



Full wwPDB EM Validation Report ⓘ

Oct 1, 2022 – 07:24 am BST

PDB ID : 8AT4
EMDB ID : EMD-15633
Title : Structure of the augmin holocomplex in closed conformation
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2022-08-22
Resolution : 33.00 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

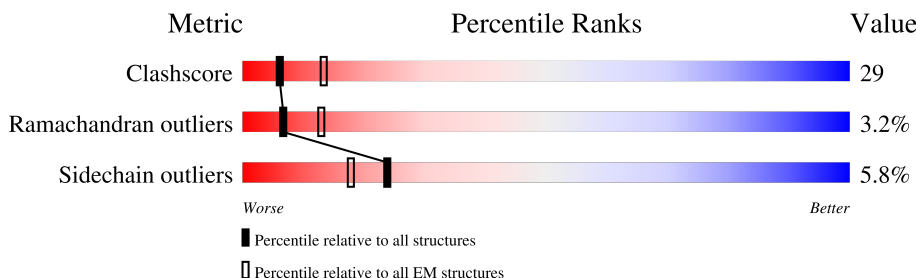
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 33.00 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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 286 | <div> <div>37%</div> <div>59%</div> <div>27%</div> <div>8%</div> <div>5%</div> </div> |
| 2 | B | 597 | <div> <div>27%</div> <div>55%</div> <div>29%</div> <div>8%</div> <div>7%</div> </div> |
| 3 | C | 353 | <div> <div>26%</div> <div>59%</div> <div>33%</div> <div>5%</div> <div>.</div> </div> |
| 4 | D | 666 | <div> <div>29%</div> <div>55%</div> <div>33%</div> <div>7%</div> <div>5%</div> </div> |
| 5 | E | 222 | <div> <div>45%</div> <div>52%</div> <div>33%</div> <div>9%</div> <div>.</div> <div>.</div> </div> |
| 6 | F | 978 | <div> <div>9%</div> <div>22%</div> <div>13%</div> <div>.</div> <div>.</div> <div>60%</div> </div> |
| 7 | G | 348 | <div> <div>24%</div> <div>47%</div> <div>36%</div> <div>9%</div> <div>5%</div> <div>.</div> </div> |
| 8 | H | 367 | <div> <div>5%</div> <div>33%</div> <div>17%</div> <div>.</div> <div>45%</div> </div> |

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24599 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 HAUS augmin-like complex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 286 | Total | C | N | O | S | 0 | 0 |
| | | | 2282 | 1436 | 380 | 453 | 13 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|------------|
| A | 156 | ARG | GLN | variant | UNP Q3B8L5 |

- Molecule 2 is a protein called HAUS augmin-like complex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | B | 597 | Total | C | N | O | S | 0 | 0 |
| | | | 4771 | 2988 | 817 | 943 | 23 | | |

- Molecule 3 is a protein called HAUS augmin like complex subunit 4 L homeolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | C | 353 | Total | C | N | O | S | 0 | 0 |
| | | | 2885 | 1807 | 508 | 554 | 16 | | |

- Molecule 4 is a protein called HAUS augmin-like complex subunit 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 4 | D | 666 | Total | C | N | O | S | 0 | 0 |
| | | | 5415 | 3362 | 1000 | 1022 | 31 | | |

- Molecule 5 is a protein called HAUS augmin like complex subunit 2 L homeolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5 | E | 217 | Total | C | N | O | S | 0 | 0 |
| | | | 1717 | 1075 | 296 | 334 | 12 | | |

- Molecule 6 is a protein called HAUS augmin like complex subunit 6 L homeolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | F | 387 | Total | C | N | O | S | 0 | 0 |
| | | | 3171 | 2020 | 574 | 558 | 19 | | |

- Molecule 7 is a protein called HAUS augmin like complex subunit 7 S homeolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | G | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2687 | 1694 | 441 | 533 | 19 | | |

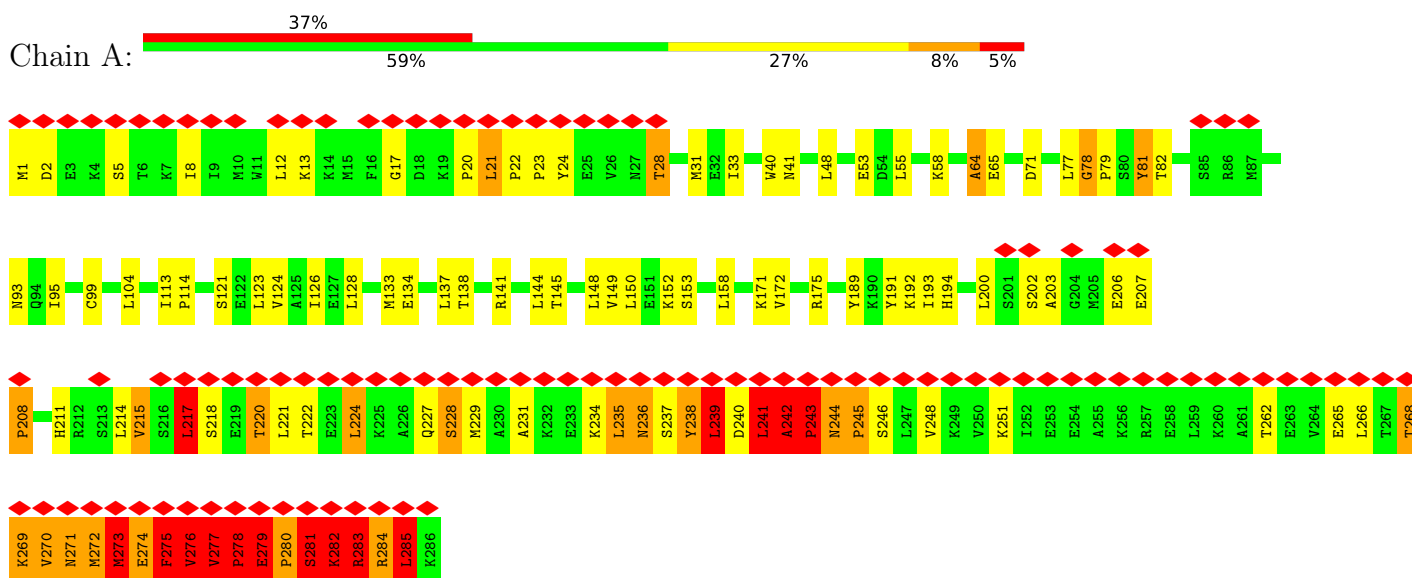
- Molecule 8 is a protein called HAUS augmin-like complex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8 | H | 203 | Total | C | N | O | S | 0 | 0 |
| | | | 1671 | 1048 | 285 | 331 | 7 | | |

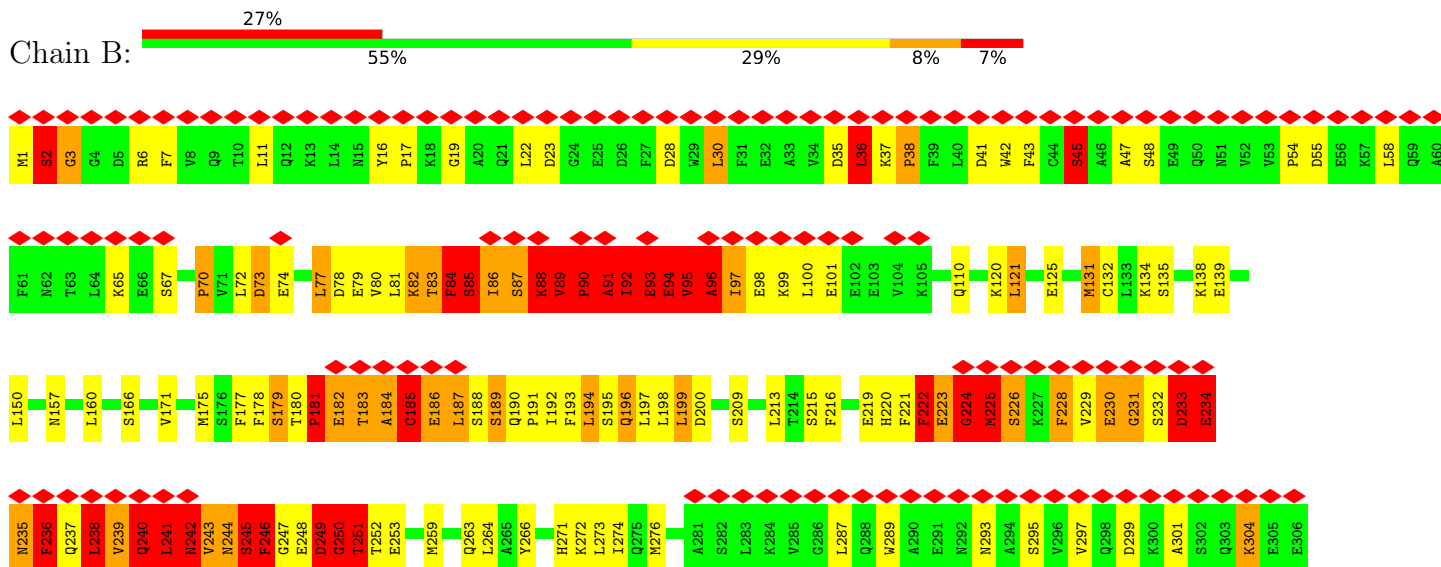
3 Residue-property plots

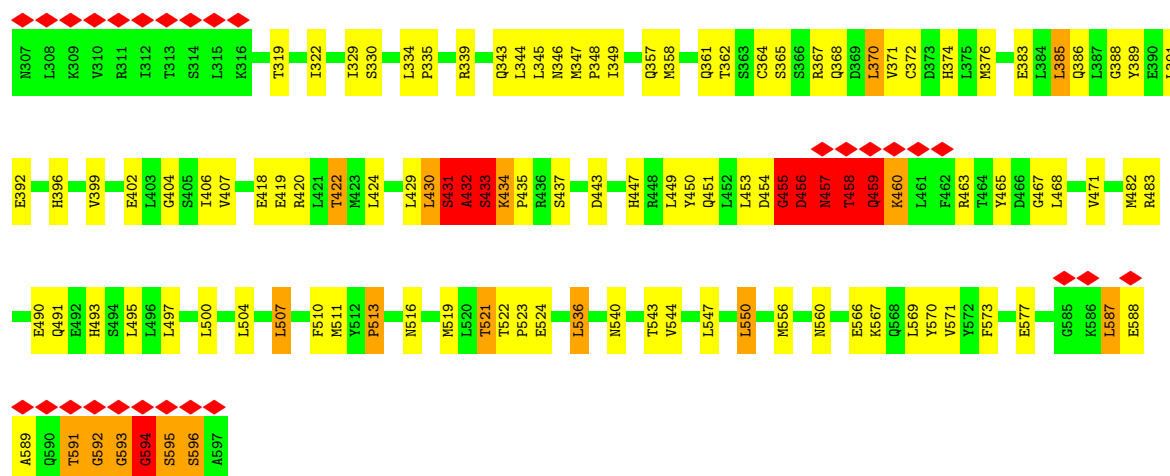
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: HAUS augmin-like complex subunit 1



• Molecule 2: HAUS augmin-like complex subunit 3



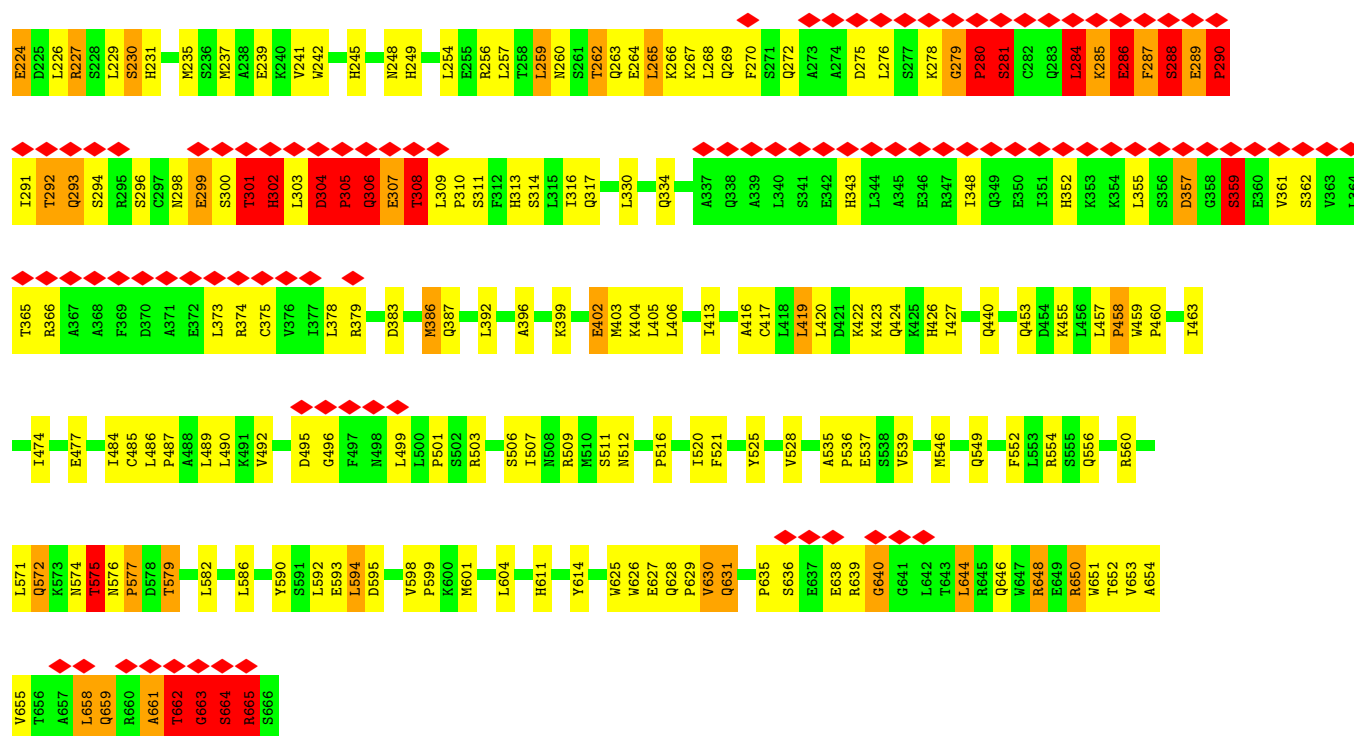


• Molecule 3: HAUS augmin like complex subunit 4 L homeolog

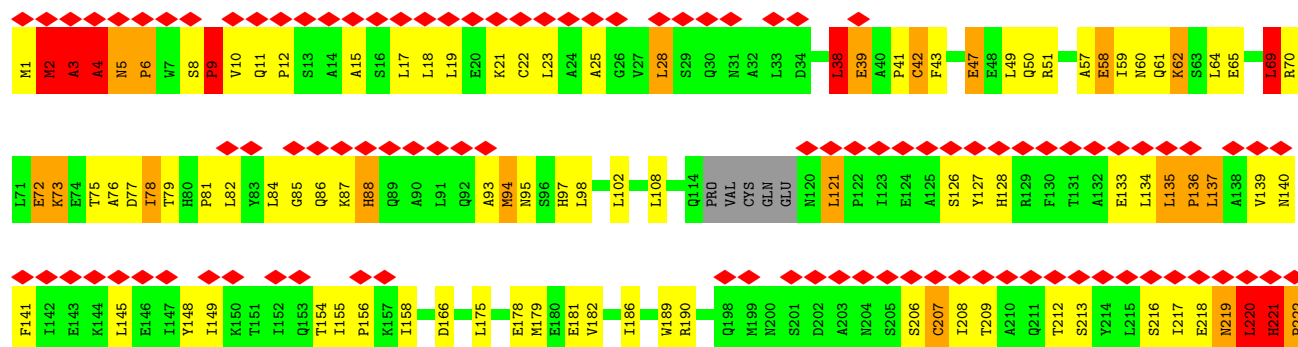
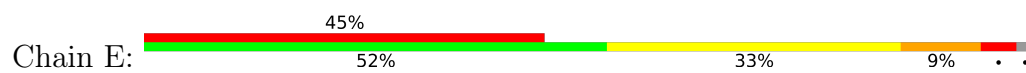


• Molecule 4: HAUS augmin-like complex subunit 5

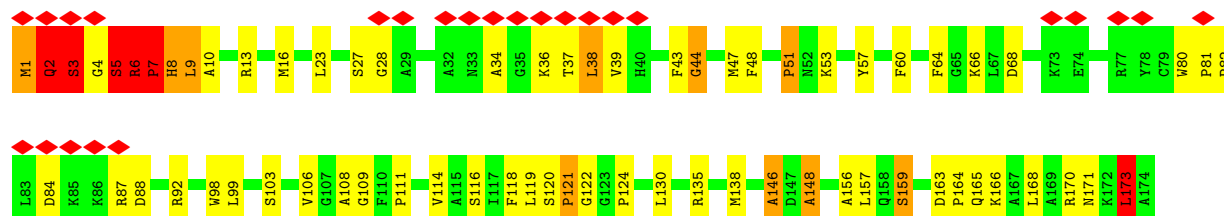


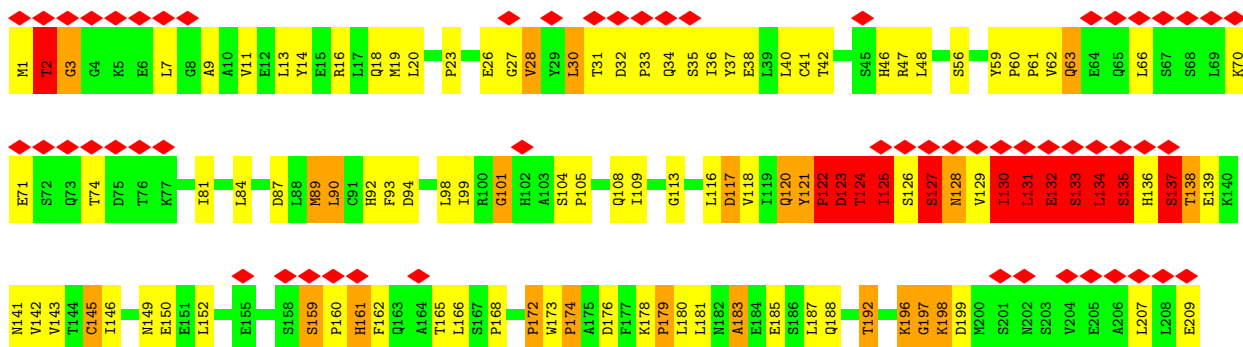


• Molecule 5: HAUS augmin like complex subunit 2 L homeolog



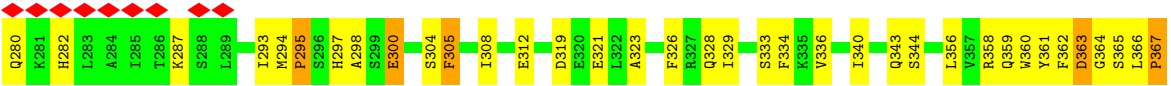
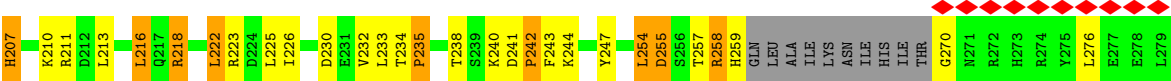
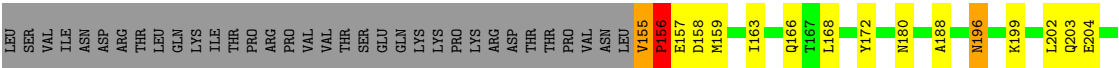
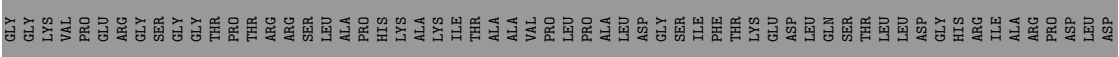
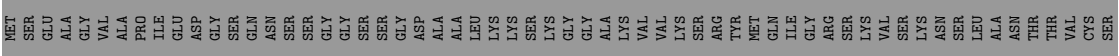
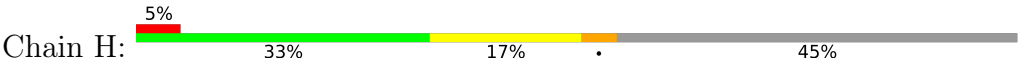
• Molecule 6: HAUS augmin like complex subunit 6 L homeolog







• Molecule 8: HAUS augmin-like complex subunit 8



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 10658 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS TALOS L120C | Depositor |
| Voltage (kV) | 120 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 101.8 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI CETA (4k x 4k) | Depositor |
| Maximum map value | 0.138 | Depositor |
| Minimum map value | -0.025 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.004 | Depositor |
| Recommended contour level | 0.0245 | Depositor |
| Map size (Å) | 601.6, 601.6, 601.6 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 2.35, 2.35, 2.35 | Depositor |

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 1.47 | 38/2309 (1.6%) | 1.41 | 48/3102 (1.5%) |
| 2 | B | 1.15 | 37/4836 (0.8%) | 1.31 | 74/6496 (1.1%) |
| 3 | C | 0.99 | 24/2920 (0.8%) | 1.18 | 29/3925 (0.7%) |
| 4 | D | 1.06 | 53/5503 (1.0%) | 1.29 | 61/7400 (0.8%) |
| 5 | E | 1.34 | 41/1743 (2.4%) | 1.08 | 16/2359 (0.7%) |
| 6 | F | 1.22 | 56/3229 (1.7%) | 1.12 | 34/4333 (0.8%) |
| 7 | G | 1.19 | 48/2736 (1.8%) | 1.30 | 38/3698 (1.0%) |
| 8 | H | 1.12 | 19/1692 (1.1%) | 0.95 | 7/2278 (0.3%) |
| All | All | 1.17 | 316/24968 (1.3%) | 1.24 | 307/33591 (0.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 15 |
| 2 | B | 0 | 68 |
| 3 | C | 0 | 11 |
| 4 | D | 0 | 41 |
| 5 | E | 0 | 11 |
| 6 | F | 0 | 19 |
| 7 | G | 0 | 27 |
| 8 | H | 0 | 1 |
| All | All | 0 | 193 |

All (316) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | B | 223 | GLU | C-N | 26.85 | 1.81 | 1.33 |
| 1 | A | 277 | VAL | C-N | 24.02 | 1.79 | 1.34 |
| 2 | B | 591 | THR | C-N | 18.64 | 1.66 | 1.33 |
| 1 | A | 280 | PRO | C-N | 17.83 | 1.75 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | A | 272 | MET | C-N | -16.41 | 0.96 | 1.34 |
| 1 | A | 283 | ARG | C-N | 15.76 | 1.70 | 1.34 |
| 1 | A | 284 | ARG | C-N | 15.51 | 1.69 | 1.34 |
| 6 | F | 34 | ALA | C-N | 14.93 | 1.59 | 1.33 |
| 3 | C | 319 | PHE | C-N | 13.88 | 1.66 | 1.34 |
| 1 | A | 276 | VAL | C-N | 13.55 | 1.65 | 1.34 |
| 2 | B | 593 | GLY | C-N | 13.20 | 1.56 | 1.33 |
| 2 | B | 17 | PRO | N-CD | -12.02 | 1.31 | 1.47 |
| 5 | E | 6 | PRO | N-CD | -11.95 | 1.31 | 1.47 |
| 2 | B | 513 | PRO | N-CD | -11.91 | 1.31 | 1.47 |
| 7 | G | 122 | PRO | N-CD | -11.87 | 1.31 | 1.47 |
| 5 | E | 9 | PRO | N-CD | -11.82 | 1.31 | 1.47 |
| 2 | B | 592 | GLY | C-N | -11.82 | 1.11 | 1.33 |
| 1 | A | 245 | PRO | N-CD | -11.81 | 1.31 | 1.47 |
| 8 | H | 367 | PRO | N-CD | -11.81 | 1.31 | 1.47 |
| 4 | D | 576 | ASN | C-N | 11.78 | 1.56 | 1.34 |
| 4 | D | 21 | PRO | N-CD | -11.75 | 1.31 | 1.47 |
| 1 | A | 22 | PRO | N-CD | -11.74 | 1.31 | 1.47 |
| 4 | D | 221 | PRO | N-CD | -11.69 | 1.31 | 1.47 |
| 4 | D | 26 | PRO | N-CD | -11.58 | 1.31 | 1.47 |
| 4 | D | 180 | PRO | N-CD | -11.49 | 1.31 | 1.47 |
| 1 | A | 208 | PRO | N-CD | -11.47 | 1.31 | 1.47 |
| 2 | B | 90 | PRO | N-CD | -11.46 | 1.31 | 1.47 |
| 2 | B | 54 | PRO | N-CD | -11.42 | 1.31 | 1.47 |
| 5 | E | 222 | PRO | N-CD | -11.40 | 1.31 | 1.47 |
| 4 | D | 280 | PRO | N-CD | -11.26 | 1.32 | 1.47 |
| 3 | C | 283 | PRO | N-CD | -11.23 | 1.32 | 1.47 |
| 3 | C | 353 | PRO | N-CD | -11.05 | 1.32 | 1.47 |
| 5 | E | 41 | PRO | N-CD | -11.03 | 1.32 | 1.47 |
| 4 | D | 290 | PRO | N-CD | -11.02 | 1.32 | 1.47 |
| 4 | D | 495 | ASP | C-N | 11.01 | 1.52 | 1.33 |
| 6 | F | 7 | PRO | N-CD | -11.01 | 1.32 | 1.47 |
| 4 | D | 190 | PRO | N-CD | -11.00 | 1.32 | 1.47 |
| 1 | A | 282 | LYS | C-N | 10.99 | 1.59 | 1.34 |
| 3 | C | 122 | PRO | N-CD | -10.97 | 1.32 | 1.47 |
| 3 | C | 322 | PRO | N-CD | -10.96 | 1.32 | 1.47 |
| 2 | B | 181 | PRO | N-CD | -10.86 | 1.32 | 1.47 |
| 2 | B | 191 | PRO | N-CD | -10.76 | 1.32 | 1.47 |
| 1 | A | 274 | GLU | C-N | 10.45 | 1.58 | 1.34 |
| 4 | D | 305 | PRO | N-CD | -10.36 | 1.33 | 1.47 |
| 6 | F | 82 | PRO | N-CD | -10.25 | 1.33 | 1.47 |
| 6 | F | 106 | VAL | C-N | 10.18 | 1.51 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 7 | G | 23 | PRO | N-CD | -10.15 | 1.33 | 1.47 |
| 1 | A | 273 | MET | C-N | 10.14 | 1.57 | 1.34 |
| 8 | H | 155 | VAL | C-N | -10.04 | 1.15 | 1.34 |
| 2 | B | 560 | ASN | C-N | 9.97 | 1.56 | 1.34 |
| 4 | D | 635 | PRO | N-CD | -9.97 | 1.33 | 1.47 |
| 6 | F | 121 | PRO | N-CD | -9.93 | 1.33 | 1.47 |
| 3 | C | 123 | PRO | N-CD | -9.92 | 1.33 | 1.47 |
| 2 | B | 70 | PRO | N-CD | -9.85 | 1.34 | 1.47 |
| 8 | H | 156 | PRO | N-CD | -9.85 | 1.34 | 1.47 |
| 6 | F | 1 | MET | C-N | -9.65 | 1.11 | 1.34 |
| 7 | G | 196 | LYS | C-N | 9.64 | 1.50 | 1.33 |
| 6 | F | 148 | ALA | C-N | 9.59 | 1.50 | 1.33 |
| 1 | A | 278 | PRO | N-CD | -9.50 | 1.34 | 1.47 |
| 6 | F | 393 | PRO | N-CD | -9.28 | 1.34 | 1.47 |
| 8 | H | 295 | PRO | N-CD | -9.27 | 1.34 | 1.47 |
| 1 | A | 269 | LYS | C-N | -9.26 | 1.12 | 1.34 |
| 1 | A | 20 | PRO | N-CD | -8.98 | 1.35 | 1.47 |
| 4 | D | 659 | GLN | C-N | 8.85 | 1.54 | 1.34 |
| 4 | D | 227 | ARG | C-N | -8.76 | 1.14 | 1.34 |
| 1 | A | 243 | PRO | N-CD | -8.67 | 1.35 | 1.47 |
| 6 | F | 121 | PRO | C-N | -8.54 | 1.17 | 1.33 |
| 6 | F | 262 | VAL | C-N | -8.55 | 1.14 | 1.34 |
| 6 | F | 281 | PRO | N-CD | -8.52 | 1.35 | 1.47 |
| 4 | D | 577 | PRO | N-CD | -8.50 | 1.35 | 1.47 |
| 4 | D | 402 | GLU | C-N | -8.47 | 1.14 | 1.34 |
| 2 | B | 38 | PRO | N-CD | -8.47 | 1.35 | 1.47 |
| 1 | A | 280 | PRO | N-CD | -8.45 | 1.36 | 1.47 |
| 1 | A | 239 | LEU | C-N | 8.45 | 1.53 | 1.34 |
| 2 | B | 587 | LEU | C-N | 8.39 | 1.53 | 1.34 |
| 5 | E | 86 | GLN | C-N | -8.31 | 1.15 | 1.34 |
| 7 | G | 275 | GLY | C-N | -8.29 | 1.18 | 1.34 |
| 6 | F | 146 | ALA | C-N | -8.27 | 1.15 | 1.34 |
| 7 | G | 315 | SER | C-N | 8.22 | 1.52 | 1.34 |
| 1 | A | 229 | MET | C-N | -8.21 | 1.15 | 1.34 |
| 5 | E | 133 | GLU | C-N | -8.20 | 1.15 | 1.34 |
| 4 | D | 72 | THR | C-N | 8.11 | 1.52 | 1.34 |
| 1 | A | 265 | GLU | C-N | -8.08 | 1.15 | 1.34 |
| 5 | E | 25 | ALA | C-N | 8.06 | 1.47 | 1.33 |
| 2 | B | 455 | GLY | C-N | 8.05 | 1.52 | 1.34 |
| 7 | G | 160 | PRO | N-CD | -8.04 | 1.36 | 1.47 |
| 6 | F | 111 | PRO | N-CD | -8.03 | 1.36 | 1.47 |
| 6 | F | 213 | LEU | C-N | -7.99 | 1.15 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | B | 434 | LYS | C-N | 7.92 | 1.49 | 1.34 |
| 1 | A | 206 | GLU | C-N | -7.90 | 1.15 | 1.34 |
| 5 | E | 12 | PRO | N-CD | -7.88 | 1.36 | 1.47 |
| 4 | D | 221 | PRO | C-N | -7.86 | 1.18 | 1.33 |
| 7 | G | 27 | GLY | C-N | 7.84 | 1.52 | 1.34 |
| 5 | E | 69 | LEU | C-N | -7.83 | 1.16 | 1.34 |
| 4 | D | 357 | ASP | C-N | 7.82 | 1.47 | 1.33 |
| 3 | C | 41 | PRO | N-CD | -7.82 | 1.36 | 1.47 |
| 1 | A | 268 | THR | C-N | -7.80 | 1.16 | 1.34 |
| 7 | G | 174 | PRO | N-CD | -7.75 | 1.36 | 1.47 |
| 7 | G | 226 | SER | C-N | 7.74 | 1.51 | 1.34 |
| 4 | D | 69 | LEU | C-N | 7.73 | 1.51 | 1.34 |
| 4 | D | 18 | MET | C-N | 7.73 | 1.47 | 1.33 |
| 7 | G | 345 | SER | C-N | 7.73 | 1.51 | 1.34 |
| 6 | F | 81 | PRO | N-CD | -7.70 | 1.37 | 1.47 |
| 6 | F | 80 | TRP | C-N | -7.69 | 1.19 | 1.34 |
| 1 | A | 242 | ALA | C-N | -7.69 | 1.19 | 1.34 |
| 4 | D | 180 | PRO | C-N | 7.67 | 1.51 | 1.34 |
| 4 | D | 662 | THR | C-N | 7.65 | 1.46 | 1.33 |
| 7 | G | 289 | PHE | C-N | -7.61 | 1.16 | 1.34 |
| 5 | E | 73 | LYS | C-N | -7.56 | 1.16 | 1.34 |
| 2 | B | 73 | ASP | C-N | -7.53 | 1.16 | 1.34 |
| 6 | F | 258 | VAL | C-N | -7.48 | 1.16 | 1.34 |
| 7 | G | 234 | VAL | C-N | -7.48 | 1.16 | 1.34 |
| 2 | B | 435 | PRO | N-CD | -7.40 | 1.37 | 1.47 |
| 1 | A | 2 | ASP | C-N | 7.35 | 1.50 | 1.34 |
| 7 | G | 122 | PRO | C-N | -7.35 | 1.17 | 1.34 |
| 4 | D | 224 | GLU | C-N | 7.34 | 1.50 | 1.34 |
| 8 | H | 242 | PRO | N-CD | -7.25 | 1.37 | 1.47 |
| 2 | B | 589 | ALA | C-N | -7.24 | 1.17 | 1.34 |
| 6 | F | 27 | SER | C-N | 7.21 | 1.46 | 1.33 |
| 5 | E | 11 | GLN | C-N | -7.18 | 1.20 | 1.34 |
| 3 | C | 113 | SER | C-N | -7.18 | 1.17 | 1.34 |
| 2 | B | 594 | GLY | C-N | -7.15 | 1.17 | 1.34 |
| 5 | E | 82 | LEU | C-N | -7.09 | 1.17 | 1.34 |
| 4 | D | 640 | GLY | C-N | 7.08 | 1.45 | 1.33 |
| 8 | H | 361 | TYR | C-N | 7.06 | 1.50 | 1.34 |
| 6 | F | 51 | PRO | C-N | -7.05 | 1.17 | 1.34 |
| 4 | D | 313 | HIS | C-N | -7.01 | 1.18 | 1.34 |
| 6 | F | 209 | GLU | C-N | -7.01 | 1.18 | 1.34 |
| 1 | A | 17 | GLY | C-N | 6.99 | 1.50 | 1.34 |
| 2 | B | 6 | ARG | C-N | -6.96 | 1.18 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6 | F | 253 | LYS | C-N | -6.95 | 1.18 | 1.34 |
| 2 | B | 215 | SER | C-N | -6.94 | 1.18 | 1.34 |
| 3 | C | 314 | LEU | C-N | -6.91 | 1.18 | 1.34 |
| 6 | F | 44 | GLY | C-N | -6.90 | 1.18 | 1.34 |
| 6 | F | 108 | ALA | C-N | -6.90 | 1.20 | 1.33 |
| 6 | F | 222 | LYS | C-N | 6.86 | 1.49 | 1.34 |
| 8 | H | 300 | GLU | C-N | -6.86 | 1.18 | 1.34 |
| 2 | B | 150 | LEU | C-N | 6.84 | 1.49 | 1.34 |
| 5 | E | 93 | ALA | C-N | -6.82 | 1.18 | 1.34 |
| 7 | G | 71 | GLU | C-N | 6.81 | 1.49 | 1.34 |
| 8 | H | 196 | ASN | C-N | -6.79 | 1.18 | 1.34 |
| 2 | B | 222 | PHE | C-N | -6.78 | 1.18 | 1.34 |
| 4 | D | 176 | SER | C-N | 6.78 | 1.49 | 1.34 |
| 7 | G | 161 | HIS | C-N | -6.77 | 1.18 | 1.34 |
| 1 | A | 270 | VAL | C-N | 6.72 | 1.49 | 1.34 |
| 3 | C | 37 | PRO | N-CD | -6.70 | 1.38 | 1.47 |
| 7 | G | 130 | ILE | C-N | 6.65 | 1.49 | 1.34 |
| 5 | E | 78 | ILE | C-N | -6.64 | 1.18 | 1.34 |
| 8 | H | 333 | SER | C-N | -6.64 | 1.18 | 1.34 |
| 7 | G | 141 | ASN | C-N | -6.62 | 1.18 | 1.34 |
| 5 | E | 58 | GLU | C-N | -6.54 | 1.19 | 1.34 |
| 3 | C | 291 | GLN | C-N | -6.54 | 1.19 | 1.34 |
| 6 | F | 260 | ALA | C-N | -6.54 | 1.19 | 1.34 |
| 6 | F | 292 | MET | C-N | 6.54 | 1.49 | 1.34 |
| 3 | C | 352 | LEU | C-N | 6.54 | 1.46 | 1.34 |
| 3 | C | 22 | LEU | C-N | 6.50 | 1.49 | 1.34 |
| 4 | D | 311 | SER | C-N | -6.50 | 1.19 | 1.34 |
| 3 | C | 313 | ILE | C-N | -6.49 | 1.19 | 1.34 |
| 2 | B | 516 | ASN | C-N | -6.48 | 1.19 | 1.34 |
| 1 | A | 81 | TYR | C-N | 6.47 | 1.49 | 1.34 |
| 4 | D | 516 | PRO | N-CD | -6.47 | 1.38 | 1.47 |
| 8 | H | 364 | GLY | C-N | 6.44 | 1.48 | 1.34 |
| 5 | E | 61 | GLN | C-N | -6.43 | 1.19 | 1.34 |
| 5 | E | 22 | CYS | C-N | -6.41 | 1.19 | 1.34 |
| 8 | H | 218 | ARG | C-N | -6.40 | 1.19 | 1.34 |
| 1 | A | 222 | THR | C-N | -6.39 | 1.19 | 1.34 |
| 3 | C | 124 | SER | C-N | 6.39 | 1.48 | 1.34 |
| 6 | F | 202 | GLN | C-N | -6.38 | 1.19 | 1.34 |
| 2 | B | 233 | ASP | C-N | 6.34 | 1.48 | 1.34 |
| 7 | G | 33 | PRO | N-CD | -6.34 | 1.39 | 1.47 |
| 2 | B | 523 | PRO | N-CD | -6.33 | 1.39 | 1.47 |
| 5 | E | 15 | ALA | C-N | -6.32 | 1.19 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6 | F | 380 | GLU | C-N | -6.30 | 1.19 | 1.34 |
| 4 | D | 652 | THR | C-N | 6.27 | 1.48 | 1.34 |
| 4 | D | 501 | PRO | C-N | -6.24 | 1.19 | 1.34 |
| 5 | E | 88 | HIS | C-N | -6.24 | 1.19 | 1.34 |
| 4 | D | 496 | GLY | C-N | 6.24 | 1.48 | 1.34 |
| 4 | D | 310 | PRO | N-CD | -6.24 | 1.39 | 1.47 |
| 1 | A | 23 | PRO | N-CD | -6.22 | 1.39 | 1.47 |
| 6 | F | 195 | LYS | C-N | -6.20 | 1.19 | 1.34 |
| 3 | C | 142 | PRO | N-CD | -6.17 | 1.39 | 1.47 |
| 7 | G | 120 | GLN | C-N | -6.14 | 1.20 | 1.34 |
| 5 | E | 8 | SER | C-N | -6.10 | 1.22 | 1.34 |
| 2 | B | 249 | ASP | C-N | 6.08 | 1.44 | 1.33 |
| 5 | E | 95 | ASN | C-N | -6.06 | 1.20 | 1.34 |
| 6 | F | 175 | ARG | C-N | -6.05 | 1.20 | 1.34 |
| 4 | D | 650 | ARG | C-N | -6.05 | 1.20 | 1.34 |
| 5 | E | 136 | PRO | C-N | -6.05 | 1.20 | 1.34 |
| 2 | B | 23 | ASP | C-N | -6.04 | 1.22 | 1.33 |
| 8 | H | 319 | ASP | C-N | -6.04 | 1.20 | 1.34 |
| 7 | G | 129 | VAL | C-N | 6.03 | 1.48 | 1.34 |
| 7 | G | 287 | THR | C-N | -6.03 | 1.20 | 1.34 |
| 5 | E | 72 | GLU | C-N | -6.03 | 1.20 | 1.34 |
| 7 | G | 26 | GLU | C-N | -6.03 | 1.22 | 1.33 |
| 4 | D | 661 | ALA | C-N | -6.02 | 1.20 | 1.34 |
| 8 | H | 297 | HIS | C-N | -6.00 | 1.20 | 1.34 |
| 5 | E | 128 | HIS | C-N | -6.00 | 1.20 | 1.34 |
| 6 | F | 173 | LEU | C-N | -5.97 | 1.20 | 1.34 |
| 3 | C | 213 | MET | C-N | -5.96 | 1.20 | 1.34 |
| 7 | G | 299 | THR | C-N | -5.95 | 1.20 | 1.34 |
| 5 | E | 51 | ARG | C-N | -5.94 | 1.20 | 1.34 |
| 4 | D | 638 | GLU | C-N | -5.93 | 1.20 | 1.34 |
| 7 | G | 179 | PRO | N-CD | -5.91 | 1.39 | 1.47 |
| 2 | B | 3 | GLY | C-N | -5.89 | 1.22 | 1.33 |
| 6 | F | 256 | ASP | C-N | -5.89 | 1.20 | 1.34 |
| 4 | D | 179 | ASP | C-N | 5.88 | 1.45 | 1.34 |
| 4 | D | 511 | SER | C-N | 5.88 | 1.47 | 1.34 |
| 5 | E | 137 | LEU | C-N | -5.88 | 1.20 | 1.34 |
| 6 | F | 329 | TYR | C-N | 5.88 | 1.47 | 1.34 |
| 1 | A | 79 | PRO | N-CD | -5.88 | 1.39 | 1.47 |
| 4 | D | 83 | GLN | C-N | 5.86 | 1.47 | 1.34 |
| 7 | G | 347 | GLN | C-N | 5.86 | 1.47 | 1.34 |
| 4 | D | 653 | VAL | C-N | -5.82 | 1.20 | 1.34 |
| 7 | G | 311 | GLU | C-N | -5.81 | 1.20 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7 | G | 290 | LYS | C-N | -5.80 | 1.20 | 1.34 |
| 5 | E | 84 | LEU | C-N | -5.79 | 1.22 | 1.33 |
| 7 | G | 159 | SER | C-N | 5.77 | 1.45 | 1.34 |
| 6 | F | 205 | ASP | C-N | -5.76 | 1.20 | 1.34 |
| 6 | F | 384 | LYS | C-N | -5.75 | 1.20 | 1.34 |
| 6 | F | 390 | GLY | C-N | 5.74 | 1.47 | 1.34 |
| 7 | G | 237 | SER | C-N | -5.74 | 1.20 | 1.34 |
| 5 | E | 9 | PRO | C-N | -5.73 | 1.20 | 1.34 |
| 7 | G | 278 | PHE | C-N | -5.73 | 1.20 | 1.34 |
| 7 | G | 89 | MET | C-N | -5.72 | 1.20 | 1.34 |
| 3 | C | 88 | LEU | C-N | 5.70 | 1.47 | 1.34 |
| 6 | F | 206 | MET | C-N | -5.67 | 1.21 | 1.34 |
| 7 | G | 32 | ASP | C-N | 5.65 | 1.45 | 1.34 |
| 3 | C | 143 | PRO | N-CD | -5.64 | 1.40 | 1.47 |
| 6 | F | 223 | VAL | C-N | 5.62 | 1.47 | 1.34 |
| 3 | C | 144 | ASN | C-N | 5.61 | 1.47 | 1.34 |
| 7 | G | 117 | ASP | C-N | -5.60 | 1.21 | 1.34 |
| 2 | B | 250 | GLY | C-N | -5.60 | 1.21 | 1.34 |
| 5 | E | 81 | PRO | C-N | -5.60 | 1.21 | 1.34 |
| 6 | F | 306 | VAL | C-N | -5.58 | 1.21 | 1.34 |
| 7 | G | 113 | GLY | C-N | -5.58 | 1.21 | 1.34 |
| 8 | H | 222 | LEU | C-N | -5.58 | 1.21 | 1.34 |
| 4 | D | 309 | LEU | C-N | -5.53 | 1.23 | 1.34 |
| 4 | D | 188 | LEU | C-N | -5.53 | 1.21 | 1.34 |
| 2 | B | 219 | GLU | C-N | -5.52 | 1.21 | 1.34 |
| 6 | F | 120 | SER | C-N | 5.51 | 1.44 | 1.34 |
| 3 | C | 325 | GLU | C-N | 5.51 | 1.43 | 1.33 |
| 4 | D | 572 | GLN | C-N | 5.49 | 1.46 | 1.34 |
| 6 | F | 251 | MET | C-N | -5.48 | 1.21 | 1.34 |
| 4 | D | 53 | HIS | C-N | -5.48 | 1.21 | 1.34 |
| 1 | A | 82 | THR | C-N | 5.42 | 1.46 | 1.34 |
| 6 | F | 43 | PHE | C-N | 5.40 | 1.42 | 1.33 |
| 4 | D | 90 | CYS | C-N | 5.38 | 1.46 | 1.34 |
| 2 | B | 45 | SER | C-N | -5.37 | 1.21 | 1.34 |
| 4 | D | 646 | GLN | C-N | -5.36 | 1.21 | 1.34 |
| 7 | G | 213 | SER | C-N | -5.36 | 1.21 | 1.34 |
| 5 | E | 140 | ASN | C-N | -5.35 | 1.21 | 1.34 |
| 8 | H | 365 | SER | C-N | 5.34 | 1.46 | 1.34 |
| 7 | G | 63 | GLN | C-N | 5.34 | 1.46 | 1.34 |
| 7 | G | 90 | LEU | C-N | 5.34 | 1.46 | 1.34 |
| 4 | D | 171 | ARG | C-N | 5.34 | 1.46 | 1.34 |
| 2 | B | 422 | THR | C-N | -5.33 | 1.21 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | D | 396 | ALA | C-N | 5.32 | 1.46 | 1.34 |
| 6 | F | 246 | GLN | C-N | -5.30 | 1.21 | 1.34 |
| 7 | G | 279 | GLN | C-N | -5.29 | 1.21 | 1.34 |
| 6 | F | 276 | ALA | C-N | 5.27 | 1.46 | 1.34 |
| 6 | F | 68 | ASP | C-N | -5.27 | 1.22 | 1.34 |
| 7 | G | 286 | SER | C-N | -5.27 | 1.22 | 1.34 |
| 3 | C | 331 | TYR | C-N | -5.26 | 1.22 | 1.34 |
| 4 | D | 644 | LEU | C-N | -5.26 | 1.22 | 1.34 |
| 5 | E | 23 | LEU | C-N | 5.26 | 1.46 | 1.34 |
| 6 | F | 237 | THR | C-N | -5.26 | 1.22 | 1.34 |
| 7 | G | 282 | HIS | C-N | -5.26 | 1.22 | 1.34 |
| 4 | D | 16 | GLU | C-N | -5.26 | 1.22 | 1.34 |
| 8 | H | 242 | PRO | C-N | -5.26 | 1.22 | 1.34 |
| 7 | G | 181 | LEU | C-N | 5.26 | 1.46 | 1.34 |
| 6 | F | 191 | GLU | C-N | -5.25 | 1.22 | 1.34 |
| 5 | E | 62 | LYS | C-N | -5.25 | 1.22 | 1.34 |
| 6 | F | 197 | GLN | C-N | -5.25 | 1.22 | 1.34 |
| 6 | F | 103 | SER | C-N | 5.24 | 1.46 | 1.34 |
| 7 | G | 317 | GLU | C-N | 5.24 | 1.46 | 1.34 |
| 5 | E | 135 | LEU | C-N | -5.23 | 1.24 | 1.34 |
| 5 | E | 2 | MET | C-N | -5.22 | 1.22 | 1.34 |
| 6 | F | 194 | ARG | C-N | -5.22 | 1.22 | 1.34 |
| 1 | A | 241 | LEU | C-N | 5.20 | 1.46 | 1.34 |
| 1 | A | 78 | GLY | C-N | -5.19 | 1.24 | 1.34 |
| 1 | A | 245 | PRO | C-N | 5.19 | 1.46 | 1.34 |
| 5 | E | 47 | GLU | C-N | -5.19 | 1.22 | 1.34 |
| 6 | F | 363 | LYS | C-N | 5.19 | 1.46 | 1.34 |
| 4 | D | 158 | ARG | C-N | -5.19 | 1.22 | 1.34 |
| 3 | C | 118 | ALA | C-N | 5.18 | 1.46 | 1.34 |
| 4 | D | 187 | PHE | C-N | 5.16 | 1.46 | 1.34 |
| 6 | F | 81 | PRO | C-N | 5.16 | 1.44 | 1.34 |
| 2 | B | 65 | LYS | C-N | 5.16 | 1.46 | 1.34 |
| 7 | G | 145 | CYS | C-N | -5.14 | 1.22 | 1.34 |
| 8 | H | 235 | PRO | N-CD | -5.14 | 1.40 | 1.47 |
| 2 | B | 36 | LEU | C-N | -5.13 | 1.22 | 1.34 |
| 7 | G | 30 | LEU | C-N | -5.13 | 1.22 | 1.34 |
| 5 | E | 65 | GLU | C-N | -5.12 | 1.22 | 1.34 |
| 5 | E | 85 | GLY | C-N | -5.11 | 1.22 | 1.34 |
| 6 | F | 257 | VAL | C-N | -5.10 | 1.22 | 1.34 |
| 6 | F | 109 | GLY | C-N | -5.09 | 1.22 | 1.34 |
| 8 | H | 207 | HIS | C-N | -5.09 | 1.22 | 1.34 |
| 4 | D | 594 | LEU | C-N | 5.08 | 1.45 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4 | D | 665 | ARG | C-N | -5.08 | 1.22 | 1.34 |
| 5 | E | 98 | LEU | C-N | -5.07 | 1.22 | 1.34 |
| 8 | H | 344 | SER | C-N | -5.07 | 1.22 | 1.34 |
| 7 | G | 124 | THR | C-N | 5.06 | 1.45 | 1.34 |
| 1 | A | 53 | GLU | C-N | -5.05 | 1.22 | 1.34 |
| 7 | G | 209 | GLU | C-N | -5.05 | 1.22 | 1.34 |
| 1 | A | 64 | ALA | C-N | -5.04 | 1.22 | 1.34 |
| 5 | E | 50 | GLN | C-N | -5.04 | 1.22 | 1.34 |
| 1 | A | 235 | LEU | C-N | 5.04 | 1.45 | 1.34 |
| 6 | F | 224 | ASP | C-N | -5.04 | 1.22 | 1.34 |
| 7 | G | 104 | SER | C-N | 5.03 | 1.43 | 1.34 |
| 1 | A | 285 | LEU | C-N | 5.02 | 1.45 | 1.34 |
| 7 | G | 98 | LEU | C-N | -5.02 | 1.22 | 1.34 |
| 2 | B | 224 | GLY | C-N | -5.01 | 1.22 | 1.34 |
| 5 | E | 126 | SER | C-N | -5.01 | 1.22 | 1.34 |
| 5 | E | 94 | MET | C-N | -5.00 | 1.22 | 1.34 |
| 6 | F | 303 | ALA | C-N | 5.00 | 1.42 | 1.33 |
| 3 | C | 19 | GLU | C-N | 5.00 | 1.45 | 1.34 |

