# Full wwPDB EM Validation Report

Mar 8, 2026 – 09:34 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 7RLB / pdb_00007rlb |
| EMDB ID | : | EMD-24524 |
| Title | : | Cryo-EM structure of human p97-A232E mutant bound to ADP |
| Authors | : | Caffrey, B.; Zhu, X.; Berezuk, A.; Tuttle, K.; Chittori, S.; Subramaniam, S. |
| Deposited on | : | 2021-07-23 |
| Resolution | : | 3.30 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.

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

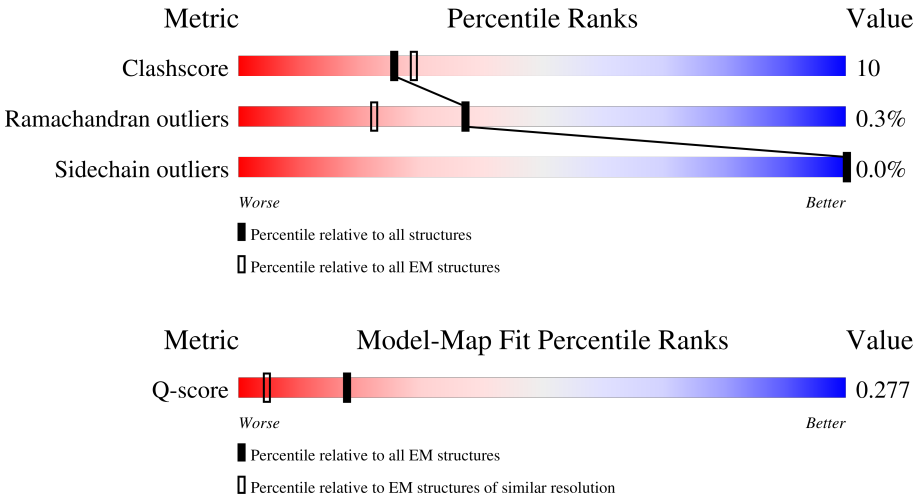
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 15087 ( 2.80 - 3.80 ) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 821 | 19% 69% 20% 10% |
| 1 | B | 821 | 20% 69% 20% 10% |
| 1 | C | 821 | 19% 69% 20% 10% |
| 1 | D | 821 | 19% 69% 21% 10% |

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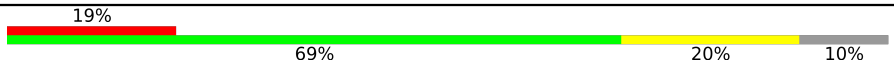
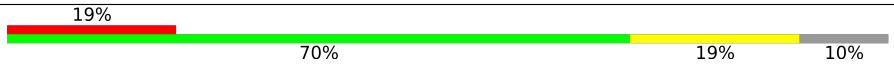
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 821 |   |
| 1 | F | 821 |   |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 34884 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 Transitional endoplasmic reticulum ATPase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 735 | Total 5760 | C 3625 | N 1015 | O 1090 | S 30 | 0 | 0 |
| 1 | B | 735 | Total 5760 | C 3625 | N 1015 | O 1090 | S 30 | 0 | 0 |
| 1 | C | 735 | Total 5760 | C 3625 | N 1015 | O 1090 | S 30 | 0 | 0 |
| 1 | D | 735 | Total 5760 | C 3625 | N 1015 | O 1090 | S 30 | 0 | 0 |
| 1 | E | 735 | Total 5760 | C 3625 | N 1015 | O 1090 | S 30 | 0 | 0 |
| 1 | F | 735 | Total 5760 | C 3625 | N 1015 | O 1090 | S 30 | 0 | 0 |

There are 102 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -14 | HIS | - | expression tag | UNP P55072 |
| A | -13 | HIS | - | expression tag | UNP P55072 |
| A | -12 | HIS | - | expression tag | UNP P55072 |
| A | -11 | HIS | - | expression tag | UNP P55072 |
| A | -10 | HIS | - | expression tag | UNP P55072 |
| A | -9 | HIS | - | expression tag | UNP P55072 |
| A | -8 | GLY | - | expression tag | UNP P55072 |
| A | -7 | THR | - | expression tag | UNP P55072 |
| A | -6 | SER | - | expression tag | UNP P55072 |
| A | -5 | GLU | - | expression tag | UNP P55072 |
| A | -4 | ASN | - | expression tag | UNP P55072 |
| A | -3 | LEU | - | expression tag | UNP P55072 |
| A | -2 | TYR | - | expression tag | UNP P55072 |
| A | -1 | PHE | - | expression tag | UNP P55072 |
| A | 0 | GLN | - | expression tag | UNP P55072 |
| A | 1 | GLY | - | expression tag | UNP P55072 |
| A | 232 | GLU | ALA | engineered mutation | UNP P55072 |
| B | -14 | HIS | - | expression tag | UNP P55072 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | -13 | HIS | - | expression tag | UNP P55072 |
| B | -12 | HIS | - | expression tag | UNP P55072 |
| B | -11 | HIS | - | expression tag | UNP P55072 |
| B | -10 | HIS | - | expression tag | UNP P55072 |
| B | -9 | HIS | - | expression tag | UNP P55072 |
| B | -8 | GLY | - | expression tag | UNP P55072 |
| B | -7 | THR | - | expression tag | UNP P55072 |
| B | -6 | SER | - | expression tag | UNP P55072 |
| B | -5 | GLU | - | expression tag | UNP P55072 |
| B | -4 | ASN | - | expression tag | UNP P55072 |
| B | -3 | LEU | - | expression tag | UNP P55072 |
| B | -2 | TYR | - | expression tag | UNP P55072 |
| B | -1 | PHE | - | expression tag | UNP P55072 |
| B | 0 | GLN | - | expression tag | UNP P55072 |
| B | 1 | GLY | - | expression tag | UNP P55072 |
| B | 232 | GLU | ALA | engineered mutation | UNP P55072 |
| C | -14 | HIS | - | expression tag | UNP P55072 |
| C | -13 | HIS | - | expression tag | UNP P55072 |
| C | -12 | HIS | - | expression tag | UNP P55072 |
| C | -11 | HIS | - | expression tag | UNP P55072 |
| C | -10 | HIS | - | expression tag | UNP P55072 |
| C | -9 | HIS | - | expression tag | UNP P55072 |
| C | -8 | GLY | - | expression tag | UNP P55072 |
| C | -7 | THR | - | expression tag | UNP P55072 |
| C | -6 | SER | - | expression tag | UNP P55072 |
| C | -5 | GLU | - | expression tag | UNP P55072 |
| C | -4 | ASN | - | expression tag | UNP P55072 |
| C | -3 | LEU | - | expression tag | UNP P55072 |
| C | -2 | TYR | - | expression tag | UNP P55072 |
| C | -1 | PHE | - | expression tag | UNP P55072 |
| C | 0 | GLN | - | expression tag | UNP P55072 |
| C | 1 | GLY | - | expression tag | UNP P55072 |
| C | 232 | GLU | ALA | engineered mutation | UNP P55072 |
| D | -14 | HIS | - | expression tag | UNP P55072 |
| D | -13 | HIS | - | expression tag | UNP P55072 |
| D | -12 | HIS | - | expression tag | UNP P55072 |
| D | -11 | HIS | - | expression tag | UNP P55072 |
| D | -10 | HIS | - | expression tag | UNP P55072 |
| D | -9 | HIS | - | expression tag | UNP P55072 |
| D | -8 | GLY | - | expression tag | UNP P55072 |
| D | -7 | THR | - | expression tag | UNP P55072 |
| D | -6 | SER | - | expression tag | UNP P55072 |

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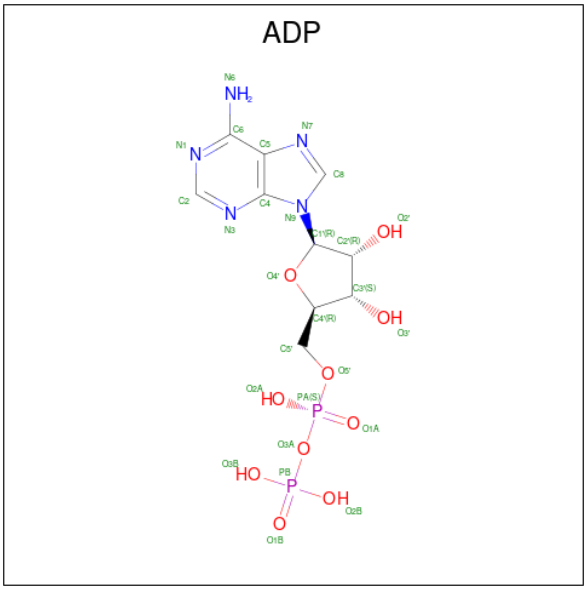
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | -5 | GLU | - | expression tag | UNP P55072 |
| D | -4 | ASN | - | expression tag | UNP P55072 |
| D | -3 | LEU | - | expression tag | UNP P55072 |
| D | -2 | TYR | - | expression tag | UNP P55072 |
| D | -1 | PHE | - | expression tag | UNP P55072 |
| D | 0 | GLN | - | expression tag | UNP P55072 |
| D | 1 | GLY | - | expression tag | UNP P55072 |
| D | 232 | GLU | ALA | engineered mutation | UNP P55072 |
| E | -14 | HIS | - | expression tag | UNP P55072 |
| E | -13 | HIS | - | expression tag | UNP P55072 |
| E | -12 | HIS | - | expression tag | UNP P55072 |
| E | -11 | HIS | - | expression tag | UNP P55072 |
| E | -10 | HIS | - | expression tag | UNP P55072 |
| E | -9 | HIS | - | expression tag | UNP P55072 |
| E | -8 | GLY | - | expression tag | UNP P55072 |
| E | -7 | THR | - | expression tag | UNP P55072 |
| E | -6 | SER | - | expression tag | UNP P55072 |
| E | -5 | GLU | - | expression tag | UNP P55072 |
| E | -4 | ASN | - | expression tag | UNP P55072 |
| E | -3 | LEU | - | expression tag | UNP P55072 |
| E | -2 | TYR | - | expression tag | UNP P55072 |
| E | -1 | PHE | - | expression tag | UNP P55072 |
| E | 0 | GLN | - | expression tag | UNP P55072 |
| E | 1 | GLY | - | expression tag | UNP P55072 |
| E | 232 | GLU | ALA | engineered mutation | UNP P55072 |
| F | -14 | HIS | - | expression tag | UNP P55072 |
| F | -13 | HIS | - | expression tag | UNP P55072 |
| F | -12 | HIS | - | expression tag | UNP P55072 |
| F | -11 | HIS | - | expression tag | UNP P55072 |
| F | -10 | HIS | - | expression tag | UNP P55072 |
| F | -9 | HIS | - | expression tag | UNP P55072 |
| F | -8 | GLY | - | expression tag | UNP P55072 |
| F | -7 | THR | - | expression tag | UNP P55072 |
| F | -6 | SER | - | expression tag | UNP P55072 |
| F | -5 | GLU | - | expression tag | UNP P55072 |
| F | -4 | ASN | - | expression tag | UNP P55072 |
| F | -3 | LEU | - | expression tag | UNP P55072 |
| F | -2 | TYR | - | expression tag | UNP P55072 |
| F | -1 | PHE | - | expression tag | UNP P55072 |
| F | 0 | GLN | - | expression tag | UNP P55072 |
| F | 1 | GLY | - | expression tag | UNP P55072 |
| F | 232 | GLU | ALA | engineered mutation | UNP P55072 |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | E | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | E | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | F | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | F | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

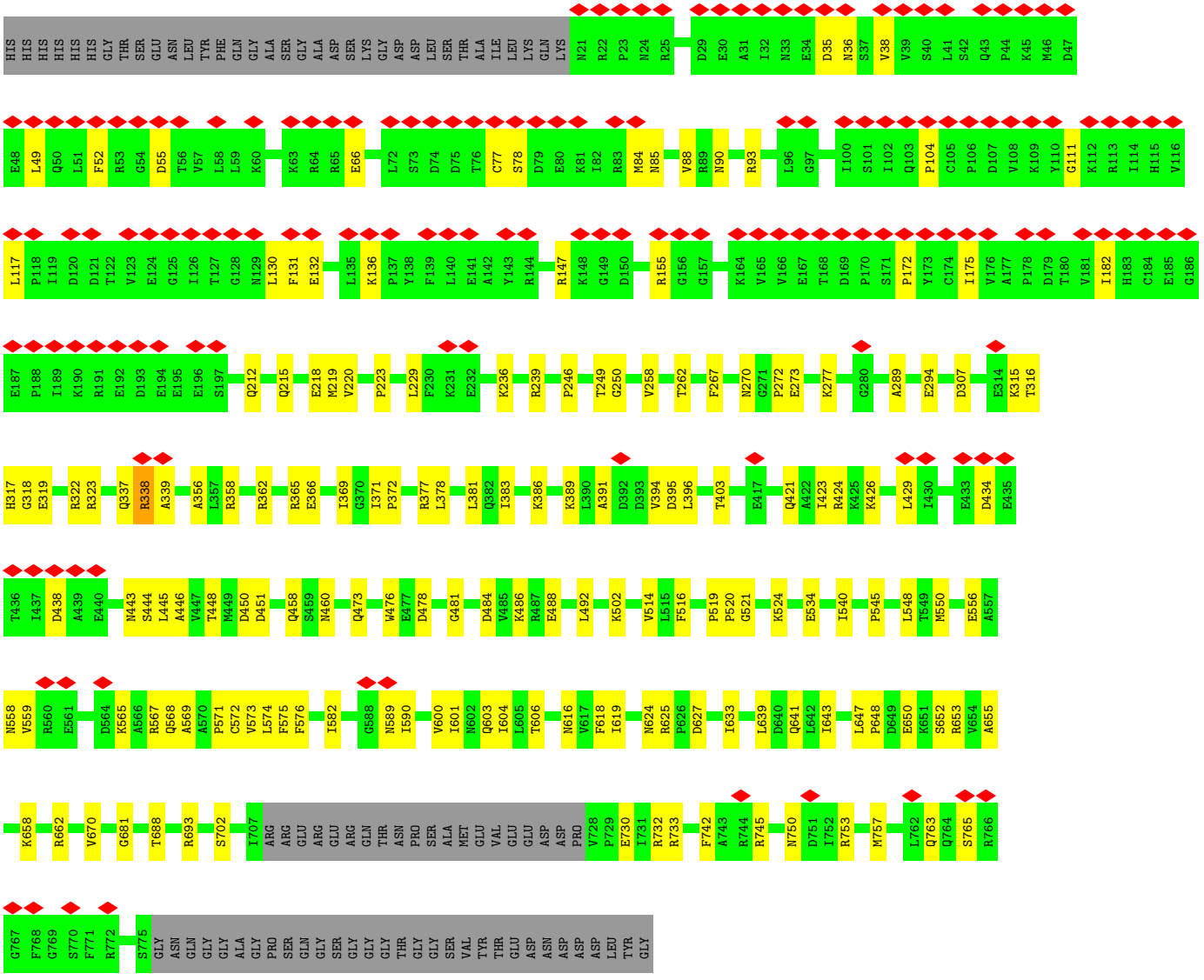
# 3 Residue-property plots (i)

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

• Molecule 1: Transitional endoplasmic reticulum ATPase

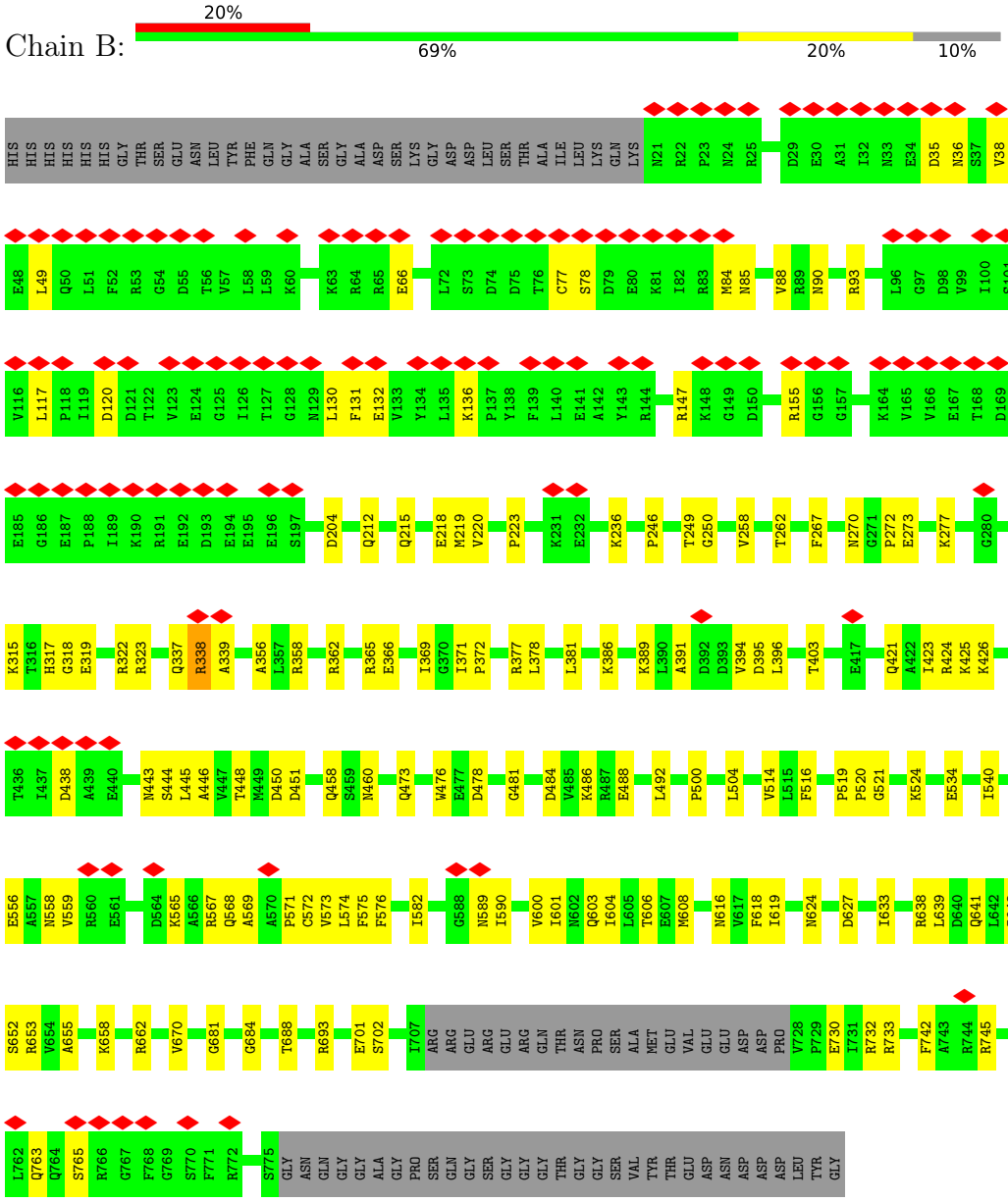
Chain A:



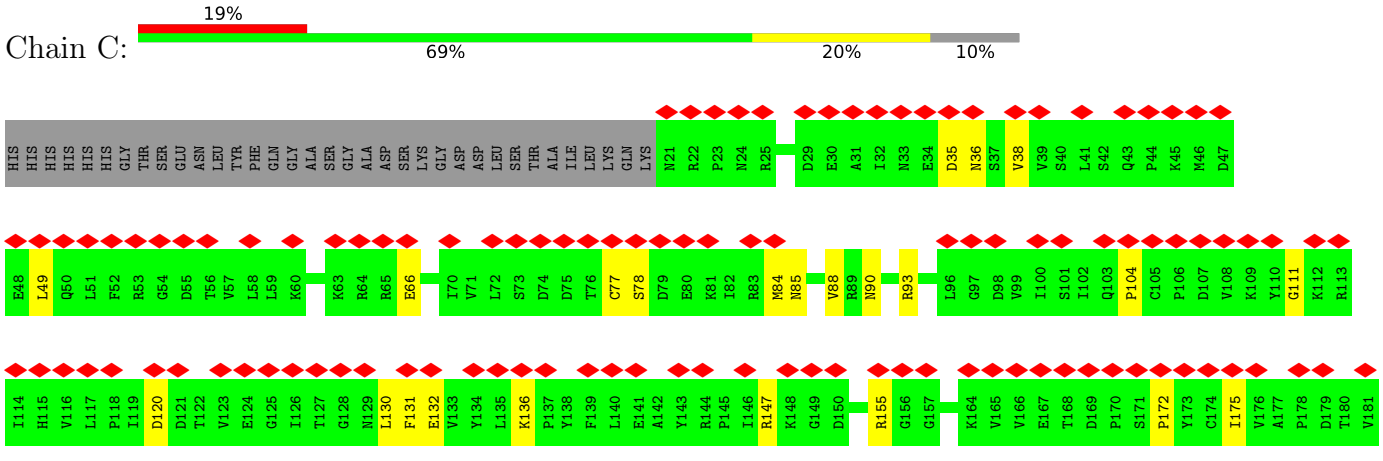
• Molecule 1: Transitional endoplasmic reticulum ATPase

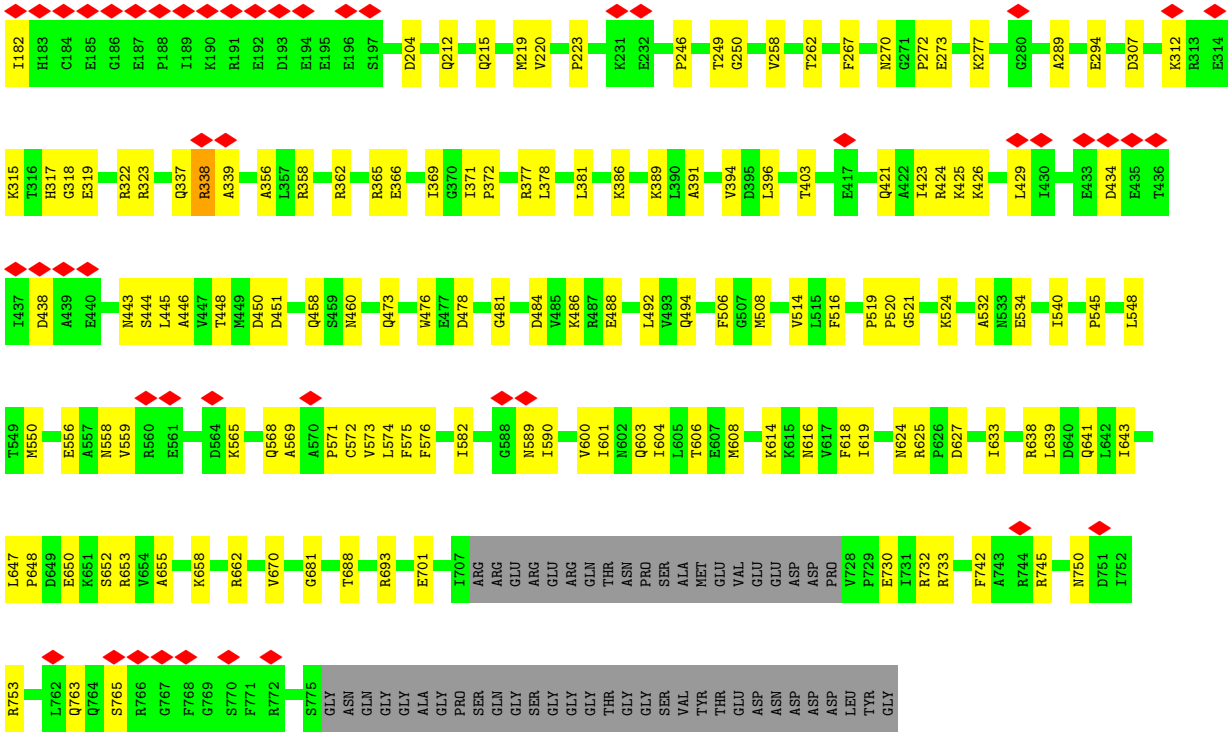
Chain B:




• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:

