



Full wwPDB EM Validation Report ⓘ

Jul 28, 2025 – 04:19 PM EDT

PDB ID : 9CDN / pdb_00009cdn
EMDB ID : EMD-45479
Title : Respiratory supercomplex I+III2 open state
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-06-25
Resolution : 3.47 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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

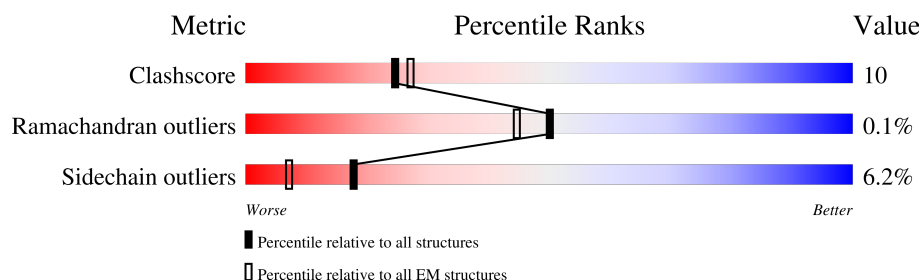
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 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.

















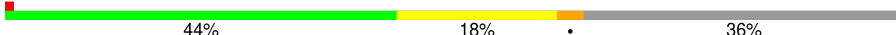
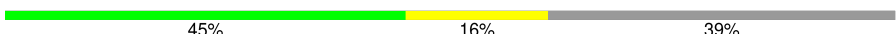









| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 | 0 | 91 | |
| 1 | Ab | 91 | |
| 2 | 1 | 64 | |
| 2 | Ac | 64 | |
| 3 | 2 | 299 | |
| 3 | 4 | 299 | |
| 3 | Ae | 299 | |
| 3 | Af | 299 | |







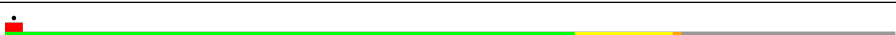
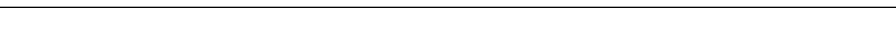
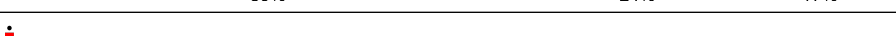
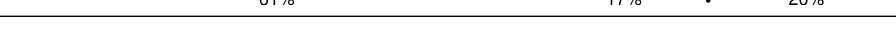
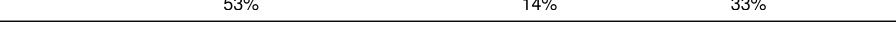
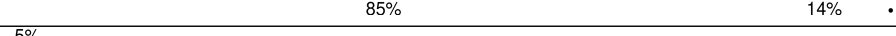



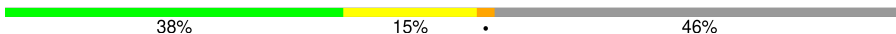









Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | 3 | 56 |  |
| 4 | Ad | 56 |  |
| 5 | 6 | 453 |  |
| 5 | v | 453 |  |
| 6 | 7 | 379 |  |
| 6 | w | 379 |  |
| 7 | 8 | 326 |  |
| 7 | x | 326 |  |
| 8 | 9 | 111 |  |
| 8 | y | 111 |  |
| 9 | a | 189 |  |
| 10 | b | 128 |  |
| 11 | c | 186 |  |
| 12 | d | 176 |  |
| 13 | e | 154 |  |
| 14 | f | 76 |  |
| 15 | g | 122 |  |
| 16 | h | 106 |  |
| 17 | i | 347 |  |
| 18 | j | 115 |  |
| 19 | k | 98 |  |
| 20 | m | 175 |  |
| 21 | n | 58 |  |
| 22 | o | 129 |  |
| 23 | p | 221 |  |









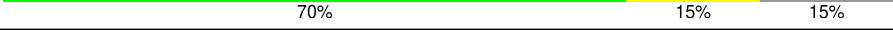
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 24 | q | 459 |  |
| 25 | r | 318 |  |
| 26 | B | 464 |  |
| 27 | C | 469 |  |
| 28 | D | 264 |  |
| 29 | E | 249 |  |
| 30 | F | 123 |  |
| 31 | H | 212 |  |
| 32 | I | 196 |  |
| 33 | J | 175 |  |
| 34 | K | 145 |  |
| 35 | L | 372 |  |
| 36 | N | 116 |  |
| 37 | O | 156 |  |
| 37 | X | 156 |  |
| 38 | P | 99 |  |
| 39 | Q | 154 |  |
| 40 | R | 110 |  |
| 41 | S | 70 |  |
| 42 | T | 169 |  |
| 43 | U | 357 |  |
| 44 | V | 141 |  |
| 45 | W | 144 |  |
| 46 | Y | 105 |  |
| 47 | Z | 114 |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 48 | l | 606 |  |
| 49 | s | 249 |  |
| 50 | t | 137 |  |
| 51 | 5 | 480 |  |
| 51 | u | 480 |  |
| 52 | Aa | 82 |  |
| 52 | z | 82 |  |
| 53 | G | 727 |  |
| 54 | M | 113 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 55 | FES | 2 | 301 | - | - | X | - |
| 55 | FES | 4 | 301 | - | - | X | - |
| 59 | SF4 | H | 301 | - | - | X | - |
| 59 | SF4 | H | 302 | - | - | X | - |

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 98319 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 Cytochrome b-c1 complex subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | 0 | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 557 | 338 | 100 | 114 | 5 | | |
| 1 | Ab | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 543 | 331 | 99 | 108 | 5 | | |

- Molecule 2 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 2 | 1 | 60 | Total | C | N | O | 0 | 0 |
| | | | 493 | 322 | 87 | 84 | | |
| 2 | Ac | 59 | Total | C | N | O | 0 | 0 |
| | | | 485 | 318 | 85 | 82 | | |

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | 2 | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 951 | 264 | 287 | 7 | | |
| 3 | 4 | 196 | Total | C | N | O | S | 0 | 0 |
| | | | 1518 | 955 | 265 | 291 | 7 | | |
| 3 | Ae | 23 | Total | C | N | O | S | 0 | 0 |
| | | | 143 | 89 | 25 | 28 | 1 | | |
| 3 | Af | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 191 | 118 | 35 | 37 | 1 | | |

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4 | 3 | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 417 | 279 | 74 | 63 | 1 | | |
| 4 | Ad | 51 | Total | C | N | O | S | 0 | 0 |
| | | | 421 | 281 | 74 | 65 | 1 | | |

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | 6 | 418 | Total | C | N | O | S | 0 | 0 |
| | | | 3140 | 1966 | 556 | 610 | 8 | | |
| 5 | v | 418 | Total | C | N | O | S | 0 | 0 |
| | | | 3140 | 1966 | 556 | 610 | 8 | | |

- Molecule 6 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | 7 | 379 | Total | C | N | O | S | 0 | 0 |
| | | | 3025 | 2031 | 471 | 502 | 21 | | |
| 6 | w | 379 | Total | C | N | O | S | 0 | 0 |
| | | | 3025 | 2031 | 471 | 502 | 21 | | |

- Molecule 7 is a protein called Cytochrome c1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | 8 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1896 | 1211 | 326 | 343 | 16 | | |
| 7 | x | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1896 | 1211 | 326 | 343 | 16 | | |

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | 9 | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 878 | 563 | 154 | 159 | 2 | | |
| 8 | y | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 893 | 572 | 157 | 162 | 2 | | |

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | a | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1151 | 754 | 195 | 199 | 3 | | |

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 10 | b | 108 | Total | C | N | O | 0 | 0 |
| | | | 900 | 591 | 156 | 153 | | |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | c | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1291 | 838 | 208 | 237 | 8 | | |

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | d | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1417 | 890 | 258 | 261 | 8 | | |

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | e | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 826 | 530 | 137 | 155 | 4 | | |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 14 | f | 46 | Total | C | N | O | 0 | 0 |
| | | | 391 | 259 | 67 | 65 | | |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | g | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 1000 | 650 | 173 | 171 | 6 | | |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | h | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 867 | 550 | 161 | 150 | 6 | | |

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17 | i | 347 | Total | C | N | O | S | 0 | 0 |
| | | | 2711 | 1782 | 420 | 463 | 46 | | |

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | j | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 793 | 537 | 116 | 135 | 5 | | |

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 19 | k | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 748 | 493 | 113 | 128 | 14 | | |

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 20 | m | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1309 | 873 | 189 | 235 | 12 | | |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 21 | n | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 475 | 308 | 87 | 79 | 1 | | |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 22 | o | 128 | Total | C | N | O | 0 | 0 |
| | | | 1058 | 688 | 181 | 189 | | |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | p | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1534 | 982 | 279 | 265 | 8 | | |

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24 | q | 459 | Total | C | N | O | S | 0 | 0 |
| | | | 3630 | 2410 | 572 | 609 | 39 | | |

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25 | r | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2508 | 1678 | 385 | 424 | 21 | | |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26 | B | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3318 | 2095 | 591 | 612 | 20 | | |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27 | C | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3454 | 2207 | 593 | 630 | 24 | | |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28 | D | 208 | Total | C | N | O | S | 0 | 0 |
| | | | 1732 | 1121 | 297 | 312 | 2 | | |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29 | E | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1658 | 1058 | 278 | 312 | 10 | | |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | F | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 727 | 444 | 136 | 144 | 3 | | |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 31 | H | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1412 | 887 | 243 | 269 | 13 | | |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 32 | I | 156 | Total | C | N | O | S | 0 | 0 |
| | | | 1248 | 794 | 227 | 213 | 14 | | |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | J | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 953 | 602 | 171 | 177 | 3 | | |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | K | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1203 | 769 | 217 | 212 | 5 | | |

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 35 | L | 340 | Total | C | N | O | S | 0 | 0 |
| | | | 2702 | 1745 | 473 | 475 | 9 | | |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 5 isoform X1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | N | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 910 | 588 | 154 | 165 | 3 | | |

- Molecule 37 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | O | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 680 | 440 | 100 | 135 | 5 | | |
| 37 | X | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 689 | 445 | 101 | 138 | 5 | | |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | P | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 669 | 419 | 125 | 123 | 2 | | |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | Q | 112 | Total | C | N | O | S | 0 | 0 |
| | | | 954 | 610 | 176 | 163 | 5 | | |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40 | R | 35 | Total | C | N | O | S | 0 | 0 |
| | | | 295 | 185 | 55 | 54 | 1 | | |

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 41 | S | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 562 | 361 | 101 | 94 | 6 | | |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | T | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 638 | 414 | 109 | 114 | 1 | | |

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43 | U | 318 | Total | C | N | O | S | 0 | 0 |
| | | | 2574 | 1638 | 437 | 489 | 10 | | |

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | V | 139 | Total | C | N | O | S | 0 | 0 |
| | | | 1016 | 648 | 173 | 189 | 6 | | |

- Molecule 45 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | W | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1162 | 749 | 201 | 203 | 9 | | |

- Molecule 46 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 46 | Y | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 531 | 352 | 88 | 90 | 1 | | |

- Molecule 47 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47 | Z | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 626 | 410 | 105 | 110 | 1 | | |

- Molecule 48 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48 | l | 603 | Total | C | N | O | S | 0 | 0 |
| | | | 4785 | 3174 | 741 | 819 | 51 | | |

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 49 | s | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1398 | 887 | 250 | 251 | 10 | | |

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | t | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 1019 | 635 | 195 | 180 | 9 | | |

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 51 | u | 446 | Total | C | N | O | S | 0 | 0 |
| | | | 3459 | 2161 | 605 | 674 | 19 | | |
| 51 | 5 | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3374 | 2105 | 594 | 656 | 19 | | |

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52 | z | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 666 | 434 | 122 | 108 | 2 | | |
| 52 | Aa | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 662 | 432 | 121 | 107 | 2 | | |

- Molecule 53 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 53 | G | 684 | Total | C | N | O | S | 0 | 0 |
| | | | 5260 | 3298 | 917 | 1006 | 39 | | |

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

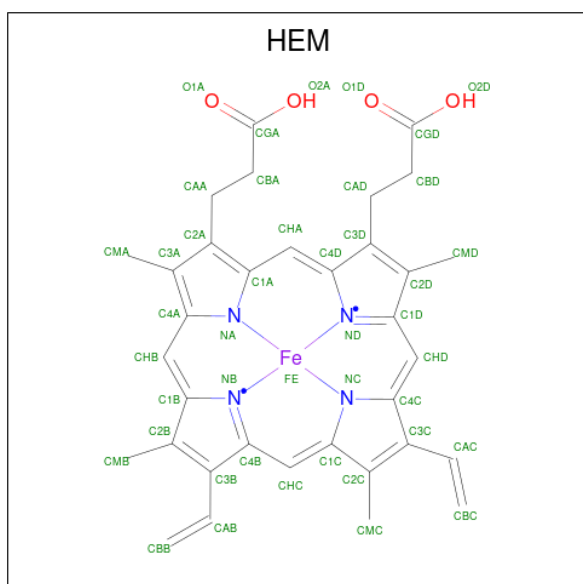
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54 | M | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 773 | 487 | 146 | 137 | 3 | | |

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



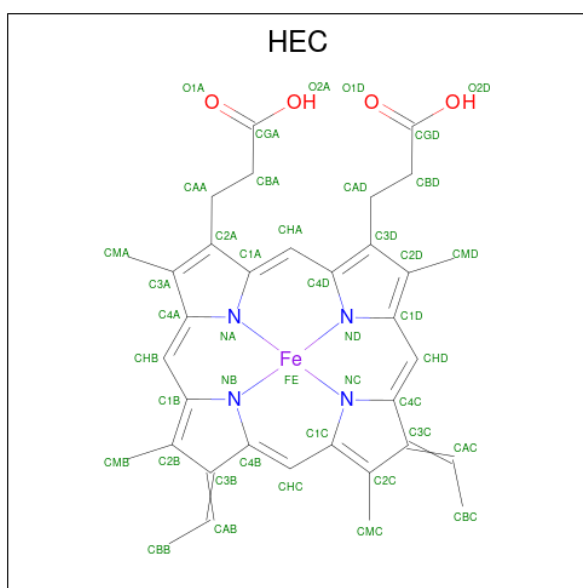
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 55 | 2 | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 55 | 4 | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 55 | E | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 55 | G | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

- Molecule 56 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



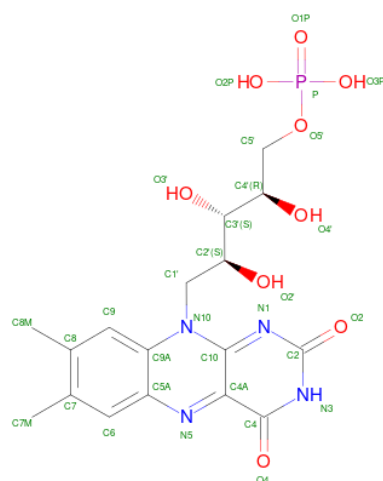
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 56 | 7 | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 56 | 7 | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 56 | w | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 56 | w | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 57 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



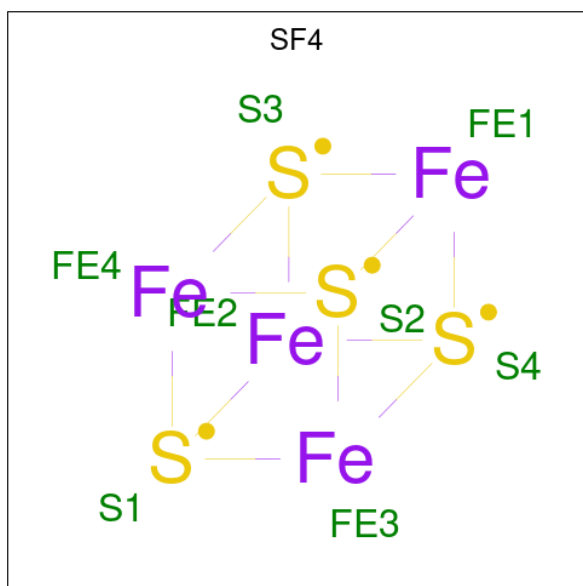
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 57 | 8 | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 57 | x | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 58 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 58 | B | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



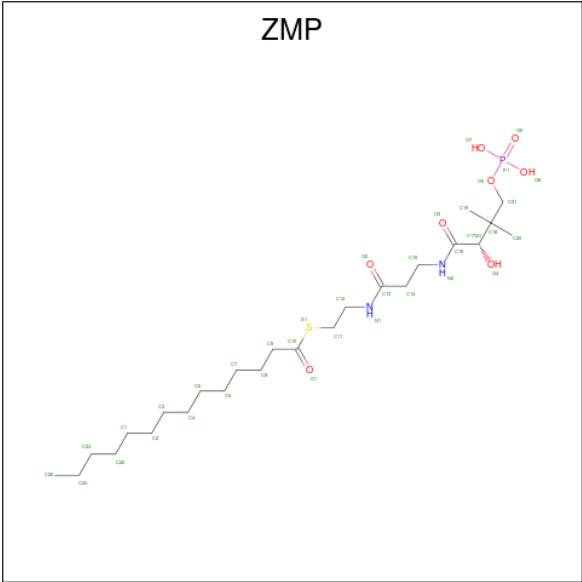
| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 59 | B | 1 | Total 8 | Fe 4 | S 4 | 0 |
| 59 | H | 1 | Total 8 | Fe 4 | S 4 | 0 |
| 59 | H | 1 | Total 8 | Fe 4 | S 4 | 0 |

Continued on next page...

| Mol | Chain | Residues | Atoms | | | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 59 | I | 1 | Total 8 | Fe 4 | S 4 | 0 |
| 59 | G | 1 | Total 8 | Fe 4 | S 4 | 0 |
| 59 | G | 1 | Total 8 | Fe 4 | S 4 | 0 |

- # NDP

- Molecule 61 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl]-}\beta\text{-alaninyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).

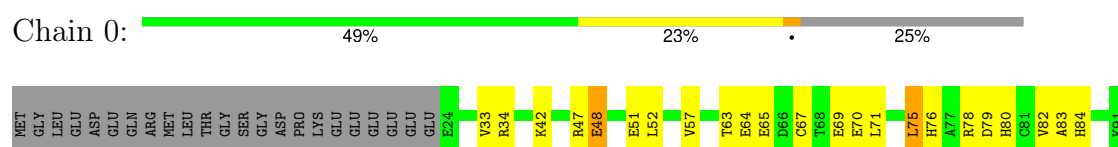


| Mol | Chain | Residues | Atoms | | | | | AltConf | |
|-----|-------|----------|-------|----|---|---|---|---------|---|
| 61 | Q | 1 | Total | C | N | O | P | S | 0 |
| | | | 30 | 18 | 2 | 8 | 1 | 1 | |

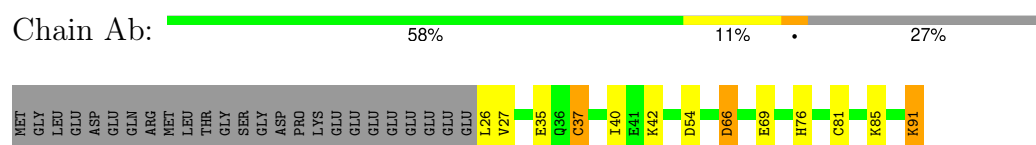
3 Residue-property plots

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.

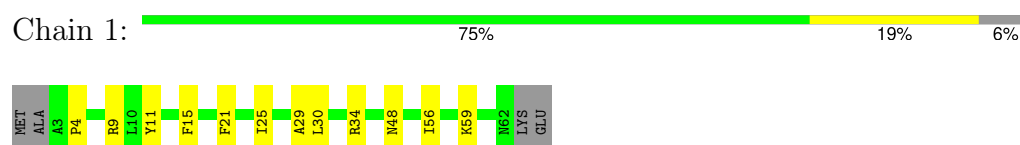
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



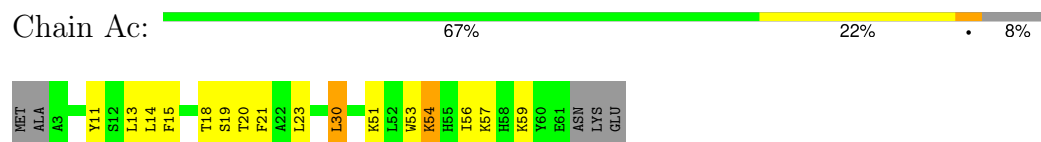
- Molecule 1: Cytochrome b-c1 complex subunit 6, mitochondrial



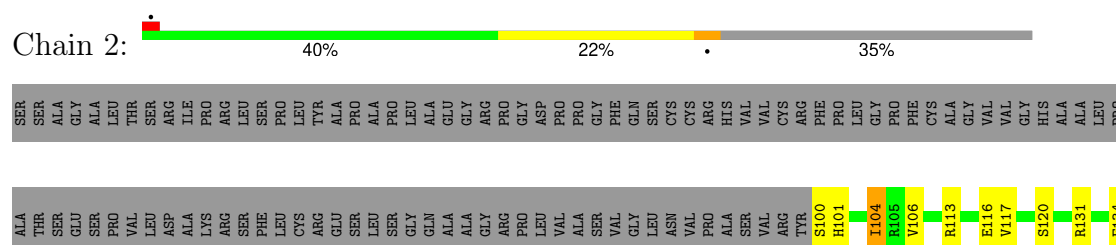
- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

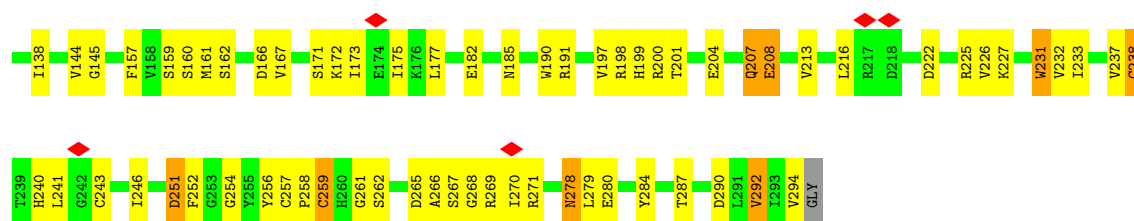


- Molecule 2: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



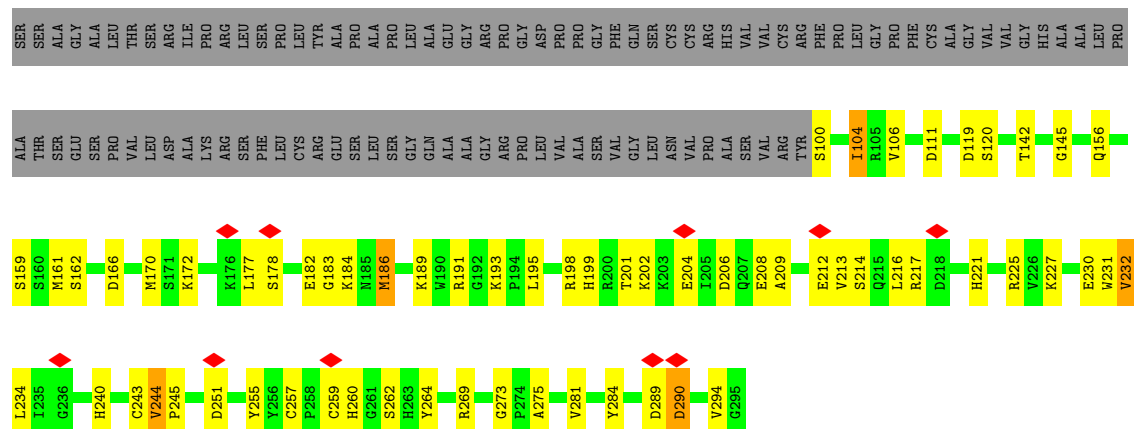
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1





- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain 4: 44% 20% 34%



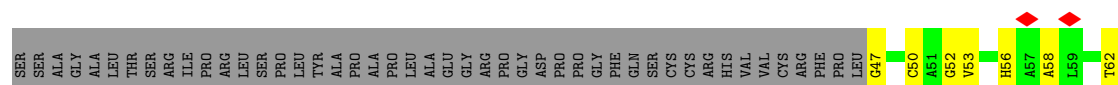
- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain Ae: 92%

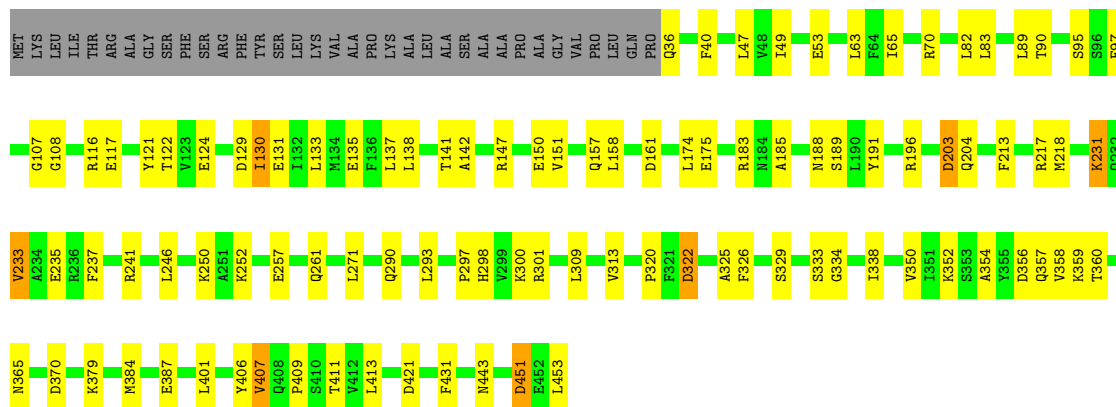


- Molecule 3: Ubiquinol-cytochrome c reductase, Rieske iron-sulfur polypeptide 1

Chain Af: 5% 90%

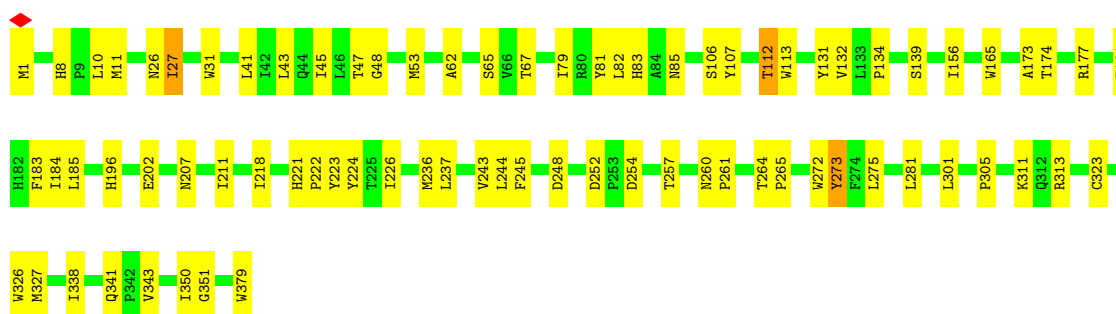






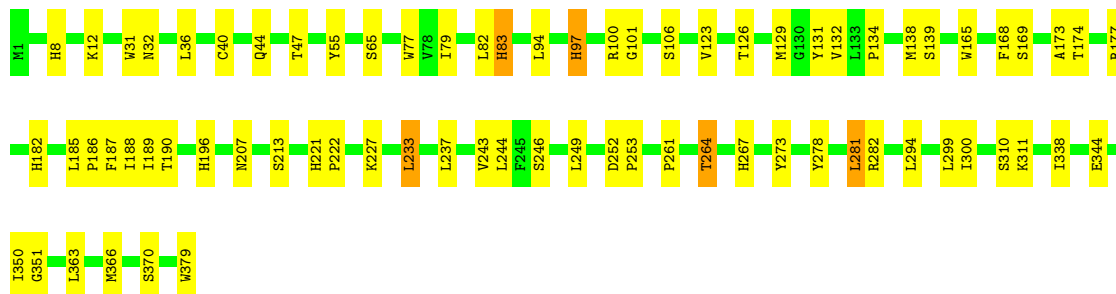
• Molecule 6: Cytochrome b

Chain 7: 79% 20% .



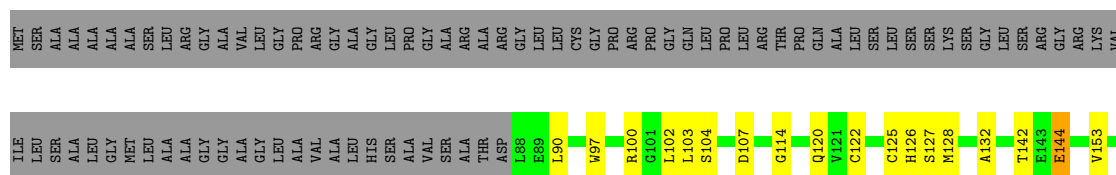
• Molecule 6: Cytochrome b

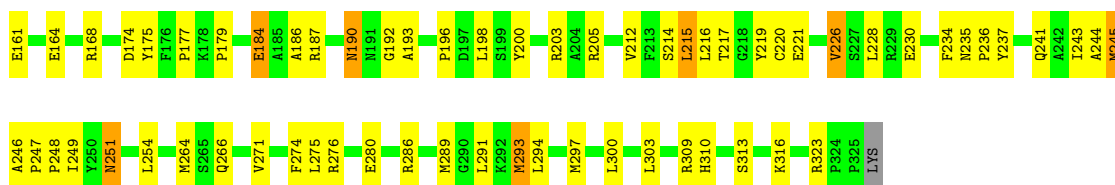
Chain w: 80% 18% .



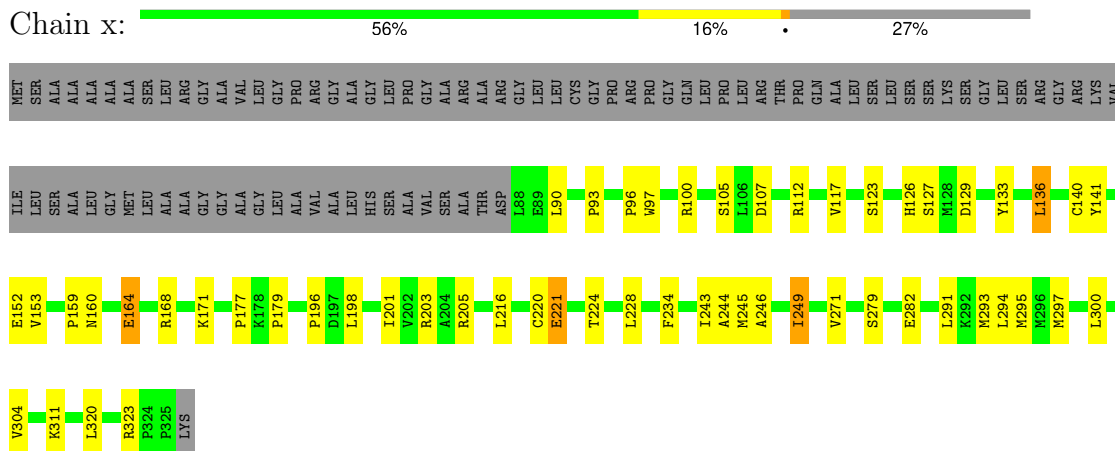
• Molecule 7: Cytochrome c1

Chain 8: 48% 22% 27% .

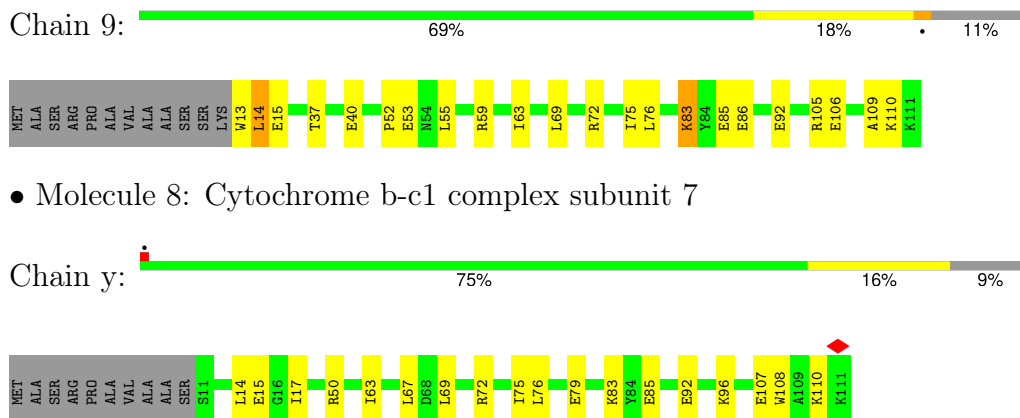




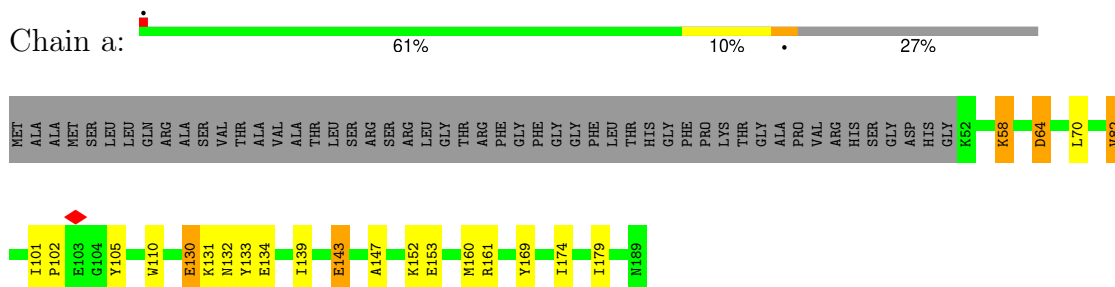
- Molecule 7: Cytochrome c1



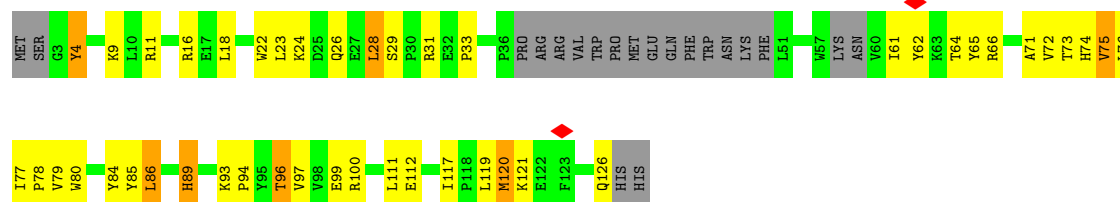
- Molecule 8: Cytochrome b-c1 complex subunit 7



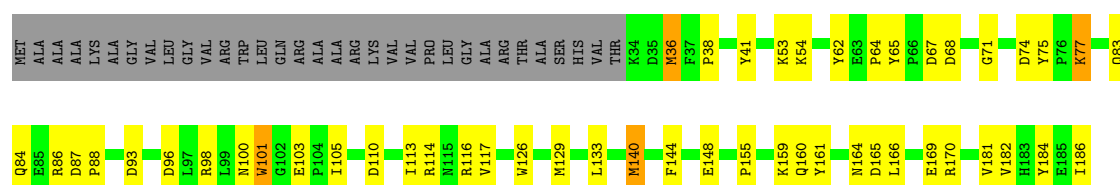
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



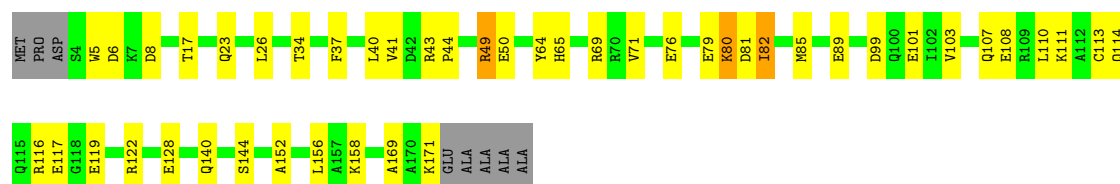
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



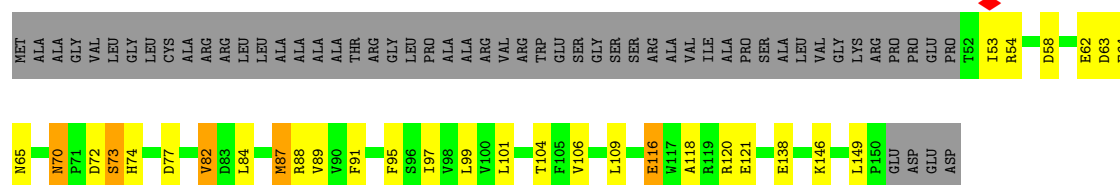
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



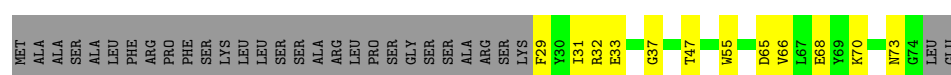
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10




- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

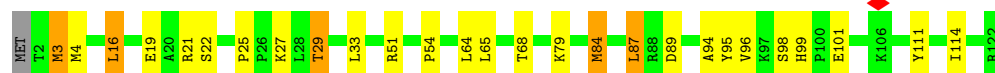


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial




- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



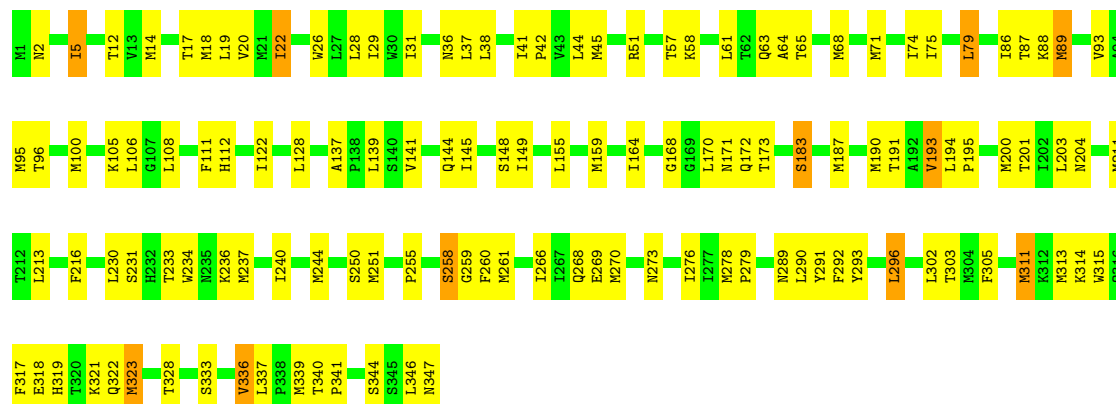
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



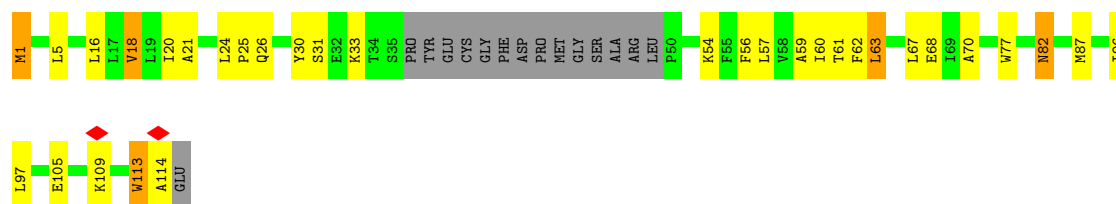
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2

Chain i: 



- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain j: 

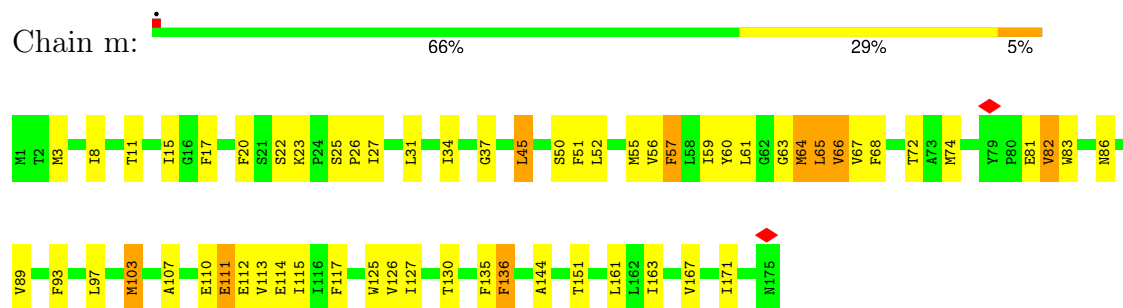


- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

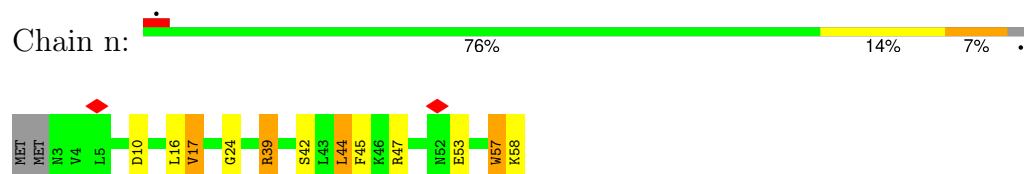
Chain k: 



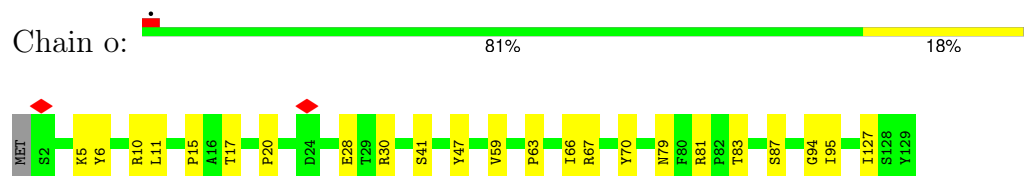
- Molecule 20: NADH-ubiquinone oxidoreductase chain 6



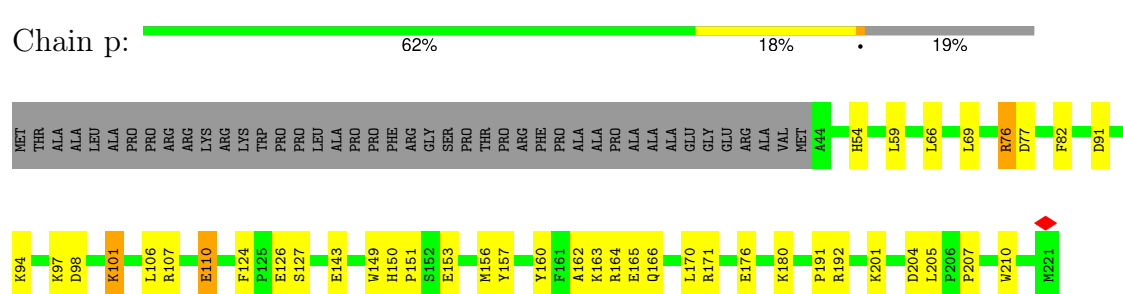
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



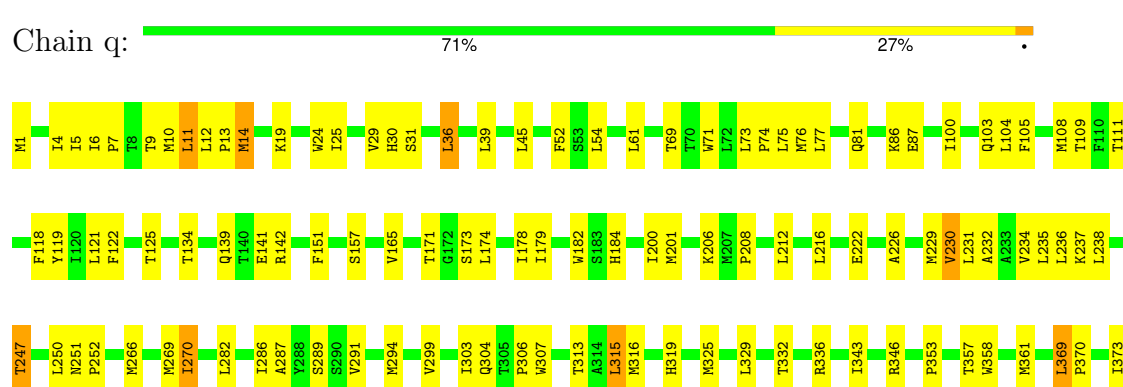
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



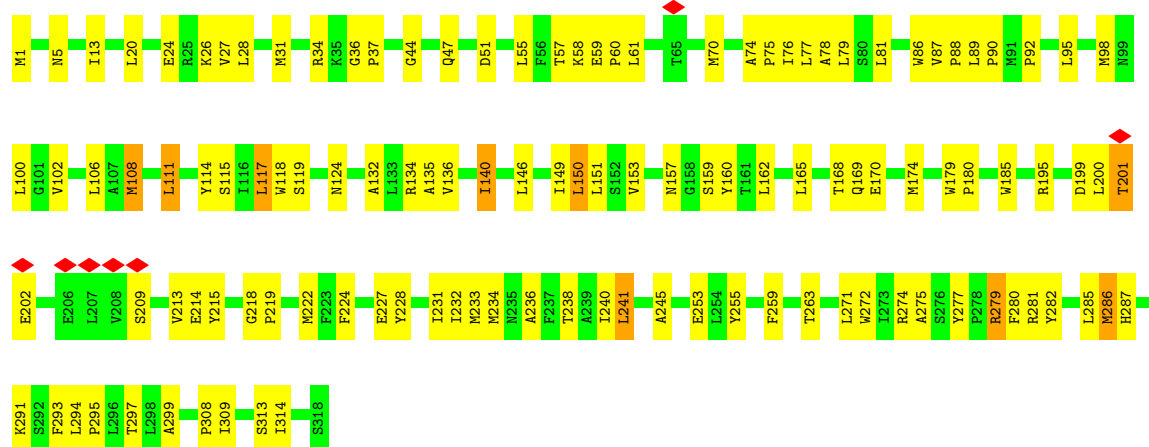
- Molecule 24: NADH-ubiquinone oxidoreductase chain 4





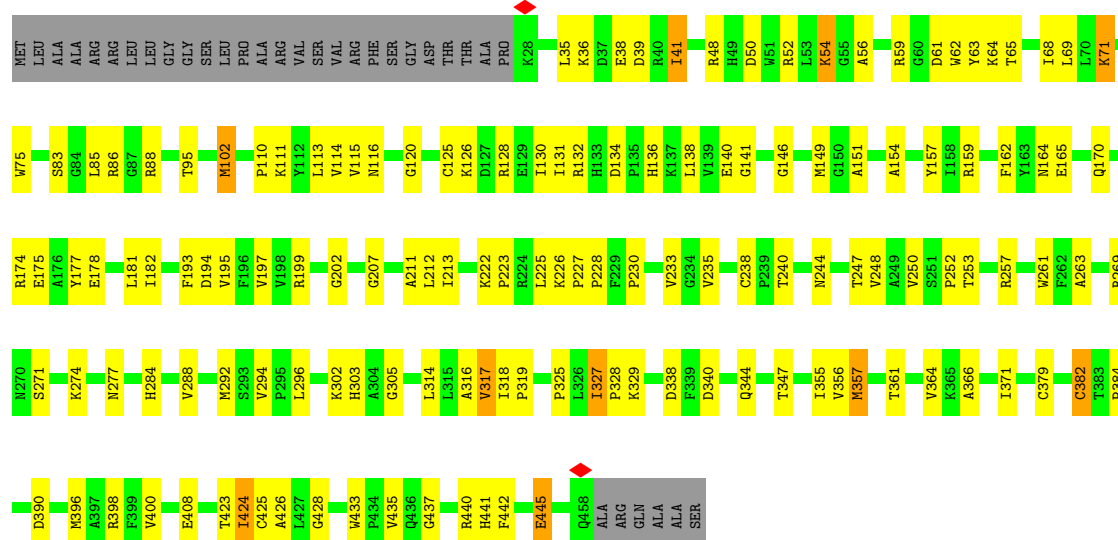
• Molecule 25: NADH-ubiquinone oxidoreductase chain 1

Chain r: 62% 35%



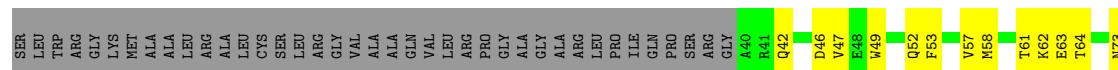
• Molecule 26: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

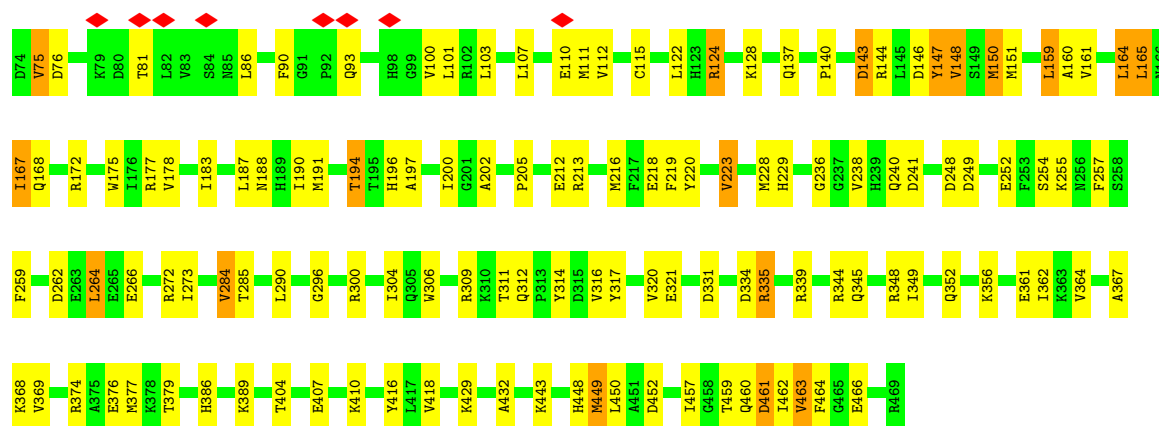
Chain B: 62% 28% 7%



• Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

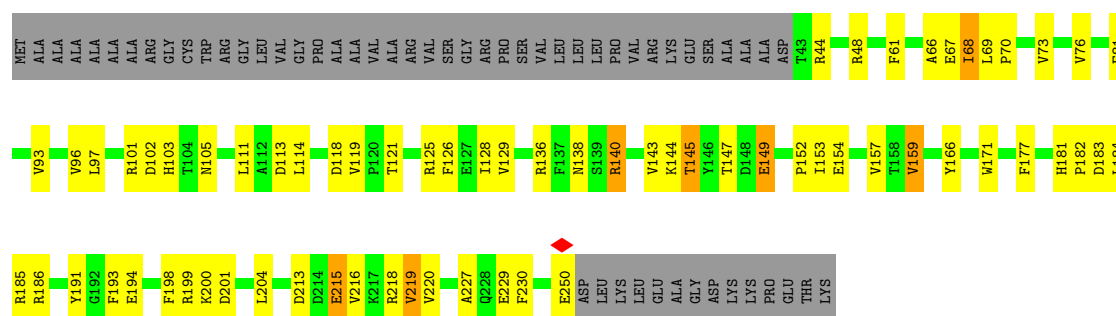
Chain C: 61% 27% 8%





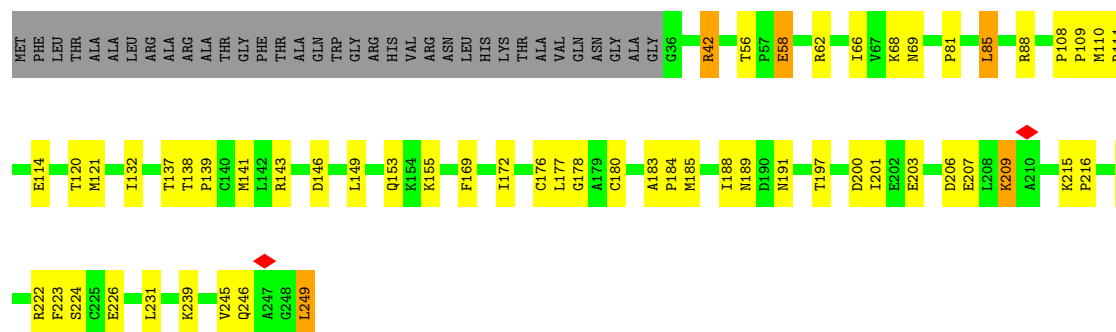
- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain D: 53% 23% 21%