All (307) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4 | D | 178 | VAL | O-C-N | -23.81 | 84.60 | 122.70 |
| 4 | D | 221 | PRO | O-C-N | -23.73 | 82.85 | 123.20 |
| 7 | G | 130 | ILE | O-C-N | -21.94 | 87.59 | 122.70 |
| 3 | C | 117 | THR | O-C-N | -21.60 | 88.14 | 122.70 |
| 4 | D | 286 | GLU | O-C-N | -21.60 | 88.14 | 122.70 |
| 3 | C | 122 | PRO | O-C-N | -21.14 | 80.93 | 121.10 |
| 1 | A | 283 | ARG | O-C-N | -20.81 | 89.40 | 122.70 |
| 7 | G | 228 | VAL | O-C-N | -20.34 | 90.15 | 122.70 |
| 4 | D | 216 | SER | O-C-N | -20.18 | 90.42 | 122.70 |
| 4 | D | 301 | THR | O-C-N | -20.06 | 90.60 | 122.70 |
| 4 | D | 306 | GLN | O-C-N | -18.98 | 92.34 | 122.70 |
| 1 | A | 282 | LYS | O-C-N | -18.61 | 92.93 | 122.70 |
| 6 | F | 1 | MET | C-N-CA | 18.57 | 168.14 | 121.70 |
| 7 | G | 127 | SER | O-C-N | -18.48 | 93.14 | 122.70 |
| 7 | G | 137 | SER | O-C-N | -18.07 | 93.78 | 122.70 |
| 4 | D | 284 | LEU | O-C-N | -18.06 | 93.80 | 122.70 |
| 2 | B | 234 | GLU | O-C-N | -17.55 | 94.62 | 122.70 |
| 2 | B | 591 | THR | O-C-N | -17.48 | 93.48 | 123.20 |
| 4 | D | 304 | ASP | O-C-N | -17.12 | 88.58 | 121.10 |
| 3 | C | 352 | LEU | O-C-N | -16.76 | 89.25 | 121.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4 | D | 186 | THR | O-C-N | -16.36 | 96.52 | 122.70 |
| 1 | A | 275 | PHE | O-C-N | -15.62 | 97.71 | 122.70 |
| 2 | B | 88 | LYS | O-C-N | -15.58 | 97.77 | 122.70 |
| 3 | C | 119 | ASP | O-C-N | -14.97 | 98.75 | 122.70 |
| 1 | A | 284 | ARG | C-N-CA | 14.57 | 158.14 | 121.70 |
| 2 | B | 594 | GLY | O-C-N | -14.44 | 99.59 | 122.70 |
| 2 | B | 236 | PHE | O-C-N | -13.88 | 100.49 | 122.70 |
| 2 | B | 596 | SER | O-C-N | -13.77 | 100.66 | 122.70 |
| 2 | B | 222 | PHE | O-C-N | -13.39 | 101.28 | 122.70 |
| 2 | B | 231 | GLY | O-C-N | -13.35 | 101.35 | 122.70 |
| 1 | A | 282 | LYS | CA-C-N | 13.23 | 146.31 | 117.20 |
| 4 | D | 662 | THR | O-C-N | -13.00 | 101.11 | 123.20 |
| 1 | A | 278 | PRO | O-C-N | -12.85 | 102.13 | 122.70 |
| 5 | E | 39 | GLU | O-C-N | -12.77 | 102.27 | 122.70 |
| 2 | B | 238 | LEU | O-C-N | -12.72 | 102.35 | 122.70 |
| 7 | G | 123 | ASP | O-C-N | -12.52 | 102.67 | 122.70 |
| 2 | B | 249 | ASP | O-C-N | -12.43 | 102.08 | 123.20 |
| 2 | B | 245 | SER | O-C-N | -12.34 | 102.96 | 122.70 |
| 4 | D | 175 | PHE | O-C-N | -12.31 | 103.01 | 122.70 |
| 1 | A | 277 | VAL | O-C-N | -12.22 | 97.88 | 121.10 |
| 2 | B | 246 | PHE | O-C-N | -12.13 | 102.58 | 123.20 |
| 4 | D | 184 | SER | O-C-N | -12.13 | 103.30 | 122.70 |
| 2 | B | 181 | PRO | O-C-N | -12.11 | 103.33 | 122.70 |
| 2 | B | 84 | PHE | O-C-N | -12.10 | 103.35 | 122.70 |
| 5 | E | 220 | LEU | O-C-N | -11.93 | 103.62 | 122.70 |
| 2 | B | 92 | ILE | O-C-N | -11.64 | 104.08 | 122.70 |
| 6 | F | 295 | LEU | O-C-N | -11.62 | 104.11 | 122.70 |
| 1 | A | 281 | SER | O-C-N | 11.44 | 141.00 | 122.70 |
| 7 | G | 196 | LYS | C-N-CA | 11.30 | 146.02 | 122.30 |
| 5 | E | 219 | ASN | O-C-N | -11.26 | 104.69 | 122.70 |
| 5 | E | 221 | HIS | O-C-N | -11.11 | 99.99 | 121.10 |
| 1 | A | 283 | ARG | C-N-CA | 11.07 | 149.38 | 121.70 |
| 2 | B | 225 | MET | O-C-N | -10.99 | 105.12 | 122.70 |
| 2 | B | 95 | VAL | O-C-N | -10.89 | 105.28 | 122.70 |
| 7 | G | 133 | SER | O-C-N | -10.80 | 105.42 | 122.70 |
| 4 | D | 280 | PRO | O-C-N | -10.80 | 105.42 | 122.70 |
| 3 | C | 320 | LEU | O-C-N | -10.73 | 104.97 | 123.20 |
| 1 | A | 278 | PRO | C-N-CA | 10.71 | 148.48 | 121.70 |
| 3 | C | 118 | ALA | O-C-N | -10.60 | 105.74 | 122.70 |
| 2 | B | 592 | GLY | O-C-N | -10.47 | 105.40 | 123.20 |
| 3 | C | 351 | SER | O-C-N | -10.40 | 106.06 | 122.70 |
| 7 | G | 129 | VAL | C-N-CA | 10.27 | 147.38 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 3 | C | 123 | PRO | O-C-N | -10.23 | 106.33 | 122.70 |
| 1 | A | 280 | PRO | C-N-CA | 9.97 | 146.63 | 121.70 |
| 4 | D | 219 | VAL | O-C-N | -9.95 | 106.78 | 122.70 |
| 4 | D | 183 | SER | O-C-N | -9.85 | 106.94 | 122.70 |
| 2 | B | 223 | GLU | C-N-CA | 9.64 | 142.56 | 122.30 |
| 2 | B | 242 | ASN | O-C-N | -9.62 | 107.31 | 122.70 |
| 6 | F | 224 | ASP | O-C-N | -9.57 | 107.39 | 122.70 |
| 4 | D | 302 | HIS | O-C-N | -9.55 | 107.42 | 122.70 |
| 2 | B | 593 | GLY | O-C-N | -9.52 | 107.02 | 123.20 |
| 1 | A | 284 | ARG | O-C-N | -9.42 | 107.63 | 122.70 |
| 2 | B | 93 | GLU | O-C-N | -9.37 | 107.71 | 122.70 |
| 2 | B | 96 | ALA | O-C-N | -9.30 | 107.83 | 122.70 |
| 4 | D | 221 | PRO | CA-C-N | 9.25 | 134.70 | 116.20 |
| 8 | H | 156 | PRO | O-C-N | -9.23 | 107.93 | 122.70 |
| 7 | G | 230 | ASP | O-C-N | -9.20 | 107.56 | 123.20 |
| 4 | D | 218 | SER | O-C-N | -9.14 | 108.07 | 122.70 |
| 7 | G | 124 | THR | C-N-CA | 9.12 | 144.51 | 121.70 |
| 1 | A | 276 | VAL | C-N-CA | 9.07 | 144.38 | 121.70 |
| 1 | A | 283 | ARG | CA-C-N | 9.05 | 137.11 | 117.20 |
| 6 | F | 8 | HIS | O-C-N | -9.02 | 108.26 | 122.70 |
| 5 | E | 2 | MET | O-C-N | -8.96 | 108.36 | 122.70 |
| 6 | F | 159 | SER | O-C-N | -8.96 | 108.36 | 122.70 |
| 1 | A | 282 | LYS | C-N-CA | 8.94 | 144.06 | 121.70 |
| 2 | B | 229 | VAL | O-C-N | -8.85 | 108.54 | 122.70 |
| 1 | A | 281 | SER | CA-C-N | -8.83 | 97.76 | 117.20 |
| 4 | D | 287 | PHE | C-N-CA | 8.81 | 143.73 | 121.70 |
| 1 | A | 281 | SER | C-N-CA | -8.81 | 99.67 | 121.70 |
| 2 | B | 456 | ASP | O-C-N | -8.73 | 108.73 | 122.70 |
| 6 | F | 6 | ARG | C-N-CD | -8.71 | 101.43 | 120.60 |
| 6 | F | 227 | ILE | O-C-N | -8.70 | 108.77 | 122.70 |
| 6 | F | 146 | ALA | O-C-N | -8.68 | 108.82 | 122.70 |
| 2 | B | 592 | GLY | CA-C-N | 8.59 | 133.38 | 116.20 |
| 2 | B | 591 | THR | C-N-CA | 8.58 | 140.31 | 122.30 |
| 7 | G | 128 | ASN | O-C-N | -8.52 | 109.06 | 122.70 |
| 1 | A | 234 | LYS | O-C-N | -8.50 | 109.09 | 122.70 |
| 4 | D | 177 | ALA | O-C-N | -8.41 | 109.25 | 122.70 |
| 7 | G | 132 | GLU | O-C-N | -8.38 | 109.30 | 122.70 |
| 2 | B | 2 | SER | O-C-N | -8.36 | 108.98 | 123.20 |
| 6 | F | 228 | SER | O-C-N | -8.35 | 109.34 | 122.70 |
| 1 | A | 236 | ASN | O-C-N | -8.32 | 109.39 | 122.70 |
| 2 | B | 595 | SER | O-C-N | -8.23 | 109.53 | 122.70 |
| 2 | B | 240 | GLN | O-C-N | -8.22 | 109.54 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6 | F | 108 | ALA | O-C-N | -8.21 | 109.25 | 123.20 |
| 2 | B | 237 | GLN | C-N-CA | 8.20 | 142.19 | 121.70 |
| 7 | G | 137 | SER | CA-C-N | 8.19 | 135.22 | 117.20 |
| 3 | C | 280 | CYS | O-C-N | -8.18 | 109.61 | 122.70 |
| 3 | C | 320 | LEU | C-N-CA | 8.14 | 139.39 | 122.30 |
| 2 | B | 241 | LEU | O-C-N | -8.12 | 109.72 | 122.70 |
| 6 | F | 6 | ARG | O-C-N | -8.07 | 105.77 | 121.10 |
| 7 | G | 199 | ASP | O-C-N | -8.03 | 109.85 | 122.70 |
| 2 | B | 230 | GLU | O-C-N | -8.02 | 109.57 | 123.20 |
| 3 | C | 344 | MET | O-C-N | -8.00 | 109.89 | 122.70 |
| 7 | G | 28 | VAL | O-C-N | -7.99 | 109.92 | 122.70 |
| 2 | B | 242 | ASN | C-N-CA | 7.92 | 141.50 | 121.70 |
| 2 | B | 432 | ALA | C-N-CA | -7.91 | 101.93 | 121.70 |
| 4 | D | 221 | PRO | C-N-CA | 7.81 | 138.70 | 122.30 |
| 2 | B | 596 | SER | CA-C-N | 7.79 | 134.35 | 117.20 |
| 4 | D | 576 | ASN | C-N-CD | -7.78 | 103.48 | 120.60 |
| 4 | D | 280 | PRO | C-N-CA | -7.75 | 102.32 | 121.70 |
| 6 | F | 3 | SER | C-N-CA | 7.75 | 138.57 | 122.30 |
| 4 | D | 280 | PRO | CA-C-N | 7.75 | 134.24 | 117.20 |
| 6 | F | 225 | ARG | O-C-N | -7.72 | 110.35 | 122.70 |
| 5 | E | 219 | ASN | CA-C-N | 7.66 | 134.06 | 117.20 |
| 2 | B | 458 | THR | O-C-N | -7.65 | 110.47 | 122.70 |
| 8 | H | 258 | ARG | O-C-N | -7.64 | 110.47 | 122.70 |
| 5 | E | 43 | PHE | O-C-N | -7.61 | 110.53 | 122.70 |
| 3 | C | 320 | LEU | CA-C-N | 7.58 | 131.36 | 116.20 |
| 6 | F | 3 | SER | O-C-N | -7.57 | 110.33 | 123.20 |
| 4 | D | 288 | SER | O-C-N | -7.54 | 110.63 | 122.70 |
| 7 | G | 137 | SER | C-N-CA | 7.54 | 140.54 | 121.70 |
| 2 | B | 223 | GLU | O-C-N | -7.52 | 110.41 | 123.20 |
| 1 | A | 238 | TYR | O-C-N | -7.52 | 110.67 | 122.70 |
| 1 | A | 285 | LEU | O-C-N | -7.51 | 110.68 | 122.70 |
| 7 | G | 197 | GLY | O-C-N | -7.51 | 110.69 | 122.70 |
| 5 | E | 221 | HIS | CA-C-N | 7.48 | 138.05 | 117.10 |
| 4 | D | 308 | THR | O-C-N | -7.48 | 110.74 | 122.70 |
| 5 | E | 4 | ALA | O-C-N | -7.47 | 110.75 | 122.70 |
| 2 | B | 459 | GLN | O-C-N | -7.46 | 110.77 | 122.70 |
| 2 | B | 228 | PHE | O-C-N | -7.40 | 110.86 | 122.70 |
| 3 | C | 348 | LEU | O-C-N | -7.40 | 110.87 | 122.70 |
| 4 | D | 458 | PRO | O-C-N | -7.32 | 110.98 | 122.70 |
| 3 | C | 351 | SER | CA-C-N | 7.28 | 133.21 | 117.20 |
| 2 | B | 591 | THR | CA-C-N | 7.27 | 130.74 | 116.20 |
| 3 | C | 119 | ASP | C-N-CA | -7.21 | 103.67 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | D | 663 | GLY | C-N-CA | -7.21 | 103.67 | 121.70 |
| 6 | F | 220 | ALA | O-C-N | -7.19 | 111.20 | 122.70 |
| 4 | D | 665 | ARG | O-C-N | -7.19 | 111.20 | 122.70 |
| 3 | C | 347 | GLU | O-C-N | -7.18 | 111.21 | 122.70 |
| 4 | D | 223 | LYS | O-C-N | -7.17 | 111.22 | 122.70 |
| 2 | B | 88 | LYS | C-N-CA | -7.17 | 103.77 | 121.70 |
| 6 | F | 223 | VAL | O-C-N | -7.14 | 111.27 | 122.70 |
| 6 | F | 5 | SER | O-C-N | -7.12 | 111.31 | 122.70 |
| 1 | A | 241 | LEU | O-C-N | -7.03 | 111.45 | 122.70 |
| 8 | H | 255 | ASP | O-C-N | -7.01 | 111.48 | 122.70 |
| 4 | D | 455 | LYS | O-C-N | -7.01 | 111.48 | 122.70 |
| 2 | B | 225 | MET | CA-C-N | 6.95 | 132.50 | 117.20 |
| 5 | E | 42 | CYS | O-C-N | -6.91 | 111.65 | 122.70 |
| 1 | A | 237 | SER | O-C-N | -6.91 | 111.65 | 122.70 |
| 1 | A | 228 | SER | O-C-N | -6.90 | 111.67 | 122.70 |
| 2 | B | 186 | GLU | O-C-N | -6.89 | 111.67 | 122.70 |
| 7 | G | 274 | MET | O-C-N | -6.83 | 111.58 | 123.20 |
| 5 | E | 3 | ALA | O-C-N | -6.77 | 111.87 | 122.70 |
| 1 | A | 274 | GLU | O-C-N | -6.76 | 111.89 | 122.70 |
| 2 | B | 16 | TYR | O-C-N | -6.75 | 108.28 | 121.10 |
| 4 | D | 665 | ARG | C-N-CA | -6.70 | 104.94 | 121.70 |
| 1 | A | 191 | TYR | O-C-N | -6.68 | 112.01 | 122.70 |
| 3 | C | 342 | ARG | O-C-N | 6.66 | 133.36 | 122.70 |
| 4 | D | 575 | THR | O-C-N | -6.66 | 112.05 | 122.70 |
| 4 | D | 216 | SER | CA-C-N | 6.65 | 131.82 | 117.20 |
| 2 | B | 91 | ALA | O-C-N | -6.62 | 112.10 | 122.70 |
| 4 | D | 216 | SER | C-N-CA | 6.61 | 138.24 | 121.70 |
| 4 | D | 303 | LEU | C-N-CA | -6.61 | 105.17 | 121.70 |
| 6 | F | 2 | GLN | C-N-CA | 6.56 | 138.09 | 121.70 |
| 2 | B | 23 | ASP | O-C-N | -6.51 | 112.13 | 123.20 |
| 1 | A | 202 | SER | O-C-N | -6.50 | 112.31 | 122.70 |
| 1 | A | 279 | GLU | O-C-N | -6.49 | 108.77 | 121.10 |
| 2 | B | 432 | ALA | O-C-N | -6.49 | 112.33 | 122.70 |
| 2 | B | 556 | MET | O-C-N | -6.49 | 112.32 | 122.70 |
| 6 | F | 226 | LYS | O-C-N | -6.47 | 112.35 | 122.70 |
| 6 | F | 1 | MET | O-C-N | -6.45 | 112.37 | 122.70 |
| 2 | B | 240 | GLN | C-N-CA | 6.45 | 137.81 | 121.70 |
| 7 | G | 196 | LYS | O-C-N | -6.39 | 112.34 | 123.20 |
| 2 | B | 23 | ASP | C-N-CA | 6.36 | 135.66 | 122.30 |
| 2 | B | 182 | GLU | O-C-N | -6.35 | 112.54 | 122.70 |
| 6 | F | 216 | GLN | O-C-N | -6.33 | 112.58 | 122.70 |
| 6 | F | 108 | ALA | CA-C-N | 6.29 | 128.77 | 116.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | D | 281 | SER | O-C-N | -6.29 | 112.64 | 122.70 |
| 6 | F | 229 | ASP | O-C-N | -6.28 | 112.65 | 122.70 |
| 7 | G | 183 | ALA | C-N-CA | 6.26 | 137.34 | 121.70 |
| 1 | A | 217 | LEU | O-C-N | -6.25 | 112.70 | 122.70 |
| 2 | B | 185 | CYS | C-N-CA | -6.21 | 106.17 | 121.70 |
| 4 | D | 175 | PHE | CA-C-N | 6.20 | 130.84 | 117.20 |
| 6 | F | 224 | ASP | CA-C-N | 6.20 | 130.83 | 117.20 |
| 7 | G | 130 | ILE | C-N-CA | 6.19 | 137.18 | 121.70 |
| 1 | A | 221 | LEU | O-C-N | -6.18 | 112.81 | 122.70 |
| 2 | B | 16 | TYR | C-N-CD | -6.18 | 107.01 | 120.60 |
| 7 | G | 273 | PRO | O-C-N | -6.17 | 112.83 | 122.70 |
| 1 | A | 243 | PRO | O-C-N | -6.17 | 112.83 | 122.70 |
| 3 | C | 316 | SER | O-C-N | -6.16 | 112.84 | 122.70 |
| 2 | B | 229 | VAL | CA-C-N | 6.16 | 130.74 | 117.20 |
| 2 | B | 82 | LYS | O-C-N | 6.14 | 132.53 | 122.70 |
| 1 | A | 224 | LEU | O-C-N | -6.11 | 112.92 | 122.70 |
| 6 | F | 8 | HIS | CA-C-N | 6.09 | 130.59 | 117.20 |
| 2 | B | 304 | LYS | O-C-N | -6.07 | 113.00 | 122.70 |
| 2 | B | 235 | ASN | C-N-CA | 6.05 | 136.84 | 121.70 |
| 2 | B | 47 | ALA | O-C-N | -6.05 | 113.03 | 122.70 |
| 4 | D | 386 | MET | O-C-N | 6.04 | 132.36 | 122.70 |
| 4 | D | 279 | GLY | C-N-CD | -6.03 | 107.34 | 120.60 |
| 4 | D | 285 | LYS | C-N-CA | 6.00 | 136.69 | 121.70 |
| 4 | D | 359 | SER | O-C-N | -5.98 | 113.13 | 122.70 |
| 4 | D | 17 | GLU | O-C-N | -5.94 | 113.20 | 122.70 |
| 2 | B | 223 | GLU | CA-C-N | 5.92 | 128.05 | 116.20 |
| 4 | D | 217 | SER | O-C-N | -5.88 | 113.30 | 122.70 |
| 5 | E | 217 | ILE | O-C-N | -5.86 | 113.33 | 122.70 |
| 1 | A | 236 | ASN | CA-C-N | 5.86 | 130.08 | 117.20 |
| 7 | G | 274 | MET | CA-C-N | 5.83 | 127.86 | 116.20 |
| 4 | D | 631 | GLN | O-C-N | -5.81 | 113.40 | 122.70 |
| 4 | D | 176 | SER | O-C-N | -5.81 | 113.40 | 122.70 |
| 2 | B | 250 | GLY | O-C-N | -5.79 | 113.43 | 122.70 |
| 3 | C | 120 | SER | C-N-CA | 5.79 | 136.18 | 121.70 |
| 2 | B | 299 | ASP | O-C-N | -5.76 | 113.48 | 122.70 |
| 4 | D | 290 | PRO | C-N-CA | -5.76 | 107.31 | 121.70 |
| 7 | G | 131 | LEU | C-N-CA | -5.76 | 107.31 | 121.70 |
| 1 | A | 231 | ALA | O-C-N | -5.75 | 113.49 | 122.70 |
| 3 | C | 280 | CYS | CA-C-N | 5.75 | 129.84 | 117.20 |
| 4 | D | 404 | LYS | O-C-N | 5.74 | 131.88 | 122.70 |
| 1 | A | 271 | ASN | O-C-N | -5.73 | 113.53 | 122.70 |
| 6 | F | 276 | ALA | O-C-N | -5.67 | 113.62 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7 | G | 20 | LEU | O-C-N | -5.67 | 113.63 | 122.70 |
| 2 | B | 244 | ASN | O-C-N | -5.64 | 113.68 | 122.70 |
| 7 | G | 272 | SER | O-C-N | -5.64 | 110.39 | 121.10 |
| 7 | G | 172 | PRO | O-C-N | -5.61 | 113.73 | 122.70 |
| 3 | C | 122 | PRO | CA-C-N | 5.60 | 132.78 | 117.10 |
| 7 | G | 126 | SER | C-N-CA | -5.60 | 107.70 | 121.70 |
| 7 | G | 133 | SER | C-N-CA | 5.60 | 135.69 | 121.70 |
| 3 | C | 344 | MET | CA-C-N | 5.59 | 129.50 | 117.20 |
| 5 | E | 42 | CYS | C-N-CA | 5.59 | 135.67 | 121.70 |
| 7 | G | 127 | SER | C-N-CA | -5.58 | 107.76 | 121.70 |
| 4 | D | 184 | SER | C-N-CA | -5.57 | 107.77 | 121.70 |
| 1 | A | 242 | ALA | O-C-N | -5.56 | 110.53 | 121.10 |
| 1 | A | 203 | ALA | O-C-N | -5.54 | 113.78 | 123.20 |
| 2 | B | 593 | GLY | C-N-CA | 5.54 | 133.93 | 122.30 |
| 2 | B | 433 | SER | O-C-N | -5.52 | 113.87 | 122.70 |
| 2 | B | 90 | PRO | O-C-N | -5.51 | 113.88 | 122.70 |
| 4 | D | 220 | HIS | C-N-CD | -5.51 | 108.49 | 120.60 |
| 5 | E | 41 | PRO | O-C-N | 5.50 | 131.50 | 122.70 |
| 3 | C | 121 | VAL | C-N-CD | -5.47 | 108.57 | 120.60 |
| 7 | G | 135 | SER | O-C-N | -5.46 | 113.96 | 122.70 |
| 1 | A | 194 | HIS | O-C-N | 5.46 | 131.43 | 122.70 |
| 2 | B | 23 | ASP | CA-C-N | 5.42 | 127.04 | 116.20 |
| 7 | G | 70 | LYS | O-C-N | -5.42 | 114.04 | 122.70 |
| 4 | D | 48 | ARG | O-C-N | -5.41 | 114.04 | 122.70 |
| 1 | A | 284 | ARG | CA-C-N | 5.40 | 129.09 | 117.20 |
| 1 | A | 234 | LYS | CA-C-N | 5.39 | 129.06 | 117.20 |
| 4 | D | 38 | GLN | O-C-N | -5.39 | 114.08 | 122.70 |
| 4 | D | 5 | SER | O-C-N | -5.37 | 114.11 | 122.70 |
| 5 | E | 43 | PHE | C-N-CA | 5.36 | 135.10 | 121.70 |
| 7 | G | 226 | SER | C-N-CA | 5.36 | 135.09 | 121.70 |
| 7 | G | 122 | PRO | O-C-N | -5.35 | 114.14 | 122.70 |
| 8 | H | 305 | PHE | O-C-N | -5.28 | 114.25 | 122.70 |
| 2 | B | 295 | SER | O-C-N | -5.28 | 114.26 | 122.70 |
| 1 | A | 234 | LYS | C-N-CA | 5.26 | 134.85 | 121.70 |
| 1 | A | 236 | ASN | C-N-CA | 5.26 | 134.85 | 121.70 |
| 3 | C | 122 | PRO | C-N-CD | 5.26 | 139.44 | 128.40 |
| 3 | C | 293 | ARG | O-C-N | 5.25 | 131.09 | 122.70 |
| 6 | F | 227 | ILE | CA-C-N | 5.24 | 128.74 | 117.20 |
| 4 | D | 289 | GLU | C-N-CD | -5.24 | 109.07 | 120.60 |
| 2 | B | 431 | SER | C-N-CA | 5.24 | 134.80 | 121.70 |
| 1 | A | 215 | VAL | O-C-N | 5.24 | 131.08 | 122.70 |
| 3 | C | 348 | LEU | CA-C-N | 5.23 | 128.70 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 521 | THR | O-C-N | 5.22 | 131.06 | 122.70 |
| 8 | H | 258 | ARG | CA-C-N | 5.20 | 128.63 | 117.20 |
| 4 | D | 175 | PHE | C-N-CA | 5.19 | 134.67 | 121.70 |
| 1 | A | 238 | TYR | CA-C-N | 5.19 | 128.61 | 117.20 |
| 6 | F | 106 | VAL | O-C-N | -5.19 | 114.38 | 123.20 |
| 1 | A | 270 | VAL | O-C-N | -5.17 | 114.43 | 122.70 |
| 3 | C | 319 | PHE | O-C-N | -5.17 | 114.44 | 122.70 |
| 6 | F | 304 | GLY | O-C-N | -5.17 | 114.43 | 122.70 |
| 4 | D | 630 | VAL | O-C-N | -5.16 | 114.45 | 122.70 |
| 4 | D | 458 | PRO | CA-C-N | 5.14 | 128.51 | 117.20 |
| 2 | B | 85 | SER | O-C-N | -5.14 | 114.48 | 122.70 |
| 6 | F | 389 | LEU | O-C-N | -5.14 | 114.47 | 123.20 |
| 7 | G | 198 | LYS | O-C-N | -5.13 | 114.50 | 122.70 |
| 8 | H | 238 | THR | O-C-N | -5.13 | 114.50 | 122.70 |
| 7 | G | 129 | VAL | O-C-N | -5.12 | 114.51 | 122.70 |
| 4 | D | 627 | GLU | O-C-N | -5.11 | 114.53 | 122.70 |
| 7 | G | 3 | GLY | O-C-N | -5.10 | 114.53 | 123.20 |
| 2 | B | 594 | GLY | CA-C-N | 5.09 | 128.40 | 117.20 |
| 4 | D | 176 | SER | C-N-CA | 5.09 | 134.42 | 121.70 |
| 1 | A | 285 | LEU | CA-C-N | 5.07 | 128.36 | 117.20 |
| 4 | D | 664 | SER | O-C-N | -5.07 | 114.58 | 122.70 |
| 5 | E | 216 | SER | O-C-N | -5.07 | 114.58 | 122.70 |
| 4 | D | 177 | ALA | C-N-CA | 5.07 | 134.37 | 121.70 |
| 2 | B | 457 | ASN | C-N-CA | -5.07 | 109.04 | 121.70 |
| 6 | F | 296 | GLN | O-C-N | -5.07 | 114.59 | 122.70 |
| 6 | F | 366 | ASP | O-C-N | -5.07 | 114.60 | 122.70 |
| 1 | A | 280 | PRO | O-C-N | 5.06 | 130.80 | 122.70 |
| 6 | F | 209 | GLU | O-C-N | -5.06 | 114.61 | 122.70 |
| 3 | C | 342 | ARG | CA-C-N | -5.04 | 106.11 | 117.20 |
| 1 | A | 244 | ASN | C-N-CD | -5.02 | 109.56 | 120.60 |
| 2 | B | 235 | ASN | O-C-N | -5.02 | 114.67 | 122.70 |
| 3 | C | 344 | MET | C-N-CA | 5.01 | 134.24 | 121.70 |
| 8 | H | 270 | GLY | O-C-N | 5.01 | 130.72 | 122.70 |
| 7 | G | 101 | GLY | O-C-N | -5.00 | 114.69 | 122.70 |
| 6 | F | 220 | ALA | CA-C-N | 5.00 | 128.21 | 117.20 |

