# Full wwPDB EM Validation Report (i)

May 12, 2024 – 06:24 am BST

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|---|---|---|
| PDB ID | : | 6REB |
| EMDB ID | : | EMD-4848 |
| Title | : | Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 3A, composite map |
| Authors | : | Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W. |
| Deposited on | : | 2019-04-12 |
| Resolution | : | 3.20 Å(reported) |

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

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

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

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

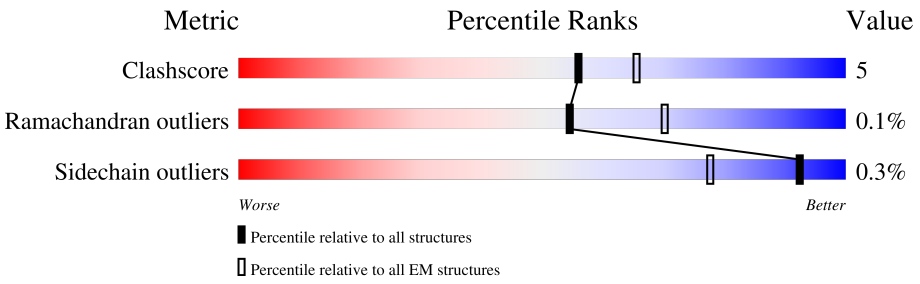
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0 | 82 | 95% |
| 2 | 1 | 618 | 85% 11% |
| 3 | 2 | 441 | 85% 15% |
| 4 | 3 | 325 | 67% 8% 25% |
| 5 | 4 | 294 | 85% 13% |
| 6 | 5 | 123 | 87% 13% |
| 7 | 6 | 151 | 73% 9% 18% |
| 8 | 7 | 190 | 78% 15% 7% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | 8 | 89 | 89% 10% • |
| 10 | 9 | 97 | 88% 12% |
| 11 | A | 127 | 51% 7% 42% |
| 11 | B | 127 | 50% 9% 42% |
| 11 | C | 127 | 50% 9% 42% |
| 11 | D | 127 | 46% 13% 42% |
| 11 | E | 127 | 48% 10% 42% |
| 11 | F | 127 | 50% 9% 42% |
| 11 | G | 127 | 50% 9% 42% |
| 11 | H | 127 | 49% 9% 42% |
| 11 | I | 127 | 46% 12% 42% |
| 11 | J | 127 | 48% 10% 42% |
| 12 | M | 327 | 58% 8% 34% |
| 13 | P | 229 | 74% 10% 16% |
| 14 | Q | 74 | 80% 18% • |
| 15 | R | 199 | 81% 8% • 11% |
| 16 | S | 317 | 73% 14% 13% |
| 17 | T | 562 | 82% 11% • 7% |
| 17 | U | 562 | 81% 12% 7% |
| 17 | V | 562 | 76% 17% 7% |
| 18 | X | 574 | 79% 14% • 6% |
| 18 | Y | 574 | 81% 10% 9% |
| 18 | Z | 574 | 79% 16% 6% |

# 2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 53756 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 0 | 81 | 607 | 388 | 107 | 110 | 2 | 0 | 0 |

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 1 | 595 | 4661 | 2958 | 798 | 900 | 5 | 0 | 0 |

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 3 | 2 | 441 | 3163 | 2020 | 532 | 611 | 0 | 0 |

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | 3 | 245 | 1874 | 1204 | 299 | 370 | 1 | 0 | 0 |

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | 4 | 290 | 2177 | 1385 | 356 | 434 | 2 | 0 | 0 |

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | 5 | 123 | 986 | 640 | 172 | 170 | 4 | 0 | 0 |

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | 6 | 124 | 926 | 599 | 154 | 172 | 1 | 0 | 0 |

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | 7 | 176 | 1347 | 860 | 227 | 259 | 1 | 0 | 0 |

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 9 | 8 | 88 | 692 | 456 | 115 | 121 | 0 | 0 |

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 10 | 9 | 97 | 776 | 514 | 124 | 132 | 6 | 0 | 0 |

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit c.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | A | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |
| 11 | B | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |
| 11 | C | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |
| 11 | D | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |
| 11 | E | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |
| 11 | F | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |
| 11 | G | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |
| 11 | H | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | I | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |
| 11 | J | 74 | 514 | 340 | 83 | 88 | 3 | 0 | 0 |

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | M | 217 | 1640 | 1077 | 267 | 288 | 8 | 0 | 0 |

- Molecule 13 is a protein called Mitochondrial ATP synthase subunit OSCP.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | P | 193 | 1532 | 988 | 250 | 290 | 4 | 0 | 0 |

- Molecule 14 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | Q | 72 | 561 | 358 | 102 | 99 | 2 | 0 | 0 |

- Molecule 15 is a protein called Mitochondrial ATP synthase subunit delta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | R | 177 | 1303 | 833 | 213 | 256 | 1 | 0 | 0 |

- Molecule 16 is a protein called ATP synthase gamma chain, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | S | 277 | 2130 | 1327 | 377 | 416 | 10 | 0 | 0 |

- Molecule 17 is a protein called ATP synthase subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | T | 523 | 3979 | 2537 | 703 | 728 | 11 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | U | 523 | 3980 | 2537 | 703 | 729 | 11 | 0 | 0 |
| 17 | V | 520 | 3962 | 2527 | 700 | 724 | 11 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| T | 266 | ARG | LYS | conflict | UNP A0ZW40 |
| U | 266 | ARG | LYS | conflict | UNP A0ZW40 |
| V | 266 | ARG | LYS | conflict | UNP A0ZW40 |

- Molecule 18 is a protein called ATP synthase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | X | 539 | 4095 | 2572 | 693 | 817 | 13 | 0 | 0 |
| 18 | Y | 521 | 3957 | 2485 | 670 | 789 | 13 | 0 | 0 |
| 18 | Z | 542 | 4115 | 2586 | 696 | 820 | 13 | 0 | 0 |

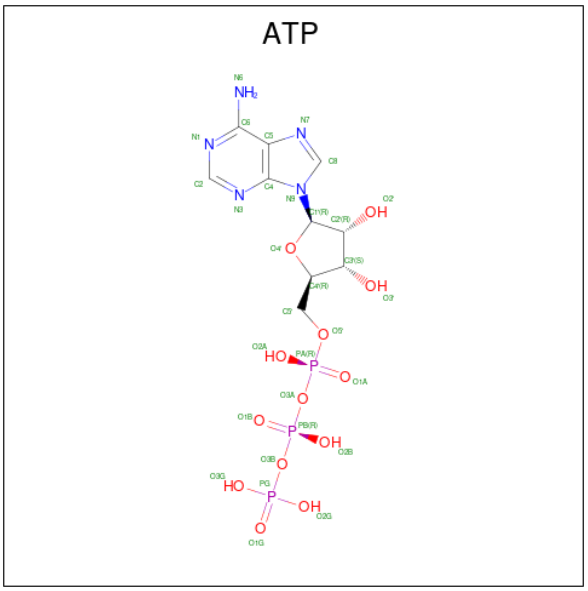
There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| X | 350 | ALA | GLY | conflict | UNP A0ZW41 |
| X | 387 | LEU | ARG | conflict | UNP A0ZW41 |
| Y | 350 | ALA | GLY | conflict | UNP A0ZW41 |
| Y | 387 | LEU | ARG | conflict | UNP A0ZW41 |
| Z | 350 | ALA | GLY | conflict | UNP A0ZW41 |
| Z | 387 | LEU | ARG | conflict | UNP A0ZW41 |

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 19 | M | 1 | 1 | 1 | 0 |

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

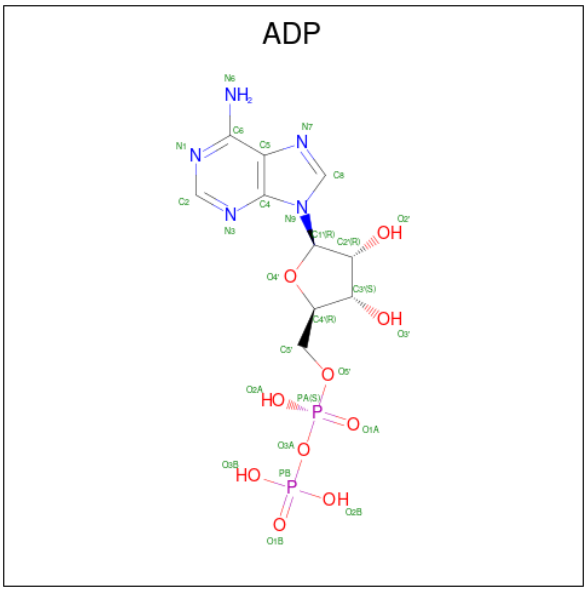



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 20 | T | 1 | 31 | 10 | 5 | 13 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 20 | U | 1 | 31 | 10 | 5 | 13 | 3 | 0 |
| | | | Total | C | N | O | P | |
| 20 | V | 1 | 31 | 10 | 5 | 13 | 3 | 0 |

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 21 | T | 1 | 1 | 1 | 0 |
| | | | Total | Mg | |
| 21 | U | 1 | 1 | 1 | 0 |
| | | | Total | Mg | |
| 21 | V | 1 | 1 | 1 | 0 |
| | | | Total | Mg | |
| 21 | X | 1 | 1 | 1 | 0 |
| | | | Total | Mg | |
| 21 | Z | 1 | 1 | 1 | 0 |

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 22 | X | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 22 | Z | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

# 3 Residue-property plots (i)

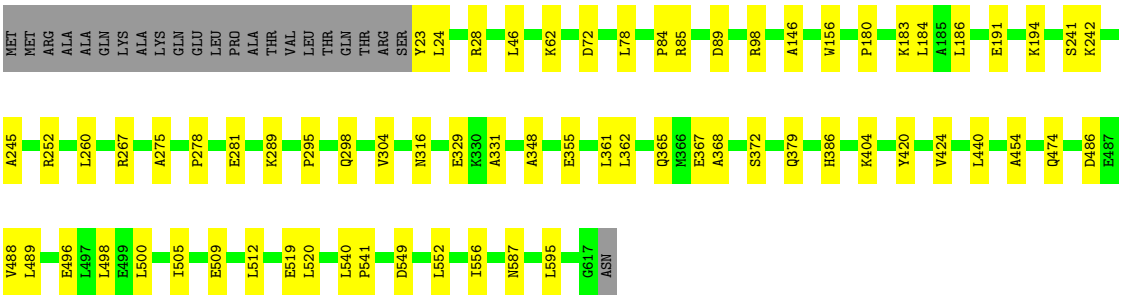
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ASA-10: Polytomella F-ATP synthase associated subunit 10

Chain 0: 95%

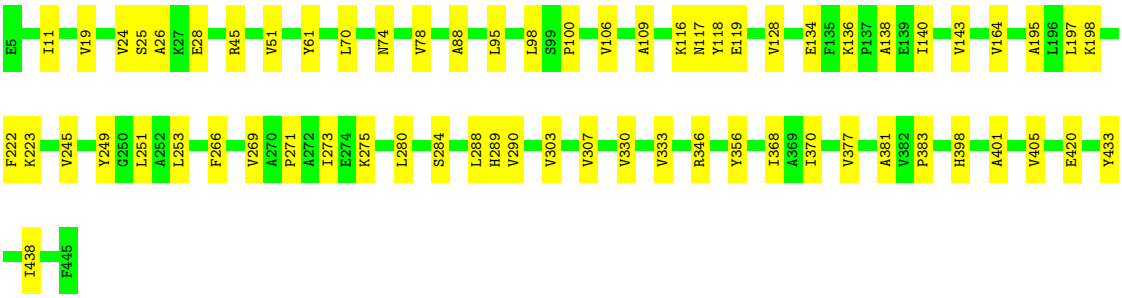
• Molecule 2: ATP synthase associated protein ASA1

Chain 1: 85% 11%



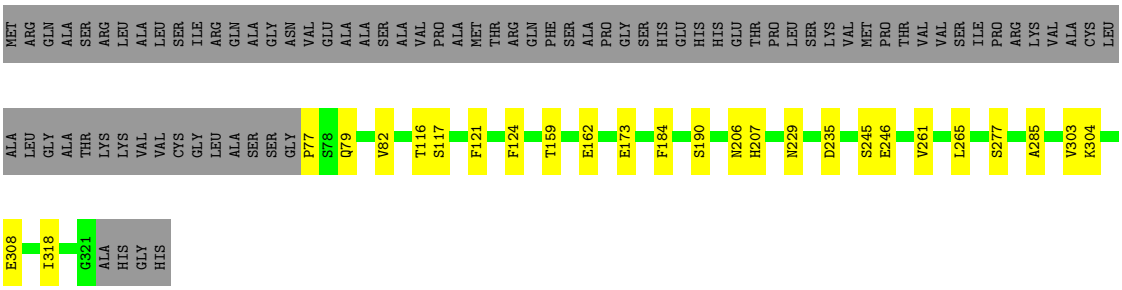

• Molecule 3: ASA-2: Polytomella F-ATP synthase associated subunit 2

Chain 2: 85% 15%



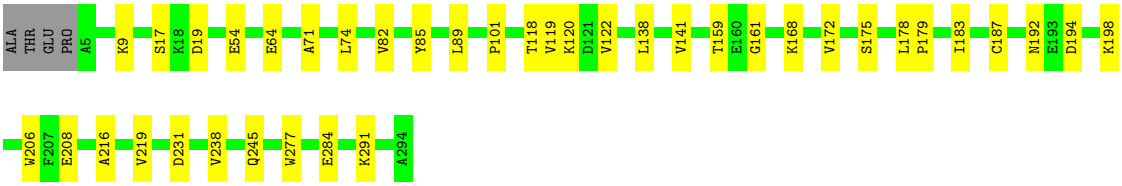

• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3: 67% 8% 25%




• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4:




• Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

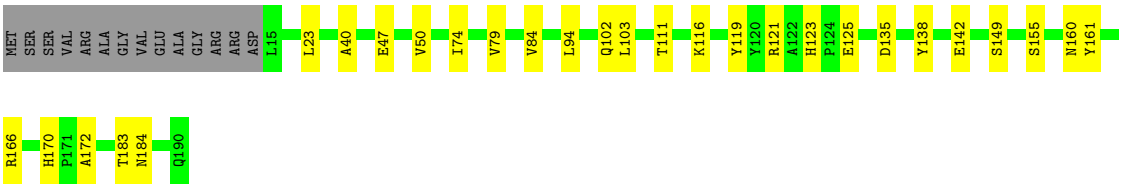
Chain 5:

• Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6:

• Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7:




• Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8:

• Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

Chain 9: 88% 12%

M1 L26 F29 L30 S31 S32 K33 P70 A71 G72 W73 Q80 A86 Y90 K94 N97

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain A: 51% 7% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 A57 K60 A70

L71 A72 L78 L85 I86 T110 L119 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain B: 50% 9% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 A70 L71 A72 G73 V74

L78 L85 I86 T110 A114 L123 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain C: 50% 9% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 A70 L71 A72 G73 V74

V80 L85 I86 P93 I113 A114 L115 F116 L119 A127

• Molecule 11: Mitochondrial ATP synthase subunit c

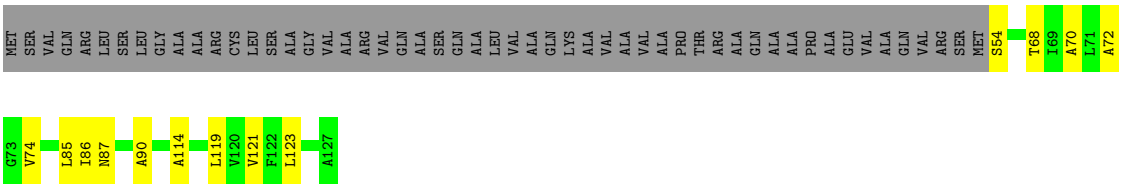
Chain D: 46% 13% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 T68 I69 A70 L71 A72

G73 V74 G75 V80 L85 I86 N87 I95 F107 E111 A114 L119 V120 V121 A127

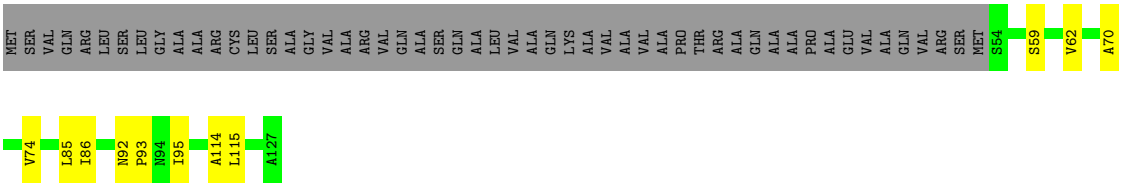
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain E: 48% 10% 42%