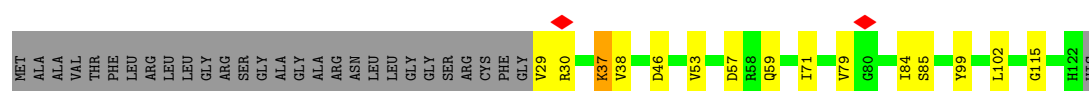
- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 63% 21% 14%



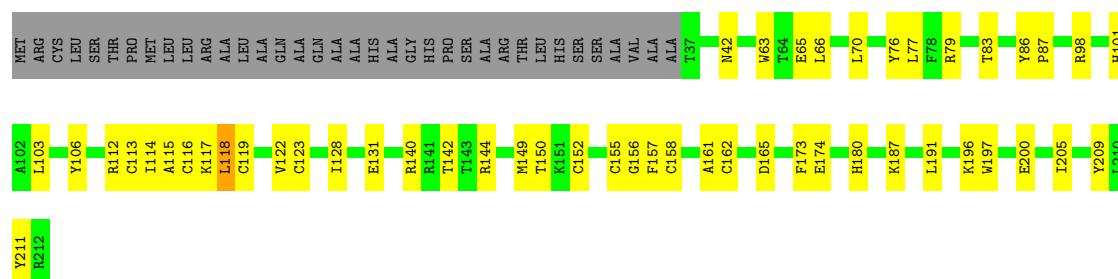
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain F: 64% 11% 24%



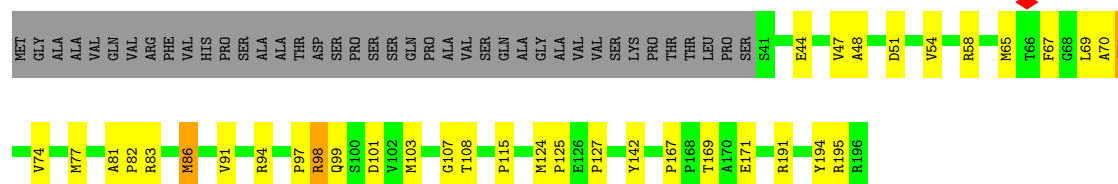
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain H: 



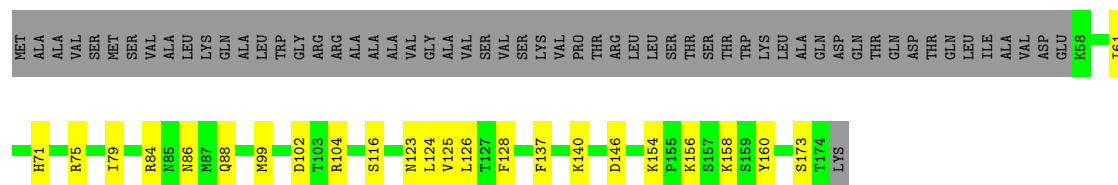
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain I: 




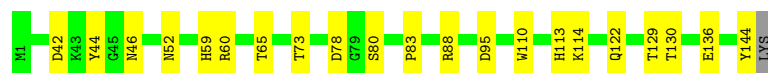
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain J: 



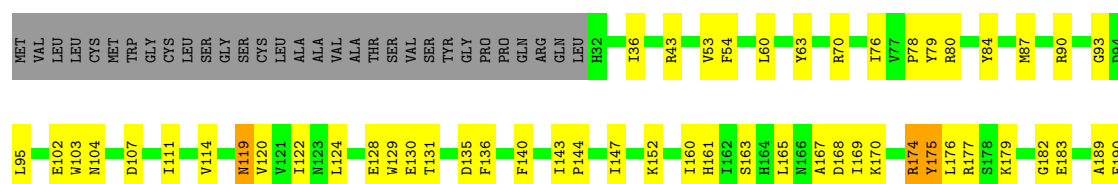
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

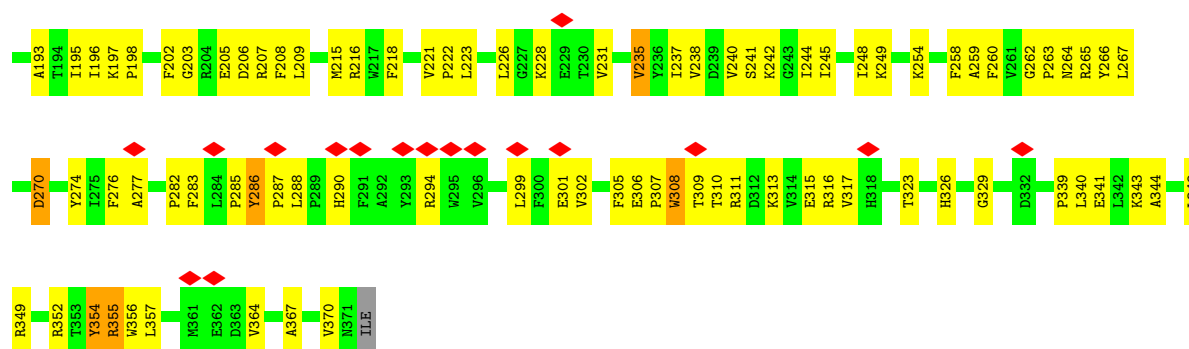
Chain K: 



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain L: 





- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain N: 76% 19%



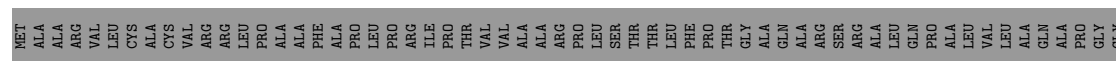
- Molecule 37: Acyl carrier protein

Chain O: 33% 17% 46%



- Molecule 37: Acyl carrier protein

Chain X: 38% 15% 46%



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P: 55% 26% 16%



LYS
ALA

- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q: 

MET ARG LYS LYS ARG ARG PRO GLN ALA ALA LEU LYS SER ARG LYS VAL LEU SER CYS GLY LEU PHE SER LYS MET MET ALA ALA SER GLY LEU PRO ARG ALA ALA ALA ALA ALA THR SER V43 I46 F47 S48 M51 N52 E53 A54 K55 K56 R57 R63 A64 Y66

R67 E68 V69 Q77 G85 R86 D87 K88 Y89 H92 P93 H94 K95 GLY A97 D101 V105 L108 V109 I110 K111 M114 E117 E118 V122 W123 K124 T127 H126 I129 F132 T136 P154


- Molecule 40: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain R: 

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

ALA ALA ALA ALA ALA GLU PRO PHE ASP ASN THR TYR ARG ASN L76 Q77 H78 H79 E80 Y81 L87 N90 V91 E92 L93 K94 K95 P96 M98 P99 Q100 H110

- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 

H1 H2 F3 E4 P7 H12 L16 P19 R37 M48 R52 H58 I69 D70

- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T: 

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

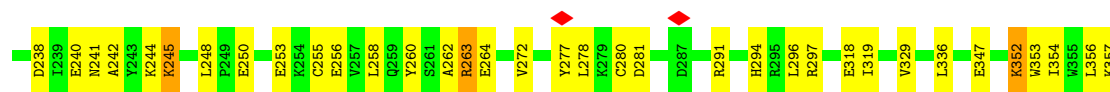
LEU GLY ARG GLN ARG CYS ALA ARG THR THR PRO ARG ALA PRO ARG VAL HIS ALA ALA GLU THR LYS MET ALA G88 K100 I110 I115 T134 P141 L142 V151 P155 L166 K167 N168 L169

- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain U: 

MET ALA LEU ARG LEU ARG LEU ALA PRO PRO ARG ARG GLY LEU GLY VAL VAL GLN ARG VAL GLY ILE HIS THR GLY ALA PRO CYS ARG LEU GLN Y40 L43 R50 V61 G66 H67 I68 C69 K72 L83 A96 D102 G103

K104 L110 E117 Y131 Y138 A139 S140 L143 A148 L149 L152 L153 G158 V159 R163 V170 F171 L172 Q178 R182 C185 V186 K193 K194 V195 P203 H204 V211 P212 V213 P214 E215 I216 Q217 S216 K223 G224 N225 E228 N229 T232



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 80% 16%



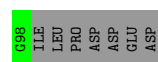
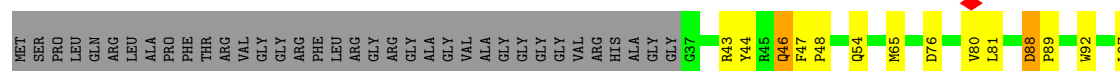
- Molecule 45: NADH:ubiquinone oxidoreductase subunit A13

Chain W: 73% 24%



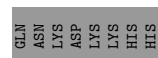
- Molecule 46: NADH:ubiquinone oxidoreductase subunit B2

Chain Y: 46% 11% 41%



- Molecule 47: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z: 54% 13% 32%



- Molecule 48: NADH-ubiquinone oxidoreductase chain 5

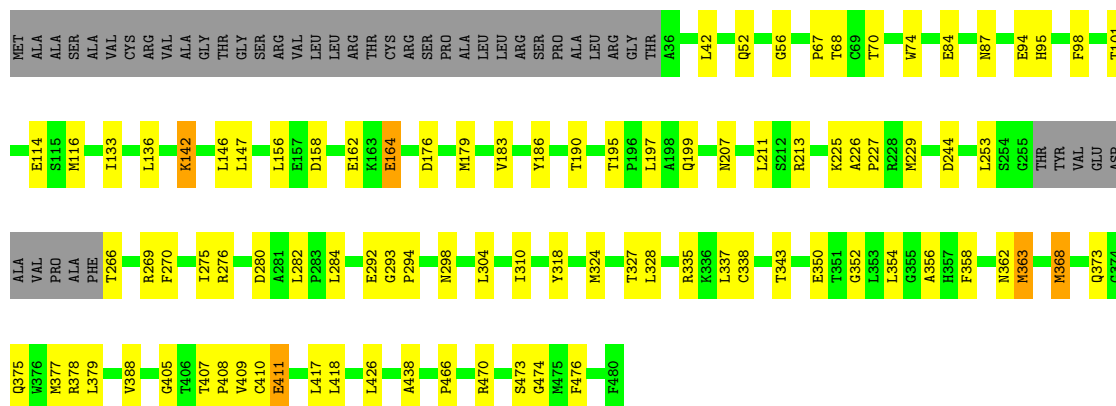
Chain I: 66% 31%





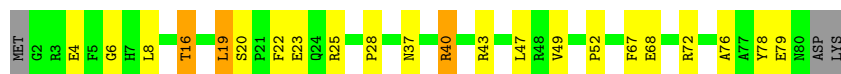
- Molecule 51: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 5: 71% 18% 9%



- Molecule 52: Cytochrome b-c1 complex subunit 8

Chain z: 70% 23% 7%



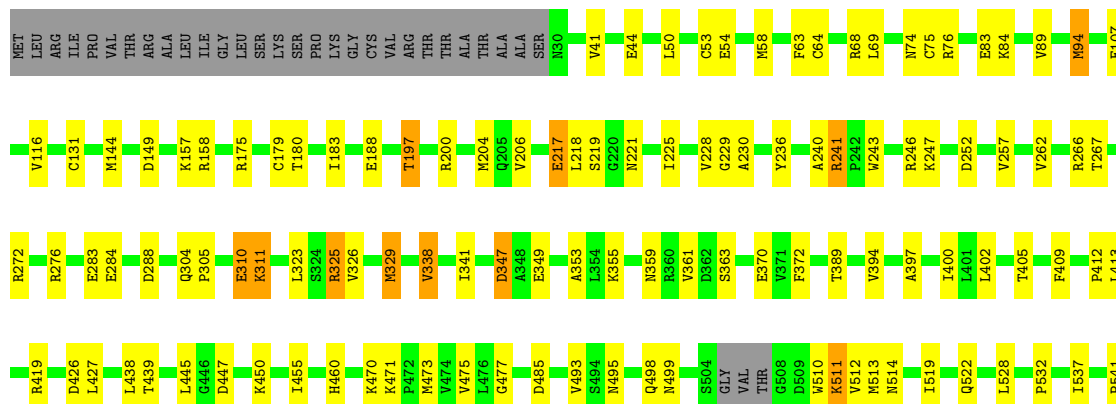
- Molecule 52: Cytochrome b-c1 complex subunit 8

Chain Aa: 71% 23% 6%



- Molecule 53: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G: 73% 19% 8%





- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 11787 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 1500 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 1.793 | Depositor |
| Minimum map value | -0.229 | Depositor |
| Average map value | 0.011 | Depositor |
| Map value standard deviation | 0.036 | Depositor |
| Recommended contour level | 0.15 | Depositor |
| Map size (Å) | 547.84, 547.84, 547.84 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.07, 1.07, 1.07 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, SF4, HEC, NDP, HEM, FMN, ZMP

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 | 0 | 0.17 | 0/563 | 0.32 | 0/755 |
| 1 | Ab | 0.17 | 0/549 | 0.27 | 0/735 |
| 2 | 1 | 0.20 | 0/506 | 0.30 | 0/683 |
| 2 | Ac | 0.15 | 0/498 | 0.23 | 0/672 |
| 3 | 2 | 0.19 | 0/1542 | 0.35 | 0/2088 |
| 3 | 4 | 0.39 | 1/1551 (0.1%) | 0.48 | 0/2098 |
| 3 | Ae | 0.28 | 0/147 | 0.64 | 0/203 |
| 3 | Af | 0.25 | 0/194 | 0.55 | 0/265 |
| 4 | 3 | 0.23 | 0/433 | 0.42 | 0/593 |
| 4 | Ad | 0.14 | 0/437 | 0.22 | 0/598 |
| 5 | 6 | 0.20 | 0/3192 | 0.32 | 0/4322 |
| 5 | v | 0.17 | 0/3192 | 0.29 | 0/4322 |
| 6 | 7 | 0.25 | 0/3123 | 0.37 | 0/4269 |
| 6 | w | 0.28 | 0/3123 | 0.41 | 0/4269 |
| 7 | 8 | 0.50 | 0/1954 | 0.64 | 0/2652 |
| 7 | x | 0.18 | 0/1954 | 0.27 | 0/2652 |
| 8 | 9 | 0.17 | 0/898 | 0.29 | 0/1204 |
| 8 | y | 0.17 | 0/913 | 0.27 | 0/1223 |
| 9 | a | 0.27 | 0/1184 | 0.36 | 0/1603 |
| 10 | b | 0.38 | 0/927 | 0.55 | 0/1264 |
| 11 | c | 0.18 | 0/1346 | 0.30 | 0/1840 |
| 12 | d | 0.23 | 0/1449 | 0.35 | 0/1953 |
| 13 | e | 0.18 | 0/849 | 0.36 | 0/1153 |
| 14 | f | 0.22 | 0/404 | 0.34 | 0/547 |
| 15 | g | 0.26 | 0/1031 | 0.37 | 0/1394 |
| 16 | h | 0.17 | 0/889 | 0.27 | 0/1190 |
| 17 | i | 0.21 | 0/2774 | 0.33 | 0/3768 |
| 18 | j | 0.42 | 0/811 | 0.62 | 0/1107 |
| 19 | k | 0.38 | 0/759 | 0.57 | 0/1029 |
| 20 | m | 0.56 | 0/1340 | 0.75 | 0/1816 |
| 21 | n | 0.16 | 0/487 | 0.32 | 0/659 |
| 22 | o | 0.17 | 0/1088 | 0.31 | 0/1477 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 23 | p | 0.21 | 0/1590 | 0.36 | 0/2155 |
| 24 | q | 0.21 | 0/3721 | 0.33 | 0/5073 |
| 25 | r | 0.45 | 0/2581 | 0.61 | 0/3529 |
| 26 | B | 0.15 | 0/3393 | 0.32 | 0/4584 |
| 27 | C | 0.30 | 0/3547 | 0.46 | 1/4809 (0.0%) |
| 28 | D | 0.18 | 0/1783 | 0.32 | 0/2428 |
| 29 | E | 0.15 | 0/1698 | 0.32 | 0/2311 |
| 30 | F | 0.14 | 0/740 | 0.26 | 0/998 |
| 31 | H | 0.42 | 0/1443 | 0.56 | 0/1952 |
| 32 | I | 0.22 | 0/1279 | 0.35 | 0/1730 |
| 33 | J | 0.14 | 0/976 | 0.26 | 0/1318 |
| 34 | K | 0.14 | 0/1244 | 0.23 | 0/1693 |
| 35 | L | 0.21 | 0/2774 | 0.38 | 0/3761 |
| 36 | N | 0.15 | 0/929 | 0.28 | 0/1258 |
| 37 | O | 0.14 | 0/692 | 0.37 | 0/934 |
| 37 | X | 0.12 | 0/701 | 0.29 | 0/946 |
| 38 | P | 0.12 | 0/680 | 0.28 | 0/916 |
| 39 | Q | 0.16 | 0/978 | 0.30 | 0/1317 |
| 40 | R | 0.11 | 0/304 | 0.25 | 0/410 |
| 41 | S | 0.18 | 0/577 | 0.32 | 0/777 |
| 42 | T | 0.15 | 0/659 | 0.26 | 0/905 |
| 43 | U | 0.38 | 0/2634 | 0.51 | 0/3565 |
| 44 | V | 0.16 | 0/1037 | 0.30 | 0/1404 |
| 45 | W | 0.20 | 0/1193 | 0.32 | 0/1609 |
| 46 | Y | 0.16 | 0/555 | 0.30 | 0/760 |
| 47 | Z | 0.12 | 0/645 | 0.23 | 0/872 |
| 48 | l | 0.19 | 0/4914 | 0.34 | 0/6683 |
| 49 | s | 0.16 | 0/1436 | 0.32 | 0/1938 |
| 50 | t | 0.28 | 0/1043 | 0.40 | 0/1396 |
| 51 | 5 | 0.18 | 0/3442 | 0.30 | 0/4667 |
| 51 | u | 0.17 | 0/3531 | 0.29 | 0/4793 |
| 52 | Aa | 0.16 | 0/684 | 0.29 | 0/926 |
| 52 | z | 0.17 | 0/688 | 0.33 | 0/931 |
| 53 | G | 0.15 | 0/5347 | 0.30 | 0/7243 |
| 54 | M | 0.14 | 0/791 | 0.29 | 0/1069 |
| All | All | 0.25 | 1/100336 (0.0%) | 0.38 | 1/136063 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7 | 8 | 0 | 1 |
| 25 | r | 0 | 1 |
| 27 | C | 0 | 2 |
| 32 | I | 0 | 1 |
| 43 | U | 0 | 1 |
| All | All | 0 | 6 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3 | 4 | 244 | VAL | N-CA | 5.10 | 1.49 | 1.45 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 27 | C | 110 | GLU | N-CA-C | -6.42 | 103.98 | 113.61 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 7 | 8 | 205 | ARG | Sidechain |
| 27 | C | 335 | ARG | Sidechain |
| 27 | C | 339 | ARG | Sidechain |
| 32 | I | 98 | ARG | Sidechain |
| 43 | U | 297 | ARG | Sidechain |
| 25 | r | 279 | ARG | Sidechain |

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 | 0 | 557 | 0 | 529 | 18 | 0 |
| 1 | Ab | 543 | 0 | 528 | 6 | 0 |
| 2 | 1 | 493 | 0 | 491 | 9 | 0 |
| 2 | Ac | 485 | 0 | 485 | 10 | 0 |
| 3 | 2 | 1509 | 0 | 1492 | 56 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 4 | 1518 | 0 | 1499 | 51 | 0 |
| 3 | Ae | 143 | 0 | 134 | 10 | 0 |
| 3 | Af | 191 | 0 | 188 | 8 | 0 |
| 4 | 3 | 417 | 0 | 414 | 7 | 0 |
| 4 | Ad | 421 | 0 | 418 | 4 | 0 |
| 5 | 6 | 3140 | 0 | 3121 | 87 | 0 |
| 5 | v | 3140 | 0 | 3121 | 60 | 0 |
| 6 | 7 | 3025 | 0 | 3090 | 55 | 0 |
| 6 | w | 3025 | 0 | 3090 | 57 | 0 |
| 7 | 8 | 1896 | 0 | 1844 | 74 | 0 |
| 7 | x | 1896 | 0 | 1843 | 38 | 0 |
| 8 | 9 | 878 | 0 | 870 | 11 | 0 |
| 8 | y | 893 | 0 | 888 | 7 | 0 |
| 9 | a | 1151 | 0 | 1164 | 25 | 0 |
| 10 | b | 900 | 0 | 903 | 44 | 0 |
| 11 | c | 1291 | 0 | 1185 | 36 | 0 |
| 12 | d | 1417 | 0 | 1393 | 35 | 0 |
| 13 | e | 826 | 0 | 789 | 18 | 0 |
| 14 | f | 391 | 0 | 392 | 12 | 0 |
| 15 | g | 1000 | 0 | 994 | 23 | 0 |
| 16 | h | 867 | 0 | 871 | 18 | 0 |
| 17 | i | 2711 | 0 | 2874 | 94 | 0 |
| 18 | j | 793 | 0 | 842 | 27 | 0 |
| 19 | k | 748 | 0 | 799 | 37 | 0 |
| 20 | m | 1309 | 0 | 1305 | 70 | 0 |
| 21 | n | 475 | 0 | 475 | 11 | 0 |
| 22 | o | 1058 | 0 | 1061 | 19 | 0 |
| 23 | p | 1534 | 0 | 1470 | 27 | 0 |
| 24 | q | 3630 | 0 | 3837 | 97 | 0 |
| 25 | r | 2508 | 0 | 2607 | 91 | 0 |
| 26 | B | 3318 | 0 | 3282 | 105 | 0 |
| 27 | C | 3454 | 0 | 3383 | 94 | 0 |
| 28 | D | 1732 | 0 | 1682 | 47 | 0 |
| 29 | E | 1658 | 0 | 1662 | 48 | 0 |
| 30 | F | 727 | 0 | 694 | 7 | 0 |
| 31 | H | 1412 | 0 | 1368 | 42 | 0 |
| 32 | I | 1248 | 0 | 1254 | 29 | 0 |
| 33 | J | 953 | 0 | 949 | 18 | 0 |
| 34 | K | 1203 | 0 | 1161 | 13 | 0 |
| 35 | L | 2702 | 0 | 2713 | 89 | 0 |
| 36 | N | 910 | 0 | 950 | 15 | 0 |
| 37 | O | 680 | 0 | 681 | 24 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 37 | X | 689 | 0 | 687 | 19 | 0 |
| 38 | P | 669 | 0 | 677 | 24 | 0 |
| 39 | Q | 954 | 0 | 960 | 27 | 0 |
| 40 | R | 295 | 0 | 279 | 14 | 0 |
| 41 | S | 562 | 0 | 557 | 8 | 0 |
| 42 | T | 638 | 0 | 637 | 6 | 0 |
| 43 | U | 2574 | 0 | 2532 | 52 | 0 |
| 44 | V | 1016 | 0 | 1022 | 19 | 0 |
| 45 | W | 1162 | 0 | 1156 | 27 | 0 |
| 46 | Y | 531 | 0 | 480 | 11 | 0 |
| 47 | Z | 626 | 0 | 607 | 11 | 0 |
| 48 | l | 4785 | 0 | 4935 | 147 | 0 |
| 49 | s | 1398 | 0 | 1374 | 31 | 0 |
| 50 | t | 1019 | 0 | 987 | 22 | 0 |
| 51 | 5 | 3374 | 0 | 3272 | 57 | 0 |
| 51 | u | 3459 | 0 | 3350 | 57 | 0 |
| 52 | Aa | 662 | 0 | 660 | 14 | 0 |
| 52 | z | 666 | 0 | 663 | 15 | 0 |
| 53 | G | 5260 | 0 | 5287 | 92 | 0 |
| 54 | M | 773 | 0 | 801 | 11 | 0 |
| 55 | 2 | 4 | 0 | 0 | 3 | 0 |
| 55 | 4 | 4 | 0 | 0 | 3 | 0 |
| 55 | E | 4 | 0 | 0 | 1 | 0 |
| 55 | G | 4 | 0 | 0 | 0 | 0 |
| 56 | 7 | 86 | 0 | 60 | 14 | 0 |
| 56 | w | 86 | 0 | 60 | 16 | 0 |
| 57 | 8 | 43 | 0 | 31 | 18 | 0 |
| 57 | x | 43 | 0 | 30 | 4 | 0 |
| 58 | B | 31 | 0 | 19 | 1 | 0 |
| 59 | B | 8 | 0 | 0 | 1 | 0 |
| 59 | G | 16 | 0 | 0 | 1 | 0 |
| 59 | H | 16 | 0 | 0 | 11 | 0 |
| 59 | I | 8 | 0 | 0 | 1 | 0 |
| 60 | L | 48 | 0 | 26 | 1 | 0 |
| 61 | Q | 30 | 0 | 30 | 3 | 0 |
| All | All | 98319 | 0 | 97964 | 2035 | 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 10.