There are no chirality outliers.

All (193) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 241 | LEU | Mainchain |
| 1 | A | 242 | ALA | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | A | 243 | PRO | Mainchain |
| 1 | A | 269 | LYS | Mainchain |
| 1 | A | 273 | MET | Peptide |
| 1 | A | 274 | GLU | Mainchain,Peptide |
| 1 | A | 275 | PHE | Mainchain,Peptide |
| 1 | A | 276 | VAL | Peptide |
| 1 | A | 278 | PRO | Mainchain,Peptide |
| 1 | A | 279 | GLU | Mainchain |
| 1 | A | 281 | SER | Peptide |
| 1 | A | 285 | LEU | Peptide |
| 2 | B | 1 | MET | Mainchain |
| 2 | B | 179 | SER | Mainchain |
| 2 | B | 181 | PRO | Mainchain |
| 2 | B | 182 | GLU | Mainchain |
| 2 | B | 183 | THR | Mainchain |
| 2 | B | 184 | ALA | Mainchain |
| 2 | B | 185 | CYS | Mainchain |
| 2 | B | 186 | GLU | Mainchain |
| 2 | B | 187 | LEU | Mainchain |
| 2 | B | 189 | SER | Mainchain |
| 2 | B | 2 | SER | Mainchain |
| 2 | B | 222 | PHE | Mainchain |
| 2 | B | 224 | GLY | Mainchain |
| 2 | B | 225 | MET | Mainchain |
| 2 | B | 230 | GLU | Mainchain,Peptide |
| 2 | B | 231 | GLY | Mainchain,Peptide |
| 2 | B | 232 | SER | Mainchain |
| 2 | B | 233 | ASP | Mainchain,Peptide |
| 2 | B | 234 | GLU | Mainchain |
| 2 | B | 235 | ASN | Mainchain |
| 2 | B | 236 | PHE | Mainchain |
| 2 | B | 238 | LEU | Mainchain |
| 2 | B | 239 | VAL | Mainchain |
| 2 | B | 240 | GLN | Mainchain |
| 2 | B | 241 | LEU | Mainchain |
| 2 | B | 242 | ASN | Mainchain |
| 2 | B | 244 | ASN | Mainchain |
| 2 | B | 245 | SER | Mainchain |
| 2 | B | 246 | PHE | Mainchain,Peptide |
| 2 | B | 247 | GLY | Mainchain |
| 2 | B | 249 | ASP | Mainchain |
| 2 | B | 250 | GLY | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 2 | B | 251 | THR | Mainchain |
| 2 | B | 304 | LYS | Mainchain |
| 2 | B | 430 | LEU | Mainchain |
| 2 | B | 432 | ALA | Mainchain |
| 2 | B | 433 | SER | Mainchain |
| 2 | B | 434 | LYS | Mainchain |
| 2 | B | 455 | GLY | Mainchain |
| 2 | B | 456 | ASP | Mainchain |
| 2 | B | 457 | ASN | Mainchain |
| 2 | B | 458 | THR | Mainchain |
| 2 | B | 459 | GLN | Mainchain |
| 2 | B | 460 | LYS | Mainchain |
| 2 | B | 593 | GLY | Mainchain |
| 2 | B | 594 | GLY | Mainchain |
| 2 | B | 595 | SER | Mainchain,Peptide |
| 2 | B | 596 | SER | Mainchain,Peptide |
| 2 | B | 67 | SER | Mainchain |
| 2 | B | 84 | PHE | Mainchain |
| 2 | B | 85 | SER | Mainchain |
| 2 | B | 86 | ILE | Mainchain |
| 2 | B | 87 | SER | Mainchain |
| 2 | B | 88 | LYS | Mainchain |
| 2 | B | 89 | VAL | Mainchain |
| 2 | B | 90 | PRO | Mainchain |
| 2 | B | 91 | ALA | Mainchain |
| 2 | B | 92 | ILE | Mainchain |
| 2 | B | 93 | GLU | Mainchain |
| 2 | B | 94 | GLU | Mainchain |
| 2 | B | 95 | VAL | Mainchain |
| 2 | B | 96 | ALA | Mainchain |
| 3 | C | 117 | THR | Mainchain |
| 3 | C | 118 | ALA | Mainchain |
| 3 | C | 119 | ASP | Mainchain |
| 3 | C | 121 | VAL | Mainchain |
| 3 | C | 122 | PRO | Mainchain |
| 3 | C | 123 | PRO | Mainchain |
| 3 | C | 124 | SER | Mainchain |
| 3 | C | 126 | SER | Mainchain |
| 3 | C | 320 | LEU | Mainchain |
| 3 | C | 352 | LEU | Mainchain,Peptide |
| 4 | D | 118 | ASP | Mainchain |
| 4 | D | 119 | LEU | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 4 | D | 120 | ASN | Mainchain |
| 4 | D | 175 | PHE | Mainchain |
| 4 | D | 177 | ALA | Mainchain |
| 4 | D | 178 | VAL | Mainchain |
| 4 | D | 180 | PRO | Mainchain |
| 4 | D | 181 | ASP | Mainchain |
| 4 | D | 182 | LEU | Mainchain |
| 4 | D | 183 | SER | Mainchain,Peptide |
| 4 | D | 184 | SER | Mainchain |
| 4 | D | 185 | SER | Mainchain |
| 4 | D | 186 | THR | Mainchain |
| 4 | D | 187 | PHE | Mainchain |
| 4 | D | 216 | SER | Mainchain |
| 4 | D | 217 | SER | Mainchain |
| 4 | D | 218 | SER | Mainchain |
| 4 | D | 219 | VAL | Mainchain |
| 4 | D | 220 | HIS | Mainchain |
| 4 | D | 221 | PRO | Mainchain |
| 4 | D | 279 | GLY | Peptide |
| 4 | D | 281 | SER | Mainchain |
| 4 | D | 284 | LEU | Mainchain |
| 4 | D | 286 | GLU | Mainchain |
| 4 | D | 288 | SER | Mainchain,Peptide |
| 4 | D | 301 | THR | Mainchain |
| 4 | D | 302 | HIS | Mainchain,Peptide |
| 4 | D | 304 | ASP | Mainchain |
| 4 | D | 305 | PRO | Mainchain |
| 4 | D | 306 | GLN | Mainchain |
| 4 | D | 307 | GLU | Mainchain |
| 4 | D | 308 | THR | Mainchain |
| 4 | D | 357 | ASP | Mainchain |
| 4 | D | 359 | SER | Mainchain |
| 4 | D | 662 | THR | Mainchain |
| 4 | D | 663 | GLY | Mainchain |
| 4 | D | 664 | SER | Mainchain |
| 4 | D | 665 | ARG | Mainchain |
| 5 | E | 1 | MET | Mainchain |
| 5 | E | 2 | MET | Mainchain |
| 5 | E | 220 | LEU | Mainchain,Peptide |
| 5 | E | 221 | HIS | Mainchain,Peptide |
| 5 | E | 3 | ALA | Mainchain |
| 5 | E | 38 | LEU | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 5 | E | 39 | GLU | Mainchain |
| 5 | E | 4 | ALA | Mainchain |
| 5 | E | 5 | ASN | Mainchain |
| 6 | F | 1 | MET | Mainchain,Peptide |
| 6 | F | 122 | GLY | Mainchain |
| 6 | F | 146 | ALA | Mainchain |
| 6 | F | 159 | SER | Mainchain |
| 6 | F | 2 | GLN | Mainchain,Peptide |
| 6 | F | 225 | ARG | Mainchain |
| 6 | F | 227 | ILE | Mainchain |
| 6 | F | 228 | SER | Mainchain |
| 6 | F | 276 | ALA | Mainchain |
| 6 | F | 295 | LEU | Mainchain |
| 6 | F | 3 | SER | Mainchain |
| 6 | F | 336 | LEU | Mainchain |
| 6 | F | 36 | LYS | Mainchain |
| 6 | F | 39 | VAL | Mainchain |
| 6 | F | 4 | GLY | Mainchain |
| 6 | F | 5 | SER | Mainchain |
| 6 | F | 6 | ARG | Mainchain |
| 7 | G | 1 | MET | Mainchain |
| 7 | G | 121 | TYR | Mainchain |
| 7 | G | 122 | PRO | Mainchain |
| 7 | G | 123 | ASP | Mainchain |
| 7 | G | 124 | THR | Mainchain |
| 7 | G | 125 | ILE | Mainchain |
| 7 | G | 127 | SER | Mainchain |
| 7 | G | 128 | ASN | Mainchain |
| 7 | G | 130 | ILE | Mainchain |
| 7 | G | 131 | LEU | Mainchain,Peptide |
| 7 | G | 132 | GLU | Mainchain |
| 7 | G | 133 | SER | Mainchain,Peptide |
| 7 | G | 134 | LEU | Mainchain |
| 7 | G | 135 | SER | Mainchain |
| 7 | G | 137 | SER | Mainchain |
| 7 | G | 196 | LYS | Mainchain |
| 7 | G | 198 | LYS | Mainchain |
| 7 | G | 2 | THR | Mainchain |
| 7 | G | 226 | SER | Mainchain |
| 7 | G | 227 | SER | Mainchain |
| 7 | G | 228 | VAL | Mainchain |
| 7 | G | 230 | ASP | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 7 | G | 272 | SER | Mainchain |
| 7 | G | 28 | VAL | Mainchain |
| 7 | G | 3 | GLY | Mainchain |
| 8 | H | 156 | PRO | Mainchain |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2282 | 0 | 2354 | 222 | 0 |
| 2 | B | 4771 | 0 | 4779 | 433 | 0 |
| 3 | C | 2885 | 0 | 2951 | 249 | 0 |
| 4 | D | 5415 | 0 | 5439 | 500 | 0 |
| 5 | E | 1717 | 0 | 1711 | 142 | 0 |
| 6 | F | 3171 | 0 | 3232 | 267 | 0 |
| 7 | G | 2687 | 0 | 2642 | 225 | 0 |
| 8 | H | 1671 | 0 | 1673 | 224 | 0 |
| All | All | 24599 | 0 | 24781 | 1440 | 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 29.