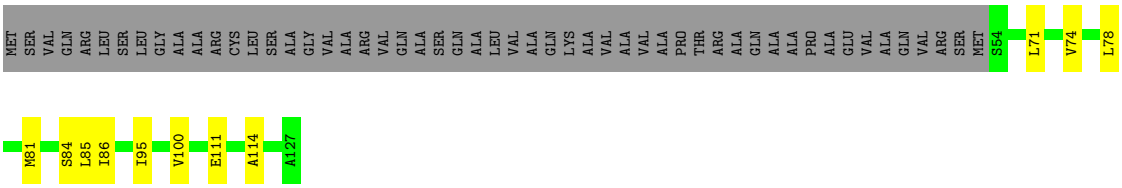

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain F: 50% 9% 42%



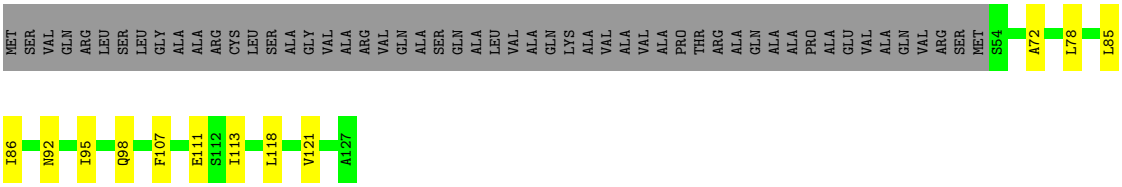

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain G: 50% 9% 42%



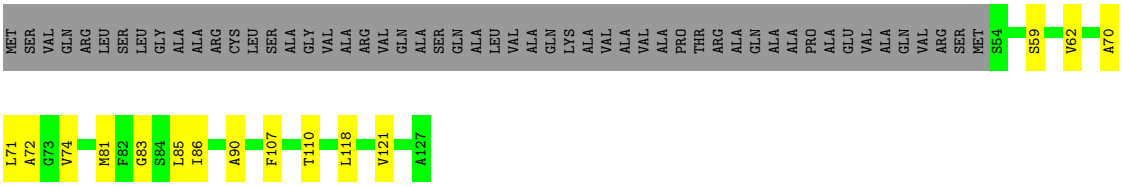

• Molecule 11: Mitochondrial ATP synthase subunit c

Chain H: 49% 9% 42%




• Molecule 11: Mitochondrial ATP synthase subunit c

Chain I: 46% 12% 42%




• Molecule 11: Mitochondrial ATP synthase subunit c

Chain J: 48% 10% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 S59 V62 A70

L71 A72 G73 V74 L78 S84 L85 I86 N92 A103 A114 A127

- Molecule 12: Mitochondrial ATP synthase subunit 6

Chain M: 58% 8% 34%

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

SER PRO LEU ASN VAL LYS LEU PRO GLY MET SER CYS SER SER ILE LEU LEU PRO LYS THR SER ARG ILE ALA VAL PRO PHE GLY ASN GLN THR MET ALA MET S95 Q120 N121 R133 R145 N163 T175 T200 G201 F202 K203 F204 P205 GLY HIS PHE ILE PRO GLY GLY

THR PRO TRP PRO MET ALA F219 Y229 R232 A233 V234 R239 N243 L250 L254 T255 S264 V271 F275 L280 L281 E288 V291 A292 T304 K321 K324 LYS ILE HIS

- Molecule 13: Mitochondrial ATP synthase subunit OSCP

Chain P: 74% 10% 16%

MET LEU ALA ARG VAL ALA SER VAL ALA LEU ARG ARG ALA GLU GLY LYS ILE MET PRO GLN MET VAL ARG ALA LEU SER VAL SER ALA ALA SER ALA ALA GLN ALA GLU L37 T49 Q52 E73 E79 Q83 S112 G113 A114 T118 E136 N140 K149

I157 P161 L162 D163 E166 D179 K189 I190 L195 V199 D208 M209 S210 T211 A212 I229

- Molecule 14: epsilon: Polytomella F-ATP synthase epsilon subunit

Chain Q: 80% 18%

MET CYS A3 P4 S5 G6 R10 S15 Y16 L17 I22 D25 R28 K32 K36 A39 D54 K71 N74

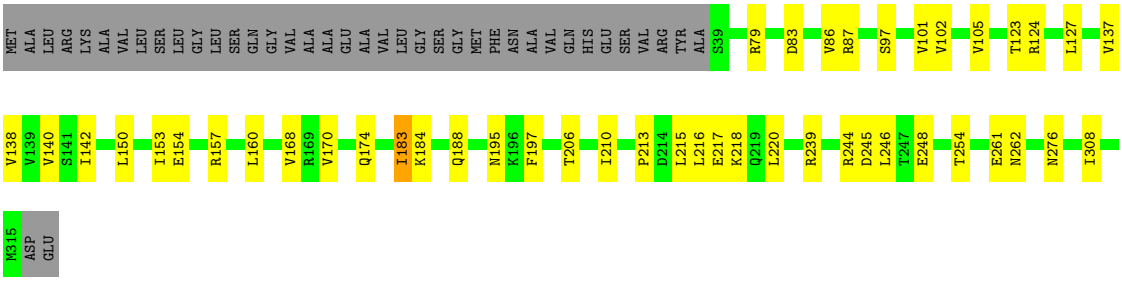
- Molecule 15: Mitochondrial ATP synthase subunit delta

Chain R: 81% 8% 11%

MET PHE GLY LEU LYS ARG ALA VAL THR VAL GLY ARG ARG PHE ILE SER THR SER ALA ALA ARG MET E23 A24 A25 E49 F50 N53 P71 V89 V90 T107 E117 L118 E125 V129 V136 V141 T142 V146 D153 A199

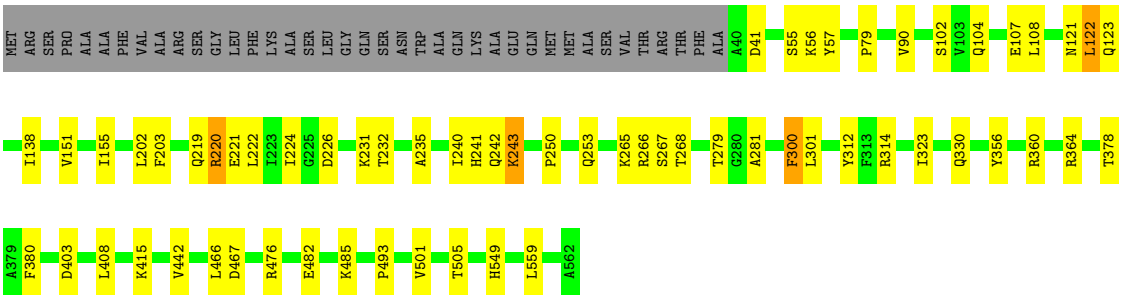
- Molecule 16: ATP synthase gamma chain, mitochondrial

Chain S: 73% 14% 13%



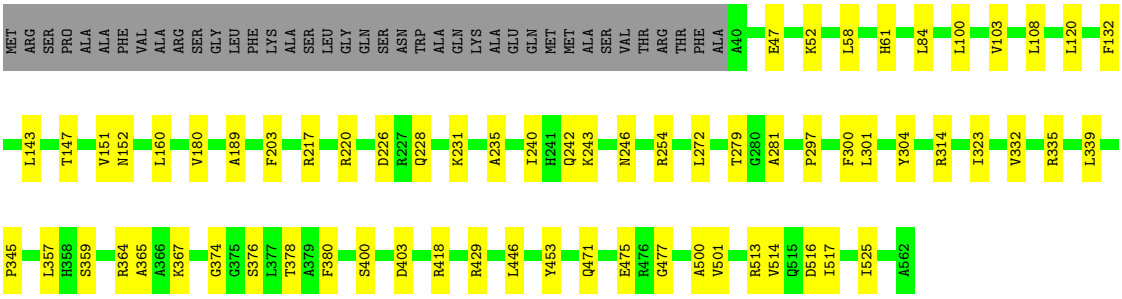

• Molecule 17: ATP synthase subunit alpha

Chain T:



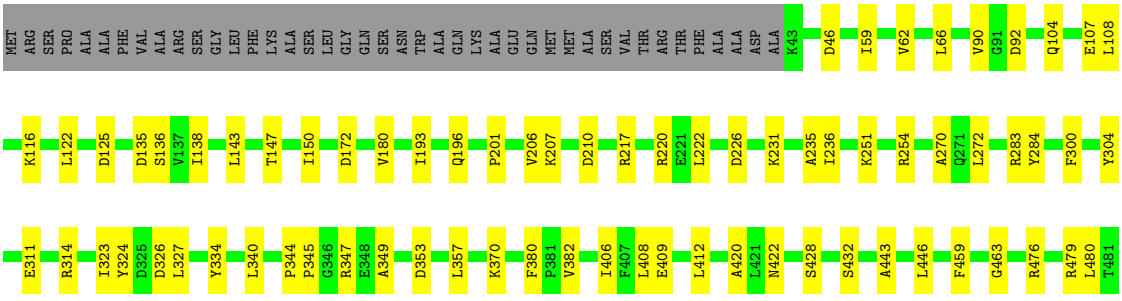

• Molecule 17: ATP synthase subunit alpha

Chain U:




• Molecule 17: ATP synthase subunit alpha

Chain V:



E482 K485 Q486 Q497 T498 V501 T505 V512 R513 V514 Q515 D516 I517 A523 Q527 V528 N529 V532 A545 L546 A552 K556 A562

- Molecule 18: ATP synthase subunit beta

Chain X: 79% 14% • 6%

MET ALA LEU ARG TYR ALA ALA GLY LEU ALA LYS ASN VAL VAL GLN ARG GLN GLY ALA SER LEU ASN ILE ALA ARG ALA PHE ALA ALA GLU PRO ALA PRO ALA ILE D36 Y39 Q42 D49 P57 V65 L72 D82 V85 R86 A89 L96 V97 R98 G99

V102 M122 N123 V124 I125 G126 D130 E131 Q132 R145 P148 V166 G180 K202 R225 V232 I233 K234 L235 N241 G249 Q250 M251 N252 A257 V261 L266 T267 R273 V284 D285 N286 I287 F288 R289 L300 A307 V308 G309 L318

R324 I325 T326 I333 T354 L358 D359 I373 A394 N398 R401 Q404 K405 V406 Y410 L420 D429 T432 R435 A436 R437 K438 L443 S444 Q445 P446 G458 K459 L474 L481 Y487 K498 A503 I506 D513 D543

V560 E563 K573 N574

- Molecule 18: ATP synthase subunit beta

Chain Y: 81% 10% 9%

MET ALA LEU ARG TYR ALA ALA GLY LEU ALA LYS ASN VAL VAL GLN ARG GLN GLY ALA SER LEU ASN ILE ALA ARG ALA PHE ALA ALA GLU PRO ALA PRO ALA ILE D36 I44 P57 S58 I59 H79 R98 V111 V124 I125 R145 T155 K165 D168 L169

L170 K202 G231 V232 I233 K234 S242 T245 L246 T264 T267 V268 F272 E276 V284 D285 N286 I304 P305 S306 A307 V308 Q337 A338 P349 T353 S365 I368 N388 V391 A394 N398 Q404 K405 V406 S426 D429

R435 I439 Q445 Q448 K459 L463 G472 G476 K477 Y478 V489 G490 D491 P525 S556 GLU THR VAL VAL LEU ASN GLU GLU GLY LYS SER VAL PRO LEU PRO LYS LYS ASN

- Molecule 18: ATP synthase subunit beta

Chain Z: 79% 16% 6%

MET ALA LEU ARG TYR ALA ALA GLY LEU ALA LYS ASN VAL VAL GLN ARG GLN GLY ALA SER LEU ASN ILE ALA ARG ALA PHE ALA ALA GLU PRO ALA P33 Q42 V43 I44 D49 P57 V65 L72 V85 A89 G95 R98 V102 K110 V111 D130

I140 W141 S142 R145 L160 K165 L170 R175 K178 I179 G180 G184 A185 L196 V200 R216 L223 Y224 R225 E226 T245 G249 Q250 V261 T264 G265 L266 T267 V268 A269 E270 L281 V284 D285 N286 I287 F288 R289 P305 S306 A307

V308 G309 L318 Q322 I325 T334 A338 V339 Y340 D348 P351 T354 L358 R366 I373 R385 A394 E395 N398 V399 Q404 K405 V406 E424 A436 I439 S444 Q445 K459 T466 I467 Q471 D480 A503 K504 D505

I506 A507 S508 E520 I524 P525 S526 L527 D528 K529 E540 D543 S556 E557 V560 N574

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 74956 | 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 ($e^-/Å^2$) | 35 | Depositor |
| Minimum defocus (nm) | -400 | Depositor |
| Maximum defocus (nm) | -5000 | Depositor |
| Magnification | 75000 | Depositor |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 35.532 | Depositor |
| Minimum map value | -21.540 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 1.034 | Depositor |
| Recommended contour level | 0.04 | Depositor |
| Map size (Å) | 505.44, 505.44, 505.44 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.053, 1.053, 1.053 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ATP, 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 | 0 | 0.50 | 0/628 | 0.52 | 0/856 |
| 2 | 1 | 0.49 | 0/4750 | 0.55 | 0/6434 |
| 3 | 2 | 0.40 | 0/3212 | 0.57 | 0/4371 |
| 4 | 3 | 0.45 | 0/1911 | 0.56 | 1/2601 (0.0%) |
| 5 | 4 | 0.47 | 0/2216 | 0.54 | 0/3000 |
| 6 | 5 | 0.58 | 0/1011 | 0.67 | 2/1376 (0.1%) |
| 7 | 6 | 0.51 | 0/946 | 0.60 | 0/1287 |
| 8 | 7 | 0.56 | 0/1374 | 0.58 | 1/1865 (0.1%) |
| 9 | 8 | 0.56 | 0/715 | 0.62 | 0/974 |
| 10 | 9 | 0.42 | 0/802 | 0.59 | 0/1084 |
| 11 | A | 0.35 | 0/520 | 0.59 | 1/704 (0.1%) |
| 11 | B | 0.35 | 0/520 | 0.56 | 0/704 |
| 11 | C | 0.39 | 0/519 | 0.60 | 1/701 (0.1%) |
| 11 | D | 0.43 | 0/520 | 0.60 | 0/704 |
| 11 | E | 0.45 | 0/520 | 0.56 | 0/704 |
| 11 | F | 0.42 | 0/520 | 0.59 | 0/704 |
| 11 | G | 0.38 | 0/520 | 0.53 | 0/704 |
| 11 | H | 0.36 | 0/520 | 0.54 | 0/704 |
| 11 | I | 0.35 | 0/520 | 0.52 | 0/704 |
| 11 | J | 0.35 | 0/520 | 0.59 | 0/704 |
| 12 | M | 0.55 | 0/1683 | 0.62 | 0/2295 |
| 13 | P | 0.44 | 0/1553 | 0.58 | 0/2093 |
| 14 | Q | 0.40 | 0/574 | 0.53 | 0/774 |
| 15 | R | 0.45 | 0/1336 | 0.57 | 1/1827 (0.1%) |
| 16 | S | 0.45 | 0/2153 | 0.59 | 1/2901 (0.0%) |
| 17 | T | 0.59 | 0/4048 | 0.62 | 2/5481 (0.0%) |
| 17 | U | 0.59 | 0/4049 | 0.62 | 1/5481 (0.0%) |
| 17 | V | 0.60 | 0/4031 | 0.60 | 0/5456 |
| 18 | X | 0.56 | 0/4155 | 0.61 | 1/5630 (0.0%) |
| 18 | Y | 0.57 | 0/4015 | 0.59 | 0/5440 |
| 18 | Z | 0.57 | 0/4176 | 0.61 | 0/5659 |
| All | All | 0.52 | 0/54537 | 0.59 | 12/73922 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 3 | 2 | 0 | 1 |
| 6 | 5 | 0 | 1 |
| 18 | X | 0 | 2 |
| 18 | Y | 0 | 1 |
| 18 | Z | 0 | 2 |
| All | All | 0 | 7 |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | 5 | 106 | LEU | CA-CB-CG | 6.62 | 130.53 | 115.30 |
| 17 | T | 559 | LEU | CA-CB-CG | 6.41 | 130.04 | 115.30 |
| 15 | R | 118 | LEU | CA-CB-CG | 6.09 | 129.32 | 115.30 |
| 4 | 3 | 77 | PRO | N-CA-CB | 5.86 | 110.33 | 103.30 |
| 6 | 5 | 106 | LEU | CB-CG-CD2 | -5.86 | 101.03 | 111.00 |
| 16 | S | 183 | ILE | CG1-CB-CG2 | -5.73 | 98.79 | 111.40 |
| 11 | A | 119 | LEU | CA-CB-CG | 5.38 | 127.68 | 115.30 |
| 17 | T | 122 | LEU | CA-CB-CG | 5.37 | 127.65 | 115.30 |
| 17 | U | 272 | LEU | CB-CG-CD2 | -5.12 | 102.30 | 111.00 |
| 18 | X | 543 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 8 | 7 | 103 | LEU | CA-CB-CG | 5.07 | 126.96 | 115.30 |
| 11 | C | 119 | LEU | CA-CB-CG | 5.06 | 126.95 | 115.30 |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | 2 | 222 | PHE | Peptide |
| 6 | 5 | 119 | LYS | Peptide |
| 18 | X | 307 | ALA | Peptide |
| 18 | X | 503 | ALA | Mainchain |
| 18 | Y | 307 | ALA | Peptide |
| 18 | Z | 307 | ALA | Peptide |
| 18 | Z | 503 | ALA | Mainchain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 0 | 607 | 0 | 584 | 3 | 0 |
| 2 | 1 | 4661 | 0 | 4695 | 46 | 0 |
| 3 | 2 | 3163 | 0 | 3262 | 35 | 0 |
| 4 | 3 | 1874 | 0 | 1826 | 16 | 0 |
| 5 | 4 | 2177 | 0 | 2169 | 28 | 0 |
| 6 | 5 | 986 | 0 | 1021 | 16 | 0 |
| 7 | 6 | 926 | 0 | 941 | 12 | 0 |
| 8 | 7 | 1347 | 0 | 1345 | 28 | 0 |
| 9 | 8 | 692 | 0 | 694 | 8 | 0 |
| 10 | 9 | 776 | 0 | 757 | 13 | 0 |
| 11 | A | 514 | 0 | 554 | 7 | 0 |
| 11 | B | 514 | 0 | 554 | 9 | 0 |
| 11 | C | 514 | 0 | 553 | 8 | 0 |
| 11 | D | 514 | 0 | 554 | 15 | 0 |
| 11 | E | 514 | 0 | 554 | 11 | 0 |
| 11 | F | 514 | 0 | 554 | 9 | 0 |
| 11 | G | 514 | 0 | 554 | 12 | 0 |
| 11 | H | 514 | 0 | 554 | 14 | 0 |
| 11 | I | 514 | 0 | 554 | 11 | 0 |
| 11 | J | 514 | 0 | 554 | 11 | 0 |
| 12 | M | 1640 | 0 | 1665 | 20 | 0 |
| 13 | P | 1532 | 0 | 1602 | 18 | 0 |
| 14 | Q | 561 | 0 | 565 | 10 | 0 |
| 15 | R | 1303 | 0 | 1266 | 11 | 0 |
| 16 | S | 2130 | 0 | 2180 | 31 | 0 |
| 17 | T | 3979 | 0 | 4119 | 42 | 0 |
| 17 | U | 3980 | 0 | 4119 | 40 | 0 |
| 17 | V | 3962 | 0 | 4105 | 63 | 0 |
| 18 | X | 4095 | 0 | 4113 | 51 | 0 |
| 18 | Y | 3957 | 0 | 3967 | 34 | 0 |
| 18 | Z | 4115 | 0 | 4138 | 57 | 0 |
| 19 | M | 1 | 0 | 0 | 0 | 0 |
| 20 | T | 31 | 0 | 12 | 1 | 0 |
| 20 | U | 31 | 0 | 12 | 0 | 0 |
| 20 | V | 31 | 0 | 12 | 0 | 0 |
| 21 | T | 1 | 0 | 0 | 0 | 0 |
| 21 | U | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 21 | V | 1 | 0 | 0 | 0 | 0 |
| 21 | X | 1 | 0 | 0 | 0 | 0 |
| 21 | Z | 1 | 0 | 0 | 0 | 0 |
| 22 | X | 27 | 0 | 12 | 0 | 0 |
| 22 | Z | 27 | 0 | 12 | 0 | 0 |
| All | All | 53756 | 0 | 54732 | 565 | 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 5.

