| 5:R:117:ARG:HA | 5:R:117:ARG:NE | 2.36 | 0.41 |
| 4:S:108:PHE:HB2 | 5:U:261:GLN:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:144:MET:HE1 | 5:U:300:THR:HB | 2.01 | 0.41 |
| 4:T:123:ILE:HG21 | 4:T:219:ALA:HB1 | 2.02 | 0.41 |
| 1:A:31:GLN:NE2 | 1:A:43:VAL:O | 2.54 | 0.41 |
| 1:A:298:LYS:O | 1:A:301:ARG:HG2 | 2.21 | 0.41 |
| 1:B:286:PRO:HD2 | 1:B:347:TRP:CE3 | 2.56 | 0.41 |
| 1:C:131:ILE:HA | 1:C:134:VAL:HG12 | 2.02 | 0.41 |
| 1:C:349:ASN:O | 1:C:350:PHE:C | 2.64 | 0.41 |
| 3:F:3:DA:C2' | 3:F:4:DT:H71 | 2.51 | 0.41 |
| 3:F:11:DA:H1' | 3:F:12:DA:C5' | 2.51 | 0.41 |
| 3:F:15:DT:H2'' | 3:F:16:DT:C6 | 2.56 | 0.41 |
| 4:G:56:ALA:HB1 | 5:I:272:CYS:CB | 2.51 | 0.41 |
| 4:G:58:LEU:O | 4:G:61:LEU:HB2 | 2.21 | 0.41 |
| 4:G:145:LEU:HD22 | 4:G:208:GLN:HG2 | 2.02 | 0.41 |
| 4:G:244:PHE:CB | 5:I:327:VAL:HG11 | 2.51 | 0.41 |
| 5:J:124:ARG:CG | 5:J:193:LEU:HD12 | 2.51 | 0.41 |
| 5:J:241:THR:O | 5:J:314:CYS:HA | 2.21 | 0.41 |
| 4:O:268:ILE:HD11 | 5:Q:321:TYR:HD2 | 1.85 | 0.41 |
| 4:T:210:LEU:O | 4:T:214:LEU:HG | 2.20 | 0.41 |
| 1:A:24:MET:HA | 1:B:206:ASN:N | 2.36 | 0.41 |
| 1:A:196:GLU:O | 1:A:199:TRP:N | 2.54 | 0.41 |
| 1:A:220:ILE:CD1 | 1:A:313:ILE:HG21 | 2.51 | 0.41 |
| 1:B:78:TYR:OH | 1:B:101:GLU:HG2 | 2.21 | 0.41 |
| 1:B:220:ILE:HG23 | 1:B:347:TRP:CD1 | 2.55 | 0.41 |
| 1:B:227:TYR:O | 1:B:231:LEU:HG | 2.20 | 0.41 |
| 1:B:267:VAL:HG12 | 1:B:268:LYS:N | 2.36 | 0.41 |
| 2:E:53:DA:C6 | 2:E:54:DA:C6 | 3.09 | 0.41 |
| 4:G:37:SER:O | 4:G:40:GLU:HG2 | 2.21 | 0.41 |
| 5:J:117:ARG:HG3 | 5:J:118:ARG:N | 2.35 | 0.41 |
| 4:K:13:THR:HG23 | 4:L:266:PHE:HD1 | 1.86 | 0.41 |
| 4:K:143:LYS:HG2 | 5:M:307:GLU:OE2 | 2.20 | 0.41 |
| 4:K:243:LEU:CD2 | 4:K:247:LYS:HG3 | 2.50 | 0.41 |
| 4:L:68:LEU:HD11 | 4:L:72:ARG:NH1 | 2.35 | 0.41 |
| 5:M:119:TYR:CG | 5:M:147:MET:SD | 3.14 | 0.41 |
| 5:M:171:ASP:O | 5:M:172:TYR:CG | 2.73 | 0.41 |
| 5:N:152:LEU:O | 5:N:162:PHE:HE1 | 2.04 | 0.41 |
| 5:N:250:ARG:O | 5:N:254:ILE:HG12 | 2.21 | 0.41 |
| 4:O:55:MET:HE1 | 4:O:209:TYR:CD1 | 2.56 | 0.41 |
| 4:O:91:ILE:HG23 | 4:O:94:ARG:NH2 | 2.36 | 0.41 |
| 4:O:132:LEU:HD21 | 4:O:226:PHE:CE1 | 2.56 | 0.41 |
| 4:T:67:LEU:HD13 | 4:T:209:TYR:CE1 | 2.56 | 0.41 |
| 4:T:138:ARG:O | 4:T:141:ILE:HG22 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:U:140:TYR:HB3 | 5:V:221:ILE:HD11 | 2.02 | 0.41 |
| 5:U:286:ASP:N | 5:U:287:PRO:HD2 | 2.36 | 0.41 |
| 5:V:243:LEU:O | 5:V:247:LEU:HD13 | 2.21 | 0.41 |
| 5:V:244:GLU:HG2 | 5:V:245:GLU:N | 2.36 | 0.41 |
| 1:A:60:LEU:HA | 1:A:103:MET:O | 2.21 | 0.41 |
| 1:A:178:TYR:HB3 | 1:A:210:SER:O | 2.21 | 0.41 |
| 1:B:9:LYS:HA | 1:B:16:VAL:O | 2.20 | 0.41 |
| 1:B:37:ARG:HD2 | 1:B:37:ARG:N | 2.36 | 0.41 |
| 1:B:132:ASP:HA | 1:B:135:ILE:HG22 | 2.03 | 0.41 |
| 1:B:154:TYR:HB2 | 1:B:229:THR:HG22 | 2.03 | 0.41 |
| 1:B:347:TRP:O | 1:B:351:MET:SD | 2.79 | 0.41 |
| 1:D:155:VAL:CG2 | 1:D:166:ILE:HD11 | 2.51 | 0.41 |
| 1:D:156:ASP:HB3 | 1:D:167:LEU:HD12 | 2.03 | 0.41 |
| 2:E:17:DA:H1' | 2:E:18:DC:O5' | 2.21 | 0.41 |
| 2:E:34:DA:P | 2:E:34:DA:H2' | 2.60 | 0.41 |
| 4:G:24:LYS:HD2 | 5:J:295:TYR:OH | 2.20 | 0.41 |
| 4:G:147:ARG:HD2 | 5:I:300:THR:OG1 | 2.21 | 0.41 |
| 4:G:203:GLU:HG2 | 5:I:293:MET:CE | 2.51 | 0.41 |
| 4:H:248:LEU:O | 4:H:248:LEU:HD23 | 2.21 | 0.41 |