All (1440) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 5:E:155:ILE:CG2 | 6:F:334:VAL:HG21 | 1.33 | 1.57 |
| 1:A:278:PRO:HB2 | 1:A:279:GLU:CB | 1.31 | 1.57 |
| 6:F:335:ARG:CZ | 8:H:259:HIS:CB | 1.81 | 1.53 |
| 2:B:490:GLU:CA | 4:D:560:ARG:NH2 | 1.71 | 1.52 |
| 6:F:335:ARG:CZ | 8:H:259:HIS:HB3 | 1.37 | 1.51 |
| 6:F:247:MET:HB2 | 8:H:240:LYS:NZ | 1.23 | 1.48 |
| 1:A:281:SER:CB | 1:A:283:ARG:HD2 | 1.41 | 1.47 |
| 2:B:402:GLU:OE2 | 4:D:158:ARG:CZ | 1.64 | 1.45 |
| 1:A:283:ARG:C | 1:A:284:ARG:N | 1.70 | 1.44 |
| 6:F:335:ARG:NH2 | 8:H:259:HIS:CG | 1.86 | 1.44 |
| 1:A:71:ASP:HB3 | 3:C:114:ARG:NH2 | 1.18 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:326:ARG:NH1 | 8:H:295:PRO:HD3 | 1.30 | 1.42 |
| 1:A:284:ARG:C | 1:A:285:LEU:N | 1.69 | 1.41 |
| 1:A:278:PRO:CG | 1:A:279:GLU:HB2 | 1.51 | 1.41 |
| 6:F:335:ARG:HH21 | 8:H:259:HIS:CA | 1.34 | 1.41 |
| 1:A:280:PRO:C | 1:A:281:SER:N | 1.75 | 1.40 |
| 5:E:155:ILE:CG2 | 6:F:334:VAL:CG2 | 1.99 | 1.40 |
| 5:E:189:TRP:CZ3 | 8:H:340:ILE:HD12 | 1.58 | 1.38 |
| 2:B:131:MET:CE | 3:C:85:VAL:HG21 | 1.51 | 1.38 |
| 6:F:335:ARG:NH2 | 8:H:259:HIS:CA | 1.85 | 1.37 |
| 2:B:138:LYS:CD | 3:C:84:GLN:NE2 | 1.86 | 1.36 |
| 2:B:138:LYS:CE | 3:C:84:GLN:HE22 | 1.37 | 1.35 |
| 1:A:277:VAL:C | 1:A:278:PRO:N | 1.79 | 1.34 |
| 5:E:189:TRP:CH2 | 8:H:340:ILE:CD1 | 2.09 | 1.34 |
| 2:B:223:GLU:C | 2:B:224:GLY:N | 1.81 | 1.34 |
| 3:C:63:ARG:NH2 | 4:D:535:ALA:HB2 | 1.43 | 1.33 |
| 1:A:138:THR:OG1 | 2:B:92:ILE:CD1 | 1.75 | 1.32 |
| 5:E:155:ILE:HG23 | 6:F:334:VAL:CG2 | 1.55 | 1.32 |
| 5:E:189:TRP:CZ3 | 8:H:340:ILE:CD1 | 2.09 | 1.32 |
| 1:A:58:LYS:NZ | 4:D:506:SER:OG | 1.62 | 1.32 |
| 2:B:404:GLY:HA2 | 4:D:459:TRP:CH2 | 1.63 | 1.32 |
| 6:F:326:ARG:HH12 | 8:H:295:PRO:CD | 1.41 | 1.31 |
| 4:D:307:GLU:CD | 7:G:324:ILE:HD11 | 1.50 | 1.31 |
| 4:D:296:SER:HB3 | 4:D:301:THR:CG2 | 1.57 | 1.31 |
| 1:A:145:THR:HG21 | 4:D:69:LEU:CD1 | 1.61 | 1.31 |
| 5:E:189:TRP:CH2 | 8:H:340:ILE:HD12 | 1.64 | 1.30 |
| 1:A:278:PRO:CB | 1:A:279:GLU:CB | 2.07 | 1.30 |
| 2:B:222:PHE:CD1 | 2:B:241:LEU:HD13 | 1.68 | 1.29 |
| 6:F:377:ARG:HH12 | 8:H:343:GLN:CB | 1.45 | 1.28 |
| 4:D:214:SER:OG | 4:D:426:HIS:CE1 | 1.86 | 1.28 |
| 8:H:259:HIS:C | 8:H:300:GLU:OE2 | 1.72 | 1.28 |
| 6:F:247:MET:SD | 8:H:240:LYS:HG3 | 1.73 | 1.28 |
| 1:A:152:LYS:NZ | 2:B:73:ASP:OD2 | 1.66 | 1.27 |
| 2:B:80:VAL:CG1 | 4:D:65:TRP:CZ3 | 2.16 | 1.27 |
| 1:A:278:PRO:CB | 1:A:279:GLU:HB2 | 1.62 | 1.27 |
| 1:A:278:PRO:HB2 | 1:A:279:GLU:CG | 1.64 | 1.26 |
| 2:B:125:GLU:OE1 | 4:D:113:GLU:OE2 | 1.53 | 1.26 |
| 2:B:132:CYS:SG | 4:D:119:LEU:HG | 1.74 | 1.26 |
| 2:B:138:LYS:NZ | 3:C:84:GLN:OE1 | 1.69 | 1.25 |
| 4:D:662:THR:C | 4:D:664:SER:H | 1.32 | 1.25 |
| 2:B:120:LYS:NZ | 3:C:171:SER:O | 1.70 | 1.25 |
| 3:C:118:ALA:C | 3:C:120:SER:H | 1.40 | 1.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:278:PRO:CB | 1:A:279:GLU:HG3 | 1.67 | 1.24 |
| 1:A:277:VAL:O | 1:A:278:PRO:C | 1.74 | 1.24 |
| 2:B:138:LYS:HD2 | 3:C:84:GLN:CD | 1.56 | 1.24 |
| 6:F:335:ARG:HH22 | 8:H:259:HIS:CG | 1.51 | 1.24 |
| 4:D:296:SER:CB | 4:D:301:THR:HG23 | 1.66 | 1.24 |
| 4:D:307:GLU:OE2 | 7:G:324:ILE:HD12 | 1.39 | 1.22 |
| 8:H:359:GLN:HG2 | 8:H:363:ASP:OD2 | 1.07 | 1.22 |
| 5:E:60:ASN:HB3 | 8:H:207:HIS:CE1 | 1.72 | 1.22 |
| 3:C:63:ARG:HH22 | 4:D:535:ALA:CB | 1.51 | 1.22 |
| 6:F:260:ALA:HB1 | 8:H:258:ARG:NH1 | 1.55 | 1.21 |
| 1:A:281:SER:OG | 1:A:283:ARG:CD | 1.89 | 1.20 |
| 2:B:138:LYS:HE3 | 3:C:84:GLN:NE2 | 1.52 | 1.20 |
| 4:D:307:GLU:CD | 7:G:324:ILE:CD1 | 2.08 | 1.20 |
| 7:G:274:MET:CE | 8:H:280:GLN:HB2 | 1.72 | 1.20 |
| 1:A:281:SER:OG | 1:A:283:ARG:NE | 1.73 | 1.20 |
| 1:A:148:LEU:HD13 | 2:B:80:VAL:CG2 | 1.72 | 1.20 |
| 6:F:260:ALA:CB | 8:H:258:ARG:HH12 | 1.55 | 1.20 |
| 6:F:173:LEU:HD12 | 7:G:118:VAL:HG21 | 1.19 | 1.19 |
| 6:F:53:LYS:HE2 | 6:F:57:TYR:OH | 1.37 | 1.19 |
| 2:B:132:CYS:CA | 4:D:119:LEU:HD21 | 1.72 | 1.18 |
| 2:B:97:ILE:HD12 | 4:D:82:GLN:CD | 1.61 | 1.18 |
| 2:B:77:LEU:HD21 | 4:D:61:GLY:HA3 | 1.20 | 1.18 |
| 4:D:352:HIS:CB | 4:D:366:ARG:HH21 | 1.56 | 1.18 |
| 4:D:307:GLU:OE2 | 7:G:324:ILE:CD1 | 1.92 | 1.17 |
| 2:B:138:LYS:CD | 3:C:84:GLN:HE22 | 1.49 | 1.17 |
| 6:F:260:ALA:CB | 8:H:258:ARG:NH1 | 2.06 | 1.17 |
| 7:G:59:TYR:CD1 | 7:G:62:VAL:HG23 | 1.80 | 1.17 |
| 8:H:294:MET:CE | 8:H:298:ALA:HB3 | 1.73 | 1.17 |
| 4:D:352:HIS:HB3 | 4:D:366:ARG:NH2 | 1.59 | 1.16 |
| 6:F:250:GLU:OE2 | 8:H:244:LYS:NZ | 1.77 | 1.16 |
| 1:A:148:LEU:CD1 | 2:B:80:VAL:CG2 | 2.23 | 1.16 |
| 2:B:138:LYS:HE3 | 3:C:84:GLN:HE22 | 1.04 | 1.16 |
| 6:F:53:LYS:CE | 6:F:57:TYR:OH | 1.92 | 1.16 |
| 6:F:359:ARG:HG3 | 8:H:328:GLN:OE1 | 1.43 | 1.15 |
| 1:A:71:ASP:CB | 3:C:114:ARG:NH2 | 2.09 | 1.15 |
| 1:A:278:PRO:CB | 1:A:279:GLU:CG | 2.17 | 1.15 |
| 2:B:132:CYS:SG | 4:D:119:LEU:CG | 2.33 | 1.15 |
| 2:B:55:ASP:OD1 | 4:D:49:HIS:CE1 | 1.99 | 1.15 |
| 3:C:118:ALA:O | 3:C:120:SER:N | 1.77 | 1.15 |
| 1:A:189:TYR:CD1 | 3:C:271:MET:HE1 | 1.82 | 1.15 |
| 2:B:138:LYS:CE | 3:C:84:GLN:NE2 | 1.98 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:377:ARG:NH1 | 8:H:343:GLN:CA | 2.10 | 1.14 |
| 1:A:148:LEU:CD1 | 2:B:80:VAL:HG22 | 1.78 | 1.14 |
| 6:F:377:ARG:HH12 | 8:H:343:GLN:CA | 1.60 | 1.14 |
| 2:B:490:GLU:HA | 4:D:560:ARG:NH2 | 0.81 | 1.14 |
| 2:B:132:CYS:HA | 4:D:119:LEU:CD2 | 1.77 | 1.13 |
| 4:D:214:SER:OG | 4:D:426:HIS:HE1 | 1.22 | 1.12 |
| 2:B:80:VAL:CG1 | 4:D:65:TRP:CH2 | 2.32 | 1.12 |
| 4:D:189:GLU:OE1 | 4:D:197:ARG:CZ | 1.98 | 1.12 |
| 1:A:278:PRO:HB2 | 1:A:279:GLU:CA | 1.78 | 1.11 |
| 6:F:10:ALA:O | 6:F:13:ARG:HG2 | 1.49 | 1.11 |
| 7:G:312:ARG:HH12 | 8:H:323:ALA:HB2 | 1.07 | 1.11 |
| 1:A:189:TYR:CD1 | 3:C:271:MET:CE | 2.34 | 1.11 |
| 1:A:278:PRO:HB3 | 1:A:279:GLU:HG3 | 1.29 | 1.11 |
| 1:A:145:THR:HG21 | 4:D:69:LEU:HD11 | 1.24 | 1.10 |
| 4:D:662:THR:C | 4:D:664:SER:N | 1.96 | 1.10 |
| 7:G:59:TYR:HD1 | 7:G:62:VAL:HG23 | 1.00 | 1.10 |
| 7:G:143:VAL:HG22 | 8:H:159:MET:CE | 1.81 | 1.10 |
| 8:H:294:MET:CE | 8:H:298:ALA:CB | 2.29 | 1.10 |
| 1:A:189:TYR:HD1 | 3:C:271:MET:HE1 | 1.00 | 1.09 |
| 8:H:259:HIS:CA | 8:H:300:GLU:OE2 | 2.00 | 1.09 |
| 2:B:55:ASP:CG | 4:D:49:HIS:HE1 | 1.56 | 1.09 |
| 7:G:274:MET:HE1 | 8:H:280:GLN:HB2 | 1.17 | 1.09 |
| 2:B:138:LYS:CG | 3:C:84:GLN:NE2 | 2.15 | 1.08 |
| 4:D:8:GLN:HG3 | 4:D:28:GLU:OE1 | 1.53 | 1.08 |
| 4:D:352:HIS:HB3 | 4:D:366:ARG:HH21 | 0.95 | 1.08 |
| 6:F:377:ARG:NH1 | 8:H:343:GLN:HA | 1.62 | 1.08 |
| 3:C:63:ARG:NH2 | 4:D:535:ALA:CB | 2.13 | 1.08 |
| 6:F:206:MET:CE | 8:H:199:LYS:HG3 | 1.84 | 1.07 |
| 2:B:80:VAL:HG12 | 4:D:65:TRP:CZ3 | 1.85 | 1.07 |
| 2:B:97:ILE:HD11 | 4:D:82:GLN:CB | 1.84 | 1.07 |
| 8:H:359:GLN:CG | 8:H:363:ASP:OD2 | 2.00 | 1.07 |
| 1:A:281:SER:CB | 1:A:283:ARG:CD | 2.30 | 1.07 |
| 2:B:175:MET:HG3 | 4:D:460:PRO:HG3 | 1.27 | 1.07 |
| 6:F:377:ARG:NH1 | 8:H:343:GLN:CB | 2.18 | 1.07 |
| 3:C:131:GLY:O | 4:D:140:LYS:NZ | 1.86 | 1.07 |
| 2:B:567:LYS:NZ | 4:D:626:TRP:O | 1.88 | 1.07 |
| 5:E:60:ASN:HB3 | 8:H:207:HIS:NE2 | 1.68 | 1.07 |
| 2:B:80:VAL:HG11 | 4:D:65:TRP:CH2 | 1.89 | 1.06 |
| 6:F:325:GLU:OE2 | 6:F:325:GLU:HA | 1.39 | 1.06 |
| 1:A:58:LYS:NZ | 4:D:506:SER:CB | 2.18 | 1.06 |
| 2:B:97:ILE:HD11 | 4:D:82:GLN:HB3 | 1.10 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:247:MET:CB | 8:H:240:LYS:NZ | 2.18 | 1.06 |
| 2:B:443:ASP:OD1 | 4:D:509:ARG:NH2 | 1.88 | 1.05 |
| 2:B:490:GLU:HA | 4:D:560:ARG:CZ | 1.85 | 1.05 |
| 2:B:138:LYS:CD | 3:C:84:GLN:CD | 2.20 | 1.05 |
| 6:F:44:GLY:H | 6:F:47:MET:HE2 | 1.16 | 1.05 |
| 7:G:280:PHE:CE1 | 8:H:287:LYS:HG3 | 1.90 | 1.05 |
| 1:A:152:LYS:NZ | 2:B:73:ASP:CG | 2.09 | 1.05 |
| 1:A:278:PRO:HG2 | 1:A:279:GLU:HB2 | 1.07 | 1.05 |
| 6:F:173:LEU:HD12 | 7:G:118:VAL:CG2 | 1.86 | 1.05 |
| 2:B:77:LEU:HD21 | 4:D:61:GLY:CA | 1.87 | 1.05 |
| 6:F:173:LEU:CD1 | 7:G:118:VAL:HG21 | 1.86 | 1.05 |
| 7:G:130:ILE:HG22 | 7:G:131:LEU:N | 1.72 | 1.05 |
| 8:H:294:MET:HE1 | 8:H:298:ALA:HB3 | 1.07 | 1.05 |
| 1:A:149:VAL:HG13 | 2:B:70:PRO:HG2 | 1.35 | 1.04 |
| 2:B:138:LYS:HG3 | 3:C:84:GLN:NE2 | 1.73 | 1.04 |
| 2:B:483:ARG:HH21 | 4:D:549:GLN:NE2 | 1.57 | 1.03 |
| 7:G:143:VAL:HG22 | 8:H:159:MET:HE3 | 1.05 | 1.03 |
| 8:H:294:MET:HE1 | 8:H:298:ALA:CB | 1.88 | 1.03 |
| 4:D:4:ARG:HG3 | 4:D:32:GLN:NE2 | 1.73 | 1.03 |
| 5:E:155:ILE:HG21 | 6:F:334:VAL:CG2 | 1.86 | 1.03 |
| 5:E:189:TRP:CH2 | 8:H:340:ILE:HD13 | 1.88 | 1.02 |
| 6:F:377:ARG:HH12 | 8:H:343:GLN:CG | 1.72 | 1.02 |
| 7:G:124:THR:HG22 | 7:G:125:ILE:HG13 | 1.39 | 1.02 |
| 4:D:296:SER:CB | 4:D:301:THR:CG2 | 2.28 | 1.02 |
| 5:E:102:LEU:CD2 | 7:G:255:ILE:HD12 | 1.88 | 1.02 |
| 3:C:63:ARG:HH22 | 4:D:535:ALA:HB2 | 0.99 | 1.01 |
| 2:B:77:LEU:CD2 | 4:D:61:GLY:HA3 | 1.89 | 1.01 |
| 2:B:131:MET:HE3 | 3:C:85:VAL:HG21 | 1.38 | 1.01 |
| 5:E:97:HIS:NE2 | 8:H:247:TYR:OH | 1.92 | 1.01 |
| 2:B:132:CYS:HA | 4:D:119:LEU:HD21 | 1.04 | 1.01 |
| 2:B:94:GLU:O | 2:B:96:ALA:N | 1.93 | 1.01 |
| 1:A:128:LEU:HD22 | 4:D:97:ARG:NH2 | 1.74 | 1.00 |
| 1:A:145:THR:HG21 | 4:D:69:LEU:HD13 | 1.40 | 1.00 |
| 2:B:138:LYS:CE | 3:C:84:GLN:OE1 | 2.09 | 1.00 |
| 6:F:206:MET:HE2 | 8:H:199:LYS:HG3 | 1.42 | 1.00 |
| 6:F:227:ILE:HA | 8:H:223:ARG:NH2 | 1.75 | 1.00 |
| 2:B:407:VAL:HG21 | 4:D:459:TRP:CZ3 | 1.95 | 1.00 |
| 5:E:49:LEU:HD23 | 8:H:196:ASN:HD22 | 1.24 | 1.00 |
| 3:C:273:GLU:OE2 | 4:D:614:TYR:OH | 1.79 | 1.00 |
| 4:D:305:PRO:O | 4:D:307:GLU:N | 1.93 | 1.00 |
| 3:C:236:ARG:HH12 | 4:D:575:THR:HA | 1.22 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:63:ARG:NH1 | 4:D:537:GLU:OE2 | 1.94 | 0.99 |
| 3:C:229:LEU:HD21 | 4:D:571:LEU:HD12 | 1.43 | 0.99 |
| 6:F:227:ILE:HA | 8:H:223:ARG:HH22 | 1.27 | 0.99 |
| 1:A:113:ILE:HG23 | 3:C:172:PHE:CZ | 1.96 | 0.99 |
| 1:A:279:GLU:CB | 1:A:280:PRO:HD3 | 1.92 | 0.99 |
| 2:B:135:SER:OG | 4:D:121:CYS:SG | 2.10 | 0.99 |
| 2:B:138:LYS:CE | 3:C:84:GLN:CD | 2.31 | 0.99 |
| 4:D:509:ARG:HD3 | 4:D:521:PHE:CE2 | 1.98 | 0.99 |
| 1:A:266:LEU:HD12 | 3:C:345:LEU:HG | 1.42 | 0.99 |
| 6:F:192:TYR:HH | 7:G:173:TRP:HE1 | 1.00 | 0.99 |
| 5:E:102:LEU:HD22 | 7:G:255:ILE:HD12 | 1.43 | 0.98 |
| 2:B:55:ASP:OD1 | 4:D:49:HIS:HE1 | 1.39 | 0.98 |
| 2:B:55:ASP:CG | 4:D:49:HIS:CE1 | 2.36 | 0.98 |
| 2:B:138:LYS:CG | 3:C:84:GLN:HE22 | 1.75 | 0.98 |
| 6:F:260:ALA:HB1 | 8:H:258:ARG:HH12 | 0.82 | 0.98 |
| 2:B:424:LEU:HD22 | 4:D:484:ILE:CD1 | 1.94 | 0.98 |
| 2:B:404:GLY:HA2 | 4:D:459:TRP:HH2 | 1.25 | 0.97 |
| 2:B:131:MET:CE | 3:C:85:VAL:CG2 | 2.42 | 0.97 |
| 1:A:138:THR:OG1 | 2:B:92:ILE:HD13 | 1.64 | 0.97 |
| 1:A:279:GLU:HB3 | 1:A:280:PRO:HD3 | 1.44 | 0.97 |
| 6:F:359:ARG:CG | 8:H:328:GLN:OE1 | 2.11 | 0.97 |
| 4:D:509:ARG:NH1 | 4:D:521:PHE:HZ | 1.61 | 0.96 |
| 6:F:326:ARG:NH1 | 8:H:295:PRO:CD | 2.12 | 0.96 |
| 2:B:407:VAL:CG2 | 4:D:459:TRP:HZ3 | 1.77 | 0.96 |
| 4:D:137:PHE:CE2 | 4:D:141:ARG:NH1 | 2.33 | 0.96 |
| 1:A:278:PRO:CG | 1:A:279:GLU:CB | 2.39 | 0.96 |
| 1:A:278:PRO:HG2 | 1:A:279:GLU:CB | 1.95 | 0.96 |
| 2:B:297:VAL:HG11 | 4:D:355:LEU:HD11 | 1.47 | 0.96 |
| 1:A:281:SER:OG | 1:A:283:ARG:HD2 | 1.56 | 0.96 |
| 4:D:189:GLU:OE1 | 4:D:197:ARG:NH1 | 1.98 | 0.96 |
| 1:A:138:THR:OG1 | 2:B:92:ILE:HD12 | 1.62 | 0.96 |
| 1:A:281:SER:HB3 | 1:A:283:ARG:HD2 | 1.00 | 0.96 |
| 1:A:12:LEU:HB3 | 1:A:21:LEU:HD21 | 1.48 | 0.95 |
| 1:A:71:ASP:HB3 | 3:C:114:ARG:HH22 | 1.16 | 0.95 |
| 4:D:374:ARG:NH1 | 5:E:218:GLU:OE1 | 1.99 | 0.95 |
| 2:B:490:GLU:HG2 | 4:D:560:ARG:CZ | 1.97 | 0.95 |
| 7:G:59:TYR:HD1 | 7:G:62:VAL:CG2 | 1.79 | 0.95 |
| 2:B:80:VAL:HG11 | 4:D:65:TRP:CZ3 | 1.97 | 0.94 |
| 6:F:247:MET:CE | 8:H:243:PHE:HD1 | 1.81 | 0.94 |
| 1:A:189:TYR:HD1 | 3:C:271:MET:CE | 1.77 | 0.94 |
| 7:G:62:VAL:HG12 | 7:G:66:LEU:CD1 | 1.96 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:274:MET:HE1 | 8:H:280:GLN:CB | 1.98 | 0.94 |
| 2:B:166:SER:CB | 4:D:152:ASN:HD21 | 1.80 | 0.94 |
| 6:F:57:TYR:OH | 6:F:88:ASP:OD1 | 1.84 | 0.94 |
| 7:G:62:VAL:HG12 | 7:G:66:LEU:HD12 | 1.47 | 0.94 |
| 7:G:47:ARG:NH1 | 7:G:108:GLN:OE1 | 2.00 | 0.94 |
| 4:D:137:PHE:HE2 | 4:D:141:ARG:NH1 | 1.67 | 0.93 |
| 2:B:84:PHE:HE2 | 4:D:65:TRP:CE3 | 1.86 | 0.93 |
| 4:D:290:PRO:O | 4:D:291:ILE:C | 1.99 | 0.93 |
| 5:E:135:LEU:HB3 | 5:E:136:PRO:HD3 | 1.51 | 0.93 |
| 2:B:175:MET:HG3 | 4:D:460:PRO:CG | 1.98 | 0.93 |
| 2:B:91:ALA:O | 2:B:93:GLU:N | 2.01 | 0.93 |
| 2:B:402:GLU:OE2 | 4:D:158:ARG:NH1 | 2.01 | 0.93 |
| 2:B:443:ASP:CG | 4:D:509:ARG:HH22 | 1.72 | 0.93 |
| 2:B:522:THR:HG23 | 4:D:590:TYR:CE2 | 2.03 | 0.92 |
| 3:C:118:ALA:C | 3:C:120:SER:N | 2.07 | 0.92 |
| 4:D:658:LEU:O | 4:D:662:THR:OG1 | 1.85 | 0.92 |
| 4:D:214:SER:HG | 4:D:426:HIS:CE1 | 1.87 | 0.92 |
| 6:F:260:ALA:HB3 | 8:H:258:ARG:NH1 | 1.84 | 0.92 |
| 2:B:2:SER:OG | 2:B:28:ASP:OD1 | 1.88 | 0.92 |
| 7:G:92:HIS:HE1 | 7:G:93:PHE:CE1 | 1.88 | 0.92 |
| 2:B:181:PRO:HG3 | 2:B:189:SER:OG | 1.70 | 0.92 |
| 2:B:166:SER:OG | 4:D:152:ASN:ND2 | 2.02 | 0.92 |
| 2:B:407:VAL:CG2 | 4:D:459:TRP:CZ3 | 2.53 | 0.92 |
| 4:D:298:ASN:O | 4:D:299:GLU:HB2 | 1.68 | 0.92 |
| 2:B:132:CYS:SG | 4:D:119:LEU:CD2 | 2.59 | 0.91 |
| 7:G:38:GLU:O | 7:G:42:THR:OG1 | 1.87 | 0.91 |
| 7:G:130:ILE:HG22 | 7:G:131:LEU:H | 1.27 | 0.91 |
| 2:B:134:LYS:CD | 3:C:85:VAL:HG13 | 2.00 | 0.91 |
| 4:D:176:SER:O | 4:D:256:ARG:NH2 | 2.04 | 0.91 |
| 5:E:49:LEU:HD23 | 8:H:196:ASN:ND2 | 1.85 | 0.91 |
| 2:B:263:GLN:NE2 | 2:B:346:ASN:ND2 | 2.19 | 0.91 |
| 2:B:483:ARG:HH21 | 4:D:549:GLN:HE22 | 1.04 | 0.91 |
| 6:F:335:ARG:CZ | 8:H:259:HIS:HB2 | 1.69 | 0.91 |
| 2:B:222:PHE:CE1 | 2:B:241:LEU:HD13 | 2.05 | 0.91 |
| 4:D:76:ARG:O | 4:D:79:GLU:HB2 | 1.70 | 0.91 |
| 4:D:122:GLU:HG3 | 4:D:512:ASN:HD21 | 1.35 | 0.91 |
| 4:D:183:SER:OG | 4:D:184:SER:N | 2.03 | 0.90 |
| 5:E:189:TRP:CZ3 | 8:H:340:ILE:HD11 | 2.06 | 0.90 |
| 2:B:35:ASP:HB3 | 4:D:30:MET:CE | 2.01 | 0.90 |
| 7:G:312:ARG:NH1 | 8:H:323:ALA:HB2 | 1.85 | 0.90 |
| 2:B:120:LYS:HZ1 | 3:C:175:PRO:HA | 1.36 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:97:ILE:CD1 | 4:D:82:GLN:HB3 | 2.01 | 0.90 |
| 2:B:131:MET:HE1 | 3:C:85:VAL:HG21 | 1.52 | 0.90 |
| 1:A:58:LYS:HZ1 | 4:D:506:SER:HB2 | 1.35 | 0.90 |
| 1:A:1:MET:CE | 1:A:28:THR:HG22 | 2.02 | 0.90 |
| 2:B:507:LEU:CD1 | 4:D:579:THR:HG22 | 2.01 | 0.90 |
| 3:C:5:LEU:HD12 | 3:C:22:LEU:CD1 | 2.01 | 0.90 |
| 2:B:500:LEU:HD21 | 4:D:571:LEU:CD1 | 2.03 | 0.89 |
| 6:F:173:LEU:CD1 | 7:G:118:VAL:CG2 | 2.47 | 0.89 |
| 3:C:4:THR:HG23 | 3:C:33:ILE:HD11 | 1.54 | 0.89 |
| 5:E:77:ASP:OD2 | 6:F:238:ARG:NE | 2.05 | 0.89 |
| 2:B:424:LEU:CD2 | 4:D:484:ILE:CD1 | 2.50 | 0.89 |
| 5:E:155:ILE:HG21 | 6:F:334:VAL:HG23 | 1.54 | 0.89 |
| 2:B:132:CYS:CB | 4:D:119:LEU:HD21 | 2.02 | 0.89 |
| 2:B:404:GLY:CA | 4:D:459:TRP:CH2 | 2.52 | 0.89 |
| 5:E:97:HIS:HE2 | 8:H:247:TYR:HH | 0.92 | 0.89 |
| 7:G:92:HIS:CE1 | 7:G:93:PHE:CE1 | 2.60 | 0.89 |
| 2:B:443:ASP:CG | 4:D:509:ARG:NH2 | 2.26 | 0.89 |
| 2:B:507:LEU:HD12 | 4:D:579:THR:HG22 | 1.55 | 0.89 |
| 1:A:145:THR:HG23 | 4:D:65:TRP:CZ2 | 2.07 | 0.88 |
| 2:B:264:LEU:HD13 | 6:F:381:TRP:CH2 | 2.07 | 0.88 |
| 1:A:149:VAL:HG13 | 2:B:70:PRO:CG | 2.02 | 0.88 |
| 6:F:241:TRP:CZ2 | 7:G:238:LEU:HD21 | 2.08 | 0.88 |
| 6:F:313:GLN:HE21 | 8:H:282:HIS:CE1 | 1.90 | 0.88 |
| 1:A:281:SER:HB3 | 1:A:283:ARG:CD | 1.95 | 0.88 |
| 4:D:189:GLU:CD | 4:D:197:ARG:HH12 | 1.77 | 0.88 |
| 2:B:74:GLU:OE1 | 4:D:54:ARG:HG3 | 1.73 | 0.88 |
| 2:B:249:ASP:O | 2:B:250:GLY:O | 1.92 | 0.88 |
| 7:G:131:LEU:O | 7:G:132:GLU:C | 2.04 | 0.88 |
| 7:G:41:CYS:HA | 7:G:47:ARG:NH1 | 1.89 | 0.88 |
| 1:A:189:TYR:CD1 | 3:C:271:MET:HE3 | 2.09 | 0.88 |
| 1:A:235:LEU:HD11 | 3:C:313:ILE:HG22 | 1.56 | 0.88 |
| 5:E:181:GLU:CD | 7:G:335:ARG:HH12 | 1.77 | 0.88 |
| 2:B:134:LYS:HD3 | 3:C:85:VAL:HG13 | 1.56 | 0.88 |
| 6:F:247:MET:CB | 8:H:240:LYS:HZ2 | 1.80 | 0.88 |
| 2:B:138:LYS:HD2 | 3:C:84:GLN:NE2 | 1.69 | 0.88 |
| 1:A:152:LYS:HZ1 | 2:B:73:ASP:CG | 1.72 | 0.87 |
| 1:A:145:THR:HG1 | 4:D:65:TRP:HZ2 | 1.22 | 0.87 |
| 3:C:236:ARG:NH2 | 4:D:579:THR:OG1 | 2.07 | 0.87 |
| 4:D:189:GLU:OE1 | 4:D:197:ARG:NH2 | 2.06 | 0.87 |
| 4:D:662:THR:O | 4:D:664:SER:N | 2.07 | 0.87 |
| 6:F:247:MET:HB2 | 8:H:240:LYS:HZ1 | 1.08 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:528:VAL:HG13 | 4:D:546:MET:SD | 2.15 | 0.87 |
| 3:C:63:ARG:HH12 | 4:D:535:ALA:HB1 | 1.39 | 0.87 |
| 4:D:189:GLU:CD | 4:D:197:ARG:NH1 | 2.28 | 0.87 |
| 2:B:424:LEU:HD22 | 4:D:484:ILE:HD12 | 1.56 | 0.87 |
| 5:E:181:GLU:CG | 7:G:335:ARG:HH12 | 1.88 | 0.86 |
| 6:F:224:ASP:OD2 | 8:H:216:LEU:HD21 | 1.75 | 0.86 |
| 3:C:129:ILE:CD1 | 4:D:489:LEU:HD13 | 2.06 | 0.86 |
| 1:A:71:ASP:HB3 | 3:C:114:ARG:HH21 | 1.37 | 0.86 |
| 6:F:326:ARG:NH2 | 7:G:291:GLU:OE2 | 2.07 | 0.86 |
| 6:F:53:LYS:HE3 | 6:F:57:TYR:OH | 1.75 | 0.85 |
| 4:D:219:VAL:O | 4:D:221:PRO:HD3 | 1.76 | 0.85 |
| 2:B:138:LYS:HD2 | 3:C:84:GLN:OE1 | 1.75 | 0.85 |
| 4:D:509:ARG:NH1 | 4:D:521:PHE:CZ | 2.38 | 0.85 |
| 4:D:352:HIS:CG | 4:D:366:ARG:HH21 | 1.95 | 0.85 |
| 1:A:148:LEU:HD13 | 2:B:80:VAL:HG21 | 1.58 | 0.85 |
| 3:C:18:ASP:OD1 | 3:C:21:ASP:CG | 2.15 | 0.85 |
| 1:A:145:THR:CG2 | 4:D:69:LEU:HD11 | 2.05 | 0.85 |
| 2:B:138:LYS:CD | 3:C:84:GLN:OE1 | 2.23 | 0.85 |
| 4:D:352:HIS:CG | 4:D:366:ARG:HE | 1.94 | 0.85 |
| 1:A:128:LEU:HD22 | 4:D:97:ARG:HH21 | 1.42 | 0.84 |
| 2:B:132:CYS:SG | 4:D:119:LEU:HD21 | 2.16 | 0.84 |
| 1:A:283:ARG:O | 1:A:284:ARG:N | 2.09 | 0.84 |
| 4:D:46:ILE:HG23 | 4:D:50:ILE:HD12 | 1.58 | 0.84 |
| 2:B:483:ARG:NH2 | 4:D:549:GLN:HE22 | 1.73 | 0.84 |
| 3:C:229:LEU:CD2 | 4:D:571:LEU:HD12 | 2.07 | 0.84 |
| 3:C:227:VAL:HG22 | 3:C:230:ARG:HH21 | 1.41 | 0.84 |
| 7:G:249:THR:HG23 | 8:H:243:PHE:CD2 | 2.12 | 0.84 |
| 1:A:58:LYS:HZ3 | 4:D:506:SER:CB | 1.81 | 0.84 |
| 2:B:522:THR:OG1 | 4:D:593:GLU:OE2 | 1.95 | 0.84 |
| 6:F:247:MET:CB | 8:H:240:LYS:HZ1 | 1.84 | 0.84 |
| 6:F:206:MET:HE1 | 8:H:199:LYS:HG3 | 1.60 | 0.84 |
| 2:B:507:LEU:CD1 | 4:D:579:THR:CG2 | 2.55 | 0.84 |
| 5:E:148:TYR:OH | 7:G:289:PHE:CD1 | 2.30 | 0.84 |
| 7:G:41:CYS:HA | 7:G:47:ARG:HH12 | 1.40 | 0.84 |
| 2:B:97:ILE:CD1 | 4:D:82:GLN:CD | 2.44 | 0.84 |
| 4:D:352:HIS:CD2 | 4:D:366:ARG:HE | 1.94 | 0.84 |
| 6:F:325:GLU:OE2 | 6:F:325:GLU:CA | 2.25 | 0.84 |
| 2:B:402:GLU:OE2 | 4:D:158:ARG:NH2 | 2.12 | 0.83 |
| 6:F:230:LYS:HE3 | 8:H:222:LEU:HD23 | 1.60 | 0.83 |
| 2:B:222:PHE:CD1 | 2:B:241:LEU:CD1 | 2.58 | 0.83 |
| 2:B:131:MET:HE2 | 3:C:85:VAL:HG21 | 1.59 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:4:ARG:HG3 | 4:D:32:GLN:HE21 | 1.43 | 0.82 |
| 2:B:490:GLU:CB | 4:D:560:ARG:NH2 | 2.41 | 0.82 |
| 1:A:171:LYS:HE2 | 1:A:175:ARG:NH2 | 1.94 | 0.82 |
| 8:H:359:GLN:HG2 | 8:H:363:ASP:CG | 1.98 | 0.82 |
| 2:B:97:ILE:CD1 | 4:D:82:GLN:CG | 2.57 | 0.82 |
| 3:C:270:ARG:HD2 | 4:D:614:TYR:OH | 1.79 | 0.82 |
| 1:A:77:LEU:HD22 | 3:C:154:LEU:CD2 | 2.10 | 0.82 |
| 1:A:266:LEU:CD1 | 3:C:345:LEU:HG | 2.09 | 0.82 |
| 2:B:30:LEU:CD2 | 4:D:34:LEU:HD23 | 2.09 | 0.82 |
| 6:F:92:ARG:NH1 | 6:F:118:PHE:O | 2.13 | 0.82 |
| 7:G:280:PHE:CD1 | 8:H:287:LYS:HG3 | 2.15 | 0.82 |
| 3:C:5:LEU:HD12 | 3:C:22:LEU:HD12 | 1.61 | 0.82 |
| 2:B:376:MET:HE1 | 4:D:211:HIS:HB2 | 1.61 | 0.81 |
| 1:A:172:VAL:HG13 | 3:C:253:ILE:HG21 | 1.61 | 0.81 |
| 2:B:216:PHE:HD2 | 4:D:269:GLN:HG2 | 1.44 | 0.81 |
| 2:B:550:LEU:HD11 | 3:C:276:VAL:HG21 | 1.59 | 0.81 |
| 6:F:377:ARG:HH22 | 8:H:343:GLN:CD | 1.83 | 0.81 |
| 7:G:143:VAL:CG2 | 8:H:159:MET:HE3 | 2.01 | 0.81 |
| 5:E:179:MET:HG2 | 8:H:329:ILE:HD11 | 1.62 | 0.81 |
| 6:F:377:ARG:HH22 | 8:H:343:GLN:CG | 1.92 | 0.81 |
| 7:G:139:GLU:HG3 | 8:H:155:VAL:HG22 | 1.61 | 0.81 |
| 1:A:145:THR:OG1 | 4:D:65:TRP:CZ2 | 2.34 | 0.81 |
| 7:G:274:MET:SD | 8:H:280:GLN:HB2 | 2.19 | 0.81 |
| 6:F:326:ARG:HH11 | 8:H:295:PRO:HD3 | 1.45 | 0.81 |
| 4:D:122:GLU:HG3 | 4:D:512:ASN:ND2 | 1.96 | 0.81 |
| 2:B:84:PHE:HE2 | 4:D:65:TRP:CZ3 | 1.97 | 0.81 |
| 3:C:18:ASP:OD1 | 3:C:21:ASP:OD2 | 1.98 | 0.81 |
| 4:D:304:ASP:C | 4:D:306:GLN:H | 1.83 | 0.81 |
| 1:A:141:ARG:HG3 | 3:C:220:GLN:NE2 | 1.96 | 0.80 |
| 1:A:235:LEU:HD11 | 3:C:313:ILE:CG2 | 2.11 | 0.80 |
| 2:B:376:MET:CE | 4:D:211:HIS:HB2 | 2.10 | 0.80 |
| 4:D:296:SER:HB3 | 4:D:301:THR:HG23 | 0.84 | 0.80 |
| 4:D:453:GLN:HA | 4:D:457:LEU:HD12 | 1.62 | 0.80 |
| 6:F:247:MET:SD | 8:H:240:LYS:CG | 2.64 | 0.80 |
| 8:H:294:MET:HE3 | 8:H:298:ALA:CB | 2.11 | 0.80 |
| 1:A:141:ARG:HG3 | 3:C:220:GLN:HE22 | 1.46 | 0.80 |
| 1:A:124:VAL:HG21 | 2:B:110:GLN:NE2 | 1.97 | 0.80 |
| 3:C:229:LEU:HD21 | 4:D:571:LEU:CD1 | 2.11 | 0.80 |
| 2:B:193:PHE:HB3 | 2:B:392:GLU:OE1 | 1.81 | 0.80 |
| 2:B:407:VAL:HG21 | 4:D:459:TRP:CE3 | 2.17 | 0.80 |
| 2:B:329:ILE:HD13 | 4:D:386:MET:SD | 2.21 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:377:ARG:HH22 | 8:H:343:GLN:HG3 | 1.46 | 0.80 |
| 7:G:249:THR:HG23 | 8:H:243:PHE:CG | 2.17 | 0.80 |
| 1:A:281:SER:OG | 1:A:283:ARG:CZ | 2.30 | 0.80 |
| 2:B:80:VAL:HG13 | 4:D:65:TRP:CH2 | 2.15 | 0.79 |
| 1:A:148:LEU:HD11 | 2:B:80:VAL:HG22 | 1.62 | 0.79 |
| 6:F:326:ARG:HH12 | 8:H:295:PRO:HD3 | 0.89 | 0.79 |
| 3:C:236:ARG:NH1 | 4:D:575:THR:HA | 1.96 | 0.79 |
| 6:F:377:ARG:HH12 | 8:H:343:GLN:HG3 | 1.44 | 0.79 |
| 7:G:239:ARG:HG3 | 8:H:232:VAL:HG21 | 1.63 | 0.79 |
| 2:B:96:ALA:C | 2:B:98:GLU:H | 1.86 | 0.79 |
| 2:B:500:LEU:HD21 | 4:D:571:LEU:HD13 | 1.62 | 0.79 |
| 1:A:211:HIS:HA | 4:D:630:VAL:HG23 | 1.65 | 0.79 |
| 2:B:513:PRO:HG2 | 2:B:519:MET:CE | 2.13 | 0.79 |
| 1:A:58:LYS:HZ1 | 4:D:506:SER:CB | 1.91 | 0.78 |
| 2:B:30:LEU:HD21 | 4:D:34:LEU:HD23 | 1.65 | 0.78 |
| 2:B:566:GLU:HA | 2:B:569:LEU:HD12 | 1.66 | 0.78 |
| 1:A:5:SER:HA | 1:A:31:MET:HE1 | 1.65 | 0.78 |
| 1:A:71:ASP:C | 3:C:114:ARG:HH21 | 1.86 | 0.78 |
| 2:B:80:VAL:HG11 | 4:D:65:TRP:CZ2 | 2.18 | 0.78 |
| 2:B:97:ILE:HD12 | 4:D:82:GLN:CG | 2.13 | 0.78 |
| 2:B:289:TRP:CE2 | 2:B:293:ASN:ND2 | 2.52 | 0.78 |
| 7:G:131:LEU:O | 7:G:132:GLU:O | 2.01 | 0.78 |
| 2:B:43:PHE:CZ | 4:D:46:ILE:HD13 | 2.18 | 0.78 |
| 1:A:277:VAL:O | 1:A:278:PRO:CA | 2.31 | 0.78 |
| 3:C:141:LEU:HG | 3:C:142:PRO:HD2 | 1.65 | 0.78 |
| 6:F:241:TRP:HZ2 | 7:G:238:LEU:HD21 | 1.48 | 0.78 |
| 6:F:335:ARG:HH21 | 8:H:259:HIS:CG | 1.73 | 0.78 |
| 2:B:94:GLU:CD | 4:D:79:GLU:OE2 | 2.17 | 0.78 |
| 4:D:189:GLU:OE2 | 4:D:197:ARG:NH1 | 2.16 | 0.78 |
| 2:B:456:ASP:C | 2:B:458:THR:H | 1.87 | 0.77 |
| 3:C:180:GLU:OE1 | 3:C:188:LYS:NZ | 2.17 | 0.77 |
| 1:A:145:THR:HG23 | 4:D:65:TRP:HZ2 | 1.48 | 0.77 |
| 4:D:117:GLN:O | 4:D:119:LEU:N | 2.17 | 0.77 |
| 4:D:211:HIS:CE1 | 4:D:215:ILE:HD11 | 2.19 | 0.77 |
| 4:D:280:PRO:O | 4:D:281:SER:C | 2.09 | 0.77 |
| 5:E:9:PRO:CB | 6:F:197:GLN:OE1 | 2.32 | 0.77 |
| 5:E:148:TYR:HH | 7:G:289:PHE:HD1 | 1.30 | 0.77 |
| 1:A:240:ASP:O | 1:A:251:LYS:NZ | 2.17 | 0.77 |
| 5:E:221:HIS:HB3 | 5:E:222:PRO:O | 1.85 | 0.77 |
| 3:C:5:LEU:CD1 | 3:C:22:LEU:HD12 | 2.15 | 0.77 |
| 2:B:96:ALA:C | 2:B:98:GLU:N | 2.34 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:399:VAL:HA | 4:D:158:ARG:NH1 | 1.99 | 0.77 |
| 2:B:522:THR:HG22 | 2:B:524:GLU:OE2 | 1.85 | 0.77 |
| 6:F:166:LYS:NZ | 7:G:87:ASP:OD2 | 2.13 | 0.77 |
| 6:F:247:MET:HB2 | 8:H:240:LYS:HZ2 | 0.96 | 0.77 |
| 5:E:9:PRO:HB3 | 6:F:197:GLN:OE1 | 1.85 | 0.77 |
| 6:F:227:ILE:CA | 8:H:223:ARG:HH22 | 1.97 | 0.77 |
| 3:C:14:MET:SD | 4:D:552:PHE:HA | 2.25 | 0.77 |
| 5:E:102:LEU:HD22 | 7:G:255:ILE:CD1 | 2.15 | 0.76 |
| 5:E:181:GLU:CD | 7:G:335:ARG:NH1 | 2.37 | 0.76 |
| 6:F:377:ARG:NH1 | 8:H:343:GLN:CG | 2.48 | 0.76 |
| 6:F:377:ARG:NH1 | 8:H:343:GLN:HG3 | 2.01 | 0.76 |
| 4:D:202:LEU:HD22 | 4:D:237:MET:HE3 | 1.67 | 0.76 |
| 2:B:94:GLU:OE1 | 4:D:79:GLU:OE2 | 2.04 | 0.76 |
| 4:D:290:PRO:O | 4:D:291:ILE:O | 2.02 | 0.76 |
| 4:D:528:VAL:CG1 | 4:D:546:MET:SD | 2.73 | 0.76 |
| 1:A:277:VAL:HG12 | 1:A:278:PRO:HA | 1.68 | 0.76 |
| 2:B:88:LYS:O | 2:B:90:PRO:HD3 | 1.86 | 0.76 |
| 6:F:326:ARG:HH12 | 8:H:295:PRO:CG | 1.99 | 0.76 |
| 2:B:424:LEU:CD2 | 4:D:484:ILE:HD11 | 2.15 | 0.76 |
| 6:F:9:LEU:HD22 | 6:F:124:PRO:HB3 | 1.68 | 0.76 |
| 1:A:138:THR:OG1 | 2:B:92:ILE:HD11 | 1.82 | 0.76 |
| 1:A:189:TYR:HA | 3:C:271:MET:CE | 2.15 | 0.76 |
| 2:B:451:GLN:HG3 | 2:B:463:ARG:HH12 | 1.50 | 0.76 |
| 1:A:152:LYS:HZ2 | 2:B:73:ASP:CG | 1.85 | 0.76 |
| 2:B:490:GLU:HG2 | 4:D:560:ARG:NH1 | 2.01 | 0.76 |
| 6:F:44:GLY:H | 6:F:47:MET:CE | 1.95 | 0.76 |
| 2:B:490:GLU:CG | 4:D:560:ARG:CZ | 2.64 | 0.76 |
| 4:D:68:GLN:O | 4:D:72:THR:OG1 | 2.04 | 0.76 |
| 4:D:296:SER:OG | 4:D:300:SER:N | 2.19 | 0.75 |
| 2:B:42:TRP:CE2 | 4:D:20:LEU:HD13 | 2.21 | 0.75 |
| 5:E:121:LEU:CD2 | 8:H:276:LEU:HD21 | 2.16 | 0.75 |
| 1:A:277:VAL:C | 1:A:278:PRO:CA | 2.55 | 0.75 |
| 6:F:44:GLY:N | 6:F:47:MET:HE2 | 2.00 | 0.75 |
| 6:F:234:ILE:HG12 | 8:H:226:ILE:HD11 | 1.68 | 0.75 |
| 1:A:99:CYS:CB | 3:C:67:MET:HE2 | 2.16 | 0.75 |
| 2:B:458:THR:O | 2:B:460:LYS:N | 2.20 | 0.75 |
| 6:F:171:ASN:OD1 | 7:G:149:ASN:ND2 | 2.19 | 0.75 |
| 3:C:121:VAL:CG1 | 3:C:122:PRO:HD2 | 2.17 | 0.75 |
| 6:F:377:ARG:NH1 | 8:H:343:GLN:HB2 | 2.00 | 0.75 |
| 1:A:141:ARG:HE | 3:C:220:GLN:NE2 | 1.85 | 0.75 |
| 2:B:87:SER:O | 2:B:89:VAL:N | 2.16 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:63:ARG:NH1 | 4:D:535:ALA:HB1 | 2.02 | 0.75 |
| 4:D:199:VAL:HG21 | 4:D:241:VAL:HG21 | 1.68 | 0.75 |
| 2:B:490:GLU:HA | 4:D:560:ARG:HH22 | 1.41 | 0.74 |
| 4:D:202:LEU:HD22 | 4:D:237:MET:CE | 2.17 | 0.74 |
| 2:B:507:LEU:HD12 | 4:D:579:THR:CG2 | 2.15 | 0.74 |
| 2:B:287:LEU:HD21 | 4:D:343:HIS:HD2 | 1.52 | 0.74 |
| 2:B:297:VAL:CG1 | 4:D:355:LEU:HD11 | 2.17 | 0.74 |
| 3:C:116:LEU:HD12 | 3:C:137:LEU:CD1 | 2.16 | 0.74 |
| 2:B:216:PHE:CD2 | 4:D:269:GLN:HG2 | 2.22 | 0.74 |
| 1:A:33:ILE:HG23 | 3:C:15:LEU:HD22 | 1.68 | 0.74 |
| 1:A:145:THR:CG2 | 4:D:65:TRP:CZ2 | 2.70 | 0.74 |
| 1:A:148:LEU:HD13 | 2:B:80:VAL:HG23 | 1.68 | 0.74 |
| 3:C:303:GLU:OE2 | 3:C:303:GLU:HA | 1.88 | 0.74 |
| 7:G:274:MET:CE | 8:H:280:GLN:CB | 2.58 | 0.74 |
| 2:B:443:ASP:OD2 | 4:D:509:ARG:NH2 | 2.21 | 0.74 |
| 4:D:571:LEU:O | 4:D:575:THR:HG23 | 1.88 | 0.74 |
| 2:B:222:PHE:CE1 | 2:B:241:LEU:CD1 | 2.70 | 0.74 |
| 6:F:377:ARG:NH2 | 8:H:343:GLN:HG3 | 2.02 | 0.74 |
| 1:A:58:LYS:NZ | 4:D:506:SER:HB2 | 1.96 | 0.73 |
| 2:B:42:TRP:CD2 | 4:D:20:LEU:HD13 | 2.23 | 0.73 |
| 2:B:84:PHE:CE2 | 4:D:65:TRP:CZ3 | 2.76 | 0.73 |
| 5:E:141:PHE:CA | 7:G:289:PHE:HZ | 2.01 | 0.73 |
| 1:A:145:THR:CG2 | 4:D:65:TRP:HZ2 | 2.01 | 0.73 |
| 1:A:211:HIS:HA | 4:D:630:VAL:CG2 | 2.17 | 0.73 |
| 5:E:148:TYR:OH | 7:G:289:PHE:CE1 | 2.39 | 0.73 |
| 8:H:259:HIS:N | 8:H:300:GLU:OE2 | 2.15 | 0.73 |
| 6:F:92:ARG:NH1 | 6:F:119:LEU:HA | 2.04 | 0.73 |
| 6:F:359:ARG:HG3 | 8:H:328:GLN:CD | 2.07 | 0.73 |
| 1:A:138:THR:HG1 | 2:B:92:ILE:CD1 | 2.01 | 0.73 |
| 2:B:132:CYS:SG | 4:D:119:LEU:CD1 | 2.76 | 0.73 |
| 7:G:274:MET:HE3 | 8:H:280:GLN:N | 2.04 | 0.73 |
| 2:B:166:SER:CB | 4:D:152:ASN:ND2 | 2.50 | 0.73 |
| 6:F:60:PHE:HE1 | 6:F:99:LEU:HD11 | 1.54 | 0.73 |
| 3:C:116:LEU:CD1 | 3:C:137:LEU:HD11 | 2.19 | 0.72 |
| 4:D:307:GLU:CG | 7:G:324:ILE:HD11 | 2.19 | 0.72 |
| 4:D:601:MET:HE2 | 4:D:604:LEU:HD12 | 1.69 | 0.72 |
| 2:B:194:LEU:HA | 2:B:197:LEU:HG | 1.70 | 0.72 |
| 2:B:521:THR:HG22 | 3:C:251:ASP:OD2 | 1.89 | 0.72 |
| 2:B:402:GLU:OE2 | 4:D:158:ARG:NE | 2.20 | 0.72 |
| 2:B:513:PRO:HG2 | 2:B:519:MET:HE2 | 1.69 | 0.72 |
| 3:C:133:ASP:OD1 | 3:C:136:ASP:CG | 2.28 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:VAL:HG13 | 3:C:253:ILE:CG2 | 2.20 | 0.72 |
| 2:B:424:LEU:HD22 | 4:D:484:ILE:HD11 | 1.70 | 0.72 |
| 6:F:247:MET:HE2 | 8:H:243:PHE:HD1 | 1.54 | 0.72 |
| 2:B:77:LEU:HD23 | 2:B:81:LEU:HD11 | 1.71 | 0.72 |
| 2:B:120:LYS:NZ | 3:C:171:SER:OG | 2.20 | 0.72 |
| 6:F:247:MET:CE | 8:H:243:PHE:CD1 | 2.70 | 0.71 |
| 1:A:113:ILE:HB | 1:A:114:PRO:HD3 | 1.72 | 0.71 |
| 2:B:209:SER:HA | 4:D:262:THR:HG23 | 1.71 | 0.71 |
| 3:C:123:PRO:C | 3:C:125:ASP:H | 1.93 | 0.71 |
| 1:A:279:GLU:CB | 1:A:280:PRO:CD | 2.56 | 0.71 |
| 2:B:87:SER:C | 2:B:89:VAL:H | 1.93 | 0.71 |
| 2:B:347:MET:HB3 | 2:B:348:PRO:HD3 | 1.72 | 0.71 |
| 3:C:129:ILE:CD1 | 4:D:489:LEU:CD1 | 2.68 | 0.71 |
| 2:B:131:MET:HE1 | 3:C:85:VAL:CG2 | 2.15 | 0.71 |
| 6:F:163:ASP:OD2 | 7:G:59:TYR:OH | 2.03 | 0.71 |
| 6:F:287:ARG:HD3 | 6:F:321:LEU:HD21 | 1.71 | 0.71 |
| 6:F:338:LEU:HD12 | 8:H:304:SER:HB3 | 1.71 | 0.71 |
| 1:A:189:TYR:HA | 3:C:271:MET:HE1 | 1.73 | 0.71 |
| 4:D:305:PRO:C | 4:D:307:GLU:H | 1.91 | 0.71 |
| 6:F:157:LEU:N | 6:F:170:ARG:HH22 | 1.89 | 0.71 |
| 6:F:247:MET:HE2 | 8:H:243:PHE:CD1 | 2.25 | 0.71 |
| 1:A:228:SER:HA | 3:C:307:LEU:HD12 | 1.71 | 0.71 |
| 2:B:266:TYR:CG | 2:B:345:LEU:HD11 | 2.25 | 0.71 |
| 6:F:176:GLN:OE1 | 7:G:117:ASP:HB3 | 1.91 | 0.71 |
| 1:A:64:ALA:HB1 | 4:D:492:VAL:CG1 | 2.21 | 0.70 |
| 3:C:63:ARG:HH22 | 4:D:535:ALA:HB1 | 1.53 | 0.70 |
| 4:D:307:GLU:OE1 | 7:G:324:ILE:HD11 | 1.90 | 0.70 |
| 2:B:386:GLN:HE22 | 4:D:440:GLN:CD | 1.95 | 0.70 |
| 5:E:108:LEU:HD22 | 8:H:254:LEU:HD11 | 1.72 | 0.70 |
| 2:B:213:LEU:HD13 | 4:D:265:LEU:HD11 | 1.73 | 0.70 |
| 6:F:173:LEU:HD21 | 7:G:90:LEU:HD21 | 1.72 | 0.70 |
| 6:F:257:VAL:HG11 | 8:H:255:ASP:HB2 | 1.72 | 0.70 |
| 1:A:133:MET:SD | 3:C:217:LEU:HD22 | 2.31 | 0.70 |
| 2:B:94:GLU:CB | 4:D:79:GLU:OE1 | 2.40 | 0.70 |
| 2:B:120:LYS:NZ | 3:C:171:SER:C | 2.45 | 0.70 |
| 4:D:317:GLN:HA | 8:H:334:PHE:CE2 | 2.27 | 0.70 |
| 7:G:56:SER:OG | 7:G:63:GLN:OE1 | 2.01 | 0.70 |
| 7:G:7:LEU:HD21 | 7:G:34:GLN:OE1 | 1.92 | 0.70 |
| 1:A:1:MET:HE3 | 1:A:28:THR:HG22 | 1.74 | 0.70 |
| 1:A:279:GLU:HB3 | 1:A:280:PRO:CD | 2.08 | 0.70 |
| 2:B:94:GLU:HB3 | 4:D:79:GLU:OE1 | 1.92 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:522:THR:HG23 | 4:D:590:TYR:HE2 | 1.53 | 0.69 |
| 4:D:601:MET:CE | 4:D:604:LEU:HD12 | 2.21 | 0.69 |
| 6:F:224:ASP:O | 6:F:225:ARG:C | 2.25 | 0.69 |
| 6:F:377:ARG:HH12 | 8:H:343:GLN:HA | 1.32 | 0.69 |
| 7:G:124:THR:HG22 | 7:G:125:ILE:H | 1.55 | 0.69 |
| 5:E:141:PHE:HB2 | 7:G:289:PHE:CZ | 2.28 | 0.69 |
| 8:H:294:MET:HE3 | 8:H:298:ALA:HB2 | 1.73 | 0.69 |
| 1:A:172:VAL:CG1 | 3:C:253:ILE:HG21 | 2.22 | 0.69 |
| 2:B:536:LEU:HD21 | 3:C:261:LYS:HG2 | 1.72 | 0.69 |
| 6:F:335:ARG:NH2 | 8:H:259:HIS:CB | 0.54 | 0.69 |
| 2:B:376:MET:HE1 | 4:D:207:LEU:O | 1.92 | 0.69 |
| 7:G:130:ILE:CG2 | 7:G:131:LEU:N | 2.49 | 0.69 |
| 3:C:75:LEU:HD11 | 3:C:162:LEU:HD23 | 1.74 | 0.69 |
| 5:E:59:ILE:HG23 | 7:G:210:ILE:HD12 | 1.75 | 0.69 |
| 6:F:28:GLY:HA2 | 6:F:38:LEU:HD11 | 1.73 | 0.69 |
| 6:F:224:ASP:CG | 6:F:227:ILE:HD11 | 2.12 | 0.69 |
| 4:D:631:GLN:HB3 | 4:D:648:ARG:NH2 | 2.07 | 0.69 |
| 6:F:261:VAL:HG21 | 8:H:254:LEU:HD23 | 1.74 | 0.69 |
| 7:G:92:HIS:CE1 | 7:G:93:PHE:CD1 | 2.80 | 0.69 |
| 7:G:62:VAL:HG12 | 7:G:66:LEU:HD11 | 1.75 | 0.69 |
| 1:A:1:MET:HE1 | 1:A:28:THR:HG22 | 1.74 | 0.68 |
| 4:D:265:LEU:O | 4:D:269:GLN:HG3 | 1.94 | 0.68 |
| 6:F:175:ARG:CZ | 7:G:152:LEU:HD22 | 2.22 | 0.68 |
| 2:B:35:ASP:HB3 | 4:D:30:MET:HE1 | 1.74 | 0.68 |
| 2:B:70:PRO:O | 4:D:66:TYR:OH | 2.10 | 0.68 |
| 2:B:577:GLU:OE1 | 4:D:640:GLY:N | 2.26 | 0.68 |
| 5:E:4:ALA:O | 5:E:6:PRO:HD3 | 1.93 | 0.68 |
| 2:B:220:HIS:CE1 | 4:D:276:LEU:HD11 | 2.27 | 0.68 |
| 4:D:4:ARG:HG3 | 4:D:32:GLN:HE22 | 1.57 | 0.68 |
| 5:E:190:ARG:CZ | 6:F:370:ILE:HG12 | 2.24 | 0.68 |
| 5:E:148:TYR:HH | 7:G:289:PHE:HE1 | 1.36 | 0.68 |
| 6:F:16:MET:SD | 6:F:130:LEU:HD23 | 2.33 | 0.68 |
| 2:B:134:LYS:HD2 | 3:C:85:VAL:HG13 | 1.74 | 0.68 |
| 6:F:224:ASP:OD1 | 6:F:227:ILE:HD11 | 1.94 | 0.68 |
| 7:G:41:CYS:HA | 7:G:108:GLN:OE1 | 1.93 | 0.68 |
| 1:A:279:GLU:HB2 | 1:A:280:PRO:HD3 | 1.75 | 0.68 |
| 2:B:80:VAL:CG1 | 4:D:65:TRP:CE3 | 2.75 | 0.68 |
| 3:C:129:ILE:HD11 | 4:D:489:LEU:HD22 | 1.76 | 0.68 |
| 1:A:240:ASP:OD2 | 3:C:335:LYS:NZ | 2.27 | 0.68 |
| 2:B:84:PHE:CE2 | 4:D:65:TRP:CE3 | 2.77 | 0.68 |
| 5:E:73:LYS:NZ | 7:G:220:GLU:OE2 | 2.26 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:334:LEU:HB3 | 2:B:335:PRO:HD3 | 1.76 | 0.68 |
| 3:C:116:LEU:HD12 | 3:C:137:LEU:HD12 | 1.75 | 0.67 |
| 2:B:536:LEU:HD22 | 3:C:261:LYS:HD3 | 1.77 | 0.67 |
| 5:E:137:LEU:HD23 | 7:G:285:LEU:HD23 | 1.76 | 0.67 |
| 5:E:179:MET:HG2 | 8:H:329:ILE:CD1 | 2.24 | 0.67 |
| 1:A:12:LEU:HB3 | 1:A:21:LEU:CD2 | 2.23 | 0.67 |
| 3:C:141:LEU:HD23 | 3:C:147:VAL:HG21 | 1.75 | 0.67 |
| 7:G:37:TYR:OH | 7:G:105:PRO:HG3 | 1.94 | 0.67 |
| 2:B:386:GLN:NE2 | 4:D:440:GLN:CD | 2.48 | 0.67 |
| 3:C:63:ARG:CZ | 4:D:535:ALA:CB | 2.71 | 0.67 |
| 5:E:189:TRP:HZ3 | 8:H:340:ILE:HD12 | 1.50 | 0.67 |
| 6:F:227:ILE:HG12 | 8:H:223:ARG:HH22 | 1.60 | 0.67 |
| 2:B:490:GLU:CA | 4:D:560:ARG:HH22 | 2.03 | 0.66 |
| 6:F:335:ARG:HH21 | 8:H:259:HIS:CB | 0.66 | 0.66 |
| 8:H:234:THR:HB | 8:H:235:PRO:HD3 | 1.77 | 0.66 |
| 2:B:456:ASP:C | 2:B:458:THR:N | 2.47 | 0.66 |
| 3:C:351:SER:O | 3:C:353:PRO:HD2 | 1.94 | 0.66 |
| 6:F:227:ILE:HG12 | 8:H:223:ARG:NH2 | 2.11 | 0.66 |
| 4:D:275:ASP:HA | 4:D:278:LYS:HE3 | 1.78 | 0.66 |
| 1:A:128:LEU:CD2 | 4:D:97:ARG:HH21 | 2.08 | 0.66 |
| 6:F:377:ARG:HH11 | 8:H:343:GLN:CA | 2.07 | 0.66 |
| 4:D:352:HIS:CG | 4:D:366:ARG:NE | 2.64 | 0.66 |
| 6:F:9:LEU:HD21 | 6:F:124:PRO:O | 1.96 | 0.66 |
| 4:D:17:GLU:O | 4:D:52:SER:HB3 | 1.96 | 0.66 |
| 6:F:259:ASP:HB3 | 6:F:263:ARG:NH2 | 2.10 | 0.66 |
| 1:A:241:LEU:HD22 | 1:A:248:VAL:HG13 | 1.78 | 0.66 |
| 1:A:266:LEU:O | 1:A:270:VAL:HG23 | 1.96 | 0.66 |
| 2:B:95:VAL:HG13 | 2:B:99:LYS:HB3 | 1.78 | 0.66 |
| 5:E:189:TRP:CZ2 | 8:H:340:ILE:HD13 | 2.31 | 0.66 |
| 5:E:9:PRO:HB2 | 6:F:197:GLN:OE1 | 1.96 | 0.65 |
| 4:D:206:PHE:CD2 | 4:D:230:SER:OG | 2.49 | 0.65 |
| 7:G:235:ILE:HD11 | 8:H:225:LEU:HD22 | 1.78 | 0.65 |
| 1:A:12:LEU:CB | 1:A:21:LEU:HD21 | 2.24 | 0.65 |
| 2:B:88:LYS:O | 2:B:90:PRO:CD | 2.43 | 0.65 |
| 2:B:175:MET:CG | 4:D:460:PRO:HG3 | 2.16 | 0.65 |
| 4:D:631:GLN:HB2 | 4:D:648:ARG:HH22 | 1.61 | 0.65 |
| 1:A:77:LEU:HD22 | 3:C:154:LEU:HD22 | 1.77 | 0.65 |
| 1:A:145:THR:CB | 4:D:65:TRP:HZ2 | 2.10 | 0.65 |
| 1:A:275:PHE:O | 1:A:276:VAL:C | 2.32 | 0.65 |
| 2:B:30:LEU:CD2 | 4:D:34:LEU:CD2 | 2.74 | 0.65 |
| 2:B:577:GLU:OE1 | 4:D:640:GLY:CA | 2.45 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:631:GLN:CB | 4:D:648:ARG:NH2 | 2.60 | 0.65 |
| 4:D:296:SER:HB2 | 4:D:301:THR:CG2 | 2.25 | 0.65 |
| 5:E:186:ILE:HG12 | 7:G:338:TYR:CZ | 2.32 | 0.65 |
| 4:D:317:GLN:HG3 | 8:H:334:PHE:CD2 | 2.32 | 0.65 |
| 7:G:301:THR:HG23 | 8:H:312:GLU:HB2 | 1.78 | 0.65 |
| 2:B:138:LYS:HG3 | 3:C:84:GLN:HE21 | 1.62 | 0.64 |
| 2:B:319:THR:HG23 | 4:D:378:LEU:HD12 | 1.78 | 0.64 |
| 5:E:42:CYS:SG | 6:F:187:LEU:HD23 | 2.37 | 0.64 |
| 2:B:97:ILE:HD11 | 4:D:82:GLN:CG | 2.22 | 0.64 |
| 2:B:383:GLU:OE2 | 4:D:203:ARG:NE | 2.30 | 0.64 |
| 1:A:77:LEU:HD22 | 3:C:154:LEU:HD21 | 1.80 | 0.64 |
| 4:D:352:HIS:CG | 4:D:366:ARG:NH2 | 2.63 | 0.64 |
| 7:G:123:ASP:O | 7:G:124:THR:O | 2.15 | 0.64 |
| 7:G:143:VAL:CG2 | 8:H:159:MET:CE | 2.68 | 0.64 |
| 1:A:215:VAL:HG21 | 4:D:629:PRO:HB2 | 1.79 | 0.64 |
| 4:D:157:TYR:CE1 | 4:D:161:GLN:NE2 | 2.64 | 0.64 |
| 5:E:155:ILE:HG23 | 6:F:334:VAL:HG21 | 0.65 | 0.64 |
| 2:B:42:TRP:CE2 | 4:D:20:LEU:CD1 | 2.80 | 0.64 |
| 2:B:507:LEU:HD11 | 4:D:579:THR:HG22 | 1.77 | 0.64 |
| 3:C:123:PRO:C | 3:C:125:ASP:N | 2.50 | 0.64 |
| 5:E:141:PHE:CA | 7:G:289:PHE:CZ | 2.81 | 0.64 |
| 2:B:36:LEU:CD2 | 4:D:34:LEU:HD21 | 2.28 | 0.64 |
| 2:B:81:LEU:O | 2:B:84:PHE:HB2 | 1.98 | 0.64 |
| 6:F:295:LEU:HD21 | 6:F:317:GLU:OE1 | 1.98 | 0.64 |
| 7:G:81:ILE:HG22 | 7:G:99:ILE:HD12 | 1.78 | 0.64 |
| 2:B:383:GLU:OE2 | 4:D:203:ARG:NH2 | 2.31 | 0.64 |
| 2:B:420:ARG:NE | 4:D:477:GLU:OE1 | 2.30 | 0.64 |
| 2:B:424:LEU:HD23 | 4:D:484:ILE:CD1 | 2.27 | 0.64 |
| 7:G:62:VAL:CG1 | 7:G:66:LEU:HD11 | 2.27 | 0.64 |
| 1:A:193:ILE:HG23 | 3:C:274:LEU:CD1 | 2.27 | 0.64 |
| 2:B:536:LEU:CD2 | 3:C:261:LYS:HD3 | 2.27 | 0.64 |
| 2:B:570:TYR:CG | 4:D:631:GLN:HG2 | 2.33 | 0.64 |
| 6:F:44:GLY:O | 6:F:47:MET:HE2 | 1.98 | 0.63 |
| 2:B:507:LEU:HD21 | 4:D:582:LEU:HD23 | 1.79 | 0.63 |
| 4:D:317:GLN:HA | 8:H:334:PHE:CD2 | 2.33 | 0.63 |
| 5:E:76:ALA:HB1 | 7:G:224:LEU:HD21 | 1.80 | 0.63 |
| 1:A:64:ALA:HB1 | 4:D:492:VAL:HG12 | 1.80 | 0.63 |
| 2:B:166:SER:HB3 | 4:D:152:ASN:ND2 | 2.12 | 0.63 |
| 2:B:190:GLN:OE1 | 4:D:169:SER:O | 2.16 | 0.63 |
| 2:B:344:LEU:HD13 | 4:D:399:LYS:HD2 | 1.80 | 0.63 |
| 3:C:86:ARG:CB | 3:C:92:LEU:HD12 | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:133:ASP:OD1 | 3:C:136:ASP:OD2 | 2.16 | 0.63 |
| 5:E:60:ASN:CB | 8:H:207:HIS:NE2 | 2.54 | 0.63 |
| 7:G:130:ILE:CG2 | 7:G:131:LEU:H | 2.00 | 0.63 |
| 2:B:120:LYS:NZ | 3:C:175:PRO:HA | 2.11 | 0.63 |
| 2:B:588:GLU:OE2 | 4:D:650:ARG:NH2 | 2.30 | 0.63 |
| 2:B:132:CYS:SG | 4:D:119:LEU:HD11 | 2.37 | 0.63 |
| 6:F:185:GLU:OE1 | 7:G:168:PRO:HB3 | 1.99 | 0.63 |
| 5:E:97:HIS:CD2 | 8:H:247:TYR:HH | 2.16 | 0.63 |
| 5:E:60:ASN:HB3 | 8:H:207:HIS:CD2 | 2.33 | 0.63 |
| 8:H:359:GLN:O | 8:H:363:ASP:HB2 | 1.98 | 0.63 |
| 2:B:35:ASP:CB | 4:D:30:MET:CE | 2.75 | 0.62 |
| 6:F:227:ILE:CG1 | 8:H:223:ARG:HH22 | 2.11 | 0.62 |
| 2:B:263:GLN:NE2 | 2:B:346:ASN:HD21 | 1.98 | 0.62 |
| 2:B:510:PHE:CE1 | 4:D:586:LEU:HB3 | 2.33 | 0.62 |
| 5:E:179:MET:CG | 8:H:329:ILE:CD1 | 2.77 | 0.62 |
| 2:B:87:SER:C | 2:B:89:VAL:N | 2.48 | 0.62 |
| 5:E:139:VAL:HG22 | 6:F:278:LEU:HD12 | 1.80 | 0.62 |
| 3:C:4:THR:CG2 | 3:C:33:ILE:HD11 | 2.26 | 0.62 |
| 4:D:184:SER:O | 4:D:185:SER:C | 2.29 | 0.62 |
| 5:E:60:ASN:CB | 8:H:207:HIS:CE1 | 2.66 | 0.62 |
| 6:F:92:ARG:HH11 | 6:F:119:LEU:HA | 1.61 | 0.62 |
| 1:A:145:THR:HG23 | 4:D:65:TRP:CE2 | 2.34 | 0.62 |
| 1:A:217:LEU:O | 1:A:220:THR:OG1 | 2.17 | 0.62 |
| 1:A:270:VAL:HG13 | 1:A:273:MET:HE3 | 1.80 | 0.62 |
| 2:B:453:LEU:HB3 | 2:B:471:VAL:HG12 | 1.80 | 0.62 |
| 4:D:485:CYS:SG | 4:D:487:PRO:HD2 | 2.39 | 0.62 |
| 4:D:598:VAL:HB | 4:D:599:PRO:HD3 | 1.82 | 0.62 |
| 3:C:5:LEU:CD1 | 3:C:22:LEU:CD1 | 2.76 | 0.62 |
| 7:G:93:PHE:CE2 | 7:G:94:ASP:OD1 | 2.53 | 0.62 |
| 1:A:145:THR:CG2 | 4:D:69:LEU:CD1 | 2.57 | 0.62 |
| 4:D:457:LEU:N | 4:D:458:PRO:CD | 2.62 | 0.62 |
| 2:B:329:ILE:CD1 | 4:D:386:MET:SD | 2.88 | 0.62 |
| 3:C:116:LEU:HD11 | 3:C:137:LEU:HD11 | 1.82 | 0.62 |
| 5:E:186:ILE:HG12 | 7:G:338:TYR:CE2 | 2.34 | 0.62 |
| 1:A:134:GLU:HG3 | 3:C:213:MET:SD | 2.40 | 0.62 |
| 2:B:194:LEU:O | 2:B:197:LEU:HB2 | 2.00 | 0.62 |
| 5:E:64:LEU:HD13 | 8:H:211:ARG:HG3 | 1.80 | 0.62 |
| 6:F:288:ILE:HD11 | 6:F:314:LEU:CD2 | 2.30 | 0.62 |
| 2:B:74:GLU:CD | 4:D:54:ARG:HG3 | 2.21 | 0.61 |
| 2:B:84:PHE:HE2 | 4:D:65:TRP:HE3 | 1.43 | 0.61 |
| 2:B:88:LYS:O | 2:B:90:PRO:N | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:184:SER:O | 4:D:186:THR:N | 2.33 | 0.61 |
| 2:B:407:VAL:CB | 4:D:459:TRP:HZ3 | 2.13 | 0.61 |
| 5:E:158:ILE:HD12 | 6:F:334:VAL:HG11 | 1.81 | 0.61 |
| 7:G:14:TYR:HB2 | 7:G:36:ILE:CG2 | 2.31 | 0.61 |
| 2:B:406:ILE:HD13 | 4:D:155:ILE:HD11 | 1.82 | 0.61 |
| 5:E:189:TRP:HZ3 | 8:H:336:VAL:HG12 | 1.65 | 0.61 |
| 3:C:116:LEU:CD1 | 3:C:137:LEU:CD1 | 2.78 | 0.61 |
| 3:C:129:ILE:HD13 | 4:D:489:LEU:CD1 | 2.30 | 0.61 |
| 4:D:535:ALA:HB1 | 4:D:537:GLU:OE2 | 2.00 | 0.61 |
| 2:B:80:VAL:HG11 | 4:D:65:TRP:CE3 | 2.32 | 0.61 |
| 5:E:47:GLU:HG3 | 6:F:195:LYS:HZ3 | 1.65 | 0.61 |
| 5:E:57:ALA:HB2 | 8:H:203:GLN:NE2 | 2.15 | 0.61 |
| 5:E:78:ILE:CD1 | 6:F:234:ILE:HG23 | 2.31 | 0.61 |
| 1:A:78:GLY:O | 1:A:81:TYR:HD1 | 1.84 | 0.61 |
| 6:F:163:ASP:OD1 | 6:F:164:PRO:HD2 | 2.00 | 0.61 |
| 6:F:335:ARG:NH2 | 8:H:259:HIS:HB2 | 0.95 | 0.61 |
| 3:C:86:ARG:HB2 | 3:C:92:LEU:HD12 | 1.81 | 0.61 |
| 3:C:282:THR:HB | 3:C:283:PRO:HD2 | 1.83 | 0.61 |
| 5:E:141:PHE:HA | 7:G:289:PHE:CZ | 2.36 | 0.61 |
| 2:B:293:ASN:O | 2:B:297:VAL:HG23 | 2.01 | 0.61 |
| 4:D:314:SER:OG | 7:G:321:GLY:N | 2.29 | 0.61 |
| 4:D:416:ALA:HA | 4:D:419:LEU:HB3 | 1.82 | 0.61 |
| 6:F:377:ARG:CZ | 8:H:343:GLN:HG3 | 2.30 | 0.61 |
| 5:E:69:LEU:HB3 | 7:G:217:LEU:HD23 | 1.82 | 0.60 |
| 6:F:319:LEU:O | 8:H:293:ILE:HD11 | 2.01 | 0.60 |
| 6:F:377:ARG:NH2 | 8:H:343:GLN:CG | 2.62 | 0.60 |
| 7:G:174:PRO:HB2 | 7:G:176:ASP:OD1 | 2.00 | 0.60 |
| 5:E:21:LYS:NZ | 7:G:159:SER:HA | 2.17 | 0.60 |
| 1:A:71:ASP:HB3 | 3:C:114:ARG:CZ | 2.19 | 0.60 |
| 2:B:536:LEU:HD21 | 3:C:261:LYS:CG | 2.30 | 0.60 |
| 4:D:157:TYR:CZ | 4:D:161:GLN:NE2 | 2.69 | 0.60 |
| 5:E:9:PRO:CA | 6:F:197:GLN:HE22 | 2.14 | 0.60 |
| 5:E:175:LEU:HD21 | 7:G:328:CYS:SG | 2.41 | 0.60 |
| 4:D:264:GLU:HA | 4:D:267:LYS:HD2 | 1.83 | 0.60 |
| 2:B:77:LEU:HD21 | 4:D:61:GLY:C | 2.21 | 0.60 |
| 3:C:129:ILE:HD11 | 4:D:489:LEU:CD2 | 2.31 | 0.60 |
| 3:C:167:PHE:HB3 | 3:C:185:ARG:NH2 | 2.16 | 0.60 |
| 5:E:62:LYS:NZ | 7:G:211:SER:OG | 2.21 | 0.60 |
| 2:B:490:GLU:CG | 4:D:560:ARG:NH2 | 2.65 | 0.60 |
| 4:D:509:ARG:HD3 | 4:D:521:PHE:CZ | 2.36 | 0.60 |
| 1:A:33:ILE:HG23 | 3:C:15:LEU:CD2 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:96:ALA:O | 2:B:99:LYS:N | 2.34 | 0.60 |
| 2:B:513:PRO:HG2 | 2:B:519:MET:HE3 | 1.83 | 0.60 |
| 5:E:59:ILE:HG23 | 7:G:210:ILE:CD1 | 2.31 | 0.60 |
| 1:A:189:TYR:HA | 3:C:271:MET:HE2 | 1.84 | 0.60 |
| 1:A:207:GLU:N | 1:A:208:PRO:CD | 2.64 | 0.60 |
| 2:B:245:SER:O | 2:B:246:PHE:C | 2.32 | 0.60 |
| 4:D:210:LEU:HD21 | 4:D:227:ARG:HD3 | 1.83 | 0.60 |
| 5:E:135:LEU:HB3 | 5:E:136:PRO:CD | 2.29 | 0.60 |
| 6:F:176:GLN:CD | 7:G:117:ASP:HB3 | 2.22 | 0.60 |
| 6:F:359:ARG:CG | 8:H:328:GLN:CD | 2.70 | 0.60 |
| 6:F:247:MET:HE1 | 8:H:243:PHE:HD1 | 1.63 | 0.59 |
| 6:F:326:ARG:NH1 | 8:H:295:PRO:CG | 2.62 | 0.59 |
| 2:B:273:LEU:HA | 4:D:330:LEU:HD13 | 1.84 | 0.59 |
| 5:E:97:HIS:CE1 | 6:F:255:VAL:HG13 | 2.37 | 0.59 |
| 5:E:221:HIS:HB3 | 5:E:222:PRO:C | 2.22 | 0.59 |
| 7:G:41:CYS:CA | 7:G:47:ARG:NH1 | 2.65 | 0.59 |
| 1:A:5:SER:HA | 1:A:31:MET:CE | 2.32 | 0.59 |
| 2:B:171:VAL:HG21 | 4:D:463:ILE:HD13 | 1.85 | 0.59 |
| 4:D:268:LEU:HB3 | 4:D:272:GLN:HE21 | 1.67 | 0.59 |
| 4:D:383:ASP:O | 4:D:387:GLN:HG3 | 2.01 | 0.59 |
| 6:F:116:SER:HA | 6:F:119:LEU:HD12 | 1.83 | 0.59 |
| 1:A:99:CYS:HB3 | 3:C:67:MET:CE | 2.32 | 0.59 |
| 2:B:120:LYS:HZ2 | 3:C:171:SER:C | 1.98 | 0.59 |
| 5:E:78:ILE:HD11 | 6:F:234:ILE:HG23 | 1.85 | 0.59 |
| 6:F:234:ILE:HG12 | 8:H:226:ILE:CD1 | 2.33 | 0.59 |
| 2:B:2:SER:OG | 2:B:28:ASP:CG | 2.40 | 0.59 |
| 2:B:91:ALA:C | 2:B:93:GLU:N | 2.56 | 0.59 |
| 2:B:97:ILE:HD12 | 4:D:82:GLN:NE2 | 2.17 | 0.59 |
| 1:A:99:CYS:HB3 | 3:C:67:MET:HE2 | 1.84 | 0.59 |
| 2:B:35:ASP:CB | 4:D:30:MET:HE3 | 2.32 | 0.59 |
| 4:D:631:GLN:OE1 | 4:D:648:ARG:NH2 | 2.35 | 0.59 |
| 6:F:377:ARG:HH11 | 8:H:343:GLN:HA | 1.59 | 0.59 |
| 2:B:376:MET:CE | 4:D:207:LEU:O | 2.50 | 0.59 |
| 2:B:391:LEU:HD11 | 4:D:239:GLU:HG2 | 1.83 | 0.59 |
| 4:D:130:ARG:NH2 | 4:D:484:ILE:O | 2.35 | 0.59 |
| 6:F:173:LEU:CD2 | 7:G:90:LEU:HD21 | 2.33 | 0.59 |
| 7:G:14:TYR:CE1 | 7:G:18:GLN:NE2 | 2.70 | 0.59 |
| 2:B:376:MET:HE1 | 4:D:211:HIS:CB | 2.32 | 0.58 |
| 5:E:141:PHE:CB | 7:G:289:PHE:CZ | 2.86 | 0.58 |
| 5:E:158:ILE:HD11 | 7:G:295:ILE:HG23 | 1.86 | 0.58 |
| 7:G:2:THR:HG21 | 7:G:37:TYR:CE1 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:550:LEU:HD11 | 3:C:276:VAL:CG2 | 2.31 | 0.58 |
| 4:D:211:HIS:CE1 | 4:D:215:ILE:CD1 | 2.85 | 0.58 |
| 5:E:148:TYR:OH | 7:G:289:PHE:HD1 | 1.75 | 0.58 |
| 6:F:168:LEU:CD1 | 7:G:145:CYS:SG | 2.91 | 0.58 |
| 1:A:266:LEU:HD12 | 3:C:345:LEU:CG | 2.24 | 0.58 |
| 2:B:344:LEU:HD22 | 2:B:347:MET:CE | 2.34 | 0.58 |
| 2:B:483:ARG:NH2 | 4:D:549:GLN:NE2 | 2.37 | 0.58 |
| 6:F:60:PHE:CE1 | 6:F:99:LEU:HD11 | 2.37 | 0.58 |
| 2:B:344:LEU:HD22 | 2:B:347:MET:HE1 | 1.85 | 0.58 |
| 2:B:385:LEU:HD12 | 4:D:254:LEU:CD1 | 2.33 | 0.58 |
| 1:A:93:ASN:OD1 | 3:C:68:ARG:NH1 | 2.36 | 0.58 |
| 2:B:92:ILE:O | 2:B:94:GLU:N | 2.37 | 0.58 |
| 1:A:145:THR:OG1 | 4:D:65:TRP:HZ2 | 1.78 | 0.58 |
| 4:D:631:GLN:HB3 | 4:D:648:ARG:HH21 | 1.68 | 0.58 |
| 5:E:72:GLU:OE1 | 8:H:218:ARG:NH1 | 2.36 | 0.58 |
| 5:E:76:ALA:CB | 7:G:224:LEU:HD21 | 2.33 | 0.58 |
| 6:F:326:ARG:HD2 | 8:H:293:ILE:HG23 | 1.86 | 0.58 |
| 2:B:80:VAL:HG12 | 4:D:65:TRP:CE3 | 2.34 | 0.58 |
| 2:B:138:LYS:HE3 | 3:C:84:GLN:CD | 2.09 | 0.58 |
| 4:D:10:LEU:HD23 | 4:D:31:LEU:HD22 | 1.86 | 0.58 |
| 2:B:139:GLU:OE1 | 4:D:123:ARG:HD3 | 2.03 | 0.57 |
| 4:D:631:GLN:CB | 4:D:648:ARG:HH22 | 2.17 | 0.57 |
| 2:B:37:LYS:HB3 | 2:B:38:PRO:HD3 | 1.85 | 0.57 |
| 5:E:139:VAL:HG22 | 6:F:278:LEU:CD1 | 2.34 | 0.57 |
| 8:H:358:ARG:HH21 | 8:H:366:LEU:CD1 | 2.18 | 0.57 |
| 1:A:141:ARG:HE | 3:C:220:GLN:HE22 | 1.51 | 0.57 |
| 1:A:278:PRO:HG2 | 1:A:280:PRO:HD3 | 1.86 | 0.57 |
| 1:A:113:ILE:HG21 | 2:B:121:LEU:HD11 | 1.87 | 0.57 |
| 3:C:63:ARG:NH2 | 4:D:535:ALA:HB1 | 2.11 | 0.57 |
| 4:D:306:GLN:C | 4:D:307:GLU:O | 2.43 | 0.57 |
| 7:G:249:THR:CG2 | 8:H:243:PHE:HB2 | 2.35 | 0.57 |
| 1:A:141:ARG:CG | 3:C:220:GLN:NE2 | 2.66 | 0.57 |
| 1:A:171:LYS:HE2 | 1:A:175:ARG:HH21 | 1.67 | 0.57 |
| 2:B:429:LEU:HB3 | 4:D:484:ILE:HG23 | 1.85 | 0.57 |
| 2:B:171:VAL:HG11 | 4:D:463:ILE:HD12 | 1.86 | 0.57 |
| 7:G:62:VAL:CG1 | 7:G:66:LEU:CD1 | 2.75 | 0.57 |
| 4:D:601:MET:HE2 | 4:D:601:MET:HA | 1.86 | 0.57 |
| 3:C:280:CYS:HB2 | 4:D:625:TRP:HD1 | 1.69 | 0.57 |
| 2:B:418:GLU:O | 2:B:422:THR:HG23 | 2.05 | 0.57 |
| 5:E:87:LYS:HD3 | 6:F:241:TRP:CE3 | 2.40 | 0.57 |
| 1:A:141:ARG:CG | 3:C:220:GLN:HE22 | 2.14 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:ILE:CG2 | 2:B:121:LEU:HD11 | 2.35 | 0.56 |
| 2:B:507:LEU:HD11 | 4:D:579:THR:CG2 | 2.32 | 0.56 |
| 5:E:166:ASP:OD1 | 6:F:340:TYR:OH | 2.23 | 0.56 |
| 7:G:142:VAL:HG13 | 8:H:163:ILE:HD11 | 1.86 | 0.56 |
| 1:A:148:LEU:HD12 | 2:B:80:VAL:HG22 | 1.80 | 0.56 |
| 2:B:72:LEU:HB2 | 2:B:77:LEU:HD12 | 1.88 | 0.56 |
| 2:B:500:LEU:HD21 | 4:D:571:LEU:HD11 | 1.84 | 0.56 |
| 4:D:307:GLU:CD | 7:G:324:ILE:HD12 | 1.97 | 0.56 |
| 7:G:123:ASP:O | 7:G:124:THR:C | 2.42 | 0.56 |
| 7:G:146:ILE:HG12 | 8:H:163:ILE:HG13 | 1.86 | 0.56 |
| 5:E:47:GLU:HG3 | 6:F:195:LYS:NZ | 2.20 | 0.56 |
| 6:F:261:VAL:HG21 | 8:H:254:LEU:CD2 | 2.34 | 0.56 |
| 1:A:141:ARG:NE | 3:C:220:GLN:HE22 | 2.04 | 0.56 |
| 2:B:399:VAL:HA | 4:D:158:ARG:HH12 | 1.70 | 0.56 |
| 6:F:92:ARG:HH12 | 6:F:119:LEU:C | 2.08 | 0.56 |
| 2:B:522:THR:CG2 | 4:D:590:TYR:CE2 | 2.84 | 0.56 |
| 4:D:216:SER:O | 4:D:218:SER:N | 2.38 | 0.56 |
| 4:D:304:ASP:C | 4:D:306:GLN:N | 2.45 | 0.56 |
| 6:F:9:LEU:HD22 | 6:F:124:PRO:CB | 2.33 | 0.56 |
| 2:B:134:LYS:HD2 | 3:C:85:VAL:CG1 | 2.35 | 0.55 |
| 2:B:177:PHE:HD1 | 2:B:192:ILE:CD1 | 2.18 | 0.55 |
| 6:F:227:ILE:HG22 | 6:F:227:ILE:O | 2.05 | 0.55 |
| 2:B:96:ALA:O | 2:B:98:GLU:N | 2.38 | 0.55 |
| 2:B:419:GLU:HB3 | 3:C:127:THR:HG21 | 1.86 | 0.55 |
| 6:F:135:ARG:HG3 | 8:H:168:LEU:CD2 | 2.36 | 0.55 |
| 6:F:241:TRP:CH2 | 7:G:238:LEU:HD21 | 2.40 | 0.55 |
| 4:D:577:PRO:HG2 | 4:D:582:LEU:HD13 | 1.89 | 0.55 |
| 1:A:228:SER:CA | 3:C:307:LEU:HD12 | 2.36 | 0.55 |
| 6:F:192:TYR:CE1 | 7:G:172:PRO:CD | 2.89 | 0.55 |
| 2:B:97:ILE:HD12 | 4:D:82:GLN:OE1 | 2.02 | 0.55 |
| 6:F:10:ALA:O | 6:F:13:ARG:CG | 2.39 | 0.55 |
| 6:F:259:ASP:HB3 | 6:F:263:ARG:HH21 | 1.71 | 0.55 |
| 1:A:71:ASP:CB | 3:C:114:ARG:HH21 | 1.98 | 0.55 |
| 2:B:157:ASN:HA | 4:D:474:ILE:HD12 | 1.89 | 0.55 |
| 2:B:376:MET:HE3 | 4:D:211:HIS:HB2 | 1.88 | 0.55 |
| 3:C:12:LEU:HB3 | 3:C:15:LEU:HD12 | 1.88 | 0.55 |
| 4:D:486:LEU:N | 4:D:487:PRO:CD | 2.69 | 0.55 |
| 6:F:175:ARG:HD3 | 7:G:121:TYR:OH | 2.07 | 0.55 |
| 6:F:209:GLU:OE1 | 8:H:210:LYS:NZ | 2.36 | 0.55 |
| 1:A:241:LEU:HD13 | 3:C:328:VAL:HG22 | 1.88 | 0.55 |
| 6:F:338:LEU:HD12 | 8:H:304:SER:CB | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:528:VAL:HG12 | 4:D:528:VAL:O | 2.07 | 0.54 |
| 3:C:129:ILE:HD13 | 4:D:489:LEU:HD11 | 1.89 | 0.54 |
| 3:C:259:GLU:HG3 | 4:D:604:LEU:HD21 | 1.88 | 0.54 |
| 2:B:588:GLU:CD | 4:D:650:ARG:HH21 | 2.11 | 0.54 |
| 3:C:239:ALA:HB1 | 4:D:586:LEU:HD11 | 1.90 | 0.54 |
| 5:E:181:GLU:CG | 7:G:335:ARG:NH1 | 2.66 | 0.54 |
| 6:F:157:LEU:CA | 6:F:170:ARG:HH22 | 2.20 | 0.54 |
| 2:B:121:LEU:HD12 | 3:C:172:PHE:CE2 | 2.43 | 0.54 |
| 6:F:23:LEU:O | 6:F:66:LYS:HE3 | 2.08 | 0.54 |
| 3:C:116:LEU:HD12 | 3:C:137:LEU:HD11 | 1.83 | 0.54 |
| 4:D:291:ILE:O | 4:D:292:THR:C | 2.45 | 0.54 |
| 5:E:141:PHE:HB2 | 7:G:289:PHE:HZ | 1.73 | 0.54 |
| 6:F:157:LEU:HG | 6:F:170:ARG:NH2 | 2.22 | 0.54 |
| 8:H:257:THR:O | 8:H:300:GLU:OE1 | 2.26 | 0.54 |
| 1:A:278:PRO:HB3 | 1:A:279:GLU:CG | 2.09 | 0.54 |
| 3:C:5:LEU:HD12 | 3:C:22:LEU:HD11 | 1.85 | 0.54 |
| 6:F:92:ARG:NH1 | 6:F:119:LEU:CA | 2.70 | 0.54 |
| 6:F:170:ARG:NE | 7:G:89:MET:HG3 | 2.23 | 0.54 |
| 7:G:7:LEU:O | 7:G:11:VAL:HG23 | 2.07 | 0.54 |
| 7:G:142:VAL:HG13 | 8:H:163:ILE:CD1 | 2.38 | 0.54 |
| 1:A:64:ALA:HB1 | 4:D:492:VAL:HG11 | 1.88 | 0.54 |
| 1:A:277:VAL:HG12 | 1:A:278:PRO:CA | 2.36 | 0.54 |
| 2:B:42:TRP:CD2 | 4:D:20:LEU:CD1 | 2.90 | 0.54 |
| 2:B:121:LEU:HD12 | 3:C:172:PHE:HE2 | 1.73 | 0.54 |
| 7:G:16:ARG:NH2 | 7:G:120:GLN:OE1 | 2.40 | 0.54 |
| 2:B:77:LEU:HD23 | 2:B:81:LEU:CD1 | 2.37 | 0.54 |
| 3:C:95:GLU:HB3 | 3:C:153:ARG:HH12 | 1.73 | 0.54 |
| 7:G:131:LEU:C | 7:G:132:GLU:O | 2.46 | 0.54 |
| 2:B:536:LEU:CD2 | 3:C:261:LYS:CD | 2.86 | 0.54 |
| 4:D:122:GLU:CG | 4:D:512:ASN:HD21 | 2.15 | 0.54 |
| 5:E:49:LEU:HD23 | 8:H:196:ASN:HB3 | 1.90 | 0.54 |
| 3:C:115:LEU:HD23 | 4:D:490:LEU:HG | 1.89 | 0.53 |
| 3:C:121:VAL:HG13 | 3:C:122:PRO:HD2 | 1.89 | 0.53 |
| 4:D:263:GLN:HA | 4:D:266:LYS:HD2 | 1.90 | 0.53 |
| 5:E:10:VAL:HG13 | 6:F:193:GLN:OE1 | 2.07 | 0.53 |
| 5:E:75:THR:O | 5:E:79:THR:OG1 | 2.13 | 0.53 |
| 5:E:17:LEU:HD13 | 7:G:161:HIS:CE1 | 2.43 | 0.53 |
| 5:E:102:LEU:HD23 | 7:G:255:ILE:HD12 | 1.86 | 0.53 |
| 5:E:141:PHE:CB | 7:G:289:PHE:HZ | 2.20 | 0.53 |
| 3:C:63:ARG:NH1 | 4:D:535:ALA:CB | 2.70 | 0.53 |
| 4:D:305:PRO:C | 4:D:307:GLU:N | 2.52 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:335:ARG:NE | 8:H:259:HIS:HB3 | 2.12 | 0.53 |
| 7:G:59:TYR:CD1 | 7:G:62:VAL:CG2 | 2.66 | 0.53 |
| 6:F:283:LEU:HD23 | 6:F:321:LEU:HD13 | 1.91 | 0.53 |
| 7:G:150:GLU:HG2 | 8:H:166:GLN:NE2 | 2.24 | 0.53 |
| 1:A:244:ASN:OD1 | 1:A:245:PRO:HD2 | 2.08 | 0.53 |
| 2:B:264:LEU:CD1 | 6:F:381:TRP:CH2 | 2.87 | 0.53 |
| 2:B:347:MET:HG3 | 4:D:406:LEU:CD1 | 2.38 | 0.53 |
| 3:C:224:TYR:N | 3:C:225:PRO:HD2 | 2.23 | 0.53 |
| 4:D:63:LEU:O | 4:D:67:GLN:HB2 | 2.09 | 0.53 |
| 2:B:41:ASP:O | 2:B:45:SER:OG | 2.25 | 0.53 |
| 2:B:347:MET:HE2 | 4:D:403:MET:SD | 2.48 | 0.53 |
| 6:F:206:MET:HE2 | 8:H:199:LYS:CG | 2.29 | 0.53 |
| 4:D:317:GLN:HG3 | 8:H:334:PHE:HB2 | 1.91 | 0.53 |
| 7:G:274:MET:HE3 | 8:H:280:GLN:H | 1.74 | 0.53 |
| 1:A:55:LEU:HD22 | 3:C:59:LEU:HD22 | 1.90 | 0.53 |
| 1:A:152:LYS:NZ | 2:B:73:ASP:OD1 | 2.40 | 0.53 |
| 2:B:213:LEU:HD22 | 2:B:374:HIS:CD2 | 2.44 | 0.53 |
| 2:B:504:LEU:HD11 | 3:C:231:CYS:HB3 | 1.91 | 0.53 |
| 3:C:121:VAL:HG12 | 3:C:122:PRO:HD2 | 1.90 | 0.53 |
| 4:D:307:GLU:OE1 | 7:G:324:ILE:CD1 | 2.53 | 0.53 |
| 4:D:348:ILE:HD11 | 4:D:373:LEU:HD21 | 1.91 | 0.53 |
| 6:F:240:MET:HE1 | 8:H:230:ASP:OD1 | 2.09 | 0.53 |
| 6:F:326:ARG:NH1 | 8:H:295:PRO:HG3 | 2.24 | 0.53 |
| 4:D:572:GLN:O | 4:D:575:THR:OG1 | 2.26 | 0.52 |
| 1:A:152:LYS:CE | 2:B:73:ASP:OD1 | 2.57 | 0.52 |
| 1:A:280:PRO:CA | 1:A:281:SER:N | 2.67 | 0.52 |
| 2:B:573:PHE:O | 4:D:639:ARG:HD2 | 2.08 | 0.52 |
| 6:F:44:GLY:O | 6:F:47:MET:CE | 2.57 | 0.52 |
| 7:G:345:SER:O | 7:G:348:ASP:HB2 | 2.09 | 0.52 |
| 1:A:48:LEU:HD22 | 3:C:52:LEU:HD22 | 1.90 | 0.52 |
| 4:D:651:TRP:O | 4:D:655:VAL:HG23 | 2.08 | 0.52 |
| 6:F:53:LYS:HE2 | 6:F:57:TYR:CZ | 2.38 | 0.52 |
| 2:B:19:GLY:HA2 | 2:B:22:LEU:HD12 | 1.92 | 0.52 |
| 2:B:482:MET:HE3 | 4:D:554:ARG:HE | 1.74 | 0.52 |
| 2:B:490:GLU:HG2 | 4:D:560:ARG:NH2 | 2.19 | 0.52 |
| 5:E:9:PRO:HA | 6:F:197:GLN:HE22 | 1.74 | 0.52 |
| 6:F:6:ARG:C | 6:F:8:HIS:H | 2.12 | 0.52 |
| 1:A:241:LEU:CD2 | 1:A:248:VAL:HG13 | 2.39 | 0.52 |
| 2:B:222:PHE:HD1 | 2:B:241:LEU:HD13 | 1.55 | 0.52 |
| 3:C:141:LEU:CD2 | 3:C:147:VAL:HG21 | 2.38 | 0.52 |
| 5:E:154:THR:HG21 | 7:G:299:THR:HG21 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:327:LEU:CD1 | 8:H:326:PHE:CD1 | 2.93 | 0.52 |
| 1:A:214:LEU:HB2 | 4:D:630:VAL:HG22 | 1.91 | 0.52 |
| 2:B:83:THR:HG22 | 3:C:220:GLN:HG2 | 1.91 | 0.52 |
| 2:B:178:PHE:HE1 | 2:B:396:HIS:CE1 | 2.28 | 0.52 |
| 5:E:87:LYS:HD3 | 6:F:241:TRP:CD2 | 2.44 | 0.52 |
| 7:G:146:ILE:HG12 | 8:H:163:ILE:CG1 | 2.40 | 0.52 |
| 4:D:175:PHE:CD1 | 4:D:193:LEU:HD13 | 2.44 | 0.52 |
| 1:A:148:LEU:HD11 | 2:B:80:VAL:CG2 | 2.28 | 0.52 |
| 1:A:171:LYS:CE | 1:A:175:ARG:NH2 | 2.72 | 0.52 |
| 2:B:90:PRO:O | 2:B:92:ILE:N | 2.43 | 0.52 |
| 2:B:195:SER:HA | 2:B:389:TYR:HE1 | 1.74 | 0.52 |
| 2:B:289:TRP:CZ2 | 2:B:293:ASN:ND2 | 2.76 | 0.52 |
| 4:D:352:HIS:CD2 | 4:D:366:ARG:NE | 2.71 | 0.52 |
| 6:F:28:GLY:HA2 | 6:F:38:LEU:CD1 | 2.40 | 0.52 |
| 8:H:241:ASP:HB2 | 8:H:242:PRO:HD3 | 1.92 | 0.52 |
| 2:B:454:ASP:O | 2:B:456:ASP:N | 2.39 | 0.52 |
| 4:D:175:PHE:CE1 | 4:D:193:LEU:HD13 | 2.45 | 0.52 |
| 6:F:168:LEU:HD11 | 7:G:145:CYS:SG | 2.50 | 0.52 |
| 6:F:377:ARG:NH2 | 8:H:343:GLN:CD | 2.60 | 0.52 |
| 2:B:95:VAL:HG12 | 2:B:100:LEU:HG | 1.93 | 0.51 |
| 2:B:349:ILE:CD1 | 4:D:316:ILE:HD12 | 2.40 | 0.51 |
| 3:C:303:GLU:OE2 | 3:C:303:GLU:CA | 2.58 | 0.51 |
| 4:D:80:GLU:HA | 4:D:83:GLN:OE1 | 2.10 | 0.51 |
| 6:F:335:ARG:HH22 | 8:H:259:HIS:HB2 | 0.78 | 0.51 |
| 1:A:145:THR:HG23 | 4:D:65:TRP:NE1 | 2.25 | 0.51 |
| 7:G:327:LEU:HD11 | 8:H:326:PHE:CG | 2.45 | 0.51 |
| 2:B:349:ILE:HD13 | 4:D:316:ILE:HD12 | 1.91 | 0.51 |
| 4:D:203:ARG:HH12 | 4:D:231:HIS:HD2 | 1.58 | 0.51 |
| 7:G:2:THR:HG21 | 7:G:37:TYR:CZ | 2.44 | 0.51 |
| 7:G:219:GLU:O | 7:G:222:VAL:HG23 | 2.10 | 0.51 |
| 2:B:7:PHE:CE1 | 2:B:11:LEU:HD11 | 2.45 | 0.51 |
| 2:B:251:THR:C | 2:B:253:GLU:N | 2.63 | 0.51 |
| 4:D:661:ALA:C | 4:D:663:GLY:H | 2.14 | 0.51 |
| 5:E:127:TYR:CD2 | 7:G:275:GLY:HA3 | 2.45 | 0.51 |
| 1:A:271:ASN:O | 1:A:273:MET:N | 2.44 | 0.51 |
| 6:F:51:PRO:HA | 6:F:121:PRO:O | 2.11 | 0.51 |
| 2:B:36:LEU:HD21 | 4:D:34:LEU:CG | 2.41 | 0.51 |
| 2:B:358:MET:O | 2:B:362:THR:HG23 | 2.11 | 0.51 |
| 6:F:166:LYS:CE | 7:G:84:LEU:HD12 | 2.40 | 0.51 |
| 2:B:80:VAL:HG11 | 4:D:65:TRP:CE2 | 2.45 | 0.51 |
| 4:D:4:ARG:CG | 4:D:32:GLN:HE21 | 2.21 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:63:ARG:CZ | 4:D:535:ALA:HB1 | 2.37 | 0.51 |
| 4:D:296:SER:HB3 | 4:D:301:THR:HG21 | 1.75 | 0.51 |
| 5:E:141:PHE:N | 7:G:289:PHE:HZ | 2.08 | 0.51 |
| 1:A:24:TYR:HB3 | 3:C:31:VAL:HG21 | 1.92 | 0.51 |
| 1:A:152:LYS:HE3 | 2:B:73:ASP:OD1 | 2.12 | 0.51 |
| 2:B:259:MET:CE | 2:B:346:ASN:HB3 | 2.41 | 0.51 |
| 4:D:202:LEU:HD22 | 4:D:237:MET:HE1 | 1.94 | 0.50 |
| 4:D:266:LYS:HB3 | 4:D:270:PHE:CZ | 2.45 | 0.50 |
| 2:B:84:PHE:CE2 | 4:D:65:TRP:HZ3 | 2.23 | 0.50 |
| 3:C:128:SER:OG | 3:C:132:LEU:O | 2.12 | 0.50 |
| 4:D:216:SER:C | 4:D:218:SER:H | 2.14 | 0.50 |
| 6:F:234:ILE:HD11 | 8:H:222:LEU:HD21 | 1.93 | 0.50 |
| 2:B:430:LEU:O | 2:B:431:SER:O | 2.30 | 0.50 |
| 5:E:219:ASN:O | 5:E:221:HIS:N | 2.45 | 0.50 |
| 6:F:260:ALA:CB | 8:H:258:ARG:HH11 | 2.13 | 0.50 |
| 2:B:37:LYS:N | 2:B:38:PRO:CD | 2.75 | 0.50 |
| 3:C:351:SER:C | 3:C:353:PRO:HD2 | 2.32 | 0.50 |
| 6:F:192:TYR:CD2 | 8:H:188:ALA:HB1 | 2.47 | 0.50 |
| 7:G:81:ILE:CG2 | 7:G:99:ILE:HD12 | 2.42 | 0.50 |
| 7:G:93:PHE:CE2 | 7:G:94:ASP:CG | 2.85 | 0.50 |
| 3:C:92:LEU:HD23 | 3:C:97:ARG:N | 2.27 | 0.50 |
| 6:F:260:ALA:HB3 | 8:H:258:ARG:HH11 | 1.69 | 0.50 |
| 1:A:171:LYS:HE2 | 1:A:175:ARG:CZ | 2.40 | 0.50 |
| 2:B:407:VAL:HB | 4:D:459:TRP:HZ3 | 1.77 | 0.50 |
| 4:D:192:VAL:HG22 | 4:D:245:HIS:ND1 | 2.27 | 0.50 |
| 4:D:8:GLN:CG | 4:D:28:GLU:OE1 | 2.44 | 0.49 |
| 7:G:30:LEU:HD22 | 7:G:35:SER:HB3 | 1.93 | 0.49 |
| 2:B:402:GLU:CD | 4:D:158:ARG:NH2 | 2.65 | 0.49 |
| 4:D:525:TYR:OH | 4:D:536:PRO:HA | 2.13 | 0.49 |
| 5:E:79:THR:HG21 | 8:H:222:LEU:CD1 | 2.42 | 0.49 |
| 1:A:278:PRO:CG | 1:A:279:GLU:CG | 2.82 | 0.49 |
| 2:B:243:VAL:HG12 | 2:B:243:VAL:O | 2.12 | 0.49 |
| 2:B:511:MET:C | 2:B:513:PRO:HD3 | 2.33 | 0.49 |
| 3:C:324:PHE:O | 3:C:328:VAL:HG23 | 2.13 | 0.49 |
| 7:G:62:VAL:O | 7:G:66:LEU:HD12 | 2.12 | 0.49 |
| 7:G:124:THR:CG2 | 7:G:125:ILE:HG13 | 2.28 | 0.49 |
| 6:F:251:MET:HE3 | 8:H:247:TYR:CD1 | 2.47 | 0.49 |
| 1:A:227:GLN:HB3 | 3:C:307:LEU:HD11 | 1.93 | 0.49 |
| 4:D:4:ARG:HA | 4:D:32:GLN:HE21 | 1.78 | 0.49 |
| 2:B:95:VAL:CG1 | 2:B:100:LEU:HG | 2.43 | 0.49 |
| 2:B:264:LEU:HD13 | 6:F:381:TRP:CZ2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:594:LEU:O | 4:D:599:PRO:HD3 | 2.13 | 0.49 |
| 1:A:1:MET:CE | 1:A:28:THR:CG2 | 2.86 | 0.49 |
| 1:A:207:GLU:N | 1:A:208:PRO:HD2 | 2.27 | 0.49 |
| 2:B:264:LEU:HD13 | 6:F:381:TRP:HH2 | 1.69 | 0.49 |
| 3:C:86:ARG:HB2 | 3:C:92:LEU:CD1 | 2.43 | 0.49 |
| 5:E:49:LEU:CD2 | 8:H:196:ASN:HD22 | 2.11 | 0.49 |
| 1:A:71:ASP:CA | 3:C:114:ARG:HH21 | 2.25 | 0.49 |
| 2:B:84:PHE:CE2 | 4:D:65:TRP:HE3 | 2.25 | 0.49 |
| 2:B:271:HIS:CE1 | 8:H:360:TRP:CE2 | 3.01 | 0.49 |
| 2:B:385:LEU:HD12 | 4:D:254:LEU:HD13 | 1.94 | 0.49 |
| 5:E:42:CYS:SG | 6:F:187:LEU:CD2 | 3.00 | 0.49 |
| 5:E:190:ARG:NH1 | 6:F:370:ILE:CG1 | 2.76 | 0.49 |
| 2:B:221:PHE:CZ | 2:B:367:ARG:HB2 | 2.48 | 0.49 |
| 2:B:587:LEU:HD23 | 4:D:654:ALA:CB | 2.42 | 0.49 |
| 7:G:14:TYR:HB2 | 7:G:36:ILE:HG21 | 1.94 | 0.49 |
| 7:G:124:THR:HG22 | 7:G:125:ILE:N | 2.26 | 0.49 |
| 7:G:178:LYS:N | 7:G:179:PRO:CD | 2.76 | 0.49 |
| 7:G:294:SER:OG | 8:H:305:PHE:HB2 | 2.13 | 0.49 |
| 2:B:37:LYS:N | 2:B:38:PRO:HD2 | 2.28 | 0.48 |
| 2:B:402:GLU:HB2 | 4:D:158:ARG:HH12 | 1.78 | 0.48 |
| 2:B:500:LEU:CD2 | 4:D:571:LEU:HD11 | 2.43 | 0.48 |
| 3:C:63:ARG:NH1 | 4:D:537:GLU:CD | 2.66 | 0.48 |
| 4:D:575:THR:O | 4:D:577:PRO:C | 2.51 | 0.48 |
| 5:E:135:LEU:CB | 5:E:136:PRO:HD3 | 2.33 | 0.48 |
| 2:B:36:LEU:HD21 | 4:D:34:LEU:HG | 1.95 | 0.48 |
| 5:E:190:ARG:CZ | 6:F:370:ILE:CG1 | 2.91 | 0.48 |
| 3:C:218:GLU:OE1 | 4:D:556:GLN:HG3 | 2.13 | 0.48 |
| 6:F:335:ARG:HH22 | 8:H:259:HIS:CD2 | 2.21 | 0.48 |
| 2:B:93:GLU:O | 2:B:94:GLU:C | 2.50 | 0.48 |
| 4:D:590:TYR:CE1 | 4:D:594:LEU:HD11 | 2.48 | 0.48 |
| 5:E:221:HIS:CB | 5:E:222:PRO:O | 2.60 | 0.48 |
| 1:A:189:TYR:CG | 3:C:271:MET:CE | 2.92 | 0.48 |
| 3:C:36:CYS:N | 3:C:37:PRO:HD2 | 2.28 | 0.48 |
| 5:E:38:LEU:HD11 | 6:F:180:LYS:HD3 | 1.95 | 0.48 |
| 1:A:145:THR:OG1 | 4:D:65:TRP:CH2 | 2.63 | 0.48 |
| 1:A:211:HIS:O | 1:A:215:VAL:HG23 | 2.14 | 0.48 |
| 2:B:83:THR:CG2 | 3:C:220:GLN:HG2 | 2.44 | 0.48 |
| 2:B:225:MET:O | 2:B:226:SER:C | 2.50 | 0.48 |
| 2:B:467:GLY:O | 2:B:471:VAL:HG23 | 2.13 | 0.48 |
| 4:D:528:VAL:HG12 | 4:D:546:MET:SD | 2.53 | 0.48 |
| 5:E:121:LEU:HD23 | 8:H:276:LEU:HD11 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:227:ILE:CB | 8:H:223:ARG:HH22 | 2.27 | 0.48 |
| 7:G:274:MET:CE | 8:H:280:GLN:N | 2.74 | 0.48 |
| 4:D:213:ASP:OD2 | 4:D:227:ARG:NH2 | 2.41 | 0.48 |
| 1:A:150:LEU:CD2 | 2:B:504:LEU:HD21 | 2.43 | 0.48 |
| 2:B:35:ASP:HB3 | 4:D:30:MET:SD | 2.53 | 0.48 |
| 5:E:158:ILE:CD1 | 6:F:334:VAL:HG11 | 2.44 | 0.48 |
| 6:F:166:LYS:HE3 | 7:G:84:LEU:CD1 | 2.44 | 0.48 |
| 4:D:293:GLN:CD | 4:D:294:SER:H | 2.17 | 0.48 |
| 6:F:60:PHE:HE1 | 6:F:99:LEU:CD1 | 2.24 | 0.48 |
| 2:B:347:MET:CE | 4:D:403:MET:SD | 3.02 | 0.47 |
| 6:F:16:MET:SD | 6:F:130:LEU:CD2 | 3.02 | 0.47 |
| 1:A:148:LEU:CD1 | 2:B:80:VAL:HG21 | 2.24 | 0.47 |
| 2:B:80:VAL:O | 2:B:83:THR:OG1 | 2.21 | 0.47 |
| 2:B:86:ILE:HG22 | 2:B:86:ILE:O | 2.14 | 0.47 |
| 2:B:263:GLN:HE21 | 2:B:346:ASN:ND2 | 2.06 | 0.47 |
| 2:B:454:ASP:C | 2:B:456:ASP:H | 2.17 | 0.47 |
| 5:E:28:LEU:HD11 | 6:F:179:LEU:HD21 | 1.96 | 0.47 |
| 7:G:239:ARG:HG3 | 8:H:232:VAL:CG2 | 2.39 | 0.47 |
| 1:A:40:TRP:CH2 | 3:C:43:GLY:HA3 | 2.48 | 0.47 |
| 2:B:89:VAL:O | 2:B:90:PRO:C | 2.49 | 0.47 |
| 7:G:274:MET:SD | 8:H:280:GLN:CB | 2.99 | 0.47 |
| 2:B:95:VAL:HA | 2:B:99:LYS:HD2 | 1.96 | 0.47 |
| 2:B:266:TYR:CD2 | 2:B:345:LEU:HD11 | 2.49 | 0.47 |
| 2:B:493:HIS:CE1 | 2:B:497:LEU:HD11 | 2.49 | 0.47 |
| 4:D:257:LEU:HA | 4:D:260:ASN:ND2 | 2.29 | 0.47 |
| 1:A:211:HIS:HB3 | 4:D:629:PRO:HG2 | 1.96 | 0.47 |
| 7:G:123:ASP:C | 7:G:124:THR:O | 2.53 | 0.47 |
| 1:A:124:VAL:HG21 | 2:B:110:GLN:HE22 | 1.78 | 0.47 |
| 1:A:137:LEU:HD21 | 3:C:217:LEU:N | 2.29 | 0.47 |
| 2:B:457:ASN:O | 2:B:459:GLN:N | 2.48 | 0.47 |
| 4:D:206:PHE:HD2 | 4:D:230:SER:HG | 1.59 | 0.47 |
| 5:E:19:LEU:HD21 | 6:F:182:LEU:HD23 | 1.96 | 0.47 |
| 6:F:277:THR:HA | 6:F:301:TYR:OH | 2.14 | 0.47 |
| 6:F:283:LEU:CD2 | 6:F:321:LEU:HD13 | 2.44 | 0.47 |
| 6:F:389:LEU:HD11 | 8:H:362:PHE:CE2 | 2.49 | 0.47 |
| 3:C:99:PHE:CE1 | 3:C:157:GLN:OE1 | 2.67 | 0.47 |
| 3:C:146:LEU:O | 3:C:150:VAL:HG23 | 2.15 | 0.47 |
| 3:C:227:VAL:HG22 | 3:C:230:ARG:NH2 | 2.20 | 0.47 |
| 3:C:280:CYS:HB2 | 4:D:625:TRP:CD1 | 2.48 | 0.47 |
| 4:D:355:LEU:O | 4:D:362:SER:HB3 | 2.15 | 0.47 |
| 5:E:178:GLU:OE2 | 7:G:331:MET:HE3 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:9:LEU:HD22 | 6:F:124:PRO:CA | 2.45 | 0.47 |
| 6:F:47:MET:HG3 | 6:F:48:PHE:CD2 | 2.50 | 0.47 |
| 6:F:309:ILE:HG23 | 8:H:282:HIS:CD2 | 2.49 | 0.47 |
| 6:F:359:ARG:HG2 | 8:H:328:GLN:OE1 | 2.05 | 0.47 |
| 1:A:284:ARG:O | 1:A:285:LEU:N | 2.38 | 0.47 |
| 3:C:12:LEU:HD13 | 3:C:15:LEU:CD1 | 2.45 | 0.47 |
| 5:E:189:TRP:CE3 | 8:H:340:ILE:HD11 | 2.50 | 0.47 |
| 1:A:99:CYS:HB2 | 3:C:67:MET:HE2 | 1.96 | 0.47 |
| 1:A:242:ALA:C | 1:A:244:ASN:H | 2.19 | 0.47 |
| 2:B:97:ILE:CD1 | 4:D:82:GLN:HG2 | 2.42 | 0.47 |
| 2:B:577:GLU:OE1 | 4:D:640:GLY:HA2 | 2.15 | 0.47 |
| 5:E:121:LEU:HD23 | 8:H:276:LEU:HD21 | 1.97 | 0.47 |
| 1:A:123:LEU:O | 1:A:126:ILE:HG22 | 2.15 | 0.47 |
| 4:D:46:ILE:CG2 | 4:D:50:ILE:HD12 | 2.38 | 0.47 |
| 6:F:261:VAL:HG22 | 8:H:258:ARG:HD2 | 1.96 | 0.47 |
| 6:F:297:MET:HE3 | 6:F:314:LEU:HG | 1.97 | 0.47 |
| 7:G:13:LEU:HD11 | 7:G:109:ILE:HG23 | 1.96 | 0.47 |
| 7:G:13:LEU:HD22 | 7:G:116:LEU:HD12 | 1.97 | 0.47 |
| 2:B:365:SER:HB2 | 4:D:423:LYS:HZ2 | 1.80 | 0.46 |
| 4:D:595:ASP:O | 4:D:599:PRO:HG2 | 2.15 | 0.46 |
| 5:E:181:GLU:HG2 | 7:G:335:ARG:HH12 | 1.77 | 0.46 |
| 1:A:192:LYS:HD2 | 3:C:271:MET:SD | 2.55 | 0.46 |
| 2:B:199:LEU:H | 2:B:199:LEU:HG | 1.43 | 0.46 |
| 2:B:273:LEU:HD13 | 4:D:330:LEU:HA | 1.98 | 0.46 |
| 4:D:307:GLU:HB3 | 7:G:318:LYS:HE3 | 1.97 | 0.46 |
| 4:D:509:ARG:CD | 4:D:521:PHE:CZ | 2.98 | 0.46 |
| 5:E:21:LYS:HZ2 | 7:G:159:SER:HA | 1.80 | 0.46 |
| 5:E:155:ILE:N | 5:E:156:PRO:CD | 2.78 | 0.46 |
| 6:F:5:SER:O | 6:F:7:PRO:HD3 | 2.15 | 0.46 |
| 7:G:139:GLU:HG3 | 8:H:155:VAL:CG2 | 2.40 | 0.46 |
| 2:B:383:GLU:OE2 | 4:D:203:ARG:CZ | 2.62 | 0.46 |
| 2:B:521:THR:HG23 | 3:C:247:GLN:CG | 2.44 | 0.46 |
| 6:F:288:ILE:CD1 | 6:F:314:LEU:CD2 | 2.93 | 0.46 |
| 5:E:69:LEU:HB3 | 7:G:217:LEU:CD2 | 2.46 | 0.46 |
| 6:F:156:ALA:C | 6:F:170:ARG:HH22 | 2.18 | 0.46 |
| 6:F:170:ARG:NH2 | 7:G:89:MET:SD | 2.82 | 0.46 |
| 1:A:121:SER:HB3 | 4:D:104:GLN:HE22 | 1.81 | 0.46 |
| 4:D:486:LEU:HB2 | 4:D:487:PRO:HD3 | 1.96 | 0.46 |
| 5:E:137:LEU:CD2 | 7:G:285:LEU:HD23 | 2.44 | 0.46 |
| 6:F:359:ARG:NE | 8:H:321:GLU:OE1 | 2.47 | 0.46 |
| 3:C:67:MET:O | 3:C:71:VAL:HG23 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:6:ARG:HD3 | 6:F:8:HIS:HD2 | 1.81 | 0.46 |
| 6:F:166:LYS:HE2 | 7:G:84:LEU:HD12 | 1.98 | 0.46 |
| 6:F:251:MET:HE1 | 8:H:243:PHE:CE1 | 2.50 | 0.46 |
| 2:B:74:GLU:OE1 | 4:D:54:ARG:CG | 2.56 | 0.46 |
| 3:C:86:ARG:HB3 | 3:C:92:LEU:HD12 | 1.97 | 0.46 |
| 4:D:459:TRP:N | 4:D:460:PRO:CD | 2.78 | 0.46 |
| 7:G:14:TYR:HB2 | 7:G:36:ILE:HG23 | 1.98 | 0.46 |
| 2:B:134:LYS:CD | 3:C:85:VAL:CG1 | 2.84 | 0.46 |
| 3:C:170:LEU:HD22 | 3:C:189:VAL:HG23 | 1.97 | 0.46 |
| 6:F:138:MET:HE2 | 8:H:172:TYR:CG | 2.51 | 0.46 |
| 2:B:357:GLN:O | 2:B:361:GLN:HG3 | 2.16 | 0.46 |
| 6:F:377:ARG:HH22 | 8:H:343:GLN:NE2 | 2.12 | 0.46 |
| 6:F:170:ARG:NE | 7:G:89:MET:SD | 2.81 | 0.46 |
| 6:F:301:TYR:CE1 | 6:F:306:VAL:HG22 | 2.51 | 0.46 |
| 2:B:330:SER:O | 2:B:335:PRO:HD3 | 2.16 | 0.45 |
| 2:B:339:ARG:CZ | 8:H:363:ASP:O | 2.64 | 0.45 |
| 2:B:458:THR:C | 2:B:460:LYS:N | 2.69 | 0.45 |
| 3:C:177:THR:HG22 | 3:C:188:LYS:HZ2 | 1.81 | 0.45 |
| 4:D:352:HIS:CB | 4:D:366:ARG:NH2 | 2.37 | 0.45 |
| 6:F:330:ASP:OD1 | 6:F:334:VAL:HG23 | 2.16 | 0.45 |
| 7:G:93:PHE:CD2 | 7:G:94:ASP:OD1 | 2.68 | 0.45 |
| 7:G:274:MET:CE | 8:H:280:GLN:H | 2.29 | 0.45 |
| 1:A:40:TRP:CH2 | 3:C:43:GLY:CA | 2.99 | 0.45 |
| 1:A:71:ASP:CA | 3:C:114:ARG:NH2 | 2.78 | 0.45 |
| 2:B:407:VAL:HG23 | 4:D:459:TRP:CZ3 | 2.50 | 0.45 |
| 3:C:28:PHE:CE1 | 3:C:32:LEU:HD11 | 2.52 | 0.45 |
| 7:G:2:THR:CG2 | 7:G:37:TYR:CZ | 2.99 | 0.45 |
| 7:G:235:ILE:HD11 | 8:H:225:LEU:CD2 | 2.44 | 0.45 |
| 2:B:132:CYS:N | 4:D:119:LEU:HD11 | 2.32 | 0.45 |
| 2:B:465:TYR:HB3 | 4:D:520:ILE:HG21 | 1.99 | 0.45 |
| 3:C:129:ILE:HD11 | 4:D:489:LEU:CD1 | 2.46 | 0.45 |
| 3:C:140:LEU:HD11 | 4:D:136:ALA:HB2 | 1.98 | 0.45 |
| 4:D:46:ILE:HA | 4:D:50:ILE:HD12 | 1.98 | 0.45 |
| 5:E:121:LEU:HD22 | 8:H:276:LEU:HD21 | 1.94 | 0.45 |
| 7:G:146:ILE:CG1 | 8:H:163:ILE:HG13 | 2.47 | 0.45 |
| 1:A:33:ILE:CG2 | 3:C:15:LEU:HD22 | 2.43 | 0.45 |
| 1:A:152:LYS:CE | 2:B:73:ASP:CG | 2.83 | 0.45 |
| 1:A:238:TYR:OH | 3:C:325:GLU:OE1 | 2.33 | 0.45 |
| 2:B:97:ILE:CD1 | 4:D:82:GLN:OE1 | 2.63 | 0.45 |
| 4:D:272:GLN:O | 4:D:276:LEU:HG | 2.16 | 0.45 |
| 7:G:132:GLU:HB3 | 7:G:133:SER:H | 1.44 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:43:PHE:CZ | 4:D:46:ILE:CD1 | 2.97 | 0.45 |
| 2:B:449:LEU:HD23 | 2:B:468:LEU:HD21 | 1.97 | 0.45 |
| 4:D:355:LEU:HD22 | 4:D:365:THR:HB | 1.98 | 0.45 |
| 5:E:88:HIS:HB2 | 7:G:238:LEU:HD12 | 1.98 | 0.45 |
| 6:F:173:LEU:HD11 | 7:G:118:VAL:HG21 | 1.87 | 0.45 |
| 7:G:139:GLU:O | 7:G:143:VAL:HG23 | 2.16 | 0.45 |
| 7:G:162:PHE:O | 7:G:165:THR:OG1 | 2.35 | 0.45 |
| 7:G:178:LYS:HB3 | 7:G:179:PRO:HD3 | 1.99 | 0.45 |
| 2:B:131:MET:HE3 | 3:C:85:VAL:CG2 | 2.28 | 0.45 |
| 2:B:521:THR:CG2 | 3:C:247:GLN:HE21 | 2.30 | 0.45 |
| 4:D:171:ARG:O | 4:D:249:HIS:NE2 | 2.46 | 0.45 |
| 5:E:148:TYR:HB3 | 7:G:292:LEU:HD13 | 1.98 | 0.45 |
| 7:G:47:ARG:CZ | 7:G:101:GLY:HA2 | 2.46 | 0.45 |
| 8:H:156:PRO:C | 8:H:158:ASP:N | 2.70 | 0.45 |
| 6:F:377:ARG:NH1 | 8:H:343:GLN:N | 2.63 | 0.45 |
| 1:A:65:GLU:OE2 | 4:D:507:ILE:HD12 | 2.17 | 0.45 |
| 1:A:271:ASN:C | 1:A:273:MET:N | 2.69 | 0.45 |
| 2:B:95:VAL:HG13 | 2:B:99:LYS:CB | 2.45 | 0.45 |
| 6:F:170:ARG:HE | 7:G:89:MET:CE | 2.30 | 0.45 |
| 2:B:407:VAL:CG2 | 4:D:459:TRP:CE3 | 2.90 | 0.45 |
| 3:C:8:VAL:HG13 | 3:C:12:LEU:HD12 | 1.99 | 0.45 |
| 8:H:294:MET:SD | 8:H:298:ALA:CB | 3.05 | 0.45 |
| 1:A:99:CYS:CB | 3:C:67:MET:CE | 2.89 | 0.45 |
| 2:B:453:LEU:HB3 | 2:B:471:VAL:CG1 | 2.47 | 0.45 |
| 7:G:340:ALA:O | 7:G:344:SER:OG | 2.34 | 0.45 |
| 4:D:661:ALA:C | 4:D:663:GLY:N | 2.69 | 0.44 |
| 7:G:41:CYS:CA | 7:G:108:GLN:OE1 | 2.62 | 0.44 |
| 1:A:215:VAL:CG2 | 4:D:629:PRO:HB2 | 2.47 | 0.44 |
| 2:B:199:LEU:HD11 | 2:B:389:TYR:OH | 2.17 | 0.44 |
| 2:B:271:HIS:CE1 | 8:H:360:TRP:NE1 | 2.85 | 0.44 |
| 2:B:536:LEU:HD11 | 3:C:262:SER:HB2 | 1.98 | 0.44 |
| 6:F:261:VAL:CG2 | 8:H:254:LEU:HD23 | 2.45 | 0.44 |
| 1:A:1:MET:HE1 | 1:A:28:THR:CG2 | 2.45 | 0.44 |
| 2:B:406:ILE:CD1 | 4:D:155:ILE:HD11 | 2.47 | 0.44 |
| 6:F:64:PHE:CD1 | 6:F:98:TRP:CE3 | 3.05 | 0.44 |
| 6:F:170:ARG:NE | 7:G:89:MET:CG | 2.81 | 0.44 |
| 7:G:188:GLN:O | 7:G:192:THR:OG1 | 2.35 | 0.44 |
| 8:H:156:PRO:C | 8:H:158:ASP:H | 2.20 | 0.44 |
| 2:B:370:LEU:HD23 | 2:B:371:VAL:HG23 | 1.99 | 0.44 |
| 1:A:207:GLU:HB3 | 1:A:208:PRO:HD3 | 2.00 | 0.44 |
| 2:B:263:GLN:NE2 | 2:B:343:GLN:HA | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:352:HIS:HB3 | 4:D:366:ARG:CZ | 2.40 | 0.44 |
| 4:D:590:TYR:CE1 | 4:D:594:LEU:CD1 | 3.01 | 0.44 |
| 5:E:97:HIS:ND1 | 6:F:255:VAL:HG13 | 2.32 | 0.44 |
| 6:F:84:ASP:OD1 | 6:F:87:ARG:HD2 | 2.17 | 0.44 |
| 1:A:145:THR:HG23 | 4:D:65:TRP:HE1 | 1.82 | 0.44 |
| 2:B:319:THR:HG23 | 4:D:378:LEU:CD1 | 2.46 | 0.44 |
| 3:C:129:ILE:HD11 | 4:D:489:LEU:HD13 | 1.96 | 0.44 |
| 5:E:149:ILE:HG23 | 6:F:325:GLU:HG3 | 1.99 | 0.44 |
| 7:G:235:ILE:CD1 | 8:H:225:LEU:CD2 | 2.95 | 0.44 |
| 7:G:298:PHE:HB2 | 8:H:308:ILE:HD13 | 2.00 | 0.44 |
| 1:A:211:HIS:CG | 4:D:629:PRO:HD2 | 2.53 | 0.44 |
| 5:E:21:LYS:HZ3 | 7:G:159:SER:HA | 1.82 | 0.44 |
| 4:D:572:GLN:HA | 4:D:575:THR:OG1 | 2.18 | 0.44 |
| 5:E:94:MET:HG2 | 7:G:245:PHE:HE2 | 1.83 | 0.44 |
| 6:F:330:ASP:OD1 | 6:F:334:VAL:N | 2.50 | 0.44 |
| 1:A:95:ILE:HG13 | 3:C:166:CYS:SG | 2.58 | 0.43 |
| 1:A:175:ARG:NH1 | 3:C:254:ASN:OD1 | 2.44 | 0.43 |
| 1:A:281:SER:O | 1:A:282:LYS:C | 2.22 | 0.43 |
| 1:A:133:MET:SD | 3:C:217:LEU:CD2 | 3.05 | 0.43 |
| 2:B:447:HIS:ND1 | 2:B:463:ARG:HD2 | 2.33 | 0.43 |
| 2:B:456:ASP:O | 2:B:458:THR:N | 2.51 | 0.43 |
| 3:C:266:PHE:CD2 | 4:D:611:HIS:CD2 | 3.06 | 0.43 |
| 5:E:179:MET:CG | 8:H:329:ILE:HD12 | 2.48 | 0.43 |
| 7:G:124:THR:CG2 | 7:G:125:ILE:H | 2.20 | 0.43 |
| 1:A:1:MET:HE3 | 1:A:28:THR:CG2 | 2.46 | 0.43 |
| 3:C:4:THR:HG23 | 3:C:33:ILE:CD1 | 2.35 | 0.43 |
| 3:C:270:ARG:HD2 | 4:D:614:TYR:CZ | 2.53 | 0.43 |
| 3:C:285:LYS:HZ1 | 4:D:628:GLN:HE22 | 1.66 | 0.43 |
| 4:D:423:LYS:O | 4:D:427:ILE:HG13 | 2.19 | 0.43 |
| 6:F:288:ILE:HD11 | 6:F:314:LEU:HD23 | 1.97 | 0.43 |
| 2:B:220:HIS:CE1 | 4:D:272:GLN:HB3 | 2.53 | 0.43 |
| 2:B:388:GLY:HA3 | 4:D:242:TRP:CZ2 | 2.53 | 0.43 |
| 3:C:180:GLU:CD | 3:C:188:LYS:HZ2 | 2.22 | 0.43 |
| 6:F:166:LYS:HE3 | 7:G:84:LEU:HD12 | 2.01 | 0.43 |
| 6:F:241:TRP:HZ2 | 7:G:238:LEU:CD2 | 2.25 | 0.43 |
| 6:F:335:ARG:HH21 | 8:H:259:HIS:HA | 1.58 | 0.43 |
| 1:A:145:THR:CB | 4:D:69:LEU:HD11 | 2.47 | 0.43 |
| 2:B:80:VAL:HG11 | 4:D:65:TRP:CD2 | 2.54 | 0.43 |
| 2:B:431:SER:O | 2:B:433:SER:N | 2.51 | 0.43 |
| 2:B:540:ASN:O | 2:B:544:VAL:HG23 | 2.18 | 0.43 |
| 3:C:12:LEU:CB | 3:C:15:LEU:HD12 | 2.47 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:296:SER:CB | 4:D:301:THR:HG21 | 2.37 | 0.43 |
| 4:D:663:GLY:O | 4:D:665:ARG:N | 2.48 | 0.43 |
| 6:F:335:ARG:NH1 | 8:H:259:HIS:HB2 | 2.23 | 0.43 |
| 1:A:78:GLY:O | 1:A:81:TYR:CD1 | 2.68 | 0.43 |
| 2:B:81:LEU:HA | 2:B:84:PHE:HD2 | 1.83 | 0.43 |
| 4:D:17:GLU:OE2 | 4:D:17:GLU:HA | 2.18 | 0.43 |
| 4:D:352:HIS:CG | 4:D:366:ARG:CZ | 3.01 | 0.43 |
| 1:A:158:LEU:HD13 | 3:C:238:ALA:HB2 | 2.00 | 0.43 |
| 2:B:30:LEU:HD23 | 4:D:34:LEU:HD23 | 1.96 | 0.43 |
| 2:B:490:GLU:C | 4:D:560:ARG:NH2 | 2.59 | 0.43 |
| 6:F:170:ARG:HE | 7:G:89:MET:CG | 2.31 | 0.43 |
| 1:A:13:LYS:HG3 | 1:A:21:LEU:HD11 | 2.00 | 0.43 |
| 2:B:193:PHE:HB2 | 2:B:196:GLN:HG3 | 2.00 | 0.43 |
| 1:A:189:TYR:CA | 3:C:271:MET:CE | 2.92 | 0.43 |
| 1:A:270:VAL:O | 1:A:273:MET:HB2 | 2.19 | 0.43 |
| 2:B:125:GLU:CD | 4:D:113:GLU:OE2 | 2.46 | 0.43 |
| 2:B:55:ASP:OD2 | 4:D:49:HIS:CE1 | 2.71 | 0.42 |
| 2:B:322:ILE:HD13 | 4:D:379:ARG:HG3 | 2.00 | 0.42 |
| 2:B:432:ALA:C | 2:B:433:SER:O | 2.57 | 0.42 |
| 2:B:571:VAL:HG13 | 3:C:288:VAL:HG21 | 2.01 | 0.42 |
| 3:C:36:CYS:N | 3:C:37:PRO:CD | 2.82 | 0.42 |
| 4:D:10:LEU:HD11 | 4:D:43:TRP:CE3 | 2.54 | 0.42 |
| 4:D:206:PHE:HD2 | 4:D:230:SER:OG | 2.00 | 0.42 |
| 4:D:298:ASN:O | 4:D:299:GLU:CB | 2.49 | 0.42 |
| 4:D:457:LEU:O | 4:D:460:PRO:HD2 | 2.19 | 0.42 |
| 5:E:137:LEU:HD23 | 7:G:285:LEU:HB3 | 2.01 | 0.42 |
| 6:F:176:GLN:NE2 | 7:G:117:ASP:HB3 | 2.34 | 0.42 |
| 6:F:341:LEU:HD21 | 7:G:298:PHE:HE2 | 1.83 | 0.42 |
| 6:F:377:ARG:HH11 | 8:H:343:GLN:N | 2.17 | 0.42 |
| 7:G:9:ALA:HB3 | 7:G:109:ILE:HD13 | 2.01 | 0.42 |
| 5:E:166:ASP:OD1 | 6:F:344:LYS:HE3 | 2.18 | 0.42 |
| 6:F:6:ARG:HA | 6:F:7:PRO:HD2 | 1.50 | 0.42 |
| 6:F:165:GLN:NE2 | 7:G:60:PRO:HD2 | 2.34 | 0.42 |
| 6:F:192:TYR:CE1 | 7:G:172:PRO:HD3 | 2.55 | 0.42 |
| 7:G:60:PRO:N | 7:G:61:PRO:CD | 2.82 | 0.42 |
| 7:G:137:SER:C | 7:G:139:GLU:H | 2.22 | 0.42 |
| 7:G:173:TRP:HA | 7:G:174:PRO:HD3 | 1.83 | 0.42 |
| 3:C:118:ALA:O | 3:C:119:ASP:C | 2.48 | 0.42 |
| 3:C:280:CYS:CB | 4:D:625:TRP:HD1 | 2.31 | 0.42 |
| 4:D:76:ARG:HA | 4:D:79:GLU:OE2 | 2.19 | 0.42 |
| 5:E:145:LEU:HD22 | 6:F:284:LEU:HD13 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:280:PHE:CE1 | 8:H:287:LYS:CG | 2.82 | 0.42 |
| 2:B:120:LYS:HZ3 | 3:C:171:SER:C | 2.21 | 0.42 |
| 4:D:46:ILE:HG23 | 4:D:50:ILE:CD1 | 2.40 | 0.42 |
| 4:D:248:ASN:OD1 | 4:D:248:ASN:O | 2.36 | 0.42 |
| 4:D:285:LYS:HD3 | 4:D:287:PHE:CZ | 2.54 | 0.42 |
| 4:D:289:GLU:HA | 4:D:290:PRO:HD3 | 1.58 | 0.42 |
| 4:D:659:GLN:O | 4:D:664:SER:O | 2.37 | 0.42 |
| 6:F:157:LEU:HG | 6:F:170:ARG:HH21 | 1.84 | 0.42 |
| 8:H:358:ARG:HH21 | 8:H:366:LEU:HD13 | 1.82 | 0.42 |
| 1:A:8:ILE:HD12 | 1:A:31:MET:CE | 2.50 | 0.42 |
| 2:B:196:GLN:HG3 | 2:B:196:GLN:H | 1.66 | 0.42 |
| 2:B:500:LEU:CD2 | 4:D:571:LEU:CD1 | 2.85 | 0.42 |
| 4:D:419:LEU:HD23 | 4:D:420:LEU:HG | 2.01 | 0.42 |
| 4:D:525:TYR:CZ | 4:D:539:VAL:CG2 | 3.03 | 0.42 |
| 6:F:244:ILE:HD12 | 8:H:233:LEU:HD22 | 2.01 | 0.42 |
| 6:F:261:VAL:CG2 | 8:H:258:ARG:HD2 | 2.50 | 0.42 |
| 1:A:172:VAL:HG21 | 3:C:250:ILE:HG23 | 2.01 | 0.42 |
| 2:B:213:LEU:HD22 | 2:B:374:HIS:NE2 | 2.35 | 0.42 |
| 2:B:570:TYR:HA | 4:D:644:LEU:HD11 | 2.02 | 0.42 |
| 3:C:75:LEU:CD1 | 3:C:162:LEU:HD23 | 2.45 | 0.42 |
| 4:D:75:GLN:O | 4:D:79:GLU:HG3 | 2.20 | 0.42 |
| 4:D:263:GLN:HB3 | 4:D:267:LYS:NZ | 2.34 | 0.42 |
| 4:D:237:MET:O | 4:D:241:VAL:HG23 | 2.19 | 0.42 |
| 4:D:268:LEU:HB3 | 4:D:272:GLN:NE2 | 2.32 | 0.42 |
| 5:E:58:GLU:HG2 | 7:G:207:LEU:HD11 | 2.02 | 0.42 |
| 7:G:135:SER:O | 7:G:136:HIS:C | 2.52 | 0.42 |
| 2:B:587:LEU:HD23 | 4:D:654:ALA:HB3 | 2.02 | 0.42 |
| 2:B:588:GLU:OE1 | 4:D:650:ARG:NE | 2.48 | 0.42 |
| 3:C:70:GLU:OE2 | 3:C:70:GLU:HA | 2.20 | 0.42 |
| 7:G:139:GLU:CG | 8:H:155:VAL:HG22 | 2.41 | 0.42 |
| 7:G:178:LYS:N | 7:G:179:PRO:HD2 | 2.34 | 0.42 |
| 1:A:193:ILE:HG23 | 3:C:274:LEU:HD12 | 2.02 | 0.42 |
| 1:A:266:LEU:HD21 | 3:C:344:MET:CE | 2.49 | 0.42 |
| 2:B:89:VAL:C | 2:B:90:PRO:O | 2.58 | 0.42 |
| 2:B:97:ILE:O | 2:B:101:GLU:HG3 | 2.19 | 0.42 |
| 2:B:347:MET:HB3 | 2:B:348:PRO:CD | 2.47 | 0.42 |
| 3:C:185:ARG:O | 3:C:189:VAL:HG23 | 2.20 | 0.42 |
| 3:C:285:LYS:NZ | 4:D:628:GLN:NE2 | 2.67 | 0.42 |
| 1:A:104:LEU:O | 3:C:63:ARG:NH2 | 2.47 | 0.42 |
| 2:B:274:ILE:CD1 | 4:D:392:LEU:HD11 | 2.50 | 0.42 |
| 7:G:176:ASP:OD1 | 7:G:176:ASP:N | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:183:ALA:HB1 | 7:G:187:LEU:HD12 | 2.02 | 0.42 |
| 2:B:450:TYR:HB3 | 2:B:463:ARG:NH1 | 2.35 | 0.41 |
| 4:D:6:LEU:HD11 | 4:D:44:LYS:HE3 | 2.01 | 0.41 |
| 5:E:78:ILE:HG13 | 5:E:79:THR:HG23 | 2.01 | 0.41 |
| 5:E:182:VAL:HG23 | 7:G:335:ARG:NH2 | 2.34 | 0.41 |
| 6:F:173:LEU:HD12 | 7:G:118:VAL:HG22 | 1.91 | 0.41 |
| 2:B:97:ILE:CD1 | 4:D:82:GLN:CB | 2.66 | 0.41 |
| 2:B:132:CYS:HA | 4:D:119:LEU:HD22 | 1.88 | 0.41 |
| 3:C:180:GLU:CD | 3:C:184:LEU:HD23 | 2.40 | 0.41 |
| 6:F:251:MET:CE | 8:H:247:TYR:CD1 | 3.03 | 0.41 |
| 2:B:570:TYR:CD1 | 4:D:631:GLN:HG2 | 2.55 | 0.41 |
| 6:F:84:ASP:OD1 | 6:F:87:ARG:CG | 2.68 | 0.41 |
| 7:G:40:LEU:O | 7:G:47:ARG:NH1 | 2.53 | 0.41 |
| 2:B:30:LEU:HD11 | 4:D:39:CYS:SG | 2.60 | 0.41 |
| 2:B:93:GLU:C | 2:B:94:GLU:O | 2.58 | 0.41 |
| 3:C:4:THR:O | 3:C:8:VAL:HG23 | 2.20 | 0.41 |
| 3:C:36:CYS:O | 3:C:39:LEU:O | 2.38 | 0.41 |
| 4:D:67:GLN:O | 4:D:71:HIS:HB2 | 2.20 | 0.41 |
| 5:E:179:MET:HG3 | 8:H:329:ILE:CD1 | 2.50 | 0.41 |
| 7:G:150:GLU:HG2 | 8:H:166:GLN:HE21 | 1.84 | 0.41 |
| 2:B:79:GLU:OE2 | 3:C:230:ARG:NH2 | 2.38 | 0.41 |
| 2:B:276:MET:CE | 4:D:334:GLN:HG2 | 2.51 | 0.41 |
| 3:C:12:LEU:HD13 | 3:C:15:LEU:HD12 | 2.02 | 0.41 |
| 3:C:285:LYS:NZ | 4:D:628:GLN:HE22 | 2.18 | 0.41 |
| 4:D:183:SER:HG | 4:D:184:SER:H | 1.63 | 0.41 |
| 6:F:168:LEU:HD12 | 7:G:145:CYS:SG | 2.60 | 0.41 |
| 4:D:215:ILE:HA | 4:D:422:LYS:CE | 2.51 | 0.41 |
| 6:F:166:LYS:HE2 | 7:G:87:ASP:HB2 | 2.02 | 0.41 |
| 2:B:85:SER:C | 2:B:87:SER:N | 2.73 | 0.41 |
| 2:B:160:LEU:HB2 | 4:D:145:CYS:SG | 2.61 | 0.41 |
| 3:C:142:PRO:CB | 3:C:146:LEU:HD23 | 2.50 | 0.41 |
| 4:D:259:LEU:O | 4:D:263:GLN:HG3 | 2.20 | 0.41 |
| 5:E:181:GLU:HG2 | 7:G:335:ARG:NH1 | 2.35 | 0.41 |
| 6:F:168:LEU:HD11 | 7:G:145:CYS:CB | 2.51 | 0.41 |
| 2:B:543:THR:OG1 | 3:C:269:LEU:HD12 | 2.20 | 0.41 |
| 4:D:215:ILE:HA | 4:D:422:LYS:HE2 | 2.01 | 0.41 |
| 4:D:260:ASN:HA | 4:D:263:GLN:OE1 | 2.21 | 0.41 |
| 4:D:525:TYR:CE2 | 4:D:539:VAL:HG21 | 2.55 | 0.41 |
| 6:F:173:LEU:HD11 | 7:G:118:VAL:CG2 | 2.45 | 0.41 |
| 1:A:236:ASN:HA | 1:A:239:LEU:HD12 | 2.02 | 0.41 |
| 2:B:35:ASP:HB2 | 4:D:30:MET:HE3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:301:ALA:O | 4:D:361:VAL:HG11 | 2.21 | 0.41 |
| 2:B:430:LEU:C | 2:B:431:SER:O | 2.58 | 0.41 |
| 4:D:34:LEU:O | 4:D:39:CYS:HB3 | 2.21 | 0.41 |
| 4:D:269:GLN:HG3 | 4:D:269:GLN:H | 1.75 | 0.41 |
| 5:E:134:LEU:HD22 | 7:G:278:PHE:HD1 | 1.85 | 0.41 |
| 5:E:179:MET:HG3 | 8:H:329:ILE:HD12 | 2.03 | 0.41 |
| 5:E:189:TRP:CZ3 | 8:H:336:VAL:HG12 | 2.50 | 0.41 |
| 1:A:211:HIS:ND1 | 4:D:630:VAL:HG23 | 2.36 | 0.40 |
| 2:B:482:MET:HE1 | 4:D:554:ARG:HG2 | 2.03 | 0.40 |
| 2:B:521:THR:HG23 | 3:C:247:GLN:HE21 | 1.86 | 0.40 |
| 5:E:207:CYS:O | 5:E:208:ILE:C | 2.58 | 0.40 |
| 6:F:84:ASP:OD1 | 6:F:87:ARG:HG3 | 2.21 | 0.40 |
| 7:G:166:LEU:O | 8:H:180:ASN:ND2 | 2.38 | 0.40 |
| 3:C:5:LEU:HD13 | 3:C:22:LEU:HD12 | 2.00 | 0.40 |
| 4:D:413:ILE:O | 4:D:417:CYS:N | 2.50 | 0.40 |
| 5:E:19:LEU:CD2 | 6:F:182:LEU:HD23 | 2.51 | 0.40 |
| 5:E:78:ILE:HD13 | 6:F:234:ILE:HG23 | 2.02 | 0.40 |
| 5:E:139:VAL:HG13 | 6:F:278:LEU:HD12 | 2.02 | 0.40 |
| 6:F:227:ILE:O | 6:F:227:ILE:CG2 | 2.68 | 0.40 |
| 1:A:144:LEU:HD13 | 3:C:224:TYR:HA | 2.04 | 0.40 |
| 1:A:145:THR:CG2 | 4:D:69:LEU:HD13 | 2.28 | 0.40 |
| 3:C:236:ARG:NH1 | 4:D:574:ASN:O | 2.54 | 0.40 |
| 4:D:117:GLN:O | 4:D:118:ASP:C | 2.54 | 0.40 |
| 7:G:274:MET:CE | 8:H:280:GLN:CA | 2.99 | 0.40 |
| 4:D:120:ASN:C | 4:D:122:GLU:H | 2.25 | 0.40 |
| 6:F:377:ARG:CZ | 8:H:343:GLN:CG | 2.94 | 0.40 |
| 7:G:318:LYS:HG3 | 7:G:324:ILE:HG12 | 2.02 | 0.40 |
| 1:A:41:ASN:ND2 | 3:C:39:LEU:CD2 | 2.85 | 0.40 |
| 2:B:78:ASP:O | 2:B:82:LYS:HG3 | 2.22 | 0.40 |
| 2:B:272:LYS:HE3 | 2:B:276:MET:HE2 | 2.03 | 0.40 |
| 2:B:368:GLN:OE1 | 4:D:423:LYS:HB2 | 2.21 | 0.40 |
| 2:B:482:MET:CE | 4:D:554:ARG:HG2 | 2.52 | 0.40 |
| 2:B:521:THR:HG23 | 3:C:247:GLN:NE2 | 2.37 | 0.40 |
| 4:D:291:ILE:HG22 | 4:D:292:THR:N | 2.37 | 0.40 |
| 7:G:146:ILE:CG1 | 8:H:163:ILE:CG1 | 3.00 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1 | A | 284/286 (99%) | 273 (96%) | 4 (1%) | 7 (2%) | 5 | 32 |
| 2 | B | 595/597 (100%) | 545 (92%) | 18 (3%) | 32 (5%) | 2 | 19 |
| 3 | C | 351/353 (99%) | 338 (96%) | 7 (2%) | 6 (2%) | 9 | 42 |
| 4 | D | 664/666 (100%) | 626 (94%) | 16 (2%) | 22 (3%) | 4 | 26 |
| 5 | E | 213/222 (96%) | 203 (95%) | 5 (2%) | 5 (2%) | 6 | 34 |
| 6 | F | 383/978 (39%) | 365 (95%) | 9 (2%) | 9 (2%) | 6 | 34 |
| 7 | G | 335/348 (96%) | 310 (92%) | 10 (3%) | 15 (4%) | 2 | 22 |
| 8 | H | 199/367 (54%) | 197 (99%) | 1 (0%) | 1 (0%) | 29 | 69 |
| All | All | 3024/3817 (79%) | 2857 (94%) | 70 (2%) | 97 (3%) | 7 | 26 |