All (565) 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) |
|---|---|---|---|
| 10:9:90:TYR:OH | 10:9:94:LYS:HE2 | 1.46 | 1.13 |
| 11:G:78:LEU:HD11 | 11:G:111:GLU:OE2 | 1.48 | 1.10 |
| 11:H:78:LEU:HD11 | 11:H:111:GLU:OE2 | 1.62 | 0.99 |
| 10:9:90:TYR:OH | 10:9:94:LYS:CE | 2.17 | 0.92 |
| 10:9:90:TYR:HH | 10:9:94:LYS:HE2 | 1.42 | 0.81 |
| 11:G:78:LEU:CD1 | 11:G:111:GLU:OE2 | 2.29 | 0.79 |
| 17:U:400:SER:HB3 | 18:X:289:ARG:HH22 | 1.49 | 0.77 |
| 15:R:129:VAL:HB | 15:R:146:VAL:HG21 | 1.68 | 0.76 |
| 11:G:111:GLU:OE2 | 11:H:113:ILE:HD11 | 1.87 | 0.74 |
| 2:1:316:ASN:HD21 | 2:1:331:ALA:H | 1.36 | 0.74 |
| 3:2:249:TYR:HH | 3:2:398:HIS:HD1 | 1.40 | 0.70 |
| 18:Z:142:SER:O | 18:Z:145:ARG:NH2 | 2.28 | 0.67 |
| 4:3:261:VAL:HG11 | 4:3:285:ALA:HB2 | 1.79 | 0.65 |
| 11:H:107:PHE:O | 11:H:111:GLU:HG2 | 1.97 | 0.65 |
| 11:C:74:VAL:HG11 | 11:C:114:ALA:HB2 | 1.79 | 0.64 |
| 17:U:471:GLN:NE2 | 17:U:475:GLU:OE2 | 2.31 | 0.64 |
| 16:S:188:GLN:HG2 | 16:S:215:LEU:HD23 | 1.80 | 0.63 |
| 11:A:110:THR:HG22 | 11:J:78:LEU:HB3 | 1.80 | 0.63 |
| 18:Z:110:LYS:HB3 | 18:Z:140:ILE:HG22 | 1.81 | 0.62 |
| 8:7:170:HIS:HD2 | 8:7:172:ALA:H | 1.46 | 0.62 |
| 17:T:151:VAL:HG11 | 17:T:301:LEU:HD21 | 1.79 | 0.62 |
| 11:H:78:LEU:CD1 | 11:H:111:GLU:OE2 | 2.43 | 0.62 |
| 17:V:254:ARG:NH1 | 18:Z:543:ASP:OD1 | 2.33 | 0.62 |
| 18:X:429:ASP:HA | 18:X:432:THR:HG22 | 1.80 | 0.62 |
| 10:9:90:TYR:CZ | 10:9:94:LYS:CE | 2.83 | 0.62 |
| 11:F:93:PRO:HB3 | 11:G:95:ILE:HD13 | 1.82 | 0.61 |
| 2:1:180:PRO:HG2 | 2:1:183:LYS:HB3 | 1.83 | 0.61 |
| 11:D:107:PHE:O | 11:D:111:GLU:HG2 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:I:72:ALA:HB2 | 11:J:70:ALA:HA | 1.84 | 0.60 |
| 2:1:295:PRO:HA | 2:1:298:GLN:HG2 | 1.83 | 0.60 |
| 15:R:107:THR:HG22 | 15:R:136:VAL:HG12 | 1.82 | 0.60 |
| 11:G:86:ILE:HG21 | 11:H:85:LEU:HA | 1.83 | 0.60 |
| 11:D:111:GLU:HB2 | 12:M:239:ARG:HH11 | 1.65 | 0.60 |
| 3:2:195:ALA:HA | 3:2:198:LYS:HE3 | 1.84 | 0.60 |
| 16:S:218:LYS:HE3 | 16:S:239:ARG:HH21 | 1.66 | 0.59 |
| 18:Z:266:LEU:HD21 | 18:Z:325:ILE:HG12 | 1.83 | 0.59 |
| 18:Z:42:GLN:HE21 | 18:Z:44:ILE:HD11 | 1.66 | 0.59 |
| 17:T:265:LYS:HE3 | 17:T:267:SER:HB2 | 1.83 | 0.59 |
| 17:T:314:ARG:NH1 | 17:T:364:ARG:O | 2.36 | 0.59 |
| 18:Z:184:GLY:O | 18:Z:366:ARG:NH2 | 2.36 | 0.59 |
| 2:1:404:LYS:NZ | 6:5:74:ASN:OD1 | 2.36 | 0.59 |
| 17:U:147:THR:HG22 | 18:X:560:VAL:HG12 | 1.85 | 0.59 |
| 17:U:189:ALA:HB3 | 18:X:252:ASN:HD22 | 1.68 | 0.59 |
| 2:1:267:ARG:NH1 | 2:1:519:GLU:OE1 | 2.35 | 0.58 |
| 15:R:49:GLU:HB2 | 16:S:206:THR:HG22 | 1.85 | 0.58 |
| 3:2:74:ASN:HD21 | 3:2:109:ALA:HA | 1.66 | 0.58 |
| 17:T:243:LYS:HG3 | 17:T:281:ALA:HA | 1.86 | 0.58 |
| 3:2:24:VAL:HG23 | 3:2:28:GLU:HB2 | 1.85 | 0.58 |
| 3:2:95:LEU:HA | 3:2:98:LEU:HD12 | 1.86 | 0.58 |
| 2:1:252:ARG:NH2 | 2:1:509:GLU:OE1 | 2.36 | 0.57 |
| 17:V:193:ILE:HG13 | 18:Z:130:ASP:HA | 1.85 | 0.57 |
| 18:Y:388:ASN:HD22 | 18:Y:391:VAL:HG23 | 1.70 | 0.57 |
| 17:U:108:LEU:HG | 17:U:151:VAL:HG22 | 1.85 | 0.57 |
| 16:S:308:ILE:HD11 | 18:Y:305:PRO:HD2 | 1.87 | 0.57 |
| 16:S:308:ILE:HD13 | 18:Y:304:ILE:HG23 | 1.87 | 0.57 |
| 18:Z:373:ILE:HG23 | 18:Z:444:SER:HB2 | 1.87 | 0.57 |
| 5:4:64:GLU:OE2 | 8:7:166:ARG:NH2 | 2.36 | 0.57 |
| 17:V:326:ASP:H | 17:V:382:VAL:HB | 1.70 | 0.57 |
| 17:V:459:PHE:HA | 17:V:463:GLY:H | 1.69 | 0.57 |
| 18:X:307:ALA:O | 18:X:309:GLY:N | 2.37 | 0.57 |
| 17:U:314:ARG:NH2 | 17:U:364:ARG:O | 2.37 | 0.57 |
| 2:1:368:ALA:O | 2:1:379:GLN:NE2 | 2.38 | 0.57 |
| 18:X:406:VAL:HG22 | 18:X:436:ALA:HB2 | 1.85 | 0.57 |
| 11:B:74:VAL:HG11 | 11:B:114:ALA:HB2 | 1.87 | 0.57 |
| 18:Z:318:LEU:HD21 | 18:Z:354:THR:HB | 1.87 | 0.56 |
| 16:S:276:ASN:ND2 | 17:V:463:GLY:O | 2.38 | 0.56 |
| 17:T:121:ASN:HB2 | 18:Y:44:ILE:HG12 | 1.87 | 0.56 |
| 11:G:111:GLU:CD | 11:H:113:ILE:HD11 | 2.24 | 0.56 |
| 16:S:154:GLU:HG2 | 16:S:157:ARG:HH11 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:I:86:ILE:HG21 | 11:J:85:LEU:HA | 1.88 | 0.56 |
| 17:U:240:ILE:HD12 | 17:U:279:THR:HG21 | 1.86 | 0.56 |
| 10:9:70:PRO:HA | 12:M:264:SER:HA | 1.88 | 0.56 |
| 16:S:97:SER:HB2 | 16:S:188:GLN:HB2 | 1.88 | 0.56 |
| 17:T:104:GLN:HB2 | 17:T:107:GLU:HB2 | 1.88 | 0.56 |
| 4:3:173:GLU:HA | 4:3:206:ASN:HD21 | 1.70 | 0.56 |
| 12:M:163:ASN:ND2 | 12:M:175:THR:OG1 | 2.38 | 0.55 |
| 14:Q:25:ASP:OD2 | 14:Q:28:ARG:NH1 | 2.39 | 0.55 |
| 17:V:210:ASP:HB2 | 17:V:497:GLN:HE22 | 1.71 | 0.55 |
| 11:I:90:ALA:O | 11:J:92:ASN:ND2 | 2.39 | 0.55 |
| 17:V:446:LEU:HD12 | 17:V:480:LEU:HD13 | 1.87 | 0.55 |
| 2:1:486:ASP:OD1 | 8:7:116:LYS:NZ | 2.39 | 0.55 |
| 18:X:373:ILE:HG23 | 18:X:444:SER:HB3 | 1.88 | 0.55 |
| 11:B:72:ALA:HB2 | 11:C:70:ALA:HA | 1.89 | 0.55 |
| 11:A:70:ALA:HA | 11:J:72:ALA:HB2 | 1.88 | 0.55 |
| 17:V:482:GLU:HA | 17:V:485:LYS:HG3 | 1.88 | 0.55 |
| 10:9:29:PHE:HB2 | 10:9:30:LEU:HD12 | 1.89 | 0.55 |
| 17:T:323:ILE:HG12 | 17:T:380:PHE:HB2 | 1.89 | 0.55 |
| 18:X:86:ARG:NH2 | 18:X:300:LEU:O | 2.40 | 0.55 |
| 2:1:156:TRP:O | 8:7:102:GLN:NE2 | 2.40 | 0.55 |
| 6:5:86:LYS:NZ | 8:7:135:ASP:OD1 | 2.38 | 0.55 |
| 2:1:186:LEU:HB3 | 2:1:440:LEU:HD22 | 1.89 | 0.55 |
| 7:6:108:LEU:HD11 | 12:M:281:LEU:HD13 | 1.88 | 0.55 |
| 18:Z:185:ALA:HB2 | 18:Z:340:TYR:HE1 | 1.71 | 0.55 |
| 11:C:80:VAL:HG12 | 11:D:80:VAL:HG11 | 1.89 | 0.55 |
| 17:T:265:LYS:NZ | 18:X:359:ASP:OD2 | 2.36 | 0.55 |
| 17:V:409:GLU:HG2 | 17:V:422:ASN:HB2 | 1.88 | 0.55 |
| 16:S:188:GLN:HB3 | 16:S:216:LEU:HD23 | 1.89 | 0.55 |
| 3:2:346:ARG:NH1 | 13:P:161:PRO:O | 2.40 | 0.54 |
| 11:H:86:ILE:HG21 | 11:I:85:LEU:HA | 1.88 | 0.54 |
| 14:Q:5:SER:OG | 14:Q:6:GLY:N | 2.41 | 0.54 |
| 4:3:190:SER:OG | 4:3:229:ASN:ND2 | 2.40 | 0.54 |
| 11:G:71:LEU:HD12 | 11:H:113:ILE:HG23 | 1.90 | 0.54 |
| 18:Y:286:ASN:H | 18:Y:338:ALA:HB3 | 1.71 | 0.54 |
| 2:1:549:ASP:HB3 | 2:1:552:LEU:HB3 | 1.89 | 0.54 |
| 7:6:104:ASN:HD22 | 12:M:255:THR:HG23 | 1.71 | 0.54 |
| 17:T:226:ASP:O | 17:T:231:LYS:NZ | 2.40 | 0.54 |
| 17:U:151:VAL:HG11 | 17:U:301:LEU:HD21 | 1.89 | 0.54 |
| 3:2:45:ARG:NH2 | 8:7:74:ILE:O | 2.37 | 0.54 |
| 5:4:17:SER:OG | 5:4:19:ASP:OD1 | 2.25 | 0.54 |
| 14:Q:15:SER:OG | 16:S:248:GLU:OE1 | 2.24 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:Z:307:ALA:O | 18:Z:309:GLY:N | 2.36 | 0.54 |
| 2:1:278:PRO:HG2 | 2:1:281:GLU:HB2 | 1.89 | 0.54 |
| 12:M:201:GLY:HA3 | 12:M:203:LYS:HE3 | 1.90 | 0.54 |
| 17:T:108:LEU:HG | 17:T:151:VAL:HG22 | 1.89 | 0.54 |
| 3:2:266:PHE:HA | 3:2:269:VAL:HG22 | 1.90 | 0.54 |
| 17:U:203:PHE:O | 17:U:242:GLN:NE2 | 2.41 | 0.54 |
| 18:X:513:ASP:OD1 | 18:X:513:ASP:N | 2.40 | 0.54 |
| 17:T:203:PHE:O | 17:T:242:GLN:NE2 | 2.40 | 0.54 |
| 4:3:318:ILE:HD11 | 12:M:321:LYS:HE2 | 1.89 | 0.54 |
| 17:T:202:LEU:HD22 | 17:T:378:THR:HG21 | 1.89 | 0.54 |
| 17:V:479:ARG:NH1 | 17:V:512:VAL:O | 2.41 | 0.54 |
| 3:2:25:SER:OG | 3:2:26:ALA:N | 2.40 | 0.53 |
| 3:2:128:VAL:HG21 | 3:2:143:VAL:HG11 | 1.90 | 0.53 |
| 17:T:122:LEU:HD23 | 18:Y:98:ARG:HG3 | 1.89 | 0.53 |
| 17:V:552:ALA:O | 17:V:556:LYS:NZ | 2.40 | 0.53 |
| 2:1:191:GLU:HA | 2:1:194:LYS:HG2 | 1.90 | 0.53 |
| 17:V:545:ALA:HA | 18:Z:524:ILE:HG22 | 1.90 | 0.53 |
| 12:M:121:ASN:O | 12:M:145:ARG:NH1 | 2.41 | 0.53 |
| 17:U:220:ARG:NH2 | 17:U:403:ASP:OD1 | 2.41 | 0.53 |
| 4:3:79:GLN:HA | 4:3:82:VAL:HG22 | 1.91 | 0.53 |
| 18:X:286:ASN:HB3 | 18:X:289:ARG:HG2 | 1.90 | 0.53 |
| 17:V:136:SER:HA | 18:Y:59:ILE:HB | 1.90 | 0.53 |
| 17:V:476:ARG:NH1 | 17:V:505:THR:O | 2.35 | 0.53 |
| 6:5:27:ASP:OD2 | 9:8:44:HIS:NE2 | 2.41 | 0.53 |
| 17:V:235:ALA:HB1 | 17:V:323:ILE:HD13 | 1.90 | 0.53 |
| 18:Y:168:ASP:HB3 | 18:Y:463:LEU:HD13 | 1.91 | 0.53 |
| 5:4:187:CYS:HB2 | 8:7:184:ASN:HD21 | 1.73 | 0.53 |
| 17:V:92:ASP:HB2 | 17:V:340:LEU:HD13 | 1.89 | 0.53 |
| 18:Y:284:VAL:HB | 18:Y:337:GLN:HG2 | 1.90 | 0.53 |
| 11:H:78:LEU:HB3 | 11:I:110:THR:HG22 | 1.90 | 0.53 |
| 17:V:532:VAL:HG23 | 17:V:546:LEU:HD11 | 1.91 | 0.53 |
| 4:3:265:LEU:HD22 | 4:3:303:VAL:HG11 | 1.91 | 0.52 |
| 8:7:40:ALA:HB3 | 8:7:47:GLU:HB2 | 1.91 | 0.52 |
| 17:T:549:HIS:NE2 | 18:Y:525:PRO:O | 2.42 | 0.52 |
| 3:2:253:LEU:HD11 | 3:2:401:ALA:HB2 | 1.91 | 0.52 |
| 17:T:266:ARG:NH1 | 18:X:148:PRO:O | 2.41 | 0.52 |
| 18:Z:72:LEU:HD11 | 18:Z:89:ALA:HB1 | 1.91 | 0.52 |
| 5:4:277:TRP:HE1 | 17:T:41:ASP:HA | 1.75 | 0.52 |
| 11:C:93:PRO:HB3 | 11:D:95:ILE:HD13 | 1.91 | 0.52 |
| 2:1:420:TYR:HB2 | 2:1:424:VAL:HG13 | 1.91 | 0.52 |
| 18:X:180:GLY:HA3 | 18:X:358:LEU:HD13 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:Y:165:LYS:NZ | 18:Y:489:VAL:O | 2.34 | 0.52 |
| 2:1:245:ALA:HB1 | 2:1:498:LEU:HD13 | 1.92 | 0.52 |
| 11:D:86:ILE:HG21 | 11:E:85:LEU:HA | 1.91 | 0.52 |
| 17:T:476:ARG:NH2 | 17:T:505:THR:O | 2.43 | 0.52 |
| 17:U:228:GLN:HE22 | 18:Z:385:ARG:HH21 | 1.58 | 0.52 |
| 9:8:26:HIS:HD2 | 9:8:28:PHE:H | 1.58 | 0.52 |
| 11:D:72:ALA:HB2 | 11:E:70:ALA:HA | 1.91 | 0.52 |
| 14:Q:22:ILE:HG12 | 14:Q:71:LYS:HG2 | 1.91 | 0.52 |
| 17:U:47:GLU:OE1 | 17:U:52:LYS:NZ | 2.40 | 0.52 |
| 18:X:202:LYS:HD3 | 18:X:232:VAL:HG22 | 1.92 | 0.52 |
| 17:U:84:LEU:HD13 | 18:X:563:GLU:HG3 | 1.91 | 0.51 |
| 18:Y:234:LYS:H | 18:Y:242:SER:HB3 | 1.75 | 0.51 |
| 16:S:140:VAL:HG22 | 16:S:160:LEU:HB3 | 1.91 | 0.51 |
| 11:F:74:VAL:HG11 | 11:F:114:ALA:HB2 | 1.93 | 0.51 |
| 17:V:125:ASP:OD1 | 17:V:125:ASP:N | 2.44 | 0.51 |
| 17:V:347:ARG:NH2 | 18:Z:348:ASP:OD2 | 2.38 | 0.51 |
| 18:X:249:GLY:HA3 | 18:X:261:VAL:HG11 | 1.92 | 0.51 |
| 18:Z:556:SER:OG | 18:Z:557:GLU:N | 2.44 | 0.51 |
| 8:7:170:HIS:CD2 | 8:7:172:ALA:H | 2.28 | 0.51 |
| 12:M:200:THR:OG1 | 12:M:201:GLY:N | 2.44 | 0.51 |
| 17:V:206:VAL:HA | 17:V:486:GLN:HE22 | 1.74 | 0.51 |
| 18:X:318:LEU:HD21 | 18:X:354:THR:HB | 1.92 | 0.51 |
| 2:1:184:LEU:HG | 2:1:488:VAL:HG21 | 1.93 | 0.51 |
| 16:S:127:LEU:HD11 | 16:S:137:VAL:HG11 | 1.93 | 0.51 |
| 17:V:201:PRO:O | 17:V:217:ARG:NH2 | 2.43 | 0.51 |
| 18:Z:286:ASN:H | 18:Z:338:ALA:HB3 | 1.75 | 0.51 |
| 18:Z:395:GLU:OE2 | 18:Z:471:GLN:NE2 | 2.44 | 0.51 |
| 18:X:65:VAL:HG22 | 18:X:102:VAL:HG22 | 1.92 | 0.51 |
| 17:V:323:ILE:HG12 | 17:V:380:PHE:HB2 | 1.92 | 0.51 |
| 18:Z:111:VAL:HG11 | 18:Z:264:THR:HG23 | 1.92 | 0.51 |
| 2:1:329:GLU:OE2 | 7:6:123:ARG:NH1 | 2.44 | 0.51 |
| 3:2:119:GLU:N | 5:4:208:GLU:OE1 | 2.44 | 0.51 |
| 17:T:235:ALA:HB1 | 17:T:323:ILE:HD13 | 1.93 | 0.51 |
| 18:Z:178:LYS:NZ | 18:Z:322:GLN:O | 2.35 | 0.51 |
| 18:Z:436:ALA:HA | 18:Z:439:ILE:HG12 | 1.93 | 0.51 |
| 3:2:140:ILE:HD12 | 3:2:164:VAL:HG11 | 1.93 | 0.51 |
| 5:4:194:ASP:O | 5:4:198:LYS:NZ | 2.35 | 0.51 |
| 16:S:210:ILE:HD11 | 16:S:254:THR:HG21 | 1.93 | 0.51 |
| 17:U:304:TYR:OH | 17:U:357:LEU:O | 2.29 | 0.51 |
| 18:Z:394:ALA:O | 18:Z:398:ASN:ND2 | 2.42 | 0.50 |
| 2:1:62:LYS:HD3 | 2:1:146:ALA:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:J:71:LEU:HA | 11:J:74:VAL:HG22 | 1.94 | 0.50 |
| 16:S:102:VAL:HG21 | 16:S:127:LEU:HD13 | 1.92 | 0.50 |
| 11:A:57:ALA:HA | 11:A:60:LYS:HG2 | 1.93 | 0.50 |
| 18:X:487:TYR:O | 18:X:498:LYS:NZ | 2.45 | 0.50 |
| 18:Z:245:THR:HG21 | 18:Z:268:VAL:HG11 | 1.92 | 0.50 |
| 17:V:236:ILE:HG21 | 17:V:272:LEU:HD11 | 1.94 | 0.50 |
| 18:Y:394:ALA:O | 18:Y:398:ASN:ND2 | 2.44 | 0.50 |
| 11:E:119:LEU:O | 11:E:123:LEU:HB2 | 2.12 | 0.50 |
| 17:U:403:ASP:O | 17:U:429:ARG:NH1 | 2.45 | 0.50 |
| 18:X:122:MET:HE3 | 18:X:126:GLY:HA2 | 1.92 | 0.50 |
| 18:Z:160:LEU:HD12 | 18:Z:175:ARG:HG3 | 1.93 | 0.50 |
| 3:2:245:VAL:HG22 | 3:2:288:LEU:HD13 | 1.93 | 0.50 |
| 4:3:277:SER:OG | 4:3:277:SER:O | 2.29 | 0.50 |
| 10:9:32:SER:OG | 10:9:33:LYS:N | 2.44 | 0.50 |
| 17:V:46:ASP:OD1 | 17:V:46:ASP:N | 2.44 | 0.50 |
| 5:4:74:LEU:HD23 | 5:4:219:VAL:HG13 | 1.94 | 0.49 |
| 5:4:119:VAL:HA | 5:4:122:VAL:HG12 | 1.94 | 0.49 |
| 13:P:112:SER:HG | 17:U:61:HIS:CD2 | 2.29 | 0.49 |
| 18:Y:445:GLN:NE2 | 18:Y:459:LYS:O | 2.43 | 0.49 |
| 17:V:108:LEU:HD21 | 17:V:116:LYS:HD2 | 1.94 | 0.49 |
| 17:V:529:ASN:HD21 | 18:Z:527:LEU:HD13 | 1.77 | 0.49 |
| 3:2:19:VAL:HG11 | 3:2:51:VAL:HG22 | 1.95 | 0.49 |
| 18:Z:503:ALA:HA | 18:Z:506:ILE:HG12 | 1.94 | 0.49 |
| 12:M:271:VAL:O | 12:M:275:PHE:HB2 | 2.12 | 0.49 |
| 17:V:428:SER:O | 17:V:432:SER:OG | 2.30 | 0.49 |
| 15:R:90:VAL:HG22 | 15:R:117:GLU:HB3 | 1.93 | 0.49 |
| 2:1:72:ASP:OD1 | 8:7:121:ARG:NH2 | 2.46 | 0.49 |
| 18:Y:170:LEU:HD22 | 18:Y:404:GLN:HG3 | 1.94 | 0.49 |
| 1:0:62:PRO:HG2 | 7:6:95:LYS:HD3 | 1.95 | 0.49 |
| 5:4:178:LEU:HD11 | 8:7:183:THR:HG21 | 1.94 | 0.49 |
| 11:C:86:ILE:HG21 | 11:D:85:LEU:HA | 1.95 | 0.49 |
| 13:P:136:GLU:O | 13:P:140:ASN:ND2 | 2.46 | 0.49 |
| 3:2:88:ALA:HB1 | 3:2:117:ASN:HD22 | 1.78 | 0.49 |
| 3:2:136:LYS:HD3 | 3:2:138:ALA:H | 1.78 | 0.49 |
| 16:S:197:PHE:N | 16:S:261:GLU:OE1 | 2.40 | 0.48 |
| 17:T:220:ARG:NH2 | 17:T:403:ASP:OD1 | 2.37 | 0.48 |
| 17:V:220:ARG:HH12 | 18:Z:216:ARG:HD3 | 1.78 | 0.48 |
| 18:Y:245:THR:HG21 | 18:Y:268:VAL:HG11 | 1.95 | 0.48 |
| 18:Z:216:ARG:O | 18:Z:250:GLN:NE2 | 2.46 | 0.48 |
| 18:Z:284:VAL:HG11 | 18:Z:287:ILE:HD13 | 1.94 | 0.48 |
| 2:1:84:PRO:HG2 | 6:5:71:VAL:HG11 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:4:284:GLU:OE1 | 5:4:291:LYS:NZ | 2.40 | 0.48 |
| 11:C:72:ALA:HB2 | 11:D:70:ALA:HA | 1.95 | 0.48 |
| 11:H:72:ALA:HB2 | 11:I:70:ALA:HA | 1.95 | 0.48 |
| 18:Y:57:PRO:O | 18:Y:79:HIS:NE2 | 2.42 | 0.48 |
| 18:Y:145:ARG:HH12 | 18:Y:267:THR:HG23 | 1.78 | 0.48 |
| 18:Z:520:GLU:HA | 18:Z:524:ILE:HD11 | 1.94 | 0.48 |
| 3:2:11:ILE:HD13 | 8:7:50:VAL:HG13 | 1.95 | 0.48 |
| 3:2:116:LYS:NZ | 3:2:118:TYR:OH | 2.44 | 0.48 |
| 17:U:513:ARG:NH1 | 17:U:516:ASP:OD1 | 2.47 | 0.48 |
| 14:Q:32:LYS:NZ | 15:R:153:ASP:O | 2.42 | 0.48 |
| 17:T:155:ILE:HD12 | 17:T:312:TYR:HB2 | 1.95 | 0.48 |
| 17:U:217:ARG:O | 17:U:376:SER:OG | 2.31 | 0.48 |
| 17:U:243:LYS:HG3 | 17:U:281:ALA:HA | 1.96 | 0.48 |
| 17:V:226:ASP:O | 17:V:231:LYS:NZ | 2.46 | 0.48 |
| 16:S:216:LEU:HD12 | 16:S:220:LEU:HD23 | 1.96 | 0.48 |
| 17:T:219:GLN:NE2 | 17:T:221:GLU:OE1 | 2.46 | 0.48 |
| 2:1:520:LEU:HD12 | 7:6:32:VAL:HG12 | 1.96 | 0.48 |
| 11:A:78:LEU:HB3 | 11:B:110:THR:HG22 | 1.96 | 0.48 |
| 11:B:123:LEU:HA | 11:B:127:ALA:HB3 | 1.96 | 0.48 |
| 11:H:118:LEU:HA | 11:H:121:VAL:HG12 | 1.96 | 0.48 |
| 6:5:62:TYR:OH | 7:6:146:PHE:O | 2.24 | 0.48 |
| 11:A:86:ILE:HG21 | 11:B:85:LEU:HA | 1.95 | 0.48 |
| 17:V:311:GLU:OE2 | 17:V:314:ARG:NH1 | 2.47 | 0.48 |
| 6:5:5:PRO:O | 9:8:65:ARG:NH1 | 2.45 | 0.48 |
| 11:F:59:SER:HA | 11:F:62:VAL:HG12 | 1.95 | 0.48 |
| 17:V:514:VAL:HA | 17:V:517:ILE:HD11 | 1.96 | 0.47 |
| 18:X:36:ASP:N | 18:X:36:ASP:OD2 | 2.45 | 0.47 |
| 18:X:57:PRO:HD2 | 18:X:85:VAL:HG11 | 1.96 | 0.47 |
| 17:U:339:LEU:HD21 | 17:U:345:PRO:HB3 | 1.96 | 0.47 |
| 18:X:273:ARG:HD3 | 18:X:333:ILE:HG13 | 1.96 | 0.47 |
| 3:2:420:GLU:OE2 | 3:2:433:TYR:OH | 2.30 | 0.47 |
| 11:J:59:SER:HA | 11:J:62:VAL:HG12 | 1.96 | 0.47 |
| 18:Y:272:PHE:HD1 | 18:Y:276:GLU:HG3 | 1.78 | 0.47 |
| 4:3:304:LYS:NZ | 4:3:308:GLU:OE2 | 2.39 | 0.47 |
| 5:4:141:VAL:HG13 | 5:4:168:LYS:HE2 | 1.95 | 0.47 |
| 17:U:100:LEU:O | 18:X:98:ARG:NH2 | 2.47 | 0.47 |
| 18:Z:399:VAL:HG11 | 18:Z:467:ILE:HG23 | 1.95 | 0.47 |
| 10:9:80:GLN:HB3 | 10:9:86:ALA:HB2 | 1.96 | 0.47 |
| 11:A:72:ALA:HB2 | 11:B:70:ALA:HA | 1.95 | 0.47 |
| 11:G:111:GLU:OE1 | 11:H:113:ILE:HD11 | 2.14 | 0.47 |
| 13:P:209:MET:HG2 | 17:T:79:PRO:HG2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:X:410:TYR:OH | 18:X:437:ARG:NH2 | 2.48 | 0.47 |
| 18:Z:42:GLN:HG2 | 18:Z:49:ASP:HB2 | 1.96 | 0.47 |
| 13:P:114:ALA:HB2 | 17:U:58:LEU:HD21 | 1.97 | 0.47 |
| 17:T:240:ILE:HG12 | 17:T:279:THR:HG21 | 1.96 | 0.47 |
| 18:X:284:VAL:HG11 | 18:X:287:ILE:HD13 | 1.96 | 0.47 |
| 2:1:28:ARG:NH2 | 8:7:160:ASN:OD1 | 2.43 | 0.47 |
| 3:2:330:VAL:HG12 | 3:2:381:ALA:HB3 | 1.96 | 0.47 |
| 5:4:9:LYS:NZ | 5:4:54:GLU:OE1 | 2.37 | 0.47 |
| 11:B:86:ILE:HG21 | 11:C:85:LEU:HA | 1.96 | 0.47 |
| 18:X:394:ALA:O | 18:X:398:ASN:ND2 | 2.47 | 0.47 |
| 11:I:83:GLY:O | 11:J:84:SER:OG | 2.33 | 0.47 |
| 2:1:355:GLU:HG3 | 7:6:48:LEU:HD23 | 1.95 | 0.47 |
| 6:5:83:THR:O | 8:7:119:TYR:OH | 2.32 | 0.47 |
| 11:E:90:ALA:HA | 11:F:95:ILE:HD11 | 1.96 | 0.47 |
| 17:T:250:PRO:HD2 | 17:T:253:GLN:HE21 | 1.80 | 0.47 |
| 17:V:122:LEU:HD23 | 18:Z:98:ARG:HG3 | 1.95 | 0.47 |
| 11:I:118:LEU:HA | 11:I:121:VAL:HG12 | 1.97 | 0.46 |
| 14:Q:32:LYS:O | 14:Q:36:LYS:N | 2.42 | 0.46 |
| 16:S:150:LEU:HA | 16:S:153:ILE:HG22 | 1.96 | 0.46 |
| 17:T:102:SER:O | 17:T:102:SER:OG | 2.30 | 0.46 |
| 14:Q:54:ASP:OD2 | 14:Q:54:ASP:N | 2.48 | 0.46 |
| 3:2:249:TYR:OH | 3:2:398:HIS:ND1 | 2.37 | 0.46 |
| 13:P:195:LEU:O | 13:P:211:THR:OG1 | 2.31 | 0.46 |
| 16:S:83:ASP:HA | 16:S:86:VAL:HG12 | 1.96 | 0.46 |
| 18:Y:491:ASP:OD1 | 18:Y:491:ASP:N | 2.49 | 0.46 |
| 18:Z:145:ARG:NH1 | 18:Z:270:GLU:OE1 | 2.48 | 0.46 |
| 18:X:438:LYS:NZ | 18:X:481:LEU:O | 2.49 | 0.46 |
| 11:D:111:GLU:CB | 12:M:239:ARG:HH11 | 2.27 | 0.46 |
| 12:M:120:GLN:HB3 | 12:M:304:THR:HG21 | 1.97 | 0.46 |
| 13:P:179:ASP:OD2 | 13:P:179:ASP:N | 2.42 | 0.46 |