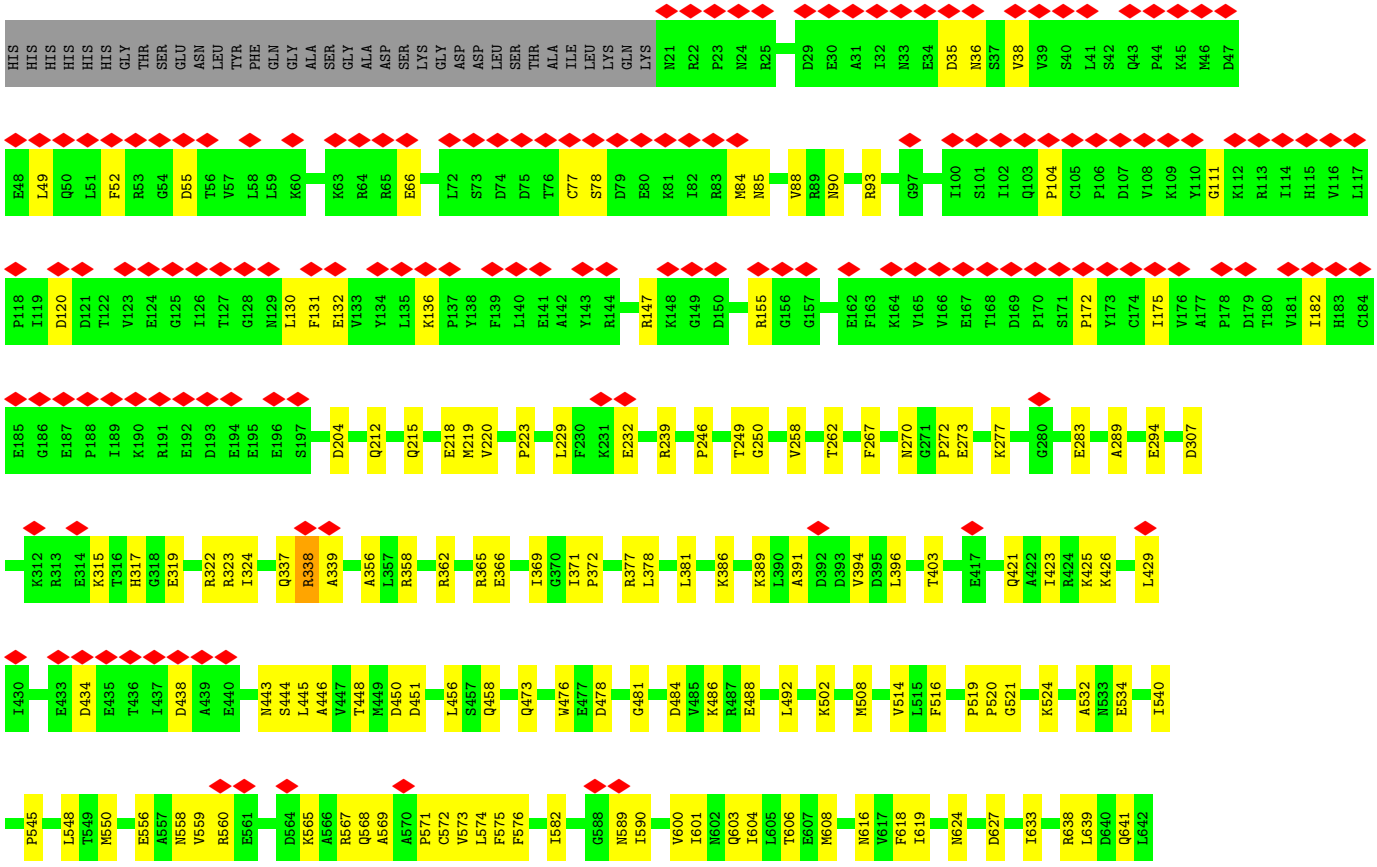


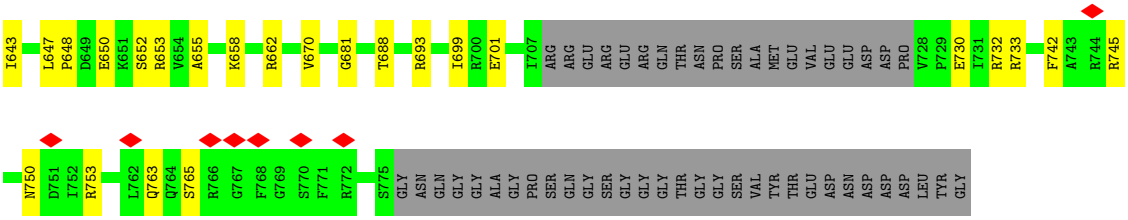


• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



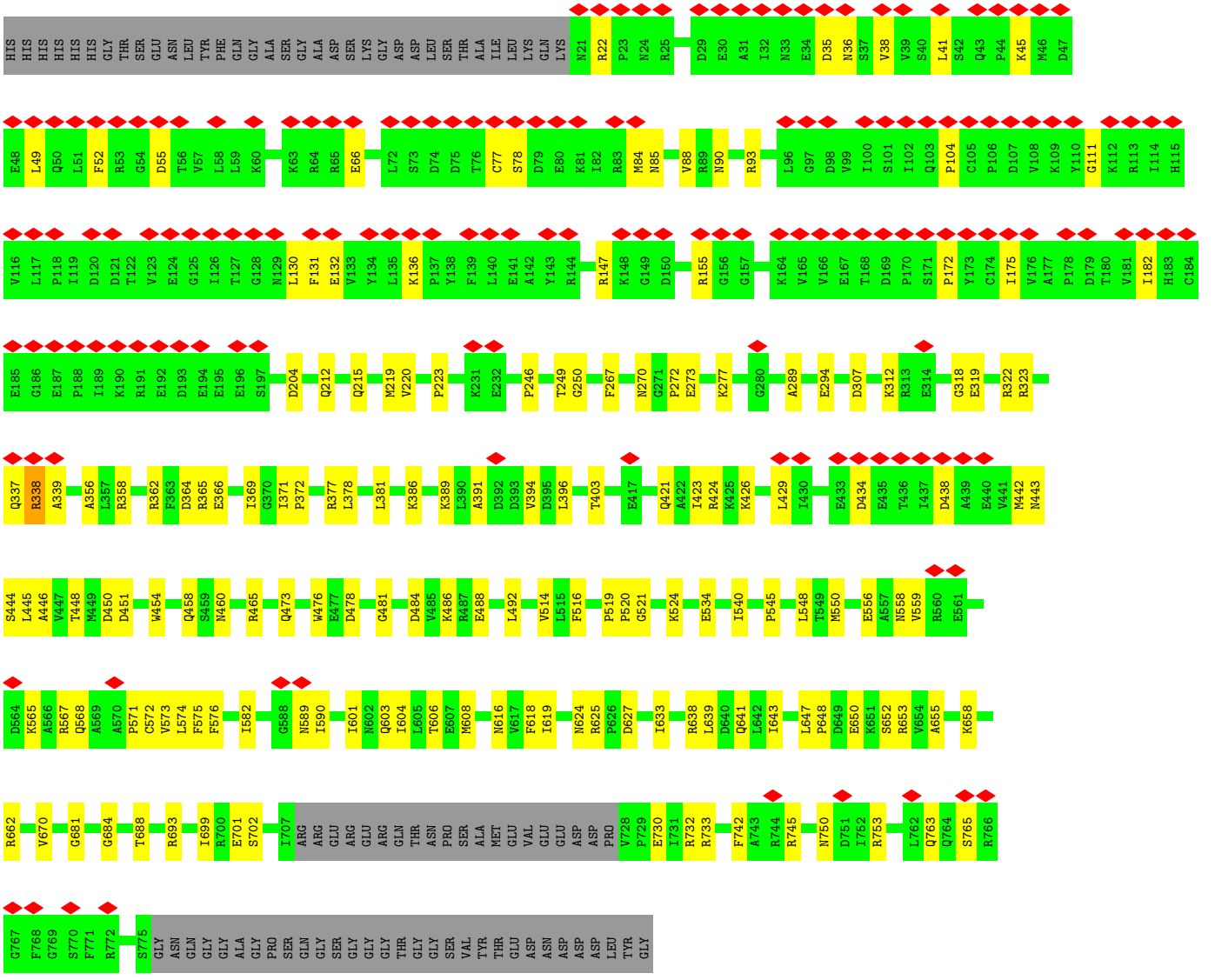






• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:

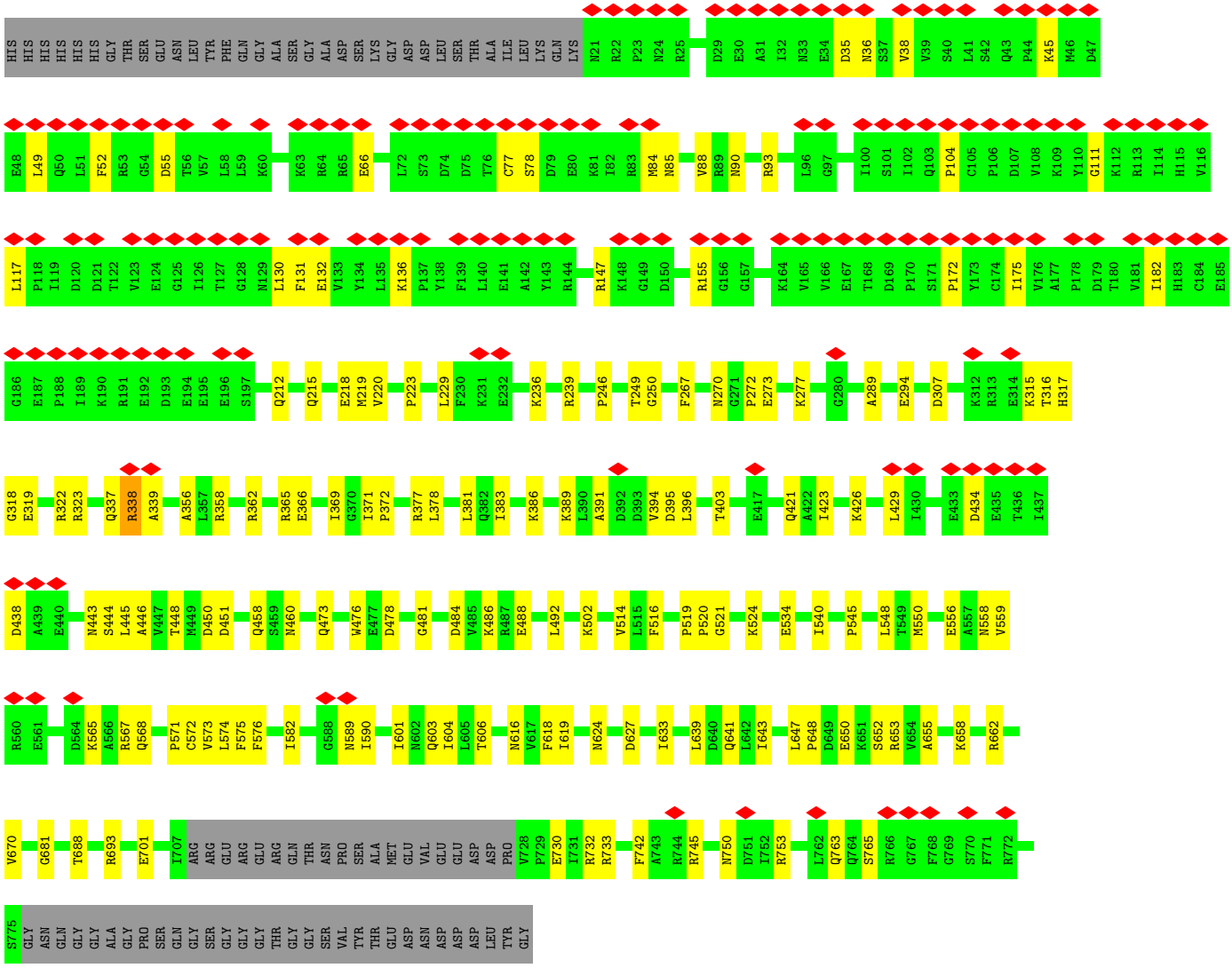



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:




HIS HIS HIS HIS HIS HIS GLY THR SER GLU ASN LEU TYR PHE GLN GLY ALA SER GLY ALA ASP SER LYS GLY ASP ASP LEU SER THR ALA ILE LEU LYS GLN LYS N21 R22 P23 N24 R25 D29 E30 A31 I32 N33 E34 D35 N36 S37 V38 V39 S40 L41 S42 Q43 P44 K45 M46 D47
E48 L49 Q50 L51 F52 R53 G54 D55 T56 V57 L58 L59 K60 K63 R64 R65 E66 L72 S73 D74 D75 T76 C77 S78 D79 E80 K81 I82 R83 M84 N85 V88 R89 N90 R93 L96 G97 I100 S101 I102 Q103 P104 C105 P106 D107 V108 K109 Y110 G111 K112 R113 I114 H115 V116
L117 P118 I119 D120 D121 T122 V123 E124 G125 I126 T127 G128 N129 L130 F131 E132 V133 Y134 L135 K136 P137 Y138 F139 L140 E141 A142 Y143 R144 R147 K148 G149 D150 R155 G156 G157 K164 V165 V166 E167 T168 D169 P170 S171 P172 Y173 C174 I175 V176 A177 P178 D179 T180 V181 I182 H183 C184 E185
G186 E187 P188 I189 K190 R191 E192 D193 E194 E195 E196 S197 Q212 Q215 E218 M219 V220 P223 L229 F230 K231 E232 K236 R239 P246 T249 G250 F267 N270 G271 P272 E273 K277 G280 A289 E294 D307 K312 R313 E314 K315 T316 H317
G318 E319 R322 R323 Q337 R338 A339 A356 L357 R358 R362 R365 E366 I369 G370 I371 P372 R377 L378 L381 Q382 I383 K386 K389 L390 A391 D392 D393 V394 D395 L396 T403 E417 Q421 A422 I423 K426 L429 I430 E433 D434 E435 T436 I437
D438 A439 E440 N443 S444 L445 A446 V447 T448 M449 D450 D451 Q458 S459 N460 Q473 W476 E477 D478 G481 D484 V485 K486 R487 E488 L492 K502 V514 L515 F516 P519 P520 G521 K524 E534 I540 P545 L548 T549 M550 E556 A557 N558 V559
R560 E561 D564 K565 A566 R567 Q568 P571 C572 V573 L574 F575 F576 I582 G588 N589 I590 I601 N602 Q603 I604 L605 T606 N616 V617 F618 I619 N624 D627 I633 L639 D640 Q641 L642 I643 L647 P648 D649 E650 K651 S652 R653 V654 A655 K658 R662
V670 G681 T688 R693 E701 I707 ARG ARG GLU ARG GLU ARG GLN THR ASN PRO SER ALA MET GLU VAL GLU GLU ASP ASP PRO V728 P729 E730 I731 R732 R733 F742 A743 R744 R745 M750 D751 I752 R753 L762 Q763 Q764 S765 R766 G767 F768 G769 S770 F771 R772
S775 GLY ASN GLN GLY GLY ALA GLY PRO SER GLN GLY SER GLY GLY GLY GLY THR GLY GLY SER VAL TYR THR GLU ASP ASN ASP ASP ASP LEU TYR GLY