All (97) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 272 | MET |
| 1 | A | 277 | VAL |
| 1 | A | 278 | PRO |
| 1 | A | 279 | GLU |
| 1 | A | 282 | LYS |
| 1 | A | 283 | ARG |
| 2 | B | 88 | LYS |
| 2 | B | 92 | ILE |
| 2 | B | 93 | GLU |
| 2 | B | 95 | VAL |
| 2 | B | 97 | ILE |
| 2 | B | 234 | GLU |
| 2 | B | 236 | PHE |
| 2 | B | 238 | LEU |
| 2 | B | 240 | GLN |
| 2 | B | 241 | LEU |
| 2 | B | 243 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 250 | GLY |
| 2 | B | 431 | SER |
| 2 | B | 432 | ALA |
| 2 | B | 457 | ASN |
| 2 | B | 459 | GLN |
| 2 | B | 594 | GLY |
| 3 | C | 118 | ALA |
| 3 | C | 119 | ASP |
| 3 | C | 122 | PRO |
| 3 | C | 124 | SER |
| 3 | C | 352 | LEU |
| 4 | D | 118 | ASP |
| 4 | D | 178 | VAL |
| 4 | D | 183 | SER |
| 4 | D | 186 | THR |
| 4 | D | 217 | SER |
| 4 | D | 219 | VAL |
| 4 | D | 284 | LEU |
| 4 | D | 304 | ASP |
| 4 | D | 305 | PRO |
| 4 | D | 306 | GLN |
| 4 | D | 308 | THR |
| 4 | D | 663 | GLY |
| 4 | D | 665 | ARG |
| 5 | E | 2 | MET |
| 5 | E | 3 | ALA |
| 6 | F | 5 | SER |
| 6 | F | 7 | PRO |
| 7 | G | 124 | THR |
| 7 | G | 130 | ILE |
| 7 | G | 132 | GLU |
| 7 | G | 134 | LEU |
| 7 | G | 138 | THR |
| 7 | G | 185 | GLU |
| 7 | G | 197 | GLY |
| 7 | G | 228 | VAL |
| 7 | G | 230 | ASP |
| 7 | G | 231 | GLY |
| 8 | H | 157 | GLU |
| 2 | B | 3 | GLY |
| 2 | B | 91 | ALA |
| 2 | B | 184 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 242 | ASN |
| 2 | B | 248 | GLU |
| 2 | B | 252 | THR |
| 2 | B | 455 | GLY |
| 2 | B | 592 | GLY |
| 4 | D | 119 | LEU |
| 4 | D | 286 | GLU |
| 4 | D | 299 | GLU |
| 5 | E | 4 | ALA |
| 5 | E | 220 | LEU |
| 6 | F | 2 | GLN |
| 6 | F | 296 | GLN |
| 7 | G | 123 | ASP |
| 1 | A | 243 | PRO |
| 2 | B | 94 | GLU |
| 2 | B | 187 | LEU |
| 4 | D | 221 | PRO |
| 4 | D | 292 | THR |
| 6 | F | 228 | SER |
| 6 | F | 337 | ASP |
| 7 | G | 2 | THR |
| 2 | B | 233 | ASP |
| 4 | D | 222 | GLY |
| 4 | D | 288 | SER |
| 7 | G | 122 | PRO |
| 7 | G | 125 | ILE |
| 4 | D | 290 | PRO |
| 5 | E | 5 | ASN |
| 6 | F | 148 | ALA |
| 6 | F | 333 | GLY |
| 2 | B | 181 | PRO |
| 2 | B | 239 | VAL |
| 2 | B | 89 | VAL |
| 2 | B | 90 | PRO |
| 3 | C | 123 | PRO |
| 7 | G | 273 | PRO |
| 4 | D | 280 | PRO |
| 6 | F | 6 | ARG |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 260/260 (100%) | 248 (95%) | 12 (5%) | 27 | 52 |
| 2 | B | 541/541 (100%) | 502 (93%) | 39 (7%) | 14 | 39 |
| 3 | C | 326/326 (100%) | 312 (96%) | 14 (4%) | 29 | 53 |
| 4 | D | 605/605 (100%) | 564 (93%) | 41 (7%) | 16 | 41 |
| 5 | E | 190/195 (97%) | 176 (93%) | 14 (7%) | 13 | 38 |
| 6 | F | 343/882 (39%) | 327 (95%) | 16 (5%) | 26 | 51 |
| 7 | G | 313/320 (98%) | 295 (94%) | 18 (6%) | 20 | 45 |
| 8 | H | 192/328 (58%) | 184 (96%) | 8 (4%) | 30 | 54 |
| All | All | 2770/3457 (80%) | 2608 (94%) | 162 (6%) | 24 | 45 |