| 5:4:64:GLU:HG2 | 17:T:55:SER:HB2 | 1.98 | 0.46 |
| 5:4:159:THR:HG22 | 5:4:161:GLY:H | 1.81 | 0.46 |
| 16:S:170:VAL:HG12 | 16:S:174:GLN:HE22 | 1.80 | 0.46 |
| 2:1:98:ARG:HH21 | 6:5:62:TYR:HD2 | 1.64 | 0.46 |
| 11:D:74:VAL:HG21 | 11:D:114:ALA:HB2 | 1.96 | 0.46 |
| 17:T:232:THR:OG1 | 20:T:1001:ATP:O2B | 2.33 | 0.46 |
| 17:V:446:LEU:HD22 | 17:V:501:VAL:HG21 | 1.98 | 0.46 |
| 18:X:132:GLN:HE22 | 18:X:235:LEU:HD22 | 1.80 | 0.46 |
| 11:F:115:LEU:HD13 | 12:M:280:LEU:HD22 | 1.98 | 0.46 |
| 18:X:145:ARG:HH12 | 18:X:267:THR:HG23 | 1.80 | 0.46 |
| 18:Z:196:LEU:O | 18:Z:200:VAL:HB | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:I:71:LEU:HA | 11:I:74:VAL:HG12 | 1.98 | 0.45 |
| 13:P:161:PRO:HD3 | 13:P:190:ILE:HD12 | 1.97 | 0.45 |
| 3:2:377:VAL:HG21 | 3:2:438:ILE:HG23 | 1.97 | 0.45 |
| 5:4:118:THR:HG22 | 5:4:120:LYS:H | 1.81 | 0.45 |
| 11:G:74:VAL:HG11 | 11:G:114:ALA:HB2 | 1.99 | 0.45 |
| 16:S:83:ASP:O | 16:S:87:ARG:HB3 | 2.17 | 0.45 |
| 18:Z:165:LYS:HG2 | 18:Z:466:THR:HG22 | 1.98 | 0.45 |
| 5:4:101:PRO:HG3 | 8:7:170:HIS:CD2 | 2.51 | 0.45 |
| 16:S:101:VAL:HG22 | 16:S:138:VAL:HB | 1.99 | 0.45 |
| 17:V:324:TYR:HB3 | 17:V:327:LEU:HD13 | 1.97 | 0.45 |
| 2:1:252:ARG:HG3 | 2:1:505:ILE:HG21 | 1.98 | 0.45 |
| 4:3:246:GLU:OE2 | 12:M:133:ARG:NH2 | 2.34 | 0.45 |
| 11:A:85:LEU:HA | 11:J:86:ILE:HG21 | 1.99 | 0.45 |
| 12:M:250:LEU:HG | 12:M:254:LEU:HD13 | 1.98 | 0.45 |
| 13:P:73:GLU:OE1 | 13:P:118:THR:OG1 | 2.30 | 0.45 |
| 17:T:231:LYS:HG2 | 17:T:408:LEU:HD12 | 1.98 | 0.45 |
| 18:X:401:ARG:NH1 | 18:X:404:GLN:OE1 | 2.48 | 0.45 |
| 2:1:556:ILE:HG21 | 6:5:36:ARG:HA | 1.99 | 0.45 |
| 5:4:85:TYR:HH | 8:7:161:TYR:HH | 1.64 | 0.45 |
| 11:F:86:ILE:HG21 | 11:G:85:LEU:HA | 1.99 | 0.45 |
| 18:X:234:LYS:HD2 | 18:X:241:ASN:HB2 | 1.98 | 0.45 |
| 11:E:72:ALA:HB2 | 11:F:70:ALA:HA | 1.99 | 0.45 |
| 11:E:74:VAL:HG11 | 11:E:114:ALA:HB2 | 1.97 | 0.45 |
| 17:U:246:ASN:O | 17:U:254:ARG:NE | 2.41 | 0.45 |
| 2:1:180:PRO:HB2 | 2:1:489:LEU:HD21 | 1.99 | 0.45 |
| 5:4:238:VAL:HG21 | 8:7:142:GLU:HB3 | 1.99 | 0.45 |
| 6:5:118:VAL:HG21 | 8:7:94:LEU:HD22 | 1.99 | 0.45 |
| 14:Q:10:ARG:NH2 | 16:S:245:ASP:OD1 | 2.46 | 0.45 |
| 2:1:260:LEU:HA | 2:1:512:LEU:HD11 | 1.99 | 0.45 |
| 11:G:85:LEU:HD21 | 11:G:100:VAL:HG12 | 1.99 | 0.45 |
| 17:V:283:ARG:NH1 | 17:V:284:TYR:OH | 2.50 | 0.45 |
| 10:9:90:TYR:OH | 10:9:94:LYS:CD | 2.65 | 0.44 |
| 15:R:89:VAL:HG12 | 15:R:118:LEU:HA | 1.98 | 0.44 |
| 16:S:213:PRO:HG3 | 16:S:244:ARG:HA | 1.98 | 0.44 |
| 17:V:344:PRO:HB3 | 18:Z:305:PRO:HG3 | 1.99 | 0.44 |
| 18:Y:233:ILE:HD11 | 18:Y:246:LEU:HD13 | 1.99 | 0.44 |
| 18:Z:445:GLN:NE2 | 18:Z:459:LYS:O | 2.45 | 0.44 |
| 18:Z:480:ASP:OD1 | 18:Z:480:ASP:N | 2.44 | 0.44 |
| 16:S:105:VAL:HG22 | 16:S:142:ILE:HD12 | 1.99 | 0.44 |
| 16:S:124:ARG:HA | 16:S:127:LEU:HB3 | 1.99 | 0.44 |
| 17:U:367:LYS:NZ | 17:U:374:GLY:O | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:Y:231:GLY:O | 18:Y:234:LYS:NZ | 2.50 | 0.44 |
| 18:Z:170:LEU:HD22 | 18:Z:404:GLN:HG3 | 2.00 | 0.44 |
| 3:2:70:LEU:HD12 | 3:2:106:VAL:HG22 | 1.99 | 0.44 |
| 17:V:135:ASP:OD1 | 17:V:135:ASP:N | 2.49 | 0.44 |
| 18:Y:124:VAL:HG13 | 18:Y:125:ILE:HG23 | 1.99 | 0.44 |
| 11:E:68:THR:HB | 11:E:121:VAL:HG21 | 1.99 | 0.44 |
| 17:T:222:LEU:HG | 17:T:224:ILE:HB | 1.98 | 0.44 |
| 18:X:42:GLN:HB3 | 18:X:49:ASP:HB2 | 1.98 | 0.44 |
| 2:1:540:LEU:HD12 | 2:1:541:PRO:HD2 | 2.00 | 0.44 |
| 17:T:55:SER:O | 17:T:57:TYR:N | 2.50 | 0.44 |
| 17:V:412:LEU:HB2 | 17:V:420:ALA:HB1 | 2.00 | 0.44 |
| 12:M:239:ARG:O | 12:M:243:ASN:ND2 | 2.43 | 0.44 |
| 15:R:50:PHE:H | 15:R:53:ASN:HD22 | 1.65 | 0.44 |
| 17:V:270:ALA:HB1 | 18:Y:155:THR:HG22 | 1.99 | 0.44 |
| 18:Z:526:SER:OG | 18:Z:527:LEU:N | 2.51 | 0.44 |
| 3:2:330:VAL:HA | 3:2:333:VAL:HG22 | 2.00 | 0.44 |
| 4:3:116:THR:OG1 | 4:3:117:SER:N | 2.50 | 0.44 |
| 5:4:183:ILE:HG22 | 8:7:184:ASN:HD22 | 1.83 | 0.44 |
| 11:E:86:ILE:HG21 | 11:F:85:LEU:HA | 2.00 | 0.44 |
| 17:U:220:ARG:HG2 | 17:U:365:ALA:HB3 | 2.00 | 0.44 |
| 18:X:124:VAL:HG21 | 18:X:257:ALA:HB1 | 2.00 | 0.44 |
| 18:Y:365:SER:HB2 | 18:Y:368:ILE:HG12 | 2.00 | 0.44 |
| 17:U:132:PHE:CE1 | 17:U:297:PRO:HB2 | 2.53 | 0.44 |
| 18:X:273:ARG:NH1 | 18:X:326:THR:O | 2.51 | 0.44 |
| 2:1:587:ASN:HD21 | 4:3:207:HIS:CD2 | 2.36 | 0.43 |
| 3:2:271:PRO:O | 3:2:275:LYS:CB | 2.66 | 0.43 |
| 5:4:192:ASN:OD1 | 5:4:192:ASN:N | 2.51 | 0.43 |
| 10:9:90:TYR:CE1 | 10:9:94:LYS:HD3 | 2.53 | 0.43 |
| 13:P:163:ASP:H | 13:P:166:GLU:HB3 | 1.83 | 0.43 |
| 17:T:482:GLU:HA | 17:T:485:LYS:HZ3 | 1.82 | 0.43 |
| 17:U:160:LEU:HD12 | 17:U:160:LEU:HA | 1.85 | 0.43 |
| 17:U:323:ILE:HG13 | 17:U:380:PHE:HB2 | 1.99 | 0.43 |
| 18:X:130:ASP:OD1 | 18:X:130:ASP:N | 2.52 | 0.43 |
| 18:X:435:ARG:NH1 | 18:X:474:LEU:O | 2.51 | 0.43 |
| 5:4:89:LEU:HB3 | 8:7:172:ALA:HB2 | 2.01 | 0.43 |
| 9:8:36:ALA:HA | 9:8:40:LEU:HB3 | 1.99 | 0.43 |
| 11:F:92:ASN:N | 11:F:92:ASN:OD1 | 2.50 | 0.43 |
| 17:V:196:GLN:HE22 | 17:V:370:LYS:HE2 | 1.83 | 0.43 |
| 18:X:503:ALA:HA | 18:X:506:ILE:HG22 | 2.00 | 0.43 |
| 18:Z:281:LEU:HD23 | 18:Z:334:THR:HB | 2.01 | 0.43 |
| 6:5:91:HIS:CG | 8:7:111:THR:HG21 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:8:26:HIS:CD2 | 9:8:28:PHE:H | 2.36 | 0.43 |
| 10:9:90:TYR:CZ | 10:9:94:LYS:HE3 | 2.53 | 0.43 |
| 17:U:120:LEU:HA | 17:U:120:LEU:HD23 | 1.75 | 0.43 |
| 17:V:516:ASP:OD2 | 17:V:516:ASP:N | 2.50 | 0.43 |
| 3:2:273:ILE:HG21 | 3:2:303:VAL:HG13 | 2.00 | 0.43 |
| 18:X:124:VAL:HG22 | 18:X:261:VAL:HB | 2.00 | 0.43 |
| 18:Z:225:ARG:HA | 18:Z:225:ARG:HD3 | 1.84 | 0.43 |
| 2:1:85:ARG:HD3 | 6:5:71:VAL:HB | 2.01 | 0.43 |
| 2:1:241:SER:OG | 2:1:242:LYS:N | 2.51 | 0.43 |
| 2:1:316:ASN:ND2 | 2:1:331:ALA:H | 2.10 | 0.43 |
| 17:V:334:TYR:OH | 17:V:353:ASP:OD2 | 2.27 | 0.43 |
| 2:1:23:TYR:O | 8:7:155:SER:OG | 2.29 | 0.43 |
| 2:1:304:VAL:HG13 | 2:1:348:ALA:HB2 | 1.99 | 0.43 |
| 2:1:595:LEU:HD23 | 6:5:58:LEU:HD13 | 2.00 | 0.43 |
| 11:D:119:LEU:HD11 | 12:M:234:VAL:HG11 | 2.01 | 0.43 |
| 14:Q:17:LEU:HD23 | 14:Q:17:LEU:HA | 1.87 | 0.43 |
| 15:R:118:LEU:HB2 | 15:R:125:GLU:HG2 | 1.99 | 0.43 |
| 18:X:166:VAL:HG23 | 18:X:443:LEU:HD22 | 2.01 | 0.43 |
| 2:1:89:ASP:OD1 | 2:1:89:ASP:N | 2.52 | 0.43 |
| 3:2:78:VAL:HG22 | 8:7:74:ILE:HG13 | 1.99 | 0.43 |
| 11:I:81:MET:HE1 | 11:I:107:PHE:HB2 | 1.99 | 0.43 |
| 17:T:90:VAL:HG21 | 17:T:138:ILE:HB | 2.01 | 0.43 |
| 17:U:152:ASN:N | 17:U:152:ASN:OD1 | 2.52 | 0.43 |
| 5:4:71:ALA:HB2 | 8:7:84:VAL:HG12 | 2.00 | 0.43 |
| 5:4:82:VAL:HG11 | 5:4:216:ALA:HB2 | 2.00 | 0.43 |
| 17:V:207:LYS:H | 17:V:486:GLN:NE2 | 2.17 | 0.43 |
| 11:G:81:MET:O | 11:G:84:SER:OG | 2.32 | 0.43 |
| 13:P:49:THR:H | 13:P:52:GLN:HG2 | 1.84 | 0.43 |
| 15:R:50:PHE:HD1 | 15:R:53:ASN:HD21 | 1.67 | 0.43 |
| 18:Y:435:ARG:HH11 | 18:Y:476:GLY:HA3 | 1.84 | 0.43 |
| 3:2:289:HIS:HB2 | 3:2:307:VAL:HB | 2.01 | 0.42 |
| 16:S:79:ARG:NH2 | 16:S:197:PHE:O | 2.47 | 0.42 |
| 18:X:420:LEU:HD23 | 18:X:420:LEU:HA | 1.84 | 0.42 |
| 2:1:362:LEU:HD23 | 2:1:362:LEU:HA | 1.87 | 0.42 |
| 2:1:367:GLU:HG3 | 2:1:372:SER:HB2 | 2.01 | 0.42 |
| 13:P:149:LYS:O | 13:P:149:LYS:HG2 | 2.19 | 0.42 |
| 7:6:72:SER:OG | 7:6:73:THR:N | 2.52 | 0.42 |
| 11:B:78:LEU:HD23 | 11:B:78:LEU:HA | 1.87 | 0.42 |
| 11:D:87:ASN:OD1 | 11:E:87:ASN:ND2 | 2.52 | 0.42 |
| 11:H:92:ASN:N | 11:H:92:ASN:OD1 | 2.51 | 0.42 |
| 13:P:209:MET:HA | 17:T:79:PRO:HG2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:S:184:LYS:HA | 16:S:184:LYS:HD3 | 1.82 | 0.42 |
| 18:X:446:PRO:HB2 | 18:X:458:GLY:HA2 | 2.01 | 0.42 |
| 18:Y:426:SER:HB3 | 18:Y:429:ASP:HB2 | 2.01 | 0.42 |
| 18:Z:504:LYS:O | 18:Z:508:SER:N | 2.52 | 0.42 |
| 18:Z:526:SER:HB3 | 18:Z:529:LYS:HG2 | 2.01 | 0.42 |
| 3:2:368:ILE:HG22 | 3:2:370:ILE:HD11 | 2.02 | 0.42 |
| 7:6:28:GLU:OE2 | 9:8:18:GLY:N | 2.44 | 0.42 |
| 7:6:144:LYS:HD3 | 7:6:144:LYS:HA | 1.90 | 0.42 |
| 10:9:26:LEU:HA | 10:9:29:PHE:HD2 | 1.84 | 0.42 |
| 11:E:54:SER:O | 11:E:54:SER:OG | 2.34 | 0.42 |
| 17:V:251:LYS:HB2 | 18:Z:540:GLU:HG3 | 2.01 | 0.42 |
| 5:4:138:LEU:HD23 | 5:4:138:LEU:HA | 1.91 | 0.42 |
| 11:D:75:GLY:HA3 | 11:E:74:VAL:HG22 | 2.01 | 0.42 |
| 18:Z:180:GLY:HA3 | 18:Z:358:LEU:HD13 | 2.02 | 0.42 |
| 6:5:44:TRP:CE3 | 7:6:142:GLY:HA3 | 2.54 | 0.42 |
| 17:T:123:GLN:O | 18:Y:98:ARG:NH2 | 2.45 | 0.42 |
| 17:V:59:ILE:HA | 17:V:62:VAL:HG22 | 2.01 | 0.42 |
| 17:V:172:ASP:N | 17:V:172:ASP:OD1 | 2.50 | 0.42 |
| 17:V:207:LYS:H | 17:V:486:GLN:HE22 | 1.66 | 0.42 |
| 18:Y:349:PRO:O | 18:Y:353:THR:OG1 | 2.34 | 0.42 |
| 5:4:172:VAL:HA | 5:4:175:SER:HB3 | 2.02 | 0.42 |
| 5:4:245:GLN:HE22 | 8:7:149:SER:HB2 | 1.85 | 0.42 |
| 8:7:123:HIS:HD2 | 8:7:125:GLU:H | 1.68 | 0.42 |
| 11:D:54:SER:O | 11:D:54:SER:OG | 2.32 | 0.42 |
| 11:J:85:LEU:HD13 | 11:J:103:ALA:HB2 | 2.01 | 0.42 |
| 13:P:79:GLU:OE2 | 13:P:83:GLN:NE2 | 2.52 | 0.42 |
| 17:U:332:VAL:HG13 | 17:U:335:ARG:HH21 | 1.85 | 0.42 |
| 17:U:500:ALA:HB2 | 17:U:525:ILE:HD11 | 2.00 | 0.42 |
| 18:X:72:LEU:HD11 | 18:X:89:ALA:HB1 | 2.02 | 0.42 |
| 18:X:266:LEU:HD21 | 18:X:324:ARG:HB2 | 2.02 | 0.42 |
| 18:Y:406:VAL:HG11 | 18:Y:439:ILE:HD12 | 2.02 | 0.42 |
| 18:Z:223:LEU:HA | 18:Z:226:GLU:HG2 | 2.00 | 0.42 |
| 11:D:68:THR:HB | 11:D:121:VAL:HG21 | 2.02 | 0.42 |
| 13:P:189:LYS:HE3 | 13:P:189:LYS:HB2 | 1.91 | 0.42 |
| 17:T:466:LEU:HB3 | 17:T:467:ASP:H | 1.60 | 0.42 |
| 18:Z:65:VAL:HG22 | 18:Z:102:VAL:HG22 | 2.02 | 0.42 |
| 2:1:454:ALA:HB2 | 2:1:474:GLN:HG3 | 2.02 | 0.42 |
| 17:V:513:ARG:HH11 | 17:V:515:GLN:HE22 | 1.67 | 0.42 |
| 2:1:365:GLN:HE21 | 2:1:386:HIS:HD2 | 1.66 | 0.42 |
| 7:6:98:GLU:HB3 | 7:6:101:VAL:HG22 | 2.01 | 0.42 |
| 17:T:442:VAL:HG12 | 17:T:501:VAL:HG12 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:U:235:ALA:HB1 | 17:U:323:ILE:HG12 | 2.01 | 0.42 |
| 18:Y:472:GLY:HA3 | 18:Y:478:TYR:HE2 | 1.85 | 0.42 |
| 1:0:59:ASP:OD1 | 1:0:59:ASP:N | 2.49 | 0.41 |
| 4:3:159:THR:HA | 4:3:162:GLU:HG2 | 2.02 | 0.41 |
| 16:S:123:THR:O | 16:S:127:LEU:HB2 | 2.20 | 0.41 |
| 16:S:213:PRO:HA | 16:S:217:GLU:HB3 | 2.01 | 0.41 |
| 17:U:453:TYR:HB2 | 17:U:477:GLY:HA3 | 2.02 | 0.41 |
| 17:V:222:LEU:O | 17:V:406:ILE:N | 2.52 | 0.41 |
| 3:2:280:LEU:HD23 | 3:2:284:SER:HB3 | 2.02 | 0.41 |
| 8:7:23:LEU:HA | 8:7:23:LEU:HD23 | 1.76 | 0.41 |
| 17:U:359:SER:HB2 | 18:X:251:MET:HB3 | 2.02 | 0.41 |
| 17:V:90:VAL:HG21 | 17:V:138:ILE:HB | 2.02 | 0.41 |
| 17:V:104:GLN:HB3 | 18:Z:95:GLY:HA2 | 2.02 | 0.41 |
| 18:X:82:ASP:OD2 | 18:X:82:ASP:N | 2.52 | 0.41 |
| 18:X:445:GLN:NE2 | 18:X:459:LYS:O | 2.47 | 0.41 |
| 10:9:71:ALA:HB3 | 10:9:73:TRP:CD1 | 2.55 | 0.41 |
| 15:R:71:PRO:HG2 | 15:R:141:VAL:HG23 | 2.02 | 0.41 |
| 18:Y:111:VAL:HG11 | 18:Y:264:THR:HG23 | 2.01 | 0.41 |
| 18:Z:249:GLY:HA3 | 18:Z:261:VAL:HG11 | 2.02 | 0.41 |
| 18:Z:286:ASN:HB3 | 18:Z:289:ARG:HG2 | 2.01 | 0.41 |
| 5:4:179:PRO:HD2 | 5:4:206:TRP:CD1 | 2.56 | 0.41 |
| 17:U:514:VAL:HA | 17:U:517:ILE:HD11 | 2.02 | 0.41 |
| 17:V:345:PRO:HB2 | 17:V:349:ALA:HA | 2.03 | 0.41 |
| 3:2:356:TYR:HB3 | 3:2:368:ILE:HA | 2.00 | 0.41 |
| 6:5:91:HIS:ND1 | 8:7:138:TYR:OH | 2.32 | 0.41 |
| 11:C:113:ILE:HA | 11:C:116:PHE:HB2 | 2.03 | 0.41 |
| 12:M:163:ASN:HB3 | 12:M:292:ALA:HB1 | 2.01 | 0.41 |
| 17:T:241:HIS:HE1 | 17:T:493:PRO:HA | 1.86 | 0.41 |
| 18:X:573:LYS:HA | 18:X:573:LYS:HD3 | 1.81 | 0.41 |
| 18:Z:424:GLU:H | 18:Z:424:GLU:HG3 | 1.77 | 0.41 |
| 9:8:26:HIS:HB3 | 9:8:29:GLN:HG3 | 2.03 | 0.41 |
| 18:X:39:TYR:HB2 | 18:X:99:GLY:HA2 | 2.02 | 0.41 |
| 2:1:46:LEU:HD22 | 5:4:231:ASP:HA | 2.02 | 0.41 |
| 3:2:251:LEU:HD23 | 3:2:251:LEU:HA | 1.92 | 0.41 |
| 13:P:195:LEU:H | 13:P:212:ALA:HB2 | 1.85 | 0.41 |
| 17:T:265:LYS:HB3 | 17:T:268:THR:HG22 | 2.02 | 0.41 |
| 17:U:446:LEU:HD22 | 17:U:501:VAL:HG21 | 2.02 | 0.41 |
| 17:V:443:ALA:HA | 17:V:446:LEU:HB3 | 2.03 | 0.41 |
| 17:V:513:ARG:HH11 | 17:V:515:GLN:NE2 | 2.19 | 0.41 |
| 18:Z:348:ASP:HB3 | 18:Z:351:PRO:HD2 | 2.03 | 0.41 |
| 2:1:275:ALA:HA | 2:1:361:LEU:HD13 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:T:415:LYS:HE3 | 17:T:415:LYS:HB2 | 1.92 | 0.41 |
| 17:U:84:LEU:HD23 | 17:U:143:LEU:HD22 | 2.02 | 0.41 |
| 17:U:100:LEU:HD13 | 17:U:103:VAL:HG11 | 2.03 | 0.41 |
| 17:V:90:VAL:HG13 | 18:Y:59:ILE:HD11 | 2.02 | 0.41 |
| 17:V:304:TYR:OH | 17:V:357:LEU:O | 2.34 | 0.41 |
| 2:1:78:LEU:N | 2:1:496:GLU:OE2 | 2.54 | 0.41 |
| 3:2:100:PRO:HG3 | 3:2:134:GLU:HG3 | 2.02 | 0.41 |
| 4:3:162:GLU:HB3 | 4:3:184:PHE:HE1 | 1.86 | 0.41 |
| 4:3:235:ASP:N | 4:3:235:ASP:OD1 | 2.54 | 0.41 |
| 11:I:59:SER:HA | 11:I:62:VAL:HG12 | 2.02 | 0.41 |
| 12:M:229:TYR:O | 12:M:232:ARG:HG2 | 2.21 | 0.41 |
| 12:M:288:GLU:HA | 12:M:291:VAL:HG12 | 2.02 | 0.41 |
| 13:P:199:VAL:HG22 | 13:P:208:ASP:HA | 2.03 | 0.41 |
| 15:R:136:VAL:HA | 15:R:142:THR:HA | 2.03 | 0.41 |
| 17:V:107:GLU:HA | 17:V:150:ILE:HA | 2.03 | 0.41 |
| 17:V:143:LEU:HD23 | 17:V:143:LEU:HA | 1.93 | 0.41 |
| 17:V:231:LYS:HG2 | 17:V:408:LEU:HD12 | 2.03 | 0.41 |
| 18:Z:406:VAL:HG12 | 18:Z:436:ALA:HB2 | 2.03 | 0.41 |
| 4:3:121:PHE:HA | 4:3:124:PHE:HB2 | 2.02 | 0.41 |
| 9:8:47:LEU:HD23 | 9:8:47:LEU:HA | 1.89 | 0.41 |
| 13:P:157:ILE:HG23 | 13:P:199:VAL:HB | 2.03 | 0.41 |
| 18:X:225:ARG:HD3 | 18:X:225:ARG:HA | 1.73 | 0.41 |
| 4:3:245:SER:OG | 4:3:246:GLU:N | 2.54 | 0.40 |
| 11:H:95:ILE:HG22 | 11:H:98:GLN:HB3 | 2.02 | 0.40 |
| 17:T:243:LYS:HE3 | 17:T:243:LYS:HB3 | 1.95 | 0.40 |
| 17:U:226:ASP:O | 17:U:231:LYS:NZ | 2.54 | 0.40 |
| 17:V:66:LEU:HD23 | 17:V:66:LEU:HA | 1.90 | 0.40 |
| 1:0:40:LYS:HE2 | 1:0:40:LYS:HB3 | 1.90 | 0.40 |
| 2:1:500:LEU:HD23 | 2:1:500:LEU:HA | 1.96 | 0.40 |
| 11:J:74:VAL:HG21 | 11:J:114:ALA:HB2 | 2.03 | 0.40 |
| 14:Q:28:ARG:HD3 | 14:Q:39:ALA:HB1 | 2.03 | 0.40 |
| 17:T:300:PHE:HA | 17:T:330:GLN:HG2 | 2.03 | 0.40 |
| 2:1:289:LYS:HA | 2:1:289:LYS:HD3 | 1.91 | 0.40 |
| 6:5:122:LEU:HA | 6:5:122:LEU:HD23 | 1.82 | 0.40 |
| 16:S:246:LEU:HD23 | 16:S:246:LEU:HA | 1.87 | 0.40 |
| 17:T:356:TYR:O | 17:T:360:ARG:HB2 | 2.21 | 0.40 |
| 17:V:147:THR:HG22 | 18:Z:560:VAL:HG12 | 2.02 | 0.40 |
| 18:X:96:LEU:HD23 | 18:X:96:LEU:HA | 1.94 | 0.40 |
| 18:Z:57:PRO:HD2 | 18:Z:85:VAL:HG11 | 2.03 | 0.40 |
| 3:2:290:VAL:HG22 | 3:2:405:VAL:HG21 | 2.04 | 0.40 |
| 11:B:54:SER:O | 11:B:54:SER:OG | 2.33 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:S:195:ASN:HD22 | 16:S:262:ASN:ND2 | 2.20 | 0.40 |
| 17:V:498:THR:HA | 17:V:501:VAL:HG12 | 2.04 | 0.40 |
| 17:V:523:ALA:O | 17:V:527:GLN:HB2 | 2.21 | 0.40 |
| 18:Y:202:LYS:NZ | 18:Y:448:GLN:OE1 | 2.44 | 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 | 0 | 79/82 (96%) | 75 (95%) | 4 (5%) | 0 | 100 | 100 |
| 2 | 1 | 593/618 (96%) | 574 (97%) | 19 (3%) | 0 | 100 | 100 |
| 3 | 2 | 439/441 (100%) | 415 (94%) | 22 (5%) | 2 (0%) | 29 | 67 |
| 4 | 3 | 243/325 (75%) | 235 (97%) | 8 (3%) | 0 | 100 | 100 |
| 5 | 4 | 288/294 (98%) | 278 (96%) | 10 (4%) | 0 | 100 | 100 |
| 6 | 5 | 121/123 (98%) | 114 (94%) | 6 (5%) | 1 (1%) | 19 | 58 |
| 7 | 6 | 122/151 (81%) | 110 (90%) | 12 (10%) | 0 | 100 | 100 |
| 8 | 7 | 174/190 (92%) | 170 (98%) | 4 (2%) | 0 | 100 | 100 |
| 9 | 8 | 86/89 (97%) | 77 (90%) | 9 (10%) | 0 | 100 | 100 |
| 10 | 9 | 95/97 (98%) | 82 (86%) | 13 (14%) | 0 | 100 | 100 |
| 11 | A | 72/127 (57%) | 71 (99%) | 1 (1%) | 0 | 100 | 100 |
| 11 | B | 72/127 (57%) | 70 (97%) | 2 (3%) | 0 | 100 | 100 |
| 11 | C | 71/127 (56%) | 70 (99%) | 1 (1%) | 0 | 100 | 100 |
| 11 | D | 72/127 (57%) | 71 (99%) | 1 (1%) | 0 | 100 | 100 |
| 11 | E | 72/127 (57%) | 71 (99%) | 1 (1%) | 0 | 100 | 100 |
| 11 | F | 72/127 (57%) | 70 (97%) | 2 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 11 | G | 72/127 (57%) | 71 (99%) | 1 (1%) | 0 | 100 | 100 |
| 11 | H | 72/127 (57%) | 71 (99%) | 1 (1%) | 0 | 100 | 100 |
| 11 | I | 72/127 (57%) | 72 (100%) | 0 | 0 | 100 | 100 |
| 11 | J | 72/127 (57%) | 70 (97%) | 2 (3%) | 0 | 100 | 100 |
| 12 | M | 213/327 (65%) | 204 (96%) | 9 (4%) | 0 | 100 | 100 |
| 13 | P | 191/229 (83%) | 178 (93%) | 13 (7%) | 0 | 100 | 100 |
| 14 | Q | 70/74 (95%) | 68 (97%) | 2 (3%) | 0 | 100 | 100 |
| 15 | R | 175/199 (88%) | 167 (95%) | 8 (5%) | 0 | 100 | 100 |
| 16 | S | 275/317 (87%) | 260 (94%) | 15 (6%) | 0 | 100 | 100 |
| 17 | T | 521/562 (93%) | 494 (95%) | 26 (5%) | 1 (0%) | 47 | 79 |
| 17 | U | 521/562 (93%) | 494 (95%) | 27 (5%) | 0 | 100 | 100 |
| 17 | V | 518/562 (92%) | 492 (95%) | 26 (5%) | 0 | 100 | 100 |
| 18 | X | 537/574 (94%) | 496 (92%) | 39 (7%) | 2 (0%) | 34 | 69 |
| 18 | Y | 519/574 (90%) | 496 (96%) | 22 (4%) | 1 (0%) | 47 | 79 |
| 18 | Z | 540/574 (94%) | 505 (94%) | 33 (6%) | 2 (0%) | 34 | 69 |
| All | All | 7039/8234 (86%) | 6691 (95%) | 339 (5%) | 9 (0%) | 54 | 83 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | X | 308 | VAL |
| 18 | Y | 308 | VAL |
| 18 | Z | 308 | VAL |
| 3 | 2 | 383 | PRO |
| 17 | T | 56 | LYS |
| 18 | Z | 307 | ALA |
| 3 | 2 | 223 | LYS |
| 6 | 5 | 120 | PRO |
| 18 | X | 309 | GLY |