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 14388 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.676 | Depositor |
| Minimum map value | -0.246 | Depositor |
| Average map value | -0.001 | Depositor |
| Map value standard deviation | 0.022 | Depositor |
| Recommended contour level | 0.1 | Depositor |
| Map size (Å) | 332.0, 332.0, 332.0 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.0375, 1.0375, 1.0375 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.15 | 0/5856 | 0.39 | 1/7906 (0.0%) |
| 1 | B | 0.15 | 0/5856 | 0.39 | 1/7906 (0.0%) |
| 1 | C | 0.15 | 0/5856 | 0.39 | 1/7906 (0.0%) |
| 1 | D | 0.15 | 0/5856 | 0.39 | 1/7906 (0.0%) |
| 1 | E | 0.15 | 0/5856 | 0.39 | 1/7906 (0.0%) |
| 1 | F | 0.15 | 0/5856 | 0.39 | 1/7906 (0.0%) |
| All | All | 0.15 | 0/35136 | 0.39 | 6/47436 (0.0%) |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 473 | GLN | CA-CB-CG | 5.34 | 124.78 | 114.10 |
| 1 | D | 473 | GLN | CA-CB-CG | 5.32 | 124.73 | 114.10 |
| 1 | F | 473 | GLN | CA-CB-CG | 5.32 | 124.73 | 114.10 |
| 1 | A | 473 | GLN | CA-CB-CG | 5.31 | 124.72 | 114.10 |
| 1 | E | 473 | GLN | CA-CB-CG | 5.31 | 124.72 | 114.10 |
| 1 | C | 473 | GLN | CA-CB-CG | 5.30 | 124.69 | 114.10 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5760 | 0 | 5821 | 136 | 0 |
| 1 | B | 5760 | 0 | 5821 | 135 | 0 |
| 1 | C | 5760 | 0 | 5821 | 129 | 0 |
| 1 | D | 5760 | 0 | 5821 | 132 | 0 |
| 1 | E | 5760 | 0 | 5821 | 129 | 0 |
| 1 | F | 5760 | 0 | 5821 | 129 | 0 |
| 2 | A | 54 | 0 | 24 | 6 | 0 |
| 2 | B | 54 | 0 | 24 | 6 | 0 |
| 2 | C | 54 | 0 | 24 | 4 | 0 |
| 2 | D | 54 | 0 | 24 | 6 | 0 |
| 2 | E | 54 | 0 | 24 | 7 | 0 |
| 2 | F | 54 | 0 | 24 | 4 | 0 |
| All | All | 34884 | 0 | 35070 | 718 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (718) 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) |
|---|---|---|---|
| 1:E:250:GLY:HA2 | 2:E:1001:ADP:O2A | 1.46 | 1.15 |
| 1:E:84:MET:CE | 1:E:88:VAL:HG23 | 1.81 | 1.10 |
| 1:F:84:MET:HE3 | 1:F:88:VAL:HG23 | 1.11 | 1.10 |
| 1:C:84:MET:CE | 1:C:88:VAL:HG23 | 1.81 | 1.10 |
| 1:F:84:MET:CE | 1:F:88:VAL:HG23 | 1.82 | 1.10 |
| 1:B:250:GLY:HA2 | 2:B:1001:ADP:O2A | 1.50 | 1.09 |
| 1:B:84:MET:CE | 1:B:88:VAL:HG23 | 1.81 | 1.09 |
| 1:D:84:MET:CE | 1:D:88:VAL:HG23 | 1.81 | 1.09 |
| 1:B:84:MET:HE3 | 1:B:88:VAL:HG23 | 1.11 | 1.08 |
| 1:A:84:MET:CE | 1:A:88:VAL:HG23 | 1.81 | 1.08 |
| 1:A:84:MET:HE3 | 1:A:88:VAL:HG23 | 1.11 | 1.08 |
| 1:C:84:MET:HE3 | 1:C:88:VAL:HG23 | 1.11 | 1.07 |
| 1:E:84:MET:HE3 | 1:E:88:VAL:HG23 | 1.11 | 1.05 |
| 1:D:84:MET:HE3 | 1:D:88:VAL:HG23 | 1.11 | 1.05 |
| 1:D:574:LEU:HD21 | 1:D:576:PHE:CE2 | 1.94 | 1.03 |
| 1:A:574:LEU:HD21 | 1:A:576:PHE:CE2 | 1.94 | 1.02 |
| 1:C:574:LEU:HD21 | 1:C:576:PHE:CE2 | 1.94 | 1.02 |
| 1:B:574:LEU:HD21 | 1:B:576:PHE:CE2 | 1.94 | 1.02 |
| 1:F:574:LEU:HD21 | 1:F:576:PHE:CE2 | 1.94 | 1.01 |
| 1:E:574:LEU:HD21 | 1:E:576:PHE:CE2 | 1.94 | 1.01 |
| 1:A:250:GLY:HA2 | 2:A:1001:ADP:O2A | 1.62 | 1.00 |
| 1:A:84:MET:HE3 | 1:A:88:VAL:CG2 | 1.95 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:84:MET:HE3 | 1:F:88:VAL:CG2 | 1.96 | 0.96 |
| 1:E:84:MET:HE3 | 1:E:88:VAL:CG2 | 1.95 | 0.96 |
| 1:B:84:MET:HE3 | 1:B:88:VAL:CG2 | 1.95 | 0.96 |
| 1:D:84:MET:HE3 | 1:D:88:VAL:CG2 | 1.95 | 0.95 |
| 1:C:84:MET:HE3 | 1:C:88:VAL:CG2 | 1.95 | 0.94 |
| 1:A:84:MET:CE | 1:A:88:VAL:CG2 | 2.47 | 0.93 |
| 1:B:84:MET:CE | 1:B:88:VAL:CG2 | 2.47 | 0.93 |
| 1:F:84:MET:CE | 1:F:88:VAL:CG2 | 2.47 | 0.92 |
| 1:A:574:LEU:HD21 | 1:A:576:PHE:CZ | 2.04 | 0.92 |
| 1:D:84:MET:CE | 1:D:88:VAL:CG2 | 2.47 | 0.92 |
| 1:F:574:LEU:HD21 | 1:F:576:PHE:CZ | 2.04 | 0.92 |
| 1:C:574:LEU:HD21 | 1:C:576:PHE:CZ | 2.04 | 0.92 |
| 1:D:574:LEU:HD21 | 1:D:576:PHE:CZ | 2.04 | 0.92 |
| 1:E:574:LEU:HD21 | 1:E:576:PHE:CZ | 2.04 | 0.92 |
| 1:B:574:LEU:HD21 | 1:B:576:PHE:CZ | 2.04 | 0.92 |
| 1:C:84:MET:CE | 1:C:88:VAL:CG2 | 2.47 | 0.91 |
| 1:E:84:MET:CE | 1:E:88:VAL:CG2 | 2.47 | 0.90 |
| 1:D:250:GLY:HA2 | 2:D:1001:ADP:O2A | 1.77 | 0.85 |
| 1:E:250:GLY:CA | 2:E:1001:ADP:O2A | 2.26 | 0.82 |
| 1:B:250:GLY:CA | 2:B:1001:ADP:O2A | 2.27 | 0.82 |
| 1:A:606:THR:HG22 | 1:B:545:PRO:HB2 | 1.63 | 0.79 |
| 1:A:545:PRO:HB2 | 1:F:606:THR:HG22 | 1.64 | 0.79 |
| 1:C:524:LYS:HG3 | 2:C:1002:ADP:O2B | 1.84 | 0.77 |
| 1:A:250:GLY:CA | 2:A:1001:ADP:O2A | 2.33 | 0.77 |
| 1:C:574:LEU:HD23 | 1:C:619:ILE:HG23 | 1.69 | 0.74 |
| 1:A:574:LEU:HD23 | 1:A:619:ILE:HG23 | 1.69 | 0.74 |
| 1:B:574:LEU:HD23 | 1:B:619:ILE:HG23 | 1.69 | 0.74 |
| 1:A:524:LYS:HG3 | 2:A:1002:ADP:O2B | 1.88 | 0.73 |
| 1:E:574:LEU:HD23 | 1:E:619:ILE:HG23 | 1.69 | 0.73 |
| 1:F:688:THR:HG21 | 2:F:1002:ADP:H1' | 1.70 | 0.73 |
| 1:E:454:TRP:CZ2 | 1:E:458:GLN:OE1 | 2.41 | 0.73 |
| 1:C:250:GLY:HA2 | 2:C:1001:ADP:O2A | 1.89 | 0.73 |
| 1:D:574:LEU:HD23 | 1:D:619:ILE:HG23 | 1.69 | 0.73 |
| 1:F:574:LEU:HD23 | 1:F:619:ILE:HG23 | 1.69 | 0.72 |
| 1:E:688:THR:HG21 | 2:E:1002:ADP:H1' | 1.71 | 0.72 |
| 1:D:606:THR:HG22 | 1:E:545:PRO:HB2 | 1.72 | 0.71 |
| 1:E:426:LYS:HZ2 | 1:E:446:ALA:H | 1.37 | 0.71 |
| 1:B:606:THR:HG22 | 1:C:545:PRO:HB2 | 1.70 | 0.71 |
| 1:B:426:LYS:HZ1 | 1:B:446:ALA:H | 1.38 | 0.71 |
| 1:E:550:MET:SD | 1:E:558:ASN:HB2 | 2.31 | 0.70 |
| 1:F:550:MET:SD | 1:F:558:ASN:HB2 | 2.31 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:550:MET:SD | 1:C:558:ASN:HB2 | 2.31 | 0.70 |
| 1:D:550:MET:SD | 1:D:558:ASN:HB2 | 2.31 | 0.70 |
| 1:A:550:MET:SD | 1:A:558:ASN:HB2 | 2.31 | 0.70 |
| 1:C:606:THR:HG22 | 1:D:545:PRO:HB2 | 1.72 | 0.70 |
| 1:B:524:LYS:HG3 | 2:B:1002:ADP:O2B | 1.92 | 0.70 |
| 1:B:550:MET:SD | 1:B:558:ASN:HB2 | 2.31 | 0.69 |
| 1:E:606:THR:HG22 | 1:F:545:PRO:HB2 | 1.73 | 0.69 |
| 1:A:545:PRO:HB2 | 1:F:606:THR:CG2 | 2.23 | 0.69 |
| 1:F:750:ASN:HA | 1:F:753:ARG:NH1 | 2.09 | 0.68 |
| 1:C:750:ASN:HA | 1:C:753:ARG:NH1 | 2.09 | 0.68 |
| 1:B:750:ASN:HA | 1:B:753:ARG:NH1 | 2.09 | 0.68 |
| 1:D:426:LYS:HZ2 | 1:D:446:ALA:H | 1.41 | 0.67 |
| 1:E:750:ASN:HA | 1:E:753:ARG:NH1 | 2.09 | 0.67 |
| 1:A:750:ASN:HA | 1:A:753:ARG:NH1 | 2.08 | 0.67 |
| 1:F:524:LYS:HG3 | 2:F:1002:ADP:O2B | 1.95 | 0.67 |
| 1:D:750:ASN:HA | 1:D:753:ARG:NH1 | 2.09 | 0.67 |
| 1:C:84:MET:HE1 | 1:C:88:VAL:CG2 | 2.25 | 0.66 |
| 1:B:84:MET:HE1 | 1:B:88:VAL:CG2 | 2.25 | 0.66 |
| 1:E:524:LYS:HG3 | 2:E:1002:ADP:O2B | 1.95 | 0.66 |
| 1:A:84:MET:HE1 | 1:A:88:VAL:CG2 | 2.26 | 0.66 |
| 1:D:84:MET:HE1 | 1:D:88:VAL:CG2 | 2.25 | 0.66 |
| 1:F:650:GLU:OE2 | 1:F:653:ARG:NH2 | 2.29 | 0.66 |
| 1:A:606:THR:CG2 | 1:B:545:PRO:HB2 | 2.26 | 0.66 |
| 1:D:524:LYS:HG3 | 2:D:1002:ADP:O2B | 1.95 | 0.66 |
| 1:A:650:GLU:OE2 | 1:A:653:ARG:NH2 | 2.29 | 0.65 |
| 1:F:84:MET:HE1 | 1:F:88:VAL:CG2 | 2.26 | 0.65 |
| 1:A:36:ASN:O | 1:A:85:ASN:ND2 | 2.30 | 0.65 |
| 1:D:250:GLY:CA | 2:D:1001:ADP:O2A | 2.44 | 0.65 |
| 1:A:426:LYS:HZ2 | 1:A:446:ALA:H | 1.42 | 0.65 |
| 1:D:650:GLU:OE2 | 1:D:653:ARG:NH2 | 2.29 | 0.65 |
| 1:E:650:GLU:OE2 | 1:E:653:ARG:NH2 | 2.29 | 0.65 |
| 1:B:650:GLU:OE2 | 1:B:653:ARG:NH2 | 2.29 | 0.65 |
| 1:C:650:GLU:OE2 | 1:C:653:ARG:NH2 | 2.29 | 0.65 |
| 1:E:36:ASN:O | 1:E:85:ASN:ND2 | 2.30 | 0.65 |
| 1:C:550:MET:SD | 1:C:558:ASN:CB | 2.85 | 0.65 |
| 1:D:36:ASN:O | 1:D:85:ASN:ND2 | 2.30 | 0.64 |
| 1:E:84:MET:HE1 | 1:E:88:VAL:CG2 | 2.25 | 0.64 |
| 1:F:36:ASN:O | 1:F:85:ASN:ND2 | 2.30 | 0.64 |
| 1:B:550:MET:SD | 1:B:558:ASN:CB | 2.85 | 0.64 |
| 1:D:550:MET:SD | 1:D:558:ASN:CB | 2.86 | 0.64 |
| 1:B:36:ASN:O | 1:B:85:ASN:ND2 | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:550:MET:SD | 1:E:558:ASN:CB | 2.85 | 0.64 |
| 1:F:426:LYS:HZ2 | 1:F:446:ALA:H | 1.44 | 0.64 |
| 1:C:36:ASN:O | 1:C:85:ASN:ND2 | 2.30 | 0.64 |
| 1:D:606:THR:CG2 | 1:E:545:PRO:HB2 | 2.28 | 0.64 |
| 1:F:478:ASP:OD1 | 1:F:662:ARG:NH2 | 2.31 | 0.63 |
| 1:A:550:MET:SD | 1:A:558:ASN:CB | 2.86 | 0.63 |
| 1:B:478:ASP:OD1 | 1:B:662:ARG:NH2 | 2.31 | 0.63 |
| 1:A:478:ASP:OD1 | 1:A:662:ARG:NH2 | 2.31 | 0.63 |
| 1:F:550:MET:SD | 1:F:558:ASN:CB | 2.86 | 0.63 |
| 1:C:426:LYS:HZ2 | 1:C:446:ALA:H | 1.46 | 0.63 |
| 1:D:478:ASP:OD1 | 1:D:662:ARG:NH2 | 2.31 | 0.63 |
| 1:B:688:THR:HG21 | 2:B:1002:ADP:H1' | 1.79 | 0.63 |
| 1:C:478:ASP:OD1 | 1:C:662:ARG:NH2 | 2.31 | 0.63 |
| 1:D:232:GLU:CD | 1:E:442:MET:HE3 | 2.23 | 0.63 |
| 1:E:478:ASP:OD1 | 1:E:662:ARG:NH2 | 2.31 | 0.63 |
| 1:A:365:ARG:HH22 | 1:B:458:GLN:HE22 | 1.47 | 0.62 |
| 1:C:322:ARG:HH12 | 1:D:317:HIS:HD2 | 1.48 | 0.62 |
| 1:C:688:THR:HG21 | 2:C:1002:ADP:H1' | 1.82 | 0.62 |
| 1:A:458:GLN:HE22 | 1:F:365:ARG:HH22 | 1.48 | 0.61 |
| 1:A:574:LEU:HB3 | 1:A:619:ILE:HA | 1.84 | 0.60 |
| 1:B:606:THR:CG2 | 1:C:545:PRO:HB2 | 2.31 | 0.60 |
| 1:C:574:LEU:HB3 | 1:C:619:ILE:HA | 1.84 | 0.60 |
| 1:D:688:THR:HG21 | 2:D:1002:ADP:H1' | 1.82 | 0.60 |
| 1:D:574:LEU:HB3 | 1:D:619:ILE:HA | 1.84 | 0.60 |
| 1:D:229:LEU:HD21 | 1:E:423:ILE:HD12 | 1.83 | 0.59 |
| 1:E:574:LEU:HB3 | 1:E:619:ILE:HA | 1.84 | 0.59 |
| 1:B:574:LEU:HB3 | 1:B:619:ILE:HA | 1.84 | 0.58 |
| 1:E:318:GLY:H | 1:F:317:HIS:CD2 | 2.21 | 0.58 |
| 1:F:574:LEU:HB3 | 1:F:619:ILE:HA | 1.84 | 0.58 |
| 1:F:389:LYS:NZ | 1:F:443:ASN:O | 2.29 | 0.58 |
| 1:A:520:PRO:HG3 | 1:A:624:ASN:HD22 | 1.69 | 0.58 |
| 1:A:381:LEU:HB3 | 1:A:396:LEU:HD13 | 1.86 | 0.58 |
| 1:A:688:THR:HG21 | 2:A:1002:ADP:H1' | 1.86 | 0.58 |
| 1:B:520:PRO:HG3 | 1:B:624:ASN:HD22 | 1.69 | 0.58 |
| 1:E:520:PRO:HG3 | 1:E:624:ASN:HD22 | 1.69 | 0.58 |
| 1:F:520:PRO:HG3 | 1:F:624:ASN:HD22 | 1.69 | 0.58 |
| 1:D:381:LEU:HB3 | 1:D:396:LEU:HD13 | 1.86 | 0.58 |
| 1:E:322:ARG:HH22 | 1:F:317:HIS:CD2 | 2.22 | 0.58 |
| 1:E:381:LEU:HB3 | 1:E:396:LEU:HD13 | 1.86 | 0.58 |
| 1:F:381:LEU:HB3 | 1:F:396:LEU:HD13 | 1.86 | 0.58 |
| 1:B:381:LEU:HB3 | 1:B:396:LEU:HD13 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:218:GLU:O | 1:E:424:ARG:NH1 | 2.37 | 0.57 |
| 1:C:381:LEU:HB3 | 1:C:396:LEU:HD13 | 1.86 | 0.57 |
| 1:E:606:THR:CG2 | 1:F:545:PRO:HB2 | 2.34 | 0.57 |
| 1:D:520:PRO:HG3 | 1:D:624:ASN:HD22 | 1.69 | 0.57 |
| 1:F:84:MET:CE | 1:F:88:VAL:HG21 | 2.35 | 0.57 |
| 1:C:520:PRO:HG3 | 1:C:624:ASN:HD22 | 1.69 | 0.56 |
| 1:E:84:MET:CE | 1:E:88:VAL:HG21 | 2.34 | 0.56 |
| 1:F:246:PRO:HG2 | 1:F:371:ILE:HD11 | 1.88 | 0.56 |
| 1:A:84:MET:CE | 1:A:88:VAL:HG21 | 2.34 | 0.56 |
| 1:C:606:THR:CG2 | 1:D:545:PRO:HB2 | 2.35 | 0.56 |
| 1:C:389:LYS:NZ | 1:C:443:ASN:O | 2.29 | 0.56 |
| 1:A:229:LEU:HD21 | 1:B:423:ILE:HD12 | 1.88 | 0.56 |
| 1:E:111:GLY:H | 1:E:175:ILE:HB | 1.71 | 0.56 |
| 1:E:312:LYS:HE2 | 1:F:315:LYS:HZ3 | 1.71 | 0.56 |
| 1:E:246:PRO:HG2 | 1:E:371:ILE:HD11 | 1.88 | 0.56 |
| 1:F:574:LEU:CD2 | 1:F:576:PHE:CE2 | 2.82 | 0.56 |
| 1:A:246:PRO:HG2 | 1:A:371:ILE:HD11 | 1.88 | 0.55 |
| 1:B:556:GLU:HG3 | 1:B:603:GLN:HG3 | 1.89 | 0.55 |
| 1:D:111:GLY:H | 1:D:175:ILE:HB | 1.71 | 0.55 |
| 1:A:317:HIS:CD2 | 1:F:318:GLY:H | 2.25 | 0.55 |
| 1:C:246:PRO:HG2 | 1:C:371:ILE:HD11 | 1.88 | 0.55 |
| 1:D:84:MET:CE | 1:D:88:VAL:HG21 | 2.34 | 0.55 |
| 1:F:111:GLY:H | 1:F:175:ILE:HB | 1.71 | 0.55 |
| 1:A:423:ILE:HD12 | 1:F:229:LEU:HD21 | 1.89 | 0.55 |
| 1:A:763:GLN:HE22 | 1:A:765:SER:HB2 | 1.72 | 0.55 |
| 1:B:111:GLY:H | 1:B:175:ILE:HB | 1.71 | 0.55 |
| 1:A:589:ASN:OD1 | 1:A:590:ILE:N | 2.40 | 0.55 |
| 1:D:246:PRO:HG2 | 1:D:371:ILE:HD11 | 1.88 | 0.55 |
| 1:C:312:LYS:HE2 | 1:D:315:LYS:HZ3 | 1.72 | 0.55 |
| 1:D:548:LEU:HD23 | 1:D:582:ILE:HD13 | 1.89 | 0.55 |
| 1:A:702:SER:OG | 1:F:502:LYS:NZ | 2.40 | 0.55 |
| 1:E:548:LEU:HD23 | 1:E:582:ILE:HD13 | 1.89 | 0.55 |
| 1:A:111:GLY:H | 1:A:175:ILE:HB | 1.71 | 0.54 |
| 1:B:589:ASN:OD1 | 1:B:590:ILE:N | 2.40 | 0.54 |
| 1:C:111:GLY:H | 1:C:175:ILE:HB | 1.71 | 0.54 |
| 1:B:84:MET:CE | 1:B:88:VAL:HG21 | 2.34 | 0.54 |
| 1:F:556:GLU:HG3 | 1:F:603:GLN:HG3 | 1.89 | 0.54 |
| 1:A:556:GLU:HG3 | 1:A:603:GLN:HG3 | 1.89 | 0.54 |
| 1:B:763:GLN:HE22 | 1:B:765:SER:HB2 | 1.72 | 0.54 |
| 1:D:49:LEU:HD13 | 1:D:104:PRO:HD3 | 1.90 | 0.54 |
| 1:F:763:GLN:HE22 | 1:F:765:SER:HB2 | 1.72 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:49:LEU:HD13 | 1:A:104:PRO:HD3 | 1.90 | 0.54 |
| 1:B:49:LEU:HD13 | 1:B:104:PRO:HD3 | 1.90 | 0.54 |
| 1:C:548:LEU:HD23 | 1:C:582:ILE:HD13 | 1.89 | 0.54 |
| 1:D:589:ASN:OD1 | 1:D:590:ILE:N | 2.40 | 0.54 |
| 1:E:556:GLU:HG3 | 1:E:603:GLN:HG3 | 1.89 | 0.54 |
| 1:C:49:LEU:HD13 | 1:C:104:PRO:HD3 | 1.90 | 0.54 |
| 1:E:589:ASN:OD1 | 1:E:590:ILE:N | 2.40 | 0.54 |
| 1:F:49:LEU:HD13 | 1:F:104:PRO:HD3 | 1.90 | 0.54 |
| 1:A:84:MET:HE1 | 1:A:88:VAL:HG21 | 1.90 | 0.54 |
| 1:B:246:PRO:HG2 | 1:B:371:ILE:HD11 | 1.88 | 0.54 |
| 1:C:556:GLU:HG3 | 1:C:603:GLN:HG3 | 1.89 | 0.54 |
| 1:C:589:ASN:OD1 | 1:C:590:ILE:N | 2.40 | 0.54 |
| 1:E:49:LEU:HD13 | 1:E:104:PRO:HD3 | 1.90 | 0.54 |
| 1:F:319:GLU:OE1 | 1:F:323:ARG:NH2 | 2.41 | 0.54 |
| 1:B:84:MET:HE1 | 1:B:88:VAL:HG21 | 1.90 | 0.54 |
| 1:F:589:ASN:OD1 | 1:F:590:ILE:N | 2.40 | 0.54 |
| 1:B:312:LYS:HE2 | 1:C:315:LYS:HZ3 | 1.73 | 0.54 |
| 1:D:132:GLU:HA | 1:D:136:LYS:HD3 | 1.90 | 0.54 |
| 1:E:389:LYS:NZ | 1:E:443:ASN:O | 2.29 | 0.54 |
| 1:B:294:GLU:HG3 | 1:B:338:ARG:HH11 | 1.74 | 0.53 |
| 1:C:763:GLN:HE22 | 1:C:765:SER:HB2 | 1.72 | 0.53 |
| 1:F:548:LEU:HD23 | 1:F:582:ILE:HD13 | 1.89 | 0.53 |
| 1:B:548:LEU:HD23 | 1:B:582:ILE:HD13 | 1.89 | 0.53 |
| 1:D:556:GLU:HG3 | 1:D:603:GLN:HG3 | 1.89 | 0.53 |
| 1:C:322:ARG:HH22 | 1:D:317:HIS:CD2 | 2.25 | 0.53 |
| 1:D:574:LEU:CD2 | 1:D:576:PHE:CE2 | 2.82 | 0.53 |
| 1:A:319:GLU:OE1 | 1:A:323:ARG:NH2 | 2.41 | 0.53 |
| 1:D:508:MET:HE3 | 1:E:699:ILE:HD12 | 1.90 | 0.53 |
| 1:E:319:GLU:OE1 | 1:E:323:ARG:NH2 | 2.41 | 0.53 |
| 1:A:132:GLU:HA | 1:A:136:LYS:HD3 | 1.91 | 0.53 |
| 1:A:426:LYS:NZ | 1:A:446:ALA:H | 2.07 | 0.53 |
| 1:A:548:LEU:HD23 | 1:A:582:ILE:HD13 | 1.89 | 0.53 |
| 1:B:365:ARG:HH22 | 1:C:458:GLN:HE22 | 1.56 | 0.53 |
| 1:E:132:GLU:HA | 1:E:136:LYS:HD3 | 1.90 | 0.53 |
| 1:E:294:GLU:HG3 | 1:E:338:ARG:HH11 | 1.74 | 0.53 |
| 1:D:763:GLN:HE22 | 1:D:765:SER:HB2 | 1.72 | 0.53 |
| 1:E:763:GLN:HE22 | 1:E:765:SER:HB2 | 1.72 | 0.53 |
| 1:C:319:GLU:OE1 | 1:C:323:ARG:NH2 | 2.41 | 0.53 |
| 1:A:502:LYS:NZ | 1:B:702:SER:OG | 2.42 | 0.53 |
| 1:D:502:LYS:NZ | 1:E:702:SER:OG | 2.41 | 0.53 |
| 1:F:84:MET:HE1 | 1:F:88:VAL:HG21 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:484:ASP:OD1 | 1:A:484:ASP:N | 2.42 | 0.53 |
| 1:A:606:THR:CG2 | 1:B:545:PRO:CB | 2.87 | 0.53 |
| 1:B:574:LEU:CD2 | 1:B:576:PHE:CE2 | 2.82 | 0.53 |
| 1:D:319:GLU:OE1 | 1:D:323:ARG:NH2 | 2.41 | 0.53 |
| 1:B:307:ASP:N | 1:B:307:ASP:OD1 | 2.42 | 0.53 |
| 1:C:294:GLU:HG3 | 1:C:338:ARG:HH11 | 1.74 | 0.53 |
| 1:D:294:GLU:HG3 | 1:D:338:ARG:HH11 | 1.73 | 0.53 |
| 1:E:84:MET:HE1 | 1:E:88:VAL:HG21 | 1.90 | 0.53 |
| 1:F:426:LYS:NZ | 1:F:446:ALA:H | 2.07 | 0.53 |
| 1:A:458:GLN:HE22 | 1:F:365:ARG:NH2 | 2.07 | 0.52 |
| 1:B:319:GLU:OE1 | 1:B:323:ARG:NH2 | 2.41 | 0.52 |
| 1:F:294:GLU:HG3 | 1:F:338:ARG:HH11 | 1.74 | 0.52 |
| 1:A:294:GLU:HG3 | 1:A:338:ARG:HH11 | 1.74 | 0.52 |
| 1:A:356:ALA:O | 1:A:362:ARG:NH1 | 2.41 | 0.52 |
| 1:C:132:GLU:HA | 1:C:136:LYS:HD3 | 1.90 | 0.52 |
| 1:C:448:THR:OG1 | 1:C:450:ASP:OD1 | 2.27 | 0.52 |
| 1:F:132:GLU:HA | 1:F:136:LYS:HD3 | 1.90 | 0.52 |
| 1:A:365:ARG:NH2 | 1:B:458:GLN:HE22 | 2.06 | 0.52 |
| 1:A:545:PRO:CB | 1:F:606:THR:CG2 | 2.87 | 0.52 |
| 1:B:132:GLU:HA | 1:B:136:LYS:HD3 | 1.90 | 0.52 |
| 1:C:574:LEU:CD2 | 1:C:576:PHE:CE2 | 2.82 | 0.52 |
| 1:E:356:ALA:O | 1:E:362:ARG:NH1 | 2.41 | 0.52 |
| 1:B:318:GLY:H | 1:C:317:HIS:CD2 | 2.28 | 0.52 |
| 1:B:484:ASP:OD1 | 1:B:484:ASP:N | 2.42 | 0.52 |
| 1:A:307:ASP:OD1 | 1:A:307:ASP:N | 2.42 | 0.52 |
| 1:A:516:PHE:HB3 | 1:A:643:ILE:HB | 1.92 | 0.52 |
| 1:B:516:PHE:HB3 | 1:B:643:ILE:HB | 1.92 | 0.52 |
| 1:C:84:MET:HE1 | 1:C:88:VAL:HG21 | 1.90 | 0.52 |
| 1:C:426:LYS:NZ | 1:C:446:ALA:H | 2.07 | 0.52 |
| 1:C:516:PHE:HB3 | 1:C:643:ILE:HB | 1.91 | 0.52 |
| 1:D:84:MET:HE1 | 1:D:88:VAL:HG21 | 1.90 | 0.52 |
| 1:E:307:ASP:OD1 | 1:E:307:ASP:N | 2.43 | 0.52 |
| 1:D:307:ASP:N | 1:D:307:ASP:OD1 | 2.42 | 0.52 |
| 1:E:448:THR:OG1 | 1:E:450:ASP:OD1 | 2.27 | 0.52 |
| 1:A:318:GLY:H | 1:B:317:HIS:CD2 | 2.28 | 0.51 |
| 1:D:426:LYS:NZ | 1:D:446:ALA:H | 2.07 | 0.51 |
| 1:F:250:GLY:HA2 | 2:F:1001:ADP:O2A | 2.10 | 0.51 |
| 1:C:307:ASP:OD1 | 1:C:307:ASP:N | 2.43 | 0.51 |
| 1:B:322:ARG:HH12 | 1:C:317:HIS:HD2 | 1.59 | 0.51 |
| 1:D:448:THR:OG1 | 1:D:450:ASP:OD1 | 2.27 | 0.51 |
| 1:E:426:LYS:NZ | 1:E:446:ALA:H | 2.07 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:476:TRP:HE1 | 1:E:534:GLU:HG3 | 1.75 | 0.51 |
| 1:A:378:LEU:HA | 1:A:381:LEU:HD23 | 1.93 | 0.51 |
| 1:A:315:LYS:HZ1 | 1:F:316:THR:HA | 1.76 | 0.51 |
| 1:B:322:ARG:HH22 | 1:C:317:HIS:CD2 | 2.29 | 0.51 |
| 1:C:378:LEU:HA | 1:C:381:LEU:HD23 | 1.92 | 0.51 |
| 1:D:627:ASP:OD1 | 1:D:627:ASP:N | 2.44 | 0.51 |
| 1:E:322:ARG:HH12 | 1:F:317:HIS:HD2 | 1.59 | 0.51 |
| 1:F:516:PHE:HB3 | 1:F:643:ILE:HB | 1.92 | 0.51 |
| 1:C:365:ARG:HH22 | 1:D:458:GLN:HE22 | 1.59 | 0.51 |
| 1:D:516:PHE:HB3 | 1:D:643:ILE:HB | 1.92 | 0.51 |
| 1:B:500:PRO:O | 1:B:504:LEU:HG | 2.11 | 0.51 |
| 1:C:84:MET:CE | 1:C:88:VAL:HG21 | 2.35 | 0.51 |
| 1:D:438:ASP:OD1 | 1:D:438:ASP:N | 2.44 | 0.51 |
| 1:C:476:TRP:HE1 | 1:C:534:GLU:HG3 | 1.75 | 0.51 |
| 1:E:648:PRO:O | 1:E:653:ARG:NH1 | 2.44 | 0.51 |
| 1:F:476:TRP:HE1 | 1:F:534:GLU:HG3 | 1.75 | 0.51 |
| 1:A:476:TRP:HE1 | 1:A:534:GLU:HG3 | 1.75 | 0.50 |
| 1:C:648:PRO:O | 1:C:653:ARG:NH1 | 2.44 | 0.50 |
| 1:A:730:GLU:O | 1:A:732:ARG:NH1 | 2.45 | 0.50 |
| 1:B:648:PRO:O | 1:B:653:ARG:NH1 | 2.44 | 0.50 |
| 1:D:476:TRP:HE1 | 1:D:534:GLU:HG3 | 1.75 | 0.50 |
| 1:E:627:ASP:N | 1:E:627:ASP:OD1 | 2.44 | 0.50 |
| 1:A:627:ASP:OD1 | 1:A:627:ASP:N | 2.44 | 0.50 |
| 1:B:356:ALA:O | 1:B:362:ARG:NH1 | 2.41 | 0.50 |
| 1:B:378:LEU:HA | 1:B:381:LEU:HD23 | 1.93 | 0.50 |
| 1:B:476:TRP:HE1 | 1:B:534:GLU:HG3 | 1.75 | 0.50 |
| 1:C:627:ASP:OD1 | 1:C:627:ASP:N | 2.44 | 0.50 |
| 1:D:730:GLU:O | 1:D:732:ARG:NH1 | 2.45 | 0.50 |
| 1:E:574:LEU:CD2 | 1:E:576:PHE:CE2 | 2.82 | 0.50 |
| 1:C:730:GLU:O | 1:C:732:ARG:NH1 | 2.45 | 0.50 |
| 1:F:730:GLU:O | 1:F:732:ARG:NH1 | 2.45 | 0.50 |
| 1:A:648:PRO:O | 1:A:653:ARG:NH1 | 2.44 | 0.50 |
| 1:D:648:PRO:O | 1:D:653:ARG:NH1 | 2.44 | 0.50 |
| 1:D:378:LEU:HA | 1:D:381:LEU:HD23 | 1.93 | 0.50 |
| 1:E:516:PHE:HB3 | 1:E:643:ILE:HB | 1.91 | 0.50 |
| 1:E:730:GLU:O | 1:E:732:ARG:NH1 | 2.45 | 0.50 |
| 1:E:454:TRP:CH2 | 1:E:458:GLN:OE1 | 2.64 | 0.50 |
| 1:E:521:GLY:N | 2:E:1002:ADP:O3B | 2.41 | 0.50 |
| 1:A:633:ILE:HG12 | 1:A:639:LEU:HD12 | 1.94 | 0.49 |
| 1:B:567:ARG:NH1 | 1:C:460:ASN:OD1 | 2.45 | 0.49 |
| 1:E:378:LEU:HA | 1:E:381:LEU:HD23 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:633:ILE:HG12 | 1:E:639:LEU:HD12 | 1.94 | 0.49 |
| 1:F:378:LEU:HA | 1:F:381:LEU:HD23 | 1.93 | 0.49 |
| 1:F:633:ILE:HG12 | 1:F:639:LEU:HD12 | 1.94 | 0.49 |
| 1:A:550:MET:SD | 1:A:558:ASN:HB3 | 2.53 | 0.49 |
| 1:A:574:LEU:CD2 | 1:A:576:PHE:CE2 | 2.82 | 0.49 |
| 1:C:550:MET:SD | 1:C:558:ASN:HB3 | 2.52 | 0.49 |
| 1:F:648:PRO:O | 1:F:653:ARG:NH1 | 2.44 | 0.49 |
| 1:B:426:LYS:NZ | 1:B:446:ALA:H | 2.07 | 0.49 |
| 1:C:204:ASP:OD1 | 1:C:204:ASP:N | 2.46 | 0.49 |
| 1:D:204:ASP:OD1 | 1:D:204:ASP:N | 2.46 | 0.49 |
| 1:D:571:PRO:HB3 | 1:D:616:ASN:ND2 | 2.28 | 0.49 |
| 1:D:633:ILE:HG12 | 1:D:639:LEU:HD12 | 1.94 | 0.49 |
| 1:E:571:PRO:HB3 | 1:E:616:ASN:ND2 | 2.28 | 0.49 |
| 1:B:730:GLU:O | 1:B:732:ARG:NH1 | 2.45 | 0.49 |
| 1:E:559:VAL:HG11 | 1:E:603:GLN:HB3 | 1.95 | 0.49 |
| 1:B:633:ILE:HG12 | 1:B:639:LEU:HD12 | 1.94 | 0.49 |
| 1:C:318:GLY:H | 1:D:317:HIS:CD2 | 2.31 | 0.49 |
| 1:A:77:CYS:SG | 1:A:78:SER:N | 2.86 | 0.49 |
| 1:A:559:VAL:HG11 | 1:A:603:GLN:HB3 | 1.95 | 0.49 |
| 1:B:559:VAL:HG11 | 1:B:603:GLN:HB3 | 1.95 | 0.49 |
| 1:C:559:VAL:HG11 | 1:C:603:GLN:HB3 | 1.95 | 0.49 |
| 1:D:377:ARG:NH2 | 1:D:403:THR:O | 2.46 | 0.49 |
| 1:D:389:LYS:NZ | 1:D:443:ASN:O | 2.29 | 0.49 |
| 1:E:567:ARG:NH1 | 1:F:460:ASN:OD1 | 2.45 | 0.49 |
| 1:F:372:PRO:O | 1:F:377:ARG:NH1 | 2.46 | 0.49 |
| 1:F:550:MET:SD | 1:F:558:ASN:HB3 | 2.52 | 0.49 |
| 1:A:481:GLY:HA3 | 1:A:652:SER:HB2 | 1.95 | 0.49 |
| 1:C:77:CYS:SG | 1:C:78:SER:N | 2.86 | 0.49 |
| 1:D:77:CYS:SG | 1:D:78:SER:N | 2.86 | 0.49 |
| 1:D:372:PRO:O | 1:D:377:ARG:NH1 | 2.46 | 0.49 |
| 1:F:559:VAL:HG11 | 1:F:603:GLN:HB3 | 1.95 | 0.49 |
| 1:B:481:GLY:HA3 | 1:B:652:SER:HB2 | 1.95 | 0.49 |
| 1:C:356:ALA:O | 1:C:362:ARG:NH1 | 2.41 | 0.49 |
| 1:C:571:PRO:HB3 | 1:C:616:ASN:ND2 | 2.28 | 0.49 |
| 1:E:550:MET:SD | 1:E:558:ASN:HB3 | 2.52 | 0.49 |
| 1:F:77:CYS:SG | 1:F:78:SER:N | 2.86 | 0.49 |
| 1:A:372:PRO:O | 1:A:377:ARG:NH1 | 2.46 | 0.48 |
| 1:A:389:LYS:NZ | 1:A:443:ASN:O | 2.29 | 0.48 |
| 1:B:77:CYS:SG | 1:B:78:SER:N | 2.86 | 0.48 |
| 1:C:484:ASP:OD1 | 1:C:484:ASP:N | 2.42 | 0.48 |
| 1:C:633:ILE:HG12 | 1:C:639:LEU:HD12 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:356:ALA:O | 1:D:362:ARG:NH1 | 2.41 | 0.48 |
| 1:D:550:MET:SD | 1:D:558:ASN:HB3 | 2.52 | 0.48 |
| 1:D:559:VAL:HG11 | 1:D:603:GLN:HB3 | 1.95 | 0.48 |
| 1:A:377:ARG:NH2 | 1:A:403:THR:O | 2.46 | 0.48 |
| 1:C:372:PRO:O | 1:C:377:ARG:NH1 | 2.46 | 0.48 |
| 1:C:426:LYS:NZ | 1:C:444:SER:O | 2.46 | 0.48 |
| 1:E:372:PRO:O | 1:E:377:ARG:NH1 | 2.46 | 0.48 |
| 1:F:377:ARG:NH2 | 1:F:403:THR:O | 2.46 | 0.48 |
| 1:B:550:MET:SD | 1:B:558:ASN:HB3 | 2.52 | 0.48 |
| 1:B:571:PRO:HB3 | 1:B:616:ASN:ND2 | 2.28 | 0.48 |
| 1:F:481:GLY:HA3 | 1:F:652:SER:HB2 | 1.95 | 0.48 |
| 1:F:571:PRO:HB3 | 1:F:616:ASN:ND2 | 2.28 | 0.48 |
| 1:E:377:ARG:NH2 | 1:E:403:THR:O | 2.46 | 0.48 |
| 1:B:372:PRO:O | 1:B:377:ARG:NH1 | 2.46 | 0.48 |
| 1:B:377:ARG:NH2 | 1:B:403:THR:O | 2.46 | 0.48 |
| 1:A:571:PRO:HB3 | 1:A:616:ASN:ND2 | 2.28 | 0.48 |
| 1:A:130:LEU:HD23 | 1:A:130:LEU:H | 1.78 | 0.48 |
| 1:B:426:LYS:NZ | 1:B:444:SER:O | 2.46 | 0.48 |
| 1:A:426:LYS:NZ | 1:A:444:SER:O | 2.47 | 0.48 |
| 1:D:521:GLY:N | 2:D:1002:ADP:O3B | 2.46 | 0.48 |
| 1:F:356:ALA:O | 1:F:362:ARG:NH1 | 2.41 | 0.48 |
| 1:A:448:THR:OG1 | 1:A:450:ASP:OD1 | 2.27 | 0.48 |
| 1:B:130:LEU:H | 1:B:130:LEU:HD23 | 1.78 | 0.48 |
| 1:A:460:ASN:OD1 | 1:F:567:ARG:NH1 | 2.47 | 0.47 |
| 1:B:627:ASP:OD1 | 1:B:627:ASP:N | 2.44 | 0.47 |
| 1:B:693:ARG:NH1 | 1:B:742:PHE:O | 2.48 | 0.47 |
| 1:C:377:ARG:NH2 | 1:C:403:THR:O | 2.46 | 0.47 |
| 1:E:77:CYS:SG | 1:E:78:SER:N | 2.86 | 0.47 |
| 1:A:693:ARG:NH1 | 1:A:742:PHE:O | 2.48 | 0.47 |
| 1:C:481:GLY:HA3 | 1:C:652:SER:HB2 | 1.95 | 0.47 |
| 1:E:481:GLY:HA3 | 1:E:652:SER:HB2 | 1.95 | 0.47 |
| 1:F:448:THR:OG1 | 1:F:450:ASP:OD1 | 2.27 | 0.47 |
| 1:C:130:LEU:HD23 | 1:C:130:LEU:H | 1.78 | 0.47 |
| 1:D:560:ARG:NH2 | 1:E:465:ARG:HD2 | 2.29 | 0.47 |
| 1:F:426:LYS:NZ | 1:F:444:SER:O | 2.46 | 0.47 |
| 1:E:365:ARG:HH22 | 1:F:458:GLN:HE22 | 1.62 | 0.47 |
| 1:F:693:ARG:NH1 | 1:F:742:PHE:O | 2.48 | 0.47 |
| 1:D:130:LEU:HD23 | 1:D:130:LEU:H | 1.79 | 0.47 |
| 1:E:426:LYS:NZ | 1:E:444:SER:O | 2.47 | 0.47 |
| 1:B:45:LYS:HD2 | 1:B:45:LYS:HA | 1.70 | 0.47 |
| 1:C:514:VAL:HG22 | 1:C:641:GLN:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:693:ARG:NH1 | 1:C:742:PHE:O | 2.48 | 0.47 |
| 1:E:688:THR:CG2 | 2:E:1002:ADP:H1' | 2.44 | 0.47 |
| 1:D:481:GLY:HA3 | 1:D:652:SER:HB2 | 1.95 | 0.47 |
| 1:C:66:GLU:HB2 | 1:C:147:ARG:NE | 2.30 | 0.47 |
| 1:E:45:LYS:HD2 | 1:E:45:LYS:HA | 1.70 | 0.47 |
| 1:A:66:GLU:HB2 | 1:A:147:ARG:NE | 2.30 | 0.47 |
| 1:D:426:LYS:NZ | 1:D:444:SER:O | 2.47 | 0.47 |
| 1:D:514:VAL:HG22 | 1:D:641:GLN:HB2 | 1.97 | 0.47 |
| 1:E:484:ASP:N | 1:E:484:ASP:OD1 | 2.42 | 0.47 |
| 1:E:693:ARG:NH1 | 1:E:742:PHE:O | 2.48 | 0.47 |
| 1:F:307:ASP:OD1 | 1:F:307:ASP:N | 2.43 | 0.47 |
| 1:F:391:ALA:HB3 | 1:F:394:VAL:HG23 | 1.97 | 0.47 |
| 1:C:258:VAL:O | 1:C:262:THR:OG1 | 2.31 | 0.46 |
| 1:D:66:GLU:HB2 | 1:D:147:ARG:NE | 2.30 | 0.46 |
| 1:F:130:LEU:HD23 | 1:F:130:LEU:H | 1.78 | 0.46 |
| 1:B:337:GLN:O | 1:B:339:ALA:N | 2.49 | 0.46 |
| 1:B:391:ALA:HB3 | 1:B:394:VAL:HG23 | 1.97 | 0.46 |
| 1:E:130:LEU:HD23 | 1:E:130:LEU:H | 1.79 | 0.46 |
| 1:F:45:LYS:HD2 | 1:F:45:LYS:HA | 1.70 | 0.46 |
| 1:B:514:VAL:HG22 | 1:B:641:GLN:HB2 | 1.97 | 0.46 |
| 1:C:337:GLN:O | 1:C:339:ALA:N | 2.49 | 0.46 |
| 1:C:701:GLU:OE1 | 1:C:732:ARG:NH2 | 2.47 | 0.46 |
| 1:D:693:ARG:NH1 | 1:D:742:PHE:O | 2.48 | 0.46 |
| 1:F:66:GLU:HB2 | 1:F:147:ARG:NE | 2.30 | 0.46 |
| 1:A:514:VAL:HG22 | 1:A:641:GLN:HB2 | 1.97 | 0.46 |
| 1:C:358:ARG:NH1 | 1:C:366:GLU:OE2 | 2.49 | 0.46 |
| 1:C:391:ALA:HB3 | 1:C:394:VAL:HG23 | 1.97 | 0.46 |
| 1:A:337:GLN:O | 1:A:339:ALA:N | 2.49 | 0.46 |
| 1:A:438:ASP:OD1 | 1:A:438:ASP:N | 2.44 | 0.46 |
| 1:E:66:GLU:HB2 | 1:E:147:ARG:NE | 2.30 | 0.46 |
| 1:F:358:ARG:NH1 | 1:F:366:GLU:OE2 | 2.49 | 0.46 |
| 1:B:358:ARG:NH1 | 1:B:366:GLU:OE2 | 2.49 | 0.46 |
| 1:B:701:GLU:OE1 | 1:B:732:ARG:NH2 | 2.47 | 0.46 |
| 1:D:391:ALA:HB3 | 1:D:394:VAL:HG23 | 1.97 | 0.46 |
| 1:E:358:ARG:NH1 | 1:E:366:GLU:OE2 | 2.49 | 0.46 |
| 1:E:514:VAL:HG22 | 1:E:641:GLN:HB2 | 1.97 | 0.46 |
| 1:E:684:GLY:HA3 | 2:E:1002:ADP:C8 | 2.51 | 0.46 |
| 1:A:358:ARG:NH1 | 1:A:366:GLU:OE2 | 2.49 | 0.46 |
| 1:B:66:GLU:HB2 | 1:B:147:ARG:NE | 2.30 | 0.46 |
| 1:B:448:THR:OG1 | 1:B:450:ASP:OD1 | 2.27 | 0.46 |
| 1:D:358:ARG:NH1 | 1:D:366:GLU:OE2 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:391:ALA:HB3 | 1:E:394:VAL:HG23 | 1.97 | 0.46 |
| 1:C:614:LYS:NZ | 1:D:456:LEU:HD21 | 2.30 | 0.46 |
| 1:F:627:ASP:OD1 | 1:F:627:ASP:N | 2.44 | 0.46 |
| 1:F:337:GLN:O | 1:F:339:ALA:N | 2.49 | 0.45 |
| 1:F:484:ASP:OD1 | 1:F:484:ASP:N | 2.43 | 0.45 |
| 1:A:90:ASN:O | 1:A:93:ARG:NH1 | 2.50 | 0.45 |
| 1:D:337:GLN:O | 1:D:339:ALA:N | 2.49 | 0.45 |
| 1:D:606:THR:CG2 | 1:E:545:PRO:CB | 2.93 | 0.45 |
| 1:F:90:ASN:O | 1:F:93:ARG:NH1 | 2.50 | 0.45 |
| 1:F:514:VAL:HG22 | 1:F:641:GLN:HB2 | 1.97 | 0.45 |
| 1:A:322:ARG:HH22 | 1:B:317:HIS:CD2 | 2.35 | 0.45 |
| 1:E:90:ASN:O | 1:E:93:ARG:NH1 | 2.50 | 0.45 |
| 1:E:131:PHE:HD2 | 1:E:182:ILE:HD11 | 1.82 | 0.45 |
| 1:E:337:GLN:O | 1:E:339:ALA:N | 2.49 | 0.45 |
| 1:B:258:VAL:O | 1:B:262:THR:OG1 | 2.31 | 0.45 |
| 1:A:521:GLY:N | 2:A:1002:ADP:O3B | 2.48 | 0.45 |
| 1:B:131:PHE:HD2 | 1:B:182:ILE:HD11 | 1.82 | 0.45 |
| 1:B:606:THR:CG2 | 1:C:545:PRO:CB | 2.94 | 0.45 |
| 1:F:438:ASP:OD1 | 1:F:438:ASP:N | 2.44 | 0.45 |
| 1:A:317:HIS:CD2 | 1:F:322:ARG:HH22 | 2.34 | 0.45 |
| 1:A:391:ALA:HB3 | 1:A:394:VAL:HG23 | 1.97 | 0.45 |
| 1:D:90:ASN:O | 1:D:93:ARG:NH1 | 2.50 | 0.45 |
| 1:B:90:ASN:O | 1:B:93:ARG:NH1 | 2.50 | 0.45 |
| 1:E:270:ASN:HB3 | 1:E:272:PRO:HD2 | 1.99 | 0.45 |
| 1:A:316:THR:HA | 1:B:315:LYS:HZ1 | 1.81 | 0.45 |
| 1:D:215:GLN:O | 1:D:219:MET:HG2 | 2.17 | 0.45 |
| 1:F:270:ASN:HB3 | 1:F:272:PRO:HD2 | 1.99 | 0.45 |
| 1:C:90:ASN:O | 1:C:93:ARG:NH1 | 2.50 | 0.45 |
| 1:C:131:PHE:HD2 | 1:C:182:ILE:HD11 | 1.82 | 0.45 |
| 1:C:625:ARG:HE | 1:C:625:ARG:HB3 | 1.68 | 0.45 |
| 1:D:131:PHE:HD2 | 1:D:182:ILE:HD11 | 1.82 | 0.45 |
| 1:D:484:ASP:OD1 | 1:D:484:ASP:N | 2.42 | 0.45 |
| 1:F:215:GLN:O | 1:F:219:MET:HG2 | 2.17 | 0.45 |
| 1:B:389:LYS:NZ | 1:B:443:ASN:O | 2.29 | 0.45 |
| 1:F:131:PHE:HD2 | 1:F:182:ILE:HD11 | 1.82 | 0.45 |
| 1:A:131:PHE:HD2 | 1:A:182:ILE:HD11 | 1.82 | 0.44 |
| 1:A:565:LYS:HA | 1:A:568:GLN:HG2 | 1.99 | 0.44 |
| 1:B:565:LYS:HA | 1:B:568:GLN:HG2 | 1.99 | 0.44 |
| 1:C:565:LYS:HA | 1:C:568:GLN:HG2 | 1.99 | 0.44 |
| 1:E:215:GLN:O | 1:E:219:MET:HG2 | 2.17 | 0.44 |
| 1:C:215:GLN:O | 1:C:219:MET:HG2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:625:ARG:HE | 1:E:625:ARG:HB3 | 1.68 | 0.44 |
| 1:F:681:GLY:HA3 | 1:F:745:ARG:HH21 | 1.83 | 0.44 |
| 1:A:270:ASN:HB3 | 1:A:272:PRO:HD2 | 1.99 | 0.44 |
| 1:B:681:GLY:HA3 | 1:B:745:ARG:HH21 | 1.83 | 0.44 |
| 1:A:215:GLN:O | 1:A:219:MET:HG2 | 2.17 | 0.44 |
| 1:A:322:ARG:HH12 | 1:B:317:HIS:HD2 | 1.66 | 0.44 |
| 1:B:438:ASP:OD1 | 1:B:438:ASP:N | 2.44 | 0.44 |
| 1:D:219:MET:HE1 | 1:D:365:ARG:HG3 | 2.00 | 0.44 |
| 1:D:270:ASN:HB3 | 1:D:272:PRO:HD2 | 1.99 | 0.44 |
| 1:A:239:ARG:HD3 | 1:A:239:ARG:HA | 1.79 | 0.44 |
| 1:A:521:GLY:HA2 | 2:A:1002:ADP:O3B | 2.17 | 0.44 |
| 1:C:219:MET:HE1 | 1:C:365:ARG:HG3 | 2.00 | 0.44 |
| 1:C:681:GLY:HA3 | 1:C:745:ARG:HH21 | 1.83 | 0.44 |
| 1:A:212:GLN:HG2 | 1:A:369:ILE:HG22 | 2.00 | 0.44 |
| 1:A:567:ARG:NH1 | 1:B:460:ASN:OD1 | 2.50 | 0.44 |
| 1:B:212:GLN:HG2 | 1:B:369:ILE:HG22 | 2.00 | 0.44 |
| 1:F:565:LYS:HA | 1:F:568:GLN:HG2 | 1.99 | 0.44 |
| 1:A:219:MET:HE1 | 1:A:365:ARG:HG3 | 2.00 | 0.44 |
| 1:A:545:PRO:HB3 | 1:F:606:THR:HG23 | 1.99 | 0.44 |
| 1:D:429:LEU:HD23 | 1:D:429:LEU:H | 1.83 | 0.44 |
| 1:E:429:LEU:HD23 | 1:E:429:LEU:H | 1.83 | 0.44 |
| 1:B:219:MET:HE1 | 1:B:365:ARG:HG3 | 2.00 | 0.44 |
| 1:D:294:GLU:HG3 | 1:D:338:ARG:HD2 | 2.00 | 0.44 |
| 1:F:429:LEU:H | 1:F:429:LEU:HD23 | 1.83 | 0.44 |
| 1:C:312:LYS:CE | 1:D:315:LYS:HZ3 | 2.31 | 0.44 |
| 1:D:239:ARG:HD3 | 1:D:239:ARG:HA | 1.79 | 0.44 |
| 1:F:35:ASP:OD2 | 1:F:38:VAL:HB | 2.18 | 0.44 |
| 1:A:35:ASP:OD2 | 1:A:38:VAL:HB | 2.18 | 0.43 |
| 1:A:681:GLY:HA3 | 1:A:745:ARG:HH21 | 1.83 | 0.43 |
| 1:B:423:ILE:HG22 | 1:B:445:LEU:HD22 | 2.00 | 0.43 |
| 1:C:35:ASP:OD2 | 1:C:38:VAL:HB | 2.18 | 0.43 |
| 1:C:212:GLN:HG2 | 1:C:369:ILE:HG22 | 2.00 | 0.43 |
| 1:D:521:GLY:HA2 | 2:D:1002:ADP:O3B | 2.17 | 0.43 |
| 1:E:219:MET:HE1 | 1:E:365:ARG:HG3 | 2.00 | 0.43 |
| 1:E:294:GLU:HG3 | 1:E:338:ARG:HD2 | 2.00 | 0.43 |
| 1:C:423:ILE:HG22 | 1:C:445:LEU:HD22 | 2.00 | 0.43 |
| 1:E:35:ASP:OD2 | 1:E:38:VAL:HB | 2.18 | 0.43 |
| 1:F:155:ARG:HH12 | 1:F:386:LYS:HZ3 | 1.66 | 0.43 |
| 1:F:212:GLN:HG2 | 1:F:369:ILE:HG22 | 2.00 | 0.43 |
| 1:F:219:MET:HE1 | 1:F:365:ARG:HG3 | 2.00 | 0.43 |
| 1:B:215:GLN:O | 1:B:219:MET:HG2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:270:ASN:HB3 | 1:C:272:PRO:HD2 | 1.99 | 0.43 |
| 1:D:35:ASP:OD2 | 1:D:38:VAL:HB | 2.19 | 0.43 |
| 1:D:246:PRO:HD2 | 1:D:249:THR:HG21 | 2.00 | 0.43 |
| 1:D:655:ALA:HA | 1:D:658:LYS:HG2 | 2.01 | 0.43 |
| 1:D:681:GLY:HA3 | 1:D:745:ARG:HH21 | 1.82 | 0.43 |
| 1:B:270:ASN:HB3 | 1:B:272:PRO:HD2 | 1.99 | 0.43 |
| 1:C:606:THR:CG2 | 1:D:545:PRO:CB | 2.96 | 0.43 |
| 1:D:565:LYS:HA | 1:D:568:GLN:HG2 | 1.99 | 0.43 |
| 1:E:155:ARG:HH12 | 1:E:386:LYS:HZ3 | 1.66 | 0.43 |
| 1:E:476:TRP:CZ3 | 1:E:486:LYS:HG2 | 2.53 | 0.43 |
| 1:E:565:LYS:HA | 1:E:568:GLN:HG2 | 1.99 | 0.43 |
| 1:F:246:PRO:HD2 | 1:F:249:THR:HG21 | 2.00 | 0.43 |
| 1:F:423:ILE:HG22 | 1:F:445:LEU:HD22 | 2.00 | 0.43 |
| 1:A:155:ARG:HH12 | 1:A:386:LYS:HZ3 | 1.66 | 0.43 |
| 1:B:476:TRP:CZ3 | 1:B:486:LYS:HG2 | 2.53 | 0.43 |
| 1:B:601:ILE:HD13 | 1:B:604:ILE:HD12 | 2.00 | 0.43 |
| 1:C:506:PHE:CD2 | 1:D:699:ILE:HG12 | 2.53 | 0.43 |
| 1:A:52:PHE:N | 1:A:55:ASP:OD2 | 2.41 | 0.43 |
| 1:A:429:LEU:H | 1:A:429:LEU:HD23 | 1.83 | 0.43 |
| 1:B:35:ASP:OD2 | 1:B:38:VAL:HB | 2.18 | 0.43 |
| 1:C:294:GLU:HG3 | 1:C:338:ARG:HD2 | 2.00 | 0.43 |
| 1:C:488:GLU:O | 1:C:492:LEU:HD12 | 2.19 | 0.43 |
| 1:D:488:GLU:O | 1:D:492:LEU:HD12 | 2.19 | 0.43 |
| 1:D:258:VAL:O | 1:D:262:THR:OG1 | 2.31 | 0.43 |
| 1:E:681:GLY:HA3 | 1:E:745:ARG:HH21 | 1.83 | 0.43 |
| 1:A:294:GLU:HG3 | 1:A:338:ARG:HD2 | 2.00 | 0.43 |
| 1:A:424:ARG:NH1 | 1:F:218:GLU:O | 2.52 | 0.43 |
| 1:A:606:THR:HG23 | 1:B:545:PRO:HB3 | 2.00 | 0.43 |
| 1:B:429:LEU:HD23 | 1:B:429:LEU:H | 1.83 | 0.43 |
| 1:C:246:PRO:HD2 | 1:C:249:THR:HG21 | 2.00 | 0.43 |
| 1:C:476:TRP:CZ3 | 1:C:486:LYS:HG2 | 2.53 | 0.43 |
| 1:D:212:GLN:HG2 | 1:D:369:ILE:HG22 | 2.00 | 0.43 |
| 1:D:423:ILE:HG22 | 1:D:445:LEU:HD22 | 2.00 | 0.43 |
| 1:E:246:PRO:HD2 | 1:E:249:THR:HG21 | 2.00 | 0.43 |
| 1:E:601:ILE:HD13 | 1:E:604:ILE:HD12 | 2.00 | 0.43 |
| 1:A:218:GLU:O | 1:B:424:ARG:NH1 | 2.51 | 0.43 |
| 1:A:601:ILE:HD13 | 1:A:604:ILE:HD12 | 2.00 | 0.43 |
| 1:B:120:ASP:OD1 | 1:B:120:ASP:N | 2.52 | 0.43 |
| 1:B:246:PRO:HD2 | 1:B:249:THR:HG21 | 2.00 | 0.43 |
| 1:B:488:GLU:O | 1:B:492:LEU:HD12 | 2.19 | 0.43 |
| 1:C:601:ILE:HD13 | 1:C:604:ILE:HD12 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:655:ALA:HA | 1:C:658:LYS:HG2 | 2.01 | 0.43 |
| 1:E:655:ALA:HA | 1:E:658:LYS:HG2 | 2.01 | 0.43 |
| 1:A:476:TRP:CZ3 | 1:A:486:LYS:HG2 | 2.53 | 0.43 |
| 1:B:655:ALA:HA | 1:B:658:LYS:HG2 | 2.01 | 0.43 |
| 1:C:429:LEU:H | 1:C:429:LEU:HD23 | 1.83 | 0.43 |
| 1:E:212:GLN:HG2 | 1:E:369:ILE:HG22 | 2.00 | 0.43 |
| 1:F:476:TRP:CZ3 | 1:F:486:LYS:HG2 | 2.53 | 0.43 |
| 1:A:246:PRO:HD2 | 1:A:249:THR:HG21 | 2.00 | 0.42 |
| 1:C:120:ASP:OD1 | 1:C:120:ASP:N | 2.52 | 0.42 |
| 1:E:574:LEU:HG | 1:E:575:PHE:N | 2.34 | 0.42 |
| 1:B:204:ASP:OD1 | 1:B:204:ASP:N | 2.46 | 0.42 |
| 1:B:521:GLY:N | 2:B:1002:ADP:O3B | 2.45 | 0.42 |
| 1:D:155:ARG:HH12 | 1:D:386:LYS:HZ3 | 1.66 | 0.42 |
| 1:D:476:TRP:CZ3 | 1:D:486:LYS:HG2 | 2.53 | 0.42 |
| 1:D:701:GLU:OE1 | 1:D:732:ARG:NH2 | 2.47 | 0.42 |
| 1:E:438:ASP:OD1 | 1:E:438:ASP:N | 2.44 | 0.42 |
| 1:F:655:ALA:HA | 1:F:658:LYS:HG2 | 2.01 | 0.42 |
| 1:B:294:GLU:HG3 | 1:B:338:ARG:HD2 | 2.00 | 0.42 |
| 1:D:567:ARG:NH1 | 1:E:460:ASN:OD1 | 2.53 | 0.42 |
| 1:E:488:GLU:O | 1:E:492:LEU:HD12 | 2.19 | 0.42 |
| 1:F:574:LEU:HG | 1:F:575:PHE:N | 2.34 | 0.42 |
| 1:A:423:ILE:HG22 | 1:A:445:LEU:HD22 | 2.00 | 0.42 |
| 1:A:572:CYS:SG | 1:A:573:VAL:N | 2.93 | 0.42 |
| 1:A:574:LEU:HG | 1:A:575:PHE:N | 2.35 | 0.42 |
| 1:D:572:CYS:SG | 1:D:573:VAL:N | 2.93 | 0.42 |
| 1:E:423:ILE:HG22 | 1:E:445:LEU:HD22 | 2.00 | 0.42 |
| 1:F:572:CYS:SG | 1:F:573:VAL:N | 2.93 | 0.42 |
| 1:A:545:PRO:CB | 1:F:606:THR:HG23 | 2.49 | 0.42 |
| 1:A:655:ALA:HA | 1:A:658:LYS:HG2 | 2.01 | 0.42 |
| 1:B:574:LEU:HG | 1:B:575:PHE:N | 2.34 | 0.42 |
| 1:C:572:CYS:SG | 1:C:573:VAL:N | 2.93 | 0.42 |
| 1:E:572:CYS:SG | 1:E:573:VAL:N | 2.93 | 0.42 |
| 1:F:277:LYS:H | 1:F:277:LYS:HG2 | 1.70 | 0.42 |
| 1:F:488:GLU:O | 1:F:492:LEU:HD12 | 2.19 | 0.42 |
| 1:C:155:ARG:HH12 | 1:C:386:LYS:HZ3 | 1.66 | 0.42 |
| 1:C:425:LYS:NZ | 1:C:450:ASP:OD2 | 2.53 | 0.42 |
| 1:B:155:ARG:HH12 | 1:B:386:LYS:HZ3 | 1.66 | 0.42 |
| 1:B:273:GLU:O | 1:B:277:LYS:HE3 | 2.20 | 0.42 |
| 1:E:204:ASP:OD1 | 1:E:204:ASP:N | 2.46 | 0.42 |
| 1:F:294:GLU:HG3 | 1:F:338:ARG:HD2 | 2.00 | 0.42 |
| 1:C:273:GLU:O | 1:C:277:LYS:HE3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:574:LEU:HG | 1:D:575:PHE:N | 2.35 | 0.42 |
| 1:D:601:ILE:HD13 | 1:D:604:ILE:HD12 | 2.00 | 0.42 |
| 1:A:434:ASP:OD1 | 1:A:434:ASP:N | 2.53 | 0.42 |
| 1:A:519:PRO:HG3 | 1:A:647:LEU:HD22 | 2.02 | 0.42 |
| 1:B:573:VAL:HG23 | 1:B:618:PHE:HB3 | 2.02 | 0.42 |
| 1:E:606:THR:CG2 | 1:F:545:PRO:CB | 2.97 | 0.42 |
| 1:F:117:LEU:HD23 | 1:F:117:LEU:HA | 1.96 | 0.42 |
| 1:B:220:VAL:O | 1:B:223:PRO:HD2 | 2.20 | 0.42 |
| 1:C:438:ASP:OD1 | 1:C:438:ASP:N | 2.44 | 0.42 |
| 1:A:488:GLU:O | 1:A:492:LEU:HD12 | 2.19 | 0.41 |
| 1:B:117:LEU:HD23 | 1:B:117:LEU:HA | 1.96 | 0.41 |
| 1:B:267:PHE:CE2 | 1:B:289:ALA:HB1 | 2.55 | 0.41 |
| 1:C:220:VAL:O | 1:C:223:PRO:HD2 | 2.20 | 0.41 |
| 1:C:267:PHE:CE2 | 1:C:289:ALA:HB1 | 2.55 | 0.41 |
| 1:D:519:PRO:HG3 | 1:D:647:LEU:HD22 | 2.02 | 0.41 |
| 1:A:573:VAL:HG23 | 1:A:618:PHE:HB3 | 2.02 | 0.41 |
| 1:B:684:GLY:HA3 | 2:B:1002:ADP:C8 | 2.55 | 0.41 |
| 1:C:434:ASP:OD1 | 1:C:434:ASP:N | 2.53 | 0.41 |
| 1:C:494:GLN:NE2 | 1:C:534:GLU:OE1 | 2.50 | 0.41 |
| 1:E:220:VAL:O | 1:E:223:PRO:HD2 | 2.20 | 0.41 |
| 1:E:421:GLN:OE1 | 1:E:451:ASP:HA | 2.20 | 0.41 |
| 1:F:220:VAL:O | 1:F:223:PRO:HD2 | 2.20 | 0.41 |
| 1:F:421:GLN:OE1 | 1:F:451:ASP:HA | 2.21 | 0.41 |
| 1:A:273:GLU:O | 1:A:277:LYS:HE3 | 2.20 | 0.41 |
| 1:B:395:ASP:OD1 | 1:B:395:ASP:N | 2.53 | 0.41 |
| 1:C:421:GLN:OE1 | 1:C:451:ASP:HA | 2.21 | 0.41 |
| 1:E:52:PHE:N | 1:E:55:ASP:OD2 | 2.41 | 0.41 |
| 1:F:573:VAL:HG23 | 1:F:618:PHE:HB3 | 2.02 | 0.41 |
| 1:F:601:ILE:HD13 | 1:F:604:ILE:HD12 | 2.00 | 0.41 |
| 1:B:425:LYS:NZ | 1:B:450:ASP:OD2 | 2.52 | 0.41 |
| 1:C:574:LEU:HG | 1:C:575:PHE:N | 2.35 | 0.41 |
| 1:D:540:ILE:HG13 | 1:D:572:CYS:SG | 2.61 | 0.41 |
| 1:E:364:ASP:OD1 | 1:E:364:ASP:N | 2.46 | 0.41 |
| 1:C:319:GLU:HA | 1:C:322:ARG:HD2 | 2.03 | 0.41 |
| 1:C:508:MET:HE3 | 1:D:699:ILE:HD12 | 2.03 | 0.41 |
| 1:C:569:ALA:O | 1:C:572:CYS:HB2 | 2.21 | 0.41 |
| 1:C:670:VAL:HA | 1:C:733:ARG:HD3 | 2.03 | 0.41 |
| 1:F:519:PRO:HG3 | 1:F:647:LEU:HD22 | 2.02 | 0.41 |
| 1:F:670:VAL:HA | 1:F:733:ARG:HD3 | 2.03 | 0.41 |
| 1:A:220:VAL:O | 1:A:223:PRO:HD2 | 2.20 | 0.41 |
| 1:A:267:PHE:CE2 | 1:A:289:ALA:HB1 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:569:ALA:O | 1:B:572:CYS:HB2 | 2.21 | 0.41 |
| 1:C:573:VAL:HG23 | 1:C:618:PHE:HB3 | 2.02 | 0.41 |
| 1:C:600:VAL:O | 1:C:604:ILE:HG13 | 2.21 | 0.41 |
| 1:D:220:VAL:O | 1:D:223:PRO:HD2 | 2.20 | 0.41 |
| 1:E:273:GLU:O | 1:E:277:LYS:HE3 | 2.20 | 0.41 |
| 1:E:573:VAL:HG23 | 1:E:618:PHE:HB3 | 2.02 | 0.41 |
| 1:F:540:ILE:HG13 | 1:F:572:CYS:SG | 2.61 | 0.41 |
| 1:A:236:LYS:HE2 | 1:A:236:LYS:HA | 2.03 | 0.41 |
| 1:A:540:ILE:HG13 | 1:A:572:CYS:SG | 2.61 | 0.41 |
| 1:A:600:VAL:O | 1:A:604:ILE:HG13 | 2.21 | 0.41 |
| 1:B:572:CYS:SG | 1:B:573:VAL:N | 2.93 | 0.41 |
| 1:D:319:GLU:HA | 1:D:322:ARG:HD2 | 2.03 | 0.41 |
| 1:F:52:PHE:N | 1:F:55:ASP:OD2 | 2.41 | 0.41 |
| 1:F:239:ARG:HD3 | 1:F:239:ARG:HA | 1.79 | 0.41 |
| 1:F:267:PHE:CE2 | 1:F:289:ALA:HB1 | 2.55 | 0.41 |
| 1:B:421:GLN:OE1 | 1:B:451:ASP:HA | 2.20 | 0.41 |
| 1:C:521:GLY:N | 2:C:1002:ADP:O3B | 2.50 | 0.41 |
| 1:D:232:GLU:OE1 | 1:E:442:MET:HE3 | 2.21 | 0.41 |
| 1:D:273:GLU:O | 1:D:277:LYS:HE3 | 2.20 | 0.41 |
| 1:F:273:GLU:O | 1:F:277:LYS:HE3 | 2.20 | 0.41 |
| 1:A:258:VAL:O | 1:A:262:THR:OG1 | 2.31 | 0.41 |
| 1:A:625:ARG:HE | 1:A:625:ARG:HB3 | 1.68 | 0.41 |
| 1:B:236:LYS:HA | 1:B:236:LYS:HE2 | 2.03 | 0.41 |
| 1:B:267:PHE:HE2 | 1:B:289:ALA:HB1 | 1.86 | 0.41 |
| 1:B:319:GLU:HA | 1:B:322:ARG:HD2 | 2.03 | 0.41 |
| 1:B:365:ARG:NH2 | 1:C:458:GLN:HE22 | 2.17 | 0.41 |
| 1:B:519:PRO:HG3 | 1:B:647:LEU:HD22 | 2.02 | 0.41 |
| 1:C:267:PHE:HE2 | 1:C:289:ALA:HB1 | 1.86 | 0.41 |
| 1:D:267:PHE:CE2 | 1:D:289:ALA:HB1 | 2.55 | 0.41 |
| 1:D:421:GLN:OE1 | 1:D:451:ASP:HA | 2.20 | 0.41 |
| 1:D:425:LYS:NZ | 1:D:450:ASP:OD2 | 2.52 | 0.41 |
| 1:E:267:PHE:CE2 | 1:E:289:ALA:HB1 | 2.55 | 0.41 |
| 1:E:319:GLU:HA | 1:E:322:ARG:HD2 | 2.03 | 0.41 |
| 1:F:236:LYS:HE2 | 1:F:236:LYS:HA | 2.03 | 0.41 |
| 1:F:267:PHE:HE2 | 1:F:289:ALA:HB1 | 1.86 | 0.41 |
| 1:F:319:GLU:HA | 1:F:322:ARG:HD2 | 2.03 | 0.41 |
| 1:F:395:ASP:OD1 | 1:F:395:ASP:N | 2.53 | 0.41 |
| 1:F:701:GLU:OE1 | 1:F:732:ARG:NH2 | 2.47 | 0.41 |
| 1:A:117:LEU:HD23 | 1:A:117:LEU:HA | 1.96 | 0.41 |
| 1:A:319:GLU:HA | 1:A:322:ARG:HD2 | 2.03 | 0.41 |
| 1:C:519:PRO:HG3 | 1:C:647:LEU:HD22 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:454:TRP:CE2 | 1:E:458:GLN:OE1 | 2.74 | 0.41 |
| 1:E:670:VAL:HA | 1:E:733:ARG:HD3 | 2.03 | 0.41 |
| 1:F:521:GLY:N | 2:F:1002:ADP:O3B | 2.52 | 0.41 |
| 1:A:267:PHE:HE2 | 1:A:289:ALA:HB1 | 1.86 | 0.40 |
| 1:A:421:GLN:OE1 | 1:A:451:ASP:HA | 2.21 | 0.40 |
| 1:B:600:VAL:O | 1:B:604:ILE:HG13 | 2.21 | 0.40 |
| 1:D:569:ALA:O | 1:D:572:CYS:HB2 | 2.21 | 0.40 |
| 1:D:573:VAL:HG23 | 1:D:618:PHE:HB3 | 2.02 | 0.40 |
| 1:D:608:MET:SD | 1:D:638:ARG:HB3 | 2.62 | 0.40 |
| 1:E:519:PRO:HG3 | 1:E:647:LEU:HD22 | 2.02 | 0.40 |
| 1:F:383:ILE:HD12 | 1:F:383:ILE:H | 1.86 | 0.40 |
| 1:A:383:ILE:H | 1:A:383:ILE:HD12 | 1.86 | 0.40 |
| 1:B:540:ILE:HG13 | 1:B:572:CYS:SG | 2.61 | 0.40 |
| 1:C:532:ALA:HB2 | 1:C:573:VAL:HG11 | 2.03 | 0.40 |
| 1:C:608:MET:SD | 1:C:638:ARG:HB3 | 2.62 | 0.40 |
| 1:D:52:PHE:N | 1:D:55:ASP:OD2 | 2.41 | 0.40 |
| 1:D:532:ALA:HB2 | 1:D:573:VAL:HG11 | 2.03 | 0.40 |
| 1:D:670:VAL:HA | 1:D:733:ARG:HD3 | 2.03 | 0.40 |
| 1:E:608:MET:SD | 1:E:638:ARG:HB3 | 2.61 | 0.40 |
| 1:A:395:ASP:OD1 | 1:A:395:ASP:N | 2.53 | 0.40 |
| 1:B:218:GLU:O | 1:C:424:ARG:NH1 | 2.55 | 0.40 |
| 1:B:434:ASP:N | 1:B:434:ASP:OD1 | 2.53 | 0.40 |
| 1:D:267:PHE:HE2 | 1:D:289:ALA:HB1 | 1.86 | 0.40 |
| 1:D:283:GLU:HG3 | 1:D:324:ILE:HD13 | 2.04 | 0.40 |
| 1:D:434:ASP:OD1 | 1:D:434:ASP:N | 2.53 | 0.40 |
| 1:E:540:ILE:HG13 | 1:E:572:CYS:SG | 2.61 | 0.40 |
| 1:E:701:GLU:OE1 | 1:E:732:ARG:NH2 | 2.47 | 0.40 |
| 1:F:434:ASP:OD1 | 1:F:434:ASP:N | 2.53 | 0.40 |
| 1:A:317:HIS:HD2 | 1:F:322:ARG:HH12 | 1.70 | 0.40 |
| 1:A:569:ALA:O | 1:A:572:CYS:HB2 | 2.21 | 0.40 |
| 1:B:608:MET:SD | 1:B:638:ARG:HB3 | 2.62 | 0.40 |
| 1:B:670:VAL:HA | 1:B:733:ARG:HD3 | 2.03 | 0.40 |
| 1:D:120:ASP:N | 1:D:120:ASP:OD1 | 2.52 | 0.40 |
| 1:D:600:VAL:O | 1:D:604:ILE:HG13 | 2.21 | 0.40 |
| 1:E:434:ASP:OD1 | 1:E:434:ASP:N | 2.53 | 0.40 |
| 1:A:670:VAL:HA | 1:A:733:ARG:HD3 | 2.03 | 0.40 |
| 1:C:540:ILE:HG13 | 1:C:572:CYS:SG | 2.61 | 0.40 |
| 1:E:22:ARG:HD3 | 1:E:22:ARG:HA | 1.94 | 0.40 |
| 1:E:41:LEU:HD23 | 1:E:45:LYS:HB3 | 2.04 | 0.40 |
| 1:F:450:ASP:OD1 | 1:F:450:ASP:N | 2.55 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 731/821 (89%) | 701 (96%) | 28 (4%) | 2 (0%) | 36 | 65 |
| 1 | B | 731/821 (89%) | 702 (96%) | 27 (4%) | 2 (0%) | 36 | 65 |
| 1 | C | 731/821 (89%) | 702 (96%) | 27 (4%) | 2 (0%) | 36 | 65 |
| 1 | D | 731/821 (89%) | 702 (96%) | 27 (4%) | 2 (0%) | 36 | 65 |
| 1 | E | 731/821 (89%) | 701 (96%) | 28 (4%) | 2 (0%) | 36 | 65 |
| 1 | F | 731/821 (89%) | 701 (96%) | 28 (4%) | 2 (0%) | 36 | 65 |
| All | All | 4386/4926 (89%) | 4209 (96%) | 165 (4%) | 12 (0%) | 37 | 65 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 172 | PRO |
| 1 | B | 172 | PRO |
| 1 | C | 172 | PRO |
| 1 | D | 172 | PRO |
| 1 | E | 172 | PRO |
| 1 | F | 172 | PRO |
| 1 | A | 338 | ARG |
| 1 | B | 338 | ARG |
| 1 | C | 338 | ARG |
| 1 | D | 338 | ARG |
| 1 | E | 338 | ARG |
| 1 | F | 338 | ARG |