All (2035) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:8:122:CYS:SG | 57:8:401:HEC:CAB | 2.22 | 1.28 |
| 31:H:116:CYS:SG | 59:H:302:SF4:FE1 | 1.44 | 1.07 |
| 7:8:122:CYS:SG | 57:8:401:HEC:C3B | 2.43 | 1.06 |
| 31:H:162:CYS:SG | 59:H:302:SF4:FE4 | 1.59 | 0.94 |
| 31:H:113:CYS:SG | 59:H:302:SF4:FE3 | 1.61 | 0.92 |
| 20:m:26:PRO:HB2 | 20:m:72:THR:HG21 | 1.52 | 0.90 |
| 31:H:113:CYS:HG | 59:H:302:SF4:FE3 | 0.67 | 0.90 |
| 16:h:81:ARG:HD2 | 20:m:111:GLU:HG3 | 1.57 | 0.86 |
| 24:q:370:PRO:HB3 | 24:q:375:LEU:HD22 | 1.59 | 0.83 |
| 17:i:38:LEU:HD23 | 19:k:73:LEU:HD12 | 1.59 | 0.83 |
| 20:m:45:LEU:HD22 | 20:m:50:SER:HA | 1.61 | 0.83 |
| 56:7:401:HEM:HHD | 56:7:401:HEM:HBC2 | 1.59 | 0.83 |
| 7:8:219:TYR:HE1 | 7:8:243:ILE:HG21 | 1.44 | 0.82 |
| 3:2:213:VAL:HA | 3:2:216:LEU:HD12 | 1.62 | 0.80 |
| 37:X:89:LEU:HD23 | 47:Z:64:ASN:HA | 1.62 | 0.80 |
| 3:2:238:CYS:HB3 | 3:2:243:CYS:SG | 2.21 | 0.80 |
| 7:8:127:SER:HB3 | 7:8:179:PRO:HD2 | 1.62 | 0.80 |
| 27:C:367:ALA:HB3 | 53:G:149:ASP:HB2 | 1.64 | 0.78 |
| 3:4:262:SER:HA | 3:4:273:GLY:HA3 | 1.65 | 0.78 |
| 56:7:401:HEM:HHC | 56:7:401:HEM:HBB2 | 1.64 | 0.78 |
| 31:H:155:CYS:SG | 59:H:301:SF4:FE3 | 1.75 | 0.78 |
| 19:k:34:GLU:HG3 | 20:m:64:MET:HE2 | 1.65 | 0.78 |
| 27:C:183:ILE:HG23 | 27:C:216:MET:HE2 | 1.63 | 0.77 |
| 7:8:97:TRP:HB2 | 7:8:100:ARG:HG3 | 1.66 | 0.77 |
| 28:D:102:ASP:HB2 | 36:N:90:LEU:HD22 | 1.67 | 0.77 |
| 18:j:21:ALA:HB1 | 25:r:218:GLY:HA3 | 1.67 | 0.76 |
| 35:L:216:ARG:HE | 35:L:282:PRO:HG2 | 1.48 | 0.76 |
| 17:i:313:MET:HE1 | 43:U:140:SER:HA | 1.67 | 0.76 |
| 17:i:42:PRO:HG3 | 20:m:167:VAL:HG22 | 1.68 | 0.75 |
| 7:8:196:PRO:HG2 | 57:8:401:HEC:HBA2 | 1.66 | 0.75 |
| 31:H:131:GLU:HB2 | 31:H:144:ARG:HB3 | 1.68 | 0.75 |
| 53:G:341:ILE:HD11 | 53:G:537:ILE:HG13 | 1.69 | 0.75 |
| 35:L:78:PRO:HB3 | 35:L:114:VAL:HG21 | 1.67 | 0.74 |
| 2:Ac:11:TYR:HA | 2:Ac:15:PHE:HB2 | 1.67 | 0.74 |
| 17:i:258:SER:HB2 | 17:i:336:VAL:HG12 | 1.67 | 0.74 |
| 3:4:208:GLU:OE1 | 3:4:269:ARG:NH2 | 2.21 | 0.74 |
| 11:c:83:GLN:HE22 | 11:c:86:ARG:HH11 | 1.33 | 0.74 |
| 6:7:41:LEU:HD12 | 56:7:401:HEM:HBB1 | 1.69 | 0.74 |
| 25:r:58:LYS:NZ | 32:I:101:ASP:OD1 | 2.20 | 0.73 |
| 27:C:374:ARG:NH2 | 31:H:165:ASP:OD1 | 2.21 | 0.73 |
| 7:8:186:ALA:O | 7:8:190:ASN:ND2 | 2.21 | 0.73 |
| 48:l:359:MET:O | 48:l:436:ARG:NH2 | 2.21 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:g:4:MET:HG3 | 17:i:347:ASN:HD21 | 1.54 | 0.73 |
| 25:r:185:TRP:HE1 | 25:r:238:THR:HG22 | 1.53 | 0.73 |
| 3:4:240:HIS:HB2 | 3:4:275:ALA:HA | 1.71 | 0.73 |
| 26:B:38:GLU:HA | 29:E:239:LYS:HE3 | 1.72 | 0.72 |
| 44:V:69:ILE:HG13 | 44:V:100:THR:HG21 | 1.72 | 0.72 |
| 3:4:177:LEU:HB2 | 3:4:290:ASP:HA | 1.72 | 0.72 |
| 51:5:293:GLY:N | 51:5:352:GLY:O | 2.21 | 0.72 |
| 3:4:255:TYR:HB2 | 3:4:264:TYR:HB2 | 1.70 | 0.72 |
| 17:i:58:LYS:HG2 | 48:l:584:ILE:HD11 | 1.72 | 0.72 |
| 6:7:338:ILE:HD13 | 6:7:351:GLY:HA2 | 1.72 | 0.71 |
| 25:r:79:LEU:HD22 | 25:r:222:MET:HG2 | 1.70 | 0.71 |
| 43:U:213:VAL:HG12 | 43:U:217:GLN:HE21 | 1.55 | 0.71 |
| 35:L:352:ARG:HG3 | 35:L:356:TRP:HB3 | 1.73 | 0.71 |
| 3:4:245:PRO:HB2 | 3:4:255:TYR:HB3 | 1.73 | 0.71 |
| 9:a:130:GLU:OE1 | 9:a:131:LYS:N | 2.24 | 0.71 |
| 7:8:186:ALA:O | 7:8:190:ASN:CG | 2.34 | 0.70 |
| 26:B:288:VAL:HG21 | 26:B:303:HIS:HB3 | 1.74 | 0.70 |
| 26:B:50:ASP:O | 26:B:59:ARG:NH1 | 2.24 | 0.70 |
| 44:V:108:TYR:OH | 52:z:43:ARG:NH1 | 2.25 | 0.70 |
| 8:y:14:LEU:HD23 | 8:y:17:ILE:HD11 | 1.74 | 0.70 |
| 28:D:186:ARG:NH2 | 28:D:193:PHE:O | 2.25 | 0.70 |
| 5:6:144:PRO:HG2 | 5:6:209:VAL:HG11 | 1.74 | 0.70 |
| 6:7:338:ILE:HD11 | 6:7:350:ILE:HG22 | 1.74 | 0.70 |
| 25:r:24:GLU:HA | 25:r:271:LEU:HD13 | 1.75 | 0.69 |
| 31:H:76:TYR:HA | 31:H:79:ARG:HD3 | 1.71 | 0.69 |
| 37:X:125:GLU:HG2 | 48:l:439:PRO:HG2 | 1.74 | 0.69 |
| 17:i:45:MET:HE1 | 20:m:171:ILE:HG23 | 1.73 | 0.69 |
| 28:D:171:TRP:HE1 | 39:Q:114:MET:HE1 | 1.56 | 0.69 |
| 51:u:470:ARG:HH21 | 6:w:222:PRO:HD3 | 1.57 | 0.69 |
| 53:G:602:ARG:HB2 | 53:G:659:VAL:HG13 | 1.74 | 0.69 |
| 14:f:65:ASP:OD2 | 15:g:79:LYS:NZ | 2.25 | 0.69 |
| 7:x:216:LEU:HB3 | 7:x:249:ILE:HD11 | 1.73 | 0.69 |
| 12:d:144:SER:O | 12:d:158:LYS:NZ | 2.26 | 0.69 |
| 18:j:70:ALA:HB2 | 20:m:59:ILE:HG21 | 1.74 | 0.69 |
| 25:r:27:VAL:HG12 | 25:r:31:MET:HE2 | 1.75 | 0.68 |
| 27:C:143:ASP:OD1 | 27:C:143:ASP:N | 2.26 | 0.68 |
| 29:E:155:LYS:NZ | 29:E:206:ASP:OD1 | 2.22 | 0.68 |
| 17:i:236:LYS:HG2 | 17:i:237:MET:HG3 | 1.75 | 0.68 |
| 25:r:157:ASN:ND2 | 25:r:159:SER:O | 2.26 | 0.68 |
| 27:C:457:ILE:HG23 | 27:C:462:ILE:HD11 | 1.76 | 0.68 |
| 5:v:65:ILE:HG12 | 5:v:218:MET:HG2 | 1.75 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:7:53:MET:HB3 | 6:w:177:ARG:HD3 | 1.75 | 0.68 |
| 10:b:117:ILE:HG22 | 10:b:119:LEU:H | 1.55 | 0.68 |
| 25:r:90:PRO:HD2 | 25:r:240:ILE:HD13 | 1.74 | 0.68 |
| 7:8:103:LEU:HD21 | 7:8:291:LEU:HB2 | 1.74 | 0.68 |
| 10:b:80:TRP:HD1 | 12:d:41:VAL:HG13 | 1.59 | 0.68 |
| 26:B:296:LEU:HD21 | 26:B:317:VAL:HG11 | 1.74 | 0.68 |
| 26:B:382:CYS:HB2 | 26:B:424:ILE:HG23 | 1.76 | 0.68 |
| 7:8:104:SER:OG | 2:Ac:51:LYS:NZ | 2.27 | 0.68 |
| 35:L:163:SER:HA | 35:L:179:LYS:HE3 | 1.76 | 0.68 |
| 51:5:335:ARG:HB2 | 51:5:337:LEU:HG | 1.76 | 0.68 |
| 3:2:225:ARG:NH2 | 3:2:279:LEU:O | 2.25 | 0.67 |
| 27:C:150:MET:SD | 27:C:150:MET:N | 2.63 | 0.67 |
| 28:D:93:VAL:HG11 | 28:D:153:ILE:HD11 | 1.73 | 0.67 |
| 43:U:148:ALA:HB1 | 43:U:159:VAL:HG11 | 1.75 | 0.67 |
| 48:l:246:LEU:HB3 | 48:l:247:LEU:HD23 | 1.75 | 0.67 |
| 48:l:372:ALA:HA | 48:l:458:LEU:HD21 | 1.76 | 0.67 |
| 3:4:184:LYS:HZ2 | 3:4:186:MET:HE1 | 1.58 | 0.67 |
| 5:6:90:THR:HG23 | 5:6:95:SER:HA | 1.77 | 0.67 |
| 20:m:37:GLY:HA3 | 20:m:61:LEU:HD11 | 1.75 | 0.67 |
| 51:u:134:LYS:HE3 | 5:v:384:MET:HE3 | 1.77 | 0.67 |
| 26:B:318:ILE:HG12 | 26:B:357:MET:HE1 | 1.76 | 0.67 |
| 17:i:128:LEU:HD11 | 17:i:213:LEU:HD23 | 1.75 | 0.67 |
| 53:G:541:PRO:HB2 | 53:G:561:PRO:HD3 | 1.76 | 0.67 |
| 17:i:108:LEU:HD11 | 17:i:191:THR:HG21 | 1.75 | 0.67 |
| 31:H:116:CYS:SG | 59:H:302:SF4:S3 | 2.92 | 0.67 |
| 34:K:95:ASP:H | 54:M:35:THR:HG23 | 1.58 | 0.67 |
| 35:L:203:GLY:H | 35:L:206:ASP:HB2 | 1.60 | 0.67 |
| 7:8:216:LEU:HD11 | 57:8:401:HEC:HMB2 | 1.77 | 0.67 |
| 10:b:126:GLN:HA | 50:t:89:TYR:CE2 | 2.30 | 0.67 |
| 26:B:357:MET:HG2 | 26:B:361:THR:HG21 | 1.75 | 0.67 |
| 46:Y:43:ARG:HB3 | 46:Y:46:GLN:HG2 | 1.76 | 0.66 |
| 28:D:181:HIS:HD2 | 28:D:183:ASP:H | 1.43 | 0.66 |
| 14:f:73:ASN:ND2 | 15:g:22:SER:O | 2.27 | 0.66 |
| 7:8:248:PRO:CB | 57:8:401:HEC:HHC | 2.26 | 0.66 |
| 1:0:69:GLU:OE2 | 52:z:72:ARG:NH1 | 2.30 | 0.65 |
| 19:k:75:LEU:HD11 | 20:m:68:PHE:HD2 | 1.60 | 0.65 |
| 45:W:105:LYS:HE3 | 45:W:108:GLU:HB2 | 1.77 | 0.65 |
| 52:z:76:ALA:HA | 52:z:79:GLU:HG2 | 1.78 | 0.65 |
| 28:D:185:ARG:HA | 39:Q:114:MET:HE3 | 1.78 | 0.65 |
| 17:i:268:GLN:HA | 24:q:165:VAL:HG11 | 1.78 | 0.65 |
| 49:s:198:ASP:N | 49:s:201:GLU:OE1 | 2.27 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:162:LYS:NZ | 5:6:194:ASP:OD1 | 2.28 | 0.65 |
| 26:B:319:PRO:HB3 | 26:B:327:ILE:HD11 | 1.78 | 0.65 |
| 31:H:142:THR:O | 31:H:187:LYS:NZ | 2.27 | 0.65 |
| 27:C:160:ALA:HA | 27:C:404:THR:HG21 | 1.78 | 0.65 |
| 17:i:18:MET:O | 17:i:22:ILE:HB | 1.97 | 0.65 |
| 25:r:157:ASN:HA | 25:r:168:THR:HG21 | 1.79 | 0.64 |
| 5:v:217:ARG:NH2 | 5:v:246:LEU:O | 2.29 | 0.64 |
| 23:p:54:HIS:NE2 | 23:p:106:LEU:HD12 | 2.12 | 0.64 |
| 12:d:76:GLU:HB3 | 13:e:146:LYS:HD3 | 1.79 | 0.64 |
| 24:q:403:THR:HA | 24:q:406:TYR:CE2 | 2.32 | 0.64 |
| 27:C:285:THR:HG23 | 36:N:13:GLY:HA3 | 1.79 | 0.64 |
| 8:9:13:TRP:CG | 8:9:14:LEU:H | 2.14 | 0.64 |
| 9:a:143:GLU:HB3 | 24:q:178:ILE:HG13 | 1.79 | 0.64 |
| 3:2:226:VAL:HG11 | 3:2:232:VAL:HA | 1.80 | 0.64 |
| 29:E:177:LEU:N | 55:E:301:FES:S1 | 2.70 | 0.64 |
| 3:4:243:CYS:HA | 6:w:264:THR:HG21 | 1.79 | 0.64 |
| 25:r:169:GLN:HG2 | 25:r:174:MET:HG3 | 1.80 | 0.64 |
| 29:E:138:THR:HA | 29:E:141:MET:HE2 | 1.80 | 0.64 |
| 11:c:101:TRP:CD1 | 22:o:47:TYR:HB2 | 2.31 | 0.64 |
| 7:8:216:LEU:HB3 | 7:8:249:ILE:HD11 | 1.80 | 0.64 |
| 29:E:69:ASN:O | 40:R:100:GLN:NE2 | 2.31 | 0.64 |
| 48:l:5:ALA:HB2 | 48:l:61:MET:HE1 | 1.79 | 0.64 |
| 48:l:319:ILE:HG13 | 48:l:399:VAL:HG22 | 1.80 | 0.64 |
| 11:c:164:ASN:HA | 11:c:181:VAL:HB | 1.80 | 0.63 |
| 32:I:94:ARG:NE | 32:I:99:GLN:OE1 | 2.32 | 0.63 |
| 35:L:136:PHE:HD2 | 35:L:174:ARG:HG2 | 1.63 | 0.63 |
| 48:l:286:LEU:HD22 | 48:l:411:MET:HG3 | 1.80 | 0.63 |
| 11:c:165:ASP:O | 11:c:170:ARG:NH1 | 2.31 | 0.63 |
| 17:i:71:MET:HE3 | 19:k:59:MET:HE1 | 1.80 | 0.63 |
| 20:m:26:PRO:CB | 20:m:72:THR:HG21 | 2.27 | 0.63 |
| 25:r:119:SER:HB2 | 25:r:215:TYR:CE1 | 2.34 | 0.63 |
| 53:G:389:THR:N | 53:G:514:ASN:OD1 | 2.31 | 0.63 |
| 9:a:101:ILE:HG12 | 12:d:64:TYR:HB3 | 1.80 | 0.63 |
| 26:B:88:ARG:HB2 | 26:B:244:ASN:HD22 | 1.63 | 0.63 |
| 26:B:211:ALA:HB2 | 26:B:223:PRO:HG3 | 1.80 | 0.63 |
| 10:b:100:ARG:HH21 | 50:t:50:GLN:HB3 | 1.63 | 0.63 |
| 19:k:27:MET:HG2 | 20:m:72:THR:HG22 | 1.80 | 0.63 |
| 25:r:149:ILE:HG21 | 25:r:185:TRP:HB2 | 1.80 | 0.63 |
| 43:U:224:GLY:HA2 | 43:U:229:MET:HE3 | 1.81 | 0.63 |
| 57:8:401:HEC:HBD1 | 57:8:401:HEC:HHA | 1.78 | 0.63 |
| 18:j:26:GLN:HA | 25:r:60:PRO:HG3 | 1.81 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:q:36:LEU:HD23 | 24:q:39:LEU:HD12 | 1.80 | 0.63 |
| 43:U:72:LYS:HE3 | 43:U:163:ARG:HG3 | 1.80 | 0.63 |
| 48:l:10:THR:HA | 48:l:13:ILE:HG22 | 1.79 | 0.63 |
| 56:w:402:HEM:HBC2 | 56:w:402:HEM:HMC1 | 1.80 | 0.63 |
| 9:a:179:ILE:HG21 | 16:h:38:LYS:HG3 | 1.80 | 0.63 |
| 53:G:338:VAL:HG12 | 53:G:544:VAL:HB | 1.81 | 0.63 |
| 35:L:122:ILE:HG23 | 35:L:160:ILE:HB | 1.81 | 0.63 |
| 5:v:89:LEU:HD22 | 5:v:150:GLU:HB3 | 1.81 | 0.63 |
| 5:6:183:ARG:NH2 | 5:v:451:ASP:OD2 | 2.32 | 0.62 |
| 53:G:63:PHE:HB2 | 53:G:75:CYS:HB2 | 1.81 | 0.62 |
| 7:8:187:ARG:HA | 7:8:190:ASN:HD21 | 1.64 | 0.62 |
| 32:I:86:MET:HB2 | 32:I:91:VAL:HB | 1.81 | 0.62 |
| 6:7:112:THR:HG22 | 6:7:196:HIS:CE1 | 2.33 | 0.62 |
| 19:k:18:GLY:O | 20:m:23:LYS:NZ | 2.21 | 0.62 |
| 19:k:23:ARG:HH21 | 20:m:86:ASN:HD22 | 1.47 | 0.62 |
| 52:Aa:19:LEU:HD22 | 52:Aa:24:GLN:HB3 | 1.79 | 0.62 |
| 48:l:400:ASN:HA | 48:l:409:LEU:HD11 | 1.80 | 0.62 |
| 8:y:92:GLU:HG2 | 8:y:96:LYS:HE3 | 1.81 | 0.62 |
| 48:l:306:THR:HG22 | 48:l:336:LYS:HG2 | 1.81 | 0.62 |
| 27:C:187:LEU:HD21 | 27:C:216:MET:HB2 | 1.81 | 0.62 |
| 35:L:290:HIS:O | 35:L:294:ARG:HB2 | 2.00 | 0.62 |
| 51:u:120:LEU:HD13 | 51:u:133:ILE:HG12 | 1.81 | 0.62 |
| 24:q:208:PRO:HD3 | 24:q:236:LEU:HD22 | 1.80 | 0.62 |
| 26:B:164:ASN:HB3 | 40:R:78:HIS:HB2 | 1.80 | 0.62 |
| 5:6:216:ALA:HB3 | 5:6:244:LEU:H | 1.65 | 0.62 |
| 5:6:272:VAL:HG12 | 5:6:337:GLY:HA3 | 1.81 | 0.62 |
| 42:T:155:PRO:HD3 | 49:s:206:THR:HG21 | 1.81 | 0.62 |
| 24:q:11:LEU:HB3 | 24:q:100:ILE:HD13 | 1.82 | 0.61 |
| 29:E:188:ILE:HG22 | 29:E:189:ASN:H | 1.64 | 0.61 |
| 29:E:191:ASN:HB3 | 29:E:216:PRO:HB3 | 1.81 | 0.61 |
| 50:t:90:CYS:HA | 50:t:93:LEU:HD12 | 1.80 | 0.61 |
| 25:r:31:MET:HG2 | 31:H:77:LEU:HB2 | 1.83 | 0.61 |
| 12:d:122:ARG:NH1 | 48:l:203:MET:O | 2.34 | 0.61 |
| 26:B:371:ILE:HD13 | 26:B:396:MET:HG3 | 1.83 | 0.61 |
| 37:X:138:LEU:HG | 37:X:144:ILE:HG12 | 1.82 | 0.61 |
| 26:B:314:LEU:HD11 | 26:B:317:VAL:HG23 | 1.81 | 0.61 |
| 37:O:104:PHE:CD2 | 37:O:139:MET:HA | 2.35 | 0.61 |
| 39:Q:47:PHE:O | 39:Q:57:ARG:NH2 | 2.34 | 0.61 |
| 27:C:344:ARG:HB3 | 45:W:21:TYR:O | 2.01 | 0.61 |
| 5:6:61:ILE:HD11 | 5:6:225:VAL:HG11 | 1.83 | 0.61 |
| 6:7:113:TRP:NE1 | 6:7:301:LEU:O | 2.26 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:i:41:ILE:HG21 | 19:k:73:LEU:HD21 | 1.82 | 0.61 |
| 35:L:231:VAL:HB | 35:L:265:ARG:HH21 | 1.66 | 0.61 |
| 17:i:96:THR:O | 17:i:100:MET:HG2 | 2.01 | 0.61 |
| 20:m:26:PRO:HB2 | 20:m:72:THR:CG2 | 2.27 | 0.61 |
| 35:L:119:ASN:HD22 | 35:L:120:VAL:HG23 | 1.66 | 0.61 |
| 16:h:86:LEU:HD23 | 16:h:92:TYR:HB2 | 1.82 | 0.61 |
| 17:i:31:ILE:HD11 | 19:k:62:ILE:HG21 | 1.83 | 0.61 |
| 53:G:341:ILE:HG12 | 53:G:545:LEU:HD11 | 1.82 | 0.61 |
| 20:m:86:ASN:HB3 | 20:m:89:VAL:HG23 | 1.83 | 0.60 |
| 28:D:128:ILE:HB | 28:D:145:THR:HG23 | 1.83 | 0.60 |
| 3:2:198:ARG:HH12 | 3:2:254:GLY:HA2 | 1.65 | 0.60 |
| 3:4:230:GLU:HG3 | 3:4:231:TRP:HD1 | 1.66 | 0.60 |
| 24:q:370:PRO:HB2 | 48:l:142:ILE:HG12 | 1.83 | 0.60 |
| 35:L:198:PRO:HA | 35:L:260:PHE:HB2 | 1.83 | 0.60 |
| 48:l:214:ILE:HG12 | 48:l:276:MET:HE1 | 1.83 | 0.60 |
| 10:b:99:GLU:HG2 | 48:l:61:MET:HG2 | 1.81 | 0.60 |
| 28:D:218:ARG:HD2 | 39:Q:127:THR:HA | 1.83 | 0.60 |
| 37:O:138:LEU:O | 37:O:139:MET:HB2 | 2.01 | 0.60 |
| 6:w:132:VAL:HA | 6:w:139:SER:HB3 | 1.82 | 0.60 |
| 7:x:96:PRO:HA | 7:x:100:ARG:HE | 1.66 | 0.60 |
| 20:m:125:TRP:HB2 | 45:W:137:THR:HG21 | 1.82 | 0.60 |
| 29:E:246:GLN:HB3 | 29:E:249:LEU:HD23 | 1.84 | 0.60 |
| 46:Y:47:PHE:HE1 | 48:l:364:LYS:HD3 | 1.66 | 0.60 |
| 52:Aa:21:PRO:HA | 52:Aa:24:GLN:HE21 | 1.65 | 0.60 |
| 7:8:187:ARG:HA | 7:8:190:ASN:ND2 | 2.16 | 0.60 |
| 7:8:228:LEU:HD11 | 7:8:234:PHE:HB2 | 1.83 | 0.60 |
| 16:h:59:GLU:OE2 | 49:s:222:ARG:NH1 | 2.33 | 0.60 |
| 48:l:504:LEU:O | 48:l:507:THR:OG1 | 2.20 | 0.60 |
| 2:Ac:20:THR:HG22 | 4:Ad:23:MET:HE2 | 1.83 | 0.60 |
| 25:r:119:SER:HB2 | 25:r:215:TYR:HE1 | 1.66 | 0.60 |
| 48:l:184:LEU:HD21 | 48:l:211:MET:HG2 | 1.84 | 0.60 |
| 24:q:104:LEU:HG | 24:q:108:MET:HE2 | 1.84 | 0.60 |
| 24:q:369:LEU:HD13 | 48:l:149:ILE:HG13 | 1.84 | 0.60 |
| 51:5:276:ARG:NH2 | 51:5:466:PRO:O | 2.32 | 0.60 |
| 24:q:247:THR:HB | 24:q:304:GLN:HE21 | 1.66 | 0.60 |
| 43:U:110:LEU:HD13 | 43:U:336:LEU:HD11 | 1.84 | 0.60 |
| 45:W:82:ARG:HG2 | 45:W:86:MET:HE2 | 1.84 | 0.60 |
| 48:l:414:ILE:O | 48:l:418:LEU:HG | 2.02 | 0.60 |
| 5:6:138:LEU:HD12 | 5:6:233:VAL:HG22 | 1.84 | 0.59 |
| 26:B:366:ALA:HA | 29:E:141:MET:HE1 | 1.84 | 0.59 |
| 5:6:151:VAL:O | 5:6:155:GLN:HG2 | 2.01 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:b:4:TYR:HD2 | 10:b:9:LYS:HG2 | 1.67 | 0.59 |
| 5:6:82:LEU:HD21 | 5:6:151:VAL:HG13 | 1.84 | 0.59 |
| 20:m:130:THR:HG21 | 45:W:124:LEU:HD12 | 1.84 | 0.59 |
| 35:L:274:TYR:HB2 | 35:L:367:ALA:HB2 | 1.85 | 0.59 |
| 27:C:172:ARG:NH1 | 27:C:241:ASP:OD2 | 2.36 | 0.59 |
| 8:y:69:LEU:HD11 | 8:y:76:LEU:HD13 | 1.84 | 0.59 |
| 5:6:111:SER:HB3 | 3:Ae:59:LEU:HG | 1.84 | 0.59 |
| 5:6:378:LEU:HD13 | 5:6:416:ILE:HD12 | 1.84 | 0.59 |
| 26:B:146:GLY:HA3 | 26:B:193:PHE:CE1 | 2.37 | 0.59 |
| 1:0:33:VAL:HG12 | 1:0:82:VAL:HG22 | 1.85 | 0.59 |
| 19:k:27:MET:HE3 | 19:k:30:LEU:HB2 | 1.83 | 0.59 |
| 23:p:76:ARG:HG2 | 47:Z:65:GLU:HB3 | 1.85 | 0.59 |
| 1:0:57:VAL:HG22 | 1:0:65:GLU:HG3 | 1.84 | 0.59 |
| 3:4:145:GLY:HA3 | 7:8:300:LEU:HD21 | 1.85 | 0.59 |
| 17:i:193:VAL:HG13 | 17:i:266:ILE:HG23 | 1.85 | 0.59 |
| 24:q:325:MET:HE2 | 24:q:329:LEU:HD11 | 1.85 | 0.59 |
| 26:B:116:ASN:ND2 | 26:B:207:GLY:O | 2.36 | 0.59 |
| 6:w:97:HIS:HE1 | 56:w:401:HEM:C1A | 2.21 | 0.59 |
| 51:5:179:MET:HE1 | 51:5:282:LEU:HD13 | 1.85 | 0.59 |
| 5:6:60:ARG:NH2 | 5:6:124:GLU:OE1 | 2.36 | 0.59 |
| 17:i:171:ASN:ND2 | 27:C:58:MET:O | 2.36 | 0.59 |
| 33:J:75:ARG:NH2 | 33:J:102:ASP:O | 2.35 | 0.58 |
| 53:G:355:LYS:NZ | 53:G:528:LEU:O | 2.30 | 0.58 |
| 24:q:401:MET:HA | 48:l:176:ARG:HG2 | 1.84 | 0.58 |
| 48:l:250:SER:HB2 | 48:l:333:ALA:HA | 1.85 | 0.58 |
| 6:w:196:HIS:HE1 | 56:w:401:HEM:ND | 2.01 | 0.58 |
| 19:k:75:LEU:HD11 | 20:m:68:PHE:CD2 | 2.38 | 0.58 |
| 20:m:17:PHE:HA | 20:m:20:PHE:CE2 | 2.38 | 0.58 |
| 29:E:169:PHE:HE2 | 29:E:209:LYS:HG3 | 1.68 | 0.58 |
| 33:J:154:LYS:HZ3 | 33:J:156:LYS:HE3 | 1.66 | 0.58 |
| 39:Q:66:TYR:CZ | 39:Q:86:ARG:HD3 | 2.38 | 0.58 |
| 17:i:57:THR:HG22 | 19:k:77:LEU:HB3 | 1.86 | 0.58 |
| 23:p:153:GLU:HA | 23:p:156:MET:HG3 | 1.85 | 0.58 |
| 25:r:236:ALA:HA | 25:r:263:THR:HG22 | 1.84 | 0.58 |
| 27:C:228:MET:HG3 | 32:I:167:PRO:HG3 | 1.84 | 0.58 |
| 35:L:161:HIS:HB3 | 35:L:195:ILE:HG12 | 1.84 | 0.58 |
| 53:G:74:ASN:HD21 | 53:G:179:CYS:HA | 1.67 | 0.58 |
| 25:r:308:PRO:HB2 | 25:r:314:ILE:HD13 | 1.84 | 0.58 |
| 28:D:215:GLU:OE1 | 35:L:70:ARG:NH2 | 2.37 | 0.58 |
| 5:6:55:TYR:HA | 5:6:127:ARG:HH12 | 1.67 | 0.58 |
| 5:6:240:MET:SD | 5:6:241:ARG:N | 2.76 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:e:106:VAL:HG13 | 24:q:453:MET:HE3 | 1.86 | 0.58 |
| 27:C:460:GLN:O | 27:C:461:ASP:C | 2.47 | 0.58 |
| 34:K:60:ARG:HH22 | 34:K:95:ASP:HA | 1.69 | 0.58 |
| 17:i:93:VAL:HG13 | 48:l:599:MET:HE1 | 1.85 | 0.58 |
| 18:j:1:MET:SD | 18:j:1:MET:N | 2.64 | 0.58 |
| 26:B:115:VAL:HG22 | 26:B:248:VAL:HG21 | 1.85 | 0.58 |
| 26:B:384:PRO:HD2 | 53:G:76:ARG:HG3 | 1.85 | 0.58 |
| 46:Y:54:GLN:HE21 | 48:l:446:ASN:HB2 | 1.68 | 0.58 |
| 48:l:562:LEU:HB2 | 48:l:563:PRO:HD3 | 1.85 | 0.58 |
| 6:w:338:ILE:HD11 | 6:w:350:ILE:HG22 | 1.84 | 0.58 |
| 10:b:85:TYR:HE2 | 48:l:65:ASN:HB2 | 1.68 | 0.58 |
| 17:i:17:THR:HG22 | 17:i:137:ALA:HB2 | 1.86 | 0.58 |
| 20:m:34:ILE:HG12 | 20:m:65:LEU:HD21 | 1.86 | 0.58 |
| 28:D:101:ARG:NH1 | 28:D:159:VAL:O | 2.37 | 0.58 |
| 6:7:132:VAL:HA | 6:7:139:SER:HB3 | 1.86 | 0.58 |
| 7:8:271:VAL:O | 7:8:275:LEU:HG | 2.04 | 0.58 |
| 11:c:159:LYS:NZ | 11:c:160:GLN:O | 2.37 | 0.58 |
| 7:x:291:LEU:HD11 | 7:x:295:MET:HE3 | 1.86 | 0.58 |
| 53:G:257:VAL:HG11 | 53:G:413:LEU:HB2 | 1.84 | 0.58 |
| 11:c:166:LEU:HB3 | 11:c:169:GLU:HB2 | 1.86 | 0.57 |
| 17:i:20:VAL:HG11 | 17:i:137:ALA:HB1 | 1.85 | 0.57 |
| 19:k:27:MET:O | 19:k:31:LEU:HG | 2.03 | 0.57 |
| 48:l:34:ASN:OD1 | 48:l:34:ASN:N | 2.37 | 0.57 |
| 13:e:82:VAL:HG23 | 24:q:25:ILE:HD11 | 1.86 | 0.57 |
| 41:S:69:ILE:HD13 | 49:s:148:PHE:HB3 | 1.86 | 0.57 |
| 3:Ae:52:GLY:HA2 | 3:Ae:61:ALA:HA | 1.87 | 0.57 |
| 5:v:90:THR:HG23 | 5:v:95:SER:HA | 1.86 | 0.57 |
| 56:w:401:HEM:HMC2 | 56:w:401:HEM:HBC2 | 1.85 | 0.57 |
| 7:8:186:ALA:O | 7:8:190:ASN:OD1 | 2.21 | 0.57 |
| 5:v:82:LEU:HD21 | 5:v:151:VAL:HG13 | 1.86 | 0.57 |
| 5:v:290:GLN:HG3 | 5:v:325:ALA:HB3 | 1.85 | 0.57 |
| 28:D:215:GLU:HG3 | 35:L:63:TYR:CD2 | 2.38 | 0.57 |
| 32:I:65:MET:HE1 | 32:I:97:PRO:HG3 | 1.85 | 0.57 |
| 33:J:75:ARG:HH12 | 33:J:104:ARG:HG3 | 1.70 | 0.57 |
| 3:4:106:VAL:HG22 | 51:5:275:ILE:HD11 | 1.87 | 0.57 |
| 11:c:169:GLU:OE1 | 11:c:169:GLU:N | 2.37 | 0.57 |
| 39:Q:51:MET:HG3 | 39:Q:55:LYS:HE2 | 1.87 | 0.57 |
| 48:l:323:HIS:ND1 | 48:l:475:MET:SD | 2.78 | 0.57 |
| 53:G:89:VAL:HB | 53:G:94:MET:HG3 | 1.87 | 0.57 |
| 1:0:34:ARG:HD2 | 1:0:78:ARG:CZ | 2.35 | 0.57 |
| 2:1:56:ILE:HB | 2:1:59:LYS:HE2 | 1.87 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:7:402:HEM:HMB1 | 56:7:402:HEM:HBB2 | 1.86 | 0.57 |
| 9:a:139:ILE:HG12 | 24:q:54:LEU:HD23 | 1.87 | 0.57 |
| 11:c:184:TYR:HD1 | 50:t:36:GLU:HA | 1.69 | 0.57 |
| 16:h:16:ARG:O | 16:h:19:THR:OG1 | 2.23 | 0.57 |
| 35:L:206:ASP:CG | 35:L:208:PHE:H | 2.12 | 0.57 |
| 48:l:223:LYS:HE3 | 48:l:252:MET:HE3 | 1.87 | 0.57 |
| 2:1:11:TYR:HA | 2:1:15:PHE:HB2 | 1.86 | 0.57 |
| 5:6:221:ILE:HG12 | 5:6:396:VAL:HG12 | 1.86 | 0.57 |
| 26:B:140:GLU:HG3 | 26:B:252:PRO:HG3 | 1.86 | 0.57 |
| 51:u:102:LYS:HG2 | 51:u:153:ASN:HB3 | 1.86 | 0.57 |
| 5:v:138:LEU:HD11 | 5:v:233:VAL:HG13 | 1.87 | 0.57 |
| 16:h:82:GLN:HE21 | 16:h:82:GLN:HA | 1.69 | 0.56 |
| 31:H:118:LEU:HD23 | 31:H:161:ALA:HB1 | 1.87 | 0.56 |
| 35:L:165:LEU:HD23 | 35:L:197:LYS:HE3 | 1.87 | 0.56 |
| 3:4:260:HIS:HB2 | 55:4:301:FES:S2 | 2.45 | 0.56 |
| 7:8:193:ALA:HB1 | 57:8:401:HEC:HAD1 | 1.88 | 0.56 |
| 25:r:102:VAL:CG1 | 25:r:150:LEU:HD21 | 2.36 | 0.56 |
| 31:H:101:HIS:H | 31:H:149:MET:HE1 | 1.69 | 0.56 |
| 48:l:481:THR:HB | 50:t:92:HIS:HD2 | 1.70 | 0.56 |
| 6:w:101:GLY:HA2 | 6:w:106:SER:HB2 | 1.87 | 0.56 |
| 53:G:266:ARG:HG2 | 53:G:267:THR:HG23 | 1.85 | 0.56 |
| 9:a:130:GLU:O | 9:a:134:GLU:HG2 | 2.05 | 0.56 |
| 10:b:16:ARG:HD2 | 37:X:146:ASP:HB2 | 1.88 | 0.56 |
| 11:c:84:GLN:HA | 11:c:98:ARG:HH21 | 1.69 | 0.56 |
| 21:n:57:TRP:CE3 | 21:n:57:TRP:HA | 2.40 | 0.56 |
| 24:q:266:MET:HE2 | 24:q:395:LEU:HD12 | 1.87 | 0.56 |
| 24:q:405:LEU:HD11 | 48:l:173:LEU:HD13 | 1.87 | 0.56 |
| 27:C:172:ARG:NH2 | 45:W:9:ASP:O | 2.37 | 0.56 |
| 29:E:85:LEU:HG | 40:R:87:LEU:HD13 | 1.86 | 0.56 |
| 31:H:162:CYS:SG | 59:H:302:SF4:S2 | 3.03 | 0.56 |
| 43:U:178:GLN:NE2 | 43:U:238:ASP:OD2 | 2.39 | 0.56 |
| 43:U:263:ARG:HD3 | 43:U:264:GLU:HG3 | 1.87 | 0.56 |
| 49:s:160:THR:HA | 49:s:163:TRP:CD1 | 2.41 | 0.56 |
| 50:t:43:GLN:HA | 50:t:46:MET:HE2 | 1.86 | 0.56 |
| 53:G:643:ARG:NH1 | 53:G:656:TYR:OH | 2.38 | 0.56 |
| 49:s:188:VAL:HG13 | 49:s:194:TRP:HB2 | 1.87 | 0.56 |
| 6:w:186:PRO:HG2 | 56:w:402:HEM:HMC3 | 1.87 | 0.56 |
| 6:w:83:HIS:NE2 | 56:w:402:HEM:NC | 2.54 | 0.56 |
| 52:Aa:19:LEU:HD21 | 52:Aa:23:GLU:HB2 | 1.88 | 0.56 |
| 7:8:215:LEU:O | 7:8:235:ASN:ND2 | 2.39 | 0.56 |
| 7:x:153:VAL:HG21 | 7:x:177:PRO:HG3 | 1.86 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:9:13:TRP:CD1 | 8:9:14:LEU:H | 2.24 | 0.56 |
| 11:c:133:LEU:HD23 | 48:l:532:ILE:HD11 | 1.88 | 0.56 |
| 18:j:67:LEU:HD11 | 19:k:68:ALA:HB3 | 1.87 | 0.56 |
| 56:w:401:HEM:HBB2 | 56:w:401:HEM:HMB2 | 1.87 | 0.56 |
| 5:6:227:HIS:CD2 | 5:6:231:LYS:HD2 | 2.40 | 0.56 |
| 7:8:122:CYS:SG | 57:8:401:HEC:CBB | 2.92 | 0.56 |
| 27:C:124:ARG:HG2 | 32:I:108:THR:HG21 | 1.87 | 0.56 |
| 6:w:253:PRO:HB3 | 7:x:203:ARG:O | 2.05 | 0.56 |
| 5:6:84:ARG:HE | 5:6:114:SER:HB3 | 1.71 | 0.56 |
| 32:I:74:VAL:HA | 32:I:77:MET:HE2 | 1.88 | 0.56 |
| 37:O:133:ILE:O | 37:O:137:LYS:HG2 | 2.05 | 0.56 |
| 12:d:140:GLN:HB2 | 22:o:127:ILE:HG22 | 1.88 | 0.56 |
| 28:D:220:VAL:HG21 | 39:Q:136:THR:HG21 | 1.88 | 0.56 |
| 26:B:114:VAL:HG11 | 26:B:212:LEU:HD22 | 1.88 | 0.55 |
| 6:w:94:LEU:HD21 | 56:w:401:HEM:HAB | 1.88 | 0.55 |
| 33:J:71:HIS:HA | 33:J:75:ARG:HG3 | 1.87 | 0.55 |
| 38:P:68:ARG:HA | 38:P:74:GLU:HG2 | 1.88 | 0.55 |
| 10:b:31:ARG:NH1 | 10:b:33:PRO:HG3 | 2.21 | 0.55 |
| 14:f:68:GLU:HG2 | 15:g:21:ARG:HE | 1.71 | 0.55 |
| 17:i:95:MET:HE2 | 17:i:149:ILE:HA | 1.88 | 0.55 |
| 25:r:185:TRP:NE1 | 25:r:238:THR:HG22 | 2.20 | 0.55 |
| 51:u:276:ARG:NH2 | 51:u:466:PRO:O | 2.30 | 0.55 |
| 53:G:68:ARG:HE | 53:G:283:GLU:HB3 | 1.71 | 0.55 |
| 5:6:89:LEU:HD22 | 5:6:150:GLU:HB3 | 1.87 | 0.55 |
| 7:8:122:CYS:SG | 57:8:401:HEC:HAB | 2.40 | 0.55 |
| 49:s:95:VAL:HG12 | 49:s:97:VAL:HG22 | 1.87 | 0.55 |
| 51:5:156:LEU:O | 51:5:213:ARG:NH1 | 2.39 | 0.55 |
| 5:6:36:GLN:HE21 | 5:6:53:GLU:HB3 | 1.71 | 0.55 |
| 5:6:63:LEU:HD23 | 5:6:141:THR:HG21 | 1.88 | 0.55 |
| 56:7:402:HEM:HBC2 | 56:7:402:HEM:HMC2 | 1.89 | 0.55 |
| 15:g:27:LYS:HG2 | 15:g:29:THR:H | 1.71 | 0.55 |
| 26:B:48:ARG:HE | 29:E:231:LEU:HD11 | 1.71 | 0.55 |
| 30:F:53:VAL:HG21 | 35:L:76:ILE:HD13 | 1.86 | 0.55 |
| 44:V:62:THR:HG22 | 44:V:104:ARG:HD3 | 1.89 | 0.55 |
| 49:s:121:MET:O | 49:s:125:TRP:HD1 | 1.89 | 0.55 |
| 3:2:257:CYS:HB3 | 3:2:262:SER:HB2 | 1.89 | 0.55 |
| 3:4:209:ALA:HA | 3:4:221:HIS:CE1 | 2.42 | 0.55 |
| 24:q:329:LEU:HD23 | 24:q:437:MET:HE3 | 1.88 | 0.55 |
| 28:D:129:VAL:HG22 | 28:D:144:LYS:HD2 | 1.87 | 0.55 |
| 35:L:130:GLU:HG3 | 35:L:135:ASP:HA | 1.88 | 0.55 |
| 6:w:32:ASN:HD21 | 6:w:227:LYS:HG2 | 1.72 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:2:269:ARG:HA | 3:2:278:ASN:HB3 | 1.89 | 0.55 |
| 6:7:47:THR:HG23 | 6:7:79:ILE:HG23 | 1.88 | 0.55 |
| 11:c:96:ASP:OD2 | 24:q:346:ARG:NH1 | 2.40 | 0.55 |
| 18:j:59:ALA:HB1 | 20:m:67:VAL:HG23 | 1.88 | 0.55 |
| 20:m:65:LEU:HA | 20:m:68:PHE:HB2 | 1.88 | 0.55 |
| 25:r:117:LEU:HG | 25:r:136:VAL:HG22 | 1.88 | 0.55 |
| 27:C:161:VAL:O | 27:C:165:LEU:HB2 | 2.07 | 0.55 |
| 29:E:111:ARG:NH1 | 33:J:173:SER:OG | 2.40 | 0.55 |
| 30:F:71:ILE:HD11 | 30:F:115:GLY:HA3 | 1.89 | 0.55 |
| 48:l:65:ASN:H | 48:l:65:ASN:HD22 | 1.54 | 0.55 |
| 5:v:320:PRO:HB3 | 3:Af:75:LEU:HB3 | 1.89 | 0.55 |
| 39:Q:48:SER:HB2 | 39:Q:53:GLU:HB3 | 1.88 | 0.55 |
| 51:u:152:GLN:HG2 | 51:u:253:LEU:HD22 | 1.88 | 0.55 |
| 7:8:245:MET:HE1 | 7:8:248:PRO:HG3 | 1.89 | 0.55 |
| 22:o:41:SER:OG | 23:p:191:PRO:O | 2.23 | 0.55 |
| 26:B:141:GLY:HA2 | 26:B:252:PRO:HD3 | 1.87 | 0.55 |
| 39:Q:118:GLU:HB3 | 39:Q:124:LYS:HG3 | 1.89 | 0.55 |
| 42:T:141:PRO:HG3 | 49:s:118:LYS:HD2 | 1.89 | 0.55 |
| 48:l:97:THR:HG22 | 48:l:246:LEU:HD21 | 1.89 | 0.55 |
| 52:z:37:ASN:OD1 | 52:z:40:ARG:NH1 | 2.39 | 0.55 |
| 25:r:199:ASP:HB3 | 25:r:279:ARG:HH21 | 1.71 | 0.54 |
| 37:O:140:CYS:HB3 | 37:O:143:GLU:HG3 | 1.89 | 0.54 |
| 48:l:566:THR:O | 48:l:570:GLN:HG2 | 2.07 | 0.54 |
| 50:t:59:CYS:HA | 50:t:61:HIS:CE1 | 2.42 | 0.54 |
| 22:o:17:THR:HB | 23:p:110:GLU:HG2 | 1.88 | 0.54 |
| 43:U:102:ASP:OD1 | 43:U:104:LYS:N | 2.40 | 0.54 |
| 5:v:231:LYS:O | 5:v:235:GLU:HG2 | 2.07 | 0.54 |
| 3:4:100:SER:N | 51:5:176:ASP:OD1 | 2.40 | 0.54 |
| 18:j:113:TRP:O | 18:j:114:ALA:C | 2.49 | 0.54 |
| 22:o:28:GLU:OE2 | 51:u:83:ASN:ND2 | 2.40 | 0.54 |
| 26:B:174:ARG:O | 26:B:178:GLU:HG2 | 2.06 | 0.54 |
| 38:P:18:GLU:HG3 | 38:P:68:ARG:HB3 | 1.89 | 0.54 |
| 6:w:237:LEU:HD13 | 7:x:297:MET:HG2 | 1.88 | 0.54 |
| 7:x:112:ARG:HB2 | 7:x:140:CYS:HB2 | 1.88 | 0.54 |
| 35:L:43:ARG:NH2 | 35:L:93:GLY:O | 2.41 | 0.54 |
| 48:l:145:GLU:OE2 | 48:l:176:ARG:NH1 | 2.40 | 0.54 |
| 48:l:536:LEU:HB3 | 48:l:537:PRO:HD3 | 1.89 | 0.54 |
| 4:3:16:ASN:HD22 | 51:u:382:SER:HA | 1.73 | 0.54 |
| 10:b:119:LEU:O | 10:b:120:MET:C | 2.50 | 0.54 |
| 20:m:103:MET:HE3 | 20:m:115:ILE:HD12 | 1.90 | 0.54 |
| 28:D:66:ALA:HA | 28:D:73:VAL:HG21 | 1.88 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:7:31:TRP:NE1 | 56:7:402:HEM:O1D | 2.39 | 0.54 |
| 13:e:97:ILE:O | 13:e:101:LEU:HB2 | 2.07 | 0.54 |
| 26:B:225:LEU:HD22 | 26:B:424:ILE:HD12 | 1.88 | 0.54 |
| 27:C:219:PHE:O | 27:C:223:VAL:HG22 | 2.08 | 0.54 |
| 31:H:116:CYS:HG | 59:H:302:SF4:FE1 | 1.23 | 0.54 |
| 6:w:300:ILE:HD11 | 6:w:363:LEU:HD21 | 1.89 | 0.54 |
| 7:8:217:THR:HA | 7:8:264:MET:HE2 | 1.89 | 0.54 |
| 6:w:281:LEU:HB2 | 6:w:294:LEU:HD12 | 1.90 | 0.54 |
| 51:5:52:GLN:HE21 | 51:5:56:GLY:HA2 | 1.72 | 0.54 |
| 53:G:219:SER:OG | 53:G:288:ASP:OD2 | 2.25 | 0.54 |
| 53:G:347:ASP:N | 53:G:347:ASP:OD1 | 2.40 | 0.54 |
| 5:6:60:ARG:HD3 | 5:6:393:LEU:HD22 | 1.89 | 0.54 |
| 17:i:237:MET:HB3 | 17:i:240:ILE:HD13 | 1.89 | 0.54 |
| 45:W:73:PRO:HG2 | 49:s:117:ASN:HB3 | 1.89 | 0.54 |
| 5:6:317:VAL:HG13 | 5:6:319:GLN:HE21 | 1.71 | 0.54 |
| 8:9:69:LEU:HD11 | 8:9:76:LEU:HD13 | 1.90 | 0.54 |
| 19:k:27:MET:HG2 | 20:m:72:THR:CG2 | 2.38 | 0.54 |
| 24:q:416:ARG:HG2 | 48:l:159:HIS:HB3 | 1.90 | 0.54 |
| 35:L:206:ASP:OD1 | 35:L:207:ARG:N | 2.41 | 0.54 |
| 35:L:270:ASP:OD1 | 35:L:270:ASP:N | 2.40 | 0.54 |
| 48:l:302:VAL:O | 48:l:306:THR:HG23 | 2.07 | 0.54 |
| 2:Ac:30:LEU:HG | 4:Ad:34:TRP:HB2 | 1.89 | 0.54 |
| 22:o:30:ARG:NH1 | 51:u:260:ASP:O | 2.41 | 0.54 |
| 48:l:245:ALA:HB2 | 48:l:340:PHE:HB3 | 1.89 | 0.54 |
| 48:l:289:ALA:HB1 | 48:l:418:LEU:HB2 | 1.89 | 0.54 |
| 6:w:344:GLU:HG3 | 52:z:67:PHE:HE1 | 1.71 | 0.54 |
| 3:2:225:ARG:NH1 | 3:2:267:SER:O | 2.41 | 0.53 |
| 7:8:216:LEU:HD21 | 57:8:401:HEC:C2B | 2.38 | 0.53 |
| 17:i:28:LEU:HD23 | 17:i:31:ILE:HD12 | 1.90 | 0.53 |
| 24:q:139:GLN:HB2 | 24:q:222:GLU:OE1 | 2.08 | 0.53 |
| 25:r:114:TYR:HA | 25:r:117:LEU:HB2 | 1.90 | 0.53 |
| 27:C:416:TYR:HB3 | 27:C:429:LYS:HB3 | 1.91 | 0.53 |
| 41:S:52:ARG:NH2 | 41:S:58:ASN:OD1 | 2.42 | 0.53 |
| 48:l:247:LEU:HD12 | 48:l:248:HIS:CE1 | 2.43 | 0.53 |
| 53:G:83:GLU:HG2 | 53:G:84:LYS:HG2 | 1.89 | 0.53 |
| 12:d:107:GLN:OE1 | 48:l:194:ASN:ND2 | 2.41 | 0.53 |
| 25:r:26:LYS:HA | 25:r:36:GLY:HA3 | 1.91 | 0.53 |
| 43:U:291:ARG:HH22 | 43:U:294:HIS:HD2 | 1.56 | 0.53 |
| 53:G:405:THR:HB | 53:G:477:GLY:HA3 | 1.91 | 0.53 |
| 3:4:216:LEU:HD13 | 3:4:269:ARG:HD2 | 1.90 | 0.53 |
| 16:h:50:ILE:O | 16:h:54:LYS:NZ | 2.39 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:J:154:LYS:NZ | 33:J:156:LYS:HE3 | 2.24 | 0.53 |
| 35:L:165:LEU:HA | 35:L:197:LYS:HE3 | 1.90 | 0.53 |
| 39:Q:97:ALA:HA | 61:Q:201:ZMP:O4 | 2.07 | 0.53 |
| 48:l:8:THR:O | 48:l:11:THR:OG1 | 2.26 | 0.53 |
| 50:t:58:TYR:O | 50:t:61:HIS:HE1 | 1.91 | 0.53 |
| 51:u:377:MET:HE3 | 51:u:475:MET:HA | 1.90 | 0.53 |
| 7:x:244:ALA:HB3 | 57:x:401:HEC:HBD2 | 1.90 | 0.53 |
| 52:z:20:SER:HB3 | 52:z:23:GLU:HG3 | 1.91 | 0.53 |
| 53:G:218:LEU:HB3 | 53:G:221:ASN:HD22 | 1.73 | 0.53 |
| 24:q:12:LEU:HB2 | 24:q:13:PRO:HD3 | 1.89 | 0.53 |
| 25:r:26:LYS:HG2 | 25:r:36:GLY:HA3 | 1.89 | 0.53 |
| 6:w:94:LEU:HD11 | 6:w:123:VAL:HG11 | 1.90 | 0.53 |
| 6:w:246:SER:HB2 | 6:w:249:LEU:HB2 | 1.89 | 0.53 |
| 25:r:24:GLU:OE2 | 25:r:274:ARG:NH1 | 2.42 | 0.53 |
| 26:B:425:CYS:SG | 26:B:426:ALA:N | 2.81 | 0.53 |
| 5:v:36:GLN:HG3 | 5:v:53:GLU:HB3 | 1.91 | 0.53 |
| 53:G:228:VAL:HG23 | 53:G:230:ALA:H | 1.74 | 0.53 |
| 21:n:57:TRP:HA | 21:n:57:TRP:HE3 | 1.74 | 0.53 |
| 35:L:197:LYS:N | 35:L:258:PHE:O | 2.40 | 0.53 |
| 47:Z:32:LEU:HD12 | 47:Z:32:LEU:H | 1.73 | 0.53 |
| 3:2:100:SER:OG | 3:2:101:HIS:N | 2.42 | 0.53 |
| 11:c:110:ASP:OD1 | 11:c:110:ASP:N | 2.42 | 0.53 |
| 35:L:190:PHE:HB3 | 35:L:193:ALA:HB2 | 1.90 | 0.53 |
| 51:u:145:GLU:HG2 | 51:u:249:HIS:CE1 | 2.44 | 0.53 |
| 5:v:407:VAL:HG23 | 5:v:411:THR:HB | 1.89 | 0.53 |
| 6:w:187:PHE:O | 6:w:190:THR:OG1 | 2.24 | 0.53 |
| 3:2:113:ARG:HH21 | 3:2:117:VAL:HB | 1.74 | 0.53 |
| 24:q:315:LEU:HD12 | 24:q:381:ILE:HD12 | 1.91 | 0.53 |
| 31:H:158:CYS:SG | 59:H:301:SF4:S1 | 2.97 | 0.53 |
| 39:Q:92:MET:SD | 39:Q:95:LYS:NZ | 2.62 | 0.53 |
| 48:l:97:THR:HG21 | 48:l:125:LEU:HD13 | 1.90 | 0.53 |
| 51:u:140:LEU:HD22 | 51:u:237:VAL:HG12 | 1.89 | 0.53 |
| 5:v:379:LYS:HG2 | 5:v:413:LEU:HD22 | 1.91 | 0.53 |
| 7:x:97:TRP:HB2 | 7:x:100:ARG:HG3 | 1.91 | 0.53 |
| 17:i:289:ASN:HA | 17:i:292:PHE:CE2 | 2.44 | 0.53 |
| 25:r:100:LEU:HD23 | 25:r:160:TYR:HB2 | 1.91 | 0.53 |
| 28:D:213:ASP:OD1 | 35:L:70:ARG:NH2 | 2.42 | 0.53 |
| 31:H:115:ALA:HB3 | 31:H:140:ARG:HG2 | 1.90 | 0.53 |
| 51:u:388:VAL:HG21 | 51:u:438:ALA:HA | 1.91 | 0.53 |
| 53:G:389:THR:OG1 | 53:G:511:LYS:O | 2.26 | 0.53 |
| 25:r:209:SER:HB3 | 25:r:213:VAL:HA | 1.91 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:C:178:VAL:HG23 | 27:C:317:TYR:CZ | 2.43 | 0.53 |
| 43:U:352:LYS:HD3 | 43:U:353:TRP:HD1 | 1.74 | 0.53 |
| 48:l:315:VAL:O | 48:l:319:ILE:HG12 | 2.09 | 0.53 |
| 6:w:182:HIS:HE1 | 56:w:402:HEM:NB | 1.99 | 0.53 |
| 53:G:229:GLY:N | 59:G:801:SF4:S2 | 2.75 | 0.53 |
| 2:1:4:PRO:HB2 | 2:1:9:ARG:HE | 1.74 | 0.52 |
| 3:4:262:SER:HA | 3:4:273:GLY:CA | 2.39 | 0.52 |
| 14:f:66:VAL:HG12 | 14:f:70:LYS:HE3 | 1.90 | 0.52 |
| 6:w:196:HIS:CE1 | 56:w:401:HEM:ND | 2.77 | 0.52 |
| 17:i:2:ASN:HB3 | 17:i:5:ILE:HD13 | 1.92 | 0.52 |
| 24:q:5:ILE:HG23 | 24:q:104:LEU:HD11 | 1.91 | 0.52 |
| 24:q:269:MET:HG3 | 24:q:270:ILE:HD12 | 1.91 | 0.52 |
| 27:C:46:ASP:OD1 | 27:C:47:VAL:N | 2.36 | 0.52 |
| 34:K:52:ASN:HB3 | 54:M:29:GLN:NE2 | 2.24 | 0.52 |
| 48:l:559:GLU:O | 48:l:563:PRO:HD2 | 2.08 | 0.52 |
| 53:G:495:ASN:HA | 53:G:498:GLN:HG2 | 1.91 | 0.52 |
| 15:g:89:ASP:OD2 | 49:s:243:ARG:NH1 | 2.35 | 0.52 |
| 6:7:112:THR:O | 6:7:196:HIS:NE2 | 2.43 | 0.52 |
| 7:8:248:PRO:HB3 | 57:8:401:HEC:HHC | 1.90 | 0.52 |
| 48:l:419:THR:HA | 48:l:422:TYR:CE2 | 2.45 | 0.52 |
| 21:n:17:VAL:HG11 | 24:q:30:HIS:CG | 2.45 | 0.52 |
| 53:G:131:CYS:SG | 53:G:175:ARG:NH1 | 2.83 | 0.52 |
| 3:2:177:LEU:HB2 | 3:2:290:ASP:HA | 1.92 | 0.52 |
| 3:2:265:ASP:OD1 | 3:2:269:ARG:N | 2.42 | 0.52 |
| 5:6:70:ARG:HH22 | 5:6:332:ASP:HB2 | 1.74 | 0.52 |
| 7:8:251:ASN:OD1 | 7:8:251:ASN:N | 2.40 | 0.52 |
| 9:a:152:LYS:HD3 | 15:g:96:VAL:HG21 | 1.91 | 0.52 |
| 10:b:97:VAL:HG13 | 48:l:61:MET:HE3 | 1.90 | 0.52 |
| 13:e:70:ASN:HD22 | 13:e:73:SER:HA | 1.75 | 0.52 |
| 17:i:44:LEU:HD22 | 17:i:122:ILE:HG21 | 1.90 | 0.52 |
| 27:C:321:GLU:O | 27:C:352:GLN:NE2 | 2.41 | 0.52 |
| 27:C:389:LYS:HG3 | 53:G:144:MET:HG3 | 1.92 | 0.52 |
| 28:D:76:VAL:HG22 | 54:M:70:MET:HB3 | 1.92 | 0.52 |
| 35:L:60:LEU:HA | 35:L:237:ILE:HD11 | 1.91 | 0.52 |
| 43:U:170:VAL:HG13 | 43:U:242:ALA:HB3 | 1.92 | 0.52 |
| 49:s:160:THR:HA | 49:s:163:TRP:NE1 | 2.23 | 0.52 |
| 2:Ac:54:LYS:HD3 | 2:Ac:54:LYS:H | 1.73 | 0.52 |
| 6:7:26:ASN:HD21 | 6:7:207:ASN:HB2 | 1.74 | 0.52 |
| 19:k:26:LEU:HB3 | 19:k:78:LEU:HD12 | 1.91 | 0.52 |
| 7:x:216:LEU:HD11 | 57:x:401:HEC:HMB2 | 1.92 | 0.52 |
| 53:G:50:LEU:O | 53:G:54:GLU:HG2 | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:d:122:ARG:NH2 | 48:l:202:PHE:O | 2.42 | 0.52 |
| 18:j:67:LEU:HD21 | 19:k:68:ALA:HB3 | 1.92 | 0.52 |
| 25:r:61:LEU:HD23 | 32:I:125:PRO:HB3 | 1.91 | 0.52 |
| 27:C:175:TRP:HA | 27:C:178:VAL:HG12 | 1.92 | 0.52 |
| 31:H:157:PHE:O | 31:H:158:CYS:HB2 | 2.08 | 0.52 |
| 53:G:326:VAL:HG23 | 53:G:626:LEU:HD13 | 1.92 | 0.52 |
| 33:J:137:PHE:HA | 33:J:140:LYS:HE3 | 1.91 | 0.52 |
| 36:N:36:GLY:O | 36:N:45:ARG:NH2 | 2.43 | 0.52 |
| 48:l:293:ILE:HD11 | 48:l:418:LEU:HD22 | 1.91 | 0.52 |
| 3:Ae:47:GLY:C | 3:Ae:49:PHE:H | 2.18 | 0.52 |
| 17:i:128:LEU:HD13 | 17:i:216:PHE:HB2 | 1.92 | 0.52 |
| 11:c:100:ASN:HB2 | 11:c:103:GLU:CD | 2.35 | 0.51 |
| 50:t:62:TYR:CE1 | 50:t:86:ASP:HB3 | 2.46 | 0.51 |
| 8:y:107:GLU:HA | 8:y:110:LYS:HD3 | 1.92 | 0.51 |
| 3:2:251:ASP:OD1 | 3:2:251:ASP:N | 2.42 | 0.51 |
| 10:b:76:LEU:O | 10:b:79:VAL:HG12 | 2.10 | 0.51 |
| 19:k:37:MET:HE3 | 19:k:67:ALA:HA | 1.93 | 0.51 |
| 20:m:31:LEU:HD11 | 25:r:70:MET:SD | 2.50 | 0.51 |
| 24:q:122:PHE:HD1 | 24:q:238:LEU:HD13 | 1.75 | 0.51 |
| 27:C:93:GLN:NE2 | 27:C:93:GLN:O | 2.44 | 0.51 |
| 31:H:162:CYS:HG | 59:H:302:SF4:FE4 | 0.40 | 0.51 |
| 35:L:349:ARG:O | 35:L:352:ARG:HB3 | 2.10 | 0.51 |
| 43:U:225:ASN:HB3 | 43:U:228:GLU:HB2 | 1.93 | 0.51 |
| 37:X:128:PHE:CZ | 37:X:148:ILE:HG12 | 2.45 | 0.51 |
| 48:l:247:LEU:HD12 | 48:l:248:HIS:HE1 | 1.76 | 0.51 |
| 3:4:183:GLY:N | 3:4:199:HIS:O | 2.29 | 0.51 |
| 5:6:421:ASP:N | 5:6:421:ASP:OD1 | 2.40 | 0.51 |
| 11:c:155:PRO:HD3 | 50:t:4:HIS:CE1 | 2.46 | 0.51 |
| 17:i:337:LEU:O | 17:i:340:THR:HG23 | 2.11 | 0.51 |
| 18:j:18:VAL:HG11 | 25:r:76:ILE:HD11 | 1.92 | 0.51 |
| 33:J:79:ILE:HG12 | 33:J:99:MET:HG3 | 1.93 | 0.51 |
| 35:L:203:GLY:N | 35:L:206:ASP:HB2 | 2.25 | 0.51 |
| 38:P:35:ASP:HA | 38:P:38:GLU:HG2 | 1.91 | 0.51 |
| 49:s:187:CYS:SG | 49:s:188:VAL:N | 2.83 | 0.51 |
| 51:5:375:GLN:OE1 | 51:5:378:ARG:NH1 | 2.39 | 0.51 |
| 3:2:120:SER:OG | 51:u:269:ARG:NH2 | 2.44 | 0.51 |
| 4:3:9:ARG:NH1 | 8:9:109:ALA:O | 2.44 | 0.51 |
| 27:C:137:GLN:O | 27:C:140:PRO:HD2 | 2.10 | 0.51 |
| 39:Q:89:VAL:HG22 | 61:Q:201:ZMP:H7 | 1.91 | 0.51 |
| 5:v:116:ARG:NH1 | 5:v:188:ASN:O | 2.42 | 0.51 |
| 53:G:64:CYS:HB3 | 53:G:75:CYS:HB3 | 1.93 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:297:PRO:HB3 | 5:6:304:ASN:HD21 | 1.75 | 0.51 |
| 6:7:67:THR:HG22 | 7:8:200:TYR:HE2 | 1.75 | 0.51 |
| 6:7:211:ILE:HD12 | 8:9:37:THR:HA | 1.92 | 0.51 |
| 26:B:263:ALA:HA | 26:B:271:SER:HB2 | 1.93 | 0.51 |
| 36:N:89:SER:OG | 36:N:93:LYS:NZ | 2.42 | 0.51 |
| 6:7:81:TYR:OH | 7:8:203:ARG:NH1 | 2.44 | 0.51 |
| 18:j:20:ILE:O | 18:j:25:PRO:HD3 | 2.11 | 0.51 |
| 25:r:200:LEU:HD21 | 25:r:280:PHE:O | 2.11 | 0.51 |
| 26:B:131:ILE:HG13 | 26:B:165:GLU:HB3 | 1.92 | 0.51 |
| 41:S:37:ARG:O | 45:W:143:TYR:OH | 2.24 | 0.51 |
| 51:5:294:PRO:HB2 | 51:5:298:ASN:HB3 | 1.93 | 0.51 |
| 3:4:193:LYS:HE3 | 6:w:169:SER:HB3 | 1.91 | 0.51 |
| 3:4:198:ARG:HB3 | 3:4:232:VAL:HG13 | 1.93 | 0.51 |
| 6:7:196:HIS:HE1 | 56:7:402:HEM:ND | 2.08 | 0.51 |
| 9:a:130:GLU:HB3 | 21:n:45:PHE:CG | 2.45 | 0.51 |
| 9:a:132:ASN:HD22 | 24:q:45:LEU:HD12 | 1.76 | 0.51 |
| 27:C:334:ASP:OD1 | 31:H:42:ASN:ND2 | 2.42 | 0.51 |
| 34:K:52:ASN:HB3 | 54:M:29:GLN:HE22 | 1.74 | 0.51 |
| 51:u:304:LEU:HD13 | 51:u:354:LEU:HD22 | 1.92 | 0.51 |
| 6:7:48:GLY:HA3 | 56:7:401:HEM:C4C | 2.46 | 0.51 |
| 8:9:52:PRO:HD2 | 8:9:55:LEU:HD12 | 1.93 | 0.51 |
| 29:E:143:ARG:HG3 | 29:E:183:ALA:HB3 | 1.92 | 0.51 |
| 43:U:258:LEU:HD21 | 43:U:278:LEU:HD21 | 1.93 | 0.51 |
| 48:l:303:ALA:O | 48:l:306:THR:OG1 | 2.25 | 0.51 |
| 7:x:112:ARG:HG3 | 7:x:141:TYR:CZ | 2.46 | 0.51 |
| 5:6:48:VAL:HG11 | 5:6:400:ALA:HB1 | 1.92 | 0.51 |
| 10:b:72:VAL:HG22 | 10:b:76:LEU:HD12 | 1.93 | 0.51 |
| 27:C:368:LYS:HG2 | 27:C:386:HIS:CE1 | 2.46 | 0.51 |
| 31:H:103:LEU:HB3 | 31:H:191:LEU:HD23 | 1.92 | 0.51 |
| 35:L:222:PRO:HB2 | 35:L:288:LEU:HD11 | 1.92 | 0.51 |
| 36:N:23:ARG:NH2 | 43:U:277:TYR:OH | 2.44 | 0.51 |
| 37:X:119:ILE:HG21 | 37:X:135:ALA:HB1 | 1.92 | 0.51 |
| 26:B:338:ASP:N | 26:B:338:ASP:OD1 | 2.44 | 0.51 |
| 26:B:340:ASP:O | 26:B:344:GLN:HG2 | 2.10 | 0.51 |
| 35:L:167:ALA:HA | 35:L:176:LEU:HB3 | 1.92 | 0.51 |
| 3:Ae:49:PHE:O | 3:Ae:51:ALA:N | 2.44 | 0.51 |
| 3:2:157:PHE:O | 3:2:160:SER:OG | 2.22 | 0.50 |
| 3:2:159:SER:O | 3:2:162:SER:OG | 2.27 | 0.50 |
| 6:7:43:LEU:HD22 | 6:7:236:MET:HE1 | 1.94 | 0.50 |
| 6:7:218:ILE:HD11 | 6:7:224:TYR:CE2 | 2.47 | 0.50 |
| 11:c:165:ASP:HB3 | 11:c:170:ARG:HH12 | 1.76 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:q:358:TRP:CE3 | 24:q:441:ILE:HD12 | 2.46 | 0.50 |
| 26:B:423:THR:HB | 59:B:502:SF4:S3 | 2.51 | 0.50 |
| 36:N:59:VAL:HG22 | 36:N:68:LEU:HD21 | 1.93 | 0.50 |
| 43:U:131:TYR:CD1 | 43:U:185:CYS:HB3 | 2.46 | 0.50 |
| 53:G:402:LEU:HD23 | 53:G:475:VAL:HB | 1.92 | 0.50 |
| 5:6:181:ALA:O | 5:6:254:ARG:N | 2.42 | 0.50 |
| 10:b:100:ARG:NH2 | 12:d:119:GLU:HG2 | 2.26 | 0.50 |
| 30:F:84:ILE:HG12 | 30:F:102:LEU:HD11 | 1.94 | 0.50 |
| 31:H:211:TYR:CZ | 54:M:39:PRO:HG3 | 2.47 | 0.50 |
| 5:v:333:SER:OG | 5:v:334:GLY:N | 2.45 | 0.50 |
| 10:b:31:ARG:HG2 | 10:b:33:PRO:HD3 | 1.93 | 0.50 |
| 25:r:200:LEU:HD13 | 25:r:282:TYR:HA | 1.93 | 0.50 |
| 25:r:228:TYR:HA | 25:r:231:ILE:HD12 | 1.93 | 0.50 |
| 27:C:197:ALA:HB1 | 27:C:202:ALA:HB3 | 1.93 | 0.50 |
| 29:E:132:ILE:HD11 | 29:E:169:PHE:HD1 | 1.76 | 0.50 |
| 31:H:119:CYS:HB3 | 31:H:158:CYS:SG | 2.52 | 0.50 |
| 51:u:170:GLN:O | 51:u:174:GLU:HG3 | 2.10 | 0.50 |
| 3:4:182:GLU:HG2 | 3:4:201:THR:HG22 | 1.92 | 0.50 |
| 5:6:194:ASP:HA | 5:6:197:ILE:HG12 | 1.94 | 0.50 |
| 5:6:372:GLN:NE2 | 5:6:376:ASN:OD1 | 2.41 | 0.50 |
| 6:7:248:ASP:OD2 | 7:8:203:ARG:NE | 2.44 | 0.50 |
| 10:b:18:LEU:HD21 | 23:p:205:LEU:HD22 | 1.92 | 0.50 |
| 11:c:126:TRP:HA | 11:c:129:MET:HE2 | 1.93 | 0.50 |
| 14:f:37:GLY:O | 43:U:357:LYS:NZ | 2.30 | 0.50 |
| 16:h:105:ARG:HH22 | 49:s:91:LYS:HA | 1.76 | 0.50 |
| 26:B:284:HIS:CD2 | 26:B:305:GLY:HA3 | 2.45 | 0.50 |
| 27:C:248:ASP:O | 27:C:252:GLU:HG2 | 2.11 | 0.50 |
| 40:R:78:HIS:HA | 40:R:81:TYR:CE2 | 2.46 | 0.50 |
| 44:V:19:HIS:CD2 | 44:V:20:ARG:HG3 | 2.46 | 0.50 |
| 50:t:46:MET:HG2 | 50:t:51:LEU:HD12 | 1.94 | 0.50 |
| 6:w:244:LEU:HD12 | 7:x:293:MET:HG2 | 1.92 | 0.50 |
| 53:G:323:LEU:HB3 | 53:G:629:ILE:HD12 | 1.93 | 0.50 |
| 6:7:260:ASN:HD22 | 6:7:261:PRO:HD2 | 1.76 | 0.50 |
| 7:8:184:GLU:OE1 | 7:x:159:PRO:HB2 | 2.10 | 0.50 |
| 9:a:169:TYR:OH | 44:V:141:VAL:HG11 | 2.12 | 0.50 |
| 25:r:132:ALA:O | 25:r:136:VAL:HG23 | 2.12 | 0.50 |
| 43:U:182:ARG:NH1 | 43:U:318:GLU:OE2 | 2.45 | 0.50 |
| 51:5:87:ASN:ND2 | 51:5:199:GLN:OE1 | 2.45 | 0.50 |
| 51:5:195:THR:HG21 | 51:5:269:ARG:H | 1.77 | 0.50 |
| 3:2:116:GLU:OE1 | 3:2:116:GLU:N | 2.32 | 0.50 |
| 5:6:138:LEU:HD13 | 5:6:237:PHE:HB2 | 1.93 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:a:161:ARG:NH2 | 17:i:195:PRO:O | 2.42 | 0.50 |
| 12:d:23:GLN:HE21 | 50:t:73:SER:HB3 | 1.75 | 0.50 |
| 24:q:71:TRP:O | 24:q:74:PRO:HD2 | 2.11 | 0.50 |
| 48:l:69:MET:HE3 | 48:l:71:LEU:HD11 | 1.93 | 0.50 |
| 51:u:310:ILE:HG21 | 51:u:379:LEU:HD21 | 1.93 | 0.50 |
| 53:G:455:ILE:HD13 | 53:G:460:HIS:HB3 | 1.93 | 0.50 |
| 3:2:175:ILE:HB | 3:2:292:VAL:HG13 | 1.93 | 0.50 |
| 5:6:116:ARG:HH12 | 5:6:189:SER:HA | 1.75 | 0.50 |
| 35:L:140:PHE:O | 35:L:182:GLY:HA3 | 2.12 | 0.50 |
| 35:L:238:VAL:HG12 | 35:L:242:LYS:HZ2 | 1.76 | 0.50 |
| 37:O:143:GLU:HA | 37:O:146:ASP:OD2 | 2.12 | 0.50 |
| 41:S:4:GLU:O | 41:S:7:PRO:HD2 | 2.10 | 0.50 |
| 3:4:161:MET:O | 6:w:177:ARG:NH2 | 2.45 | 0.50 |
| 7:8:293:MET:HG3 | 7:8:294:LEU:N | 2.26 | 0.50 |
| 20:m:15:ILE:HG12 | 20:m:97:LEU:HD22 | 1.92 | 0.50 |
| 26:B:257:ARG:HG2 | 26:B:261:TRP:CD2 | 2.46 | 0.50 |
| 26:B:284:HIS:HD2 | 26:B:305:GLY:HA3 | 1.77 | 0.50 |
| 27:C:90:PHE:HB3 | 27:C:103:LEU:HB3 | 1.94 | 0.50 |
| 43:U:153:LEU:HD11 | 43:U:296:LEU:HD23 | 1.94 | 0.50 |
| 5:6:255:GLY:HA2 | 5:6:437:SER:HB3 | 1.94 | 0.50 |
| 6:7:41:LEU:CD1 | 56:7:401:HEM:HBB1 | 2.39 | 0.50 |
| 10:b:28:LEU:HD11 | 23:p:157:TYR:CD2 | 2.47 | 0.50 |
| 18:j:33:LYS:HE2 | 25:r:59:GLU:CD | 2.37 | 0.50 |
| 24:q:75:LEU:HD23 | 24:q:440:HIS:CE1 | 2.46 | 0.50 |
| 24:q:457:PRO:HG2 | 24:q:458:LEU:HD12 | 1.93 | 0.50 |
| 26:B:52:ARG:HB3 | 26:B:54:LYS:HZ2 | 1.77 | 0.50 |
| 35:L:263:PRO:HG3 | 35:L:339:PRO:HA | 1.93 | 0.50 |
| 37:O:110:LEU:HB2 | 37:O:114:ASP:HB3 | 1.93 | 0.50 |
| 37:O:120:MET:HE1 | 39:Q:66:TYR:HB3 | 1.93 | 0.50 |
| 51:u:121:ASN:ND2 | 51:u:132:TYR:OH | 2.45 | 0.50 |
| 51:u:141:PRO:O | 51:u:145:GLU:HG3 | 2.12 | 0.50 |
| 5:v:70:ARG:HD2 | 5:v:117:GLU:HG2 | 1.93 | 0.50 |
| 5:v:196:ARG:HH12 | 5:v:204:GLN:HE22 | 1.59 | 0.50 |
| 51:5:328:LEU:HB2 | 51:5:375:GLN:HG3 | 1.94 | 0.50 |
| 3:4:199:HIS:HB2 | 3:4:231:TRP:CZ3 | 2.47 | 0.49 |
| 7:8:212:VAL:HA | 7:8:215:LEU:HD23 | 1.93 | 0.49 |
| 18:j:96:ILE:HD11 | 42:T:115:ILE:HD11 | 1.94 | 0.49 |
| 26:B:364:VAL:HG12 | 26:B:400:VAL:HG12 | 1.93 | 0.49 |
| 27:C:159:LEU:HD22 | 27:C:177:ARG:HH21 | 1.77 | 0.49 |
| 48:l:272:LEU:O | 48:l:275:THR:OG1 | 2.26 | 0.49 |
| 3:4:182:GLU:HA | 3:4:199:HIS:HB3 | 1.93 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:r:234:MET:O | 25:r:238:THR:HG23 | 2.12 | 0.49 |
| 38:P:32:GLY:HA3 | 38:P:82:PHE:O | 2.12 | 0.49 |
| 24:q:118:PHE:O | 24:q:122:PHE:HB3 | 2.12 | 0.49 |
| 26:B:41:ILE:HG22 | 26:B:253:THR:HG21 | 1.94 | 0.49 |
| 41:S:37:ARG:HD2 | 41:S:48:MET:HG2 | 1.94 | 0.49 |
| 53:G:400:ILE:HG13 | 53:G:427:LEU:HD11 | 1.93 | 0.49 |
| 3:4:240:HIS:HB3 | 55:4:301:FES:S1 | 2.52 | 0.49 |
| 8:9:13:TRP:CG | 8:9:14:LEU:N | 2.81 | 0.49 |
| 9:a:58:LYS:O | 23:p:149:TRP:NE1 | 2.43 | 0.49 |
| 10:b:89:HIS:NE2 | 10:b:96:THR:HB | 2.27 | 0.49 |
| 11:c:54:LYS:NZ | 11:c:74:ASP:OD2 | 2.43 | 0.49 |
| 14:f:31:ILE:HG13 | 14:f:32:ARG:H | 1.78 | 0.49 |
| 22:o:11:LEU:HD13 | 48:l:535:ARG:HB3 | 1.94 | 0.49 |
| 26:B:228:PRO:HG3 | 33:J:160:TYR:HD2 | 1.78 | 0.49 |
| 44:V:41:ILE:HD12 | 44:V:46:PRO:HG3 | 1.94 | 0.49 |
| 48:l:529:TYR:O | 48:l:533:MET:HB2 | 2.12 | 0.49 |
| 5:6:233:VAL:HG23 | 5:6:236:ARG:HH12 | 1.76 | 0.49 |
| 7:8:244:ALA:H | 57:8:401:HEC:HBD2 | 1.77 | 0.49 |
| 11:c:75:TYR:OH | 11:c:105:ILE:O | 2.30 | 0.49 |
| 17:i:57:THR:HA | 19:k:77:LEU:HD13 | 1.94 | 0.49 |
| 19:k:2:PRO:HG3 | 20:m:127:ILE:HD13 | 1.94 | 0.49 |
| 25:r:81:LEU:HD22 | 25:r:108:MET:HG3 | 1.94 | 0.49 |
| 25:r:165:LEU:HD23 | 25:r:241:LEU:HA | 1.93 | 0.49 |
| 28:D:68:ILE:HD13 | 36:N:44:TYR:HA | 1.95 | 0.49 |
| 48:l:49:VAL:HB | 48:l:50:PRO:HD3 | 1.95 | 0.49 |
| 48:l:397:GLU:HG3 | 48:l:482:MET:HE1 | 1.93 | 0.49 |
| 51:5:388:VAL:HG21 | 51:5:438:ALA:HA | 1.94 | 0.49 |
| 3:4:213:VAL:HA | 3:4:216:LEU:HD12 | 1.95 | 0.49 |
| 5:6:214:THR:HG21 | 5:6:245:GLY:HA3 | 1.93 | 0.49 |
| 6:7:196:HIS:HE1 | 56:7:402:HEM:C1D | 2.30 | 0.49 |
| 56:7:402:HEM:HBD1 | 56:7:402:HEM:HHA | 1.93 | 0.49 |
| 7:8:220:CYS:SG | 7:8:221:GLU:N | 2.86 | 0.49 |
| 10:b:79:VAL:HG23 | 48:l:10:THR:HG21 | 1.94 | 0.49 |
| 12:d:85:MET:HE1 | 24:q:182:TRP:CD1 | 2.47 | 0.49 |
| 26:B:41:ILE:HD12 | 26:B:250:VAL:HG12 | 1.93 | 0.49 |
| 27:C:167:ILE:HD12 | 27:C:369:VAL:HG21 | 1.95 | 0.49 |
| 27:C:312:GLN:OE1 | 28:D:140:ARG:NH1 | 2.45 | 0.49 |
| 37:O:133:ILE:HG12 | 37:O:134:ASP:N | 2.28 | 0.49 |
| 44:V:90:TYR:CE1 | 44:V:126:LYS:HD3 | 2.48 | 0.49 |
| 45:W:108:GLU:HA | 49:s:81:ILE:HD13 | 1.94 | 0.49 |
| 21:n:39:ARG:HD3 | 21:n:58:LYS:H | 1.78 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:C:73:ASN:HB2 | 43:U:195:VAL:HG13 | 1.93 | 0.49 |
| 48:l:90:ILE:HD11 | 48:l:133:THR:HG21 | 1.95 | 0.49 |
| 51:u:74:TRP:CZ2 | 51:u:411:GLU:HA | 2.48 | 0.49 |
| 3:Af:47:GLY:C | 3:Af:66:PRO:HA | 2.37 | 0.49 |
| 15:g:4:MET:HE1 | 15:g:87:LEU:HB3 | 1.95 | 0.49 |
| 17:i:12:THR:HG21 | 20:m:163:ILE:HG21 | 1.95 | 0.49 |
| 25:r:169:GLN:NE2 | 25:r:241:LEU:O | 2.46 | 0.49 |
| 32:I:81:ALA:HB1 | 32:I:82:PRO:HD2 | 1.95 | 0.49 |
| 35:L:286:TYR:HD1 | 35:L:286:TYR:H | 1.60 | 0.49 |
| 48:l:124:PHE:HE1 | 48:l:252:MET:HB2 | 1.78 | 0.49 |
| 5:6:324:SER:OG | 3:Ae:67:VAL:O | 2.31 | 0.49 |
| 6:7:85:ASN:HD22 | 6:7:243:VAL:HG22 | 1.78 | 0.49 |
| 18:j:61:THR:HG21 | 18:j:105:GLU:OE2 | 2.13 | 0.49 |
| 19:k:35:GLY:HA3 | 20:m:20:PHE:CZ | 2.48 | 0.49 |
| 23:p:149:TRP:CE3 | 23:p:153:GLU:HB3 | 2.47 | 0.49 |
| 32:I:71:CYS:HB2 | 59:I:201:SF4:S2 | 2.53 | 0.49 |
| 51:u:315:ASP:OD1 | 51:u:316:SER:N | 2.46 | 0.49 |
| 52:z:49:VAL:O | 52:z:52:PRO:HD2 | 2.13 | 0.49 |
| 53:G:471:LYS:HG3 | 53:G:510:TRP:CD2 | 2.48 | 0.49 |
| 3:4:284:TYR:HB3 | 3:4:294:VAL:HA | 1.94 | 0.49 |
| 18:j:77:TRP:HB2 | 20:m:144:ALA:HB2 | 1.95 | 0.49 |
| 38:P:46:LYS:HZ2 | 53:G:674:LEU:HD21 | 1.77 | 0.49 |
| 40:R:95:LYS:HE2 | 40:R:96:PHE:CZ | 2.48 | 0.49 |
| 3:2:182:GLU:HG2 | 3:2:201:THR:HG22 | 1.94 | 0.48 |
| 3:4:177:LEU:HD13 | 3:4:231:TRP:CD2 | 2.48 | 0.48 |
| 11:c:93:ASP:HB2 | 11:c:100:ASN:HA | 1.95 | 0.48 |
| 12:d:34:THR:HG22 | 48:l:3:PRO:HG2 | 1.94 | 0.48 |
| 24:q:108:MET:HB3 | 24:q:121:LEU:HD13 | 1.95 | 0.48 |
| 28:D:103:HIS:CE1 | 28:D:105:ASN:HA | 2.48 | 0.48 |
| 43:U:256:GLU:HG3 | 43:U:278:LEU:HD22 | 1.95 | 0.48 |
| 48:l:182:PHE:O | 48:l:185:SER:OG | 2.30 | 0.48 |
| 6:w:32:ASN:O | 6:w:36:LEU:HG | 2.13 | 0.48 |
| 3:Ae:48:PRO:HA | 3:Ae:65:SER:C | 2.38 | 0.48 |
| 3:4:217:ARG:HH22 | 3:4:273:GLY:H | 1.61 | 0.48 |
| 17:i:193:VAL:HG23 | 17:i:201:THR:HG22 | 1.95 | 0.48 |
| 25:r:57:THR:HB | 32:I:58:ARG:HH21 | 1.78 | 0.48 |
| 48:l:37:LYS:NZ | 48:l:102:GLU:OE2 | 2.41 | 0.48 |
| 48:l:346:ILE:HG12 | 48:l:366:MET:HE1 | 1.95 | 0.48 |
| 5:v:121:TYR:HB3 | 5:v:137:LEU:HD11 | 1.94 | 0.48 |
| 5:v:131:GLU:O | 5:v:135:GLU:HG2 | 2.13 | 0.48 |
| 14:f:55:TRP:CD1 | 15:g:68:THR:HG22 | 2.48 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:i:340:THR:N | 17:i:341:PRO:HD2 | 2.29 | 0.48 |
| 24:q:171:THR:HG22 | 24:q:184:HIS:HE1 | 1.78 | 0.48 |
| 25:r:136:VAL:HG12 | 25:r:140:ILE:HD12 | 1.95 | 0.48 |
| 25:r:287:HIS:HD2 | 25:r:291:LYS:HB2 | 1.78 | 0.48 |
| 25:r:299:ALA:HB1 | 42:T:110:ILE:HB | 1.95 | 0.48 |
| 31:H:117:LYS:HE2 | 53:G:240:ALA:HA | 1.95 | 0.48 |
| 36:N:94:MET:HE3 | 36:N:99:PRO:HG2 | 1.95 | 0.48 |
| 3:2:161:MET:O | 6:7:177:ARG:NH1 | 2.46 | 0.48 |
| 19:k:64:LEU:HD23 | 20:m:59:ILE:HD11 | 1.96 | 0.48 |
| 28:D:126:PHE:HZ | 28:D:199:ARG:HE | 1.61 | 0.48 |
| 35:L:221:VAL:HG11 | 35:L:283:PHE:HE1 | 1.78 | 0.48 |
| 46:Y:47:PHE:CE1 | 48:l:364:LYS:HD3 | 2.48 | 0.48 |
| 47:Z:48:VAL:HG22 | 48:l:511:LEU:HD21 | 1.95 | 0.48 |
| 53:G:690:THR:OG1 | 53:G:692:LYS:NZ | 2.46 | 0.48 |
| 3:2:225:ARG:HH12 | 3:2:268:GLY:C | 2.22 | 0.48 |
| 9:a:82:VAL:HG11 | 13:e:104:THR:HG21 | 1.95 | 0.48 |
| 10:b:28:LEU:CD2 | 10:b:29:SER:H | 2.26 | 0.48 |
| 25:r:81:LEU:HD11 | 25:r:111:LEU:HD13 | 1.94 | 0.48 |
| 31:H:200:GLU:HG3 | 34:K:88:ARG:HD2 | 1.96 | 0.48 |
| 38:P:38:GLU:HG3 | 38:P:39:LYS:HG2 | 1.94 | 0.48 |
| 10:b:84:TYR:HE1 | 12:d:49:ARG:HG2 | 1.77 | 0.48 |
| 14:f:29:PHE:CE1 | 43:U:102:ASP:HB3 | 2.49 | 0.48 |
| 27:C:218:GLU:OE2 | 32:I:83:ARG:NH1 | 2.47 | 0.48 |
| 29:E:132:ILE:HD11 | 29:E:169:PHE:CD1 | 2.49 | 0.48 |
| 43:U:152:LEU:HD12 | 43:U:158:GLY:HA2 | 1.95 | 0.48 |
| 43:U:204:HIS:CE1 | 43:U:280:CYS:HB3 | 2.49 | 0.48 |
| 37:X:115:GLN:O | 37:X:118:ILE:HG13 | 2.13 | 0.48 |
| 6:w:186:PRO:HA | 6:w:189:ILE:HD12 | 1.96 | 0.48 |
| 1:0:67:CYS:SG | 7:x:224:THR:OG1 | 2.68 | 0.48 |
| 7:8:168:ARG:HH22 | 7:8:174:ASP:CG | 2.21 | 0.48 |
| 8:9:106:GLU:O | 8:9:110:LYS:HG3 | 2.14 | 0.48 |
| 25:r:259:PHE:O | 25:r:263:THR:HG23 | 2.14 | 0.48 |
| 28:D:216:VAL:HG13 | 28:D:218:ARG:HB3 | 1.94 | 0.48 |
| 53:G:394:VAL:HG13 | 53:G:400:ILE:HD11 | 1.96 | 0.48 |
| 2:1:30:LEU:HD11 | 4:3:48:ILE:HG21 | 1.94 | 0.48 |
| 3:2:173:ILE:HD13 | 3:2:190:TRP:HB2 | 1.96 | 0.48 |
| 3:2:254:GLY:HA3 | 3:2:265:ASP:C | 2.39 | 0.48 |
| 3:4:104:ILE:HG22 | 7:8:323:ARG:NH1 | 2.29 | 0.48 |
| 7:8:153:VAL:HG21 | 7:8:177:PRO:HG2 | 1.95 | 0.48 |
| 9:a:110:TRP:CD1 | 9:a:110:TRP:H | 2.31 | 0.48 |
| 9:a:134:GLU:OE1 | 21:n:42:SER:HB3 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:c:161:TYR:HB2 | 11:c:165:ASP:HA | 1.94 | 0.48 |
| 17:i:79:LEU:HD23 | 19:k:47:ILE:HG12 | 1.95 | 0.48 |
| 20:m:61:LEU:HA | 20:m:65:LEU:HD23 | 1.96 | 0.48 |
| 20:m:125:TRP:HH2 | 45:W:126:GLY:HA2 | 1.78 | 0.48 |
| 25:r:24:GLU:HG3 | 25:r:271:LEU:HD22 | 1.96 | 0.48 |
| 26:B:177:TYR:CD1 | 26:B:182:ILE:HG13 | 2.49 | 0.48 |
| 35:L:53:VAL:HG22 | 35:L:122:ILE:HD12 | 1.95 | 0.48 |
| 43:U:215:GLU:O | 43:U:218:SER:OG | 2.22 | 0.48 |
| 45:W:100:ASP:OD1 | 45:W:100:ASP:N | 2.41 | 0.48 |
| 51:u:165:ARG:HD3 | 51:u:209:ARG:HA | 1.95 | 0.48 |
| 6:7:326:TRP:NE1 | 52:Aa:49:VAL:HG22 | 2.28 | 0.48 |
| 15:g:94:ALA:HB1 | 49:s:232:GLU:HG3 | 1.96 | 0.48 |
| 15:g:111:TYR:HA | 15:g:114:ILE:HG12 | 1.94 | 0.48 |
| 25:r:31:MET:HE1 | 25:r:272:TRP:HA | 1.96 | 0.48 |
| 27:C:190:ILE:HD11 | 27:C:257:PHE:CZ | 2.48 | 0.48 |
| 28:D:69:LEU:HD22 | 28:D:96:VAL:HG22 | 1.95 | 0.48 |
| 32:I:48:ALA:HA | 32:I:191:ARG:HE | 1.78 | 0.48 |
| 35:L:183:GLU:HG3 | 35:L:195:ILE:HG21 | 1.96 | 0.48 |
| 38:P:92:GLU:HG2 | 38:P:93:ASN:N | 2.27 | 0.48 |
| 39:Q:85:GLY:O | 39:Q:89:VAL:HG23 | 2.14 | 0.48 |
| 48:l:162:THR:O | 48:l:166:THR:HG23 | 2.13 | 0.48 |
| 51:5:42:LEU:HD22 | 51:5:426:LEU:HB3 | 1.95 | 0.48 |
| 51:5:74:TRP:CZ2 | 51:5:411:GLU:HA | 2.48 | 0.48 |
| 53:G:241:ARG:HG2 | 53:G:243:TRP:CH2 | 2.48 | 0.48 |
| 13:e:74:HIS:ND1 | 24:q:431:THR:HG21 | 2.29 | 0.48 |
| 17:i:106:LEU:HD22 | 17:i:187:MET:HE2 | 1.95 | 0.48 |
| 25:r:294:LEU:HB3 | 25:r:295:PRO:HD3 | 1.96 | 0.48 |
| 48:l:251:THR:O | 48:l:254:VAL:HG22 | 2.14 | 0.48 |
| 50:t:22:MET:HE3 | 50:t:105:GLU:HG3 | 1.95 | 0.48 |
| 3:2:100:SER:HB2 | 51:u:176:ASP:HB2 | 1.96 | 0.47 |
| 3:2:197:VAL:HG13 | 3:2:233:ILE:HG12 | 1.95 | 0.47 |
| 3:2:197:VAL:HG22 | 3:2:233:ILE:HG23 | 1.96 | 0.47 |
| 9:a:161:ARG:HH11 | 44:V:141:VAL:HB | 1.78 | 0.47 |
| 16:h:17:TRP:CD1 | 16:h:17:TRP:H | 2.32 | 0.47 |
| 24:q:400:MET:HE1 | 48:l:183:VAL:HG21 | 1.95 | 0.47 |
| 26:B:202:GLY:HA3 | 29:E:121:MET:HG3 | 1.95 | 0.47 |
| 28:D:200:LYS:O | 33:J:126:LEU:HD21 | 2.13 | 0.47 |
| 35:L:80:ARG:HD2 | 60:L:401:NDP:C2A | 2.43 | 0.47 |
| 35:L:128:GLU:OE2 | 35:L:313:LYS:HE2 | 2.14 | 0.47 |
| 38:P:74:GLU:OE2 | 53:G:645:ARG:NH2 | 2.47 | 0.47 |
| 48:l:356:ILE:HA | 48:l:359:MET:HE2 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:l:368:PHE:HE2 | 48:l:454:ILE:HB | 1.78 | 0.47 |
| 53:G:370:GLU:HB2 | 53:G:522:GLN:OE1 | 2.14 | 0.47 |
| 52:Aa:79:GLU:HG2 | 52:Aa:80:ASN:N | 2.27 | 0.47 |
| 3:4:120:SER:HA | 51:5:269:ARG:HE | 1.79 | 0.47 |
| 17:i:65:THR:HG22 | 19:k:19:LEU:HD21 | 1.96 | 0.47 |
| 17:i:111:PHE:HA | 48:l:591:PHE:CE1 | 2.50 | 0.47 |
| 24:q:24:TRP:CD2 | 24:q:81:GLN:HG2 | 2.50 | 0.47 |
| 25:r:28:LEU:HD22 | 25:r:275:ALA:HB2 | 1.97 | 0.47 |
| 26:B:193:PHE:N | 40:R:98:MET:HE1 | 2.29 | 0.47 |
| 27:C:190:ILE:O | 27:C:194:THR:HB | 2.13 | 0.47 |
| 35:L:84:TYR:HA | 35:L:87:MET:HE2 | 1.95 | 0.47 |
| 5:v:271:LEU:HD22 | 5:v:453:LEU:HD13 | 1.95 | 0.47 |
| 56:7:402:HEM:HHA | 56:7:402:HEM:HBA1 | 1.95 | 0.47 |
| 7:8:187:ARG:HB3 | 7:8:192:GLY:HA2 | 1.96 | 0.47 |
| 9:a:169:TYR:CE2 | 15:g:3:MET:HG2 | 2.49 | 0.47 |
| 17:i:200:MET:HG3 | 17:i:269:GLU:HG3 | 1.95 | 0.47 |
| 25:r:219:PRO:HA | 25:r:222:MET:HE3 | 1.96 | 0.47 |
| 27:C:122:LEU:HD11 | 32:I:70:ALA:HB2 | 1.97 | 0.47 |
| 27:C:410:LYS:NZ | 27:C:461:ASP:HB2 | 2.29 | 0.47 |
| 32:I:98:ARG:HA | 32:I:125:PRO:HD3 | 1.95 | 0.47 |
| 39:Q:65:TRP:O | 39:Q:69:VAL:HG23 | 2.14 | 0.47 |
| 44:V:22:ALA:O | 44:V:26:THR:OG1 | 2.31 | 0.47 |
| 45:W:66:GLU:OE2 | 49:s:201:GLU:N | 2.46 | 0.47 |
| 5:6:446:HIS:H | 5:6:446:HIS:CD2 | 2.32 | 0.47 |
| 10:b:62:TYR:HA | 10:b:66:ARG:HB2 | 1.97 | 0.47 |
| 17:i:311:MET:HE3 | 17:i:314:LYS:HD3 | 1.95 | 0.47 |
| 24:q:11:LEU:HA | 24:q:14:MET:HE3 | 1.96 | 0.47 |
| 25:r:58:LYS:HD2 | 32:I:127:PRO:HD2 | 1.96 | 0.47 |
| 28:D:61:PHE:CE1 | 54:M:97:PRO:HD3 | 2.49 | 0.47 |
| 28:D:230:PHE:O | 33:J:123:ASN:ND2 | 2.47 | 0.47 |
| 42:T:167:LYS:HA | 45:W:59:ARG:HD3 | 1.96 | 0.47 |
| 45:W:30:LEU:HD23 | 45:W:34:SER:OG | 2.14 | 0.47 |
| 48:l:8:THR:HB | 48:l:82:MET:HE3 | 1.96 | 0.47 |
| 48:l:296:ASN:O | 48:l:356:ILE:HG12 | 2.14 | 0.47 |
| 2:Ac:18:THR:HA | 2:Ac:21:PHE:HB3 | 1.96 | 0.47 |
| 3:2:240:HIS:HB3 | 55:2:301:FES:S2 | 2.55 | 0.47 |
| 17:i:112:HIS:CE1 | 17:i:164:ILE:HD13 | 2.49 | 0.47 |
| 23:p:201:LYS:HE2 | 23:p:201:LYS:HB3 | 1.74 | 0.47 |
| 25:r:168:THR:HG22 | 45:W:57:ARG:NH2 | 2.29 | 0.47 |
| 32:I:51:ASP:HA | 32:I:54:VAL:HG22 | 1.96 | 0.47 |
| 35:L:226:LEU:HB3 | 35:L:228:LYS:HD3 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 45:W:10:MET:HE3 | 45:W:11:PRO:HD2 | 1.97 | 0.47 |
| 48:l:428:PHE:CE2 | 48:l:505:ASN:HB3 | 2.50 | 0.47 |
| 10:b:84:TYR:CE1 | 12:d:49:ARG:HG2 | 2.50 | 0.47 |
| 24:q:208:PRO:HG3 | 24:q:216:LEU:HD13 | 1.96 | 0.47 |
| 35:L:277:ALA:HB1 | 35:L:364:VAL:HG11 | 1.97 | 0.47 |
| 51:u:192:PHE:HB3 | 51:u:195:THR:OG1 | 2.14 | 0.47 |
| 3:2:100:SER:HB2 | 51:u:176:ASP:OD2 | 2.15 | 0.47 |
| 7:8:216:LEU:HD11 | 57:8:401:HEC:CMB | 2.45 | 0.47 |
| 17:i:250:SER:O | 17:i:259:GLY:HA3 | 2.15 | 0.47 |
| 23:p:124:PHE:O | 23:p:127:SER:OG | 2.29 | 0.47 |
| 23:p:150:HIS:CD2 | 23:p:151:PRO:HD2 | 2.50 | 0.47 |
| 24:q:358:TRP:HE3 | 24:q:441:ILE:HD12 | 1.80 | 0.47 |
| 26:B:52:ARG:HG2 | 26:B:175:GLU:OE2 | 2.15 | 0.47 |
| 26:B:445:GLU:H | 26:B:445:GLU:HG2 | 1.47 | 0.47 |
| 27:C:53:PHE:HD1 | 27:C:58:MET:HE1 | 1.79 | 0.47 |
| 34:K:44:TYR:HE2 | 34:K:83:PRO:HB3 | 1.80 | 0.47 |
| 35:L:163:SER:O | 35:L:197:LYS:HA | 2.14 | 0.47 |
| 37:O:104:PHE:HD2 | 37:O:139:MET:HA | 1.75 | 0.47 |
| 38:P:31:GLN:OE1 | 38:P:34:ARG:NH1 | 2.48 | 0.47 |
| 44:V:90:TYR:CD1 | 44:V:126:LYS:HD3 | 2.49 | 0.47 |
| 46:Y:44:TYR:HD2 | 47:Z:33:PRO:HD2 | 1.79 | 0.47 |
| 48:l:362:LEU:HD22 | 48:l:366:MET:HE2 | 1.96 | 0.47 |
| 48:l:587:TYR:O | 48:l:590:SER:OG | 2.25 | 0.47 |
| 5:v:63:LEU:HD11 | 5:v:218:MET:HB3 | 1.96 | 0.47 |
| 6:w:182:HIS:HE1 | 56:w:402:HEM:C1B | 2.33 | 0.47 |
| 8:y:63:ILE:O | 8:y:67:LEU:HG | 2.14 | 0.47 |
| 53:G:310:GLU:OE1 | 53:G:311:LYS:HG2 | 2.14 | 0.47 |
| 53:G:438:LEU:O | 53:G:439:THR:OG1 | 2.31 | 0.47 |
| 53:G:575:VAL:O | 53:G:578:PRO:HD2 | 2.15 | 0.47 |
| 3:2:190:TRP:CE2 | 3:2:191:ARG:HG2 | 2.49 | 0.47 |
| 3:4:199:HIS:HE1 | 3:4:230:GLU:HB2 | 1.80 | 0.47 |
| 5:6:131:GLU:HA | 5:6:134:MET:HE3 | 1.97 | 0.47 |
| 7:8:246:ALA:O | 7:8:247:PRO:C | 2.57 | 0.47 |
| 26:B:85:LEU:HD21 | 26:B:247:THR:HG23 | 1.95 | 0.47 |
| 28:D:118:ASP:OD1 | 28:D:125:ARG:NE | 2.42 | 0.47 |
| 35:L:349:ARG:NH1 | 39:Q:77:GLN:O | 2.47 | 0.47 |
| 36:N:23:ARG:NH2 | 36:N:27:LEU:HD21 | 2.30 | 0.47 |
| 41:S:16:LEU:O | 41:S:19:PRO:HD2 | 2.14 | 0.47 |
| 48:l:95:PHE:CZ | 48:l:456:ARG:HB3 | 2.50 | 0.47 |
| 51:u:276:ARG:HB2 | 52:z:16:THR:HG23 | 1.96 | 0.47 |
| 3:2:284:TYR:HB3 | 3:2:294:VAL:HG22 | 1.95 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:e:87:MET:HE3 | 13:e:88:ARG:HG3 | 1.97 | 0.47 |
| 24:q:6:ILE:O | 24:q:9:THR:OG1 | 2.27 | 0.47 |
| 24:q:73:LEU:HD22 | 24:q:103:GLN:OE1 | 2.14 | 0.47 |
| 26:B:86:ARG:NH1 | 26:B:269:ARG:O | 2.46 | 0.47 |
| 27:C:147:TYR:HB3 | 32:I:71:CYS:HB3 | 1.96 | 0.47 |
| 31:H:106:TYR:CE2 | 31:H:112:ARG:HA | 2.49 | 0.47 |
| 3:2:177:LEU:HD22 | 3:2:231:TRP:CD2 | 2.49 | 0.47 |
| 5:6:358:VAL:HG11 | 5:6:431:PHE:CD2 | 2.50 | 0.47 |
| 7:8:198:LEU:HD13 | 7:8:275:LEU:HD21 | 1.96 | 0.47 |
| 9:a:147:ALA:HB2 | 24:q:173:SER:HB2 | 1.97 | 0.47 |
| 10:b:4:TYR:CD2 | 10:b:9:LYS:HG2 | 2.48 | 0.47 |
| 11:c:41:TYR:CG | 11:c:67:ASP:HB2 | 2.50 | 0.47 |
| 16:h:26:PRO:HD3 | 19:k:55:LEU:HD13 | 1.97 | 0.47 |
| 20:m:64:MET:O | 20:m:67:VAL:HG12 | 2.14 | 0.47 |
| 22:o:87:SER:HA | 48:l:557:TRP:CZ2 | 2.49 | 0.47 |
| 26:B:102:MET:HG2 | 26:B:149:MET:HB3 | 1.97 | 0.47 |
| 27:C:212:GLU:O | 27:C:216:MET:HG3 | 2.14 | 0.47 |
| 38:P:42:VAL:HG12 | 38:P:46:LYS:HE2 | 1.97 | 0.47 |
| 48:l:391:SER:O | 48:l:395:ILE:HG12 | 2.15 | 0.47 |
| 53:G:397:ALA:HA | 53:G:471:LYS:HB3 | 1.96 | 0.47 |
| 53:G:624:ARG:NH1 | 53:G:628:GLU:HB2 | 2.30 | 0.47 |
| 5:6:176:ASN:ND2 | 5:6:260:ASP:OD2 | 2.48 | 0.46 |
| 10:b:28:LEU:HD23 | 10:b:29:SER:H | 1.79 | 0.46 |
| 12:d:37:PHE:CD2 | 48:l:3:PRO:HG3 | 2.50 | 0.46 |
| 20:m:8:ILE:O | 20:m:11:THR:OG1 | 2.30 | 0.46 |
| 23:p:171:ARG:HD2 | 23:p:210:TRP:CD2 | 2.50 | 0.46 |
| 24:q:216:LEU:HD22 | 24:q:291:VAL:HG23 | 1.97 | 0.46 |
| 26:B:325:PRO:HG3 | 26:B:433:TRP:HB3 | 1.97 | 0.46 |
| 27:C:432:ALA:HB1 | 27:C:466:GLU:HB3 | 1.97 | 0.46 |
| 31:H:128:ILE:CD1 | 31:H:158:CYS:SG | 3.03 | 0.46 |
| 35:L:104:ASN:HB3 | 35:L:107:ASP:HB3 | 1.97 | 0.46 |
| 43:U:263:ARG:HD3 | 43:U:264:GLU:N | 2.30 | 0.46 |
| 51:u:80:ARG:NH2 | 51:u:266:THR:O | 2.48 | 0.46 |
| 6:w:126:THR:HA | 6:w:129:MET:HE2 | 1.96 | 0.46 |
| 3:Ae:56:HIS:C | 3:Ae:58:ALA:H | 2.23 | 0.46 |
| 5:6:70:ARG:NH1 | 5:6:117:GLU:OE2 | 2.47 | 0.46 |
| 5:6:221:ILE:HD13 | 5:6:397:GLY:HA2 | 1.97 | 0.46 |
| 5:6:233:VAL:HG23 | 5:6:236:ARG:NH1 | 2.30 | 0.46 |
| 6:7:165:TRP:O | 6:7:174:THR:OG1 | 2.26 | 0.46 |
| 7:8:219:TYR:CE1 | 7:8:243:ILE:HG21 | 2.35 | 0.46 |
| 17:i:137:ALA:O | 17:i:141:VAL:HG23 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:p:91:ASP:HA | 23:p:94:LYS:HB2 | 1.96 | 0.46 |
| 24:q:226:ALA:O | 24:q:230:VAL:HG22 | 2.15 | 0.46 |
| 29:E:66:ILE:HD13 | 29:E:81:PRO:HB2 | 1.97 | 0.46 |
| 43:U:241:ASN:O | 43:U:245:LYS:HB2 | 2.16 | 0.46 |
| 45:W:23:ARG:HG3 | 45:W:25:LEU:HD13 | 1.97 | 0.46 |
| 46:Y:97:LEU:H | 50:t:111:ARG:HH21 | 1.62 | 0.46 |
| 51:u:447:LYS:HE3 | 51:u:448:TYR:CE2 | 2.50 | 0.46 |
| 53:G:372:PHE:H | 53:G:532:PRO:HB2 | 1.79 | 0.46 |
| 52:Aa:73:LYS:NZ | 1:Ab:66:ASP:H | 2.13 | 0.46 |
| 3:4:243:CYS:SG | 3:4:244:VAL:N | 2.88 | 0.46 |
| 7:8:245:MET:HG2 | 57:8:401:HEC:C4D | 2.46 | 0.46 |
| 11:c:96:ASP:N | 11:c:96:ASP:OD1 | 2.47 | 0.46 |
| 19:k:21:MET:O | 20:m:23:LYS:NZ | 2.44 | 0.46 |
| 20:m:25:SER:HB3 | 20:m:81:GLU:N | 2.30 | 0.46 |
| 25:r:153:VAL:HB | 25:r:174:MET:HE1 | 1.98 | 0.46 |
| 26:B:71:LYS:HG2 | 26:B:75:TRP:CD2 | 2.49 | 0.46 |
| 28:D:67:GLU:O | 28:D:70:PRO:HD3 | 2.15 | 0.46 |
| 32:I:191:ARG:O | 32:I:195:ARG:HG3 | 2.16 | 0.46 |
| 35:L:152:LYS:HG3 | 35:L:189:ALA:O | 2.15 | 0.46 |
| 46:Y:65:MET:HE2 | 48:l:375:ILE:HG12 | 1.98 | 0.46 |
| 48:l:76:LEU:HD21 | 48:l:196:TRP:HE3 | 1.80 | 0.46 |
| 6:w:165:TRP:O | 6:w:174:THR:OG1 | 2.28 | 0.46 |
| 6:w:278:TYR:CE2 | 6:w:282:ARG:HD3 | 2.51 | 0.46 |
| 53:G:445:LEU:HD22 | 53:G:460:HIS:HE1 | 1.79 | 0.46 |
| 3:2:256:TYR:CZ | 3:2:258:PRO:HA | 2.51 | 0.46 |
| 5:6:109:LYS:HE2 | 5:6:124:GLU:HG3 | 1.97 | 0.46 |
| 10:b:94:PRO:HB3 | 12:d:5:TRP:CG | 2.50 | 0.46 |
| 11:c:38:PRO:HD2 | 22:o:70:TYR:CD1 | 2.51 | 0.46 |
| 17:i:230:LEU:O | 17:i:233:THR:OG1 | 2.31 | 0.46 |
| 18:j:113:TRP:HB2 | 25:r:286:MET:HE3 | 1.98 | 0.46 |
| 19:k:22:TYR:HA | 20:m:23:LYS:HE2 | 1.97 | 0.46 |
| 24:q:7:PRO:O | 24:q:11:LEU:HD23 | 2.15 | 0.46 |
| 25:r:61:LEU:HD13 | 32:I:98:ARG:HH11 | 1.79 | 0.46 |
| 27:C:317:TYR:HA | 27:C:320:VAL:HG22 | 1.97 | 0.46 |
| 35:L:221:VAL:HB | 35:L:285:PRO:HA | 1.97 | 0.46 |
| 37:O:115:GLN:O | 37:O:119:ILE:HG12 | 2.15 | 0.46 |
| 43:U:50:ARG:HA | 43:U:50:ARG:HD3 | 1.79 | 0.46 |
| 48:l:118:PHE:O | 48:l:122:VAL:HG23 | 2.16 | 0.46 |
| 5:v:338:ILE:HG21 | 5:v:354:ALA:HB1 | 1.97 | 0.46 |
| 51:5:275:ILE:HG12 | 52:Aa:17:TYR:HD2 | 1.80 | 0.46 |
| 5:6:421:ASP:O | 5:6:425:ILE:HG13 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:7:245:PHE:HE2 | 7:8:102:LEU:HB3 | 1.81 | 0.46 |
| 11:c:65:TYR:CE1 | 11:c:77:LYS:HG2 | 2.51 | 0.46 |
| 13:e:101:LEU:O | 13:e:104:THR:OG1 | 2.33 | 0.46 |
| 20:m:83:TRP:HA | 20:m:89:VAL:HG12 | 1.98 | 0.46 |
| 24:q:119:TYR:HE1 | 24:q:157:SER:HB2 | 1.81 | 0.46 |
| 24:q:134:THR:O | 24:q:142:ARG:NH1 | 2.49 | 0.46 |
| 26:B:68:ILE:HG23 | 26:B:75:TRP:HZ3 | 1.80 | 0.46 |
| 43:U:291:ARG:HH22 | 43:U:294:HIS:CD2 | 2.33 | 0.46 |
| 45:W:66:GLU:OE2 | 49:s:202:LEU:N | 2.48 | 0.46 |
| 5:v:65:ILE:HG21 | 5:v:213:PHE:CD1 | 2.51 | 0.46 |
| 51:5:133:ILE:HG13 | 51:5:147:LEU:HD21 | 1.96 | 0.46 |
| 53:G:669:ASN:O | 53:G:672:SER:OG | 2.29 | 0.46 |
| 1:0:34:ARG:HG2 | 1:0:82:VAL:HG21 | 1.96 | 0.46 |
| 1:0:80:HIS:CE1 | 1:0:84:HIS:HE2 | 2.34 | 0.46 |
| 3:2:200:ARG:NH1 | 3:2:222:ASP:OD1 | 2.48 | 0.46 |
| 5:6:171:ALA:O | 5:6:175:GLU:HG2 | 2.15 | 0.46 |
| 10:b:89:HIS:CD2 | 10:b:96:THR:HB | 2.51 | 0.46 |
| 19:k:97:GLN:HA | 48:l:582:GLY:HA3 | 1.96 | 0.46 |
| 24:q:1:MET:HG2 | 24:q:52:PHE:CD2 | 2.50 | 0.46 |
| 24:q:122:PHE:HE1 | 24:q:206:LYS:HG3 | 1.81 | 0.46 |
| 26:B:442:PHE:HB3 | 26:B:445:GLU:HG3 | 1.97 | 0.46 |
| 27:C:128:LYS:HB2 | 28:D:198:PHE:CE1 | 2.51 | 0.46 |
| 48:l:154:LEU:HD13 | 48:l:243:VAL:HG22 | 1.97 | 0.46 |
| 51:u:42:LEU:HD22 | 51:u:426:LEU:HB3 | 1.98 | 0.46 |
| 51:5:186:TYR:O | 51:5:190:THR:HG22 | 2.16 | 0.46 |
| 51:5:318:TYR:CE1 | 3:Ae:55:GLY:HA2 | 2.51 | 0.46 |
| 3:4:142:THR:OG1 | 7:8:303:LEU:HB3 | 2.16 | 0.46 |
| 3:4:159:SER:O | 3:4:162:SER:OG | 2.29 | 0.46 |
| 11:c:36:MET:HG2 | 22:o:67:ARG:HE | 1.81 | 0.46 |
| 17:i:26:TRP:CE2 | 17:i:86:ILE:HG13 | 2.51 | 0.46 |
| 17:i:244:MET:HE2 | 17:i:244:MET:HB3 | 1.76 | 0.46 |
| 26:B:355:ILE:HD13 | 29:E:139:PRO:HG3 | 1.97 | 0.46 |
| 29:E:222:ARG:NH2 | 29:E:226:GLU:O | 2.49 | 0.46 |
| 38:P:68:ARG:HH11 | 53:G:359:ASN:HD21 | 1.63 | 0.46 |
| 48:l:86:SER:HB3 | 48:l:133:THR:HG22 | 1.98 | 0.46 |
| 49:s:115:LYS:HE3 | 49:s:119:GLU:CD | 2.41 | 0.46 |
| 51:u:316:SER:N | 51:u:339:GLN:O | 2.48 | 0.46 |
| 6:w:82:LEU:HD23 | 6:w:243:VAL:HG21 | 1.98 | 0.46 |
| 1:0:76:HIS:HB2 | 7:x:90:LEU:HD11 | 1.98 | 0.46 |
| 1:0:79:ASP:HB3 | 7:x:93:PRO:HG2 | 1.98 | 0.46 |
| 3:2:227:LYS:HG3 | 3:2:284:TYR:HE1 | 1.81 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2:241:LEU:HB2 | 55:2:301:FES:S1 | 2.56 | 0.46 |
| 5:6:449:PHE:CZ | 5:v:183:ARG:HB2 | 2.51 | 0.46 |
| 20:m:107:ALA:HA | 20:m:113:VAL:HB | 1.98 | 0.46 |
| 24:q:174:LEU:HA | 24:q:179:ILE:HD11 | 1.97 | 0.46 |
| 29:E:146:ASP:OD1 | 29:E:146:ASP:N | 2.49 | 0.46 |
| 35:L:209:LEU:HD21 | 35:L:340:LEU:HD11 | 1.97 | 0.46 |
| 38:P:42:VAL:O | 38:P:46:LYS:HG3 | 2.16 | 0.46 |
| 51:u:270:PHE:CG | 51:u:292:GLU:HB2 | 2.51 | 0.46 |
| 3:2:182:GLU:HA | 3:2:199:HIS:HB3 | 1.98 | 0.46 |
| 5:6:271:LEU:HD11 | 5:6:436:LYS:HB3 | 1.97 | 0.46 |
| 7:8:236:PRO:HA | 7:8:241:GLN:HG3 | 1.97 | 0.46 |
| 9:a:169:TYR:CZ | 15:g:3:MET:HG2 | 2.50 | 0.46 |
| 11:c:113:ILE:HD11 | 11:c:116:ARG:HG3 | 1.98 | 0.46 |
| 13:e:91:PHE:HA | 13:e:95:PHE:HD2 | 1.81 | 0.46 |
| 17:i:173:THR:HG22 | 27:C:58:MET:HE2 | 1.98 | 0.46 |
| 24:q:121:LEU:O | 24:q:125:THR:HG23 | 2.16 | 0.46 |
| 35:L:111:ILE:HG21 | 35:L:147:ILE:HA | 1.97 | 0.46 |
| 35:L:264:ASN:HB2 | 35:L:266:TYR:CZ | 2.51 | 0.46 |
| 39:Q:55:LYS:HZ2 | 61:Q:201:ZMP:H21 | 1.81 | 0.46 |
| 39:Q:63:ARG:O | 39:Q:67:ARG:HG2 | 2.16 | 0.46 |
| 43:U:353:TRP:HZ3 | 43:U:356:LEU:HD12 | 1.81 | 0.46 |
| 48:l:253:VAL:HB | 48:l:310:LEU:HD11 | 1.98 | 0.46 |
| 51:u:343:THR:HG22 | 51:u:356:ALA:HB2 | 1.98 | 0.46 |
| 6:w:77:TRP:CD2 | 7:x:282:GLU:HG3 | 2.51 | 0.46 |
| 7:x:198:LEU:HA | 7:x:201:ILE:HB | 1.98 | 0.46 |
| 51:5:142:LYS:O | 51:5:146:LEU:HG | 2.15 | 0.46 |
| 53:G:262:VAL:HG23 | 53:G:276:ARG:HB2 | 1.98 | 0.46 |
| 3:2:270:ILE:HG22 | 3:2:278:ASN:OD1 | 2.16 | 0.46 |
| 7:8:216:LEU:HD21 | 57:8:401:HEC:HMB2 | 1.96 | 0.46 |
| 17:i:63:GLN:OE1 | 17:i:105:LYS:HG2 | 2.15 | 0.46 |
| 17:i:270:MET:HE1 | 17:i:278:MET:HG2 | 1.98 | 0.46 |
| 23:p:160:TYR:HA | 23:p:163:LYS:HE2 | 1.97 | 0.46 |
| 28:D:152:PRO:HD3 | 39:Q:46:ILE:HG12 | 1.97 | 0.46 |
| 28:D:171:TRP:HH2 | 39:Q:111:LYS:HZ2 | 1.63 | 0.46 |
| 29:E:143:ARG:O | 29:E:184:PRO:HG3 | 2.16 | 0.46 |
| 44:V:59:TYR:O | 44:V:62:THR:OG1 | 2.31 | 0.46 |
| 7:x:117:VAL:HG11 | 7:x:271:VAL:HB | 1.97 | 0.46 |
| 53:G:75:CYS:SG | 53:G:76:ARG:N | 2.89 | 0.46 |
| 3:Af:50:CYS:O | 3:Af:52:GLY:N | 2.49 | 0.46 |
| 3:2:106:VAL:HG21 | 51:u:190:THR:HA | 1.97 | 0.45 |
| 3:2:145:GLY:HA3 | 7:x:300:LEU:HD21 | 1.97 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:91:THR:HG21 | 5:6:140:VAL:HA | 1.98 | 0.45 |
| 5:6:104:GLU:OE2 | 51:5:324:MET:HG3 | 2.17 | 0.45 |
| 5:6:375:LYS:HD3 | 5:6:417:ASP:HA | 1.97 | 0.45 |
| 17:i:170:LEU:HD22 | 17:i:291:TYR:HD2 | 1.81 | 0.45 |
| 22:o:20:PRO:HA | 23:p:107:ARG:HH12 | 1.81 | 0.45 |
| 26:B:317:VAL:HG22 | 26:B:356:VAL:HG22 | 1.98 | 0.45 |
| 27:C:101:LEU:HB2 | 27:C:464:PHE:CZ | 2.51 | 0.45 |
| 30:F:99:TYR:CD1 | 53:G:157:LYS:HB2 | 2.50 | 0.45 |
| 51:u:342:GLN:HE21 | 51:u:342:GLN:HB2 | 1.62 | 0.45 |
| 6:w:97:HIS:CE1 | 6:w:100:ARG:HH22 | 2.34 | 0.45 |
| 53:G:236:TYR:CZ | 53:G:272:ARG:HD3 | 2.51 | 0.45 |
| 3:4:227:LYS:NZ | 3:4:284:TYR:O | 2.39 | 0.45 |
| 5:6:129:ASP:OD1 | 5:6:129:ASP:N | 2.48 | 0.45 |
| 5:6:155:GLN:O | 5:6:158:LEU:HB2 | 2.17 | 0.45 |
| 7:8:122:CYS:SG | 57:8:401:HEC:C4B | 3.04 | 0.45 |
| 7:8:132:ALA:HB2 | 7:8:175:TYR:CD2 | 2.51 | 0.45 |
| 17:i:64:ALA:O | 17:i:68:MET:HG2 | 2.17 | 0.45 |
| 24:q:122:PHE:CE1 | 24:q:206:LYS:HG3 | 2.52 | 0.45 |
| 24:q:216:LEU:HD23 | 24:q:287:ALA:HB1 | 1.98 | 0.45 |
| 25:r:20:LEU:HD13 | 41:S:12:MET:HE1 | 1.98 | 0.45 |
| 34:K:65:THR:O | 34:K:73:THR:OG1 | 2.31 | 0.45 |
| 35:L:168:ASP:OD1 | 35:L:169:ILE:N | 2.50 | 0.45 |
| 48:l:232:TRP:HZ3 | 48:l:248:HIS:HD2 | 1.64 | 0.45 |
| 48:l:249:SER:O | 48:l:332:HIS:HE1 | 1.99 | 0.45 |
| 5:v:142:ALA:HA | 5:v:241:ARG:HH22 | 1.81 | 0.45 |
| 53:G:338:VAL:O | 53:G:363:SER:OG | 2.30 | 0.45 |
| 54:M:46:SER:O | 54:M:52:ASN:ND2 | 2.50 | 0.45 |
| 3:4:225:ARG:HH12 | 3:4:269:ARG:HG2 | 1.81 | 0.45 |
| 6:7:1:MET:O | 51:5:335:ARG:NH1 | 2.50 | 0.45 |
| 6:7:244:LEU:O | 7:8:286:ARG:NH1 | 2.33 | 0.45 |
| 13:e:65:ASN:HB3 | 24:q:427:LYS:HE3 | 1.97 | 0.45 |
| 17:i:211:MET:HG2 | 17:i:333:SER:HB2 | 1.98 | 0.45 |
| 17:i:302:LEU:HD13 | 24:q:134:THR:OG1 | 2.16 | 0.45 |
| 18:j:67:LEU:HD21 | 19:k:68:ALA:CB | 2.47 | 0.45 |
| 20:m:3:MET:HE1 | 45:W:133:ILE:HG21 | 1.97 | 0.45 |
| 23:p:98:ASP:HB3 | 23:p:101:LYS:HB2 | 1.98 | 0.45 |
| 23:p:180:LYS:HE3 | 23:p:180:LYS:HB3 | 1.87 | 0.45 |
| 26:B:314:LEU:HB3 | 26:B:329:LYS:HG3 | 1.98 | 0.45 |
| 31:H:86:TYR:CD1 | 31:H:87:PRO:HA | 2.51 | 0.45 |
| 44:V:18:CYS:SG | 44:V:75:CYS:HB3 | 2.56 | 0.45 |
| 47:Z:49:GLN:HE22 | 47:Z:59:ASP:HB3 | 1.81 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:v:138:LEU:HD13 | 5:v:237:PHE:HB2 | 1.97 | 0.45 |
| 6:w:338:ILE:HD13 | 6:w:351:GLY:HA2 | 1.99 | 0.45 |
| 7:x:245:MET:HG2 | 7:x:246:ALA:O | 2.16 | 0.45 |
| 51:5:417:LEU:HD23 | 51:5:417:LEU:HA | 1.82 | 0.45 |
| 3:2:171:SER:O | 3:2:190:TRP:NE1 | 2.48 | 0.45 |
| 3:2:204:GLU:O | 3:2:207:GLN:HG3 | 2.17 | 0.45 |
| 6:7:27:ILE:HG12 | 6:7:224:TYR:CZ | 2.51 | 0.45 |
| 7:8:310:HIS:CE1 | 52:Aa:21:PRO:HB2 | 2.52 | 0.45 |
| 13:e:116:GLU:HB3 | 13:e:120:ARG:NH1 | 2.31 | 0.45 |
| 24:q:373:ILE:HA | 24:q:376:ILE:HD12 | 1.99 | 0.45 |
| 27:C:103:LEU:HD22 | 27:C:457:ILE:HD11 | 1.99 | 0.45 |
| 37:O:138:LEU:HB3 | 37:O:139:MET:H | 1.66 | 0.45 |
| 51:u:92:PHE:O | 51:u:96:LEU:HG | 2.16 | 0.45 |
| 5:v:189:SER:OG | 5:v:191:TYR:O | 2.27 | 0.45 |
| 3:4:156:GLN:HE22 | 7:8:289:MET:HE3 | 1.81 | 0.45 |
| 20:m:34:ILE:HG23 | 20:m:61:LEU:HD23 | 1.98 | 0.45 |
| 25:r:34:ARG:HG2 | 32:I:82:PRO:HA | 1.98 | 0.45 |
| 26:B:174:ARG:HA | 40:R:93:LEU:HD21 | 1.98 | 0.45 |
| 26:B:235:VAL:HG12 | 26:B:240:THR:OG1 | 2.17 | 0.45 |
| 27:C:196:HIS:O | 27:C:200:ILE:HG12 | 2.16 | 0.45 |
| 43:U:69:CYS:HG | 43:U:223:LYS:HZ3 | 1.61 | 0.45 |
| 46:Y:47:PHE:HA | 47:Z:73:PHE:CZ | 2.52 | 0.45 |
| 48:l:419:THR:HA | 48:l:422:TYR:CZ | 2.52 | 0.45 |
| 7:8:103:LEU:HD11 | 7:8:291:LEU:HD13 | 1.99 | 0.45 |
| 23:p:170:LEU:HG | 23:p:205:LEU:HD11 | 1.98 | 0.45 |
| 24:q:232:ALA:O | 24:q:237:LYS:NZ | 2.49 | 0.45 |
| 24:q:353:PRO:O | 24:q:357:THR:HG23 | 2.17 | 0.45 |
| 25:r:200:LEU:CD1 | 25:r:282:TYR:HA | 2.47 | 0.45 |
| 34:K:78:ASP:OD1 | 34:K:80:SER:OG | 2.28 | 0.45 |
| 48:l:375:ILE:HD12 | 48:l:458:LEU:HD22 | 1.99 | 0.45 |
| 49:s:178:ARG:HD3 | 49:s:178:ARG:HA | 1.68 | 0.45 |
| 51:u:54:ASP:OD1 | 51:u:54:ASP:N | 2.49 | 0.45 |
| 5:v:49:ILE:HD13 | 5:v:231:LYS:HA | 1.99 | 0.45 |
| 7:x:160:ASN:OD1 | 7:x:164:GLU:HG3 | 2.16 | 0.45 |
| 51:5:280:ASP:OD2 | 52:Aa:10:ARG:HA | 2.17 | 0.45 |
| 2:Ac:56:ILE:HB | 2:Ac:59:LYS:HE2 | 1.99 | 0.45 |
| 7:8:309:ARG:HG3 | 52:Aa:27:PHE:CE1 | 2.52 | 0.45 |
| 10:b:11:ARG:NH2 | 23:p:207:PRO:O | 2.49 | 0.45 |
| 25:r:281:ARG:HD2 | 27:C:449:MET:HE3 | 1.98 | 0.45 |
| 32:I:103:MET:HB2 | 32:I:124:MET:HE1 | 1.99 | 0.45 |
| 48:l:37:LYS:HD2 | 48:l:105:MET:HE1 | 1.98 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:u:341:PHE:HB2 | 51:u:358:PHE:HB3 | 1.99 | 0.45 |
| 53:G:627:SER:HB3 | 53:G:632:MET:O | 2.15 | 0.45 |
| 16:h:3:PHE:HB2 | 17:i:144:GLN:CD | 2.41 | 0.45 |
| 20:m:34:ILE:HD11 | 20:m:65:LEU:HD11 | 1.98 | 0.45 |
| 21:n:24:GLY:HA2 | 24:q:6:ILE:HD12 | 1.99 | 0.45 |
| 27:C:107:LEU:HD23 | 27:C:112:VAL:HA | 1.98 | 0.45 |
| 36:N:38:ILE:O | 36:N:45:ARG:NH2 | 2.48 | 0.45 |
| 42:T:151:VAL:O | 49:s:207:LYS:NZ | 2.40 | 0.45 |
| 48:l:62:ILE:HG21 | 48:l:199:GLN:HE22 | 1.81 | 0.45 |
| 48:l:561:ILE:O | 48:l:565:THR:OG1 | 2.35 | 0.45 |
| 51:5:116:MET:SD | 51:5:142:LYS:HG2 | 2.57 | 0.45 |
| 3:2:131:ARG:NH1 | 52:z:22:PHE:O | 2.48 | 0.45 |
| 6:7:106:SER:HA | 6:7:313:ARG:HH21 | 1.82 | 0.45 |
| 16:h:38:LYS:HE2 | 49:s:219:TYR:CZ | 2.52 | 0.45 |
| 24:q:251:ASN:HB2 | 24:q:252:PRO:HD3 | 1.99 | 0.45 |
| 26:B:213:ILE:HG23 | 26:B:235:VAL:HA | 1.98 | 0.45 |
| 26:B:257:ARG:HG2 | 26:B:261:TRP:CG | 2.52 | 0.45 |
| 26:B:327:ILE:HG12 | 26:B:347:THR:HG21 | 1.98 | 0.45 |
| 26:B:371:ILE:HD11 | 26:B:435:VAL:HG22 | 1.99 | 0.45 |
| 27:C:236:GLY:O | 27:C:364:VAL:HG23 | 2.17 | 0.45 |
| 39:Q:47:PHE:HB3 | 39:Q:57:ARG:CZ | 2.47 | 0.45 |
| 43:U:138:TYR:OH | 43:U:193:LYS:HA | 2.16 | 0.45 |
| 48:l:241:THR:HG22 | 48:l:299:LYS:HD2 | 1.99 | 0.45 |
| 5:v:322:ASP:C | 3:Af:68:LEU:HD11 | 2.42 | 0.45 |
| 53:G:485:ASP:HA | 53:G:677:GLN:NE2 | 2.32 | 0.45 |
| 3:4:259:CYS:SG | 3:4:260:HIS:N | 2.89 | 0.45 |
| 6:7:183:PHE:CE2 | 56:7:401:HEM:HBC1 | 2.52 | 0.45 |
| 7:8:243:ILE:HD11 | 57:8:401:HEC:HHA | 1.98 | 0.45 |
| 9:a:174:ILE:HG21 | 16:h:20:ILE:HG21 | 1.99 | 0.45 |
| 14:f:33:GLU:OE1 | 14:f:33:GLU:N | 2.48 | 0.45 |
| 17:i:51:ARG:HH11 | 27:C:75:VAL:HG22 | 1.81 | 0.45 |
| 17:i:313:MET:HE2 | 43:U:143:LEU:HD22 | 1.99 | 0.45 |
| 25:r:74:ALA:HB3 | 25:r:75:PRO:HD3 | 1.99 | 0.45 |
| 35:L:326:HIS:H | 35:L:326:HIS:CD2 | 2.35 | 0.45 |
| 48:l:15:LEU:O | 48:l:18:PRO:HD2 | 2.16 | 0.45 |
| 48:l:416:THR:O | 48:l:419:THR:OG1 | 2.26 | 0.45 |
| 48:l:428:PHE:CD2 | 48:l:505:ASN:HB3 | 2.52 | 0.45 |
| 51:u:206:GLU:CD | 51:u:206:GLU:H | 2.24 | 0.45 |
| 5:v:108:GLY:HA3 | 5:v:133:LEU:HD21 | 1.99 | 0.45 |
| 5:v:360:THR:HG22 | 5:v:365:ASN:HB3 | 1.98 | 0.45 |
| 6:w:131:TYR:O | 6:w:134:PRO:HD2 | 2.16 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:x:168:ARG:NH1 | 7:x:171:LYS:HE3 | 2.32 | 0.45 |
| 51:5:304:LEU:HD23 | 51:5:304:LEU:HA | 1.86 | 0.45 |
| 1:0:34:ARG:HD2 | 1:0:78:ARG:NE | 2.31 | 0.44 |
| 5:6:254:ARG:O | 5:6:435:ARG:NH1 | 2.50 | 0.44 |
| 17:i:251:MET:HE2 | 17:i:293:TYR:OH | 2.17 | 0.44 |
| 20:m:51:PHE:CZ | 20:m:55:MET:HE2 | 2.53 | 0.44 |
| 22:o:59:VAL:HG22 | 24:q:423:ILE:HG23 | 1.99 | 0.44 |
| 24:q:77:LEU:O | 24:q:81:GLN:HG3 | 2.17 | 0.44 |
| 26:B:120:GLY:HA2 | 26:B:159:ARG:HH21 | 1.81 | 0.44 |
| 28:D:227:ALA:O | 33:J:116:SER:OG | 2.22 | 0.44 |
| 35:L:87:MET:HA | 35:L:90:ARG:HE | 1.81 | 0.44 |
| 35:L:267:LEU:HG | 35:L:370:VAL:HG21 | 1.99 | 0.44 |
| 36:N:35:LEU:HD23 | 36:N:38:ILE:HD12 | 2.00 | 0.44 |
| 43:U:172:LEU:HD21 | 43:U:186:VAL:HG13 | 1.99 | 0.44 |
| 45:W:129:THR:HG23 | 45:W:132:GLU:H | 1.82 | 0.44 |
| 2:1:34:ARG:HH21 | 4:3:50:GLY:HA3 | 1.83 | 0.44 |
| 17:i:255:PRO:HG3 | 17:i:260:PHE:CD1 | 2.52 | 0.44 |
| 18:j:82:ASN:OD1 | 18:j:82:ASN:N | 2.50 | 0.44 |
| 24:q:1:MET:HE2 | 24:q:111:THR:HG21 | 1.99 | 0.44 |
| 24:q:25:ILE:O | 24:q:29:VAL:HG23 | 2.16 | 0.44 |
| 24:q:306:PRO:HA | 24:q:458:LEU:HD22 | 1.98 | 0.44 |
| 26:B:423:THR:HG21 | 26:B:428:GLY:HA3 | 1.99 | 0.44 |
| 27:C:187:LEU:HD22 | 27:C:213:ARG:HE | 1.82 | 0.44 |
| 33:J:158:LYS:NZ | 53:G:69:LEU:O | 2.35 | 0.44 |
| 35:L:54:PHE:O | 35:L:124:LEU:HB2 | 2.18 | 0.44 |
| 36:N:77:ILE:O | 36:N:81:ILE:HG23 | 2.17 | 0.44 |
| 37:O:112:SER:O | 37:O:116:VAL:HG23 | 2.16 | 0.44 |
| 43:U:66:GLY:O | 43:U:163:ARG:NH2 | 2.43 | 0.44 |
| 48:l:332:HIS:HA | 48:l:335:PHE:CZ | 2.51 | 0.44 |
| 5:v:203:ASP:OD1 | 5:v:203:ASP:N | 2.47 | 0.44 |
| 51:5:407:THR:HB | 51:5:408:PRO:HD3 | 2.00 | 0.44 |
| 3:2:104:ILE:HG23 | 7:x:323:ARG:HE | 1.81 | 0.44 |
| 3:2:134:PHE:CZ | 3:2:138:ILE:HD11 | 2.53 | 0.44 |
| 7:8:214:SER:HB3 | 7:8:237:TYR:CE2 | 2.52 | 0.44 |
| 10:b:86:LEU:HD21 | 48:l:9:LEU:HD12 | 2.00 | 0.44 |
| 11:c:36:MET:HE3 | 11:c:36:MET:HB3 | 1.69 | 0.44 |
| 17:i:61:LEU:O | 17:i:65:THR:HG23 | 2.17 | 0.44 |
| 17:i:75:ILE:HD12 | 19:k:40:LEU:HD22 | 1.99 | 0.44 |
| 17:i:89:MET:HB2 | 17:i:95:MET:HG2 | 1.98 | 0.44 |
| 26:B:126:LYS:HB3 | 26:B:277:ASN:HD21 | 1.81 | 0.44 |
| 27:C:463:VAL:HG13 | 27:C:466:GLU:HB2 | 1.98 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:E:185:MET:HE3 | 29:E:185:MET:HB3 | 1.70 | 0.44 |
| 5:v:138:LEU:HD12 | 5:v:233:VAL:HG22 | 1.99 | 0.44 |
| 5:v:196:ARG:NH2 | 5:v:204:GLN:OE1 | 2.42 | 0.44 |
| 5:v:358:VAL:HG11 | 5:v:431:PHE:CD2 | 2.53 | 0.44 |
| 51:5:253:LEU:HD12 | 51:5:253:LEU:HA | 1.81 | 0.44 |
| 53:G:325:ARG:HE | 53:G:325:ARG:HB2 | 1.53 | 0.44 |
| 5:6:313:VAL:HG11 | 5:6:350:VAL:HG13 | 1.99 | 0.44 |
| 12:d:40:LEU:HD23 | 12:d:40:LEU:HA | 1.87 | 0.44 |
| 12:d:110:LEU:HD21 | 48:l:204:LEU:HD21 | 2.00 | 0.44 |
| 20:m:57:PHE:HD1 | 20:m:57:PHE:HA | 1.72 | 0.44 |
| 22:o:87:SER:HA | 48:l:557:TRP:HZ2 | 1.81 | 0.44 |
| 28:D:219:VAL:HG21 | 32:I:115:PRO:HG3 | 2.00 | 0.44 |
| 29:E:42:ARG:HB2 | 29:E:42:ARG:HH11 | 1.83 | 0.44 |
| 37:O:110:LEU:HD13 | 37:O:114:ASP:HB3 | 1.98 | 0.44 |
| 37:O:147:TYR:O | 37:O:151:LYS:HG2 | 2.17 | 0.44 |
| 43:U:149:LEU:HD13 | 43:U:296:LEU:HD21 | 1.99 | 0.44 |
| 5:v:70:ARG:HG3 | 5:v:185:ALA:HB1 | 2.00 | 0.44 |
| 56:w:402:HEM:HBB2 | 56:w:402:HEM:HMB1 | 2.00 | 0.44 |
| 53:G:305:PRO:HA | 53:G:585:PRO:HD3 | 1.99 | 0.44 |
| 5:6:49:ILE:HB | 5:6:230:LEU:HD23 | 2.00 | 0.44 |
| 6:7:8:HIS:ND1 | 6:7:11:MET:HG2 | 2.32 | 0.44 |
| 10:b:28:LEU:HD11 | 23:p:157:TYR:HD2 | 1.82 | 0.44 |
| 25:r:162:LEU:HA | 25:r:165:LEU:HD13 | 1.99 | 0.44 |
| 26:B:111:LYS:HB2 | 26:B:151:ALA:HA | 1.99 | 0.44 |
| 26:B:128:ARG:HG2 | 26:B:132:ARG:NH1 | 2.31 | 0.44 |
| 35:L:129:TRP:CZ3 | 35:L:131:THR:HG22 | 2.53 | 0.44 |
| 6:w:310:SER:HB2 | 6:w:370:SER:HB3 | 1.99 | 0.44 |
| 51:5:310:ILE:HG21 | 51:5:379:LEU:HD21 | 1.99 | 0.44 |
| 6:7:131:TYR:O | 6:7:134:PRO:HD2 | 2.18 | 0.44 |
| 6:7:275:LEU:HD23 | 6:7:275:LEU:HA | 1.82 | 0.44 |
| 57:8:401:HEC:HBD1 | 57:8:401:HEC:CHA | 2.48 | 0.44 |
| 16:h:82:GLN:OE1 | 45:W:101:VAL:HG23 | 2.17 | 0.44 |
| 17:i:203:LEU:HD21 | 17:i:261:MET:HE2 | 1.99 | 0.44 |
| 20:m:3:MET:HE3 | 20:m:125:TRP:NE1 | 2.32 | 0.44 |
| 20:m:56:VAL:O | 20:m:60:TYR:HB3 | 2.17 | 0.44 |
| 23:p:59:LEU:HD21 | 37:X:112:SER:HB2 | 1.99 | 0.44 |
| 23:p:66:LEU:HB3 | 37:X:120:MET:HE1 | 1.99 | 0.44 |
| 24:q:76:MET:SD | 24:q:230:VAL:HG13 | 2.58 | 0.44 |
| 24:q:231:LEU:O | 24:q:236:LEU:HG | 2.17 | 0.44 |
| 24:q:329:LEU:O | 24:q:332:THR:OG1 | 2.35 | 0.44 |
| 27:C:103:LEU:HD11 | 27:C:115:CYS:SG | 2.58 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:E:223:PHE:H | 29:E:226:GLU:CD | 2.26 | 0.44 |
| 35:L:216:ARG:HB2 | 35:L:276:PHE:CE2 | 2.53 | 0.44 |
| 47:Z:46:GLU:HG2 | 47:Z:50:GLU:OE2 | 2.18 | 0.44 |
| 50:t:34:ARG:NH1 | 50:t:104:ARG:HH12 | 2.14 | 0.44 |
| 50:t:99:MET:HE2 | 50:t:99:MET:HB3 | 1.87 | 0.44 |
| 7:x:196:PRO:HG2 | 57:x:401:HEC:HBA1 | 1.99 | 0.44 |
| 51:5:207:ASN:O | 51:5:211:LEU:HG | 2.17 | 0.44 |
| 51:5:473:SER:HA | 51:5:476:PHE:CE1 | 2.53 | 0.44 |
| 53:G:68:ARG:NH1 | 53:G:284:GLU:OE2 | 2.51 | 0.44 |
| 53:G:600:GLU:OE1 | 53:G:602:ARG:NH2 | 2.48 | 0.44 |
| 3:4:161:MET:HE2 | 3:4:161:MET:HB3 | 1.82 | 0.44 |
| 6:7:45:ILE:HA | 56:7:401:HEM:HMC2 | 2.00 | 0.44 |
| 6:7:47:THR:HB | 6:7:83:HIS:HD1 | 1.83 | 0.44 |
| 7:8:249:ILE:O | 7:8:264:MET:HG3 | 2.17 | 0.44 |
| 11:c:88:PRO:HA | 11:c:98:ARG:HD3 | 2.00 | 0.44 |
| 11:c:184:TYR:HB3 | 50:t:34:ARG:HB3 | 1.98 | 0.44 |
| 26:B:52:ARG:HB3 | 26:B:54:LYS:NZ | 2.32 | 0.44 |
| 26:B:62:TRP:CZ3 | 26:B:181:LEU:HB3 | 2.53 | 0.44 |
| 31:H:211:TYR:CE2 | 54:M:39:PRO:HG3 | 2.52 | 0.44 |
| 35:L:240:VAL:HG13 | 35:L:260:PHE:HD2 | 1.83 | 0.44 |
| 43:U:244:LYS:HA | 43:U:248:LEU:HD12 | 1.99 | 0.44 |
| 51:u:397:ASN:ND2 | 5:v:107:GLY:O | 2.51 | 0.44 |
| 53:G:217:GLU:HG2 | 53:G:412:PRO:HB3 | 1.99 | 0.44 |
| 3:4:177:LEU:O | 3:4:178:SER:OG | 2.32 | 0.44 |
| 5:6:106:VAL:HG21 | 5:6:133:LEU:HD13 | 1.99 | 0.44 |
| 6:7:223:TYR:O | 6:7:226:ILE:HG22 | 2.17 | 0.44 |
| 12:d:80:LYS:HD2 | 24:q:182:TRP:CE2 | 2.53 | 0.44 |
| 20:m:103:MET:N | 20:m:103:MET:SD | 2.91 | 0.44 |
| 24:q:375:LEU:HD11 | 48:l:141:PHE:HE2 | 1.83 | 0.44 |
| 26:B:199:ARG:NH1 | 29:E:88:ARG:HH12 | 2.16 | 0.44 |
| 27:C:140:PRO:HB2 | 32:I:142:TYR:CE2 | 2.53 | 0.44 |
| 27:C:144:ARG:NH1 | 27:C:229:HIS:HB3 | 2.33 | 0.44 |
| 39:Q:88:LYS:HD3 | 39:Q:132:PHE:HB3 | 2.00 | 0.44 |
| 7:x:123:SER:O | 7:x:179:PRO:HB3 | 2.18 | 0.44 |
| 51:5:362:ASN:ND2 | 51:5:363:MET:SD | 2.90 | 0.44 |
| 53:G:498:GLN:HG3 | 53:G:499:ASN:N | 2.32 | 0.44 |
| 1:0:71:LEU:HG | 1:0:75:LEU:HD12 | 2.00 | 0.44 |
| 6:7:173:ALA:O | 6:7:177:ARG:HG3 | 2.17 | 0.44 |
| 6:7:272:TRP:HA | 6:7:275:LEU:HD12 | 2.00 | 0.44 |
| 7:8:294:LEU:HD23 | 7:8:294:LEU:HA | 1.88 | 0.44 |
| 16:h:47:ILE:HA | 49:s:228:ASN:HD21 | 1.83 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:i:88:LYS:HD2 | 17:i:148:SER:HB3 | 1.99 | 0.44 |
| 17:i:231:SER:O | 17:i:234:TRP:HD1 | 1.99 | 0.44 |
| 20:m:82:VAL:HG12 | 20:m:83:TRP:H | 1.82 | 0.44 |
| 20:m:110:GLU:O | 20:m:111:GLU:C | 2.61 | 0.44 |
| 24:q:357:THR:O | 24:q:361:MET:HG3 | 2.18 | 0.44 |
| 27:C:284:VAL:HG22 | 27:C:335:ARG:NH2 | 2.33 | 0.44 |
| 29:E:177:LEU:HD12 | 29:E:185:MET:SD | 2.58 | 0.44 |
| 34:K:110:TRP:CZ3 | 34:K:114:LYS:HE2 | 2.53 | 0.44 |
| 50:t:29:TYR:HD1 | 50:t:29:TYR:HA | 1.69 | 0.44 |
| 5:v:130:ILE:HD13 | 5:v:130:ILE:HA | 1.85 | 0.44 |
| 6:w:31:TRP:NE1 | 56:w:401:HEM:O2D | 2.51 | 0.44 |
| 7:x:220:CYS:SG | 7:x:221:GLU:N | 2.91 | 0.44 |
| 51:5:304:LEU:HD13 | 51:5:354:LEU:HD22 | 2.00 | 0.44 |
| 53:G:338:VAL:HG23 | 53:G:363:SER:HB2 | 2.00 | 0.44 |
| 53:G:562:LYS:HA | 53:G:562:LYS:HD3 | 1.85 | 0.44 |
| 1:0:65:GLU:HB3 | 52:z:78:TYR:CG | 2.52 | 0.43 |
| 6:7:221:HIS:HB3 | 6:7:222:PRO:HD3 | 1.99 | 0.43 |
| 10:b:73:THR:HA | 10:b:77:ILE:HD12 | 2.00 | 0.43 |
| 10:b:74:HIS:O | 10:b:78:PRO:HG2 | 2.18 | 0.43 |
| 11:c:62:TYR:CE2 | 11:c:64:PRO:HD3 | 2.53 | 0.43 |
| 11:c:186:ILE:HB | 50:t:97:LYS:HG3 | 1.99 | 0.43 |
| 24:q:313:THR:HA | 24:q:316:MET:HE2 | 2.00 | 0.43 |
| 25:r:77:LEU:HD22 | 25:r:118:TRP:CZ3 | 2.53 | 0.43 |
| 27:C:205:PRO:HB3 | 27:C:264:LEU:HD12 | 1.99 | 0.43 |
| 29:E:203:GLU:O | 29:E:207:GLU:HG3 | 2.17 | 0.43 |
| 31:H:63:TRP:HB3 | 31:H:66:LEU:HD12 | 1.99 | 0.43 |
| 31:H:65:GLU:OE1 | 31:H:65:GLU:N | 2.51 | 0.43 |
| 37:O:100:VAL:HG12 | 37:O:142:GLN:HB2 | 1.99 | 0.43 |
| 37:O:120:MET:HA | 37:O:123:GLU:HG2 | 2.00 | 0.43 |
| 38:P:68:ARG:HD2 | 53:G:359:ASN:ND2 | 2.33 | 0.43 |
| 43:U:245:LYS:HB2 | 43:U:245:LYS:HE3 | 1.85 | 0.43 |
| 48:l:79:SER:OG | 48:l:135:ASN:HB3 | 2.18 | 0.43 |
| 3:2:252:PHE:CZ | 3:2:271:ARG:HB2 | 2.53 | 0.43 |
| 5:6:79:THR:HG23 | 5:6:205:LEU:HD23 | 2.00 | 0.43 |
| 5:6:438:MET:HE2 | 5:6:440:ALA:HB2 | 1.99 | 0.43 |
| 7:8:316:LYS:HA | 7:8:316:LYS:HD3 | 1.79 | 0.43 |
| 25:r:280:PHE:CZ | 27:C:273:ILE:HG12 | 2.53 | 0.43 |
| 37:X:120:MET:O | 37:X:123:GLU:HG2 | 2.18 | 0.43 |
| 6:w:8:HIS:O | 6:w:12:LYS:N | 2.46 | 0.43 |
| 1:Ab:40:ILE:HG22 | 1:Ab:42:LYS:HD2 | 2.01 | 0.43 |
| 10:b:22:TRP:O | 10:b:26:GLN:HG2 | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:b:71:ALA:O | 10:b:75:VAL:HG22 | 2.18 | 0.43 |
| 12:d:82:ILE:H | 12:d:82:ILE:HG13 | 1.46 | 0.43 |
| 14:f:31:ILE:HG13 | 14:f:32:ARG:N | 2.33 | 0.43 |
| 15:g:98:SER:OG | 15:g:99:HIS:ND1 | 2.49 | 0.43 |
| 19:k:64:LEU:HD12 | 19:k:64:LEU:HA | 1.83 | 0.43 |
| 21:n:47:ARG:HH22 | 21:n:53:GLU:CD | 2.26 | 0.43 |
| 25:r:92:PRO:HB3 | 25:r:255:TYR:CD1 | 2.53 | 0.43 |
| 26:B:194:ASP:OD2 | 40:R:98:MET:HG2 | 2.17 | 0.43 |
| 27:C:296:GLY:O | 27:C:300:ARG:HG3 | 2.18 | 0.43 |
| 29:E:219:ARG:HD2 | 29:E:219:ARG:HA | 1.78 | 0.43 |
| 36:N:88:LEU:HD22 | 36:N:92:ARG:NH1 | 2.33 | 0.43 |
| 43:U:211:VAL:HG22 | 43:U:262:ALA:HB2 | 1.99 | 0.43 |
| 48:l:124:PHE:CD2 | 48:l:247:LEU:HD22 | 2.53 | 0.43 |
| 49:s:208:VAL:HG12 | 49:s:210:THR:HG23 | 2.00 | 0.43 |
| 5:v:63:LEU:HD23 | 5:v:141:THR:HG21 | 1.99 | 0.43 |
| 3:2:256:TYR:HE1 | 3:2:261:GLY:HA2 | 1.82 | 0.43 |
| 5:6:359:LYS:HA | 5:6:432:VAL:HG21 | 2.00 | 0.43 |
| 5:6:371:VAL:HG12 | 5:6:375:LYS:HE3 | 2.01 | 0.43 |
| 5:6:383:LEU:HD13 | 51:5:67:PRO:HB2 | 2.00 | 0.43 |
| 9:a:70:LEU:HD22 | 13:e:87:MET:HE1 | 2.01 | 0.43 |
| 17:i:273:ASN:HD21 | 44:V:141:VAL:HG23 | 1.84 | 0.43 |
| 24:q:299:VAL:O | 24:q:303:ILE:HG13 | 2.19 | 0.43 |
| 26:B:157:TYR:CB | 26:B:212:LEU:HD21 | 2.48 | 0.43 |
| 48:l:190:LEU:HD22 | 48:l:196:TRP:CZ2 | 2.54 | 0.43 |
| 5:v:40:PHE:CE1 | 5:v:406:TYR:HB2 | 2.53 | 0.43 |
| 1:Ab:37:CYS:O | 1:Ab:40:ILE:N | 2.51 | 0.43 |
| 10:b:77:ILE:HB | 10:b:78:PRO:HD3 | 2.00 | 0.43 |
| 17:i:139:LEU:HD23 | 17:i:139:LEU:HA | 1.86 | 0.43 |
| 17:i:291:TYR:HA | 24:q:151:PHE:HZ | 1.83 | 0.43 |
| 20:m:110:GLU:O | 20:m:112:GLU:N | 2.51 | 0.43 |
| 25:r:233:MET:HE3 | 25:r:233:MET:HB3 | 1.74 | 0.43 |
| 26:B:62:TRP:HE1 | 26:B:136:HIS:HB3 | 1.84 | 0.43 |
| 35:L:129:TRP:H | 35:L:129:TRP:CD1 | 2.37 | 0.43 |
| 48:l:37:LYS:NZ | 48:l:98:TRP:HE1 | 2.16 | 0.43 |
| 7:x:228:LEU:HD11 | 7:x:234:PHE:HB2 | 1.99 | 0.43 |
| 7:x:311:LYS:HD3 | 7:x:311:LYS:HA | 1.86 | 0.43 |
| 51:5:318:TYR:CD1 | 3:Ae:55:GLY:HA2 | 2.54 | 0.43 |
| 3:2:278:ASN:OD1 | 3:2:278:ASN:N | 2.50 | 0.43 |
| 20:m:126:VAL:HG13 | 45:W:122:GLY:HA3 | 2.00 | 0.43 |
| 24:q:31:SER:HB2 | 24:q:74:PRO:HG3 | 2.01 | 0.43 |
| 26:B:115:VAL:HG11 | 26:B:138:LEU:HD11 | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:B:226:LYS:O | 26:B:227:PRO:C | 2.62 | 0.43 |
| 26:B:292:MET:HE3 | 26:B:292:MET:HB3 | 1.84 | 0.43 |
| 27:C:309:ARG:HG3 | 27:C:407:GLU:HB3 | 2.01 | 0.43 |
| 37:X:133:ILE:HD13 | 37:X:133:ILE:H | 1.82 | 0.43 |
| 51:u:317:THR:HA | 5:v:157:GLN:NE2 | 2.34 | 0.43 |
| 51:u:406:THR:HG1 | 5:v:387:GLU:CD | 2.25 | 0.43 |
| 51:5:225:LYS:O | 51:5:229:MET:HG3 | 2.19 | 0.43 |
| 51:5:373:GLN:O | 51:5:377:MET:HG2 | 2.18 | 0.43 |
| 53:G:76:ARG:O | 53:G:116:VAL:HG21 | 2.18 | 0.43 |
| 5:6:301:ARG:HH22 | 51:5:94:GLU:HG2 | 1.83 | 0.43 |
| 7:8:128:MET:HE3 | 7:8:198:LEU:HB3 | 2.01 | 0.43 |
| 9:a:160:MET:HE2 | 15:g:95:TYR:CD1 | 2.54 | 0.43 |
| 18:j:87:MET:HE1 | 25:r:309:ILE:HD11 | 2.01 | 0.43 |
| 19:k:23:ARG:HD3 | 20:m:23:LYS:HB2 | 2.00 | 0.43 |
| 20:m:63:GLY:O | 20:m:66:VAL:HG12 | 2.18 | 0.43 |
| 20:m:66:VAL:HG23 | 25:r:114:TYR:CZ | 2.54 | 0.43 |
| 24:q:336:ARG:NH2 | 24:q:429:SER:HA | 2.33 | 0.43 |
| 26:B:371:ILE:CD1 | 26:B:396:MET:HG3 | 2.47 | 0.43 |
| 31:H:98:ARG:HD2 | 31:H:156:GLY:CA | 2.49 | 0.43 |
| 31:H:196:LYS:HD3 | 34:K:113:HIS:CE1 | 2.54 | 0.43 |
| 35:L:120:VAL:HG11 | 35:L:248:ILE:HD13 | 2.01 | 0.43 |
| 35:L:306:GLU:O | 35:L:308:TRP:N | 2.45 | 0.43 |
| 38:P:85:ASP:OD1 | 38:P:85:ASP:N | 2.41 | 0.43 |
| 51:u:407:THR:HB | 51:u:408:PRO:HD3 | 1.99 | 0.43 |
| 7:x:205:ARG:NE | 57:x:401:HEC:O2A | 2.43 | 0.43 |
| 3:2:166:ASP:OD1 | 3:2:167:VAL:N | 2.52 | 0.43 |
| 3:4:257:CYS:SG | 3:4:259:CYS:SG | 3.17 | 0.43 |
| 5:6:65:ILE:HG21 | 5:6:213:PHE:CD1 | 2.53 | 0.43 |
| 16:h:85:LYS:O | 16:h:89:GLU:HG2 | 2.19 | 0.43 |
| 17:i:190:MET:HG2 | 17:i:204:ASN:HB3 | 2.01 | 0.43 |
| 17:i:337:LEU:C | 17:i:339:MET:H | 2.27 | 0.43 |
| 20:m:55:MET:O | 20:m:59:ILE:HG12 | 2.18 | 0.43 |
| 22:o:10:ARG:NH2 | 48:l:539:TYR:OH | 2.51 | 0.43 |
| 23:p:162:ALA:O | 23:p:166:GLN:HG3 | 2.18 | 0.43 |
| 24:q:10:MET:O | 24:q:13:PRO:HD2 | 2.19 | 0.43 |
| 24:q:14:MET:HE3 | 24:q:14:MET:HB3 | 1.80 | 0.43 |
| 24:q:231:LEU:HA | 24:q:235:LEU:HB2 | 2.01 | 0.43 |
| 26:B:325:PRO:HD2 | 26:B:347:THR:HA | 1.99 | 0.43 |
| 27:C:63:GLU:H | 27:C:63:GLU:CD | 2.26 | 0.43 |
| 27:C:345:GLN:O | 27:C:349:ILE:HG13 | 2.18 | 0.43 |
| 28:D:149:GLU:HG3 | 33:J:61:ILE:HD12 | 2.01 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:E:224:SER:C | 29:E:226:GLU:H | 2.27 | 0.43 |
| 30:F:30:ARG:O | 30:F:38:VAL:HG12 | 2.19 | 0.43 |
| 37:O:110:LEU:HB2 | 37:O:114:ASP:CB | 2.48 | 0.43 |
| 5:v:261:GLN:NE2 | 5:v:443:ASN:O | 2.48 | 0.43 |
| 51:5:343:THR:HG22 | 51:5:356:ALA:HB2 | 1.99 | 0.43 |
| 3:4:212:GLU:HG2 | 3:4:214:SER:H | 1.82 | 0.43 |
| 12:d:79:GLU:C | 12:d:81:ASP:H | 2.27 | 0.43 |
| 12:d:79:GLU:C | 12:d:81:ASP:N | 2.76 | 0.43 |
| 14:f:47:THR:HG23 | 15:g:65:LEU:HD22 | 2.01 | 0.43 |
| 16:h:81:ARG:HD2 | 20:m:111:GLU:CG | 2.40 | 0.43 |
| 18:j:87:MET:HE3 | 18:j:87:MET:HB3 | 1.92 | 0.43 |
| 24:q:235:LEU:HD23 | 24:q:235:LEU:HA | 1.84 | 0.43 |
| 26:B:225:LEU:HB2 | 33:J:160:TYR:CE2 | 2.54 | 0.43 |
| 27:C:62:LYS:HE3 | 27:C:62:LYS:HB2 | 1.78 | 0.43 |
| 29:E:149:LEU:HG | 29:E:153:GLN:HE21 | 1.82 | 0.43 |
| 31:H:116:CYS:SG | 59:H:302:SF4:S2 | 3.11 | 0.43 |
| 38:P:62:GLN:HB2 | 38:P:80:ASN:HB2 | 2.01 | 0.43 |
| 38:P:65:LEU:HB2 | 38:P:79:LEU:HD11 | 2.01 | 0.43 |
| 37:X:82:ARG:HH21 | 37:X:125:GLU:CD | 2.27 | 0.43 |
| 46:Y:88:ASP:N | 46:Y:89:PRO:HD2 | 2.34 | 0.43 |
| 49:s:121:MET:HE2 | 49:s:121:MET:HA | 2.00 | 0.43 |
| 51:u:75:ILE:HG12 | 51:u:229:MET:HG2 | 2.01 | 0.43 |
| 51:u:453:CYS:HA | 51:u:472:ARG:HD3 | 1.99 | 0.43 |
| 53:G:587:ALA:O | 53:G:592:LYS:NZ | 2.49 | 0.43 |
| 5:6:149:TRP:CE2 | 8:y:50:ARG:HD3 | 2.54 | 0.43 |
| 14:f:65:ASP:HB3 | 15:g:25:PRO:HB3 | 2.01 | 0.43 |
| 26:B:424:ILE:HG22 | 53:G:76:ARG:CZ | 2.49 | 0.43 |
| 26:B:437:GLY:HA2 | 26:B:440:ARG:NH2 | 2.34 | 0.43 |
| 27:C:229:HIS:NE2 | 32:I:71:CYS:HB3 | 2.34 | 0.43 |
| 27:C:259:PHE:CD1 | 54:M:23:LYS:HD2 | 2.54 | 0.43 |
| 27:C:448:HIS:HB3 | 27:C:452:ASP:HB2 | 2.01 | 0.43 |
| 48:l:88:MET:O | 48:l:91:PRO:HD2 | 2.19 | 0.43 |
| 7:8:313:SER:HA | 7:8:316:LYS:HB2 | 2.00 | 0.42 |
| 10:b:16:ARG:HD3 | 37:X:150:ASP:OD2 | 2.18 | 0.42 |
| 10:b:93:LYS:HD2 | 10:b:94:PRO:HD2 | 2.00 | 0.42 |
| 12:d:113:CYS:SG | 12:d:116:ARG:NH2 | 2.92 | 0.42 |
| 17:i:317:PHE:HZ | 43:U:143:LEU:HD21 | 1.84 | 0.42 |
| 21:n:10:ASP:HB2 | 24:q:19:LYS:HD2 | 2.01 | 0.42 |
| 24:q:69:THR:HG22 | 24:q:234:VAL:HG21 | 2.00 | 0.42 |
| 26:B:398:ARG:HH22 | 26:B:408:GLU:CD | 2.27 | 0.42 |
| 28:D:125:ARG:NH2 | 28:D:199:ARG:O | 2.52 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:D:184:LEU:HA | 28:D:184:LEU:HD23 | 1.80 | 0.42 |
| 31:H:180:HIS:CE1 | 35:L:95:LEU:HD21 | 2.54 | 0.42 |
| 43:U:61:VAL:HG12 | 43:U:203:PRO:HB3 | 2.01 | 0.42 |
| 7:x:203:ARG:HG3 | 7:x:279:SER:HB3 | 1.99 | 0.42 |
| 5:6:317:VAL:HG13 | 5:6:319:GLN:NE2 | 2.35 | 0.42 |
| 6:7:27:ILE:HG12 | 6:7:224:TYR:CE1 | 2.54 | 0.42 |
| 6:7:207:ASN:ND2 | 6:7:211:ILE:O | 2.48 | 0.42 |
| 15:g:51:ARG:HD3 | 17:i:322:GLN:HG3 | 1.99 | 0.42 |
| 30:F:59:GLN:HG2 | 34:K:122:GLN:HA | 2.01 | 0.42 |
| 31:H:205:ILE:O | 31:H:209:TYR:HB3 | 2.19 | 0.42 |
| 35:L:355:ARG:HA | 35:L:355:ARG:HD2 | 1.61 | 0.42 |
| 38:P:16:LEU:HD11 | 38:P:94:VAL:HG12 | 2.01 | 0.42 |
| 43:U:256:GLU:OE2 | 43:U:278:LEU:HB3 | 2.19 | 0.42 |
| 37:X:140:CYS:HB3 | 37:X:143:GLU:HG2 | 1.99 | 0.42 |
| 48:l:59:GLN:HE22 | 48:l:61:MET:HG3 | 1.84 | 0.42 |
| 48:l:241:THR:OG1 | 48:l:242:PRO:HD3 | 2.19 | 0.42 |
| 51:u:119:HIS:ND1 | 5:v:384:MET:HE1 | 2.33 | 0.42 |
| 6:w:47:THR:HG23 | 6:w:79:ILE:CG2 | 2.49 | 0.42 |
| 51:5:158:ASP:O | 51:5:162:GLU:HG2 | 2.18 | 0.42 |
| 53:G:310:GLU:H | 53:G:310:GLU:HG3 | 1.57 | 0.42 |
| 53:G:598:ASN:OD1 | 53:G:602:ARG:N | 2.49 | 0.42 |
| 3:4:189:LYS:HE2 | 3:4:189:LYS:HB2 | 1.89 | 0.42 |
| 17:i:68:MET:HE2 | 19:k:36:MET:HB3 | 2.00 | 0.42 |
| 17:i:231:SER:HB2 | 17:i:305:PHE:HB2 | 2.01 | 0.42 |
| 25:r:179:TRP:CG | 25:r:180:PRO:HD3 | 2.54 | 0.42 |
| 26:B:328:PRO:HD3 | 26:B:441:HIS:CG | 2.54 | 0.42 |
| 26:B:340:ASP:OD1 | 26:B:340:ASP:N | 2.51 | 0.42 |
| 58:B:501:FMN:HM81 | 58:B:501:FMN:HM73 | 1.84 | 0.42 |
| 27:C:168:GLN:HB2 | 28:D:48:ARG:HA | 2.01 | 0.42 |
| 28:D:44:ARG:NH2 | 54:M:62:GLU:OE1 | 2.45 | 0.42 |
| 31:H:196:LYS:HD2 | 31:H:197:TRP:NE1 | 2.34 | 0.42 |
| 38:P:17:ARG:HB3 | 38:P:68:ARG:HH21 | 1.84 | 0.42 |
| 45:W:63:GLU:OE2 | 49:s:196:ARG:NH1 | 2.46 | 0.42 |
| 37:X:128:PHE:HZ | 37:X:148:ILE:HG12 | 1.84 | 0.42 |
| 48:l:60:GLU:OE1 | 48:l:84:TYR:N | 2.51 | 0.42 |
| 48:l:76:LEU:HD23 | 48:l:76:LEU:HA | 1.91 | 0.42 |
| 48:l:415:ALA:O | 48:l:419:THR:HG23 | 2.19 | 0.42 |
| 5:v:352:LYS:HD2 | 5:v:352:LYS:HA | 1.84 | 0.42 |
| 52:z:25:ARG:NH1 | 52:z:28:PRO:HA | 2.34 | 0.42 |
| 2:Ac:23:LEU:HD22 | 4:Ad:23:MET:HE3 | 2.01 | 0.42 |
| 2:1:29:ALA:HA | 3:2:144:VAL:HG13 | 2.01 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3:47:TYR:N | 4:3:49:ASN:OD1 | 2.52 | 0.42 |
| 5:6:259:ARG:NH2 | 5:6:447:THR:O | 2.52 | 0.42 |
| 6:7:185:LEU:HD23 | 6:7:185:LEU:HA | 1.73 | 0.42 |
| 7:8:216:LEU:HB3 | 7:8:249:ILE:CD1 | 2.47 | 0.42 |
| 18:j:77:TRP:CH2 | 25:r:100:LEU:HD21 | 2.55 | 0.42 |
| 25:r:195:ARG:HD3 | 25:r:231:ILE:HD11 | 2.01 | 0.42 |
| 26:B:56:ALA:HB1 | 26:B:61:ASP:HB2 | 2.02 | 0.42 |
| 27:C:190:ILE:HG21 | 27:C:213:ARG:HG3 | 2.01 | 0.42 |
| 36:N:78:GLU:O | 36:N:81:ILE:HG12 | 2.18 | 0.42 |
| 37:O:114:ASP:O | 37:O:118:ILE:HG23 | 2.18 | 0.42 |
| 51:5:405:GLY:O | 51:5:409:VAL:HG23 | 2.19 | 0.42 |
| 51:5:418:LEU:HD23 | 51:5:418:LEU:HA | 1.84 | 0.42 |
| 2:Ac:53:TRP:O | 2:Ac:57:LYS:N | 2.51 | 0.42 |
| 1:0:65:GLU:HB3 | 52:z:78:TYR:CD1 | 2.54 | 0.42 |
| 3:2:226:VAL:HA | 3:2:284:TYR:OH | 2.19 | 0.42 |
| 5:6:298:HIS:HB2 | 51:5:114:GLU:HG2 | 2.01 | 0.42 |
| 20:m:52:LEU:O | 20:m:55:MET:HB2 | 2.19 | 0.42 |
| 20:m:114:GLU:HA | 20:m:117:PHE:O | 2.19 | 0.42 |
| 23:p:54:HIS:CD2 | 23:p:106:LEU:HD12 | 2.54 | 0.42 |
| 25:r:89:LEU:HD22 | 25:r:240:ILE:HD12 | 2.01 | 0.42 |
| 26:B:35:LEU:HD11 | 26:B:39:ASP:HB2 | 2.02 | 0.42 |
| 26:B:316:ALA:HA | 26:B:327:ILE:O | 2.19 | 0.42 |
| 27:C:146:ASP:HB2 | 27:C:466:GLU:HG3 | 2.00 | 0.42 |
| 35:L:175:TYR:CE1 | 35:L:316:ARG:HD2 | 2.55 | 0.42 |
| 35:L:241:SER:O | 35:L:245:ILE:HG12 | 2.20 | 0.42 |
| 35:L:311:ARG:O | 35:L:315:GLU:HG2 | 2.18 | 0.42 |
| 43:U:131:TYR:CG | 43:U:185:CYS:HB3 | 2.54 | 0.42 |
| 48:l:63:ILE:O | 48:l:79:SER:HA | 2.20 | 0.42 |
| 52:z:4:GLU:O | 52:z:8:LEU:HG | 2.20 | 0.42 |
| 51:5:276:ARG:O | 52:Aa:15:ILE:HA | 2.20 | 0.42 |
| 3:2:237:VAL:HA | 3:2:243:CYS:O | 2.19 | 0.42 |
| 5:6:123:VAL:HB | 5:6:133:LEU:HD23 | 2.01 | 0.42 |
| 9:a:64:ASP:OD1 | 9:a:64:ASP:N | 2.50 | 0.42 |
| 17:i:145:ILE:O | 17:i:149:ILE:HG13 | 2.19 | 0.42 |
| 17:i:313:MET:HE3 | 43:U:96:ALA:HB2 | 2.01 | 0.42 |
| 18:j:68:GLU:HG3 | 20:m:161:LEU:HD13 | 2.00 | 0.42 |
| 19:k:26:LEU:O | 19:k:29:SER:OG | 2.28 | 0.42 |
| 25:r:146:LEU:HG | 25:r:185:TRP:CZ3 | 2.54 | 0.42 |
| 26:B:63:TYR:CE2 | 29:E:245:VAL:HG21 | 2.54 | 0.42 |
| 26:B:88:ARG:HD2 | 26:B:274:LYS:HE2 | 2.02 | 0.42 |
| 26:B:230:PRO:HA | 26:B:233:VAL:O | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 35:L:79:TYR:CZ | 35:L:102:GLU:HB2 | 2.54 | 0.42 |
| 39:Q:124:LYS:HE3 | 39:Q:129:ILE:HD13 | 2.00 | 0.42 |
| 48:l:291:CYS:O | 48:l:295:GLN:HG2 | 2.19 | 0.42 |
| 48:l:383:MET:SD | 48:l:384:PRO:HD2 | 2.59 | 0.42 |
| 5:v:300:LYS:HG2 | 5:v:301:ARG:HG3 | 2.01 | 0.42 |
| 5:v:326:PHE:CE2 | 3:Af:65:SER:HB2 | 2.55 | 0.42 |
| 6:7:237:LEU:HD13 | 7:8:297:MET:HG2 | 2.01 | 0.42 |
| 6:7:327:MET:HA | 52:Aa:52:PRO:HB3 | 2.02 | 0.42 |
| 7:8:120:GLN:NE2 | 7:8:254:LEU:HB2 | 2.35 | 0.42 |
| 7:8:245:MET:HB2 | 7:8:245:MET:HE3 | 1.54 | 0.42 |
| 9:a:102:PRO:HG2 | 9:a:105:TYR:HB3 | 2.02 | 0.42 |
| 15:g:33:LEU:HD12 | 15:g:33:LEU:HA | 1.83 | 0.42 |
| 18:j:16:LEU:O | 18:j:20:ILE:HG13 | 2.19 | 0.42 |
| 26:B:170:GLN:OE1 | 26:B:197:VAL:HB | 2.20 | 0.42 |
| 27:C:348:ARG:HB2 | 45:W:21:TYR:CD2 | 2.54 | 0.42 |
| 29:E:56:THR:OG1 | 29:E:58:GLU:HG3 | 2.19 | 0.42 |
| 31:H:173:PHE:CE1 | 32:I:171:GLU:HB3 | 2.55 | 0.42 |
| 32:I:70:ALA:H | 32:I:107:GLY:HA3 | 1.85 | 0.42 |
| 37:O:104:PHE:CE1 | 37:O:141:PRO:HG3 | 2.55 | 0.42 |
| 37:O:104:PHE:HD1 | 37:O:108:LEU:HD12 | 1.84 | 0.42 |
| 44:V:118:MET:HE3 | 44:V:118:MET:HB2 | 1.95 | 0.42 |
| 48:l:264:TYR:N | 48:l:265:PRO:HD2 | 2.35 | 0.42 |
| 49:s:180:GLN:HA | 49:s:183:LYS:HD3 | 2.02 | 0.42 |
| 6:w:138:MET:HE3 | 6:w:252:ASP:CG | 2.45 | 0.42 |
| 1:0:83:ALA:HB2 | 7:x:93:PRO:HB2 | 2.00 | 0.42 |
| 5:6:55:TYR:HA | 5:6:127:ARG:NH1 | 2.34 | 0.42 |
| 10:b:93:LYS:HB3 | 10:b:96:THR:HG23 | 2.01 | 0.42 |
| 20:m:60:TYR:HA | 20:m:64:MET:CG | 2.50 | 0.42 |
| 27:C:306:TRP:CE3 | 27:C:311:THR:HG21 | 2.55 | 0.42 |
| 27:C:410:LYS:HZ2 | 27:C:461:ASP:HB2 | 1.83 | 0.42 |
| 28:D:114:LEU:HB3 | 28:D:166:TYR:HB3 | 2.02 | 0.42 |
| 29:E:111:ARG:HD2 | 33:J:173:SER:HB2 | 2.02 | 0.42 |
| 33:J:84:ARG:NH2 | 33:J:88:GLN:O | 2.45 | 0.42 |
| 43:U:223:LYS:HZ1 | 43:U:228:GLU:CD | 2.27 | 0.42 |
| 37:X:122:MET:HG3 | 37:X:144:ILE:HD13 | 2.01 | 0.42 |
| 49:s:87:LEU:O | 49:s:91:LYS:HG3 | 2.20 | 0.42 |
| 49:s:149:ARG:O | 49:s:153:ARG:HG3 | 2.19 | 0.42 |
| 5:v:370:ASP:N | 5:v:370:ASP:OD1 | 2.53 | 0.42 |
| 6:w:196:HIS:HE1 | 56:w:401:HEM:NA | 2.18 | 0.42 |
| 7:x:126:HIS:HE1 | 7:x:196:PRO:HD2 | 1.85 | 0.42 |
| 5:6:168:ASN:H | 5:6:168:ASN:HD22 | 1.68 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:254:ARG:HH21 | 5:v:257:GLU:HG3 | 1.85 | 0.42 |
| 6:7:222:PRO:HG3 | 51:5:470:ARG:HE | 1.84 | 0.42 |
| 10:b:61:ILE:HB | 10:b:65:TYR:HB3 | 2.01 | 0.42 |
| 18:j:18:VAL:HA | 25:r:222:MET:HE1 | 2.02 | 0.42 |
| 25:r:294:LEU:O | 25:r:297:THR:OG1 | 2.33 | 0.42 |
| 26:B:64:LYS:HZ3 | 29:E:245:VAL:HG11 | 1.85 | 0.42 |
| 26:B:65:THR:O | 26:B:69:LEU:HG | 2.19 | 0.42 |
| 26:B:110:PRO:O | 26:B:238:CYS:HB3 | 2.20 | 0.42 |
| 27:C:252:GLU:O | 27:C:255:LYS:HG2 | 2.20 | 0.42 |
| 43:U:258:LEU:HD11 | 43:U:278:LEU:HD11 | 2.02 | 0.42 |
| 6:7:272:TRP:CE2 | 6:7:273:TYR:HD1 | 2.37 | 0.42 |
| 10:b:61:ILE:HG22 | 10:b:64:THR:H | 1.85 | 0.42 |
| 11:c:140:MET:HE3 | 48:l:286:LEU:HD23 | 2.01 | 0.42 |
| 17:i:26:TRP:HB3 | 17:i:74:ILE:HD13 | 2.01 | 0.42 |
| 24:q:75:LEU:HB3 | 24:q:229:MET:HE1 | 2.01 | 0.42 |
| 24:q:141:GLU:HB2 | 24:q:222:GLU:CD | 2.45 | 0.42 |
| 24:q:307:TRP:CZ3 | 48:l:190:LEU:HD21 | 2.54 | 0.42 |
| 26:B:225:LEU:HB3 | 26:B:227:PRO:HD2 | 2.01 | 0.42 |
| 28:D:183:ASP:OD2 | 28:D:185:ARG:NH1 | 2.50 | 0.42 |
| 35:L:313:LYS:O | 35:L:317:VAL:HG23 | 2.19 | 0.42 |
| 48:l:217:LEU:HD13 | 48:l:276:MET:HE3 | 2.02 | 0.42 |
| 51:u:70:THR:HG21 | 51:u:407:THR:HA | 2.02 | 0.42 |
| 6:w:182:HIS:CD2 | 56:w:402:HEM:C4C | 3.08 | 0.42 |
| 2:Ac:19:SER:HB3 | 4:Ad:23:MET:HB3 | 2.01 | 0.42 |
| 2:1:21:PHE:O | 2:1:25:ILE:HG13 | 2.20 | 0.41 |
| 3:4:191:ARG:HG2 | 6:w:168:PHE:CD2 | 2.55 | 0.41 |
| 16:h:103:ASP:OD1 | 16:h:103:ASP:N | 2.52 | 0.41 |
| 17:i:37:LEU:O | 17:i:41:ILE:HG12 | 2.20 | 0.41 |
| 17:i:296:LEU:HD23 | 17:i:296:LEU:HA | 1.85 | 0.41 |
| 20:m:22:SER:HB2 | 20:m:89:VAL:HG13 | 2.02 | 0.41 |
| 23:p:143:GLU:HB2 | 23:p:164:ARG:HH12 | 1.85 | 0.41 |
| 25:r:47:GLN:HE21 | 25:r:51:ASP:CG | 2.28 | 0.41 |
| 25:r:55:LEU:HA | 25:r:55:LEU:HD23 | 1.84 | 0.41 |
| 25:r:228:TYR:O | 25:r:232:ILE:HG13 | 2.19 | 0.41 |
| 25:r:313:SER:HB3 | 45:W:51:MET:HA | 2.01 | 0.41 |
| 26:B:162:PHE:CZ | 29:E:178:GLY:HA3 | 2.55 | 0.41 |
| 31:H:144:ARG:HB2 | 34:K:130:THR:HG23 | 2.01 | 0.41 |
| 39:Q:101:ASP:O | 39:Q:105:VAL:HG23 | 2.20 | 0.41 |
| 46:Y:47:PHE:CD1 | 46:Y:48:PRO:HD2 | 2.54 | 0.41 |
| 48:l:280:LEU:O | 48:l:284:THR:HG23 | 2.20 | 0.41 |
| 3:2:185:ASN:HB2 | 3:2:198:ARG:HE | 1.84 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:d:101:GLU:HG3 | 13:e:118:ALA:HB1 | 2.02 | 0.41 |
| 17:i:276:ILE:C | 17:i:279:PRO:HD2 | 2.45 | 0.41 |
| 25:r:135:ALA:O | 25:r:136:VAL:C | 2.63 | 0.41 |
| 25:r:201:THR:OG1 | 25:r:202:GLU:N | 2.53 | 0.41 |
| 27:C:151:MET:HG3 | 27:C:220:TYR:CE2 | 2.55 | 0.41 |
| 29:E:215:LYS:HE2 | 29:E:215:LYS:HB2 | 1.91 | 0.41 |
| 32:I:67:PHE:CZ | 32:I:69:LEU:HD21 | 2.54 | 0.41 |
| 35:L:143:ILE:HB | 35:L:144:PRO:HD3 | 2.02 | 0.41 |
| 47:Z:41:GLU:H | 47:Z:41:GLU:HG3 | 1.67 | 0.41 |
| 48:l:21:MET:O | 48:l:24:SER:OG | 2.31 | 0.41 |
| 51:u:302:VAL:HB | 51:u:303:PRO:HD3 | 2.01 | 0.41 |
| 5:v:183:ARG:HG2 | 5:v:252:LYS:HB2 | 2.03 | 0.41 |
| 5:v:356:ASP:HA | 5:v:359:LYS:HD3 | 2.02 | 0.41 |
| 51:5:358:PHE:CD2 | 51:5:368:MET:HG2 | 2.56 | 0.41 |
| 53:G:53:CYS:O | 53:G:58:MET:N | 2.53 | 0.41 |
| 53:G:217:GLU:OE2 | 53:G:409:PHE:HA | 2.20 | 0.41 |
| 1:0:63:THR:OG1 | 1:0:65:GLU:HG2 | 2.20 | 0.41 |
| 3:4:204:GLU:O | 3:4:208:GLU:HG2 | 2.19 | 0.41 |
| 7:8:90:LEU:HD11 | 1:Ab:76:HIS:HB2 | 2.02 | 0.41 |
| 7:8:168:ARG:NH1 | 7:8:174:ASP:OD2 | 2.53 | 0.41 |
| 9:a:133:TYR:CZ | 21:n:44:LEU:HD12 | 2.55 | 0.41 |
| 11:c:71:GLY:HA2 | 22:o:79:ASN:O | 2.20 | 0.41 |
| 13:e:65:ASN:OD1 | 13:e:65:ASN:N | 2.53 | 0.41 |
| 17:i:323:MET:HE2 | 17:i:323:MET:HB3 | 1.89 | 0.41 |
| 27:C:331:ASP:OD1 | 27:C:331:ASP:N | 2.53 | 0.41 |
| 28:D:186:ARG:NH1 | 28:D:191:TYR:O | 2.54 | 0.41 |
| 29:E:141:MET:HE2 | 29:E:141:MET:HB3 | 1.87 | 0.41 |
| 35:L:216:ARG:HH11 | 35:L:216:ARG:HG3 | 1.85 | 0.41 |
| 37:O:130:ILE:HG12 | 37:O:147:TYR:HE2 | 1.85 | 0.41 |
| 37:X:138:LEU:HD13 | 37:X:138:LEU:HA | 1.85 | 0.41 |
| 48:l:437:PHE:HE1 | 48:l:441:VAL:HG22 | 1.85 | 0.41 |
| 51:u:304:LEU:HD23 | 51:u:304:LEU:HA | 1.78 | 0.41 |
| 53:G:183:ILE:HD11 | 53:G:206:VAL:HG13 | 2.01 | 0.41 |
| 5:6:60:ARG:CZ | 5:6:390:GLU:HG2 | 2.49 | 0.41 |
| 5:6:253:TYR:HE2 | 5:6:435:ARG:HB3 | 1.85 | 0.41 |
| 6:7:338:ILE:HD13 | 6:7:351:GLY:CA | 2.46 | 0.41 |
| 15:g:16:LEU:HD13 | 15:g:16:LEU:HA | 1.80 | 0.41 |
| 17:i:155:LEU:HD22 | 17:i:278:MET:HE2 | 2.01 | 0.41 |
| 18:j:54:LYS:HD2 | 18:j:54:LYS:HA | 1.87 | 0.41 |
| 18:j:60:ILE:O | 18:j:63:LEU:HB2 | 2.21 | 0.41 |
| 27:C:352:GLN:O | 27:C:356:LYS:HG2 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:I:44:GLU:HG2 | 32:I:194:TYR:CE2 | 2.55 | 0.41 |
| 37:O:113:LEU:HD12 | 39:Q:94:MET:HE2 | 2.01 | 0.41 |
| 48:l:54:PHE:CZ | 48:l:84:TYR:HB2 | 2.56 | 0.41 |
| 48:l:257:VAL:HG11 | 48:l:313:MET:HB3 | 2.02 | 0.41 |
| 48:l:305:SER:O | 48:l:309:GLN:HG2 | 2.19 | 0.41 |
| 48:l:368:PHE:HZ | 48:l:455:LYS:HG3 | 1.85 | 0.41 |
| 50:t:7:ARG:NH1 | 50:t:16:GLU:OE2 | 2.52 | 0.41 |
| 6:w:299:LEU:HD23 | 6:w:299:LEU:HA | 1.86 | 0.41 |
| 51:5:373:GLN:OE1 | 51:5:474:GLY:HA3 | 2.20 | 0.41 |
| 6:7:264:THR:HG22 | 6:7:265:PRO:O | 2.21 | 0.41 |
| 6:7:323:CYS:SG | 6:7:327:MET:HE3 | 2.61 | 0.41 |
| 10:b:75:VAL:HG12 | 48:l:14:ILE:HD13 | 2.03 | 0.41 |
| 10:b:93:LYS:NZ | 12:d:108:GLU:OE2 | 2.49 | 0.41 |
| 12:d:89:GLU:CD | 12:d:152:ALA:H | 2.28 | 0.41 |
| 12:d:169:ALA:O | 12:d:171:LYS:HG3 | 2.20 | 0.41 |
| 17:i:168:GLY:O | 17:i:172:GLN:HG2 | 2.19 | 0.41 |
| 22:o:94:GLY:HA2 | 48:l:553:LEU:HD21 | 2.01 | 0.41 |
| 24:q:105:PHE:O | 24:q:109:THR:HG23 | 2.19 | 0.41 |
| 25:r:1:MET:HE2 | 25:r:1:MET:HB3 | 1.80 | 0.41 |
| 25:r:245:ALA:HB3 | 25:r:255:TYR:CE2 | 2.54 | 0.41 |
| 25:r:293:PHE:O | 25:r:294:LEU:C | 2.63 | 0.41 |
| 26:B:125:CYS:SG | 29:E:180:CYS:N | 2.93 | 0.41 |
| 29:E:197:THR:H | 29:E:200:ASP:HB2 | 1.84 | 0.41 |
| 35:L:223:LEU:O | 35:L:287:PRO:HA | 2.21 | 0.41 |
| 38:P:16:LEU:HD21 | 38:P:67:ALA:HB1 | 2.03 | 0.41 |
| 40:R:87:LEU:O | 40:R:91:VAL:HG23 | 2.20 | 0.41 |
| 43:U:319:ILE:H | 43:U:319:ILE:HG13 | 1.75 | 0.41 |
| 44:V:17:GLU:HB3 | 44:V:20:ARG:HD3 | 2.03 | 0.41 |
| 46:Y:54:GLN:NE2 | 48:l:446:ASN:HB2 | 2.34 | 0.41 |
| 48:l:12:LEU:HD22 | 48:l:129:MET:HB3 | 2.03 | 0.41 |
| 48:l:94:LEU:HD23 | 48:l:125:LEU:HD21 | 2.01 | 0.41 |
| 48:l:100:ILE:O | 48:l:104:SER:OG | 2.31 | 0.41 |
| 49:s:175:ARG:H | 49:s:175:ARG:HG3 | 1.53 | 0.41 |
| 51:u:293:GLY:N | 51:u:352:GLY:O | 2.51 | 0.41 |
| 51:u:373:GLN:HE22 | 51:u:471:ILE:HG23 | 1.86 | 0.41 |
| 6:w:207:ASN:ND2 | 6:w:213:SER:HB3 | 2.36 | 0.41 |
| 51:5:70:THR:HB | 51:5:410:CYS:SG | 2.61 | 0.41 |
| 51:5:95:HIS:HB3 | 51:5:164:GLU:HG3 | 2.03 | 0.41 |
| 53:G:710:CYS:O | 53:G:714:VAL:HG12 | 2.20 | 0.41 |
| 1:0:47:ARG:O | 1:0:51:GLU:HG2 | 2.20 | 0.41 |
| 6:7:82:LEU:HD23 | 6:7:243:VAL:HG21 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:d:65:HIS:CE1 | 13:e:121:GLU:HG2 | 2.55 | 0.41 |
| 12:d:79:GLU:O | 12:d:81:ASP:N | 2.54 | 0.41 |
| 19:k:65:VAL:HG13 | 20:m:161:LEU:HD21 | 2.03 | 0.41 |
| 22:o:6:TYR:CE2 | 22:o:15:PRO:HD3 | 2.55 | 0.41 |
| 25:r:87:VAL:HG13 | 25:r:95:LEU:HD23 | 2.03 | 0.41 |
| 27:C:61:THR:N | 27:C:64:THR:OG1 | 2.53 | 0.41 |
| 27:C:164:LEU:HD12 | 27:C:164:LEU:HA | 1.82 | 0.41 |
| 30:F:37:LYS:HE3 | 30:F:37:LYS:HB2 | 1.78 | 0.41 |
| 31:H:122:VAL:O | 31:H:123:CYS:C | 2.64 | 0.41 |
| 34:K:42:ASP:OD1 | 34:K:46:ASN:N | 2.54 | 0.41 |
| 35:L:78:PRO:HB2 | 35:L:103:TRP:CD1 | 2.55 | 0.41 |
| 38:P:65:LEU:O | 38:P:76:ASN:HA | 2.21 | 0.41 |
| 38:P:68:ARG:NH1 | 53:G:359:ASN:HD21 | 2.18 | 0.41 |
| 39:Q:67:ARG:HE | 39:Q:67:ARG:HB3 | 1.28 | 0.41 |
| 43:U:83:LEU:HG | 43:U:272:VAL:HG13 | 2.02 | 0.41 |
| 45:W:95:ALA:HA | 45:W:106:VAL:HG11 | 2.02 | 0.41 |
| 47:Z:40:ILE:O | 47:Z:43:THR:OG1 | 2.37 | 0.41 |
| 48:l:233:LEU:HB3 | 48:l:234:PRO:HD3 | 2.01 | 0.41 |
| 48:l:336:LYS:HA | 48:l:336:LYS:HD3 | 1.71 | 0.41 |
| 3:2:213:VAL:O | 3:2:216:LEU:HB2 | 2.20 | 0.41 |
| 5:6:180:ALA:HB2 | 5:6:258:ILE:HG13 | 2.03 | 0.41 |
| 7:8:142:THR:HG23 | 7:8:144:GLU:HG2 | 2.02 | 0.41 |
| 10:b:119:LEU:O | 10:b:121:LYS:N | 2.53 | 0.41 |
| 12:d:43:ARG:HB3 | 12:d:44:PRO:HD3 | 2.02 | 0.41 |
| 12:d:113:CYS:O | 12:d:117:GLU:HG2 | 2.21 | 0.41 |
| 17:i:315:TRP:HZ3 | 43:U:329:VAL:HG12 | 1.85 | 0.41 |
| 20:m:27:ILE:O | 20:m:31:LEU:HG | 2.20 | 0.41 |
| 20:m:136:PHE:HD1 | 20:m:136:PHE:HA | 1.77 | 0.41 |
| 25:r:37:PRO:O | 25:r:44:GLY:HA3 | 2.20 | 0.41 |
| 27:C:262:ASP:CG | 27:C:344:ARG:HH22 | 2.29 | 0.41 |
| 27:C:449:MET:HE3 | 27:C:449:MET:HB2 | 1.80 | 0.41 |
| 35:L:36:ILE:HD11 | 53:G:304:GLN:HE21 | 1.84 | 0.41 |
| 35:L:235:VAL:HG22 | 35:L:262:GLY:N | 2.34 | 0.41 |
| 35:L:245:ILE:O | 35:L:249:LYS:HG3 | 2.20 | 0.41 |
| 35:L:259:ALA:O | 35:L:329:GLY:HA2 | 2.20 | 0.41 |
| 38:P:20:ARG:HB2 | 38:P:66:TRP:HB2 | 2.02 | 0.41 |
| 38:P:20:ARG:NH2 | 38:P:74:GLU:OE1 | 2.43 | 0.41 |
| 47:Z:52:LEU:HA | 47:Z:55:ARG:HG2 | 2.02 | 0.41 |
| 51:u:477:TRP:HB3 | 51:u:479:ARG:HG2 | 2.02 | 0.41 |
| 5:v:309:LEU:HD23 | 5:v:357:GLN:HB3 | 2.03 | 0.41 |
| 51:5:197:LEU:HD23 | 51:5:197:LEU:HA | 1.85 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:5:338:CYS:SG | 51:5:358:PHE:HB2 | 2.60 | 0.41 |
| 53:G:179:CYS:O | 53:G:180:THR:OG1 | 2.33 | 0.41 |
| 2:1:48:ASN:OD1 | 7:x:105:SER:N | 2.53 | 0.41 |
| 5:6:423:ASP:OD1 | 5:6:423:ASP:N | 2.52 | 0.41 |
| 6:7:181:PHE:HA | 6:7:184:ILE:HG22 | 2.02 | 0.41 |
| 8:9:83:LYS:H | 8:9:86:GLU:HG2 | 1.85 | 0.41 |
| 12:d:26:LEU:HD12 | 50:t:76:ASN:HB2 | 2.02 | 0.41 |
| 12:d:128:GLU:H | 12:d:128:GLU:HG2 | 1.64 | 0.41 |
| 17:i:14:MET:O | 17:i:18:MET:HG2 | 2.20 | 0.41 |
| 21:n:16:LEU:HB3 | 24:q:10:MET:HE3 | 2.02 | 0.41 |
| 22:o:63:PRO:O | 22:o:67:ARG:HG3 | 2.20 | 0.41 |
| 25:r:88:PRO:HB3 | 25:r:98:MET:HE3 | 2.03 | 0.41 |
| 26:B:63:TYR:CE2 | 26:B:64:LYS:HG3 | 2.55 | 0.41 |
| 26:B:63:TYR:CZ | 26:B:64:LYS:HG3 | 2.56 | 0.41 |
| 27:C:290:LEU:HD23 | 27:C:290:LEU:HA | 1.90 | 0.41 |
| 28:D:177:PHE:CE1 | 39:Q:110:ILE:HD13 | 2.55 | 0.41 |
| 35:L:36:ILE:HG23 | 53:G:615:LEU:HG | 2.02 | 0.41 |
| 44:V:9:TYR:CE1 | 44:V:21:LYS:HE3 | 2.55 | 0.41 |
| 51:u:118:ALA:O | 5:v:298:HIS:HB3 | 2.20 | 0.41 |
| 51:u:470:ARG:NH2 | 6:w:221:HIS:HB3 | 2.36 | 0.41 |
| 5:v:293:LEU:HB3 | 5:v:309:LEU:HG | 2.02 | 0.41 |
| 5:v:313:VAL:HG11 | 5:v:350:VAL:HG13 | 2.03 | 0.41 |
| 52:z:19:LEU:HD23 | 52:z:19:LEU:HA | 1.93 | 0.41 |
| 53:G:197:THR:HB | 53:G:204:MET:HE3 | 2.03 | 0.41 |
| 53:G:445:LEU:HD22 | 53:G:460:HIS:CE1 | 2.55 | 0.41 |
| 3:2:207:GLN:HE21 | 3:2:207:GLN:HB2 | 1.61 | 0.41 |
| 4:3:9:ARG:HH11 | 4:3:9:ARG:HB3 | 1.86 | 0.41 |
| 3:4:195:LEU:HD21 | 3:4:294:VAL:HG21 | 2.03 | 0.41 |
| 3:4:257:CYS:SG | 55:4:301:FES:S2 | 3.19 | 0.41 |
| 5:6:394:ASP:OD1 | 5:6:395:GLU:N | 2.54 | 0.41 |
| 6:7:107:TYR:HB2 | 6:7:305:PRO:HG3 | 2.03 | 0.41 |
| 11:c:96:ASP:O | 11:c:114:ARG:HD3 | 2.21 | 0.41 |
| 12:d:107:GLN:O | 12:d:111:LYS:HG3 | 2.21 | 0.41 |
| 13:e:53:ILE:H | 13:e:53:ILE:HG12 | 1.70 | 0.41 |
| 15:g:84:MET:HB3 | 17:i:344:SER:HB3 | 2.03 | 0.41 |
| 17:i:31:ILE:HG23 | 19:k:66:PHE:CZ | 2.56 | 0.41 |
| 17:i:204:ASN:HD22 | 17:i:204:ASN:C | 2.27 | 0.41 |
| 18:j:30:TYR:HB3 | 18:j:31:SER:H | 1.72 | 0.41 |
| 19:k:75:LEU:CD1 | 20:m:67:VAL:HG13 | 2.51 | 0.41 |
| 20:m:83:TRP:HA | 20:m:89:VAL:CG1 | 2.51 | 0.41 |
| 23:p:69:LEU:HD21 | 23:p:82:PHE:HB3 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:q:86:LYS:HE2 | 24:q:86:LYS:HB3 | 1.89 | 0.41 |
| 24:q:405:LEU:HD23 | 24:q:405:LEU:HA | 1.78 | 0.41 |
| 26:B:136:HIS:O | 26:B:140:GLU:HG2 | 2.21 | 0.41 |
| 27:C:49:TRP:NE1 | 27:C:53:PHE:HE2 | 2.19 | 0.41 |
| 27:C:443:LYS:HE2 | 27:C:443:LYS:HB2 | 1.93 | 0.41 |
| 28:D:157:VAL:HG11 | 28:D:182:PRO:HG2 | 2.02 | 0.41 |
| 28:D:181:HIS:CD2 | 28:D:183:ASP:H | 2.32 | 0.41 |
| 35:L:60:LEU:HD21 | 35:L:244:ILE:HD11 | 2.02 | 0.41 |
| 35:L:161:HIS:O | 35:L:196:ILE:N | 2.54 | 0.41 |
| 35:L:215:MET:HA | 35:L:218:PHE:CD2 | 2.56 | 0.41 |
| 37:X:104:PHE:HA | 37:X:108:LEU:HB2 | 2.01 | 0.41 |
| 48:l:210:ASN:OD1 | 48:l:270:ASN:ND2 | 2.43 | 0.41 |
| 50:t:110:GLN:O | 50:t:114:ARG:HG2 | 2.21 | 0.41 |
| 51:u:363:MET:HE3 | 52:z:6:GLY:HA3 | 2.03 | 0.41 |
| 6:w:138:MET:HE1 | 6:w:267:HIS:O | 2.21 | 0.41 |
| 7:x:127:SER:HB2 | 7:x:179:PRO:HD2 | 2.03 | 0.41 |
| 53:G:188:GLU:O | 53:G:419:ARG:NE | 2.50 | 0.41 |
| 53:G:353:ALA:HA | 53:G:636:TYR:OH | 2.21 | 0.41 |
| 17:i:100:MET:HE3 | 17:i:111:PHE:CZ | 2.56 | 0.41 |
| 20:m:61:LEU:HA | 20:m:65:LEU:CD2 | 2.50 | 0.41 |
| 24:q:201:MET:HE1 | 24:q:212:LEU:HD11 | 2.03 | 0.41 |
| 29:E:68:LYS:HE2 | 29:E:68:LYS:HB3 | 1.78 | 0.41 |
| 29:E:108:PRO:HA | 29:E:109:PRO:HD3 | 1.97 | 0.41 |
| 41:S:1:MET:HB2 | 41:S:3:PHE:CZ | 2.56 | 0.41 |
| 44:V:95:CYS:HA | 44:V:115:CYS:HA | 2.02 | 0.41 |
| 45:W:116:TRP:HB2 | 49:s:129:ASP:OD2 | 2.21 | 0.41 |
| 6:w:40:CYS:O | 6:w:44:GLN:HG2 | 2.21 | 0.41 |
| 6:w:55:TYR:HA | 6:w:65:SER:OG | 2.21 | 0.41 |
| 6:w:185:LEU:HD23 | 6:w:185:LEU:HA | 1.79 | 0.41 |
| 51:5:68:THR:HG22 | 51:5:136:LEU:HD23 | 2.02 | 0.41 |
| 53:G:329:MET:HG2 | 53:G:565:PHE:CD2 | 2.56 | 0.41 |
| 53:G:400:ILE:HD12 | 53:G:427:LEU:HD21 | 2.03 | 0.41 |
| 2:1:34:ARG:NH2 | 4:3:50:GLY:HA3 | 2.36 | 0.40 |
| 3:2:259:CYS:HB2 | 55:2:301:FES:S1 | 2.60 | 0.40 |
| 5:6:293:LEU:HD12 | 5:6:336:PHE:HZ | 1.85 | 0.40 |
| 7:8:114:GLY:HA3 | 7:8:274:PHE:HB2 | 2.02 | 0.40 |
| 7:8:203:ARG:CZ | 7:8:280:GLU:HG2 | 2.52 | 0.40 |
| 7:8:266:GLN:HE22 | 1:Ab:91:LYS:H | 1.69 | 0.40 |
| 10:b:79:VAL:HA | 48:l:10:THR:HG21 | 2.03 | 0.40 |
| 15:g:87:LEU:HD23 | 15:g:87:LEU:HA | 1.87 | 0.40 |
| 17:i:112:HIS:CE1 | 17:i:164:ILE:HG21 | 2.56 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:i:128:LEU:HD11 | 17:i:213:LEU:HA | 2.02 | 0.40 |
| 25:r:78:ALA:HB2 | 25:r:115:SER:HB2 | 2.02 | 0.40 |
| 25:r:134:ARG:NH2 | 25:r:282:TYR:HB2 | 2.36 | 0.40 |
| 26:B:170:GLN:HE22 | 40:R:93:LEU:HD12 | 1.86 | 0.40 |
| 29:E:110:MET:O | 29:E:114:GLU:HG3 | 2.20 | 0.40 |
| 29:E:169:PHE:CE2 | 29:E:209:LYS:HG3 | 2.51 | 0.40 |
| 35:L:183:GLU:HG3 | 35:L:195:ILE:HD13 | 2.03 | 0.40 |
| 35:L:222:PRO:HA | 35:L:288:LEU:HD21 | 2.04 | 0.40 |
| 48:l:154:LEU:HD23 | 48:l:154:LEU:HA | 1.91 | 0.40 |
| 5:v:409:PRO:O | 5:v:413:LEU:HG | 2.21 | 0.40 |
| 6:w:173:ALA:O | 6:w:177:ARG:HG2 | 2.21 | 0.40 |
| 6:w:185:LEU:HD23 | 6:w:188:ILE:HD12 | 2.03 | 0.40 |
| 53:G:400:ILE:HG12 | 53:G:473:MET:HB3 | 2.02 | 0.40 |
| 53:G:618:GLU:O | 53:G:622:ILE:HG13 | 2.20 | 0.40 |
| 1:0:79:ASP:HA | 1:0:82:VAL:HB | 2.03 | 0.40 |
| 3:4:189:LYS:HZ1 | 6:w:261:PRO:HB2 | 1.85 | 0.40 |
| 5:6:138:LEU:HD22 | 5:6:238:LEU:HD21 | 2.03 | 0.40 |
| 6:7:62:ALA:O | 6:7:65:SER:OG | 2.24 | 0.40 |
| 7:8:226:VAL:HG23 | 1:Ab:66:ASP:OD2 | 2.22 | 0.40 |
| 8:9:59:ARG:O | 8:9:63:ILE:HG13 | 2.22 | 0.40 |
| 13:e:109:LEU:HD12 | 13:e:109:LEU:HA | 1.91 | 0.40 |
| 17:i:89:MET:HE3 | 17:i:89:MET:HB3 | 1.91 | 0.40 |
| 17:i:183:SER:O | 17:i:187:MET:HG2 | 2.21 | 0.40 |
| 24:q:142:ARG:NH2 | 27:C:42:GLN:HE21 | 2.20 | 0.40 |
| 28:D:121:THR:OG1 | 33:J:128:PHE:HA | 2.22 | 0.40 |
| 28:D:229:GLU:OE2 | 53:G:246:ARG:NH2 | 2.55 | 0.40 |
| 29:E:66:ILE:HD11 | 40:R:87:LEU:HD22 | 2.04 | 0.40 |
| 35:L:340:LEU:O | 35:L:344:ALA:N | 2.54 | 0.40 |
| 35:L:354:TYR:HA | 35:L:357:LEU:HB3 | 2.03 | 0.40 |
| 37:O:104:PHE:HE2 | 37:O:144:ILE:HD11 | 1.87 | 0.40 |
| 37:O:115:GLN:O | 37:O:118:ILE:HG13 | 2.21 | 0.40 |
| 43:U:67:ASN:OD1 | 43:U:68:ILE:N | 2.45 | 0.40 |
| 43:U:258:LEU:HB3 | 43:U:260:TYR:CE2 | 2.57 | 0.40 |
| 6:w:97:HIS:HE1 | 56:w:401:HEM:CHA | 2.34 | 0.40 |
| 7:x:294:LEU:HD23 | 7:x:294:LEU:HA | 1.95 | 0.40 |
| 51:5:426:LEU:HD23 | 51:5:426:LEU:HA | 1.91 | 0.40 |
| 54:M:9:GLN:HA | 54:M:12:ARG:HG2 | 2.03 | 0.40 |
| 1:0:48:GLU:O | 1:0:52:LEU:HG | 2.21 | 0.40 |
| 3:4:202:LYS:NZ | 3:4:206:ASP:OD1 | 2.47 | 0.40 |
| 5:6:132:ILE:H | 5:6:132:ILE:HG13 | 1.64 | 0.40 |
| 5:6:168:ASN:HB2 | 5:6:170:GLN:HE22 | 1.86 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:6:177:LEU:HD21 | 5:6:272:VAL:HG11 | 2.02 | 0.40 |
| 5:6:290:GLN:HB2 | 5:6:336:PHE:HE1 | 1.86 | 0.40 |
| 8:9:105:ARG:HG2 | 5:v:97:PHE:CE1 | 2.57 | 0.40 |
| 17:i:273:ASN:HA | 44:V:140:LYS:HD2 | 2.02 | 0.40 |
| 20:m:93:PHE:O | 20:m:97:LEU:HG | 2.21 | 0.40 |
| 25:r:86:TRP:NE1 | 25:r:233:MET:HB2 | 2.36 | 0.40 |
| 25:r:277:TYR:HB3 | 27:C:273:ILE:HD12 | 2.04 | 0.40 |
| 26:B:36:LYS:HE3 | 26:B:36:LYS:HB3 | 1.88 | 0.40 |
| 26:B:85:LEU:HD23 | 26:B:95:THR:HG21 | 2.03 | 0.40 |
| 26:B:154:ALA:HB3 | 26:B:195:VAL:HG12 | 2.04 | 0.40 |
| 27:C:159:LEU:HD13 | 27:C:159:LEU:HA | 1.91 | 0.40 |
| 27:C:272:ARG:HH22 | 31:H:63:TRP:HA | 1.87 | 0.40 |
| 27:C:285:THR:HA | 36:N:12:VAL:HG23 | 2.04 | 0.40 |
| 28:D:93:VAL:O | 28:D:97:LEU:HB2 | 2.21 | 0.40 |
| 29:E:69:ASN:OD1 | 40:R:90:ASN:ND2 | 2.48 | 0.40 |
| 35:L:301:GLU:HA | 35:L:307:PRO:HB3 | 2.02 | 0.40 |
| 40:R:98:MET:HE2 | 40:R:98:MET:HB3 | 1.74 | 0.40 |
| 37:X:93:ILE:HD11 | 37:X:110:LEU:HD11 | 2.03 | 0.40 |
| 48:l:13:ILE:HD12 | 48:l:13:ILE:HA | 1.93 | 0.40 |
| 48:l:293:ILE:O | 48:l:425:ARG:HD2 | 2.22 | 0.40 |
| 5:v:297:PRO:CD | 3:Af:70:ALA:HB1 | 2.51 | 0.40 |
| 5:v:297:PRO:HD3 | 3:Af:70:ALA:HB1 | 2.04 | 0.40 |
| 6:w:129:MET:HE3 | 6:w:129:MET:HB2 | 1.91 | 0.40 |
| 6:w:233:LEU:CD1 | 7:x:304:VAL:HG21 | 2.52 | 0.40 |
| 3:2:208:GLU:OE1 | 3:2:266:ALA:HB3 | 2.21 | 0.40 |
| 5:6:101:ARG:HB3 | 8:y:108:TRP:CZ2 | 2.56 | 0.40 |
| 5:6:168:ASN:H | 5:6:168:ASN:ND2 | 2.19 | 0.40 |
| 5:6:170:GLN:HG2 | 3:Ae:67:VAL:HG11 | 2.04 | 0.40 |
| 18:j:62:PHE:CG | 25:r:140:ILE:HG23 | 2.55 | 0.40 |
| 22:o:81:ARG:O | 22:o:83:THR:HG23 | 2.22 | 0.40 |
| 24:q:286:ILE:O | 24:q:289:SER:OG | 2.27 | 0.40 |
| 24:q:294:MET:HE3 | 24:q:319:HIS:ND1 | 2.37 | 0.40 |
| 26:B:62:TRP:CD2 | 26:B:181:LEU:HD13 | 2.57 | 0.40 |
| 26:B:113:LEU:HD13 | 26:B:149:MET:HE1 | 2.02 | 0.40 |
| 26:B:126:LYS:O | 26:B:130:ILE:HG13 | 2.21 | 0.40 |
| 26:B:222:LYS:HG2 | 26:B:379:CYS:SG | 2.62 | 0.40 |
| 29:E:120:THR:HG23 | 53:G:200:ARG:HH11 | 1.86 | 0.40 |
| 35:L:202:PHE:HE2 | 35:L:343:LYS:HB2 | 1.86 | 0.40 |
| 35:L:209:LEU:HB3 | 35:L:348:LEU:HD21 | 2.04 | 0.40 |
| 44:V:140:LYS:HE2 | 44:V:140:LYS:HB2 | 1.92 | 0.40 |
| 48:l:105:MET:HB3 | 48:l:449:LEU:HD13 | 2.03 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:u:158:ASP:O | 51:u:162:GLU:HG2 | 2.21 | 0.40 |
| 51:u:274:GLU:CD | 51:u:276:ARG:HE | 2.28 | 0.40 |
| 51:u:324:MET:HE3 | 51:u:324:MET:HB2 | 1.91 | 0.40 |
| 51:5:226:ALA:N | 51:5:227:PRO:HD2 | 2.36 | 0.40 |
| 53:G:679:LEU:H | 53:G:679:LEU:HG | 1.61 | 0.40 |
| 3:4:111:ASP:OD1 | 52:Aa:29:HIS:NE2 | 2.55 | 0.40 |
| 3:4:201:THR:HG1 | 3:4:204:GLU:HG3 | 1.87 | 0.40 |
| 5:6:168:ASN:HB2 | 5:6:170:GLN:NE2 | 2.36 | 0.40 |
| 11:c:117:VAL:HG21 | 48:l:539:TYR:HA | 2.04 | 0.40 |
| 11:c:144:PHE:O | 11:c:148:GLU:HG2 | 2.21 | 0.40 |
| 12:d:99:ASP:O | 12:d:103:VAL:HG23 | 2.21 | 0.40 |
| 15:g:54:PRO:HG2 | 43:U:354:ILE:HG21 | 2.03 | 0.40 |
| 20:m:57:PHE:HA | 20:m:61:LEU:HD13 | 2.04 | 0.40 |
| 27:C:148:VAL:HG12 | 27:C:188:ASN:HA | 2.04 | 0.40 |
| 27:C:376:GLU:HA | 27:C:379:THR:HG22 | 2.04 | 0.40 |
| 28:D:138:ASN:ND2 | 28:D:138:ASN:O | 2.54 | 0.40 |
| 29:E:62:ARG:HD3 | 40:R:87:LEU:HB2 | 2.03 | 0.40 |
| 31:H:205:ILE:O | 31:H:209:TYR:N | 2.55 | 0.40 |
| 35:L:356:TRP:O | 35:L:356:TRP:CD1 | 2.74 | 0.40 |
| 38:P:20:ARG:HG3 | 38:P:54:LEU:HB2 | 2.04 | 0.40 |
| 48:l:7:LEU:HD13 | 48:l:7:LEU:HA | 1.83 | 0.40 |
| 7:x:133:TYR:HA | 7:x:136:LEU:HD12 | 2.03 | 0.40 |
| 51:5:270:PHE:CG | 51:5:292:GLU:HB2 | 2.56 | 0.40 |
| 3:Af:56:HIS:C | 3:Af:58:ALA:H | 2.30 | 0.40 |
| 52:Aa:68:GLU:O | 52:Aa:72:ARG:HG2 | 2.22 | 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 | 0 | 66/91 (72%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | Ab | 64/91 (70%) | 64 (100%) | 0 | 0 | 100 | 100 |
| 2 | 1 | 58/64 (91%) | 58 (100%) | 0 | 0 | 100 | 100 |
| 2 | Ac | 57/64 (89%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 3 | 2 | 193/299 (64%) | 188 (97%) | 5 (3%) | 0 | 100 | 100 |
| 3 | 4 | 194/299 (65%) | 184 (95%) | 9 (5%) | 1 (0%) | 25 | 59 |
| 3 | Ae | 21/299 (7%) | 13 (62%) | 7 (33%) | 1 (5%) | 2 | 17 |
| 3 | Af | 27/299 (9%) | 20 (74%) | 7 (26%) | 0 | 100 | 100 |
| 4 | 3 | 49/56 (88%) | 47 (96%) | 2 (4%) | 0 | 100 | 100 |
| 4 | Ad | 49/56 (88%) | 46 (94%) | 3 (6%) | 0 | 100 | 100 |
| 5 | 6 | 416/453 (92%) | 412 (99%) | 4 (1%) | 0 | 100 | 100 |
| 5 | v | 416/453 (92%) | 412 (99%) | 4 (1%) | 0 | 100 | 100 |
| 6 | 7 | 377/379 (100%) | 365 (97%) | 12 (3%) | 0 | 100 | 100 |
| 6 | w | 377/379 (100%) | 372 (99%) | 5 (1%) | 0 | 100 | 100 |
| 7 | 8 | 236/326 (72%) | 227 (96%) | 8 (3%) | 1 (0%) | 30 | 64 |
| 7 | x | 236/326 (72%) | 231 (98%) | 5 (2%) | 0 | 100 | 100 |
| 8 | 9 | 97/111 (87%) | 97 (100%) | 0 | 0 | 100 | 100 |
| 8 | y | 99/111 (89%) | 99 (100%) | 0 | 0 | 100 | 100 |
| 9 | a | 136/189 (72%) | 135 (99%) | 1 (1%) | 0 | 100 | 100 |
| 10 | b | 102/128 (80%) | 93 (91%) | 8 (8%) | 1 (1%) | 13 | 46 |
| 11 | c | 151/186 (81%) | 147 (97%) | 4 (3%) | 0 | 100 | 100 |
| 12 | d | 166/176 (94%) | 165 (99%) | 0 | 1 (1%) | 22 | 55 |
| 13 | e | 97/154 (63%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 14 | f | 44/76 (58%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 15 | g | 119/122 (98%) | 117 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | h | 103/106 (97%) | 102 (99%) | 1 (1%) | 0 | 100 | 100 |
| 17 | i | 345/347 (99%) | 341 (99%) | 4 (1%) | 0 | 100 | 100 |
| 18 | j | 96/115 (84%) | 92 (96%) | 4 (4%) | 0 | 100 | 100 |
| 19 | k | 96/98 (98%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | m | 173/175 (99%) | 162 (94%) | 10 (6%) | 1 (1%) | 22 | 55 |
| 21 | n | 54/58 (93%) | 49 (91%) | 5 (9%) | 0 | 100 | 100 |
| 22 | o | 126/129 (98%) | 122 (97%) | 4 (3%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|------------|---------|----------|-------------|-----|
| 23 | p | 176/221 (80%) | 175 (99%) | 1 (1%) | 0 | 100 | 100 |
| 24 | q | 457/459 (100%) | 451 (99%) | 6 (1%) | 0 | 100 | 100 |
| 25 | r | 316/318 (99%) | 298 (94%) | 17 (5%) | 1 (0%) | 37 | 69 |
| 26 | B | 429/464 (92%) | 418 (97%) | 11 (3%) | 0 | 100 | 100 |
| 27 | C | 428/469 (91%) | 411 (96%) | 16 (4%) | 1 (0%) | 44 | 76 |
| 28 | D | 206/264 (78%) | 197 (96%) | 9 (4%) | 0 | 100 | 100 |
| 29 | E | 212/249 (85%) | 204 (96%) | 8 (4%) | 0 | 100 | 100 |
| 30 | F | 92/123 (75%) | 91 (99%) | 1 (1%) | 0 | 100 | 100 |
| 31 | H | 174/212 (82%) | 170 (98%) | 4 (2%) | 0 | 100 | 100 |
| 32 | I | 154/196 (79%) | 151 (98%) | 3 (2%) | 0 | 100 | 100 |
| 33 | J | 115/175 (66%) | 115 (100%) | 0 | 0 | 100 | 100 |
| 34 | K | 142/145 (98%) | 142 (100%) | 0 | 0 | 100 | 100 |
| 35 | L | 338/372 (91%) | 324 (96%) | 14 (4%) | 0 | 100 | 100 |
| 36 | N | 110/116 (95%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 37 | O | 82/156 (53%) | 79 (96%) | 2 (2%) | 1 (1%) | 11 | 43 |
| 37 | X | 83/156 (53%) | 80 (96%) | 3 (4%) | 0 | 100 | 100 |
| 38 | P | 81/99 (82%) | 80 (99%) | 1 (1%) | 0 | 100 | 100 |
| 39 | Q | 110/154 (71%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 40 | R | 33/110 (30%) | 33 (100%) | 0 | 0 | 100 | 100 |
| 41 | S | 68/70 (97%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 42 | T | 80/169 (47%) | 78 (98%) | 2 (2%) | 0 | 100 | 100 |
| 43 | U | 316/357 (88%) | 307 (97%) | 9 (3%) | 0 | 100 | 100 |
| 44 | V | 137/141 (97%) | 135 (98%) | 2 (2%) | 0 | 100 | 100 |
| 45 | W | 138/144 (96%) | 135 (98%) | 3 (2%) | 0 | 100 | 100 |
| 46 | Y | 60/105 (57%) | 55 (92%) | 5 (8%) | 0 | 100 | 100 |
| 47 | Z | 76/114 (67%) | 76 (100%) | 0 | 0 | 100 | 100 |
| 48 | l | 601/606 (99%) | 578 (96%) | 23 (4%) | 0 | 100 | 100 |
| 49 | s | 169/249 (68%) | 167 (99%) | 2 (1%) | 0 | 100 | 100 |
| 50 | t | 117/137 (85%) | 115 (98%) | 2 (2%) | 0 | 100 | 100 |
| 51 | 5 | 431/480 (90%) | 423 (98%) | 8 (2%) | 0 | 100 | 100 |
| 51 | u | 444/480 (92%) | 437 (98%) | 7 (2%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 52 | Aa | 76/82 (93%) | 76 (100%) | 0 | 0 | 100 | 100 |
| 52 | z | 77/82 (94%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |
| 53 | G | 680/727 (94%) | 668 (98%) | 12 (2%) | 0 | 100 | 100 |
| 54 | M | 92/113 (81%) | 89 (97%) | 3 (3%) | 0 | 100 | 100 |
| All | All | 12140/14729 (82%) | 11826 (97%) | 305 (2%) | 9 (0%) | 50 | 79 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | b | 120 | MET |
| 25 | r | 201 | THR |
| 27 | C | 461 | ASP |
| 3 | Ae | 50 | CYS |
| 12 | d | 80 | LYS |
| 20 | m | 111 | GLU |
| 3 | 4 | 289 | ASP |
| 7 | 8 | 126 | HIS |
| 37 | O | 138 | LEU |