| 5:J:126:LEU:HD22 | 5:J:148:THR:CG2 | 2.45 | 0.41 |
| 5:J:164:LEU:HD23 | 5:J:210:ARG:HE | 1.85 | 0.41 |
| 5:J:167:THR:O | 5:J:173:THR:HG21 | 2.21 | 0.41 |
| 4:P:261:LEU:HD12 | 4:P:262:SER:N | 2.36 | 0.41 |
| 5:U:226:LYS:HE2 | 5:U:226:LYS:HA | 2.03 | 0.41 |
| 1:A:95:ASN:HB3 | 1:A:98:SER:OG | 2.21 | 0.40 |
| 1:B:221:TYR:CD1 | 1:B:296:TYR:HD2 | 2.39 | 0.40 |
| 1:C:87:ALA:HB2 | 1:C:165:ILE:HD11 | 2.03 | 0.40 |
| 1:C:120:GLY:HA2 | 1:C:234:ILE:O | 2.21 | 0.40 |
| 1:C:244:ILE:O | 1:C:244:ILE:CG2 | 2.68 | 0.40 |
| 1:C:270:CYS:HA | 1:C:280:GLY:HA2 | 2.03 | 0.40 |
| 1:D:22:LYS:HB2 | 1:D:95:ASN:OD1 | 2.20 | 0.40 |
| 3:F:39:DA:H2'' | 3:F:40:DG:O5' | 2.21 | 0.40 |
| 5:J:174:CYS:SG | 5:U:176:PRO:HA | 2.61 | 0.40 |
| 5:M:295:TYR:O | 5:M:299:ASN:OD1 | 2.39 | 0.40 |
| 4:O:126:THR:O | 4:O:126:THR:HG23 | 2.21 | 0.40 |
| 4:O:127:GLU:HA | 4:O:132:LEU:HA | 2.04 | 0.40 |
| 5:Q:122:ALA:HA | 5:Q:125:LYS:HG2 | 2.04 | 0.40 |
| 4:S:51:LEU:HB3 | 4:S:55:MET:HE1 | 2.03 | 0.40 |
| 4:T:116:THR:HG21 | 5:V:257:LEU:HD11 | 2.03 | 0.40 |
| 5:U:251:GLY:HA2 | 5:U:254:ILE:HG22 | 2.03 | 0.40 |
| 5:U:254:ILE:HG23 | 5:U:255:GLN:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:35:HIS:HA | 1:B:38:ARG:NH2 | 2.35 | 0.40 |
| 1:B:148:LEU:HD13 | 1:B:300:VAL:HA | 2.03 | 0.40 |
| 1:B:198:PRO:O | 1:B:202:ILE:HD12 | 2.21 | 0.40 |
| 1:B:260:CYS:HB3 | 1:B:263:ASN:O | 2.21 | 0.40 |
| 1:B:310:SER:OG | 1:B:311:GLU:OE1 | 2.39 | 0.40 |
| 1:C:90:ARG:HB3 | 1:C:101:GLU:OE2 | 2.21 | 0.40 |
| 1:C:157:LEU:HA | 1:C:167:LEU:HG | 2.02 | 0.40 |
| 1:C:224:PHE:HD2 | 1:C:293:PHE:HB2 | 1.87 | 0.40 |
| 1:D:198:PRO:O | 1:D:201:LEU:HG | 2.21 | 0.40 |
| 1:D:235:LEU:HD22 | 1:D:237:GLN:NE2 | 2.36 | 0.40 |
| 3:F:10:DT:C1' | 3:F:11:DA:O5' | 2.63 | 0.40 |
| 3:F:14:DT:H6 | 3:F:14:DT:H2' | 1.65 | 0.40 |
| 3:F:28:DA:C4 | 3:F:29:DC:C4 | 3.09 | 0.40 |
| 3:F:51:DT:C2' | 3:F:52:DT:H72 | 2.51 | 0.40 |
| 5:I:242:THR:CG2 | 5:I:315:LYS:HZ3 | 2.34 | 0.40 |
| 5:M:205:THR:HA | 5:M:208:ILE:HD12 | 2.03 | 0.40 |
| 5:R:152:LEU:HG | 5:R:162:PHE:HB2 | 2.03 | 0.40 |
| 4:S:10:ARG:HH11 | 4:S:12:VAL:HG23 | 1.87 | 0.40 |
| 4:S:71:PHE:O | 4:S:138:ARG:HD2 | 2.20 | 0.40 |
| 5:U:124:ARG:O | 5:U:128:HIS:CG | 2.75 | 0.40 |
| 5:U:132:LEU:HD11 | 5:U:303:TYR:CE1 | 2.55 | 0.40 |
| 5:U:277:PHE:CZ | 5:U:281:LEU:HD21 | 2.55 | 0.40 |
| 5:V:277:PHE:O | 5:V:280:ARG:HG2 | 2.22 | 0.40 |
| 1:A:175:LYS:HG2 | 1:A:192:CYS:SG | 2.62 | 0.40 |
| 1:B:250:ILE:HD12 | 1:B:253:ILE:HB | 2.03 | 0.40 |
| 1:B:264:LYS:HD2 | 1:B:265:ASP:N | 2.37 | 0.40 |
| 1:C:128:LYS:O | 1:C:132:ASP:CG | 2.64 | 0.40 |
| 1:C:268:LYS:HG3 | 1:C:268:LYS:O | 2.21 | 0.40 |
| 1:D:153:MET:HE1 | 1:D:297:ALA:CB | 2.51 | 0.40 |
| 1:D:198:PRO:HG2 | 1:D:199:TRP:CE3 | 2.56 | 0.40 |
| 2:E:45:DA:OP2 | 2:E:45:DA:H8 | 2.03 | 0.40 |
| 3:F:21:DT:H1' | 3:F:22:DT:C5' | 2.52 | 0.40 |
| 4:G:222:HIS:CE1 | 4:G:238:LEU:HD23 | 2.56 | 0.40 |
| 5:J:183:THR:HG23 | 5:J:203:LEU:HD21 | 2.03 | 0.40 |
| 4:K:244:PHE:HB2 | 5:M:327:VAL:HG11 | 2.03 | 0.40 |
| 5:N:140:TYR:C | 5:N:141:LYS:HD3 | 2.47 | 0.40 |
| 5:N:306:MET:HA | 5:N:306:MET:HE2 | 2.02 | 0.40 |
| 5:Q:295:TYR:CD1 | 5:Q:299:ASN:OD1 | 2.74 | 0.40 |
| 5:R:168:THR:HG21 | 5:R:210:ARG:HG3 | 2.03 | 0.40 |
| 4:S:144:MET:CE | 5:U:301:MET:SD | 3.09 | 0.40 |