### 5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 626/692 (90%) | 625 (100%) | 1 (0%) | 87 88 |
| 1 | B | 626/692 (90%) | 626 (100%) | 0 | 100 100 |
| 1 | C | 626/692 (90%) | 626 (100%) | 0 | 100 100 |
| 1 | D | 626/692 (90%) | 626 (100%) | 0 | 100 100 |
| 1 | E | 626/692 (90%) | 626 (100%) | 0 | 100 100 |
| 1 | F | 626/692 (90%) | 626 (100%) | 0 | 100 100 |
| All | All | 3756/4152 (90%) | 3755 (100%) | 1 (0%) | 100 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 757 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 296 | ASN |
| 1 | A | 317 | HIS |
| 1 | A | 384 | HIS |
| 1 | A | 458 | GLN |
| 1 | A | 603 | GLN |
| 1 | B | 43 | GLN |
| 1 | B | 296 | ASN |
| 1 | B | 317 | HIS |
| 1 | B | 382 | GLN |
| 1 | B | 384 | HIS |
| 1 | B | 458 | GLN |
| 1 | C | 43 | GLN |
| 1 | C | 296 | ASN |
| 1 | C | 317 | HIS |
| 1 | C | 382 | GLN |
| 1 | C | 384 | HIS |
| 1 | C | 458 | GLN |
| 1 | D | 43 | GLN |
| 1 | D | 296 | ASN |
| 1 | D | 317 | HIS |
| 1 | D | 382 | GLN |
| 1 | D | 384 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 458 | GLN |
| 1 | E | 296 | ASN |
| 1 | E | 382 | GLN |
| 1 | E | 384 | HIS |
| 1 | F | 296 | ASN |
| 1 | F | 317 | HIS |
| 1 | F | 382 | GLN |
| 1 | F | 384 | HIS |
| 1 | F | 458 | GLN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | ADP | B | 1002 | - | 28,29,29 | 1.44 | 4 (14%) | 43,45,45 | 1.84 | 8 (18%) |
| 2 | ADP | B | 1001 | - | 28,29,29 | 1.51 | 4 (14%) | 43,45,45 | 1.86 | 10 (23%) |
| 2 | ADP | E | 1002 | - | 28,29,29 | 1.44 | 4 (14%) | 43,45,45 | 1.84 | 8 (18%) |
| 2 | ADP | C | 1001 | - | 28,29,29 | 1.55 | 4 (14%) | 43,45,45 | 1.84 | 9 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | ADP | C | 1002 | - | 28,29,29 | 1.46 | 4 (14%) | 43,45,45 | 1.90 | 9 (20%) |
| 2 | ADP | F | 1002 | - | 28,29,29 | 1.47 | 4 (14%) | 43,45,45 | 1.90 | 9 (20%) |
| 2 | ADP | D | 1002 | - | 28,29,29 | 1.46 | 4 (14%) | 43,45,45 | 1.87 | 8 (18%) |
| 2 | ADP | D | 1001 | - | 28,29,29 | 1.54 | 5 (17%) | 43,45,45 | 1.88 | 10 (23%) |
| 2 | ADP | E | 1001 | - | 28,29,29 | 1.51 | 4 (14%) | 43,45,45 | 1.87 | 10 (23%) |
| 2 | ADP | F | 1001 | - | 28,29,29 | 1.55 | 4 (14%) | 43,45,45 | 1.84 | 9 (20%) |
| 2 | ADP | A | 1001 | - | 28,29,29 | 1.54 | 5 (17%) | 43,45,45 | 1.88 | 10 (23%) |
| 2 | ADP | A | 1002 | - | 28,29,29 | 1.45 | 4 (14%) | 43,45,45 | 1.87 | 8 (18%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | ADP | B | 1002 | - | - | 4/16/32/32 | 0/3/3/3 |
| 2 | ADP | B | 1001 | - | - | 7/16/32/32 | 0/3/3/3 |
| 2 | ADP | E | 1002 | - | - | 4/16/32/32 | 0/3/3/3 |
| 2 | ADP | C | 1001 | - | - | 6/16/32/32 | 0/3/3/3 |
| 2 | ADP | C | 1002 | - | - | 5/16/32/32 | 0/3/3/3 |
| 2 | ADP | F | 1002 | - | - | 5/16/32/32 | 0/3/3/3 |
| 2 | ADP | D | 1002 | - | - | 4/16/32/32 | 0/3/3/3 |
| 2 | ADP | D | 1001 | - | - | 7/16/32/32 | 0/3/3/3 |
| 2 | ADP | E | 1001 | - | - | 7/16/32/32 | 0/3/3/3 |
| 2 | ADP | F | 1001 | - | - | 5/16/32/32 | 0/3/3/3 |
| 2 | ADP | A | 1001 | - | - | 7/16/32/32 | 0/3/3/3 |
| 2 | ADP | A | 1002 | - | - | 4/16/32/32 | 0/3/3/3 |