### 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 | 0 | 63/64 (98%) | 63 (100%) | 0 | 100 | 100 |
| 2 | 1 | 493/512 (96%) | 492 (100%) | 1 (0%) | 93 | 98 |
| 3 | 2 | 312/312 (100%) | 310 (99%) | 2 (1%) | 86 | 94 |
| 4 | 3 | 195/258 (76%) | 195 (100%) | 0 | 100 | 100 |
| 5 | 4 | 220/223 (99%) | 220 (100%) | 0 | 100 | 100 |
| 6 | 5 | 107/107 (100%) | 107 (100%) | 0 | 100 | 100 |
| 7 | 6 | 96/115 (84%) | 96 (100%) | 0 | 100 | 100 |
| 8 | 7 | 140/150 (93%) | 139 (99%) | 1 (1%) | 84 | 94 |
| 9 | 8 | 71/72 (99%) | 71 (100%) | 0 | 100 | 100 |
| 10 | 9 | 79/79 (100%) | 79 (100%) | 0 | 100 | 100 |
| 11 | A | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | B | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | C | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | D | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | E | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | F | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | G | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | H | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | I | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 11 | J | 50/86 (58%) | 50 (100%) | 0 | 100 | 100 |
| 12 | M | 178/272 (65%) | 178 (100%) | 0 | 100 | 100 |
| 13 | P | 171/196 (87%) | 171 (100%) | 0 | 100 | 100 |
| 14 | Q | 56/58 (97%) | 56 (100%) | 0 | 100 | 100 |
| 15 | R | 134/151 (89%) | 134 (100%) | 0 | 100 | 100 |
| 16 | S | 235/265 (89%) | 233 (99%) | 2 (1%) | 78 | 91 |
| 17 | T | 419/448 (94%) | 416 (99%) | 3 (1%) | 84 | 94 |
| 17 | U | 419/448 (94%) | 415 (99%) | 4 (1%) | 76 | 90 |
| 17 | V | 418/448 (93%) | 416 (100%) | 2 (0%) | 88 | 95 |
| 18 | X | 447/469 (95%) | 447 (100%) | 0 | 100 | 100 |
| 18 | Y | 430/469 (92%) | 430 (100%) | 0 | 100 | 100 |
| 18 | Z | 449/469 (96%) | 449 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| All | All | 5632/6445 (87%) | 5617 (100%) | 15 (0%) | 92 96 |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 24 | LEU |
| 3 | 2 | 61 | TYR |
| 3 | 2 | 197 | LEU |
| 8 | 7 | 79 | VAL |
| 16 | S | 168 | VAL |
| 16 | S | 183 | ILE |
| 17 | T | 220 | ARG |
| 17 | T | 243 | LYS |
| 17 | T | 300 | PHE |
| 17 | U | 180 | VAL |
| 17 | U | 300 | PHE |
| 17 | U | 378 | THR |
| 17 | U | 418 | ARG |
| 17 | V | 180 | VAL |
| 17 | V | 300 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 65 | GLN |
| 2 | 1 | 257 | HIS |
| 2 | 1 | 298 | GLN |
| 2 | 1 | 316 | ASN |
| 2 | 1 | 365 | GLN |
| 2 | 1 | 482 | ASN |
| 2 | 1 | 587 | ASN |
| 2 | 1 | 606 | ASN |
| 3 | 2 | 68 | ASN |
| 3 | 2 | 243 | GLN |
| 3 | 2 | 289 | HIS |
| 3 | 2 | 380 | GLN |
| 4 | 3 | 87 | ASN |
| 4 | 3 | 164 | ASN |
| 4 | 3 | 206 | ASN |
| 4 | 3 | 229 | ASN |
| 5 | 4 | 135 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | 4 | 240 | GLN |
| 6 | 5 | 29 | GLN |
| 6 | 5 | 107 | ASN |
| 7 | 6 | 40 | ASN |
| 7 | 6 | 74 | GLN |
| 8 | 7 | 98 | ASN |
| 8 | 7 | 123 | HIS |
| 8 | 7 | 170 | HIS |
| 8 | 7 | 184 | ASN |
| 9 | 8 | 26 | HIS |
| 10 | 9 | 97 | ASN |
| 11 | A | 94 | ASN |
| 11 | B | 94 | ASN |
| 11 | E | 94 | ASN |
| 11 | G | 92 | ASN |
| 12 | M | 108 | ASN |
| 12 | M | 163 | ASN |
| 13 | P | 220 | ASN |
| 13 | P | 223 | ASN |
| 15 | R | 38 | ASN |
| 15 | R | 53 | ASN |
| 15 | R | 66 | HIS |
| 15 | R | 83 | GLN |
| 15 | R | 85 | GLN |
| 15 | R | 137 | HIS |
| 15 | R | 154 | GLN |
| 16 | S | 98 | ASN |
| 16 | S | 174 | GLN |
| 16 | S | 262 | ASN |
| 17 | T | 64 | GLN |
| 17 | T | 241 | HIS |
| 17 | T | 441 | GLN |
| 17 | T | 497 | GLN |
| 17 | U | 123 | GLN |
| 17 | U | 386 | GLN |
| 17 | U | 497 | GLN |
| 17 | V | 139 | HIS |
| 17 | V | 152 | ASN |
| 17 | V | 196 | GLN |
| 17 | V | 241 | HIS |
| 17 | V | 244 | ASN |
| 17 | V | 386 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | V | 435 | GLN |
| 17 | V | 486 | GLN |
| 17 | V | 497 | GLN |
| 18 | X | 198 | ASN |
| 18 | X | 390 | ASN |
| 18 | X | 398 | ASN |
| 18 | Y | 83 | ASN |
| 18 | Y | 199 | ASN |
| 18 | Y | 278 | GLN |
| 18 | Y | 294 | ASN |
| 18 | Y | 388 | ASN |
| 18 | Y | 390 | ASN |
| 18 | Y | 398 | ASN |
| 18 | Y | 404 | GLN |
| 18 | Z | 42 | GLN |
| 18 | Z | 199 | ASN |
| 18 | Z | 278 | GLN |
| 18 | Z | 337 | 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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 | $\#\|Z\| > 2$ |
| 20 | ATP | U | 1001 | 21 | 26,33,33 | 0.95 | 0 | 31,52,52 | 1.42 | 5 (16%) |
| 20 | ATP | T | 1001 | 21 | 26,33,33 | 0.93 | 0 | 31,52,52 | 1.43 | 5 (16%) |
| 20 | ATP | V | 1001 | 21 | 26,33,33 | 0.95 | 0 | 31,52,52 | 1.45 | 4 (12%) |
| 22 | ADP | X | 601 | 21 | 24,29,29 | 0.95 | 1 (4%) | 29,45,45 | 1.44 | 4 (13%) |
| 22 | ADP | Z | 601 | 21 | 24,29,29 | 0.98 | 1 (4%) | 29,45,45 | 1.38 | 4 (13%) |