| 1:B:135:ILE:HD11 | 1:B:364:ASN:OD1 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:69:PHE:CE2 | 1:C:170:SER:HB2 | 2.57 | 0.40 |
| 2:E:2:DA:C2' | 2:E:3:DT:H71 | 2.52 | 0.40 |
| 2:E:53:DA:O5' | 2:E:53:DA:C8 | 2.74 | 0.40 |
| 3:F:54:DG:P | 3:F:54:DG:H2' | 2.61 | 0.40 |
| 4:G:66:PRO:HD2 | 4:G:69:GLU:OE2 | 2.22 | 0.40 |
| 4:G:118:ILE:HG21 | 4:G:124:LEU:HD11 | 2.03 | 0.40 |
| 4:G:233:GLU:HA | 4:G:236:LYS:HG2 | 2.03 | 0.40 |
| 4:H:138:ARG:HD2 | 4:H:138:ARG:C | 2.47 | 0.40 |
| 5:I:115:ASN:O | 5:I:119:TYR:HD1 | 2.03 | 0.40 |
| 5:I:124:ARG:O | 5:I:128:HIS:CD2 | 2.75 | 0.40 |
| 4:K:141:ILE:O | 4:K:144:MET:HB2 | 2.22 | 0.40 |
| 4:K:212:LEU:HD12 | 4:K:213:LEU:N | 2.36 | 0.40 |
| 4:O:111:THR:HB | 4:O:116:THR:HG23 | 2.02 | 0.40 |
| 5:Q:152:LEU:HD11 | 5:Q:161:LEU:CB | 2.51 | 0.40 |
| 5:Q:227:ILE:CD1 | 5:R:223:ARG:HD3 | 2.52 | 0.40 |
| 4:T:80:ILE:HG22 | 4:T:136:VAL:HG11 | 2.02 | 0.40 |
| 4:T:221:LEU:HD21 | 4:T:259:LEU:HD12 | 2.04 | 0.40 |
| 5:U:128:HIS:CD2 | 5:U:194:LEU:HG | 2.56 | 0.40 |
| 5:U:289:PRO:HB2 | 5:U:292:ARG:HG2 | 2.04 | 0.40 |
| 5:U:299:ASN:OD1 | 5:V:226:LYS:HG2 | 2.21 | 0.40 |
| 5:V:302:PHE:O | 5:V:306:MET:HG2 | 2.21 | 0.40 |
| 1:A:260:CYS:HA | 1:A:268:LYS:HG2 | 2.03 | 0.40 |
| 1:A:299:TRP:CG | 1:A:309:TYR:HB2 | 2.57 | 0.40 |
| 1:B:114:ARG:NH1 | 1:B:115:SER:O | 2.54 | 0.40 |
| 1:B:154:TYR:CE1 | 1:B:242:ASP:HB3 | 2.57 | 0.40 |
| 1:B:224:PHE:HB3 | 1:B:293:PHE:CE1 | 2.56 | 0.40 |
| 1:D:47:ARG:C | 4:G:275:ASN:HB3 | 2.47 | 0.40 |
| 5:Q:114:ILE:HG23 | 5:R:166:GLU:OE1 | 2.22 | 0.40 |
| 5:Q:252:GLU:HA | 5:Q:255:GLN:HG3 | 2.04 | 0.40 |
| 5:Q:309:TYR:HE1 | 5:Q:314:CYS:HG | 1.67 | 0.40 |
| 4:S:55:MET:HA | 4:S:58:LEU:HG | 2.04 | 0.40 |
| 4:T:145:LEU:HD12 | 4:T:208:GLN:CG | 2.44 | 0.40 |
| 5:U:153:LEU:HB2 | 5:U:162:PHE:CE1 | 2.57 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 | A | 328/365 (90%) | 296 (90%) | 32 (10%) | 0 | 100 | 100 |
| 1 | B | 331/365 (91%) | 305 (92%) | 26 (8%) | 0 | 100 | 100 |
| 1 | C | 318/365 (87%) | 283 (89%) | 35 (11%) | 0 | 100 | 100 |
| 1 | D | 317/365 (87%) | 286 (90%) | 31 (10%) | 0 | 100 | 100 |
| 4 | G | 232/290 (80%) | 219 (94%) | 13 (6%) | 0 | 100 | 100 |
| 4 | H | 146/290 (50%) | 141 (97%) | 5 (3%) | 0 | 100 | 100 |
| 4 | K | 218/290 (75%) | 206 (94%) | 12 (6%) | 0 | 100 | 100 |
| 4 | L | 112/290 (39%) | 111 (99%) | 1 (1%) | 0 | 100 | 100 |
| 4 | O | 230/290 (79%) | 216 (94%) | 14 (6%) | 0 | 100 | 100 |
| 4 | P | 146/290 (50%) | 140 (96%) | 6 (4%) | 0 | 100 | 100 |
| 4 | S | 216/290 (74%) | 204 (94%) | 12 (6%) | 0 | 100 | 100 |
| 4 | T | 166/290 (57%) | 161 (97%) | 4 (2%) | 1 (1%) | 22 | 61 |
| 5 | I | 207/361 (57%) | 196 (95%) | 11 (5%) | 0 | 100 | 100 |
| 5 | J | 184/361 (51%) | 172 (94%) | 12 (6%) | 0 | 100 | 100 |
| 5 | M | 207/361 (57%) | 194 (94%) | 13 (6%) | 0 | 100 | 100 |
| 5 | N | 165/361 (46%) | 159 (96%) | 6 (4%) | 0 | 100 | 100 |
| 5 | Q | 207/361 (57%) | 195 (94%) | 12 (6%) | 0 | 100 | 100 |
| 5 | R | 164/361 (45%) | 156 (95%) | 8 (5%) | 0 | 100 | 100 |
| 5 | U | 207/361 (57%) | 194 (94%) | 13 (6%) | 0 | 100 | 100 |
| 5 | V | 186/361 (52%) | 174 (94%) | 12 (6%) | 0 | 100 | 100 |
| All | All | 4287/6668 (64%) | 4008 (94%) | 278 (6%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | T | 247 | LYS |