All (162) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 21 | LEU |
| 1 | A | 28 | THR |
| 1 | A | 153 | SER |
| 1 | A | 200 | LEU |
| 1 | A | 217 | LEU |
| 1 | A | 218 | SER |
| 1 | A | 220 | THR |
| 1 | A | 224 | LEU |
| 1 | A | 239 | LEU |
| 1 | A | 246 | SER |
| 1 | A | 262 | THR |
| 1 | A | 268 | THR |
| 2 | B | 30 | LEU |
| 2 | B | 36 | LEU |
| 2 | B | 45 | SER |
| 2 | B | 48 | SER |
| 2 | B | 58 | LEU |
| 2 | B | 77 | LEU |
| 2 | B | 83 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 94 | GLU |
| 2 | B | 121 | LEU |
| 2 | B | 131 | MET |
| 2 | B | 179 | SER |
| 2 | B | 180 | THR |
| 2 | B | 183 | THR |
| 2 | B | 185 | CYS |
| 2 | B | 188 | SER |
| 2 | B | 194 | LEU |
| 2 | B | 196 | GLN |
| 2 | B | 198 | LEU |
| 2 | B | 199 | LEU |
| 2 | B | 200 | ASP |
| 2 | B | 225 | MET |
| 2 | B | 226 | SER |
| 2 | B | 228 | PHE |
| 2 | B | 238 | LEU |
| 2 | B | 246 | PHE |
| 2 | B | 251 | THR |
| 2 | B | 364 | CYS |
| 2 | B | 370 | LEU |
| 2 | B | 372 | CYS |
| 2 | B | 385 | LEU |
| 2 | B | 437 | SER |
| 2 | B | 456 | ASP |
| 2 | B | 491 | GLN |
| 2 | B | 495 | LEU |
| 2 | B | 507 | LEU |
| 2 | B | 536 | LEU |
| 2 | B | 547 | LEU |
| 2 | B | 550 | LEU |
| 2 | B | 591 | THR |
| 3 | C | 60 | LEU |
| 3 | C | 92 | LEU |
| 3 | C | 120 | SER |
| 3 | C | 141 | LEU |
| 3 | C | 158 | LEU |
| 3 | C | 176 | GLU |
| 3 | C | 218 | GLU |
| 3 | C | 269 | LEU |
| 3 | C | 303 | GLU |
| 3 | C | 309 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 314 | LEU |
| 3 | C | 315 | SER |
| 3 | C | 330 | GLU |
| 3 | C | 352 | LEU |
| 4 | D | 1 | MET |
| 4 | D | 64 | LEU |
| 4 | D | 69 | LEU |
| 4 | D | 72 | THR |
| 4 | D | 77 | THR |
| 4 | D | 83 | GLN |
| 4 | D | 122 | GLU |
| 4 | D | 164 | GLU |
| 4 | D | 174 | MET |
| 4 | D | 179 | ASP |
| 4 | D | 182 | LEU |
| 4 | D | 186 | THR |
| 4 | D | 188 | LEU |
| 4 | D | 202 | LEU |
| 4 | D | 214 | SER |
| 4 | D | 224 | GLU |
| 4 | D | 226 | LEU |
| 4 | D | 229 | LEU |
| 4 | D | 230 | SER |
| 4 | D | 235 | MET |
| 4 | D | 259 | LEU |
| 4 | D | 262 | THR |
| 4 | D | 265 | LEU |
| 4 | D | 293 | GLN |
| 4 | D | 302 | HIS |
| 4 | D | 359 | SER |
| 4 | D | 375 | CYS |
| 4 | D | 402 | GLU |
| 4 | D | 405 | LEU |
| 4 | D | 419 | LEU |
| 4 | D | 424 | GLN |
| 4 | D | 499 | LEU |
| 4 | D | 503 | ARG |
| 4 | D | 575 | THR |
| 4 | D | 579 | THR |
| 4 | D | 592 | LEU |
| 4 | D | 636 | SER |
| 4 | D | 648 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 658 | LEU |
| 4 | D | 662 | THR |
| 4 | D | 664 | SER |
| 5 | E | 9 | PRO |
| 5 | E | 18 | LEU |
| 5 | E | 28 | LEU |
| 5 | E | 38 | LEU |
| 5 | E | 69 | LEU |
| 5 | E | 70 | ARG |
| 5 | E | 121 | LEU |
| 5 | E | 206 | SER |
| 5 | E | 207 | CYS |
| 5 | E | 209 | THR |
| 5 | E | 212 | THR |
| 5 | E | 213 | SER |
| 5 | E | 220 | LEU |
| 5 | E | 221 | HIS |
| 6 | F | 3 | SER |
| 6 | F | 9 | LEU |
| 6 | F | 37 | THR |
| 6 | F | 38 | LEU |
| 6 | F | 114 | VAL |
| 6 | F | 173 | LEU |
| 6 | F | 187 | LEU |
| 6 | F | 219 | LEU |
| 6 | F | 224 | ASP |
| 6 | F | 278 | LEU |
| 6 | F | 283 | LEU |
| 6 | F | 293 | HIS |
| 6 | F | 325 | GLU |
| 6 | F | 331 | CYS |
| 6 | F | 338 | LEU |
| 6 | F | 360 | HIS |
| 7 | G | 2 | THR |
| 7 | G | 19 | MET |
| 7 | G | 31 | THR |
| 7 | G | 46 | HIS |
| 7 | G | 48 | LEU |
| 7 | G | 74 | THR |
| 7 | G | 124 | THR |
| 7 | G | 127 | SER |
| 7 | G | 134 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | G | 135 | SER |
| 7 | G | 138 | THR |
| 7 | G | 180 | LEU |
| 7 | G | 192 | THR |
| 7 | G | 226 | SER |
| 7 | G | 229 | THR |
| 7 | G | 230 | ASP |
| 7 | G | 322 | SER |
| 7 | G | 344 | SER |
| 8 | H | 202 | LEU |
| 8 | H | 204 | GLU |
| 8 | H | 213 | LEU |
| 8 | H | 216 | LEU |
| 8 | H | 254 | LEU |
| 8 | H | 356 | LEU |
| 8 | H | 363 | ASP |
| 8 | H | 367 | PRO |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 114 | HIS |
| 2 | B | 220 | HIS |
| 2 | B | 263 | GLN |
| 2 | B | 346 | ASN |
| 2 | B | 386 | GLN |
| 2 | B | 493 | HIS |
| 3 | C | 220 | GLN |
| 3 | C | 247 | GLN |
| 4 | D | 32 | GLN |
| 4 | D | 49 | HIS |
| 4 | D | 68 | GLN |
| 4 | D | 70 | GLN |
| 4 | D | 104 | GLN |
| 4 | D | 152 | ASN |
| 4 | D | 161 | GLN |
| 4 | D | 231 | HIS |
| 4 | D | 272 | GLN |
| 4 | D | 334 | GLN |
| 4 | D | 343 | HIS |
| 4 | D | 352 | HIS |
| 4 | D | 426 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 542 | HIS |
| 4 | D | 549 | GLN |
| 4 | D | 628 | GLN |
| 4 | D | 631 | GLN |
| 6 | F | 313 | GLN |
| 7 | G | 18 | GLN |
| 7 | G | 92 | HIS |
| 7 | G | 161 | HIS |
| 8 | H | 196 | ASN |
| 8 | H | 207 | HIS |
| 8 | H | 282 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 5 | E | 17 |