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 |
|---|---|---|---|---|---|---|---|
| 20 | ATP | U | 1001 | 21 | - | 0/18/38/38 | 0/3/3/3 |
| 20 | ATP | T | 1001 | 21 | - | 0/18/38/38 | 0/3/3/3 |
| 20 | ATP | V | 1001 | 21 | - | 2/18/38/38 | 0/3/3/3 |
| 22 | ADP | X | 601 | 21 | - | 0/12/32/32 | 0/3/3/3 |
| 22 | ADP | Z | 601 | 21 | - | 8/12/32/32 | 0/3/3/3 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 22 | X | 601 | ADP | C5-C4 | 2.06 | 1.46 | 1.40 |
| 22 | Z | 601 | ADP | C5-C4 | 2.01 | 1.46 | 1.40 |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 22 | X | 601 | ADP | C3'-C2'-C1' | 3.61 | 106.41 | 100.98 |
| 22 | Z | 601 | ADP | C3'-C2'-C1' | 3.60 | 106.39 | 100.98 |
| 20 | V | 1001 | ATP | N3-C2-N1 | -3.57 | 123.09 | 128.68 |
| 20 | U | 1001 | ATP | N3-C2-N1 | -3.47 | 123.25 | 128.68 |
| 20 | T | 1001 | ATP | N3-C2-N1 | -3.38 | 123.40 | 128.68 |
| 20 | V | 1001 | ATP | PB-O3B-PG | -3.10 | 122.18 | 132.83 |
| 22 | X | 601 | ADP | N3-C2-N1 | -3.06 | 123.90 | 128.68 |
| 20 | T | 1001 | ATP | PB-O3B-PG | -3.01 | 122.51 | 132.83 |
| 22 | Z | 601 | ADP | N3-C2-N1 | -2.95 | 124.06 | 128.68 |
| 20 | U | 1001 | ATP | C3'-C2'-C1' | 2.67 | 105.00 | 100.98 |
| 20 | U | 1001 | ATP | PA-O3A-PB | -2.63 | 123.81 | 132.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | V | 1001 | ATP | C3'-C2'-C1' | 2.59 | 104.88 | 100.98 |
| 22 | X | 601 | ADP | PA-O3A-PB | -2.53 | 124.14 | 132.83 |
| 20 | U | 1001 | ATP | PB-O3B-PG | -2.49 | 124.30 | 132.83 |
| 20 | V | 1001 | ATP | C4-C5-N7 | -2.35 | 106.95 | 109.40 |
| 20 | U | 1001 | ATP | C4-C5-N7 | -2.32 | 106.98 | 109.40 |
| 20 | T | 1001 | ATP | PA-O3A-PB | -2.27 | 125.05 | 132.83 |
| 20 | T | 1001 | ATP | C3'-C2'-C1' | 2.21 | 104.30 | 100.98 |
| 22 | Z | 601 | ADP | PA-O3A-PB | -2.20 | 125.27 | 132.83 |
| 22 | X | 601 | ADP | C4-C5-N7 | -2.20 | 107.11 | 109.40 |
| 22 | Z | 601 | ADP | C4-C5-N7 | -2.18 | 107.13 | 109.40 |
| 20 | T | 1001 | ATP | C4-C5-N7 | -2.16 | 107.15 | 109.40 |