5.3.2 Protein sidechains ⓘ

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 | A | 303/331 (92%) | 303 (100%) | 0 | 100 | 100 |
| 1 | B | 308/331 (93%) | 308 (100%) | 0 | 100 | 100 |
| 1 | C | 296/331 (89%) | 296 (100%) | 0 | 100 | 100 |
| 1 | D | 297/331 (90%) | 297 (100%) | 0 | 100 | 100 |
| 4 | G | 224/273 (82%) | 224 (100%) | 0 | 100 | 100 |
| 4 | H | 148/273 (54%) | 148 (100%) | 0 | 100 | 100 |
| 4 | K | 213/273 (78%) | 213 (100%) | 0 | 100 | 100 |
| 4 | L | 120/273 (44%) | 120 (100%) | 0 | 100 | 100 |
| 4 | O | 222/273 (81%) | 222 (100%) | 0 | 100 | 100 |
| 4 | P | 148/273 (54%) | 148 (100%) | 0 | 100 | 100 |
| 4 | S | 209/273 (77%) | 207 (99%) | 2 (1%) | 73 | 82 |
| 4 | T | 164/273 (60%) | 164 (100%) | 0 | 100 | 100 |
| 5 | I | 201/326 (62%) | 201 (100%) | 0 | 100 | 100 |
| 5 | J | 184/326 (56%) | 184 (100%) | 0 | 100 | 100 |
| 5 | M | 201/326 (62%) | 201 (100%) | 0 | 100 | 100 |
| 5 | N | 171/326 (52%) | 171 (100%) | 0 | 100 | 100 |
| 5 | Q | 201/326 (62%) | 201 (100%) | 0 | 100 | 100 |
| 5 | R | 168/326 (52%) | 168 (100%) | 0 | 100 | 100 |
| 5 | U | 201/326 (62%) | 201 (100%) | 0 | 100 | 100 |
| 5 | V | 186/326 (57%) | 186 (100%) | 0 | 100 | 100 |
| All | All | 4165/6116 (68%) | 4163 (100%) | 2 (0%) | 100 | 100 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | S | 69 | GLU |
| 4 | S | 70 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 31 | GLN |
| 1 | A | 80 | HIS |
| 1 | A | 112 | HIS |
| 1 | A | 187 | GLN |
| 1 | A | 273 | ASN |
| 1 | A | 281 | HIS |
| 1 | A | 343 | HIS |
| 1 | A | 361 | HIS |
| 1 | B | 48 | ASN |
| 1 | B | 73 | HIS |
| 1 | B | 295 | HIS |
| 1 | C | 48 | ASN |
| 1 | C | 218 | GLN |
| 1 | C | 238 | ASN |
| 1 | C | 343 | HIS |
| 1 | D | 35 | HIS |
| 1 | D | 57 | ASN |
| 1 | D | 237 | GLN |
| 1 | D | 281 | HIS |
| 4 | G | 35 | ASN |
| 4 | G | 241 | HIS |
| 4 | H | 208 | GLN |
| 5 | I | 128 | HIS |
| 5 | J | 121 | ASN |
| 5 | J | 313 | ASN |
| 5 | M | 218 | ASN |
| 5 | M | 296 | ASN |
| 5 | M | 299 | ASN |
| 5 | N | 159 | HIS |
| 4 | O | 92 | HIS |
| 4 | O | 96 | HIS |
| 4 | O | 101 | ASN |
| 4 | O | 258 | ASN |
| 4 | P | 241 | HIS |
| 5 | Q | 159 | HIS |
| 5 | R | 129 | HIS |
| 5 | R | 284 | HIS |
| 4 | T | 93 | ASN |
| 4 | T | 114 | ASN |
| 5 | U | 261 | GLN |
| 5 | U | 322 | ASN |

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](#)

There are no ligands in this entry.

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.

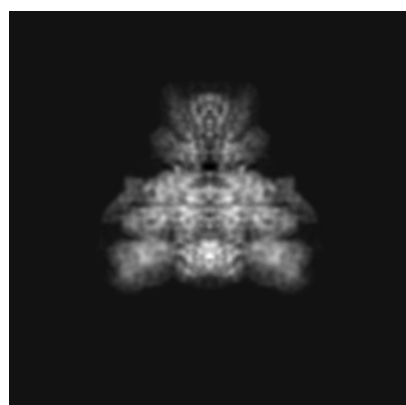
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51803. These allow visual inspection of the internal detail of the map and identification of artifacts.

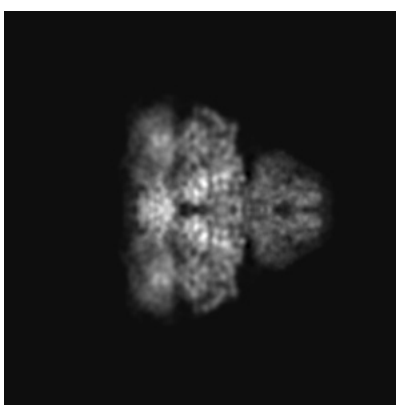
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

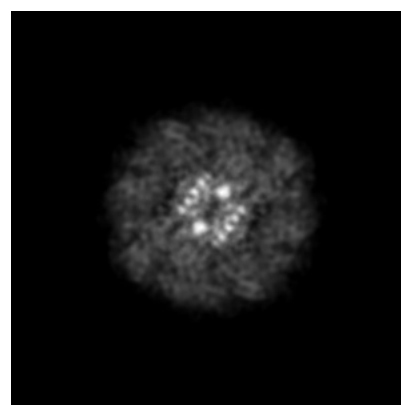
6.1.1 Primary map



X



Y

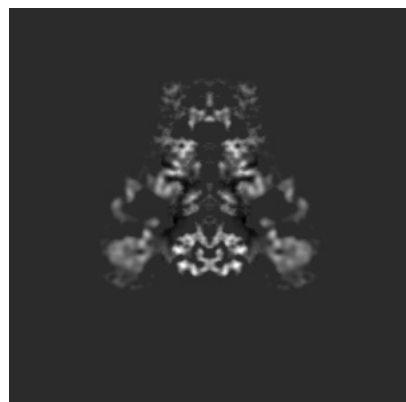


Z

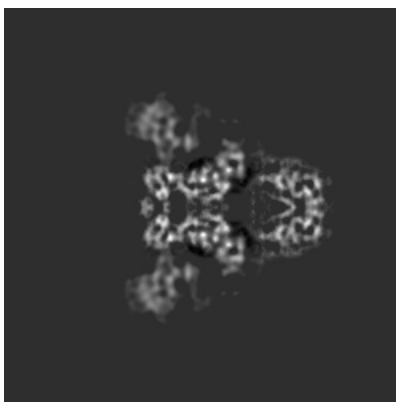
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

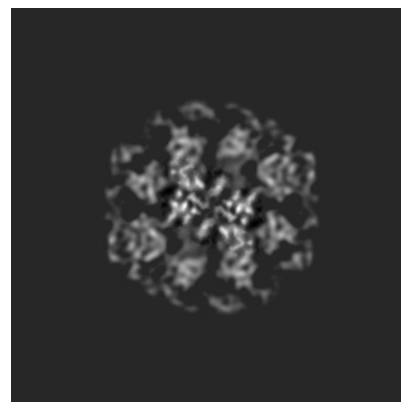
6.2.1 Primary map



X Index: 150



Y Index: 150

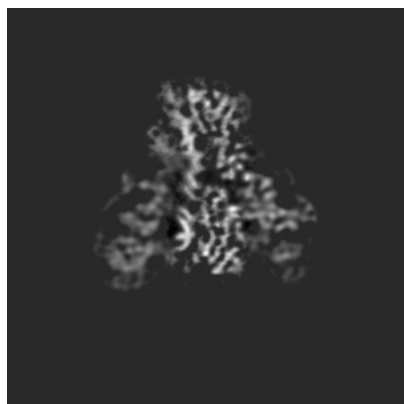


Z Index: 150

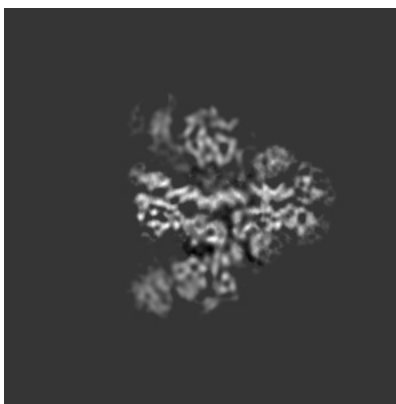
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