All (50) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 1002 | ADP | C5-N7 | -3.71 | 1.32 | 1.39 |
| 2 | F | 1002 | ADP | C5-N7 | -3.71 | 1.32 | 1.39 |
| 2 | F | 1001 | ADP | C5-N7 | -3.71 | 1.32 | 1.39 |
| 2 | C | 1001 | ADP | C5-N7 | -3.70 | 1.32 | 1.39 |
| 2 | B | 1001 | ADP | C5-N7 | -3.68 | 1.32 | 1.39 |
| 2 | E | 1001 | ADP | C5-N7 | -3.64 | 1.32 | 1.39 |
| 2 | A | 1001 | ADP | C5-N7 | -3.57 | 1.32 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | D | 1001 | ADP | C5-N7 | -3.57 | 1.32 | 1.39 |
| 2 | A | 1002 | ADP | C5-N7 | -3.56 | 1.32 | 1.39 |
| 2 | D | 1002 | ADP | C5-N7 | -3.56 | 1.32 | 1.39 |
| 2 | B | 1002 | ADP | C5-N7 | -3.55 | 1.32 | 1.39 |
| 2 | E | 1002 | ADP | C5-N7 | -3.55 | 1.32 | 1.39 |
| 2 | F | 1002 | ADP | C5-C4 | 3.13 | 1.44 | 1.39 |
| 2 | C | 1002 | ADP | C5-C4 | 3.12 | 1.44 | 1.39 |
| 2 | D | 1002 | ADP | C5-C4 | 3.12 | 1.44 | 1.39 |
| 2 | A | 1002 | ADP | C5-C4 | 3.12 | 1.44 | 1.39 |
| 2 | E | 1001 | ADP | C4-N9 | -3.10 | 1.31 | 1.37 |
| 2 | E | 1002 | ADP | C5-C4 | 3.10 | 1.44 | 1.39 |
| 2 | F | 1001 | ADP | C4-N9 | -3.09 | 1.31 | 1.37 |
| 2 | F | 1001 | ADP | C5-C4 | 3.09 | 1.44 | 1.39 |
| 2 | B | 1002 | ADP | C5-C4 | 3.09 | 1.44 | 1.39 |
| 2 | D | 1001 | ADP | C5-C4 | 3.07 | 1.44 | 1.39 |
| 2 | B | 1001 | ADP | C4-N9 | -3.07 | 1.31 | 1.37 |
| 2 | A | 1001 | ADP | C4-N9 | -3.06 | 1.31 | 1.37 |
| 2 | C | 1001 | ADP | C5-C4 | 3.05 | 1.44 | 1.39 |
| 2 | C | 1001 | ADP | C4-N9 | -3.04 | 1.31 | 1.37 |
| 2 | D | 1001 | ADP | C4-N9 | -3.04 | 1.31 | 1.37 |
| 2 | A | 1001 | ADP | C5-C4 | 3.04 | 1.44 | 1.39 |
| 2 | C | 1001 | ADP | C8-N9 | -3.02 | 1.32 | 1.37 |
| 2 | F | 1001 | ADP | C8-N9 | -2.97 | 1.32 | 1.37 |
| 2 | B | 1001 | ADP | C5-C4 | 2.96 | 1.44 | 1.39 |
| 2 | E | 1001 | ADP | C5-C4 | 2.96 | 1.44 | 1.39 |
| 2 | D | 1001 | ADP | C8-N9 | -2.94 | 1.32 | 1.37 |
| 2 | A | 1001 | ADP | C8-N9 | -2.94 | 1.32 | 1.37 |
| 2 | A | 1002 | ADP | C4-N9 | -2.86 | 1.31 | 1.37 |
| 2 | D | 1002 | ADP | C4-N9 | -2.86 | 1.31 | 1.37 |
| 2 | B | 1001 | ADP | C8-N9 | -2.85 | 1.32 | 1.37 |
| 2 | E | 1002 | ADP | C4-N9 | -2.84 | 1.31 | 1.37 |
| 2 | B | 1002 | ADP | C4-N9 | -2.82 | 1.31 | 1.37 |
| 2 | F | 1002 | ADP | C4-N9 | -2.81 | 1.31 | 1.37 |
| 2 | E | 1001 | ADP | C8-N9 | -2.79 | 1.32 | 1.37 |
| 2 | C | 1002 | ADP | C4-N9 | -2.78 | 1.31 | 1.37 |
| 2 | D | 1002 | ADP | C8-N9 | -2.73 | 1.32 | 1.37 |
| 2 | C | 1002 | ADP | C8-N9 | -2.71 | 1.32 | 1.37 |
| 2 | A | 1002 | ADP | C8-N9 | -2.70 | 1.32 | 1.37 |
| 2 | F | 1002 | ADP | C8-N9 | -2.68 | 1.33 | 1.37 |
| 2 | B | 1002 | ADP | C8-N9 | -2.61 | 1.33 | 1.37 |
| 2 | E | 1002 | ADP | C8-N9 | -2.60 | 1.33 | 1.37 |
| 2 | D | 1001 | ADP | PA-O3A | -2.09 | 1.57 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 1001 | ADP | PA-O3A | -2.06 | 1.57 | 1.59 |