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 22 | Z | 601 | ADP | PA-O3A-PB-O2B |
| 22 | Z | 601 | ADP | PA-O3A-PB-O3B |
| 22 | Z | 601 | ADP | C5'-O5'-PA-O1A |
| 22 | Z | 601 | ADP | C5'-O5'-PA-O3A |
| 20 | V | 1001 | ATP | O4'-C4'-C5'-O5' |
| 22 | Z | 601 | ADP | O4'-C4'-C5'-O5' |
| 22 | Z | 601 | ADP | C3'-C4'-C5'-O5' |
| 20 | V | 1001 | ATP | C3'-C4'-C5'-O5' |
| 22 | Z | 601 | ADP | C5'-O5'-PA-O2A |
| 22 | Z | 601 | ADP | PA-O3A-PB-O1B |

There are no ring outliers.

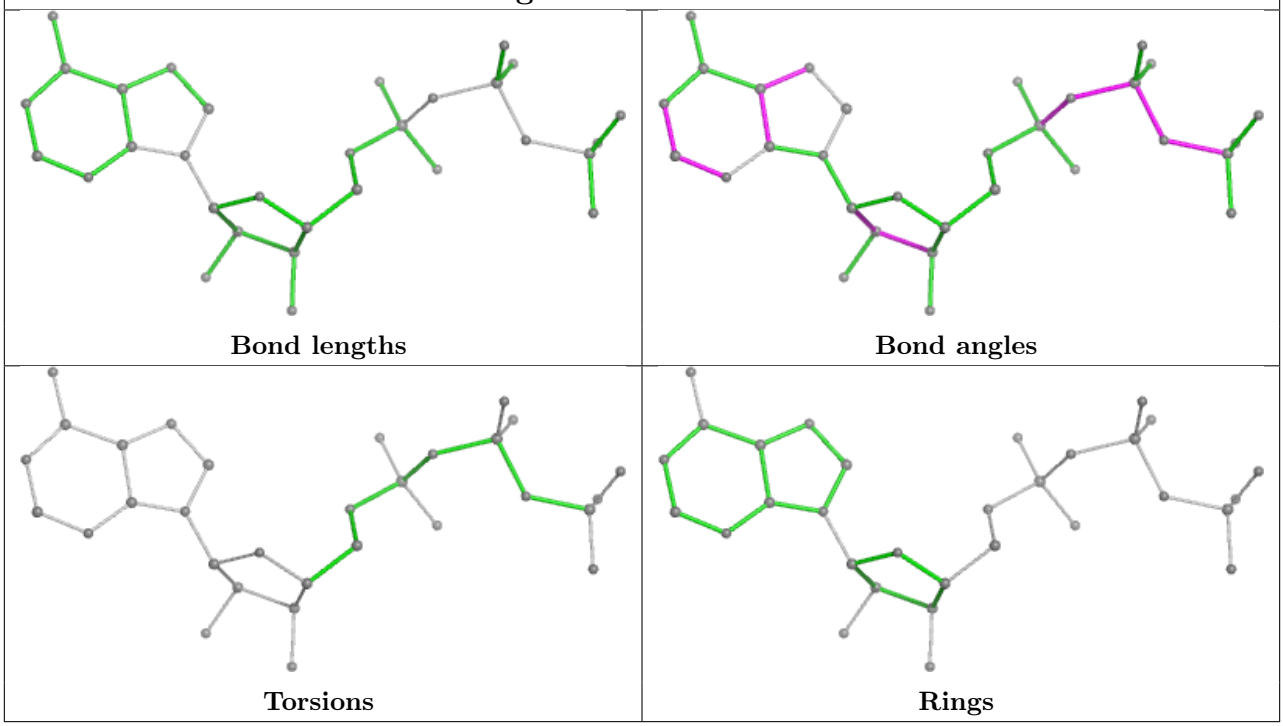
1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 20 | T | 1001 | ATP | 1 | 0 |

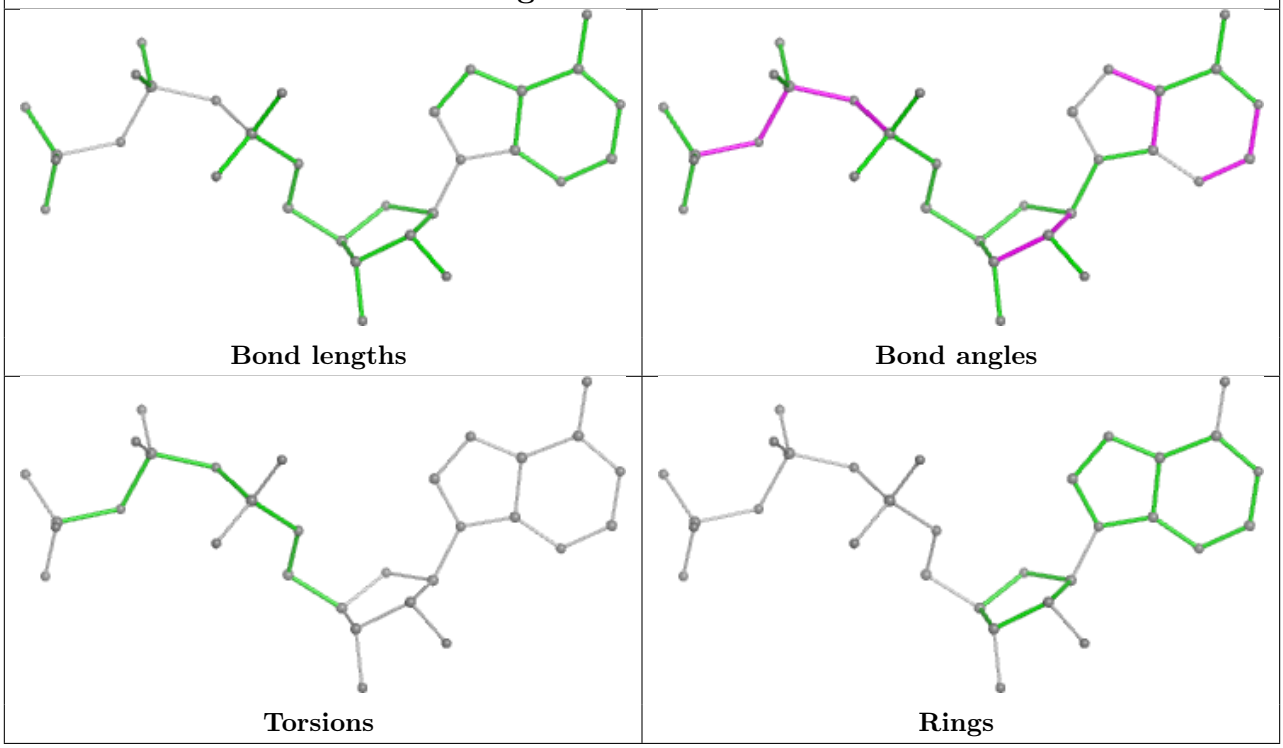
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