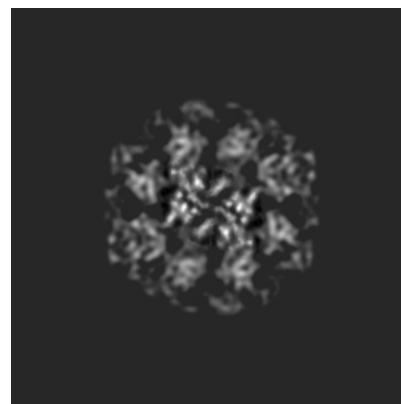
6.3.1 Primary map



X Index: 139



Y Index: 164

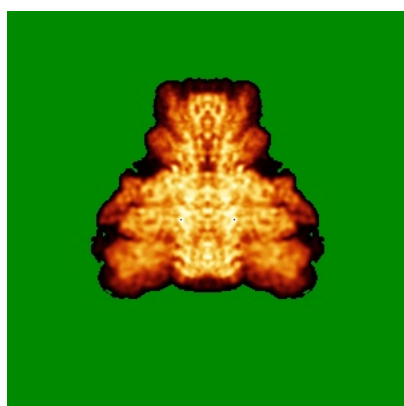


Z Index: 149

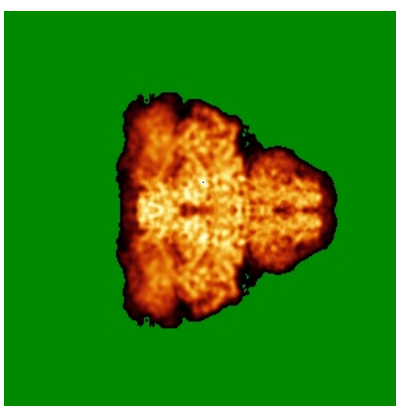
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

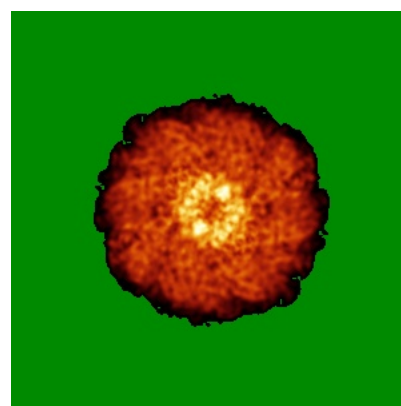
6.4.1 Primary map



X



Y

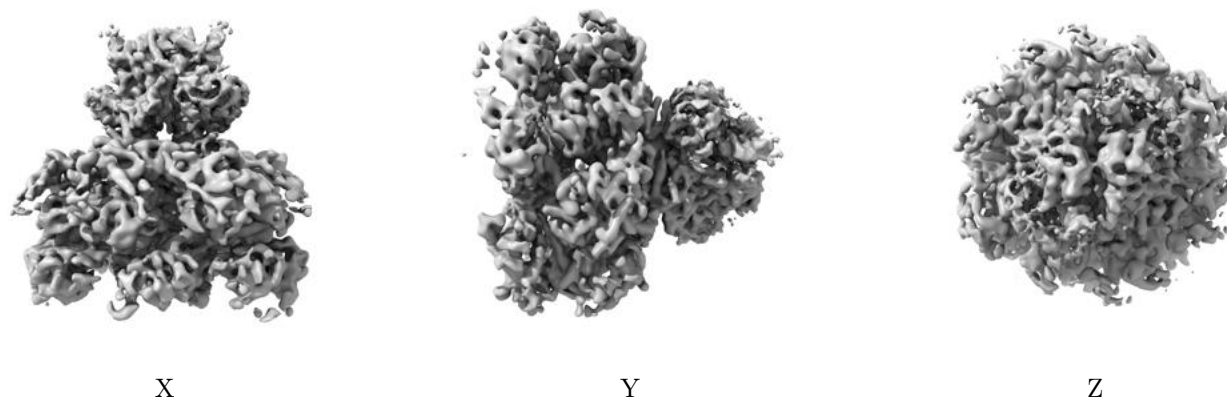


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

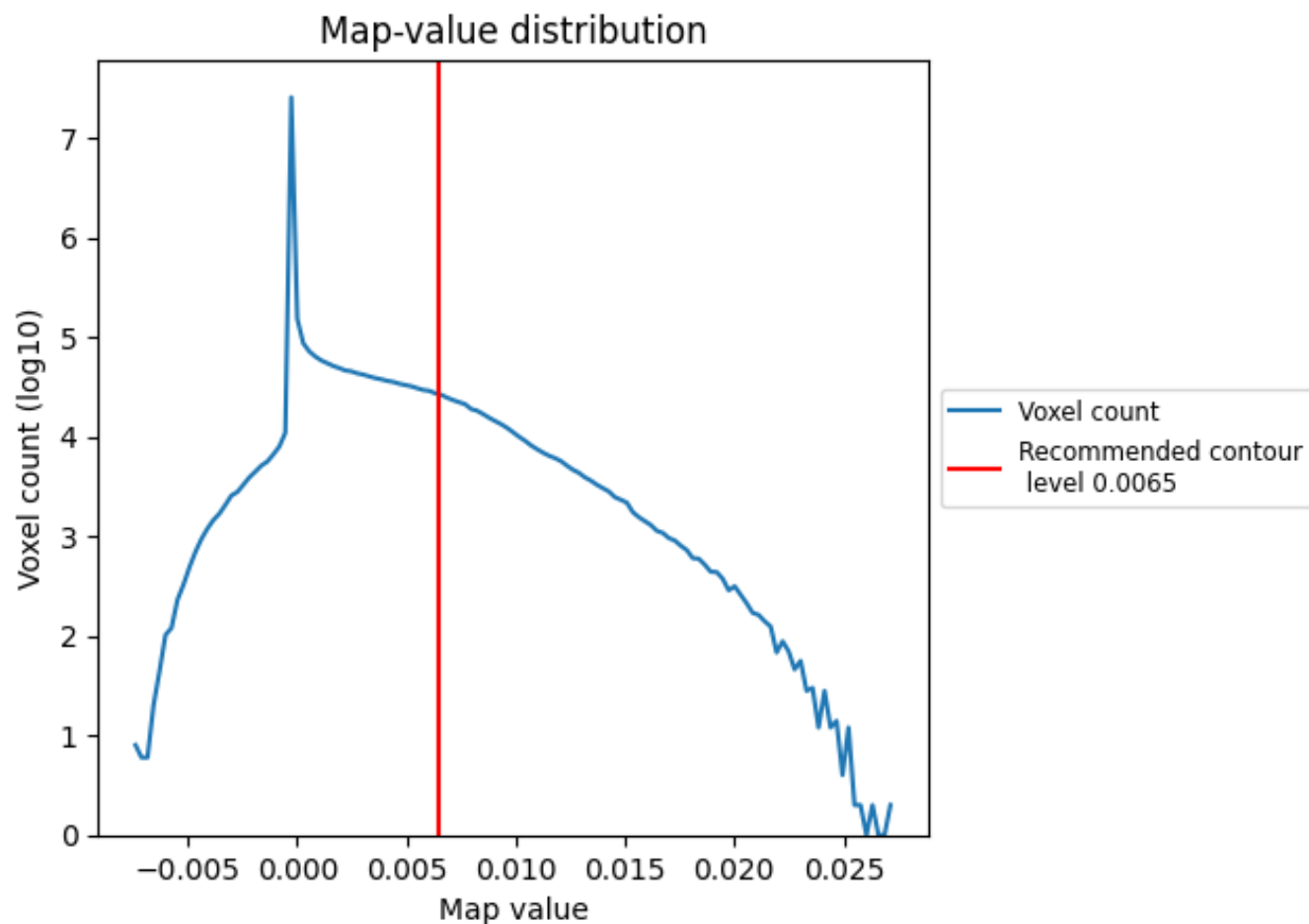
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