Continued on next page...

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| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 6 | F | 17 |
| 1 | A | 13 |
| 2 | B | 10 |
| 4 | D | 9 |
| 7 | G | 9 |
| 8 | H | 7 |
| 3 | C | 6 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | B | 223:GLU | C | 224:GLY | N | 1.81 |
| 1 | A | 277:VAL | C | 278:PRO | N | 1.79 |
| 1 | A | 280:PRO | C | 281:SER | N | 1.75 |
| 1 | A | 283:ARG | C | 284:ARG | N | 1.70 |
| 1 | A | 284:ARG | C | 285:LEU | N | 1.69 |
| 1 | B | 591:THR | C | 592:GLY | N | 1.66 |
| 1 | C | 319:PHE | C | 320:LEU | N | 1.66 |
| 1 | A | 276:VAL | C | 277:VAL | N | 1.65 |
| 1 | C | 213:MET | C | 214:ARG | N | 1.20 |
| 1 | D | 638:GLU | C | 639:ARG | N | 1.20 |
| 1 | D | 650:ARG | C | 651:TRP | N | 1.20 |
| 1 | D | 661:ALA | C | 662:THR | N | 1.20 |
| 1 | E | 51:ARG | C | 52:ILE | N | 1.20 |
| 1 | E | 72:GLU | C | 73:LYS | N | 1.20 |
| 1 | E | 95:ASN | C | 96:SER | N | 1.20 |
| 1 | E | 128:HIS | C | 129:ARG | N | 1.20 |
| 1 | E | 136:PRO | C | 137:LEU | N | 1.20 |
| 1 | F | 173:LEU | C | 174:ALA | N | 1.20 |
| 1 | F | 175:ARG | C | 176:GLN | N | 1.20 |
| 1 | G | 287:THR | C | 288:CYS | N | 1.20 |
| 1 | G | 299:THR | C | 300:GLU | N | 1.20 |
| 1 | H | 297:HIS | C | 298:ALA | N | 1.20 |
| 1 | H | 319:ASP | C | 320:GLU | N | 1.20 |
| 1 | A | 222:THR | C | 223:GLU | N | 1.19 |
| 1 | A | 242:ALA | C | 243:PRO | N | 1.19 |
| 1 | B | 516:ASN | C | 517:THR | N | 1.19 |
| 1 | C | 291:GLN | C | 292:ILE | N | 1.19 |
| 1 | C | 313:ILE | C | 314:LEU | N | 1.19 |
| 1 | D | 311:SER | C | 312:PHE | N | 1.19 |
| 1 | D | 501:PRO | C | 502:SER | N | 1.19 |
| 1 | E | 15:ALA | C | 16:SER | N | 1.19 |
| 1 | E | 22:CYS | C | 23:LEU | N | 1.19 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | E | 58:GLU | C | 59:ILE | N | 1.19 |
| 1 | E | 61:GLN | C | 62:LYS | N | 1.19 |
| 1 | E | 88:HIS | C | 89:GLN | N | 1.19 |
| 1 | F | 80:TRP | C | 81:PRO | N | 1.19 |
| 1 | F | 195:LYS | C | 196:ALA | N | 1.19 |
| 1 | F | 202:GLN | C | 203:ILE | N | 1.19 |
| 1 | F | 260:ALA | C | 261:VAL | N | 1.19 |
| 1 | F | 380:GLU | C | 381:TRP | N | 1.19 |
| 1 | G | 120:GLN | C | 121:TYR | N | 1.19 |
| 1 | H | 218:ARG | C | 219:GLU | N | 1.19 |
| 1 | B | 6:ARG | C | 7:PHE | N | 1.18 |
| 1 | B | 215:SER | C | 216:PHE | N | 1.18 |
| 1 | B | 222:PHE | C | 223:GLU | N | 1.18 |
| 1 | C | 314:LEU | C | 315:SER | N | 1.18 |
| 1 | D | 221:PRO | C | 222:GLY | N | 1.18 |
| 1 | E | 78:ILE | C | 79:THR | N | 1.18 |
| 1 | E | 93:ALA | C | 94:MET | N | 1.18 |
| 1 | F | 44:GLY | C | 45:VAL | N | 1.18 |
| 1 | F | 253:LYS | C | 254:GLU | N | 1.18 |
| 1 | G | 141:ASN | C | 142:VAL | N | 1.18 |
| 1 | G | 161:HIS | C | 162:PHE | N | 1.18 |
| 1 | G | 275:GLY | C | 276:PRO | N | 1.18 |
| 1 | H | 196:ASN | C | 197:ASP | N | 1.18 |
| 1 | H | 300:GLU | C | 301:ASN | N | 1.18 |
| 1 | H | 333:SER | C | 334:PHE | N | 1.18 |
| 1 | B | 589:ALA | C | 590:GLN | N | 1.17 |
| 1 | B | 594:GLY | C | 595:SER | N | 1.17 |
| 1 | C | 113:SER | C | 114:ARG | N | 1.17 |
| 1 | D | 313:HIS | C | 314:SER | N | 1.17 |
| 1 | E | 82:LEU | C | 83:TYR | N | 1.17 |
| 1 | F | 51:PRO | C | 52:ASN | N | 1.17 |
| 1 | F | 121:PRO | C | 122:GLY | N | 1.17 |
| 1 | F | 209:GLU | C | 210:HIS | N | 1.17 |
| 1 | G | 122:PRO | C | 123:ASP | N | 1.17 |
| 1 | A | 268:THR | C | 269:LYS | N | 1.16 |
| 1 | B | 73:ASP | C | 74:GLU | N | 1.16 |
| 1 | E | 69:LEU | C | 70:ARG | N | 1.16 |
| 1 | E | 73:LYS | C | 74:GLU | N | 1.16 |
| 1 | F | 258:VAL | C | 259:ASP | N | 1.16 |
| 1 | G | 234:VAL | C | 235:ILE | N | 1.16 |
| 1 | G | 289:PHE | C | 290:LYS | N | 1.16 |
| 1 | A | 206:GLU | C | 207:GLU | N | 1.15 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | A | 229:MET | C | 230:ALA | N | 1.15 |
| 1 | A | 265:GLU | C | 266:LEU | N | 1.15 |
| 1 | E | 133:GLU | C | 134:LEU | N | 1.15 |
| 1 | F | 146:ALA | C | 147:ASP | N | 1.15 |
| 1 | F | 213:LEU | C | 214:GLN | N | 1.15 |
| 1 | H | 155:VAL | C | 156:PRO | N | 1.15 |
| 1 | D | 402:GLU | C | 403:MET | N | 1.14 |
| 1 | E | 86:GLN | C | 87:LYS | N | 1.14 |
| 1 | F | 262:VAL | C | 263:ARG | N | 1.14 |
| 1 | D | 227:ARG | C | 228:SER | N | 1.13 |
| 1 | A | 269:LYS | C | 270:VAL | N | 1.12 |
| 1 | B | 592:GLY | C | 593:GLY | N | 1.11 |
| 1 | F | 1:MET | C | 2:GLN | N | 1.11 |
| 1 | A | 272:MET | C | 273:MET | N | 0.96 |