All (108) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | F | 1002 | ADP | C5-C4-N3 | -6.06 | 118.38 | 126.72 |
| 2 | C | 1002 | ADP | C5-C4-N3 | -6.05 | 118.38 | 126.72 |
| 2 | A | 1002 | ADP | C5-C4-N3 | -6.05 | 118.39 | 126.72 |
| 2 | D | 1002 | ADP | C5-C4-N3 | -6.04 | 118.41 | 126.72 |
| 2 | B | 1002 | ADP | C5-C4-N3 | -5.98 | 118.48 | 126.72 |
| 2 | E | 1002 | ADP | C5-C4-N3 | -5.97 | 118.50 | 126.72 |
| 2 | A | 1001 | ADP | C5-C4-N3 | -5.87 | 118.63 | 126.72 |
| 2 | D | 1001 | ADP | C5-C4-N3 | -5.83 | 118.68 | 126.72 |
| 2 | B | 1001 | ADP | C5-C4-N3 | -5.79 | 118.74 | 126.72 |
| 2 | E | 1001 | ADP | C5-C4-N3 | -5.78 | 118.76 | 126.72 |
| 2 | F | 1001 | ADP | C5-C4-N3 | -5.76 | 118.78 | 126.72 |
| 2 | C | 1001 | ADP | C5-C4-N3 | -5.73 | 118.82 | 126.72 |
| 2 | A | 1002 | ADP | N3-C4-N9 | 5.08 | 135.81 | 127.17 |
| 2 | C | 1002 | ADP | N3-C4-N9 | 5.07 | 135.80 | 127.17 |
| 2 | D | 1002 | ADP | N3-C4-N9 | 5.07 | 135.78 | 127.17 |
| 2 | F | 1002 | ADP | N3-C4-N9 | 5.05 | 135.75 | 127.17 |
| 2 | B | 1002 | ADP | N3-C4-N9 | 4.76 | 135.26 | 127.17 |
| 2 | E | 1002 | ADP | N3-C4-N9 | 4.74 | 135.22 | 127.17 |
| 2 | F | 1001 | ADP | N3-C4-N9 | 4.57 | 134.94 | 127.17 |
| 2 | C | 1001 | ADP | N3-C4-N9 | 4.56 | 134.91 | 127.17 |
| 2 | B | 1001 | ADP | N3-C4-N9 | 4.44 | 134.72 | 127.17 |
| 2 | A | 1001 | ADP | N3-C4-N9 | 4.43 | 134.71 | 127.17 |
| 2 | E | 1001 | ADP | N3-C4-N9 | 4.42 | 134.69 | 127.17 |
| 2 | D | 1001 | ADP | N3-C4-N9 | 4.42 | 134.69 | 127.17 |
| 2 | A | 1001 | ADP | C2-N3-C4 | 3.73 | 120.93 | 111.83 |
| 2 | D | 1001 | ADP | C2-N3-C4 | 3.72 | 120.91 | 111.83 |
| 2 | A | 1002 | ADP | C2-N3-C4 | 3.69 | 120.85 | 111.83 |
| 2 | D | 1002 | ADP | C2-N3-C4 | 3.69 | 120.85 | 111.83 |
| 2 | F | 1002 | ADP | C2-N3-C4 | 3.67 | 120.80 | 111.83 |
| 2 | C | 1002 | ADP | C2-N3-C4 | 3.66 | 120.78 | 111.83 |
| 2 | B | 1002 | ADP | C2-N3-C4 | 3.64 | 120.73 | 111.83 |
| 2 | E | 1002 | ADP | C2-N3-C4 | 3.61 | 120.65 | 111.83 |
| 2 | F | 1001 | ADP | C2-N3-C4 | 3.55 | 120.50 | 111.83 |
| 2 | B | 1001 | ADP | C2-N3-C4 | 3.55 | 120.50 | 111.83 |
| 2 | E | 1001 | ADP | C2-N3-C4 | 3.55 | 120.50 | 111.83 |
| 2 | C | 1001 | ADP | C2-N3-C4 | 3.54 | 120.48 | 111.83 |
| 2 | D | 1001 | ADP | C4-C5-N7 | -3.52 | 106.56 | 110.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 1001 | ADP | C4-C5-N7 | -3.48 | 106.60 | 110.58 |
| 2 | A | 1001 | ADP | N3-C2-N1 | -3.37 | 123.48 | 128.58 |
| 2 | E | 1001 | ADP | C4-C5-N7 | -3.36 | 106.74 | 110.58 |
| 2 | D | 1001 | ADP | N3-C2-N1 | -3.36 | 123.49 | 128.58 |
| 2 | C | 1002 | ADP | N3-C2-N1 | -3.35 | 123.51 | 128.58 |
| 2 | F | 1002 | ADP | N3-C2-N1 | -3.34 | 123.53 | 128.58 |
| 2 | B | 1001 | ADP | C4-C5-N7 | -3.33 | 106.77 | 110.58 |
| 2 | E | 1002 | ADP | C4-C5-N7 | -3.32 | 106.79 | 110.58 |
| 2 | B | 1002 | ADP | C4-C5-N7 | -3.31 | 106.80 | 110.58 |
| 2 | F | 1001 | ADP | N3-C2-N1 | -3.31 | 123.58 | 128.58 |
| 2 | C | 1001 | ADP | N3-C2-N1 | -3.28 | 123.62 | 128.58 |
| 2 | F | 1001 | ADP | C4-C5-N7 | -3.28 | 106.84 | 110.58 |
| 2 | C | 1001 | ADP | C4-C5-N7 | -3.27 | 106.84 | 110.58 |
| 2 | D | 1002 | ADP | N3-C2-N1 | -3.27 | 123.64 | 128.58 |
| 2 | A | 1002 | ADP | N3-C2-N1 | -3.26 | 123.65 | 128.58 |
| 2 | B | 1001 | ADP | N3-C2-N1 | -3.22 | 123.70 | 128.58 |
| 2 | E | 1001 | ADP | N3-C2-N1 | -3.22 | 123.70 | 128.58 |
| 2 | A | 1002 | ADP | C4-N9-C8 | 3.17 | 109.07 | 105.74 |
| 2 | D | 1002 | ADP | C4-N9-C8 | 3.16 | 109.06 | 105.74 |
| 2 | B | 1002 | ADP | N3-C2-N1 | -3.10 | 123.90 | 128.58 |
| 2 | E | 1002 | ADP | N3-C2-N1 | -3.06 | 123.95 | 128.58 |
| 2 | C | 1001 | ADP | C4-N9-C8 | 2.96 | 108.85 | 105.74 |
| 2 | F | 1001 | ADP | C4-N9-C8 | 2.95 | 108.84 | 105.74 |
| 2 | C | 1002 | ADP | C4-N9-C8 | 2.94 | 108.83 | 105.74 |
| 2 | E | 1002 | ADP | C4-N9-C8 | 2.94 | 108.82 | 105.74 |
| 2 | D | 1002 | ADP | C4-C5-N7 | -2.94 | 107.22 | 110.58 |
| 2 | B | 1002 | ADP | C4-N9-C8 | 2.92 | 108.80 | 105.74 |
| 2 | F | 1002 | ADP | C4-N9-C8 | 2.92 | 108.80 | 105.74 |
| 2 | A | 1002 | ADP | C4-C5-N7 | -2.90 | 107.26 | 110.58 |
| 2 | F | 1002 | ADP | C4-C5-N7 | -2.84 | 107.34 | 110.58 |
| 2 | C | 1002 | ADP | C4-C5-N7 | -2.81 | 107.36 | 110.58 |
| 2 | E | 1001 | ADP | C4-N9-C8 | 2.78 | 108.65 | 105.74 |
| 2 | D | 1001 | ADP | C4-N9-C8 | 2.77 | 108.64 | 105.74 |
| 2 | B | 1001 | ADP | C4-N9-C8 | 2.76 | 108.64 | 105.74 |
| 2 | A | 1001 | ADP | C4-N9-C8 | 2.75 | 108.62 | 105.74 |
| 2 | E | 1001 | ADP | C2'-C1'-N9 | -2.71 | 106.57 | 113.30 |
| 2 | B | 1002 | ADP | C5-N7-C8 | 2.67 | 107.65 | 103.45 |
| 2 | E | 1002 | ADP | C5-N7-C8 | 2.67 | 107.65 | 103.45 |
| 2 | B | 1001 | ADP | C2'-C1'-N9 | -2.67 | 106.68 | 113.30 |
| 2 | D | 1001 | ADP | C5-N7-C8 | 2.52 | 107.42 | 103.45 |
| 2 | E | 1001 | ADP | C5-N7-C8 | 2.52 | 107.40 | 103.45 |
| 2 | B | 1001 | ADP | C5-N7-C8 | 2.49 | 107.36 | 103.45 |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 1001 | ADP | C5-N7-C8 | 2.48 | 107.35 | 103.45 |
| 2 | C | 1001 | ADP | C5-N7-C8 | 2.48 | 107.34 | 103.45 |
| 2 | F | 1001 | ADP | C5-N7-C8 | 2.46 | 107.32 | 103.45 |
| 2 | E | 1002 | ADP | N9-C8-N7 | -2.45 | 110.46 | 113.94 |
| 2 | B | 1002 | ADP | N9-C8-N7 | -2.43 | 110.49 | 113.94 |
| 2 | D | 1002 | ADP | C5-N7-C8 | 2.42 | 107.26 | 103.45 |
| 2 | A | 1002 | ADP | C5-N7-C8 | 2.41 | 107.24 | 103.45 |
| 2 | C | 1002 | ADP | C3'-C2'-C1' | 2.38 | 105.97 | 101.46 |
| 2 | C | 1002 | ADP | C5-N7-C8 | 2.36 | 107.17 | 103.45 |
| 2 | F | 1002 | ADP | C5-N7-C8 | 2.36 | 107.17 | 103.45 |
| 2 | F | 1002 | ADP | C3'-C2'-C1' | 2.36 | 105.92 | 101.46 |
| 2 | A | 1002 | ADP | N9-C8-N7 | -2.33 | 110.64 | 113.94 |
| 2 | D | 1002 | ADP | N9-C8-N7 | -2.31 | 110.65 | 113.94 |
| 2 | E | 1001 | ADP | N9-C8-N7 | -2.31 | 110.66 | 113.94 |
| 2 | B | 1001 | ADP | N9-C8-N7 | -2.29 | 110.69 | 113.94 |
| 2 | C | 1001 | ADP | N9-C8-N7 | -2.28 | 110.71 | 113.94 |
| 2 | F | 1001 | ADP | N9-C8-N7 | -2.26 | 110.73 | 113.94 |
| 2 | D | 1001 | ADP | N9-C8-N7 | -2.25 | 110.75 | 113.94 |
| 2 | C | 1001 | ADP | C2'-C1'-N9 | -2.24 | 107.75 | 113.30 |
| 2 | A | 1001 | ADP | N9-C8-N7 | -2.24 | 110.76 | 113.94 |
| 2 | C | 1002 | ADP | N9-C8-N7 | -2.19 | 110.82 | 113.94 |
| 2 | A | 1001 | ADP | C2'-C1'-N9 | -2.19 | 107.86 | 113.30 |
| 2 | F | 1002 | ADP | N9-C8-N7 | -2.19 | 110.83 | 113.94 |
| 2 | D | 1001 | ADP | C2'-C1'-N9 | -2.19 | 107.87 | 113.30 |
| 2 | F | 1001 | ADP | C2'-C1'-N9 | -2.16 | 107.94 | 113.30 |
| 2 | D | 1001 | ADP | O2A-PA-O1A | 2.11 | 122.24 | 112.44 |
| 2 | B | 1001 | ADP | O2A-PA-O1A | 2.10 | 122.23 | 112.44 |
| 2 | E | 1001 | ADP | O2A-PA-O1A | 2.10 | 122.22 | 112.44 |
| 2 | A | 1001 | ADP | O2A-PA-O1A | 2.10 | 122.20 | 112.44 |

There are no chirality outliers.

All (65) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 1001 | ADP | C5'-O5'-PA-O1A |
| 2 | A | 1001 | ADP | C5'-O5'-PA-O3A |
| 2 | A | 1001 | ADP | O4'-C4'-C5'-O5' |
| 2 | A | 1002 | ADP | C5'-O5'-PA-O3A |
| 2 | B | 1001 | ADP | C5'-O5'-PA-O1A |
| 2 | B | 1001 | ADP | C5'-O5'-PA-O3A |
| 2 | B | 1001 | ADP | O4'-C4'-C5'-O5' |
| 2 | B | 1002 | ADP | C5'-O5'-PA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | B | 1002 | ADP | C5'-O5'-PA-O2A |
| 2 | B | 1002 | ADP | C5'-O5'-PA-O3A |
| 2 | C | 1001 | ADP | C5'-O5'-PA-O1A |
| 2 | C | 1001 | ADP | C5'-O5'-PA-O3A |
| 2 | C | 1002 | ADP | C5'-O5'-PA-O1A |
| 2 | C | 1002 | ADP | C5'-O5'-PA-O2A |
| 2 | C | 1002 | ADP | C5'-O5'-PA-O3A |
| 2 | D | 1001 | ADP | C5'-O5'-PA-O1A |
| 2 | D | 1001 | ADP | C5'-O5'-PA-O3A |
| 2 | D | 1001 | ADP | O4'-C4'-C5'-O5' |
| 2 | D | 1002 | ADP | C5'-O5'-PA-O3A |
| 2 | E | 1001 | ADP | C5'-O5'-PA-O1A |
| 2 | E | 1001 | ADP | C5'-O5'-PA-O3A |
| 2 | E | 1001 | ADP | O4'-C4'-C5'-O5' |
| 2 | E | 1002 | ADP | C5'-O5'-PA-O1A |
| 2 | E | 1002 | ADP | C5'-O5'-PA-O2A |
| 2 | E | 1002 | ADP | C5'-O5'-PA-O3A |
| 2 | F | 1001 | ADP | C5'-O5'-PA-O1A |
| 2 | F | 1002 | ADP | C5'-O5'-PA-O1A |
| 2 | F | 1002 | ADP | C5'-O5'-PA-O2A |
| 2 | F | 1002 | ADP | C5'-O5'-PA-O3A |
| 2 | B | 1001 | ADP | C3'-C4'-C5'-O5' |
| 2 | E | 1001 | ADP | C3'-C4'-C5'-O5' |
| 2 | A | 1001 | ADP | C3'-C4'-C5'-O5' |
| 2 | D | 1001 | ADP | C3'-C4'-C5'-O5' |
| 2 | A | 1002 | ADP | PB-O3A-PA-O1A |
| 2 | D | 1002 | ADP | PB-O3A-PA-O1A |
| 2 | B | 1001 | ADP | PB-O3A-PA-O2A |
| 2 | C | 1002 | ADP | PB-O3A-PA-O2A |
| 2 | E | 1001 | ADP | PB-O3A-PA-O2A |
| 2 | C | 1001 | ADP | O4'-C4'-C5'-O5' |
| 2 | A | 1001 | ADP | C5'-O5'-PA-O2A |
| 2 | A | 1002 | ADP | C5'-O5'-PA-O1A |
| 2 | B | 1001 | ADP | C5'-O5'-PA-O2A |
| 2 | C | 1001 | ADP | C5'-O5'-PA-O2A |
| 2 | D | 1001 | ADP | C5'-O5'-PA-O2A |
| 2 | D | 1002 | ADP | C5'-O5'-PA-O1A |
| 2 | E | 1001 | ADP | C5'-O5'-PA-O2A |
| 2 | F | 1001 | ADP | C5'-O5'-PA-O2A |
| 2 | F | 1001 | ADP | C5'-O5'-PA-O3A |
| 2 | A | 1001 | ADP | PB-O3A-PA-O2A |
| 2 | A | 1002 | ADP | PB-O3A-PA-O2A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | D | 1001 | ADP | PB-O3A-PA-O2A |
| 2 | D | 1002 | ADP | PB-O3A-PA-O2A |
| 2 | F | 1002 | ADP | PB-O3A-PA-O2A |
| 2 | B | 1002 | ADP | PB-O3A-PA-O2A |
| 2 | E | 1002 | ADP | PB-O3A-PA-O2A |
| 2 | F | 1001 | ADP | PB-O3A-PA-O2A |
| 2 | A | 1001 | ADP | PB-O3A-PA-O1A |
| 2 | C | 1001 | ADP | PB-O3A-PA-O1A |
| 2 | C | 1001 | ADP | PB-O3A-PA-O2A |
| 2 | C | 1002 | ADP | PB-O3A-PA-O1A |
| 2 | D | 1001 | ADP | PB-O3A-PA-O1A |
| 2 | F | 1002 | ADP | PB-O3A-PA-O1A |
| 2 | B | 1001 | ADP | PB-O3A-PA-O1A |
| 2 | E | 1001 | ADP | PB-O3A-PA-O1A |
| 2 | F | 1001 | ADP | PB-O3A-PA-O1A |

There are no ring outliers.

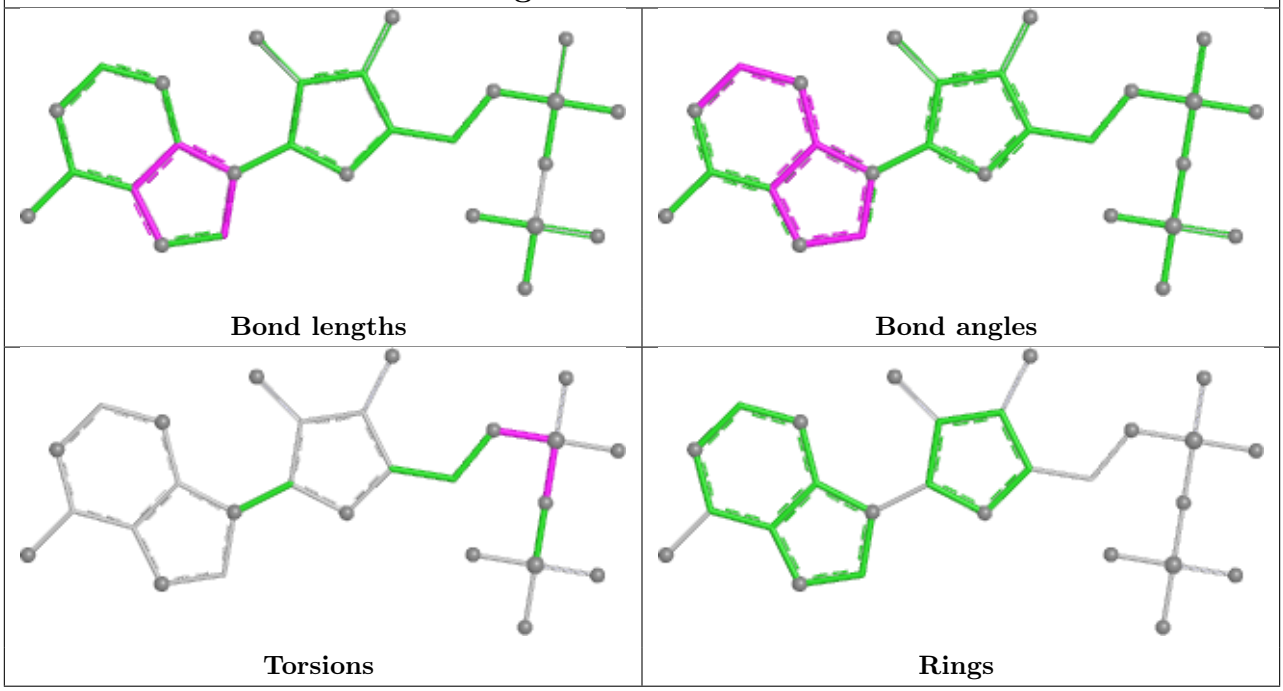
12 monomers are involved in 33 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 1002 | ADP | 4 | 0 |
| 2 | B | 1001 | ADP | 2 | 0 |
| 2 | E | 1002 | ADP | 5 | 0 |
| 2 | C | 1001 | ADP | 1 | 0 |
| 2 | C | 1002 | ADP | 3 | 0 |
| 2 | F | 1002 | ADP | 3 | 0 |
| 2 | D | 1002 | ADP | 4 | 0 |
| 2 | D | 1001 | ADP | 2 | 0 |
| 2 | E | 1001 | ADP | 2 | 0 |
| 2 | F | 1001 | ADP | 1 | 0 |
| 2 | A | 1001 | ADP | 2 | 0 |
| 2 | A | 1002 | ADP | 4 | 0 |

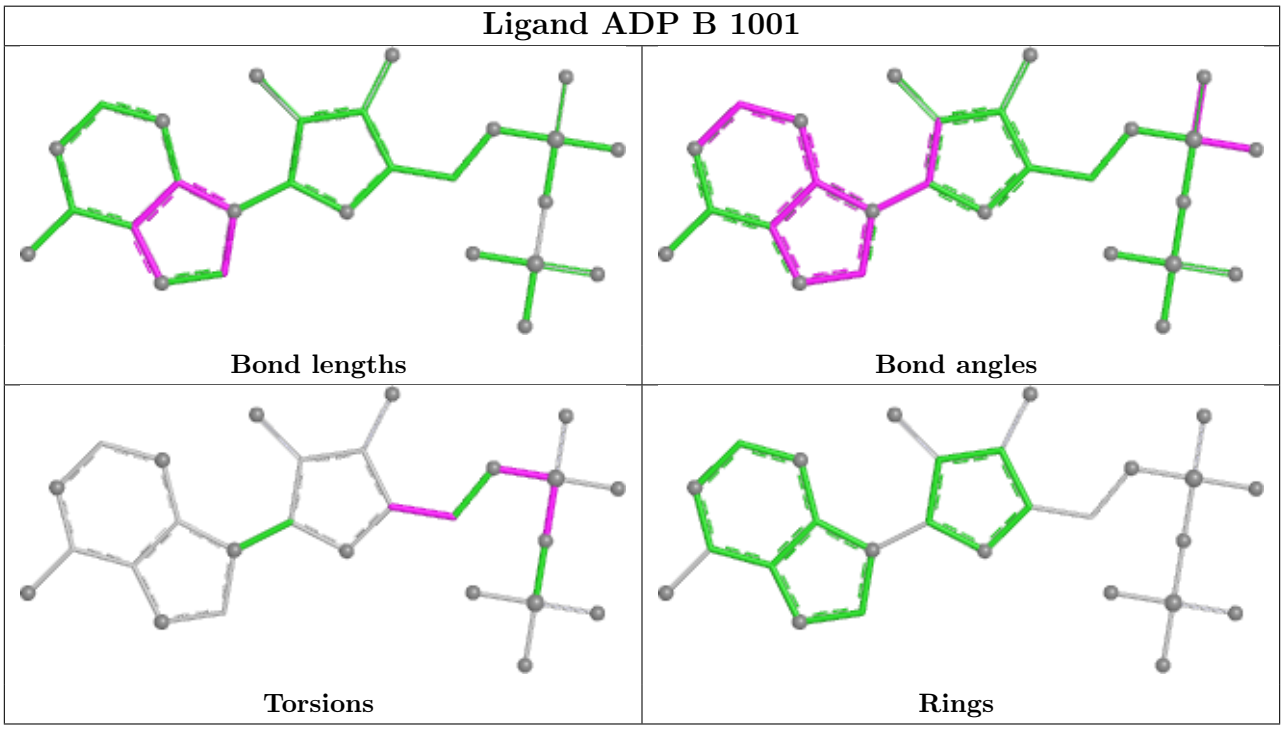
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

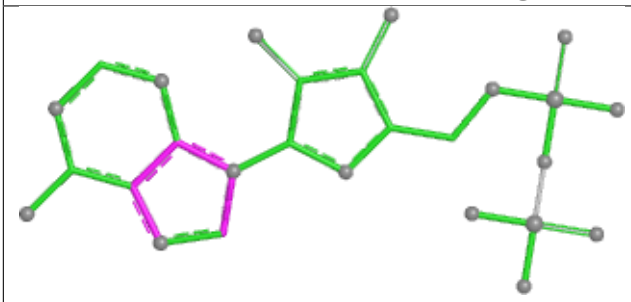
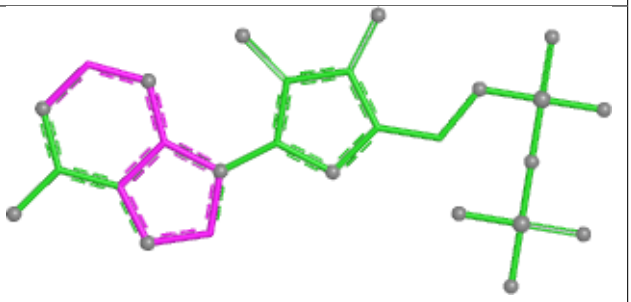
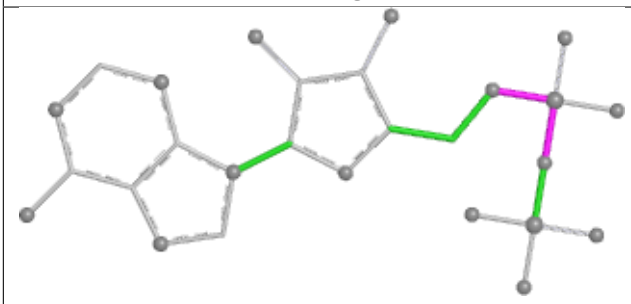
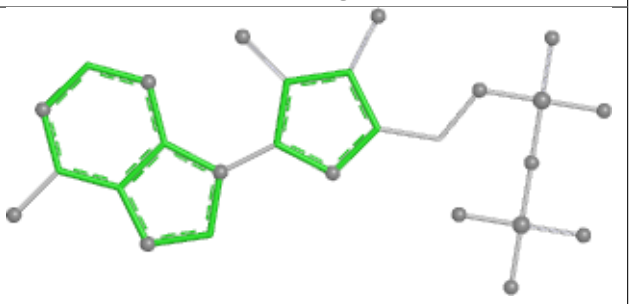
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

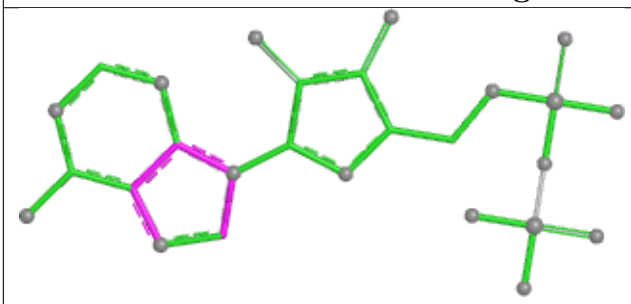
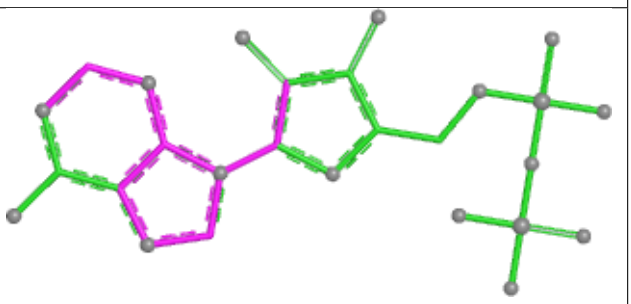
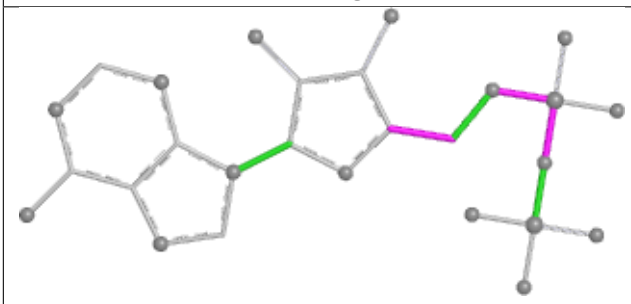
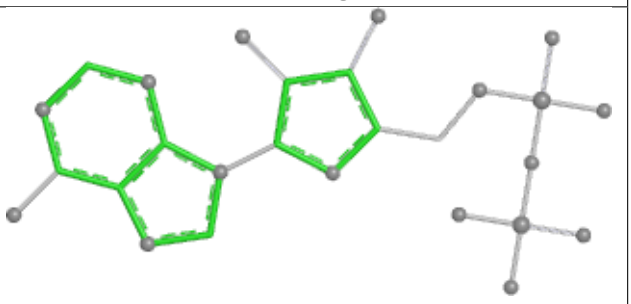
**Ligand ADP B 1002**