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 | 0 | 64/85 (75%) | 59 (92%) | 5 (8%) | 10 | 34 |
| 1 | Ab | 63/85 (74%) | 53 (84%) | 10 (16%) | 2 | 12 |
| 2 | 1 | 49/52 (94%) | 49 (100%) | 0 | 100 | 100 |
| 2 | Ac | 48/52 (92%) | 44 (92%) | 4 (8%) | 9 | 32 |
| 3 | 2 | 165/245 (67%) | 152 (92%) | 13 (8%) | 10 | 34 |
| 3 | 4 | 166/245 (68%) | 155 (93%) | 11 (7%) | 14 | 41 |
| 3 | Ae | 14/245 (6%) | 12 (86%) | 2 (14%) | 2 | 16 |
| 3 | Af | 19/245 (8%) | 15 (79%) | 4 (21%) | 1 | 5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 4 | 3 | 40/46 (87%) | 39 (98%) | 1 (2%) | 42 | 68 |
| 4 | Ad | 41/46 (89%) | 40 (98%) | 1 (2%) | 44 | 68 |
| 5 | 6 | 329/355 (93%) | 310 (94%) | 19 (6%) | 17 | 44 |
| 5 | v | 329/355 (93%) | 308 (94%) | 21 (6%) | 14 | 42 |
| 6 | 7 | 332/332 (100%) | 318 (96%) | 14 (4%) | 25 | 54 |
| 6 | w | 332/332 (100%) | 323 (97%) | 9 (3%) | 40 | 65 |
| 7 | 8 | 203/259 (78%) | 189 (93%) | 14 (7%) | 13 | 39 |
| 7 | x | 203/259 (78%) | 194 (96%) | 9 (4%) | 24 | 54 |
| 8 | 9 | 91/99 (92%) | 82 (90%) | 9 (10%) | 6 | 26 |
| 8 | y | 93/99 (94%) | 87 (94%) | 6 (6%) | 14 | 41 |
| 9 | a | 121/158 (77%) | 115 (95%) | 6 (5%) | 20 | 49 |
| 10 | b | 97/121 (80%) | 87 (90%) | 10 (10%) | 6 | 26 |
| 11 | c | 138/160 (86%) | 130 (94%) | 8 (6%) | 17 | 44 |
| 12 | d | 152/156 (97%) | 142 (93%) | 10 (7%) | 14 | 41 |
| 13 | e | 91/129 (70%) | 74 (81%) | 17 (19%) | 1 | 7 |
| 14 | f | 42/66 (64%) | 42 (100%) | 0 | 100 | 100 |
| 15 | g | 108/109 (99%) | 100 (93%) | 8 (7%) | 11 | 36 |
| 16 | h | 93/94 (99%) | 88 (95%) | 5 (5%) | 18 | 46 |
| 17 | i | 311/311 (100%) | 287 (92%) | 24 (8%) | 10 | 35 |
| 18 | j | 87/100 (87%) | 76 (87%) | 11 (13%) | 3 | 19 |
| 19 | k | 85/85 (100%) | 80 (94%) | 5 (6%) | 16 | 44 |
| 20 | m | 136/141 (96%) | 125 (92%) | 11 (8%) | 9 | 34 |
| 21 | n | 52/55 (94%) | 48 (92%) | 4 (8%) | 10 | 35 |
| 22 | o | 112/114 (98%) | 109 (97%) | 3 (3%) | 40 | 65 |
| 23 | p | 159/190 (84%) | 149 (94%) | 10 (6%) | 15 | 43 |
| 24 | q | 409/409 (100%) | 391 (96%) | 18 (4%) | 24 | 54 |
| 25 | r | 275/275 (100%) | 257 (94%) | 18 (6%) | 14 | 41 |
| 26 | B | 345/368 (94%) | 330 (96%) | 15 (4%) | 25 | 54 |
| 27 | C | 370/398 (93%) | 332 (90%) | 38 (10%) | 6 | 26 |
| 28 | D | 188/228 (82%) | 169 (90%) | 19 (10%) | 6 | 26 |
| 29 | E | 183/207 (88%) | 174 (95%) | 9 (5%) | 21 | 50 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|------------|----------|-------------|----|
| 30 | F | 78/97 (80%) | 72 (92%) | 6 (8%) | 10 | 35 |
| 31 | H | 151/176 (86%) | 144 (95%) | 7 (5%) | 23 | 52 |
| 32 | I | 132/163 (81%) | 128 (97%) | 4 (3%) | 36 | 63 |
| 33 | J | 106/152 (70%) | 102 (96%) | 4 (4%) | 28 | 57 |
| 34 | K | 130/131 (99%) | 126 (97%) | 4 (3%) | 35 | 63 |
| 35 | L | 289/320 (90%) | 269 (93%) | 20 (7%) | 13 | 39 |
| 36 | N | 99/101 (98%) | 94 (95%) | 5 (5%) | 20 | 49 |
| 37 | O | 78/132 (59%) | 69 (88%) | 9 (12%) | 4 | 22 |
| 37 | X | 79/132 (60%) | 74 (94%) | 5 (6%) | 15 | 43 |
| 38 | P | 74/82 (90%) | 69 (93%) | 5 (7%) | 13 | 40 |
| 39 | Q | 105/134 (78%) | 100 (95%) | 5 (5%) | 21 | 51 |
| 40 | R | 34/92 (37%) | 32 (94%) | 2 (6%) | 16 | 44 |
| 41 | S | 58/58 (100%) | 57 (98%) | 1 (2%) | 56 | 75 |
| 42 | T | 69/134 (52%) | 64 (93%) | 5 (7%) | 12 | 38 |
| 43 | U | 281/307 (92%) | 266 (95%) | 15 (5%) | 19 | 47 |
| 44 | V | 101/102 (99%) | 95 (94%) | 6 (6%) | 16 | 44 |
| 45 | W | 122/124 (98%) | 117 (96%) | 5 (4%) | 26 | 55 |
| 46 | Y | 54/84 (64%) | 48 (89%) | 6 (11%) | 5 | 23 |
| 47 | Z | 60/90 (67%) | 56 (93%) | 4 (7%) | 13 | 41 |
| 48 | l | 537/540 (99%) | 503 (94%) | 34 (6%) | 15 | 43 |
| 49 | s | 153/206 (74%) | 144 (94%) | 9 (6%) | 16 | 44 |
| 50 | t | 107/120 (89%) | 97 (91%) | 10 (9%) | 7 | 29 |
| 51 | 5 | 363/397 (91%) | 349 (96%) | 14 (4%) | 27 | 57 |
| 51 | u | 372/397 (94%) | 353 (95%) | 19 (5%) | 20 | 49 |
| 52 | Aa | 70/73 (96%) | 65 (93%) | 5 (7%) | 12 | 38 |
| 52 | z | 70/73 (96%) | 65 (93%) | 5 (7%) | 12 | 38 |
| 53 | G | 576/610 (94%) | 539 (94%) | 37 (6%) | 14 | 42 |
| 54 | M | 86/98 (88%) | 80 (93%) | 6 (7%) | 12 | 39 |
| All | All | 10569/12435 (85%) | 9911 (94%) | 658 (6%) | 18 | 43 |