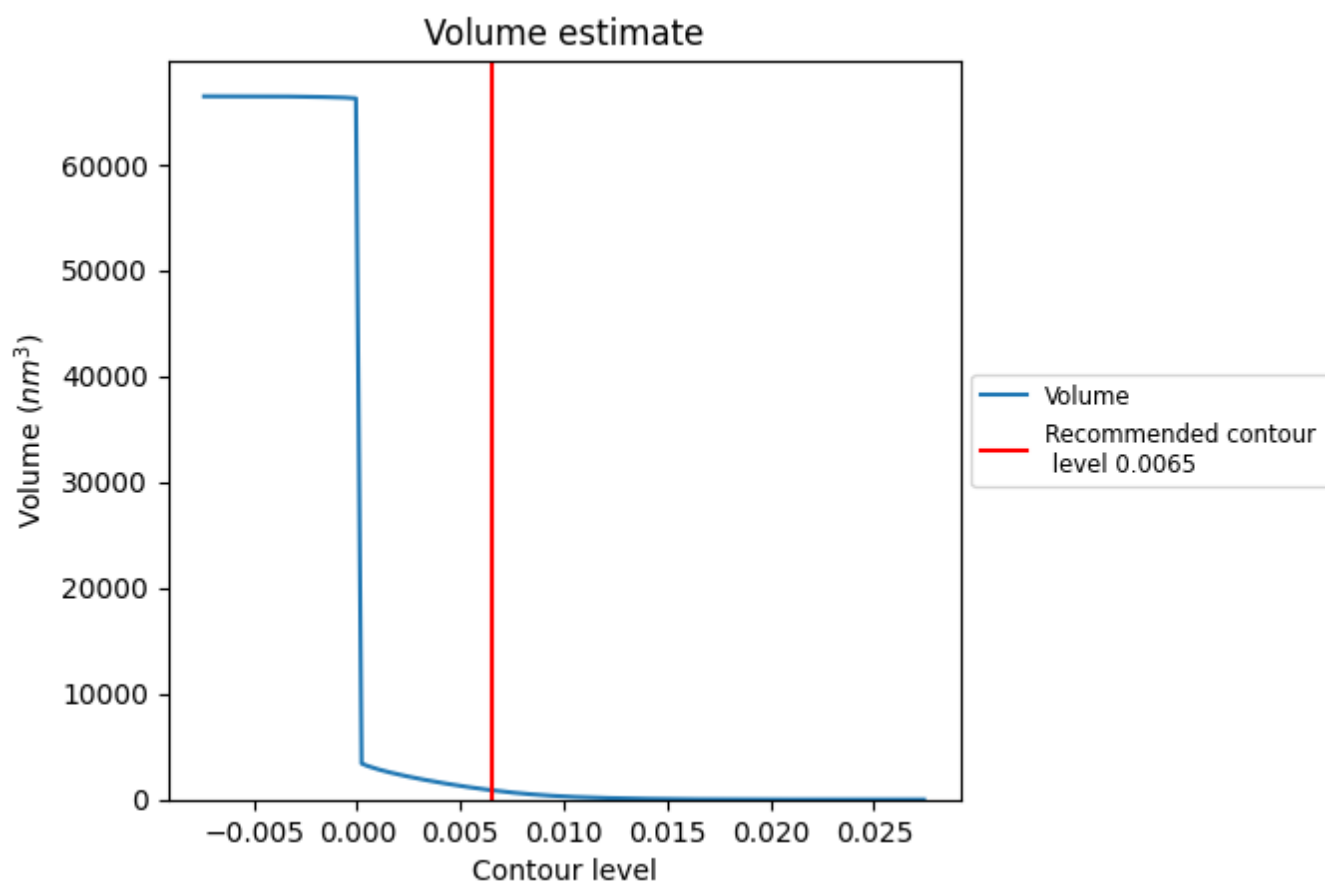
This section contains the results of statistical analysis of the map.

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.

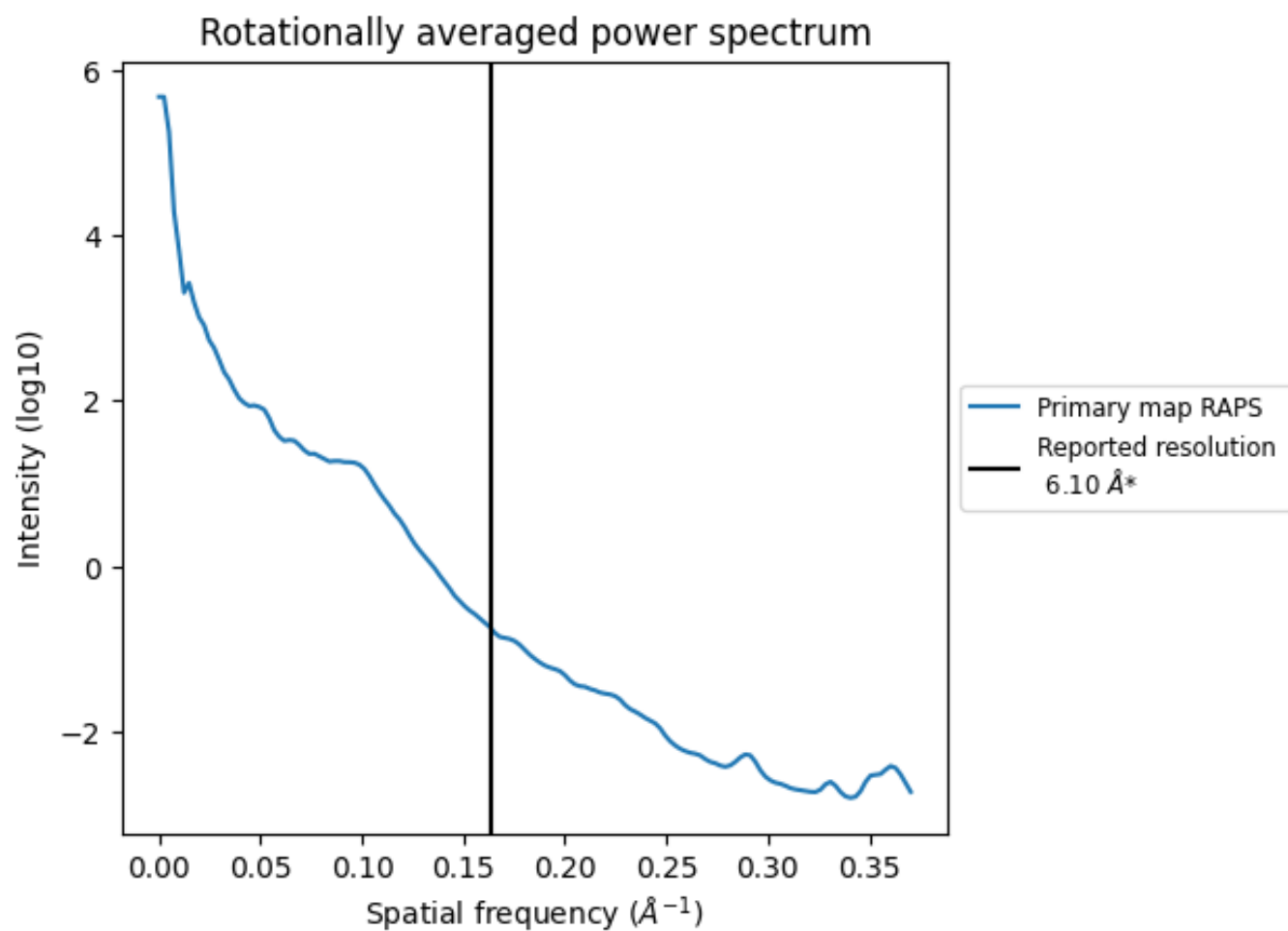
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 886 nm³; this corresponds to an approximate mass of 800 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.164 Å⁻¹