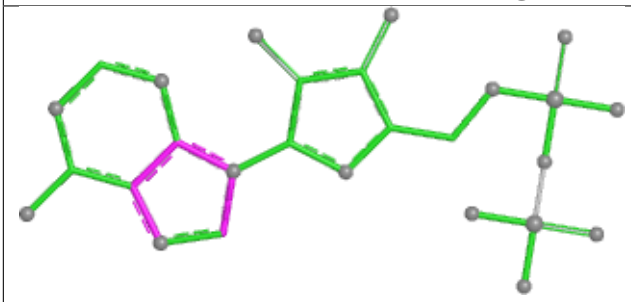
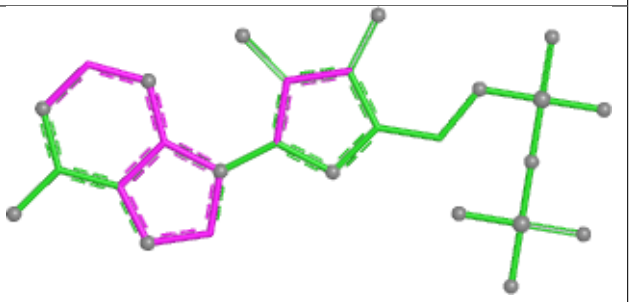
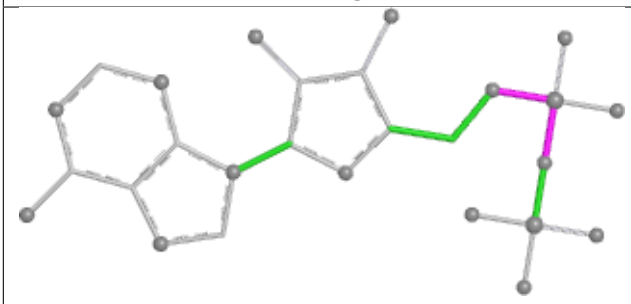
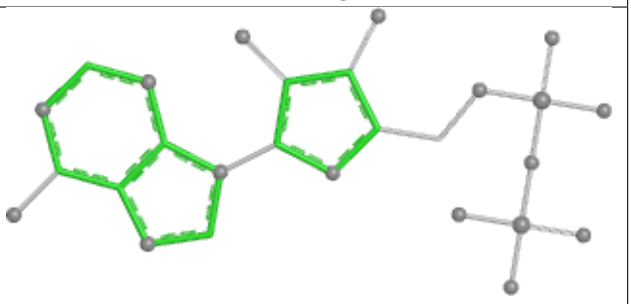


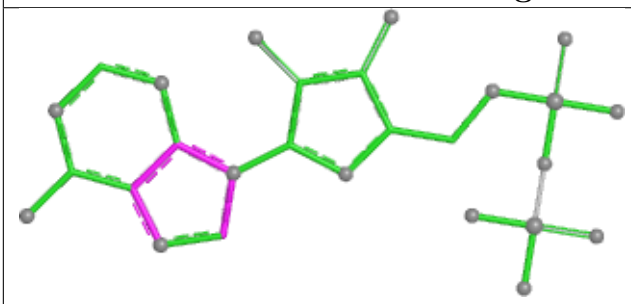
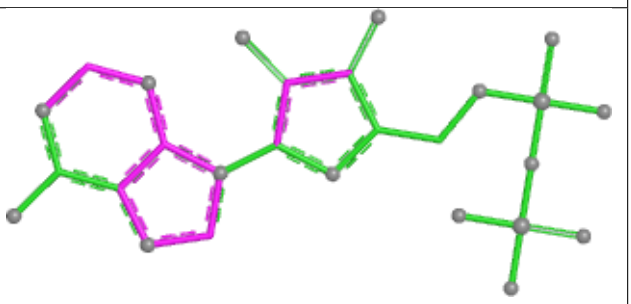
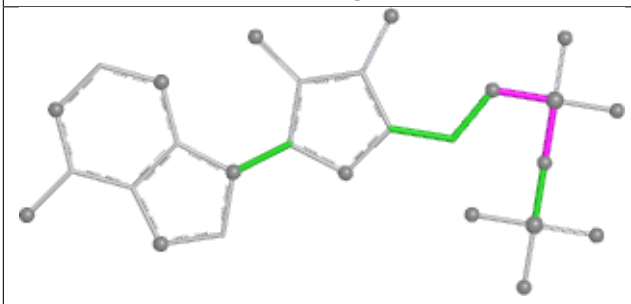
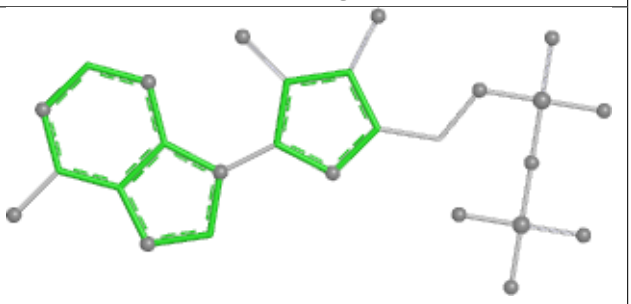

**Ligand ADP B 1001**

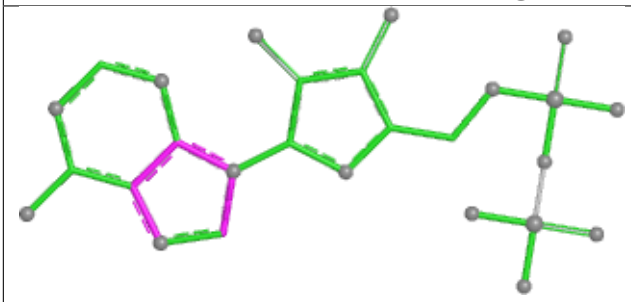
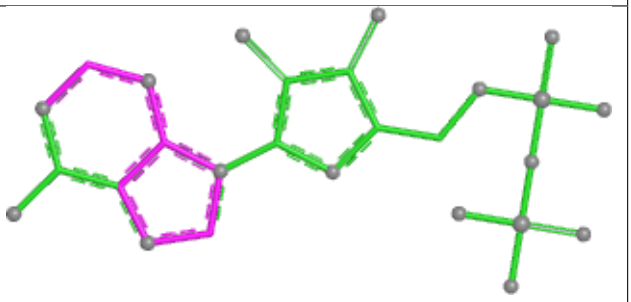
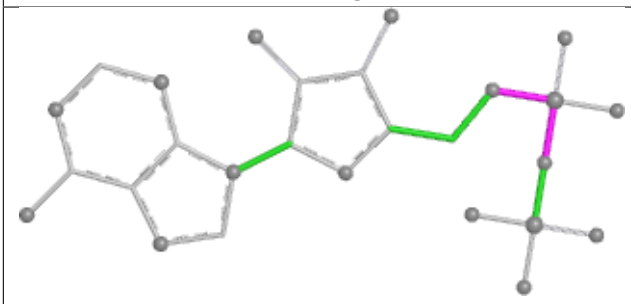
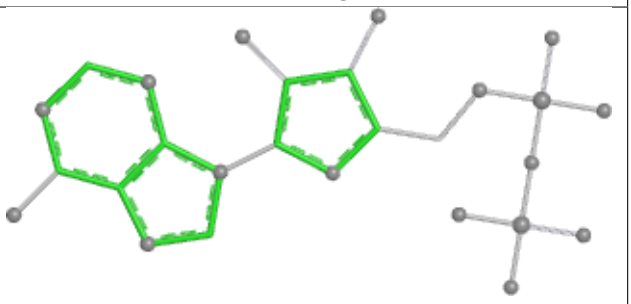


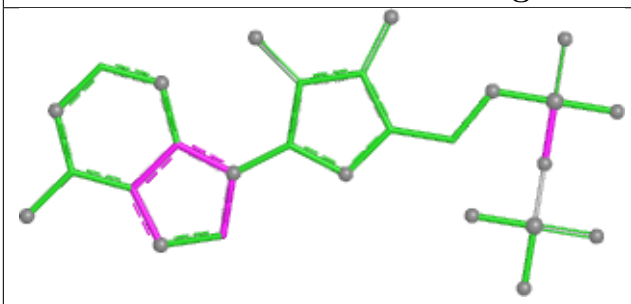
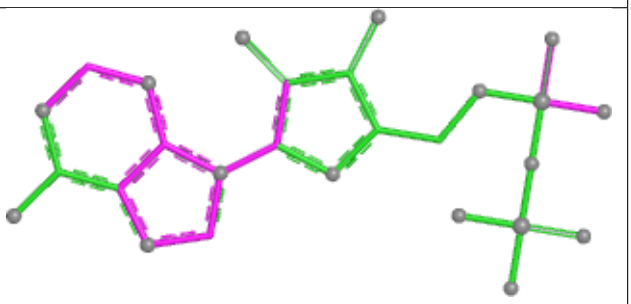
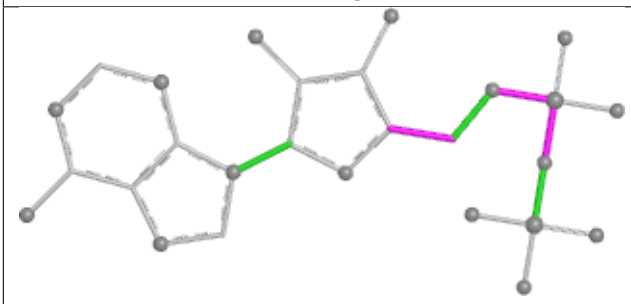
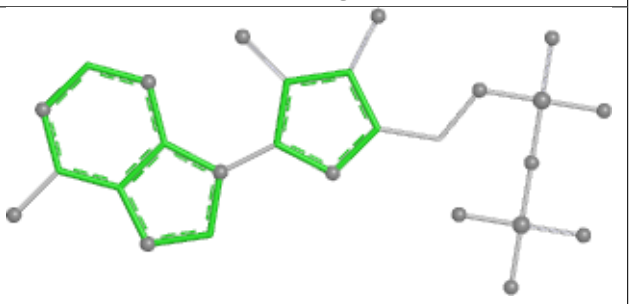
| Ligand ADP E 1002 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

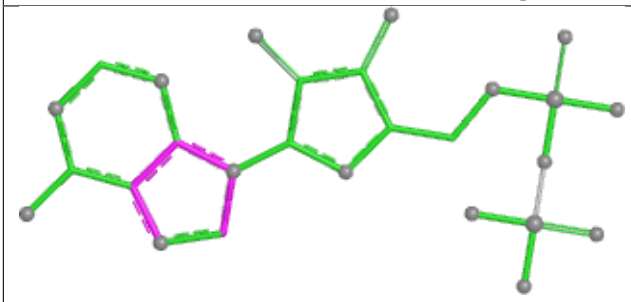
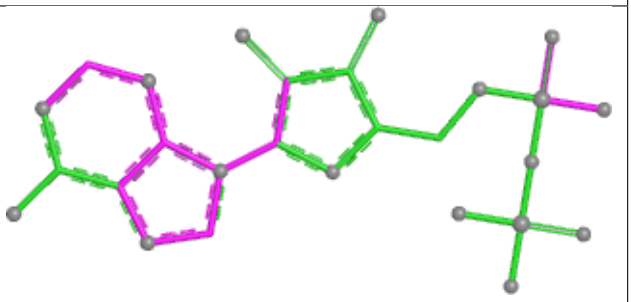
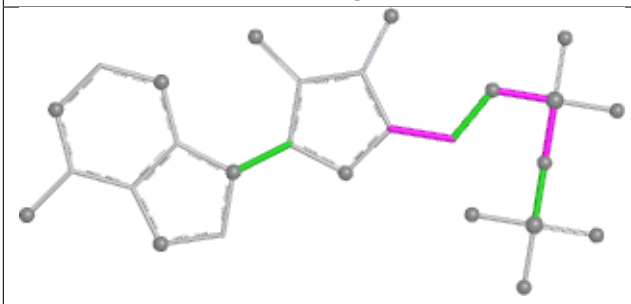
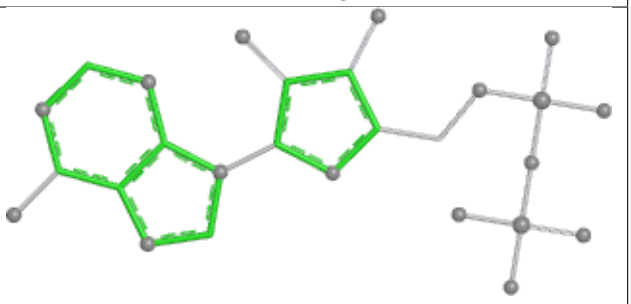
| Ligand ADP C 1001 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

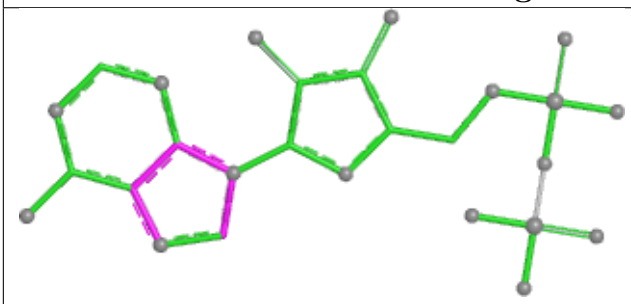
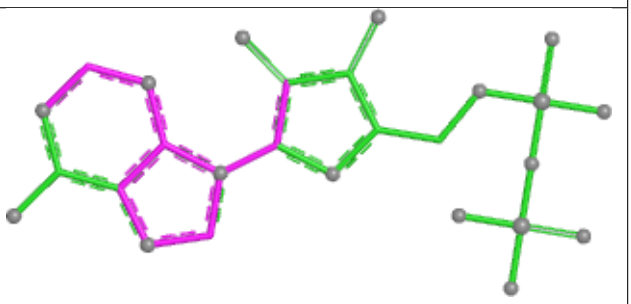
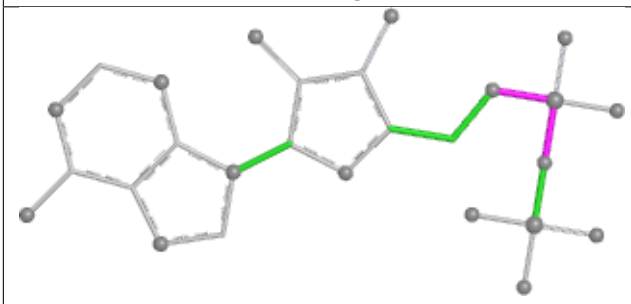
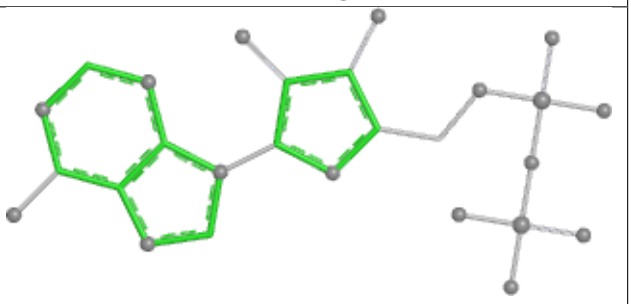
| Ligand ADP C 1002 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP F 1002 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

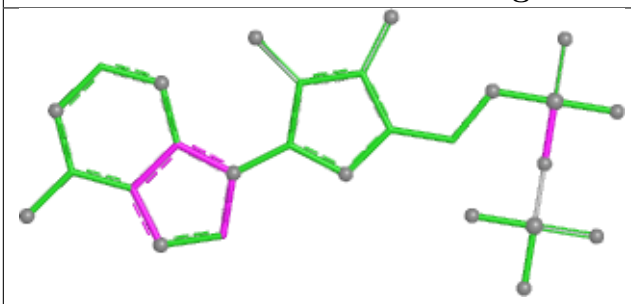
| Ligand ADP D 1002 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP D 1001 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

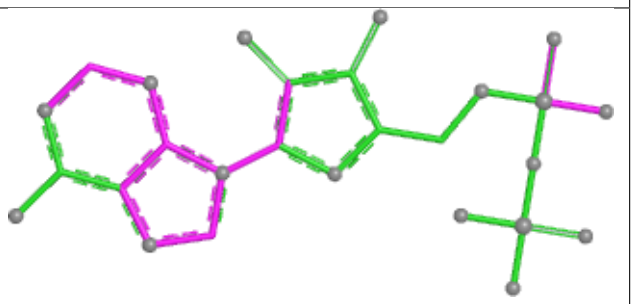
| Ligand ADP E 1001 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ADP F 1001 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

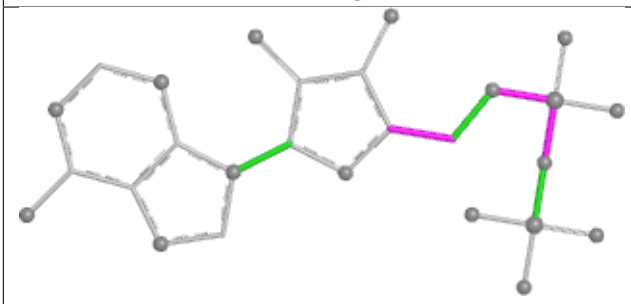
**Ligand ADP A 1001**



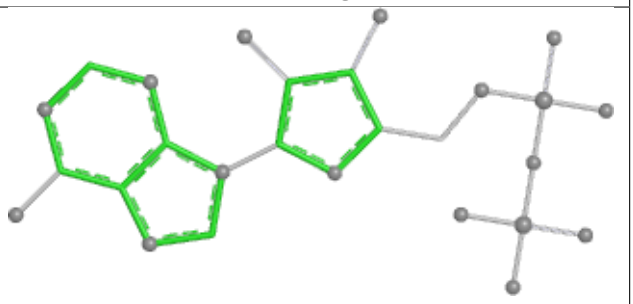
Bond lengths



Bond angles

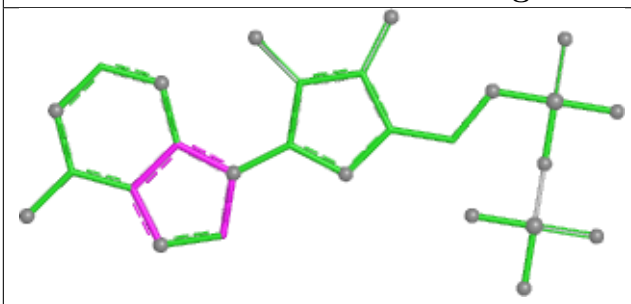


Torsions

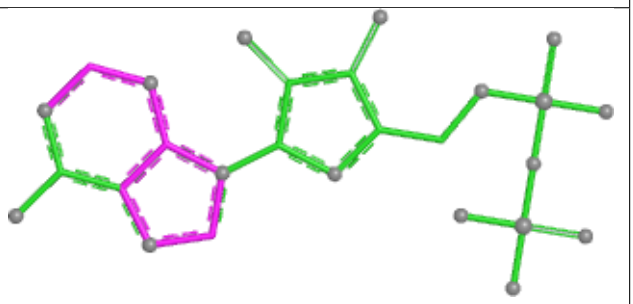


Rings

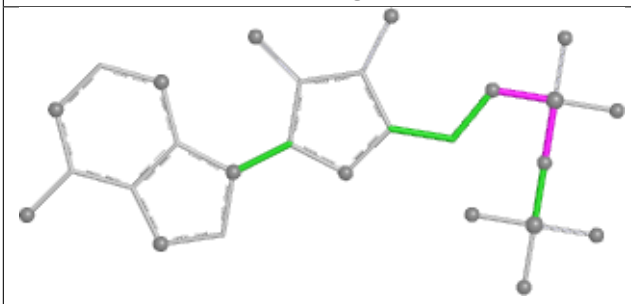
**Ligand ADP A 1002**



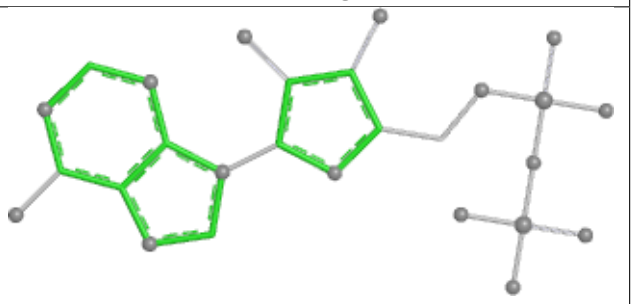
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

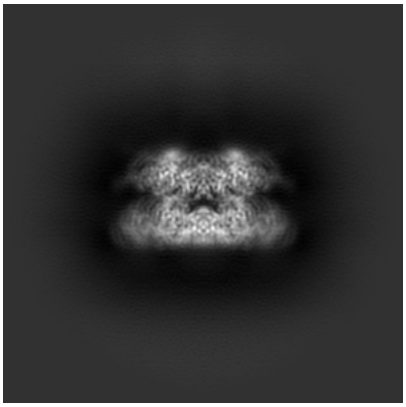
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24524. These allow visual inspection of the internal detail of the map and identification of artifacts.

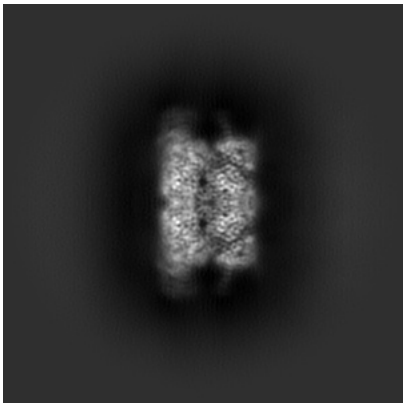
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

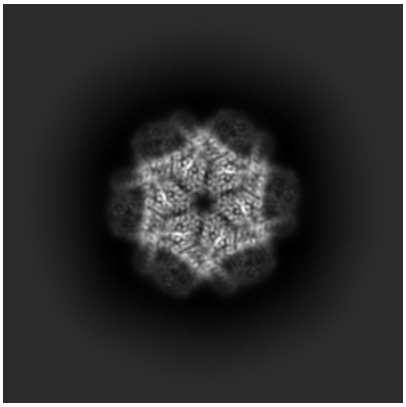
### 6.1.1 Primary map



X



Y

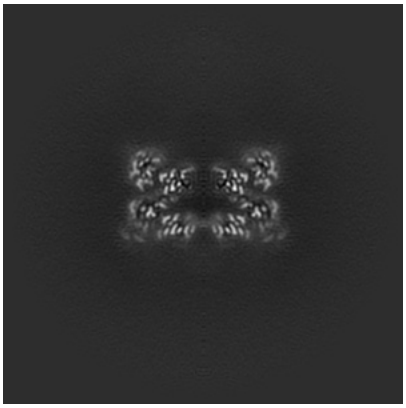


Z

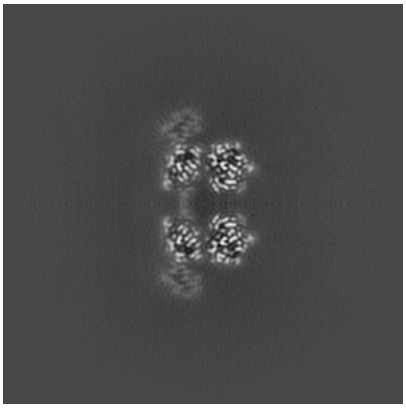
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

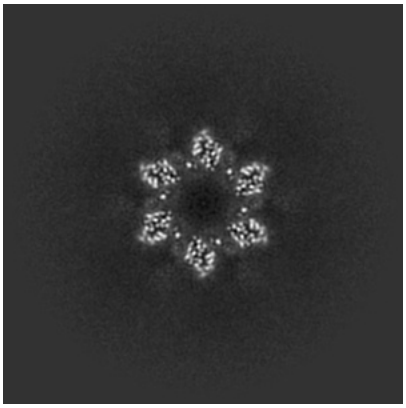
### 6.2.1 Primary map



X Index: 160



Y Index: 160

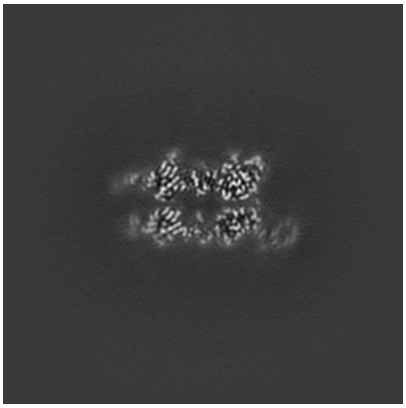


Z Index: 160

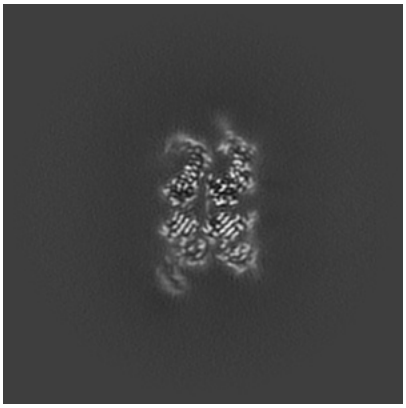
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

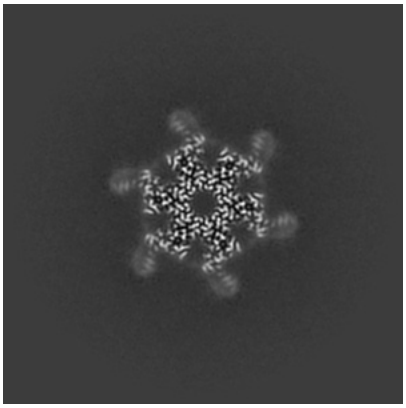
### 6.3.1 Primary map



X Index: 175



Y Index: 135

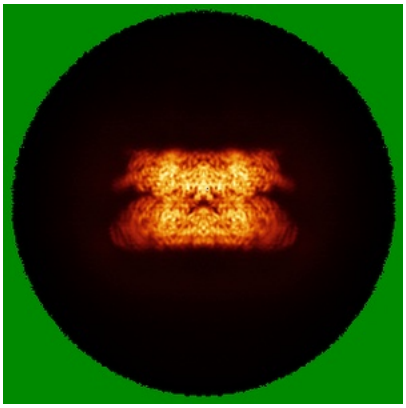


Z Index: 175

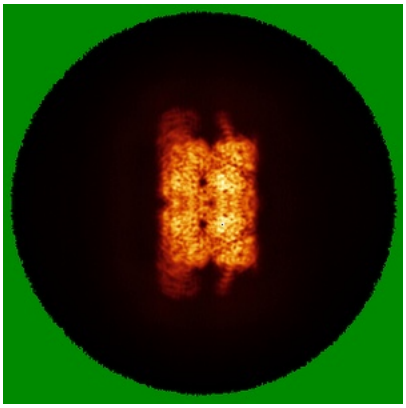
The images above show the largest variance slices of the map in three orthogonal directions.