All (658) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 42 | LYS |
| 1 | 0 | 48 | GLU |
| 1 | 0 | 64 | GLU |
| 1 | 0 | 70 | GLU |
| 1 | 0 | 75 | LEU |
| 3 | 2 | 104 | ILE |
| 3 | 2 | 172 | LYS |
| 3 | 2 | 207 | GLN |
| 3 | 2 | 208 | GLU |
| 3 | 2 | 231 | TRP |
| 3 | 2 | 238 | CYS |
| 3 | 2 | 246 | ILE |
| 3 | 2 | 251 | ASP |
| 3 | 2 | 259 | CYS |
| 3 | 2 | 278 | ASN |
| 3 | 2 | 280 | GLU |
| 3 | 2 | 287 | THR |
| 3 | 2 | 292 | VAL |
| 4 | 3 | 9 | ARG |
| 3 | 4 | 104 | ILE |
| 3 | 4 | 119 | ASP |
| 3 | 4 | 166 | ASP |
| 3 | 4 | 170 | MET |
| 3 | 4 | 172 | LYS |
| 3 | 4 | 186 | MET |
| 3 | 4 | 232 | VAL |
| 3 | 4 | 234 | LEU |
| 3 | 4 | 251 | ASP |
| 3 | 4 | 281 | VAL |
| 3 | 4 | 290 | ASP |
| 5 | 6 | 49 | ILE |
| 5 | 6 | 115 | THR |
| 5 | 6 | 122 | THR |
| 5 | 6 | 132 | ILE |
| 5 | 6 | 133 | LEU |
| 5 | 6 | 138 | LEU |
| 5 | 6 | 203 | ASP |
| 5 | 6 | 240 | MET |
| 5 | 6 | 244 | LEU |
| 5 | 6 | 246 | LEU |
| 5 | 6 | 319 | GLN |
| 5 | 6 | 323 | VAL |
| 5 | 6 | 370 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 6 | 378 | LEU |
| 5 | 6 | 421 | ASP |
| 5 | 6 | 423 | ASP |
| 5 | 6 | 435 | ARG |
| 5 | 6 | 451 | ASP |
| 5 | 6 | 453 | LEU |
| 6 | 7 | 10 | LEU |
| 6 | 7 | 27 | ILE |
| 6 | 7 | 112 | THR |
| 6 | 7 | 156 | ILE |
| 6 | 7 | 202 | GLU |
| 6 | 7 | 252 | ASP |
| 6 | 7 | 254 | ASP |
| 6 | 7 | 257 | THR |
| 6 | 7 | 273 | TYR |
| 6 | 7 | 281 | LEU |
| 6 | 7 | 311 | LYS |
| 6 | 7 | 341 | GLN |
| 6 | 7 | 343 | VAL |
| 6 | 7 | 379 | TRP |
| 7 | 8 | 107 | ASP |
| 7 | 8 | 125 | CYS |
| 7 | 8 | 144 | GLU |
| 7 | 8 | 161 | GLU |
| 7 | 8 | 164 | GLU |
| 7 | 8 | 184 | GLU |
| 7 | 8 | 190 | ASN |
| 7 | 8 | 215 | LEU |
| 7 | 8 | 226 | VAL |
| 7 | 8 | 230 | GLU |
| 7 | 8 | 245 | MET |
| 7 | 8 | 251 | ASN |
| 7 | 8 | 276 | ARG |
| 7 | 8 | 293 | MET |
| 8 | 9 | 14 | LEU |
| 8 | 9 | 15 | GLU |
| 8 | 9 | 40 | GLU |
| 8 | 9 | 53 | GLU |
| 8 | 9 | 72 | ARG |
| 8 | 9 | 75 | ILE |
| 8 | 9 | 83 | LYS |
| 8 | 9 | 85 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | 9 | 92 | GLU |
| 9 | a | 58 | LYS |
| 9 | a | 64 | ASP |
| 9 | a | 82 | VAL |
| 9 | a | 130 | GLU |
| 9 | a | 143 | GLU |
| 9 | a | 153 | GLU |
| 10 | b | 4 | TYR |
| 10 | b | 23 | LEU |
| 10 | b | 24 | LYS |
| 10 | b | 28 | LEU |
| 10 | b | 75 | VAL |
| 10 | b | 86 | LEU |
| 10 | b | 89 | HIS |
| 10 | b | 96 | THR |
| 10 | b | 111 | LEU |
| 10 | b | 112 | GLU |
| 11 | c | 36 | MET |
| 11 | c | 53 | LYS |
| 11 | c | 68 | ASP |
| 11 | c | 77 | LYS |
| 11 | c | 87 | ASP |
| 11 | c | 101 | TRP |
| 11 | c | 140 | MET |
| 11 | c | 182 | VAL |
| 12 | d | 6 | ASP |
| 12 | d | 8 | ASP |
| 12 | d | 17 | THR |
| 12 | d | 49 | ARG |
| 12 | d | 50 | GLU |
| 12 | d | 69 | ARG |
| 12 | d | 71 | VAL |
| 12 | d | 82 | ILE |
| 12 | d | 114 | GLN |
| 12 | d | 156 | LEU |
| 13 | e | 54 | ARG |
| 13 | e | 58 | ASP |
| 13 | e | 62 | GLU |
| 13 | e | 63 | ASP |
| 13 | e | 64 | GLU |
| 13 | e | 70 | ASN |
| 13 | e | 72 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | e | 73 | SER |
| 13 | e | 77 | ASP |
| 13 | e | 82 | VAL |
| 13 | e | 84 | LEU |
| 13 | e | 87 | MET |
| 13 | e | 89 | VAL |
| 13 | e | 99 | LEU |
| 13 | e | 116 | GLU |
| 13 | e | 138 | GLU |
| 13 | e | 149 | LEU |
| 15 | g | 3 | MET |
| 15 | g | 16 | LEU |
| 15 | g | 19 | GLU |
| 15 | g | 29 | THR |
| 15 | g | 64 | LEU |
| 15 | g | 84 | MET |
| 15 | g | 87 | LEU |
| 15 | g | 101 | GLU |
| 16 | h | 75 | ARG |
| 16 | h | 82 | GLN |
| 16 | h | 86 | LEU |
| 16 | h | 91 | LYS |
| 16 | h | 101 | LYS |
| 17 | i | 5 | ILE |
| 17 | i | 19 | LEU |
| 17 | i | 22 | ILE |
| 17 | i | 29 | ILE |
| 17 | i | 36 | ASN |
| 17 | i | 79 | LEU |
| 17 | i | 87 | THR |
| 17 | i | 89 | MET |
| 17 | i | 159 | MET |
| 17 | i | 183 | SER |
| 17 | i | 193 | VAL |
| 17 | i | 194 | LEU |
| 17 | i | 258 | SER |
| 17 | i | 290 | LEU |
| 17 | i | 296 | LEU |
| 17 | i | 303 | THR |
| 17 | i | 311 | MET |
| 17 | i | 318 | GLU |
| 17 | i | 319 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | i | 321 | LYS |
| 17 | i | 323 | MET |
| 17 | i | 328 | THR |
| 17 | i | 336 | VAL |
| 17 | i | 346 | LEU |
| 18 | j | 1 | MET |
| 18 | j | 5 | LEU |
| 18 | j | 18 | VAL |
| 18 | j | 24 | LEU |
| 18 | j | 56 | PHE |
| 18 | j | 57 | LEU |
| 18 | j | 63 | LEU |
| 18 | j | 82 | ASN |
| 18 | j | 97 | LEU |
| 18 | j | 109 | LYS |
| 18 | j | 113 | TRP |
| 19 | k | 3 | LEU |
| 19 | k | 4 | VAL |
| 19 | k | 26 | LEU |
| 19 | k | 43 | MET |
| 19 | k | 59 | MET |
| 20 | m | 45 | LEU |
| 20 | m | 57 | PHE |
| 20 | m | 64 | MET |
| 20 | m | 65 | LEU |
| 20 | m | 66 | VAL |
| 20 | m | 74 | MET |
| 20 | m | 82 | VAL |
| 20 | m | 103 | MET |
| 20 | m | 135 | PHE |
| 20 | m | 136 | PHE |
| 20 | m | 151 | THR |
| 21 | n | 17 | VAL |
| 21 | n | 39 | ARG |
| 21 | n | 44 | LEU |
| 21 | n | 57 | TRP |
| 22 | o | 5 | LYS |
| 22 | o | 66 | ILE |
| 22 | o | 95 | ILE |
| 23 | p | 76 | ARG |
| 23 | p | 77 | ASP |
| 23 | p | 97 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | p | 101 | LYS |
| 23 | p | 110 | GLU |
| 23 | p | 126 | GLU |
| 23 | p | 165 | GLU |
| 23 | p | 176 | GLU |
| 23 | p | 192 | ARG |
| 23 | p | 204 | ASP |
| 24 | q | 4 | ILE |
| 24 | q | 11 | LEU |
| 24 | q | 14 | MET |
| 24 | q | 36 | LEU |
| 24 | q | 61 | LEU |
| 24 | q | 87 | GLU |
| 24 | q | 200 | ILE |
| 24 | q | 230 | VAL |
| 24 | q | 247 | THR |
| 24 | q | 250 | LEU |
| 24 | q | 270 | ILE |
| 24 | q | 282 | LEU |
| 24 | q | 315 | LEU |
| 24 | q | 343 | ILE |
| 24 | q | 369 | LEU |
| 24 | q | 375 | LEU |
| 24 | q | 426 | ILE |
| 24 | q | 454 | ILE |
| 25 | r | 5 | ASN |
| 25 | r | 13 | ILE |
| 25 | r | 106 | LEU |
| 25 | r | 108 | MET |
| 25 | r | 111 | LEU |
| 25 | r | 117 | LEU |
| 25 | r | 124 | ASN |
| 25 | r | 140 | ILE |
| 25 | r | 150 | LEU |
| 25 | r | 151 | LEU |
| 25 | r | 170 | GLU |
| 25 | r | 214 | GLU |
| 25 | r | 224 | PHE |
| 25 | r | 227 | GLU |
| 25 | r | 241 | LEU |
| 25 | r | 253 | GLU |
| 25 | r | 285 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | r | 286 | MET |
| 26 | B | 41 | ILE |
| 26 | B | 54 | LYS |
| 26 | B | 71 | LYS |
| 26 | B | 83 | SER |
| 26 | B | 102 | MET |
| 26 | B | 134 | ASP |
| 26 | B | 294 | VAL |
| 26 | B | 302 | LYS |
| 26 | B | 317 | VAL |
| 26 | B | 327 | ILE |
| 26 | B | 357 | MET |
| 26 | B | 382 | CYS |
| 26 | B | 390 | ASP |
| 26 | B | 424 | ILE |
| 26 | B | 445 | GLU |
| 27 | C | 52 | GLN |
| 27 | C | 57 | VAL |
| 27 | C | 75 | VAL |
| 27 | C | 76 | ASP |
| 27 | C | 81 | THR |
| 27 | C | 86 | LEU |
| 27 | C | 100 | VAL |
| 27 | C | 111 | MET |
| 27 | C | 124 | ARG |
| 27 | C | 143 | ASP |
| 27 | C | 147 | TYR |
| 27 | C | 148 | VAL |
| 27 | C | 150 | MET |
| 27 | C | 159 | LEU |
| 27 | C | 164 | LEU |
| 27 | C | 165 | LEU |
| 27 | C | 167 | ILE |
| 27 | C | 191 | MET |
| 27 | C | 194 | THR |
| 27 | C | 223 | VAL |
| 27 | C | 238 | VAL |
| 27 | C | 240 | GLN |
| 27 | C | 249 | ASP |
| 27 | C | 254 | SER |
| 27 | C | 264 | LEU |
| 27 | C | 266 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27 | C | 284 | VAL |
| 27 | C | 304 | ILE |
| 27 | C | 314 | TYR |
| 27 | C | 316 | VAL |
| 27 | C | 361 | GLU |
| 27 | C | 362 | ILE |
| 27 | C | 377 | MET |
| 27 | C | 418 | VAL |
| 27 | C | 449 | MET |
| 27 | C | 450 | LEU |
| 27 | C | 459 | THR |
| 27 | C | 463 | VAL |
| 28 | D | 68 | ILE |
| 28 | D | 81 | PHE |
| 28 | D | 111 | LEU |
| 28 | D | 113 | ASP |
| 28 | D | 119 | VAL |
| 28 | D | 136 | ARG |
| 28 | D | 140 | ARG |
| 28 | D | 143 | VAL |
| 28 | D | 145 | THR |
| 28 | D | 147 | THR |
| 28 | D | 149 | GLU |
| 28 | D | 154 | GLU |
| 28 | D | 159 | VAL |
| 28 | D | 194 | GLU |
| 28 | D | 201 | ASP |
| 28 | D | 204 | LEU |
| 28 | D | 215 | GLU |
| 28 | D | 219 | VAL |
| 28 | D | 250 | GLU |
| 29 | E | 42 | ARG |
| 29 | E | 58 | GLU |
| 29 | E | 85 | LEU |
| 29 | E | 137 | THR |
| 29 | E | 172 | ILE |
| 29 | E | 176 | CYS |
| 29 | E | 201 | ILE |
| 29 | E | 209 | LYS |
| 29 | E | 249 | LEU |
| 30 | F | 29 | VAL |
| 30 | F | 37 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | F | 46 | ASP |
| 30 | F | 57 | ASP |
| 30 | F | 79 | VAL |
| 30 | F | 85 | SER |
| 31 | H | 70 | LEU |
| 31 | H | 83 | THR |
| 31 | H | 114 | ILE |
| 31 | H | 118 | LEU |
| 31 | H | 150 | THR |
| 31 | H | 152 | CYS |
| 31 | H | 174 | GLU |
| 32 | I | 47 | VAL |
| 32 | I | 71 | CYS |
| 32 | I | 86 | MET |
| 32 | I | 169 | THR |
| 33 | J | 86 | ASN |
| 33 | J | 124 | LEU |
| 33 | J | 125 | VAL |
| 33 | J | 146 | ASP |
| 34 | K | 59 | HIS |
| 34 | K | 129 | THR |
| 34 | K | 136 | GLU |
| 34 | K | 144 | TYR |
| 35 | L | 119 | ASN |
| 35 | L | 170 | LYS |
| 35 | L | 174 | ARG |
| 35 | L | 175 | TYR |
| 35 | L | 177 | ARG |
| 35 | L | 205 | GLU |
| 35 | L | 235 | VAL |
| 35 | L | 254 | LYS |
| 35 | L | 270 | ASP |
| 35 | L | 286 | TYR |
| 35 | L | 299 | LEU |
| 35 | L | 302 | VAL |
| 35 | L | 305 | PHE |
| 35 | L | 308 | TRP |
| 35 | L | 309 | THR |
| 35 | L | 310 | THR |
| 35 | L | 323 | THR |
| 35 | L | 341 | GLU |
| 35 | L | 354 | TYR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | L | 355 | ARG |
| 36 | N | 5 | LEU |
| 36 | N | 40 | LYS |
| 36 | N | 87 | GLU |
| 36 | N | 88 | LEU |
| 36 | N | 94 | MET |
| 37 | O | 76 | LEU |
| 37 | O | 96 | GLU |
| 37 | O | 98 | LEU |
| 37 | O | 106 | LYS |
| 37 | O | 114 | ASP |
| 37 | O | 115 | GLN |
| 37 | O | 118 | ILE |
| 37 | O | 124 | ASP |
| 37 | O | 133 | ILE |
| 38 | P | 19 | ILE |
| 38 | P | 20 | ARG |
| 38 | P | 45 | LYS |
| 38 | P | 85 | ASP |
| 38 | P | 92 | GLU |
| 39 | Q | 67 | ARG |
| 39 | Q | 108 | LEU |
| 39 | Q | 117 | GLU |
| 39 | Q | 122 | VAL |
| 39 | Q | 127 | THR |
| 40 | R | 76 | LEU |
| 40 | R | 80 | GLU |
| 41 | S | 3 | PHE |
| 42 | T | 100 | LYS |
| 42 | T | 134 | THR |
| 42 | T | 142 | LEU |
| 42 | T | 151 | VAL |
| 42 | T | 166 | LEU |
| 43 | U | 43 | LEU |
| 43 | U | 69 | CYS |
| 43 | U | 117 | GLU |
| 43 | U | 152 | LEU |
| 43 | U | 172 | LEU |
| 43 | U | 232 | THR |
| 43 | U | 240 | GLU |
| 43 | U | 245 | LYS |
| 43 | U | 250 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | U | 253 | GLU |
| 43 | U | 255 | CYS |
| 43 | U | 263 | ARG |
| 43 | U | 281 | ASP |
| 43 | U | 347 | GLU |
| 43 | U | 352 | LYS |
| 44 | V | 3 | LYS |
| 44 | V | 6 | LEU |
| 44 | V | 104 | ARG |
| 44 | V | 115 | CYS |
| 44 | V | 140 | LYS |
| 44 | V | 141 | VAL |
| 45 | W | 80 | ASP |
| 45 | W | 99 | LYS |
| 45 | W | 101 | VAL |
| 45 | W | 110 | VAL |
| 45 | W | 131 | GLU |
| 37 | X | 76 | LEU |
| 37 | X | 89 | LEU |
| 37 | X | 129 | GLU |
| 37 | X | 133 | ILE |
| 37 | X | 138 | LEU |
| 46 | Y | 46 | GLN |
| 46 | Y | 76 | ASP |
| 46 | Y | 80 | VAL |
| 46 | Y | 81 | LEU |
| 46 | Y | 88 | ASP |
| 46 | Y | 92 | TRP |
| 47 | Z | 41 | GLU |
| 47 | Z | 59 | ASP |
| 47 | Z | 67 | TRP |
| 47 | Z | 101 | GLU |
| 48 | l | 7 | LEU |
| 48 | l | 34 | ASN |
| 48 | l | 36 | VAL |
| 48 | l | 59 | GLN |
| 48 | l | 60 | GLU |
| 48 | l | 62 | ILE |
| 48 | l | 65 | ASN |
| 48 | l | 70 | THR |
| 48 | l | 105 | MET |
| 48 | l | 169 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | l | 246 | LEU |
| 48 | l | 247 | LEU |
| 48 | l | 268 | GLU |
| 48 | l | 271 | LYS |
| 48 | l | 314 | MET |
| 48 | l | 321 | GLN |
| 48 | l | 340 | PHE |
| 48 | l | 351 | ASN |
| 48 | l | 364 | LYS |
| 48 | l | 383 | MET |
| 48 | l | 387 | THR |
| 48 | l | 397 | GLU |
| 48 | l | 407 | TRP |
| 48 | l | 411 | MET |
| 48 | l | 434 | LYS |
| 48 | l | 440 | LEU |
| 48 | l | 445 | GLU |
| 48 | l | 481 | THR |
| 48 | l | 486 | MET |
| 48 | l | 502 | LEU |
| 48 | l | 554 | ASP |
| 48 | l | 559 | GLU |
| 48 | l | 565 | THR |
| 48 | l | 589 | LEU |
| 49 | s | 83 | GLU |
| 49 | s | 88 | GLU |
| 49 | s | 129 | ASP |
| 49 | s | 135 | GLU |
| 49 | s | 175 | ARG |
| 49 | s | 188 | VAL |
| 49 | s | 191 | LYS |
| 49 | s | 214 | LEU |
| 49 | s | 216 | GLU |
| 50 | t | 21 | ARG |
| 50 | t | 29 | TYR |
| 50 | t | 31 | PHE |
| 50 | t | 33 | GLU |
| 50 | t | 39 | MET |
| 50 | t | 42 | THR |
| 50 | t | 65 | GLN |
| 50 | t | 83 | GLU |
| 50 | t | 88 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | t | 91 | GLU |
| 51 | u | 35 | THR |
| 51 | u | 84 | GLU |
| 51 | u | 94 | GLU |
| 51 | u | 95 | HIS |
| 51 | u | 138 | LYS |
| 51 | u | 181 | ASP |
| 51 | u | 206 | GLU |
| 51 | u | 256 | THR |
| 51 | u | 259 | GLU |
| 51 | u | 274 | GLU |
| 51 | u | 341 | PHE |
| 51 | u | 342 | GLN |
| 51 | u | 350 | GLU |
| 51 | u | 363 | MET |
| 51 | u | 368 | MET |
| 51 | u | 375 | GLN |
| 51 | u | 384 | THR |
| 51 | u | 411 | GLU |
| 51 | u | 467 | ASP |
| 5 | v | 47 | LEU |
| 5 | v | 83 | LEU |
| 5 | v | 122 | THR |
| 5 | v | 124 | GLU |
| 5 | v | 129 | ASP |
| 5 | v | 130 | ILE |
| 5 | v | 147 | ARG |
| 5 | v | 158 | LEU |
| 5 | v | 161 | ASP |
| 5 | v | 174 | LEU |
| 5 | v | 175 | GLU |
| 5 | v | 203 | ASP |
| 5 | v | 231 | LYS |
| 5 | v | 233 | VAL |
| 5 | v | 250 | LYS |
| 5 | v | 322 | ASP |
| 5 | v | 329 | SER |
| 5 | v | 401 | LEU |
| 5 | v | 407 | VAL |
| 5 | v | 421 | ASP |
| 5 | v | 451 | ASP |
| 6 | w | 83 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | w | 97 | HIS |
| 6 | w | 233 | LEU |
| 6 | w | 264 | THR |
| 6 | w | 273 | TYR |
| 6 | w | 281 | LEU |
| 6 | w | 311 | LYS |
| 6 | w | 366 | MET |
| 6 | w | 379 | TRP |
| 7 | x | 107 | ASP |
| 7 | x | 129 | ASP |
| 7 | x | 136 | LEU |
| 7 | x | 152 | GLU |
| 7 | x | 164 | GLU |
| 7 | x | 221 | GLU |
| 7 | x | 243 | ILE |
| 7 | x | 249 | ILE |
| 7 | x | 320 | LEU |
| 8 | y | 15 | GLU |
| 8 | y | 72 | ARG |
| 8 | y | 75 | ILE |
| 8 | y | 79 | GLU |
| 8 | y | 83 | LYS |
| 8 | y | 85 | GLU |
| 52 | z | 16 | THR |
| 52 | z | 19 | LEU |
| 52 | z | 40 | ARG |
| 52 | z | 47 | LEU |
| 52 | z | 68 | GLU |
| 51 | 5 | 84 | GLU |
| 51 | 5 | 98 | PHE |
| 51 | 5 | 101 | THR |
| 51 | 5 | 142 | LYS |
| 51 | 5 | 164 | GLU |
| 51 | 5 | 183 | VAL |
| 51 | 5 | 244 | ASP |
| 51 | 5 | 266 | THR |
| 51 | 5 | 284 | LEU |
| 51 | 5 | 327 | THR |
| 51 | 5 | 350 | GLU |
| 51 | 5 | 363 | MET |
| 51 | 5 | 368 | MET |
| 51 | 5 | 411 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | G | 41 | VAL |
| 53 | G | 44 | GLU |
| 53 | G | 94 | MET |
| 53 | G | 107 | GLU |
| 53 | G | 158 | ARG |
| 53 | G | 197 | THR |
| 53 | G | 217 | GLU |
| 53 | G | 225 | ILE |
| 53 | G | 241 | ARG |
| 53 | G | 247 | LYS |
| 53 | G | 252 | ASP |
| 53 | G | 310 | GLU |
| 53 | G | 311 | LYS |
| 53 | G | 325 | ARG |
| 53 | G | 329 | MET |
| 53 | G | 338 | VAL |
| 53 | G | 347 | ASP |
| 53 | G | 349 | GLU |
| 53 | G | 361 | VAL |
| 53 | G | 426 | ASP |
| 53 | G | 447 | ASP |
| 53 | G | 450 | LYS |
| 53 | G | 470 | LYS |
| 53 | G | 493 | VAL |
| 53 | G | 511 | LYS |
| 53 | G | 512 | VAL |
| 53 | G | 513 | MET |
| 53 | G | 519 | ILE |
| 53 | G | 592 | LYS |
| 53 | G | 617 | ARG |
| 53 | G | 632 | MET |
| 53 | G | 636 | TYR |
| 53 | G | 657 | ASP |
| 53 | G | 659 | VAL |
| 53 | G | 671 | LEU |
| 53 | G | 679 | LEU |
| 53 | G | 680 | LEU |
| 54 | M | 10 | LEU |
| 54 | M | 25 | GLN |
| 54 | M | 31 | ILE |
| 54 | M | 64 | MET |
| 54 | M | 69 | VAL |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | M | 91 | GLU |
| 3 | Ae | 50 | CYS |
| 3 | Ae | 59 | LEU |
| 3 | Af | 53 | VAL |
| 3 | Af | 62 | THR |
| 3 | Af | 68 | LEU |
| 3 | Af | 72 | ARG |
| 52 | Aa | 5 | PHE |
| 52 | Aa | 32 | THR |
| 52 | Aa | 47 | LEU |
| 52 | Aa | 48 | ARG |
| 52 | Aa | 79 | GLU |
| 1 | Ab | 26 | LEU |
| 1 | Ab | 27 | VAL |
| 1 | Ab | 35 | GLU |
| 1 | Ab | 37 | CYS |
| 1 | Ab | 54 | ASP |
| 1 | Ab | 66 | ASP |
| 1 | Ab | 69 | GLU |
| 1 | Ab | 81 | CYS |
| 1 | Ab | 85 | LYS |
| 1 | Ab | 91 | LYS |
| 2 | Ac | 13 | LEU |
| 2 | Ac | 14 | LEU |
| 2 | Ac | 30 | LEU |
| 2 | Ac | 54 | LYS |
| 4 | Ad | 13 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 0 | 39 | GLN |
| 1 | 0 | 62 | GLN |
| 3 | 2 | 156 | GLN |
| 3 | 2 | 207 | GLN |
| 4 | 3 | 16 | ASN |
| 3 | 4 | 156 | GLN |
| 3 | 4 | 215 | GLN |
| 3 | 4 | 240 | HIS |
| 5 | 6 | 36 | GLN |
| 5 | 6 | 139 | ASN |
| 5 | 6 | 168 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 6 | 170 | GLN |
| 5 | 6 | 176 | ASN |
| 5 | 6 | 268 | HIS |
| 5 | 6 | 291 | HIS |
| 5 | 6 | 304 | ASN |
| 5 | 6 | 311 | GLN |
| 5 | 6 | 318 | HIS |
| 5 | 6 | 319 | GLN |
| 5 | 6 | 446 | HIS |
| 6 | 7 | 85 | ASN |
| 6 | 7 | 137 | GLN |
| 6 | 7 | 196 | HIS |
| 6 | 7 | 201 | HIS |
| 6 | 7 | 260 | ASN |
| 6 | 7 | 286 | ASN |
| 6 | 7 | 312 | GLN |
| 6 | 7 | 374 | ASN |
| 7 | 8 | 116 | GLN |
| 7 | 8 | 120 | GLN |
| 7 | 8 | 126 | HIS |
| 7 | 8 | 190 | ASN |
| 7 | 8 | 191 | ASN |
| 7 | 8 | 206 | HIS |
| 7 | 8 | 283 | HIS |
| 7 | 8 | 310 | HIS |
| 8 | 9 | 23 | ASN |
| 9 | a | 170 | GLN |
| 11 | c | 83 | GLN |
| 11 | c | 94 | HIS |
| 12 | d | 23 | GLN |
| 12 | d | 55 | GLN |
| 12 | d | 114 | GLN |
| 13 | e | 70 | ASN |
| 15 | g | 81 | GLN |
| 16 | h | 25 | GLN |
| 16 | h | 82 | GLN |
| 16 | h | 97 | HIS |
| 17 | i | 49 | ASN |
| 17 | i | 112 | HIS |
| 17 | i | 171 | ASN |
| 17 | i | 197 | ASN |
| 17 | i | 221 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | i | 289 | ASN |
| 18 | j | 26 | GLN |
| 20 | m | 86 | ASN |
| 21 | n | 40 | ASN |
| 23 | p | 75 | HIS |
| 23 | p | 93 | HIS |
| 24 | q | 180 | HIS |
| 24 | q | 184 | HIS |
| 24 | q | 279 | GLN |
| 24 | q | 304 | GLN |
| 24 | q | 338 | HIS |
| 24 | q | 366 | ASN |
| 24 | q | 390 | ASN |
| 25 | r | 247 | HIS |
| 25 | r | 287 | HIS |
| 26 | B | 133 | HIS |
| 26 | B | 170 | GLN |
| 26 | B | 244 | ASN |
| 26 | B | 376 | HIS |
| 26 | B | 418 | GLN |
| 26 | B | 456 | GLN |
| 27 | C | 240 | GLN |
| 27 | C | 305 | GLN |
| 27 | C | 386 | HIS |
| 27 | C | 448 | HIS |
| 28 | D | 51 | ASN |
| 28 | D | 77 | GLN |
| 28 | D | 124 | ASN |
| 28 | D | 138 | ASN |
| 28 | D | 181 | HIS |
| 28 | D | 228 | GLN |
| 29 | E | 87 | GLN |
| 29 | E | 123 | ASN |
| 29 | E | 133 | GLN |
| 29 | E | 153 | GLN |
| 30 | F | 63 | ASN |
| 30 | F | 120 | GLN |
| 32 | I | 111 | ASN |
| 33 | J | 86 | ASN |
| 35 | L | 32 | HIS |
| 35 | L | 74 | GLN |
| 35 | L | 117 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | L | 123 | ASN |
| 35 | L | 264 | ASN |
| 35 | L | 326 | HIS |
| 36 | N | 21 | HIS |
| 36 | N | 73 | GLN |
| 39 | Q | 74 | HIS |
| 39 | Q | 96 | ASN |
| 39 | Q | 98 | HIS |
| 40 | R | 79 | HIS |
| 41 | S | 25 | HIS |
| 41 | S | 44 | GLN |
| 41 | S | 68 | ASN |
| 42 | T | 125 | ASN |
| 43 | U | 204 | HIS |
| 43 | U | 217 | GLN |
| 45 | W | 8 | GLN |
| 45 | W | 76 | GLN |
| 46 | Y | 54 | GLN |
| 48 | l | 56 | HIS |
| 48 | l | 59 | GLN |
| 48 | l | 65 | ASN |
| 48 | l | 72 | GLN |
| 48 | l | 135 | ASN |
| 48 | l | 170 | GLN |
| 48 | l | 309 | GLN |
| 48 | l | 354 | GLN |
| 48 | l | 470 | ASN |
| 48 | l | 506 | ASN |
| 49 | s | 108 | HIS |
| 49 | s | 112 | GLN |
| 49 | s | 181 | GLN |
| 49 | s | 240 | HIS |
| 50 | t | 4 | HIS |
| 50 | t | 44 | GLN |
| 50 | t | 61 | HIS |
| 50 | t | 82 | HIS |
| 50 | t | 92 | HIS |
| 51 | u | 160 | GLN |
| 51 | u | 323 | HIS |
| 51 | u | 342 | GLN |
| 51 | u | 397 | ASN |
| 5 | v | 157 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | v | 168 | ASN |
| 5 | v | 212 | HIS |
| 5 | v | 268 | HIS |
| 5 | v | 311 | GLN |
| 5 | v | 372 | GLN |
| 6 | w | 3 | ASN |
| 6 | w | 196 | HIS |
| 6 | w | 255 | ASN |
| 7 | x | 120 | GLN |
| 7 | x | 241 | GLN |
| 7 | x | 283 | HIS |
| 8 | y | 23 | ASN |
| 51 | 5 | 52 | GLN |
| 51 | 5 | 119 | HIS |
| 51 | 5 | 277 | HIS |
| 51 | 5 | 362 | ASN |
| 53 | G | 30 | ASN |
| 53 | G | 74 | ASN |
| 53 | G | 123 | ASN |
| 53 | G | 142 | GLN |
| 53 | G | 278 | HIS |
| 53 | G | 304 | GLN |
| 53 | G | 359 | ASN |
| 53 | G | 425 | ASN |
| 53 | G | 569 | GLN |
| 53 | G | 604 | GLN |
| 53 | G | 666 | GLN |
| 53 | G | 678 | GLN |
| 3 | Af | 56 | HIS |
| 52 | Aa | 13 | HIS |
| 1 | Ab | 76 | HIS |
| 2 | Ac | 48 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 56 | HEM | w | 401 | - | 42,50,50 | 1.46 | 4 (9%) | 46,82,82 | 1.28 | 4 (8%) |
| 55 | FES | E | 301 | 29 | 0,4,4 | - | - | - | - | - |
| 58 | FMN | B | 501 | - | 33,33,33 | 1.11 | 3 (9%) | 48,50,50 | 1.23 | 8 (16%) |
| 56 | HEM | 7 | 401 | 6 | 42,50,50 | 1.35 | 7 (16%) | 46,82,82 | 1.83 | 10 (21%) |
| 59 | SF4 | H | 302 | 31 | 0,12,12 | - | - | - | - | - |
| 59 | SF4 | B | 502 | 26 | 0,12,12 | - | - | - | - | - |
| 59 | SF4 | G | 801 | 53 | 0,12,12 | - | - | - | - | - |
| 59 | SF4 | G | 802 | 53 | 0,12,12 | - | - | - | - | - |
| 61 | ZMP | Q | 201 | - | 27,29,36 | 1.86 | 5 (18%) | 34,38,45 | 1.74 | 8 (23%) |
| 59 | SF4 | I | 201 | 32 | 0,12,12 | - | - | - | - | - |
| 57 | HEC | 8 | 401 | 7 | 32,50,50 | 2.63 | 12 (37%) | 30,82,82 | 1.99 | 7 (23%) |
| 59 | SF4 | H | 301 | 31 | 0,12,12 | - | - | - | - | - |
| 55 | FES | G | 803 | 53 | 0,4,4 | - | - | - | - | - |
| 55 | FES | 4 | 301 | 3 | 0,4,4 | - | - | - | - | - |
| 55 | FES | 2 | 301 | 3 | 0,4,4 | - | - | - | - | - |
| 56 | HEM | w | 402 | 6 | 42,50,50 | 1.46 | 5 (11%) | 46,82,82 | 1.17 | 2 (4%) |
| 56 | HEM | 7 | 402 | - | 42,50,50 | 1.50 | 4 (9%) | 46,82,82 | 1.24 | 7 (15%) |
| 60 | NDP | L | 401 | - | 47,52,52 | 0.64 | 0 | 61,80,80 | 0.99 | 3 (4%) |
| 57 | HEC | x | 401 | 7 | 32,50,50 | 2.14 | 3 (9%) | 30,82,82 | 2.37 | 7 (23%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 56 | HEM | w | 401 | - | - | 0/12/54/54 | - |
| 55 | FES | E | 301 | 29 | - | - | 0/1/1/1 |
| 58 | FMN | B | 501 | - | - | 0/18/18/18 | 0/3/3/3 |
| 56 | HEM | 7 | 401 | 6 | - | 4/12/54/54 | - |
| 59 | SF4 | H | 302 | 31 | - | - | 0/6/5/5 |
| 59 | SF4 | B | 502 | 26 | - | - | 0/6/5/5 |
| 59 | SF4 | G | 801 | 53 | - | - | 0/6/5/5 |
| 59 | SF4 | G | 802 | 53 | - | - | 0/6/5/5 |
| 61 | ZMP | Q | 201 | - | - | 11/36/36/43 | - |
| 59 | SF4 | I | 201 | 32 | - | - | 0/6/5/5 |
| 57 | HEC | 8 | 401 | 7 | - | 7/10/54/54 | - |
| 59 | SF4 | H | 301 | 31 | - | - | 0/6/5/5 |
| 55 | FES | G | 803 | 53 | - | - | 0/1/1/1 |
| 55 | FES | 4 | 301 | 3 | - | - | 0/1/1/1 |
| 55 | FES | 2 | 301 | 3 | - | - | 0/1/1/1 |
| 56 | HEM | w | 402 | 6 | - | 1/12/54/54 | - |
| 56 | HEM | 7 | 402 | - | - | 6/12/54/54 | - |
| 60 | NDP | L | 401 | - | - | 4/30/77/77 | 0/5/5/5 |
| 57 | HEC | x | 401 | 7 | - | 4/10/54/54 | - |