8 Fourier-Shell correlation ⓘ

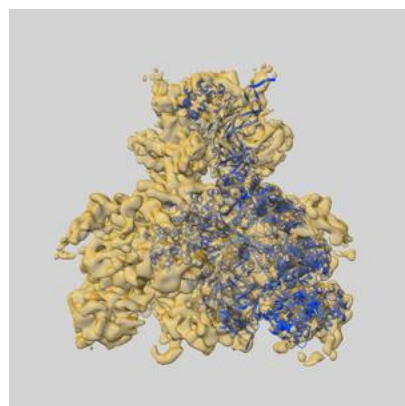
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

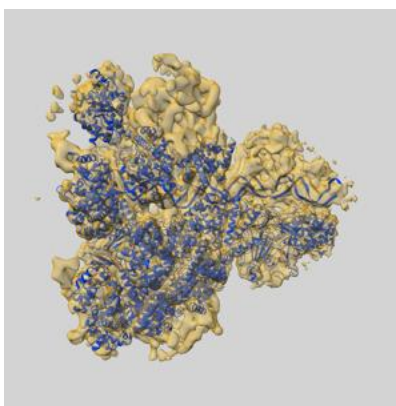
This section contains information regarding the fit between EMDB map EMD-51803 and PDB model 9H2H. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

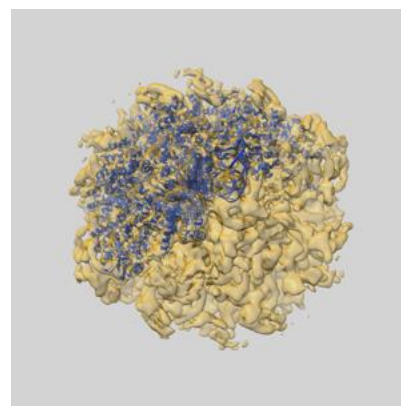
9.1.1 Map-model overlay [i](#)



X

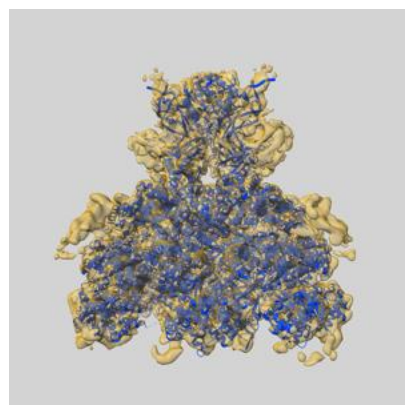


Y

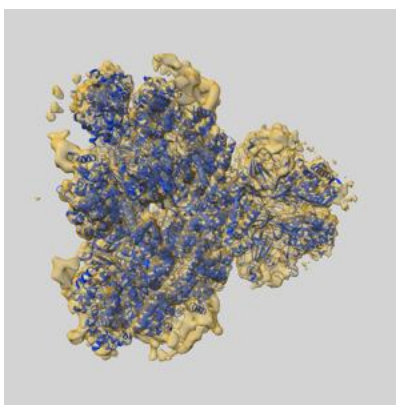


Z

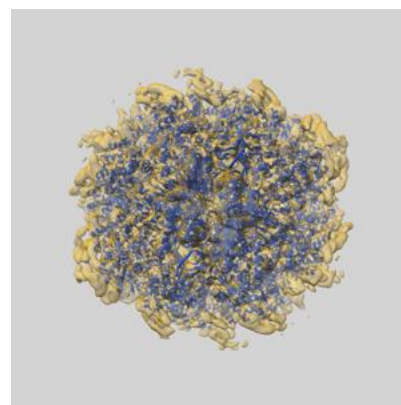
9.1.2 Map-model assembly overlay [i](#)