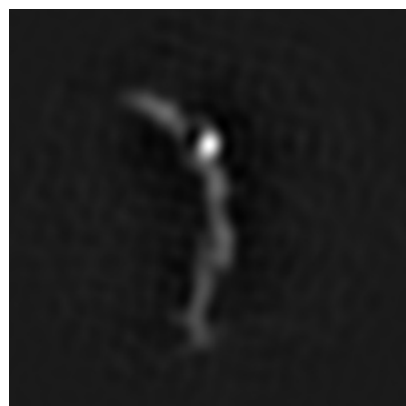
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15633. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

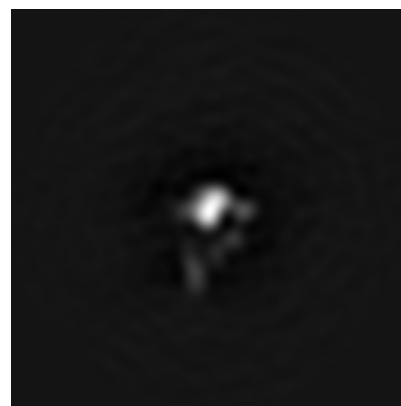
6.1.1 Primary map



X

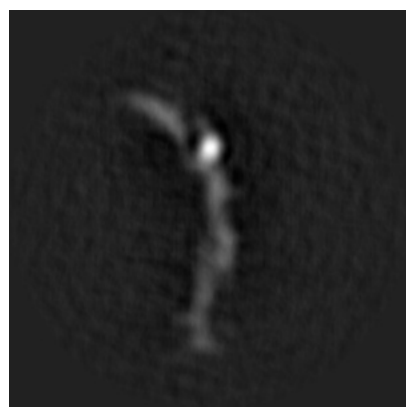


Y

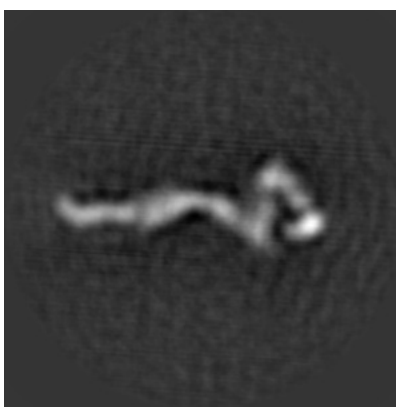


Z

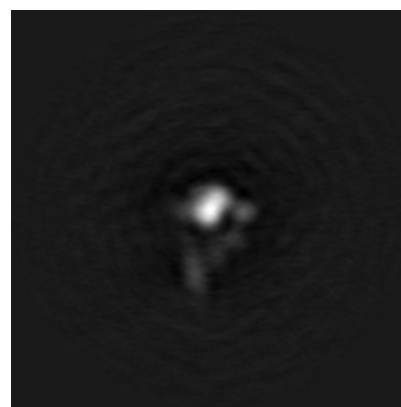
6.1.2 Raw map



X



Y

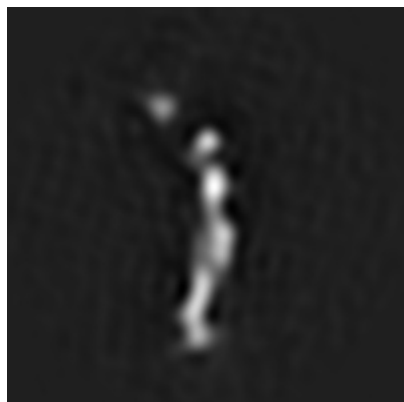


Z

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

6.2 Central slices [i](#)

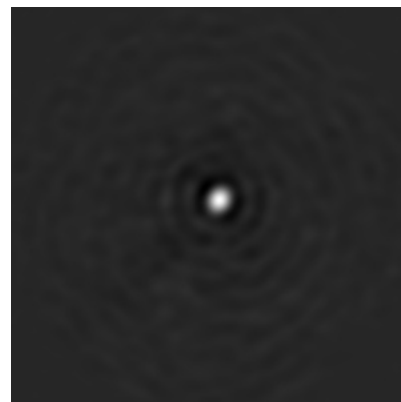
6.2.1 Primary map



X Index: 128

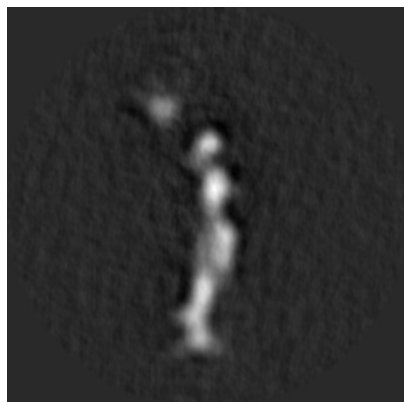


Y Index: 128

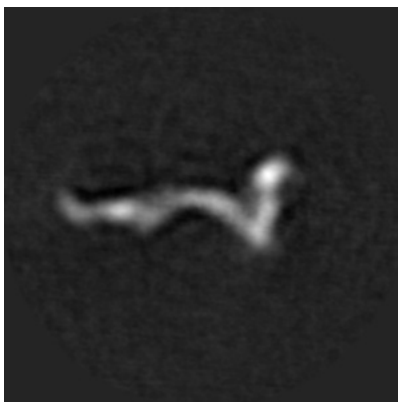


Z Index: 128

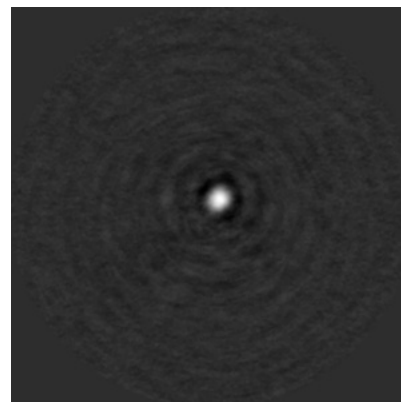
6.2.2 Raw map



X Index: 128



Y Index: 128

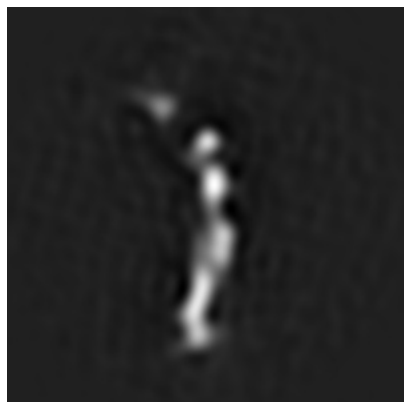


Z Index: 128

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

6.3 Largest variance slices [i](#)

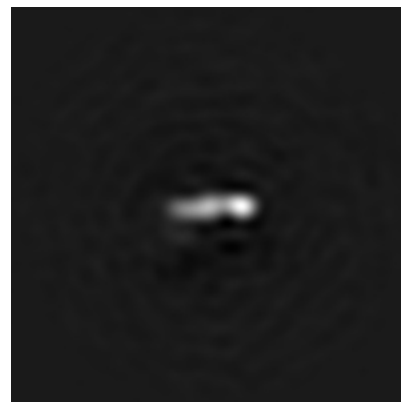
6.3.1 Primary map



X Index: 127

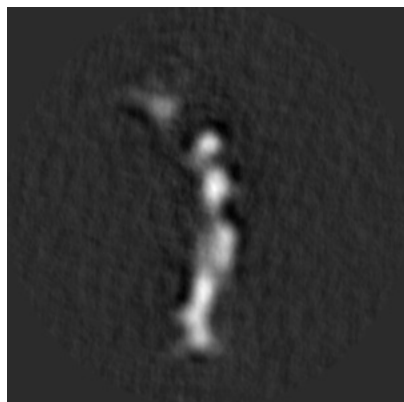


Y Index: 128

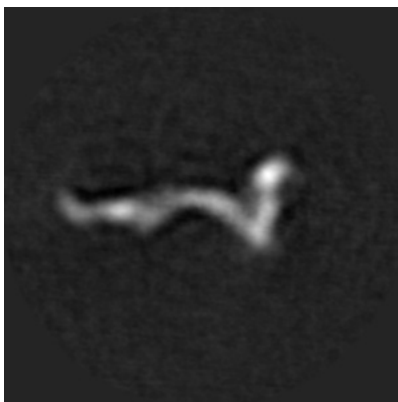


Z Index: 169

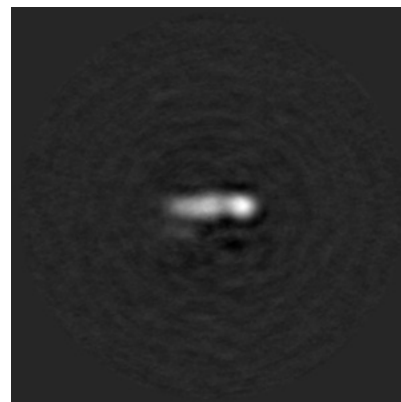
6.3.2 Raw map



X Index: 127



Y Index: 128

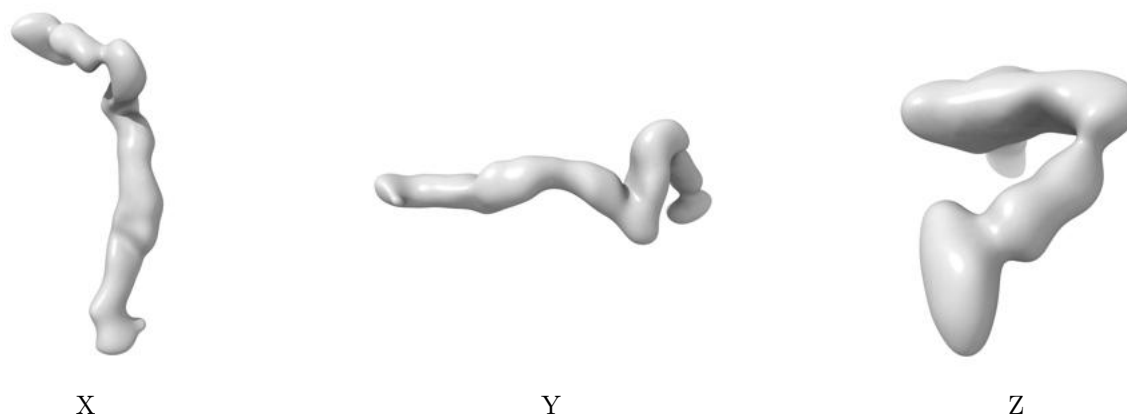


Z Index: 167

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

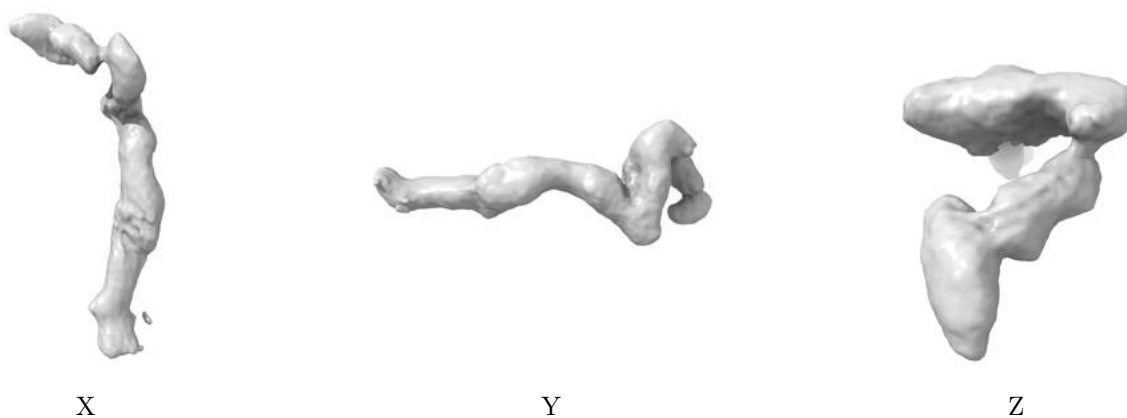
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

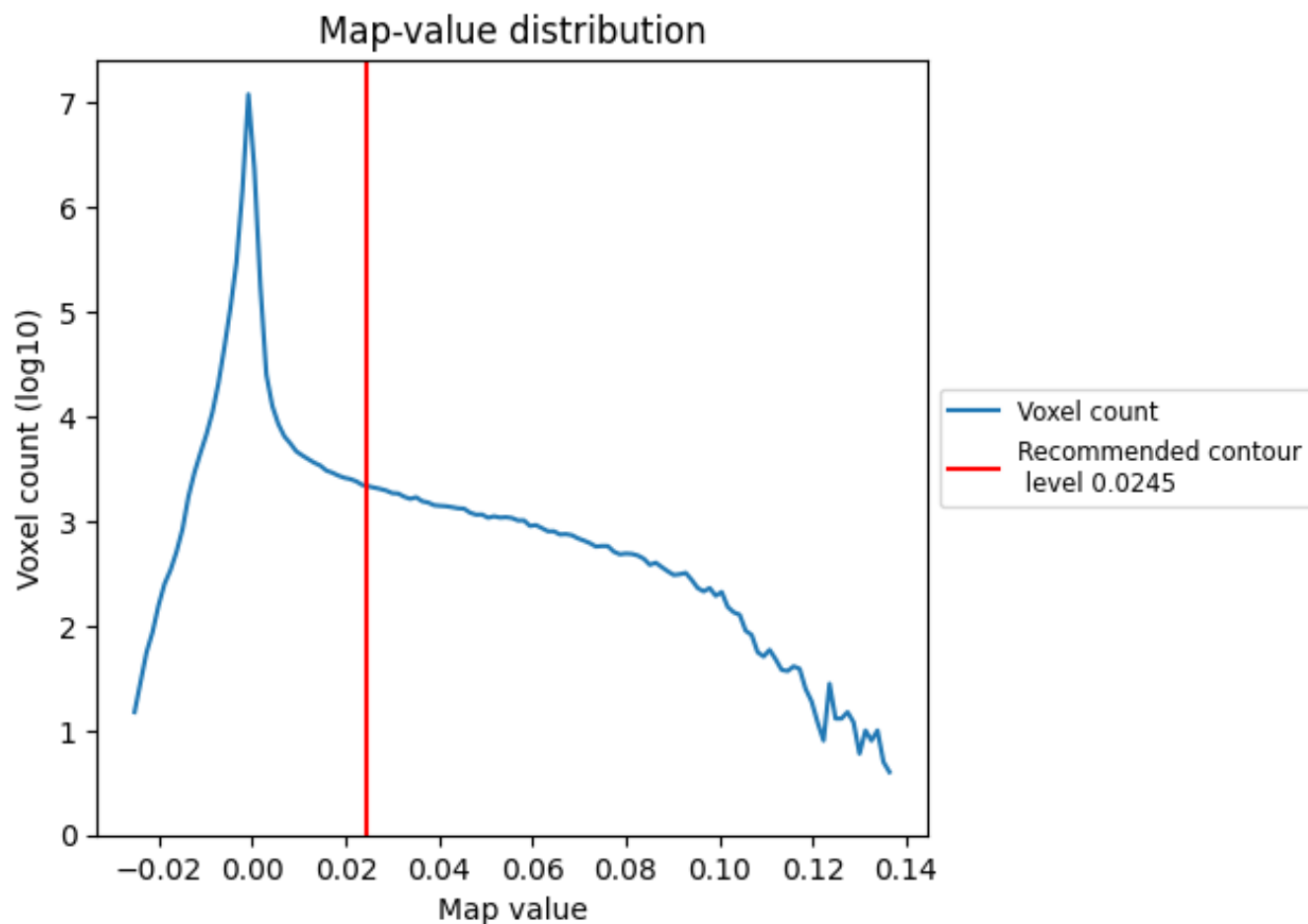
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

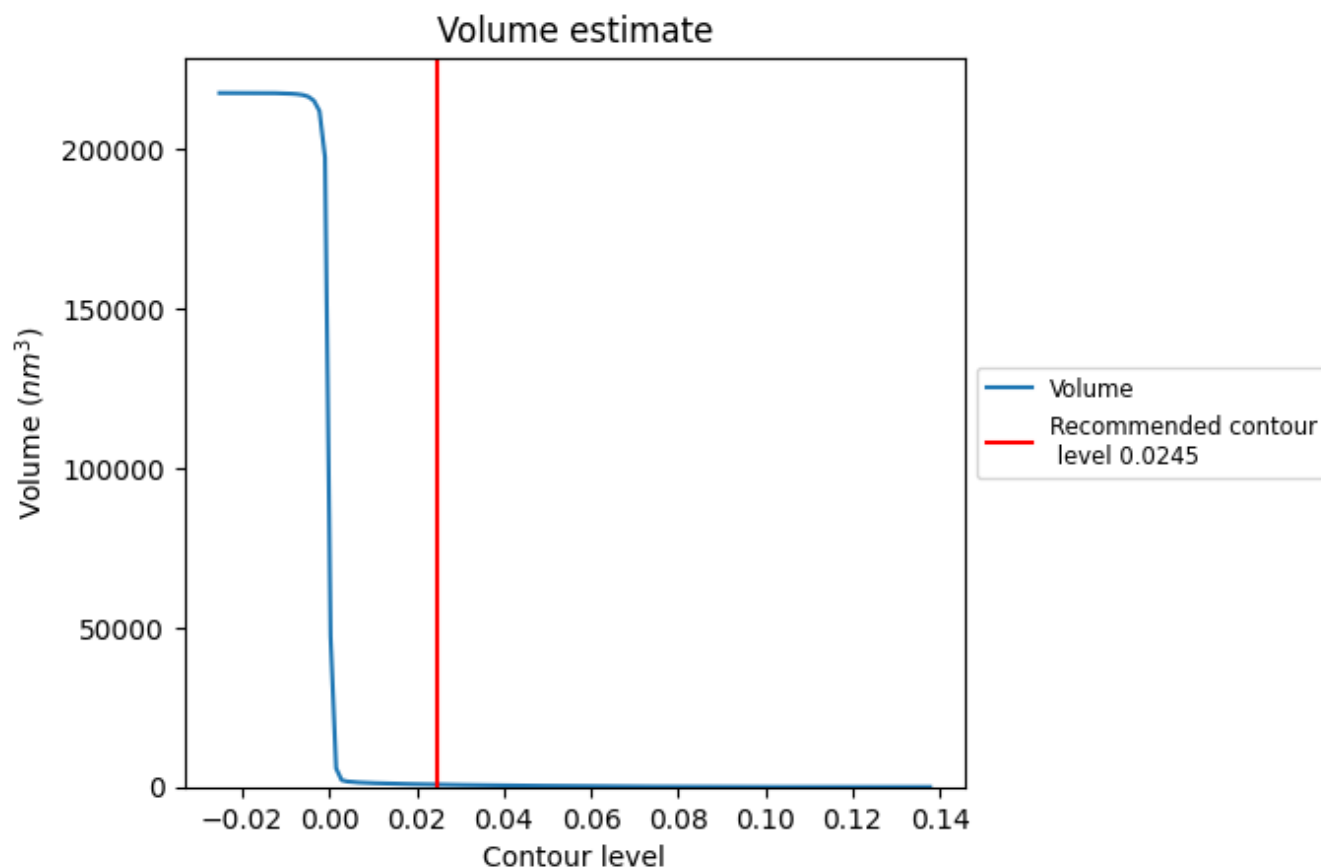
This section contains the results of statistical analysis of the map.

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.

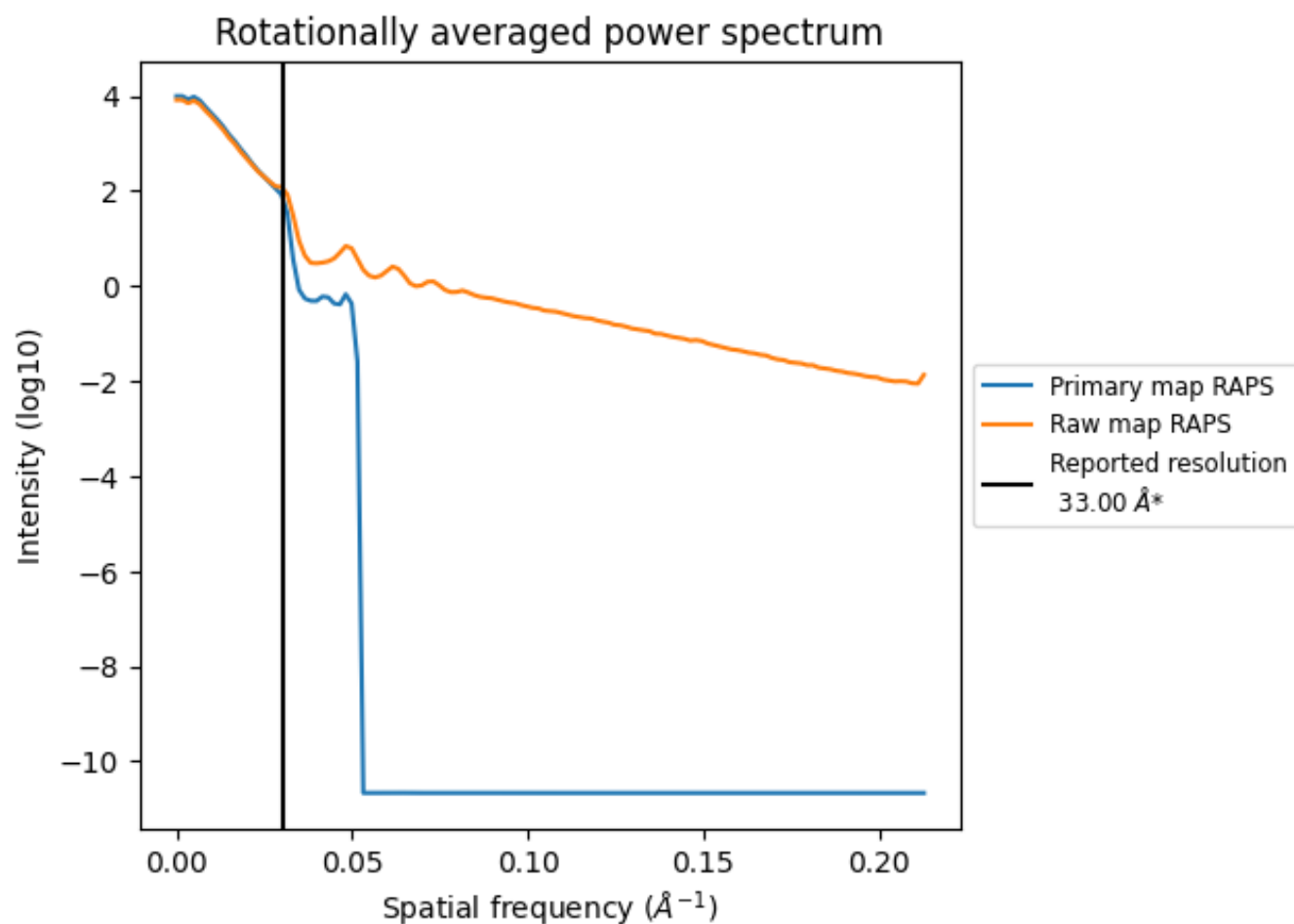
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 753 nm^3 ; this corresponds to an approximate mass of 680 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 ⓘ

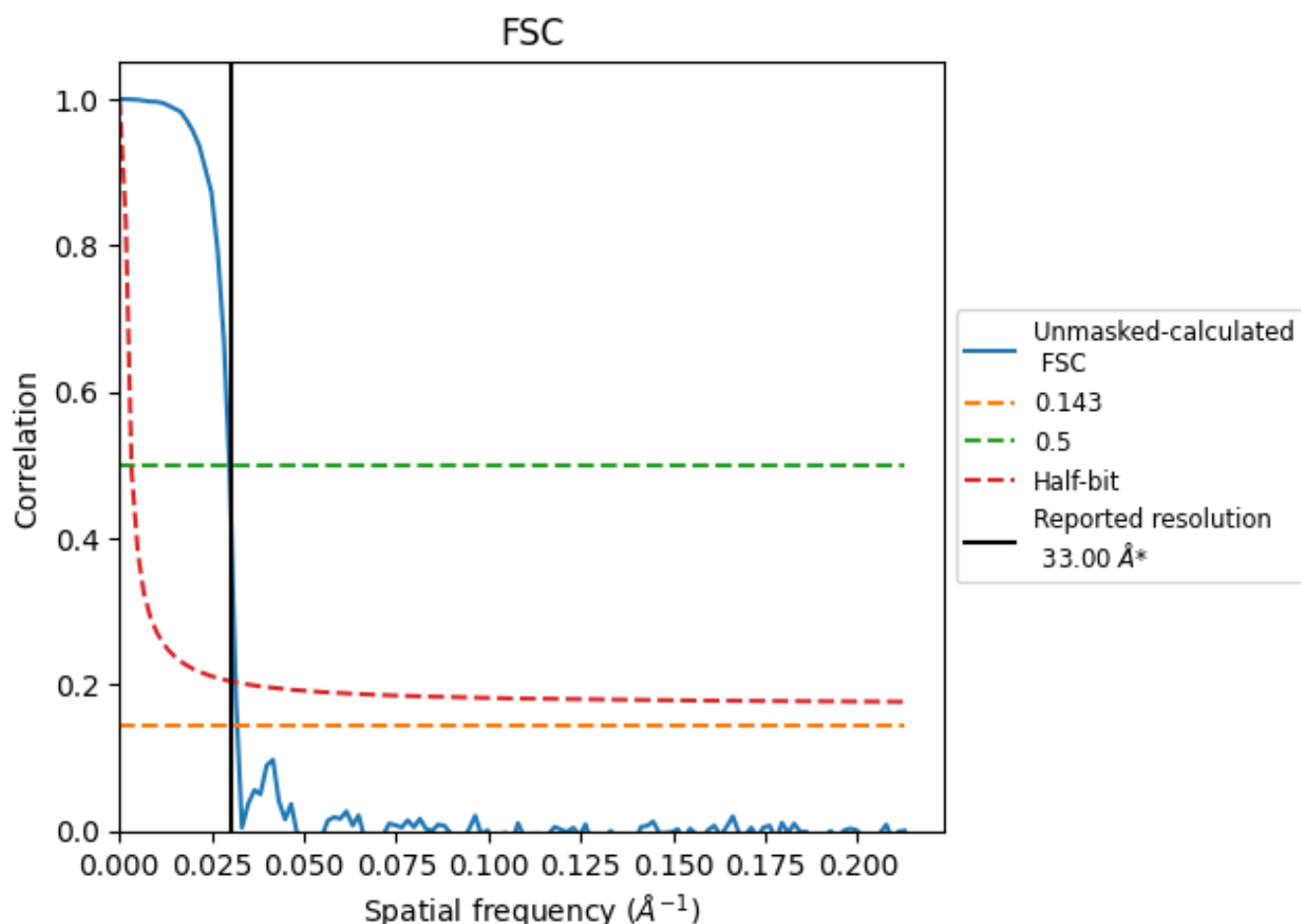


*Reported resolution corresponds to spatial frequency of 0.030 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.030 \AA^{-1}

8.2 Resolution estimates [i](#)

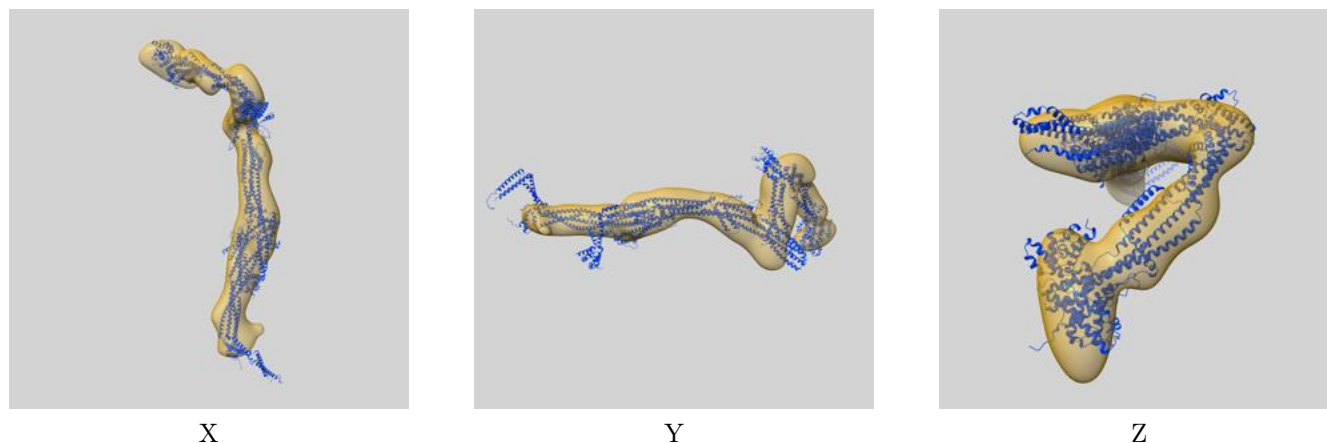
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|-------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 33.00 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 31.35 | 33.56 | 31.75 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

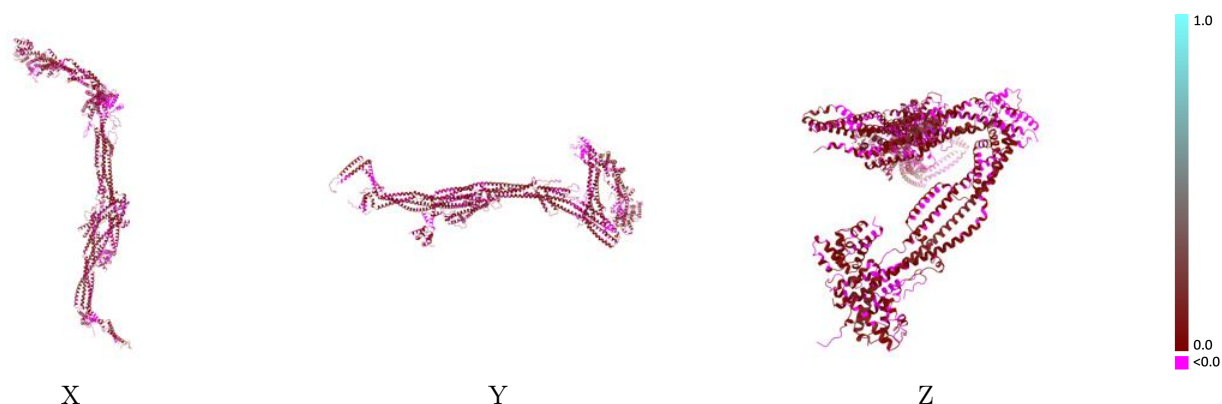
This section contains information regarding the fit between EMDB map EMD-15633 and PDB model 8AT4. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



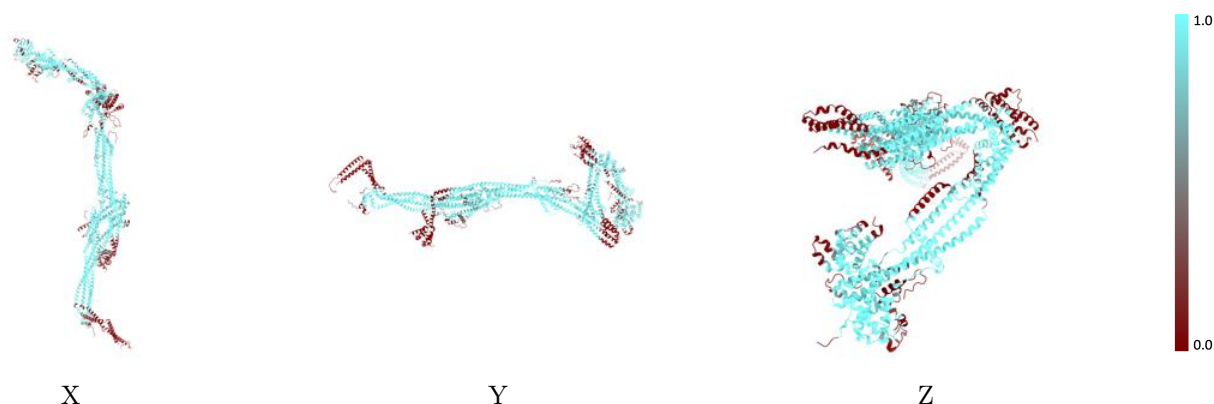
The images above show the 3D surface view of the map at the recommended contour level 0.0245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



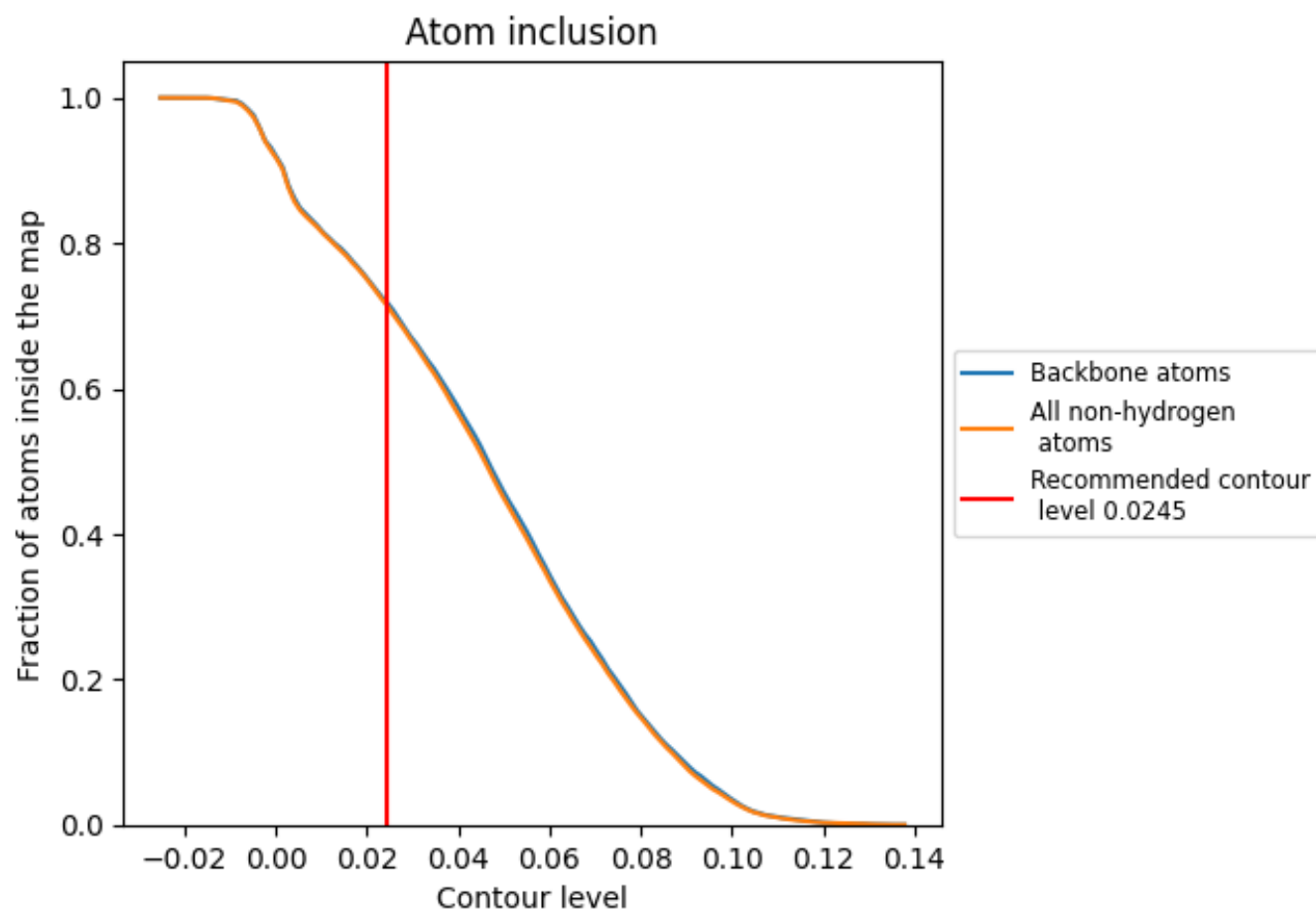
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0245).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.0245) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------|--------------------|
| All | <div></div> 0.7134 | <div></div> 0.0400 |
| A | <div></div> 0.6228 | <div></div> 0.0480 |
| B | <div></div> 0.7177 | <div></div> 0.0410 |
| C | <div></div> 0.7251 | <div></div> 0.0530 |
| D | <div></div> 0.6985 | <div></div> 0.0330 |
| E | <div></div> 0.5387 | <div></div> 0.0190 |
| F | <div></div> 0.7652 | <div></div> 0.0340 |
| G | <div></div> 0.7347 | <div></div> 0.0310 |
| H | <div></div> 0.9013 | <div></div> 0.0710 |

1.0

0.0

<0.0