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

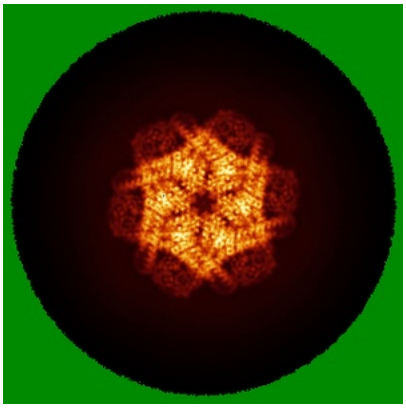
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

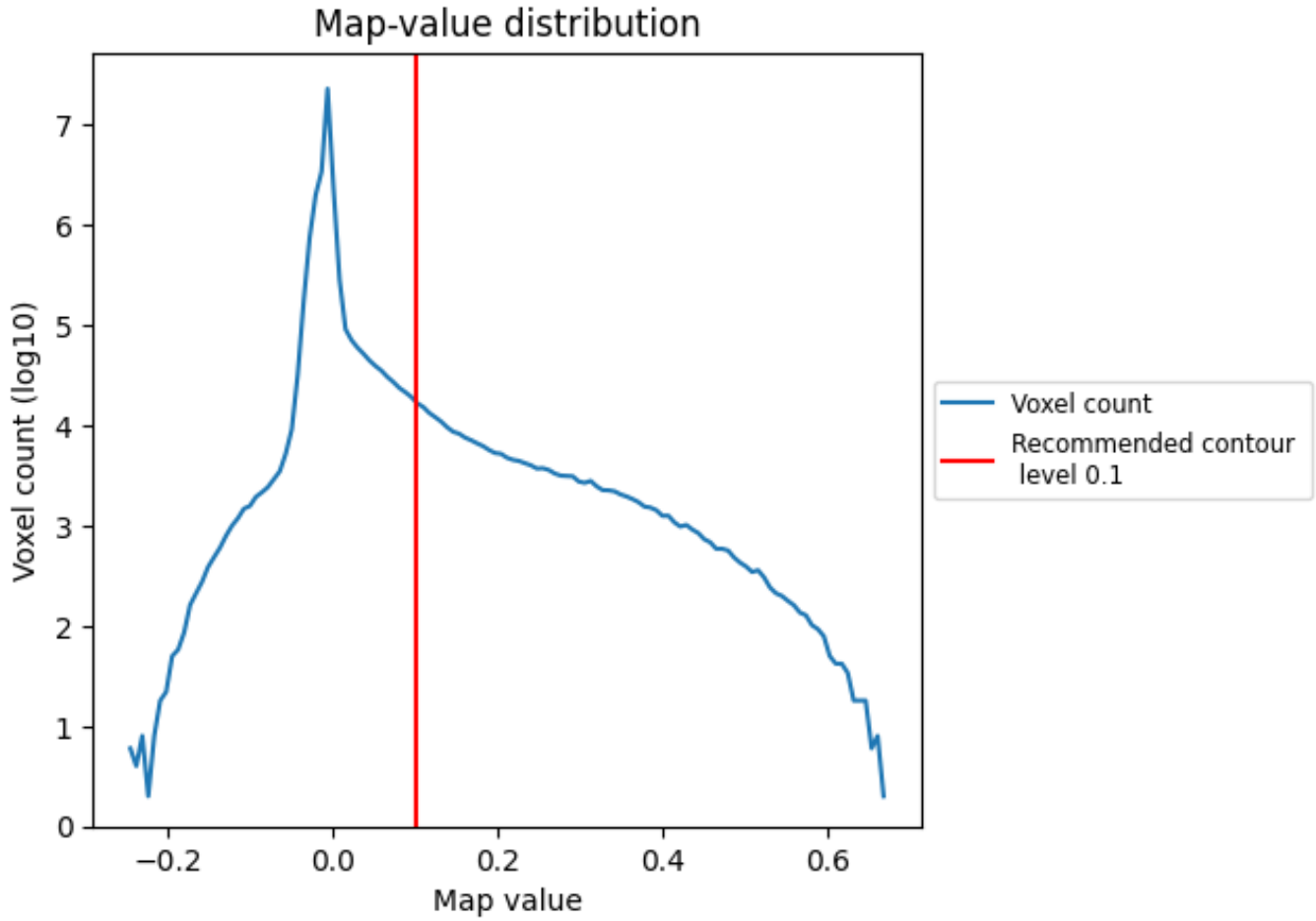
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

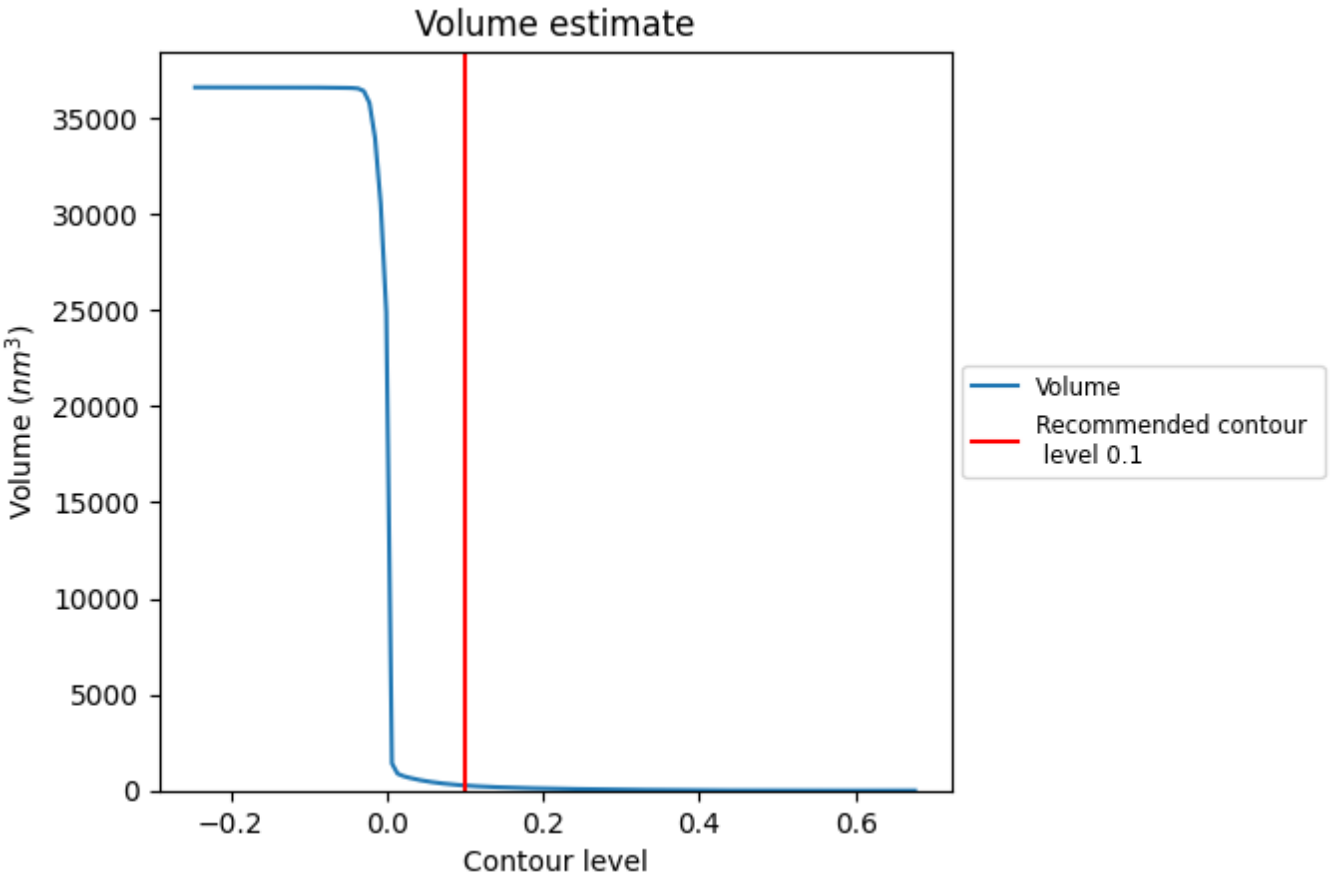
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

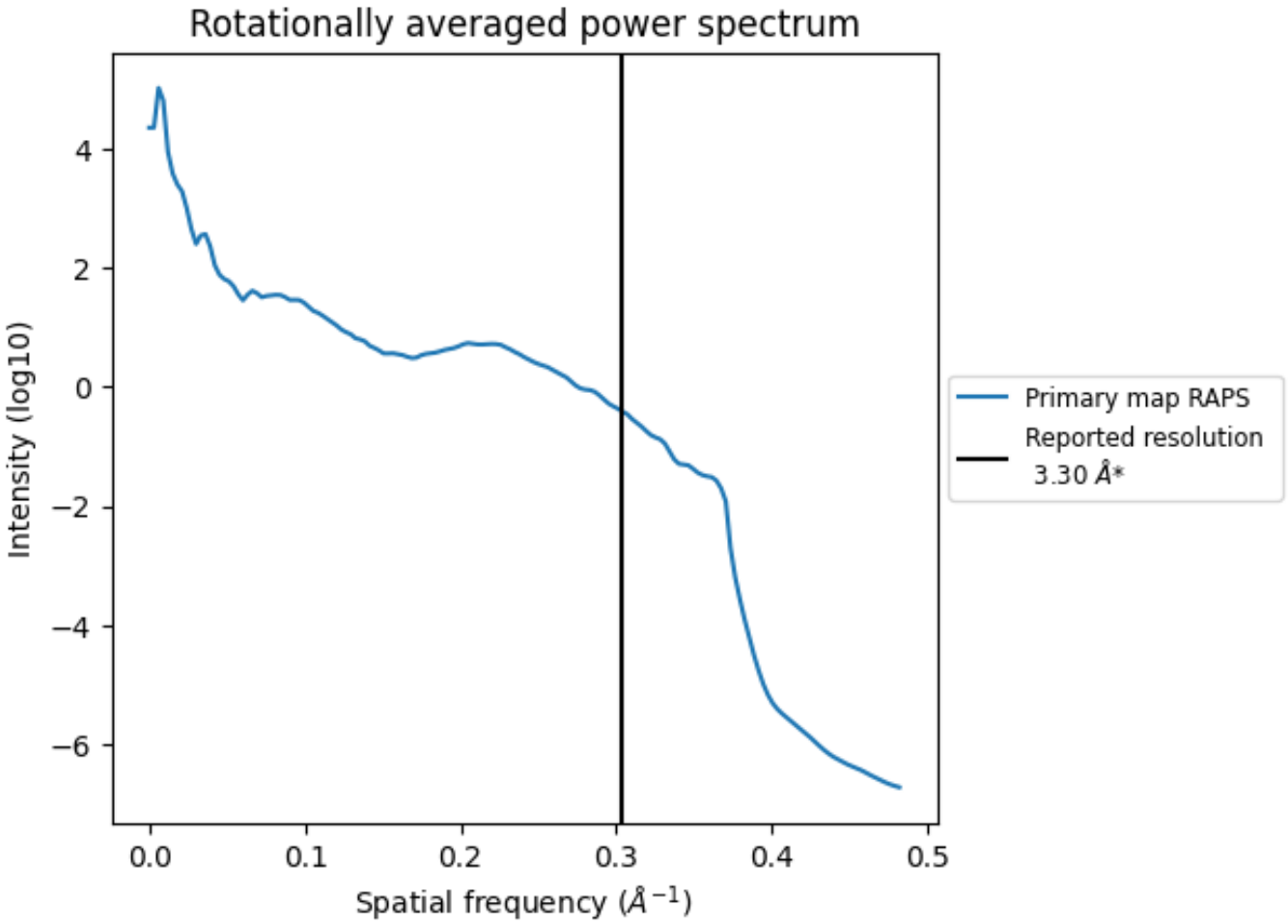
## 7.2 Volume estimate




The volume at the recommended contour level is 264 $nm^3$; this corresponds to an approximate mass of 238 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

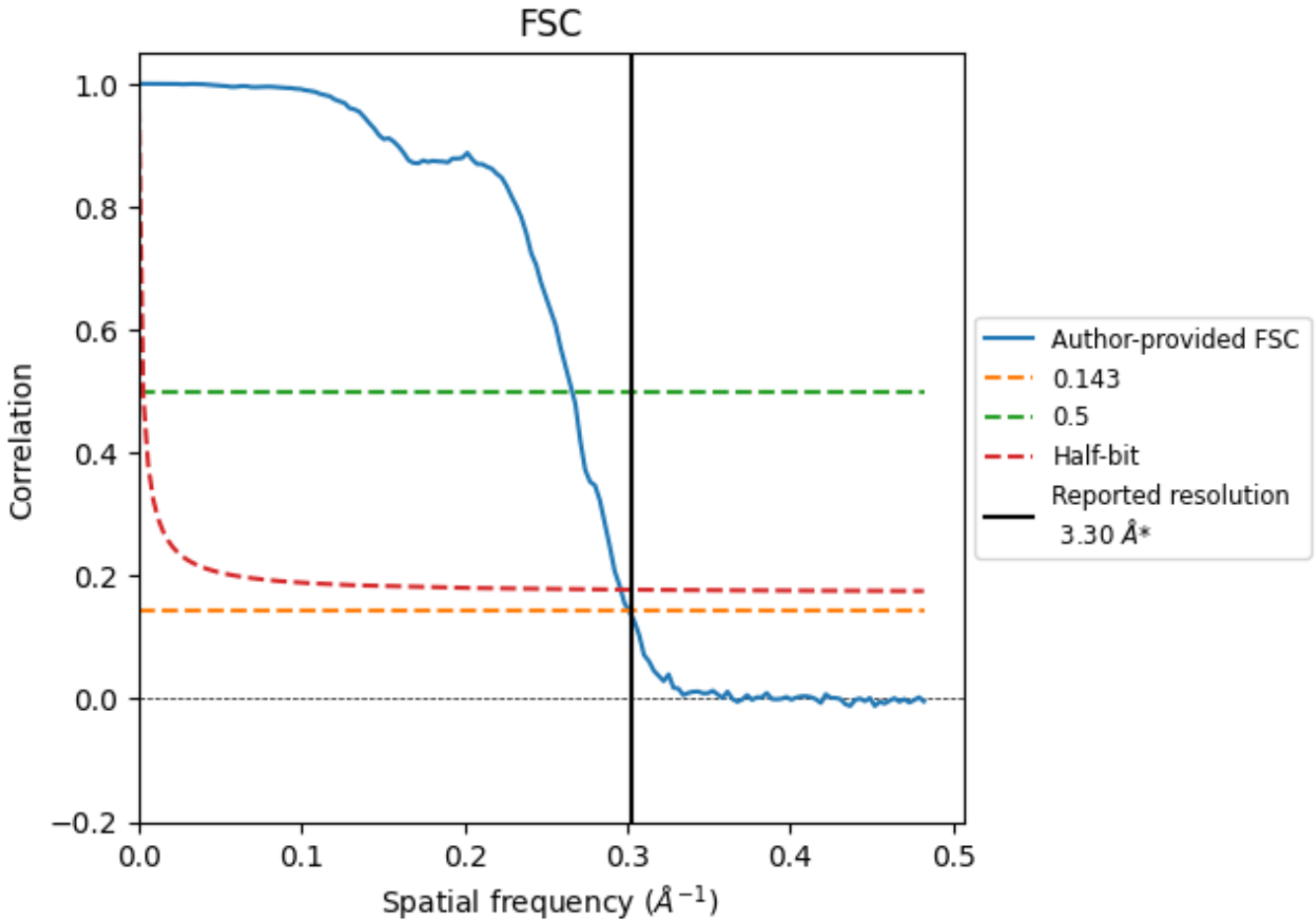



*Reported resolution corresponds to spatial frequency of 0.303 Å$^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

## 8.2 Resolution estimates (i)

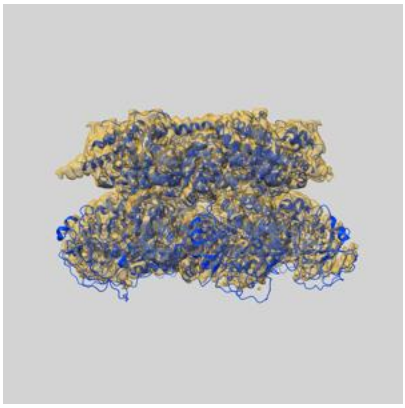
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.30 | - | - |
| Author-provided FSC curve | 3.32 | 3.76 | 3.38 |
| Unmasked-calculated* | - | - | - |

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

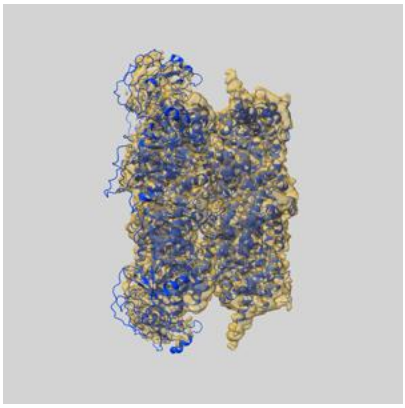
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24524 and PDB model 7RLB. Per-residue inclusion information can be found in section 3 on page 8.

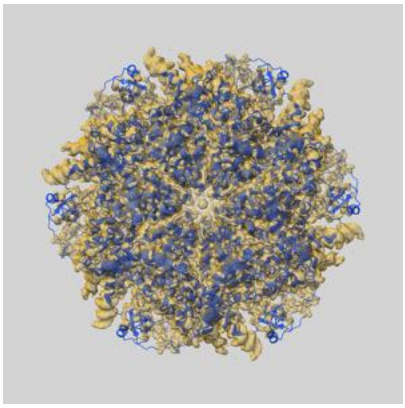
## 9.1 Map-model overlay



X



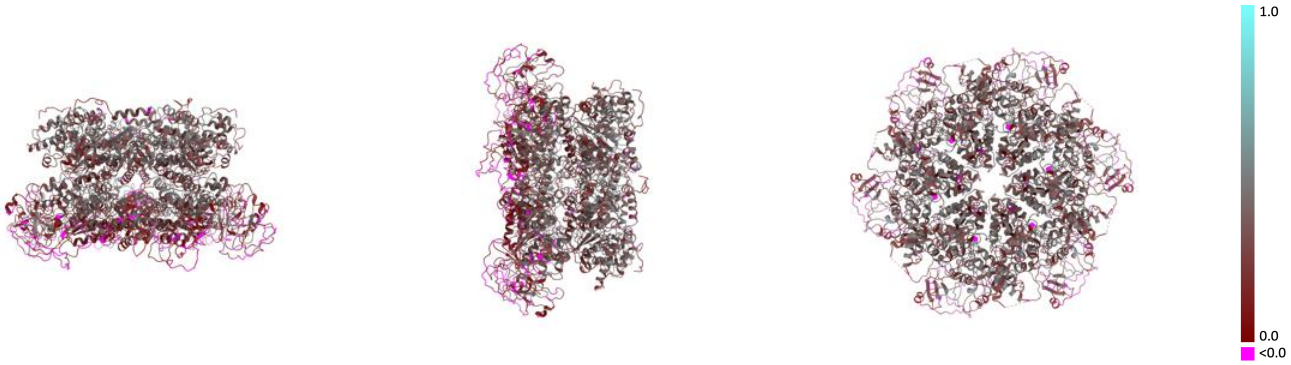
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

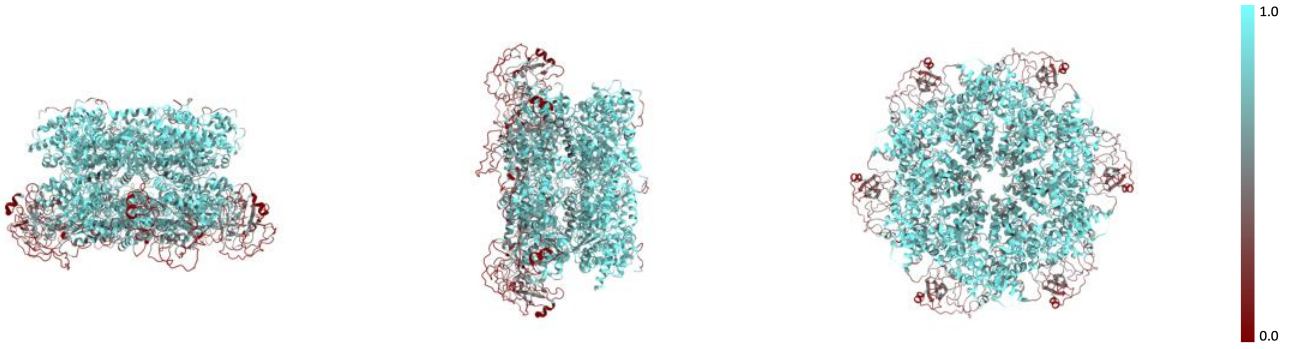
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

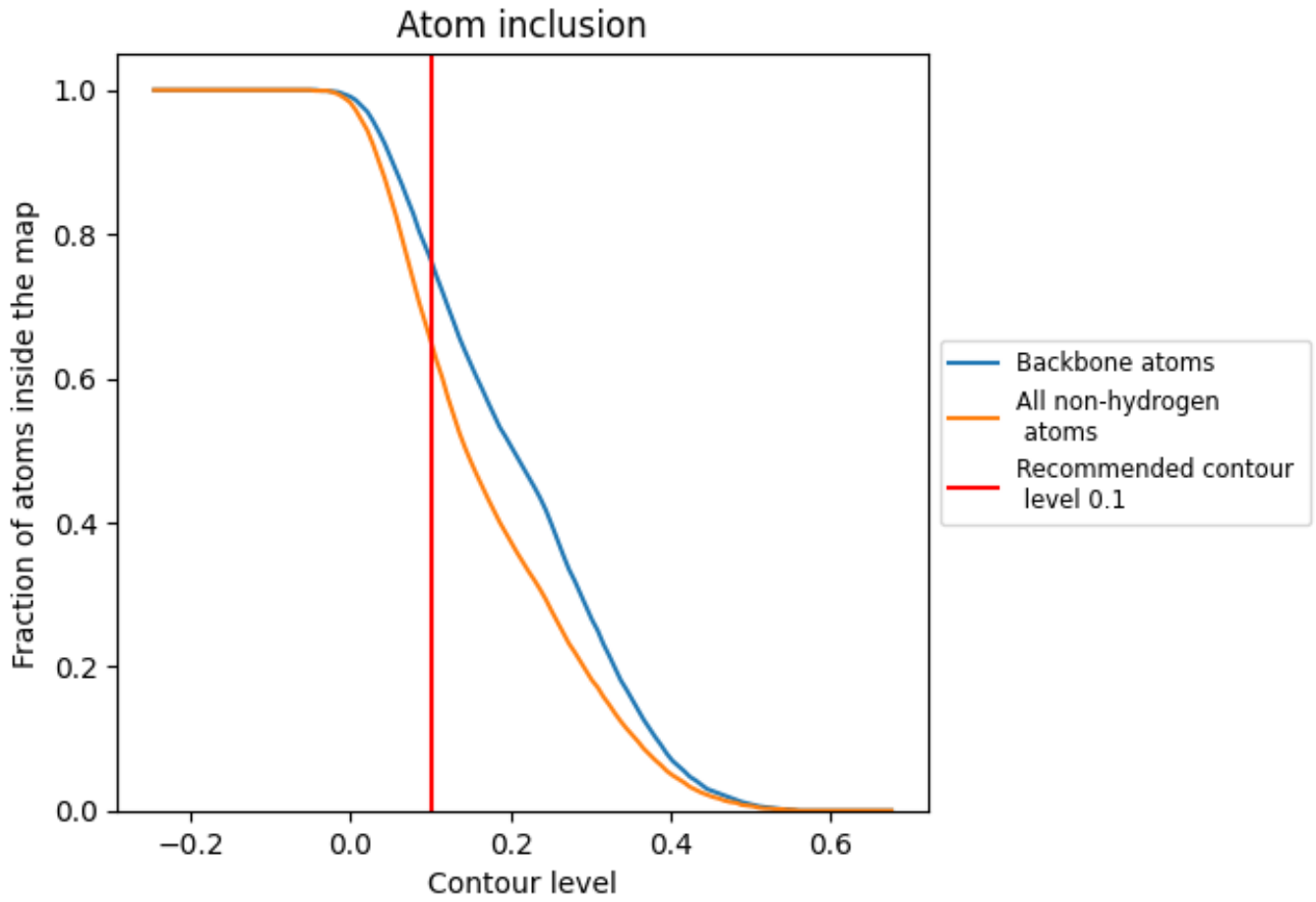
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

## 9.4 Atom inclusion (i)




At the recommended contour level, 76% of all backbone atoms, 65% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6530 | 0.2770 |
| A | 0.6560 | 0.2810 |
| B | 0.6480 | 0.2720 |
| C | 0.6510 | 0.2770 |
| D | 0.6540 | 0.2770 |
| E | 0.6480 | 0.2700 |
| F | 0.6570 | 0.2840 |