X



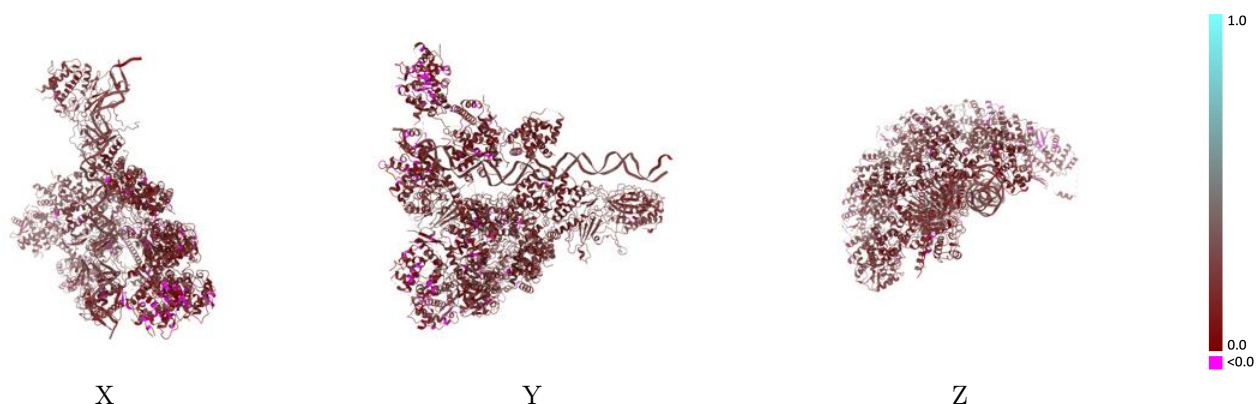
Y



Z

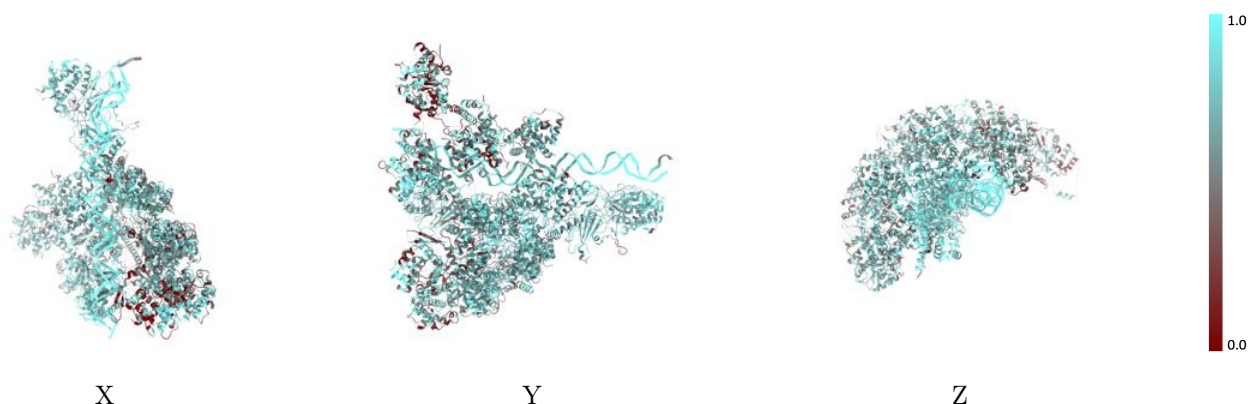
The images above show the 3D surface view of the map at the recommended contour level 0.0065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



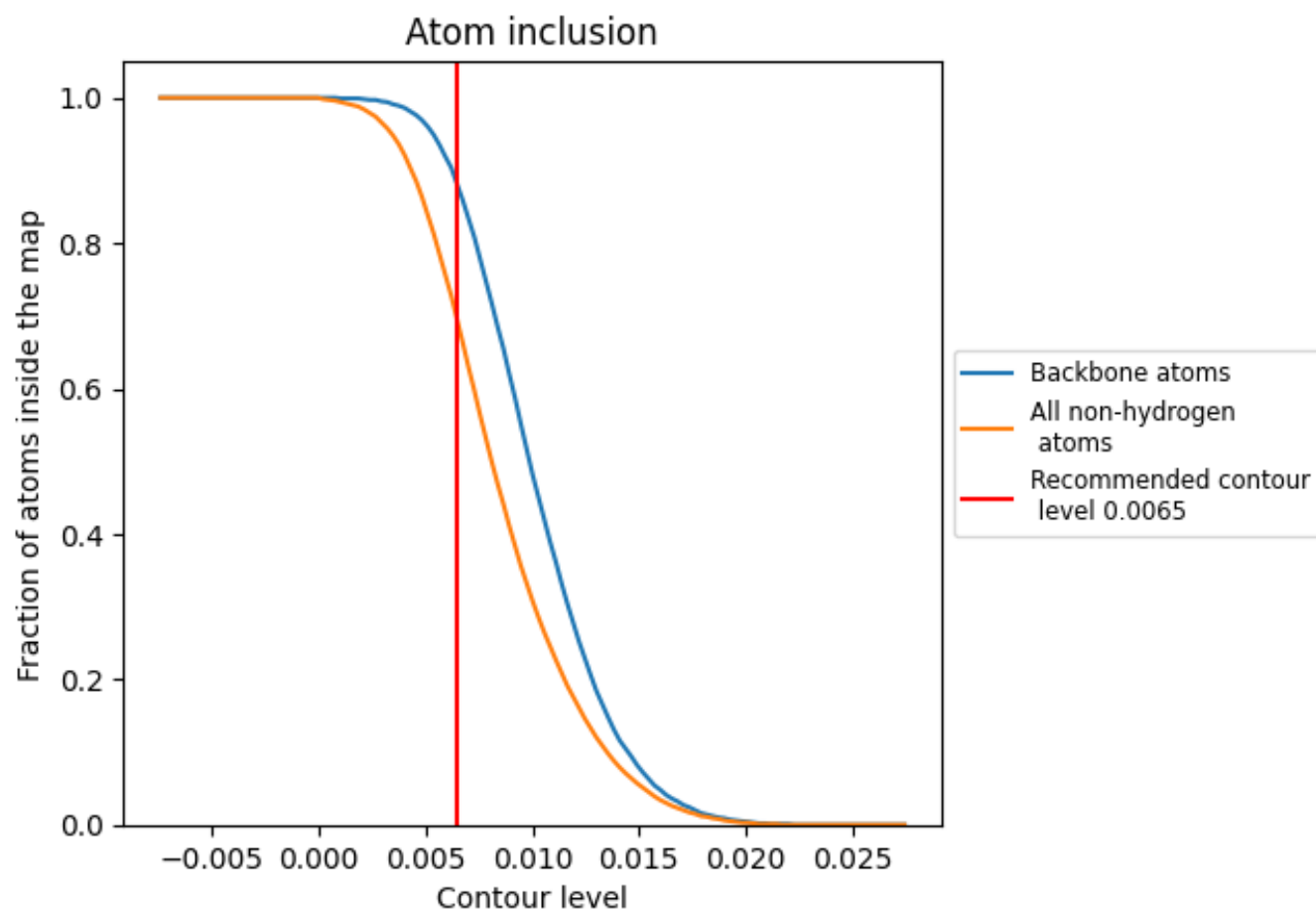
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.0065).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0065) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.6930 |  0.1920 |
| A |  0.7500 |  0.2170 |
| B |  0.7680 |  0.2250 |
| C |  0.7900 |  0.2300 |
| D |  0.7850 |  0.2170 |
| E |  0.9240 |  0.2670 |
| F |  0.9520 |  0.2780 |
| G |  0.6420 |  0.1770 |
| H |  0.6240 |  0.1580 |
| I |  0.7220 |  0.1970 |
| J |  0.7100 |  0.1790 |
| K |  0.6480 |  0.1760 |
| L |  0.7210 |  0.1580 |
| M |  0.7060 |  0.1870 |
| N |  0.7010 |  0.1780 |
| O |  0.5770 |  0.1710 |
| P |  0.6370 |  0.1540 |
| Q |  0.6640 |  0.1880 |
| R |  0.6730 |  0.1840 |
| S |  0.4990 |  0.1580 |
| T |  0.5360 |  0.1260 |
| U |  0.6310 |  0.1760 |
| V |  0.5370 |  0.1650 |