All (43) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 57 | 8 | 401 | HEC | C3C-C2C | 7.58 | 1.49 | 1.40 |
| 57 | 8 | 401 | HEC | C2B-C3B | 7.09 | 1.48 | 1.40 |
| 57 | x | 401 | HEC | C3C-C2C | -6.59 | 1.33 | 1.40 |
| 57 | x | 401 | HEC | C2B-C3B | -5.63 | 1.34 | 1.40 |
| 61 | Q | 201 | ZMP | C13-N1 | 5.36 | 1.46 | 1.33 |
| 57 | x | 401 | HEC | C3D-C2D | 5.24 | 1.53 | 1.37 |
| 61 | Q | 201 | ZMP | C16-N2 | 5.17 | 1.45 | 1.33 |
| 56 | w | 402 | HEM | C3C-C2C | -4.56 | 1.34 | 1.40 |
| 56 | 7 | 402 | HEM | C3C-C2C | -4.39 | 1.34 | 1.40 |
| 56 | w | 401 | HEM | C3C-C2C | -4.38 | 1.34 | 1.40 |
| 57 | 8 | 401 | HEC | C4B-C3B | 3.59 | 1.49 | 1.43 |
| 57 | 8 | 401 | HEC | C3D-C2D | 3.53 | 1.48 | 1.37 |
| 57 | 8 | 401 | HEC | C2A-C3A | 3.53 | 1.48 | 1.37 |
| 56 | 7 | 402 | HEM | C3C-CAC | 3.47 | 1.55 | 1.47 |
| 57 | 8 | 401 | HEC | C1C-CHC | 3.46 | 1.50 | 1.41 |
| 56 | w | 401 | HEM | C3C-CAC | 3.45 | 1.55 | 1.47 |
| 58 | B | 501 | FMN | C4A-N5 | 3.41 | 1.38 | 1.30 |
| 57 | 8 | 401 | HEC | C3C-C4C | 3.31 | 1.49 | 1.43 |
| 56 | 7 | 401 | HEM | C1B-NB | -3.29 | 1.34 | 1.40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 56 | w | 402 | HEM | C3C-CAC | 3.29 | 1.55 | 1.47 |
| 56 | 7 | 401 | HEM | C4D-ND | -3.21 | 1.34 | 1.40 |
| 57 | 8 | 401 | HEC | C2A-C1A | 3.10 | 1.49 | 1.42 |
| 56 | w | 401 | HEM | CAB-C3B | 3.01 | 1.55 | 1.47 |
| 56 | 7 | 402 | HEM | CAB-C3B | 2.99 | 1.55 | 1.47 |
| 57 | 8 | 401 | HEC | C4D-CHA | 2.98 | 1.49 | 1.41 |
| 56 | w | 402 | HEM | CAB-C3B | 2.86 | 1.55 | 1.47 |
| 57 | 8 | 401 | HEC | C3A-C4A | 2.71 | 1.48 | 1.42 |
| 61 | Q | 201 | ZMP | O2-C13 | -2.65 | 1.18 | 1.23 |
| 57 | 8 | 401 | HEC | C1B-CHB | 2.58 | 1.48 | 1.41 |
| 61 | Q | 201 | ZMP | C10-S1 | 2.56 | 1.82 | 1.76 |
| 61 | Q | 201 | ZMP | O3-C16 | -2.53 | 1.18 | 1.23 |
| 56 | 7 | 402 | HEM | C3C-C4C | 2.52 | 1.45 | 1.41 |
| 57 | 8 | 401 | HEC | C1D-CHD | 2.51 | 1.48 | 1.41 |
| 56 | 7 | 401 | HEM | FE-NB | 2.50 | 2.11 | 1.98 |
| 56 | w | 401 | HEM | C3C-C4C | 2.40 | 1.44 | 1.41 |
| 56 | 7 | 401 | HEM | C1D-ND | -2.28 | 1.34 | 1.38 |
| 56 | 7 | 401 | HEM | CHB-C1B | 2.27 | 1.40 | 1.34 |
| 56 | w | 402 | HEM | C3C-C4C | 2.21 | 1.44 | 1.41 |
| 56 | 7 | 401 | HEM | C3B-C4B | 2.19 | 1.49 | 1.44 |
| 58 | B | 501 | FMN | C10-N1 | 2.10 | 1.37 | 1.33 |
| 56 | 7 | 401 | HEM | C4B-NB | -2.06 | 1.34 | 1.38 |
| 56 | w | 402 | HEM | CMB-C2B | 2.03 | 1.54 | 1.50 |
| 58 | B | 501 | FMN | C4A-C10 | -2.01 | 1.38 | 1.44 |

All (56) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 57 | x | 401 | HEC | CBC-CAC-C3C | -8.47 | 107.66 | 127.49 |
| 57 | 8 | 401 | HEC | CMB-C2B-C3B | 5.84 | 132.69 | 125.82 |
| 57 | x | 401 | HEC | CBB-CAB-C3B | -5.49 | 114.65 | 127.49 |
| 60 | L | 401 | NDP | P2B-O2B-C2B | -5.38 | 109.06 | 123.43 |
| 57 | 8 | 401 | HEC | C1D-C2D-C3D | -5.06 | 103.48 | 107.00 |
| 61 | Q | 201 | ZMP | C9-C10-S1 | 4.81 | 119.13 | 113.40 |
| 56 | 7 | 401 | HEM | CHD-C1D-ND | 4.44 | 129.22 | 124.44 |
| 56 | 7 | 401 | HEM | CHC-C4B-NB | 4.17 | 128.92 | 124.44 |
| 57 | x | 401 | HEC | CMB-C2B-C1B | -4.00 | 122.59 | 128.46 |
| 56 | 7 | 401 | HEM | CHB-C1B-NB | 3.75 | 129.02 | 124.37 |
| 61 | Q | 201 | ZMP | O1-C10-C9 | -3.62 | 119.81 | 123.98 |
| 56 | 7 | 401 | HEM | C1B-NB-C4B | 3.51 | 109.36 | 105.21 |
| 58 | B | 501 | FMN | C4-N3-C2 | -3.25 | 119.86 | 125.64 |
| 56 | 7 | 401 | HEM | CHA-C4D-ND | 3.19 | 128.32 | 124.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 57 | x | 401 | HEC | CMC-C2C-C1C | -3.10 | 123.91 | 128.46 |
| 56 | 7 | 401 | HEM | C3B-C4B-NB | -2.98 | 107.33 | 109.47 |
| 61 | Q | 201 | ZMP | O3-C16-N2 | -2.97 | 116.69 | 122.98 |
| 61 | Q | 201 | ZMP | C11-S1-C10 | 2.95 | 110.57 | 101.84 |
| 57 | 8 | 401 | HEC | C4C-C3C-C2C | -2.93 | 103.19 | 106.35 |
| 58 | B | 501 | FMN | C4A-C10-N10 | 2.88 | 120.61 | 116.48 |
| 56 | 7 | 401 | HEM | CHD-C1D-C2D | -2.85 | 120.52 | 125.03 |
| 56 | 7 | 401 | HEM | CBA-CAA-C2A | -2.82 | 107.80 | 112.54 |
| 56 | w | 402 | HEM | C4B-CHC-C1C | 2.78 | 126.23 | 122.56 |
| 57 | 8 | 401 | HEC | CMD-C2D-C3D | 2.78 | 130.19 | 124.94 |
| 61 | Q | 201 | ZMP | C14-C15-N2 | -2.71 | 106.23 | 112.00 |
| 58 | B | 501 | FMN | C4A-C4-N3 | 2.49 | 119.60 | 113.25 |
| 56 | w | 401 | HEM | C4D-ND-C1D | 2.45 | 108.11 | 105.21 |
| 57 | 8 | 401 | HEC | CAD-CBD-CGD | -2.45 | 107.23 | 113.83 |
| 57 | x | 401 | HEC | CBD-CAD-C3D | -2.45 | 108.42 | 112.54 |
| 58 | B | 501 | FMN | O4-C4-C4A | -2.39 | 120.22 | 126.53 |
| 61 | Q | 201 | ZMP | C15-C14-C13 | -2.39 | 108.42 | 112.39 |
| 56 | 7 | 402 | HEM | CMC-C2C-C3C | 2.38 | 129.44 | 124.68 |
| 57 | x | 401 | HEC | CAA-CBA-CGA | -2.36 | 107.48 | 113.83 |
| 56 | 7 | 402 | HEM | CAD-C3D-C2D | -2.35 | 123.46 | 127.87 |
| 58 | B | 501 | FMN | C5A-C9A-N10 | 2.34 | 120.08 | 117.97 |
| 57 | 8 | 401 | HEC | CMC-C2C-C3C | 2.33 | 128.56 | 125.82 |
| 56 | w | 401 | HEM | C3D-C4D-ND | -2.30 | 107.64 | 110.17 |
| 56 | w | 402 | HEM | CBA-CAA-C2A | -2.30 | 108.67 | 112.54 |
| 56 | w | 401 | HEM | CBA-CAA-C2A | -2.29 | 108.69 | 112.54 |
| 61 | Q | 201 | ZMP | C12-N1-C13 | -2.27 | 118.59 | 122.82 |
| 60 | L | 401 | NDP | C5A-C6A-N6A | 2.27 | 123.77 | 120.31 |
| 58 | B | 501 | FMN | C10-C4A-N5 | -2.26 | 120.19 | 124.81 |
| 57 | x | 401 | HEC | CMB-C2B-C3B | 2.24 | 128.46 | 125.82 |
| 56 | 7 | 402 | HEM | CAD-C3D-C4D | 2.24 | 128.60 | 124.70 |
| 56 | 7 | 402 | HEM | CAD-CBD-CGD | -2.17 | 107.90 | 113.67 |
| 56 | w | 401 | HEM | CMC-C2C-C3C | 2.17 | 129.02 | 124.68 |
| 56 | 7 | 401 | HEM | CHB-C1B-C2B | -2.11 | 120.97 | 126.94 |
| 56 | 7 | 402 | HEM | C3D-C4D-ND | -2.09 | 107.88 | 110.17 |
| 60 | L | 401 | NDP | O4D-C1D-C2D | -2.07 | 102.20 | 106.62 |
| 58 | B | 501 | FMN | C9A-C5A-N5 | -2.06 | 120.27 | 122.45 |
| 57 | 8 | 401 | HEC | CMA-C3A-C2A | 2.05 | 128.81 | 124.94 |
| 56 | 7 | 402 | HEM | C3B-C2B-C1B | 2.05 | 107.95 | 106.41 |
| 61 | Q | 201 | ZMP | C17-C16-N2 | 2.04 | 120.34 | 116.48 |
| 58 | B | 501 | FMN | C4'-C3'-C2' | -2.02 | 110.21 | 113.57 |
| 56 | 7 | 402 | HEM | C4D-ND-C1D | 2.02 | 107.60 | 105.21 |
| 56 | 7 | 401 | HEM | CAD-C3D-C4D | 2.02 | 128.21 | 124.70 |

There are no chirality outliers.

All (37) torsion outliers are listed below:

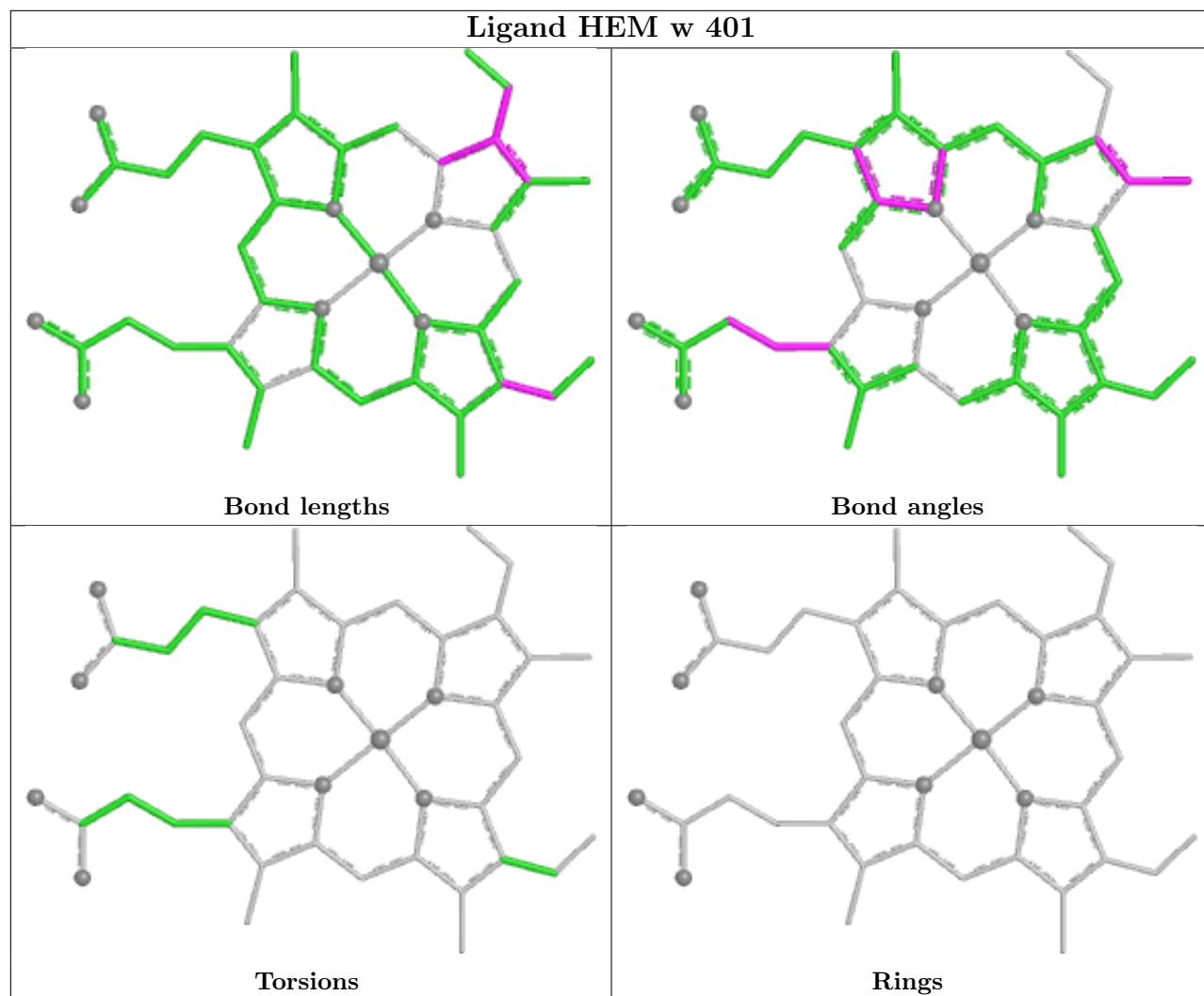
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 56 | 7 | 402 | HEM | C1A-C2A-CAA-CBA |
| 56 | 7 | 402 | HEM | C3A-C2A-CAA-CBA |
| 57 | 8 | 401 | HEC | C2D-C3D-CAD-CBD |
| 57 | 8 | 401 | HEC | C4D-C3D-CAD-CBD |
| 61 | Q | 201 | ZMP | C17-C16-N2-C15 |
| 61 | Q | 201 | ZMP | S1-C11-C12-N1 |
| 61 | Q | 201 | ZMP | C12-C11-S1-C10 |
| 61 | Q | 201 | ZMP | O3-C16-N2-C15 |
| 60 | L | 401 | NDP | O4D-C1D-N1N-C6N |
| 57 | 8 | 401 | HEC | C3D-CAD-CBD-CGD |
| 60 | L | 401 | NDP | O4B-C4B-C5B-O5B |
| 56 | 7 | 402 | HEM | C4D-C3D-CAD-CBD |
| 61 | Q | 201 | ZMP | O3-C16-C17-O4 |
| 56 | 7 | 402 | HEM | C2D-C3D-CAD-CBD |
| 56 | 7 | 401 | HEM | C3D-CAD-CBD-CGD |
| 61 | Q | 201 | ZMP | N2-C16-C17-O4 |
| 61 | Q | 201 | ZMP | O1-C10-S1-C11 |
| 60 | L | 401 | NDP | C3B-C4B-C5B-O5B |
| 61 | Q | 201 | ZMP | C9-C10-S1-C11 |
| 56 | 7 | 401 | HEM | C4B-C3B-CAB-CBB |
| 60 | L | 401 | NDP | O4D-C4D-C5D-O5D |
| 61 | Q | 201 | ZMP | C6-C7-C8-C9 |
| 61 | Q | 201 | ZMP | O3-C16-C17-C18 |
| 61 | Q | 201 | ZMP | N2-C16-C17-C18 |
| 56 | 7 | 401 | HEM | CAA-CBA-CGA-O1A |
| 56 | w | 402 | HEM | C3D-CAD-CBD-CGD |
| 57 | 8 | 401 | HEC | CAD-CBD-CGD-O2D |
| 56 | 7 | 401 | HEM | CAA-CBA-CGA-O2A |
| 57 | 8 | 401 | HEC | CAA-CBA-CGA-O2A |
| 57 | x | 401 | HEC | CAD-CBD-CGD-O2D |
| 57 | x | 401 | HEC | CAA-CBA-CGA-O2A |
| 57 | 8 | 401 | HEC | CAD-CBD-CGD-O1D |
| 57 | x | 401 | HEC | CAA-CBA-CGA-O1A |
| 57 | x | 401 | HEC | CAD-CBD-CGD-O1D |
| 57 | 8 | 401 | HEC | CAA-CBA-CGA-O1A |
| 56 | 7 | 402 | HEM | CAD-CBD-CGD-O1D |
| 56 | 7 | 402 | HEM | CAA-CBA-CGA-O2A |

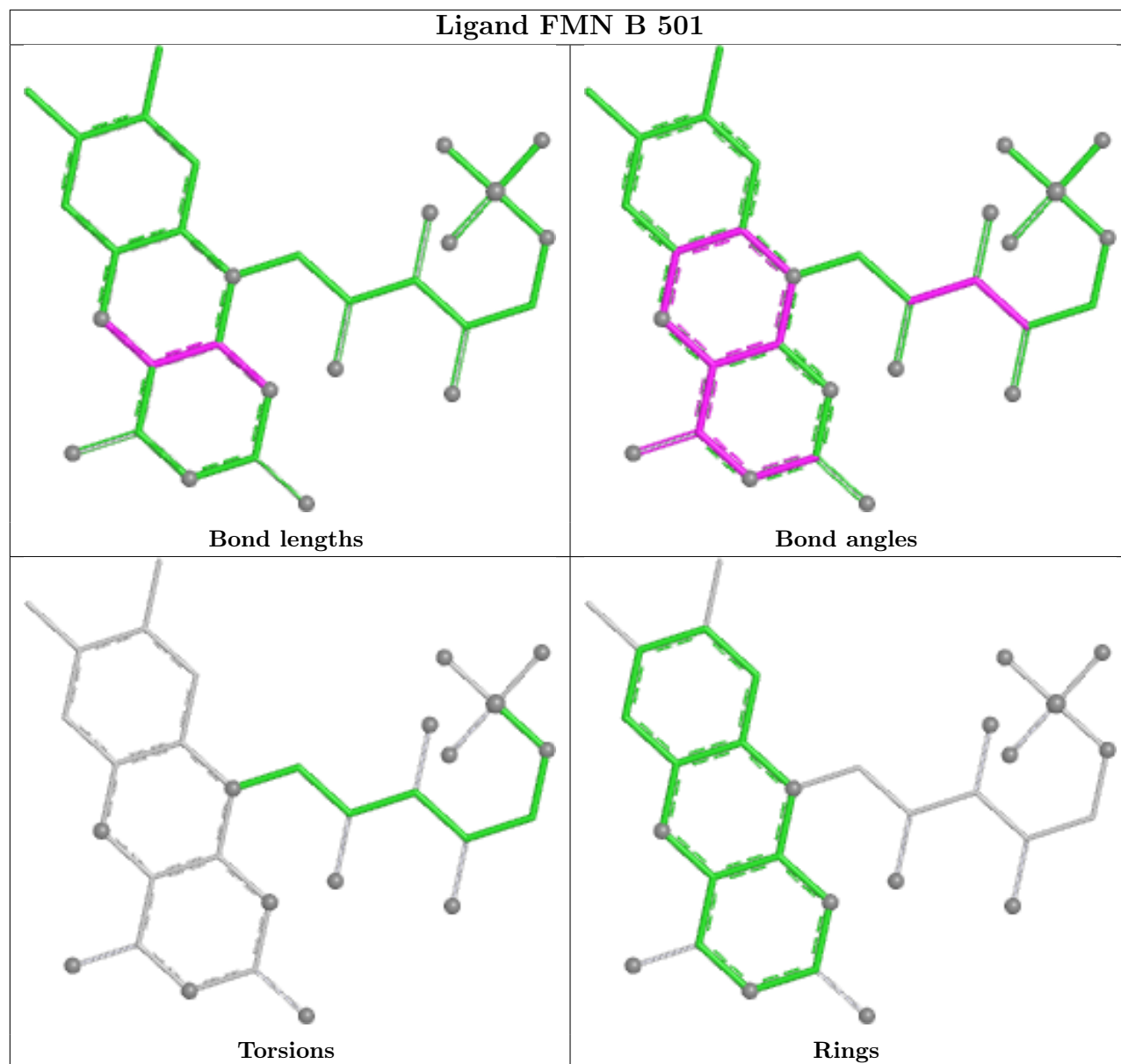
There are no ring outliers.

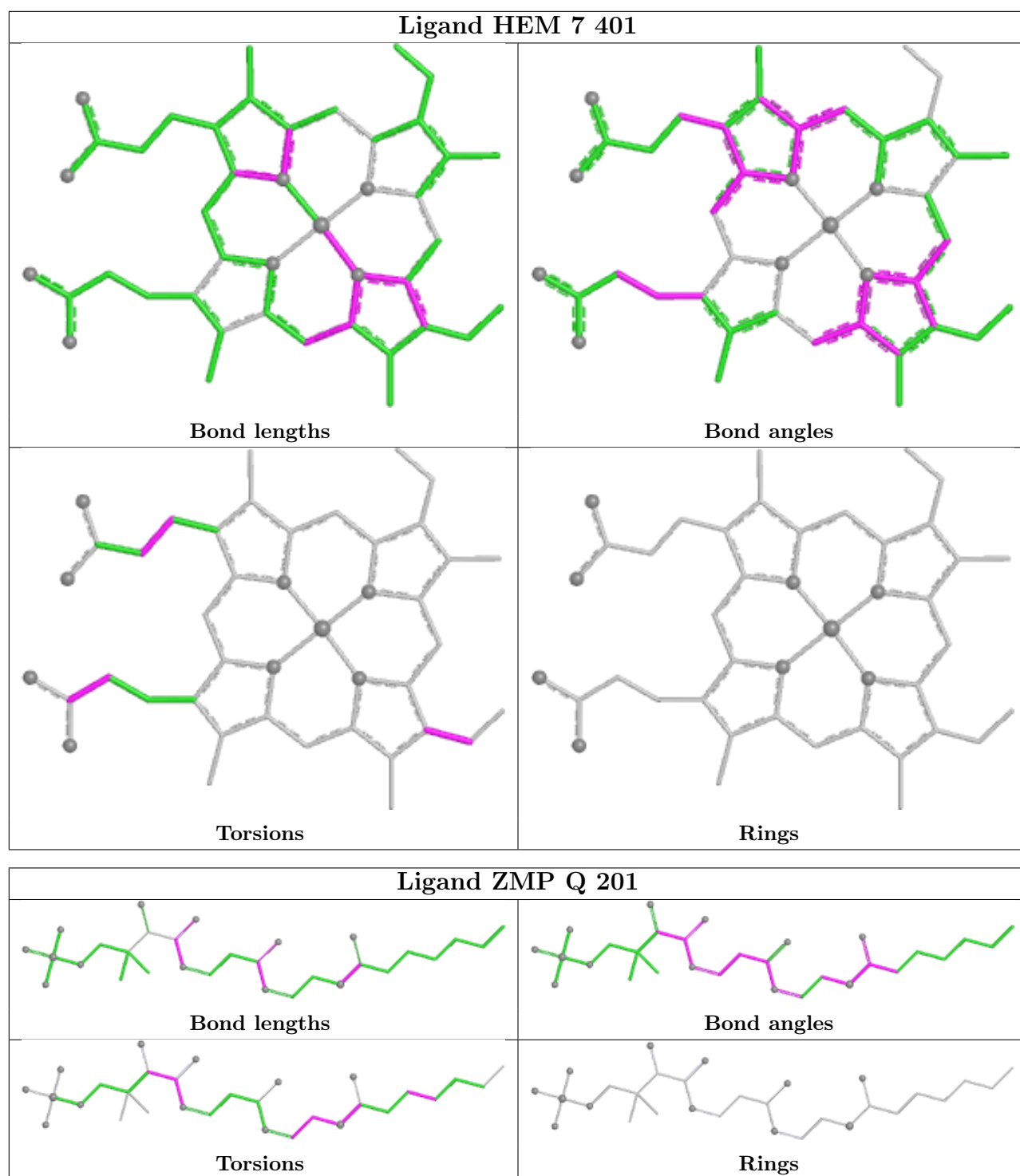
17 monomers are involved in 78 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 56 | w | 401 | HEM | 9 | 0 |
| 55 | E | 301 | FES | 1 | 0 |
| 58 | B | 501 | FMN | 1 | 0 |
| 56 | 7 | 401 | HEM | 7 | 0 |
| 59 | H | 302 | SF4 | 9 | 0 |
| 59 | B | 502 | SF4 | 1 | 0 |
| 59 | G | 801 | SF4 | 1 | 0 |
| 61 | Q | 201 | ZMP | 3 | 0 |
| 59 | I | 201 | SF4 | 1 | 0 |
| 57 | 8 | 401 | HEC | 18 | 0 |
| 59 | H | 301 | SF4 | 2 | 0 |
| 55 | 4 | 301 | FES | 3 | 0 |
| 55 | 2 | 301 | FES | 3 | 0 |
| 56 | w | 402 | HEM | 7 | 0 |
| 56 | 7 | 402 | HEM | 7 | 0 |
| 60 | L | 401 | NDP | 1 | 0 |
| 57 | x | 401 | HEC | 4 | 0 |

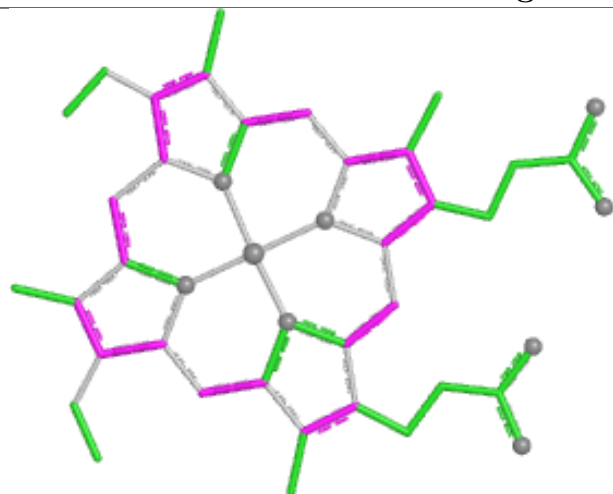
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



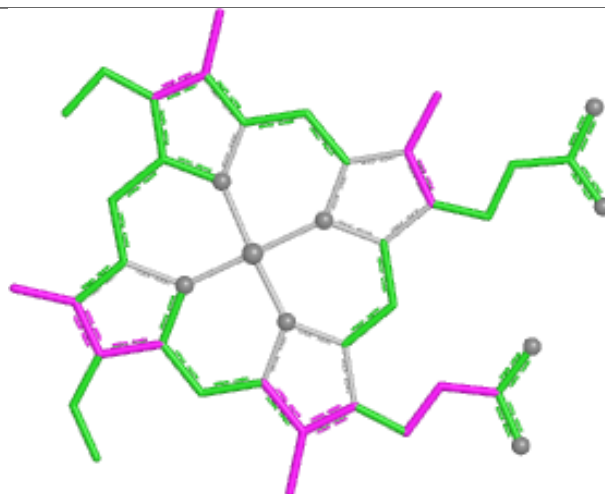




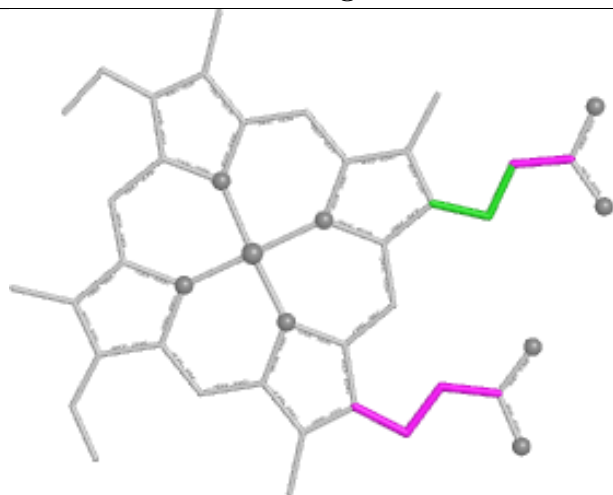
Ligand HEC 8 401



Bond lengths



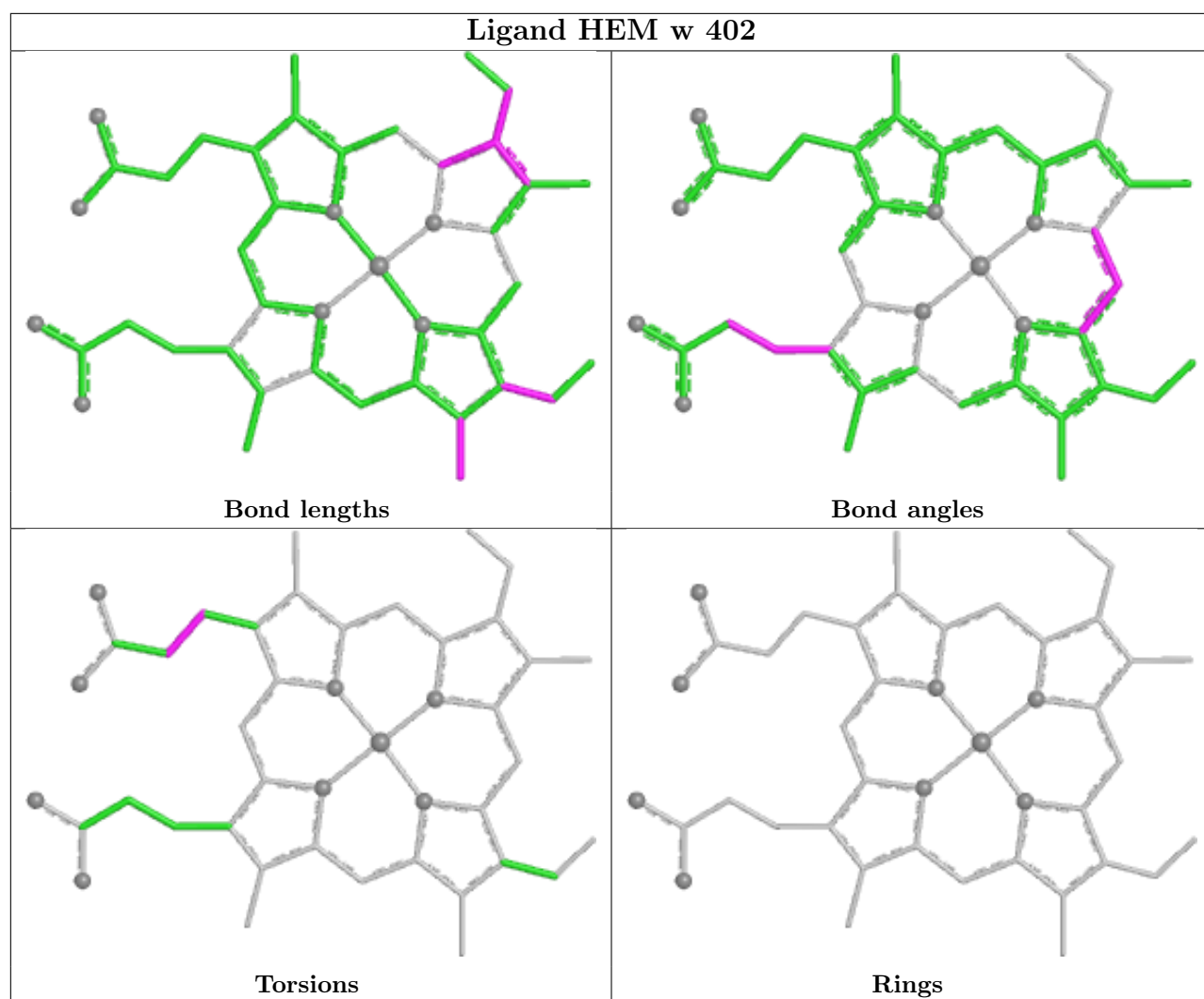
Bond angles

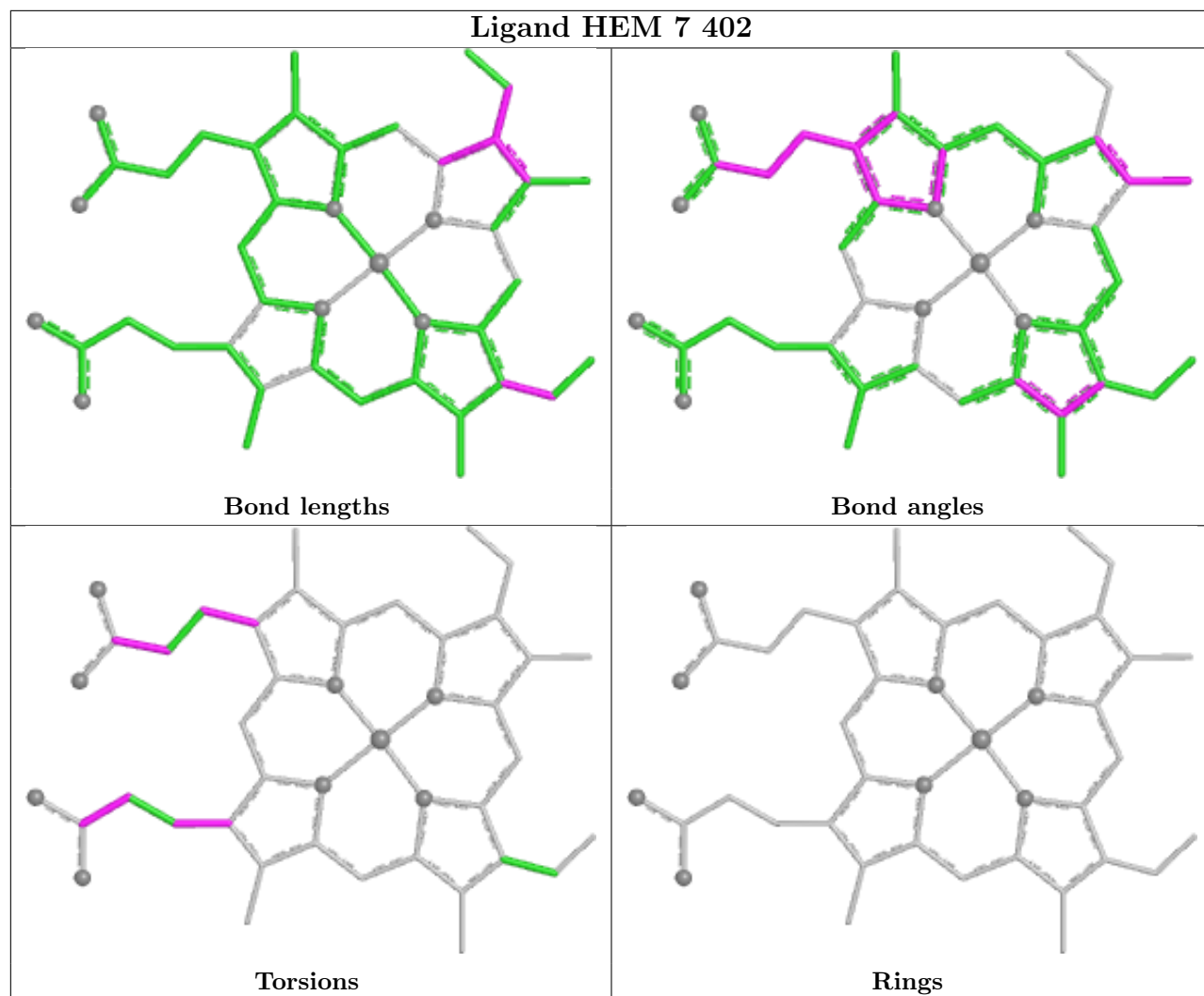


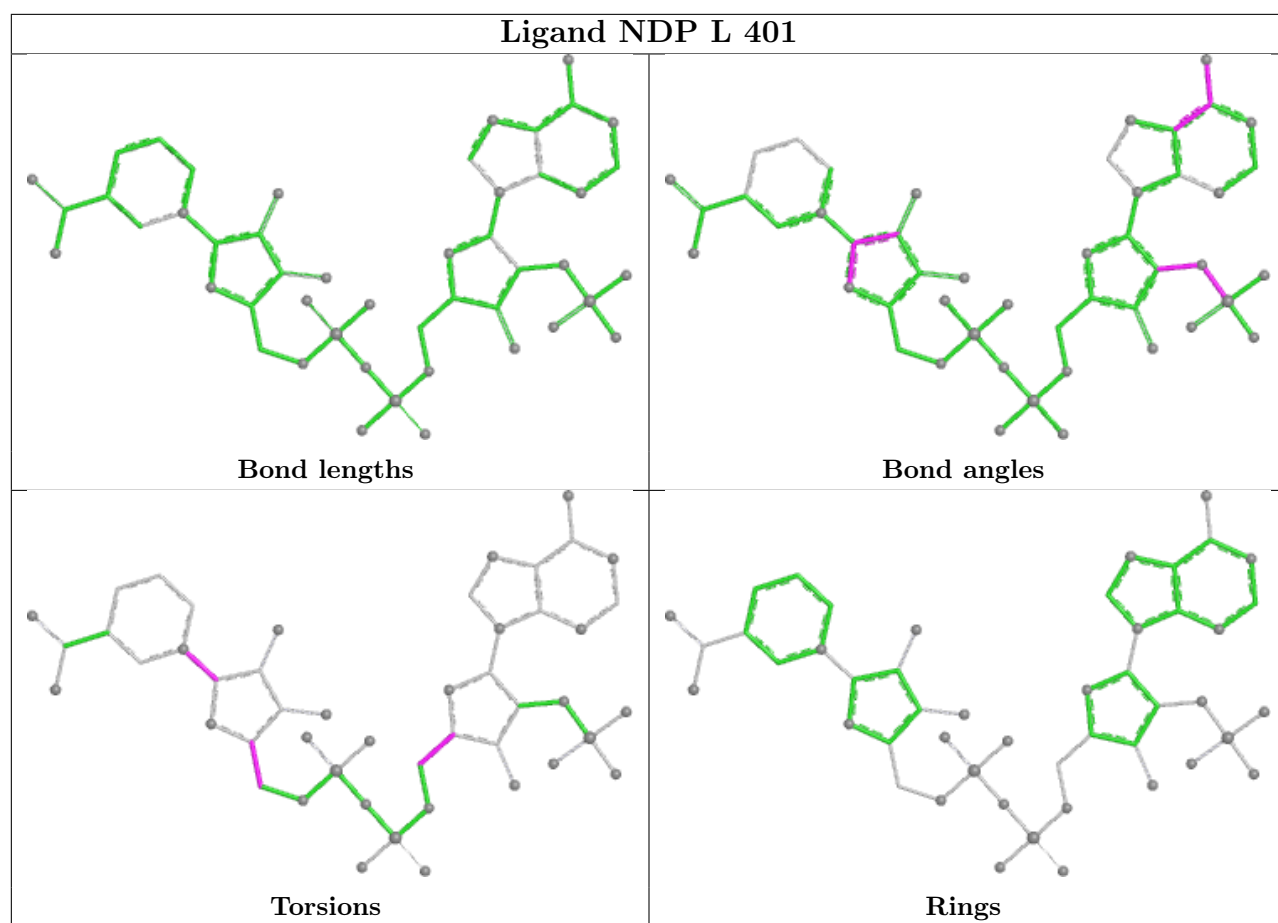
Torsions

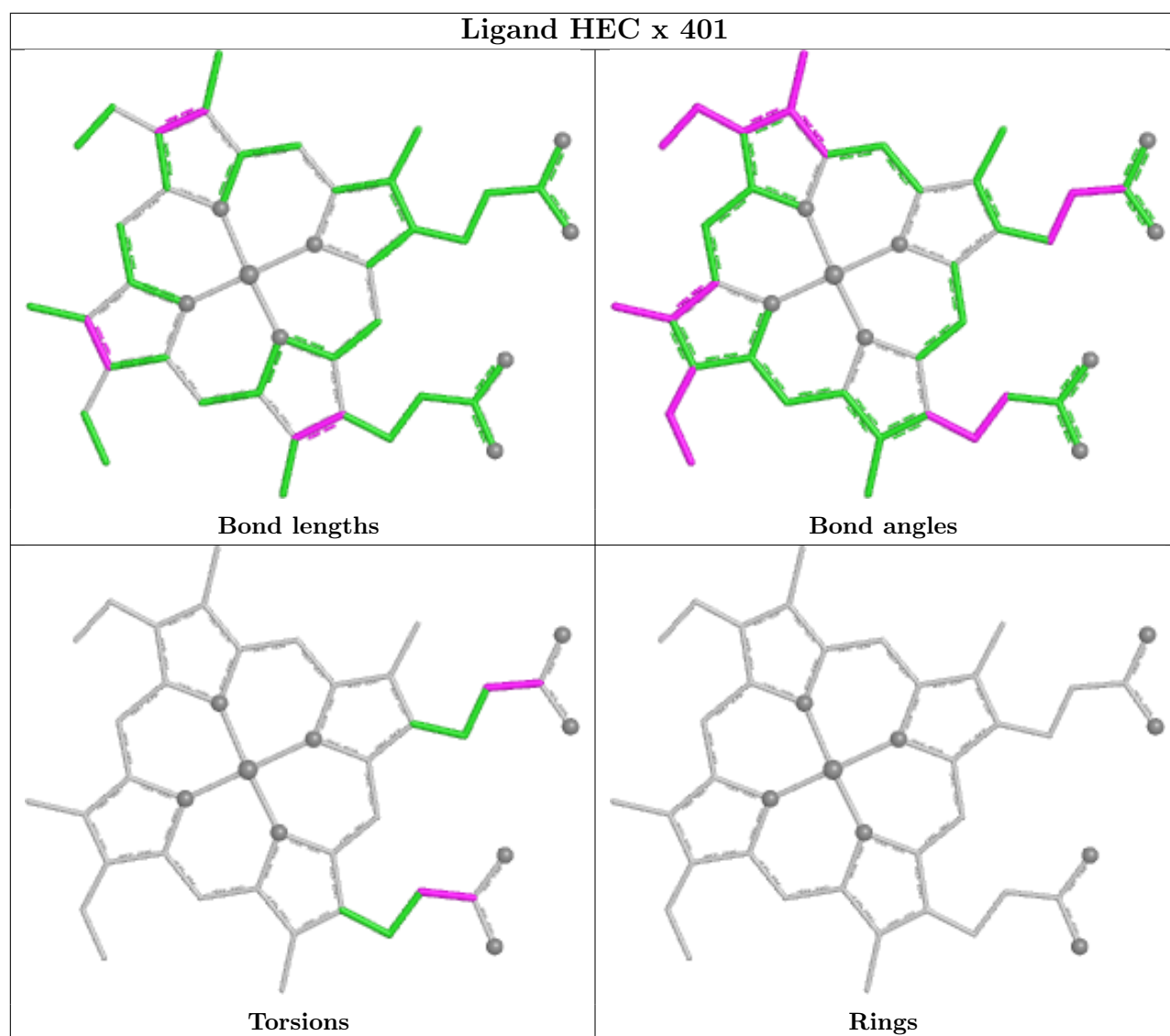


Rings









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.

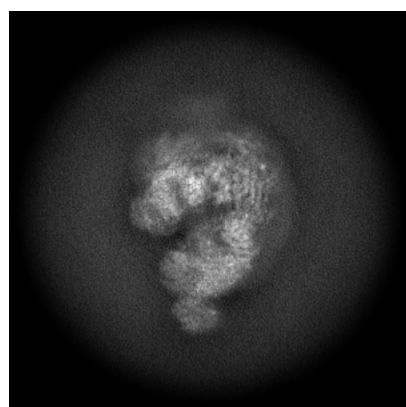
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45479. These allow visual inspection of the internal detail of the map and identification of artifacts.

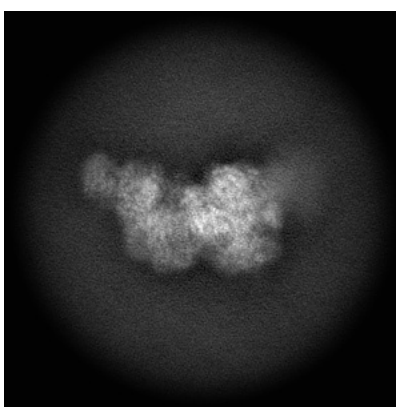
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

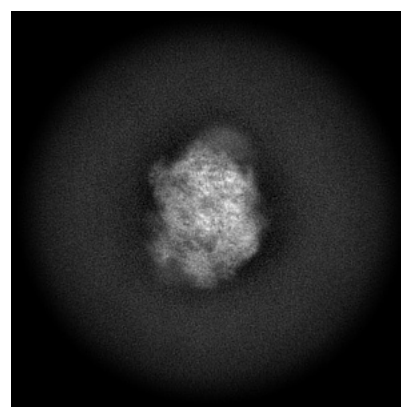
6.1.1 Primary map



X



Y

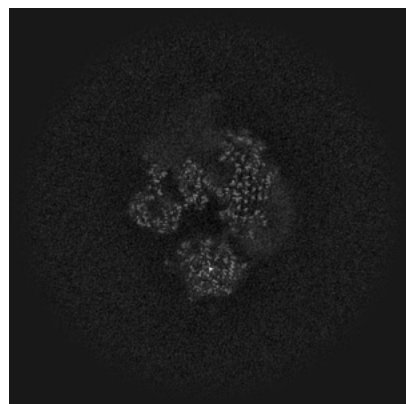


Z

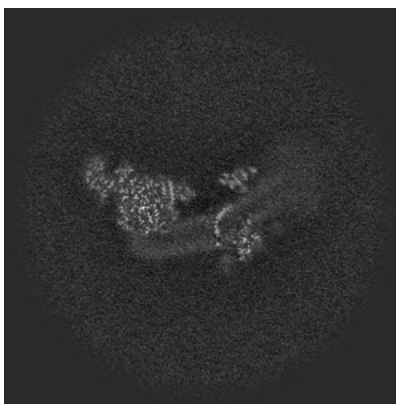
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

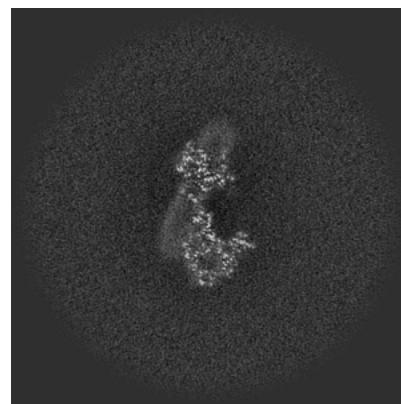
6.2.1 Primary map



X Index: 256



Y Index: 256

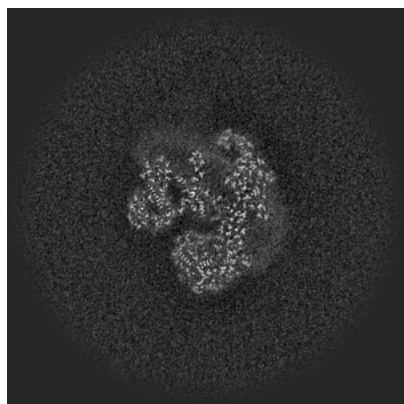


Z Index: 256

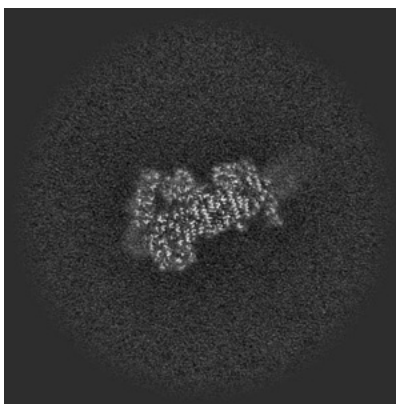
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

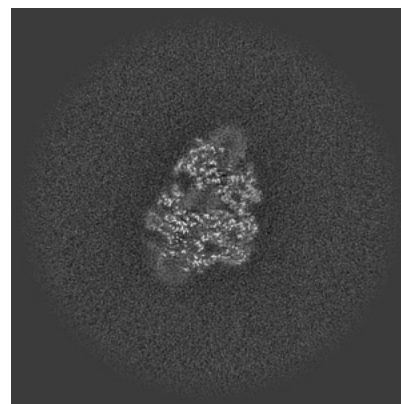
6.3.1 Primary map



X Index: 244



Y Index: 291

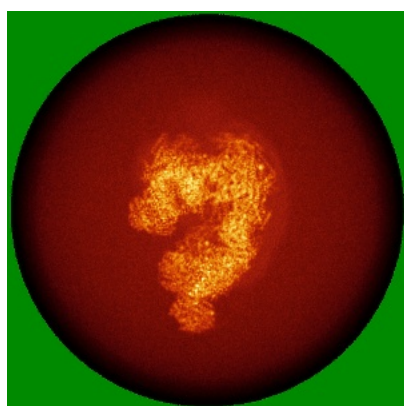


Z Index: 294

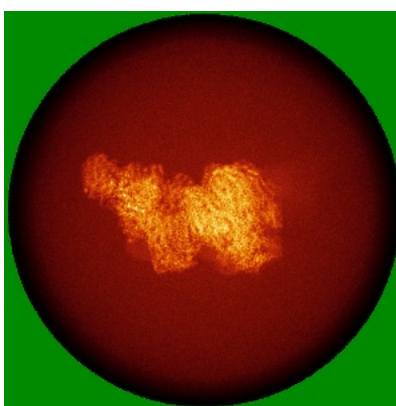
The images above show the largest variance slices of the map in three orthogonal directions.

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

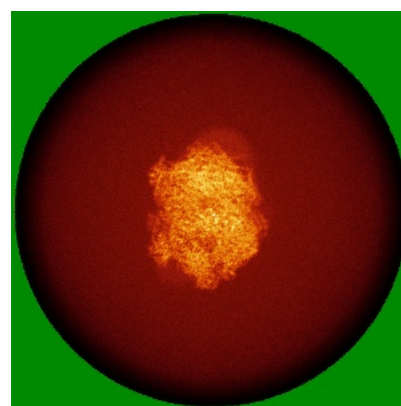
6.4.1 Primary map



X



Y



Z

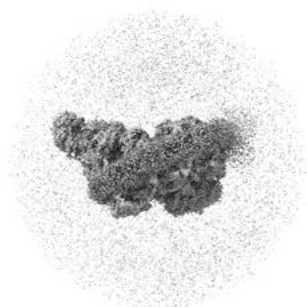
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

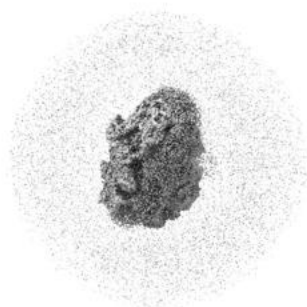
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

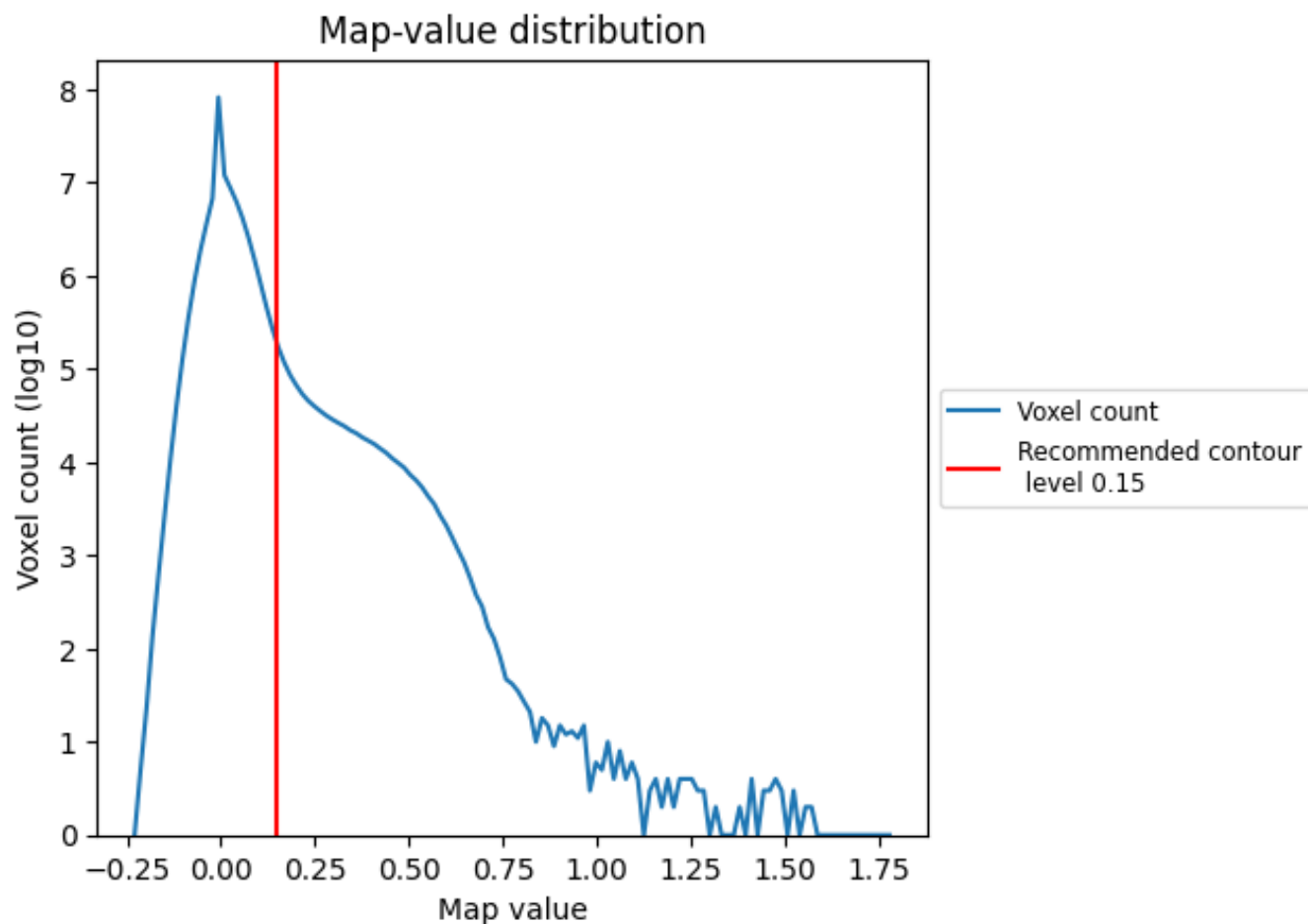
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

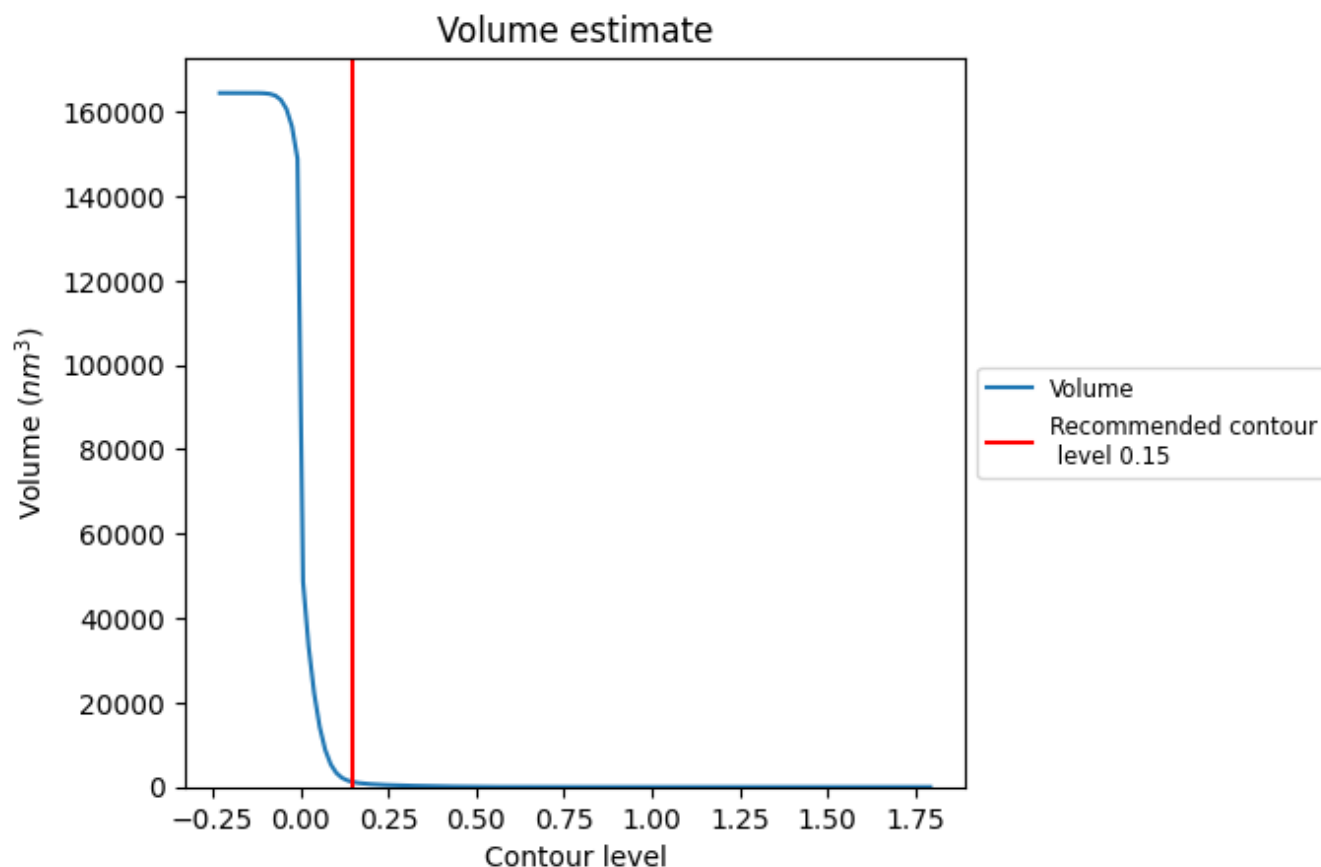
This section contains the results of statistical analysis of the map.

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.

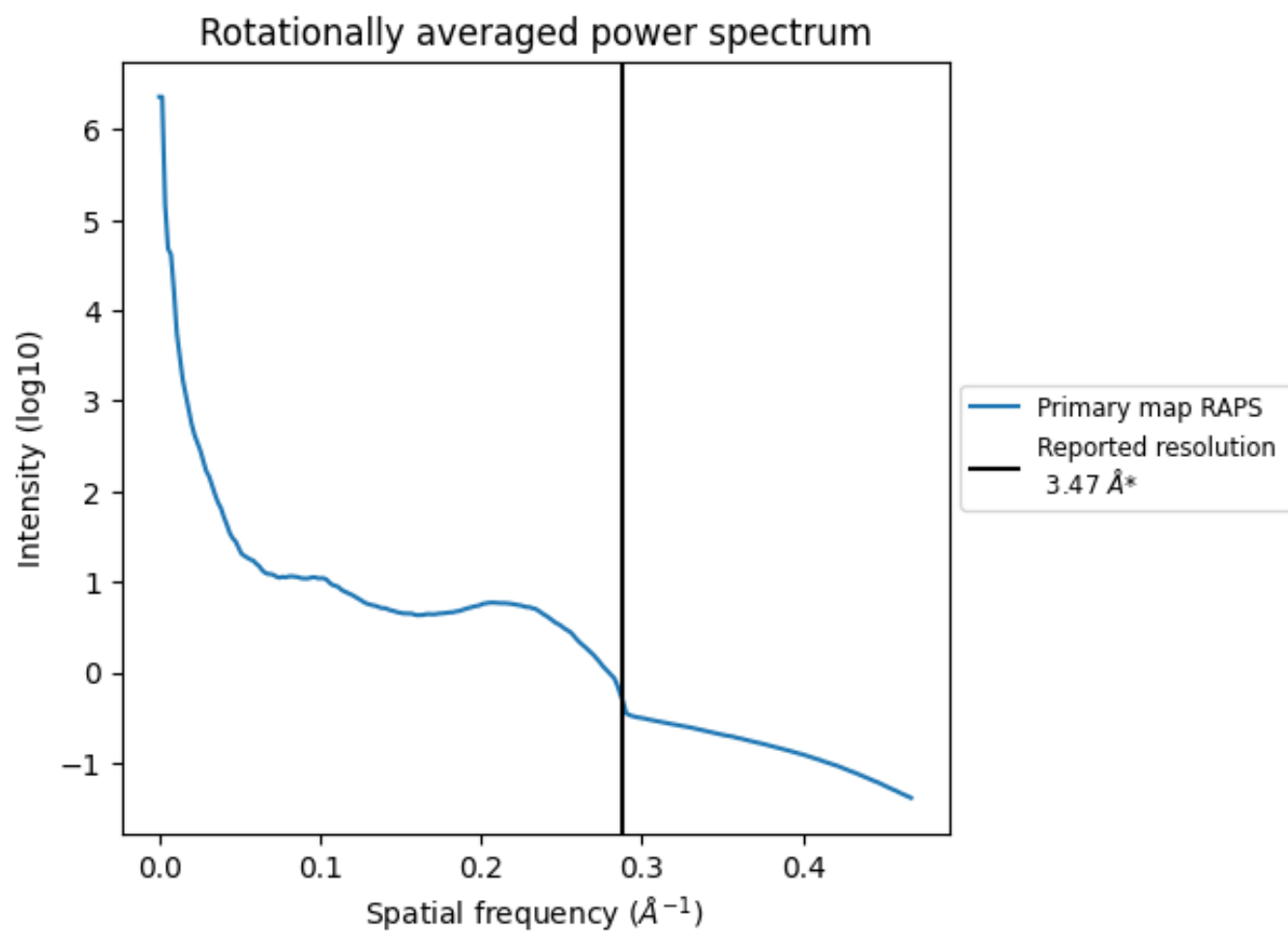
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1168 nm³; this corresponds to an approximate mass of 1055 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 0.288 Å⁻¹

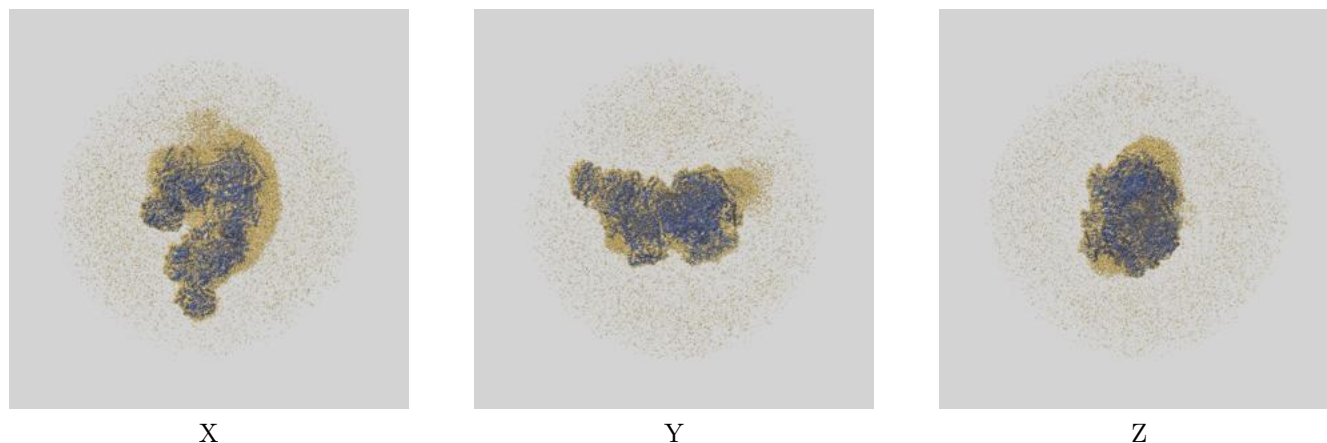
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

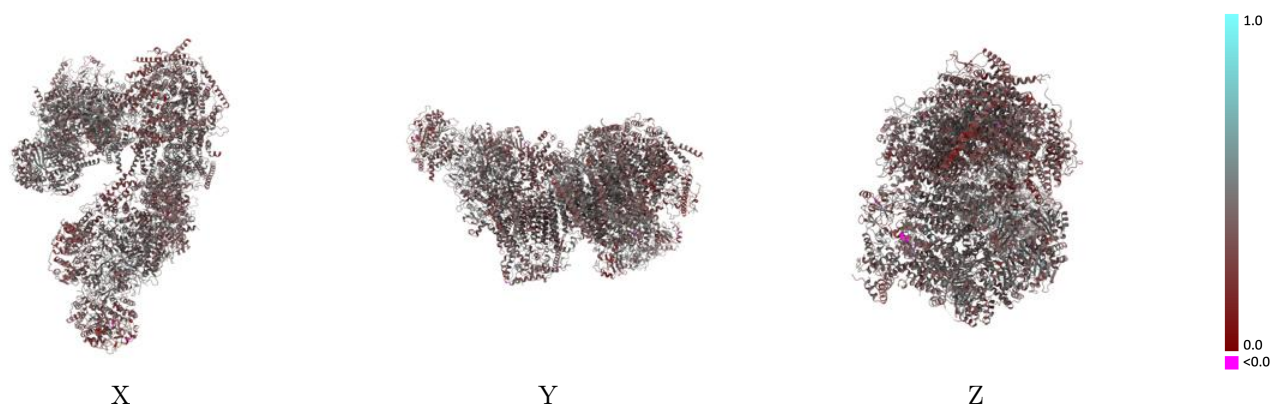
This section contains information regarding the fit between EMDB map EMD-45479 and PDB model 9CDN. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



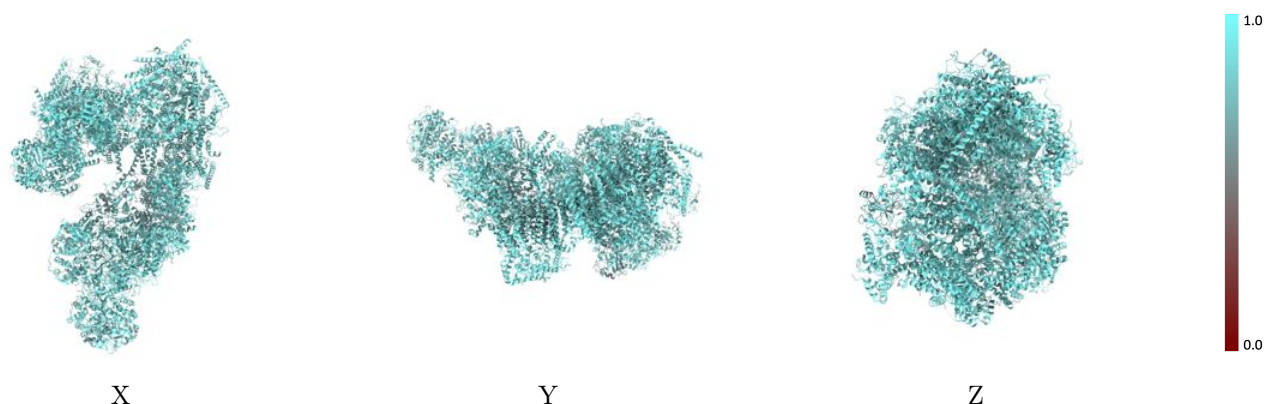
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



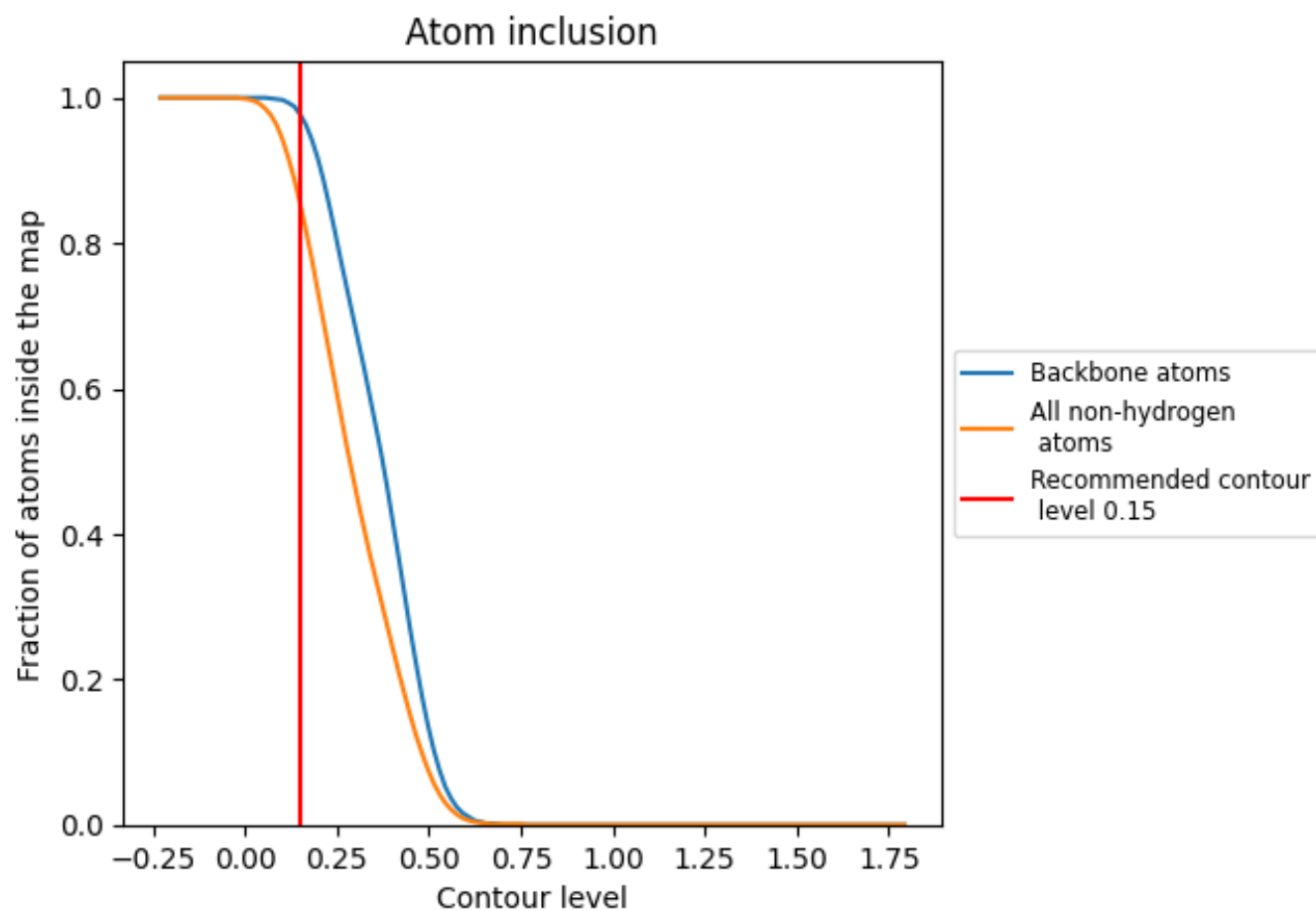
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 85% 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 (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8540 |  0.3920 |
| 0 |  0.8330 |  0.3460 |
| 1 |  0.8810 |  0.3980 |
| 2 |  0.7930 |  0.3530 |
| 3 |  0.8900 |  0.4090 |
| 4 |  0.7490 |  0.3420 |
| 5 |  0.8900 |  0.4250 |
| 6 |  0.8730 |  0.4220 |
| 7 |  0.8850 |  0.4340 |
| 8 |  0.8860 |  0.4220 |
| 9 |  0.8750 |  0.4170 |
| Aa |  0.8720 |  0.4260 |
| Ab |  0.8290 |  0.3390 |
| Ac |  0.8250 |  0.3840 |
| Ad |  0.8590 |  0.4140 |
| Ae |  0.7060 |  0.2910 |
| Af |  0.7040 |  0.3210 |
| B |  0.8240 |  0.3410 |
| C |  0.8710 |  0.4090 |
| D |  0.8850 |  0.4230 |
| E |  0.8250 |  0.3620 |
| F |  0.8160 |  0.4170 |
| G |  0.8470 |  0.3850 |
| H |  0.8980 |  0.4290 |
| I |  0.8800 |  0.4120 |
| J |  0.8540 |  0.4240 |
| K |  0.8360 |  0.4160 |
| L |  0.7840 |  0.3420 |
| M |  0.8600 |  0.4160 |
| N |  0.8510 |  0.3720 |
| O |  0.7540 |  0.2820 |
| P |  0.7980 |  0.3090 |
| Q |  0.8090 |  0.3610 |
| R |  0.7730 |  0.3480 |
| S |  0.8940 |  0.4280 |



Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| T |  0.8770 |  0.4100 |
| U |  0.8420 |  0.3610 |
| V |  0.8460 |  0.3630 |
| W |  0.8790 |  0.3790 |
| X |  0.8240 |  0.3320 |
| Y |  0.8510 |  0.3340 |
| Z |  0.8440 |  0.3300 |
| a |  0.8690 |  0.3640 |
| b |  0.8480 |  0.3240 |
| c |  0.8770 |  0.3890 |
| d |  0.8670 |  0.3560 |
| e |  0.8120 |  0.3640 |
| f |  0.8000 |  0.3520 |
| g |  0.8910 |  0.4140 |
| h |  0.8690 |  0.4010 |
| i |  0.8750 |  0.4290 |
| j |  0.7880 |  0.3740 |
| k |  0.8420 |  0.3990 |
| l |  0.8400 |  0.3940 |
| m |  0.7880 |  0.3420 |
| n |  0.8150 |  0.3460 |
| o |  0.8250 |  0.3500 |
| p |  0.8710 |  0.3620 |
| q |  0.8620 |  0.4250 |
| r |  0.8290 |  0.3930 |
| s |  0.8710 |  0.3890 |
| t |  0.8560 |  0.2930 |
| u |  0.8910 |  0.4220 |
| v |  0.8890 |  0.4220 |
| w |  0.8890 |  0.4370 |
| x |  0.9040 |  0.4310 |
| y |  0.8850 |  0.4220 |
| z |  0.9100 |  0.4220 |