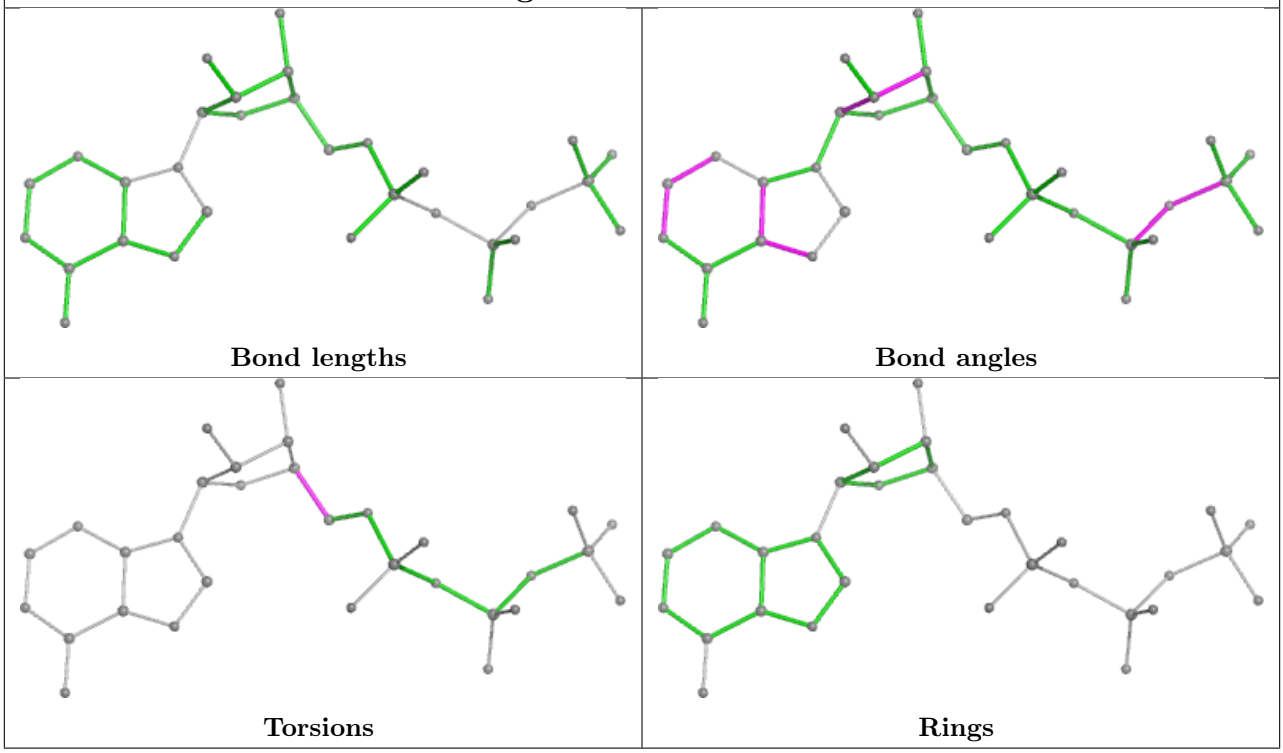
**Ligand ATP U 1001**



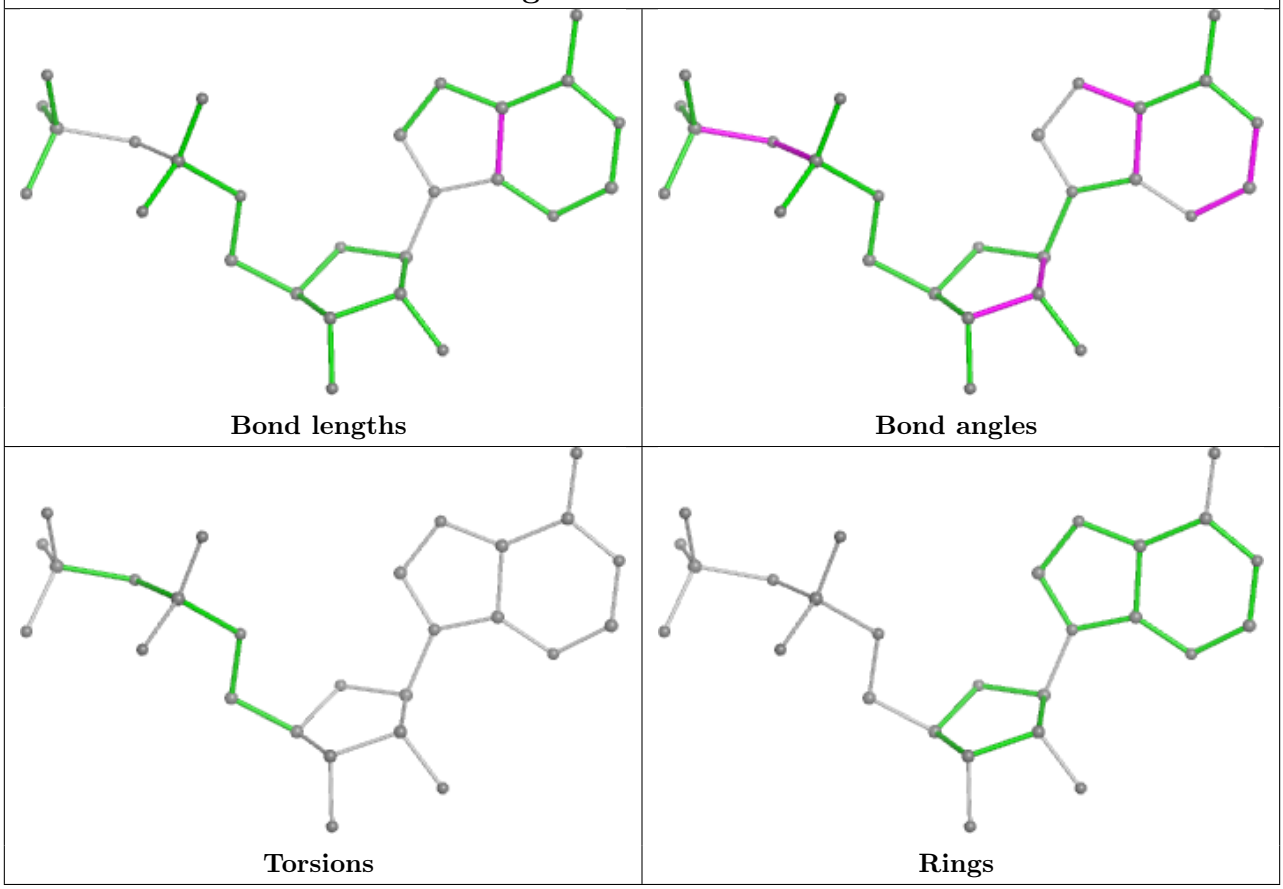

**Ligand ATP T 1001**

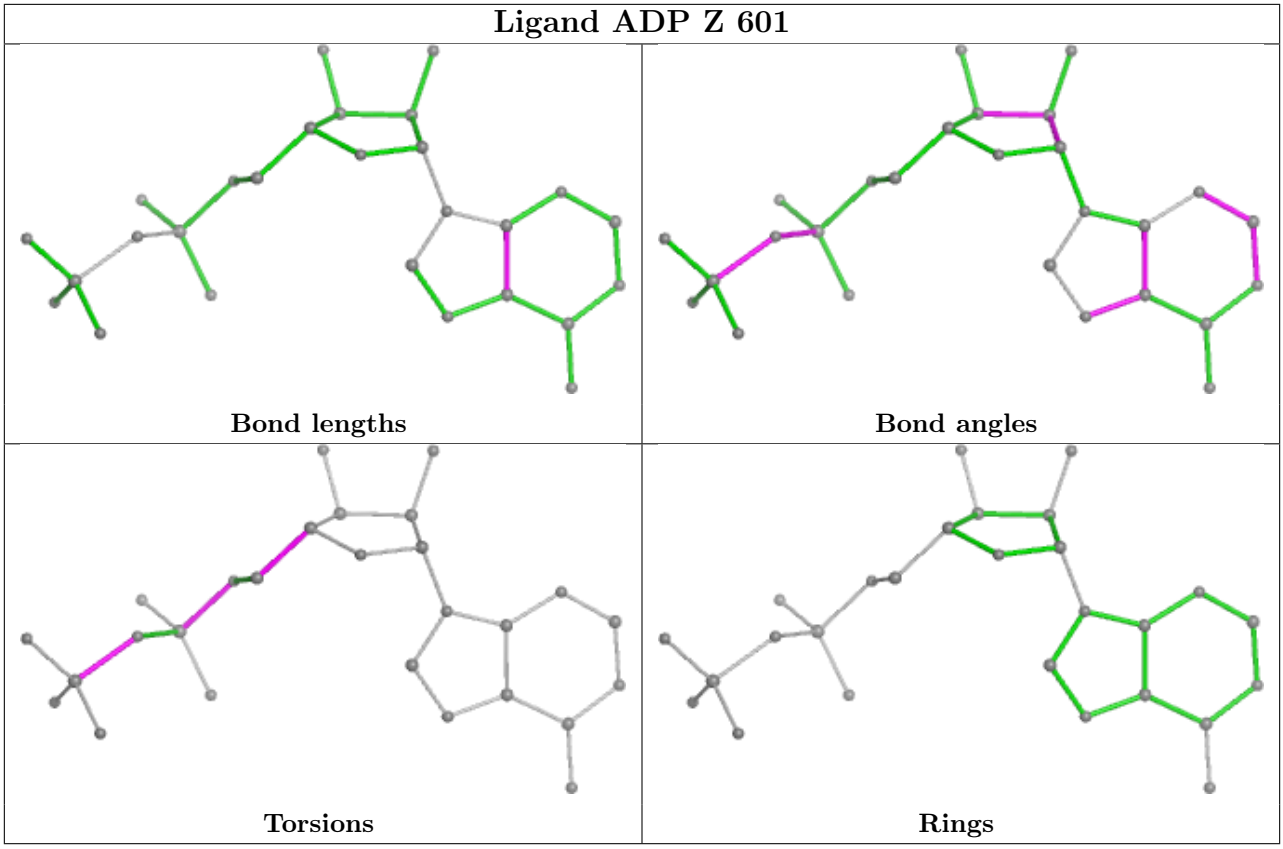


## Ligand ATP V 1001




## Ligand ADP X 601






## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 11 | C | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | C | 126:PHE | C | 127:ALA | N | 4.35 |

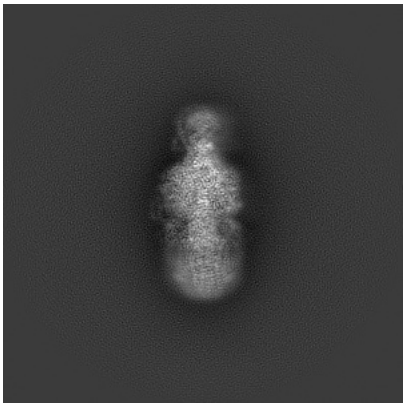
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4848. These allow visual inspection of the internal detail of the map and identification of artifacts.

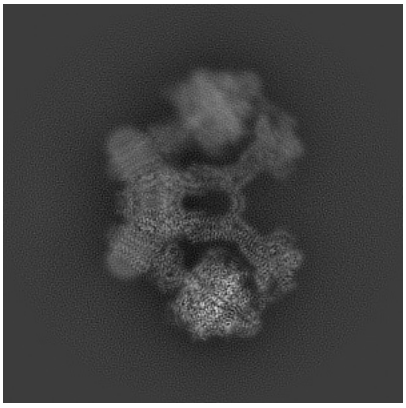
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

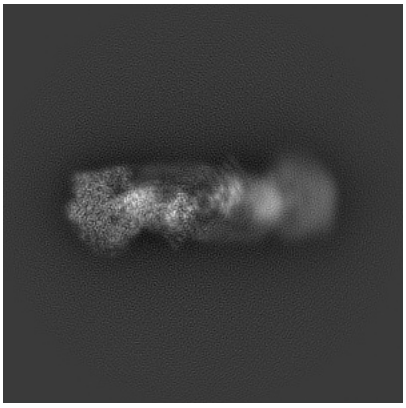
### 6.1.1 Primary map



X



Y

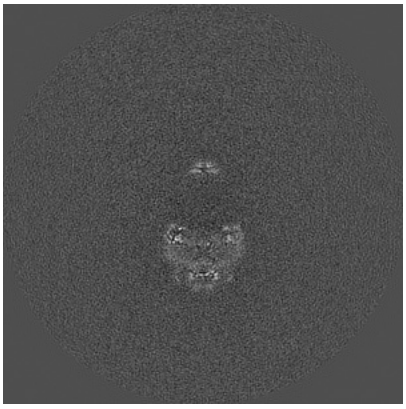


Z

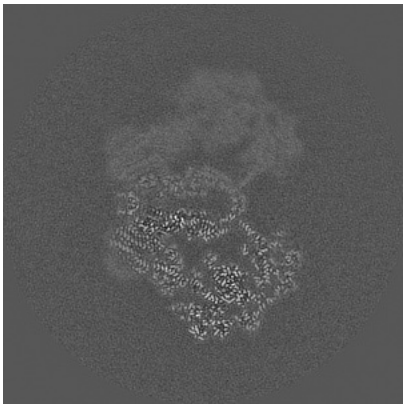
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

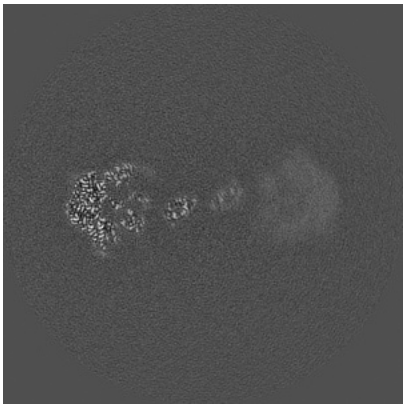
### 6.2.1 Primary map



X Index: 240



Y Index: 240

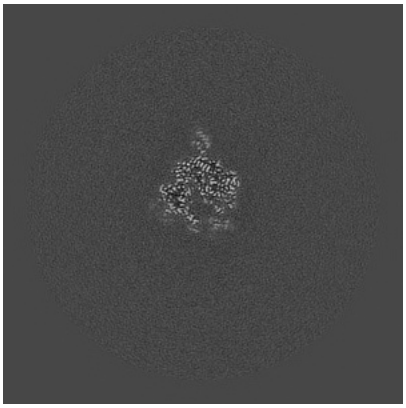


Z Index: 240

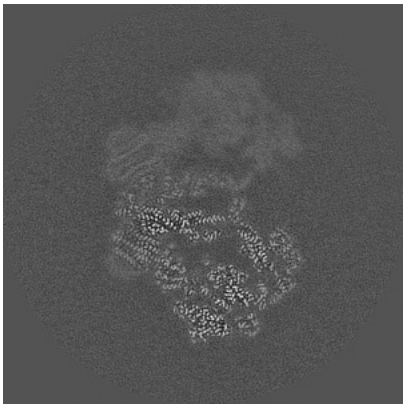
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

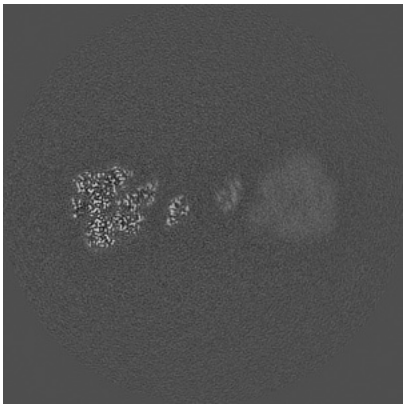
### 6.3.1 Primary map



X Index: 124



Y Index: 235

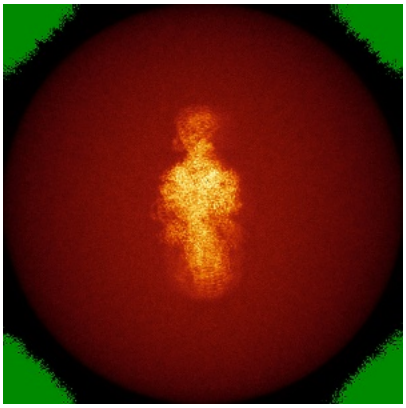


Z Index: 255

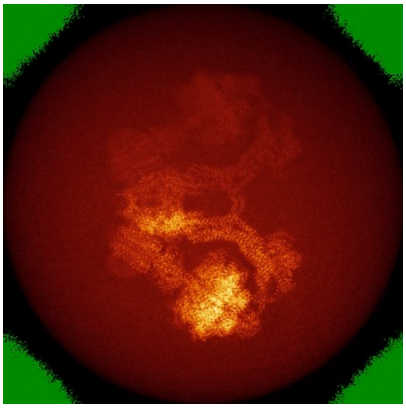
The images above show the largest variance slices of the map in three orthogonal directions.

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

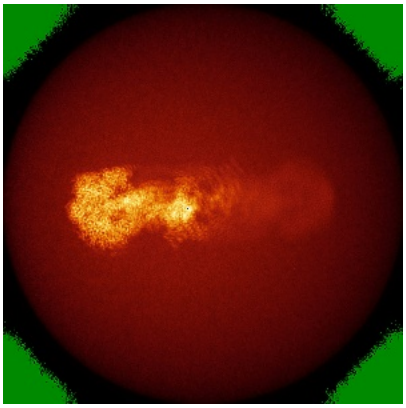
### 6.4.1 Primary map



X



Y

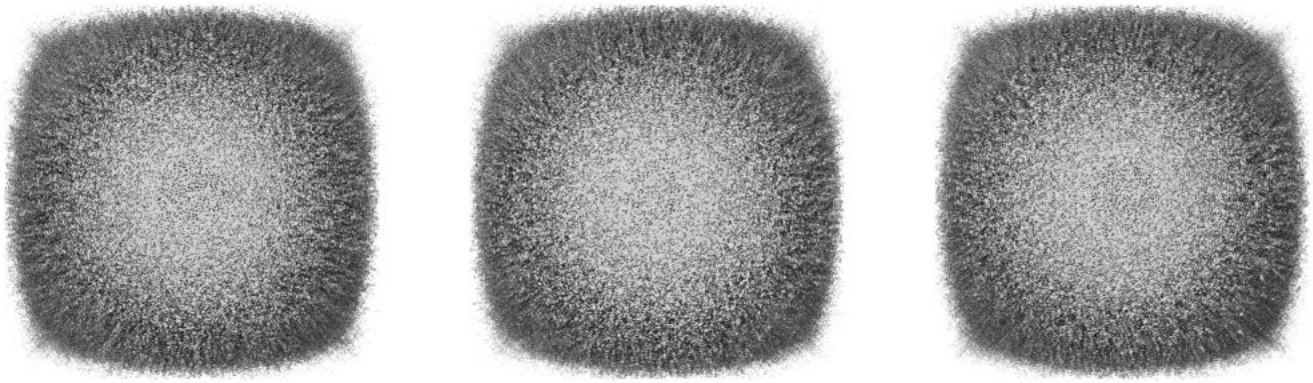


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

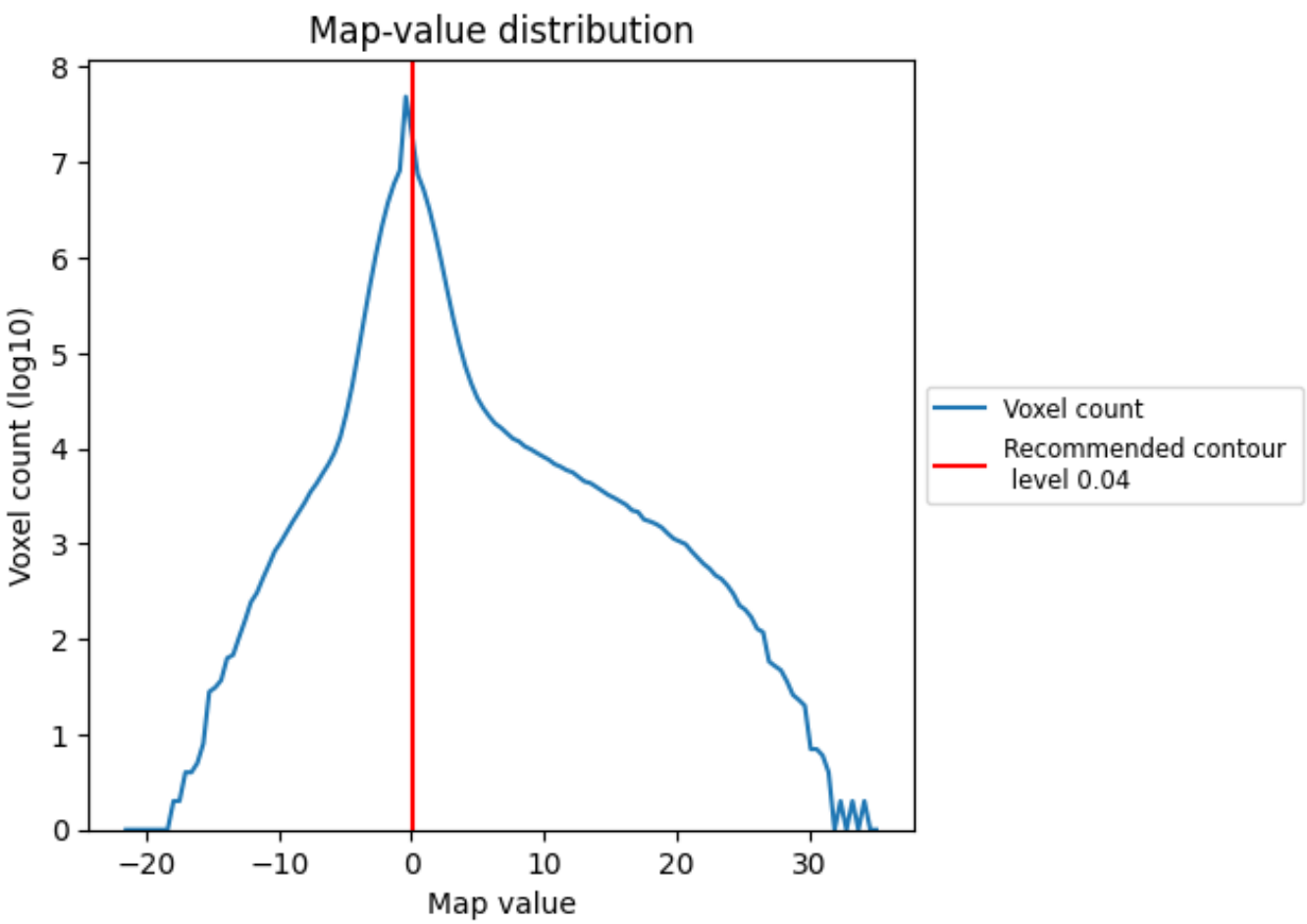
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

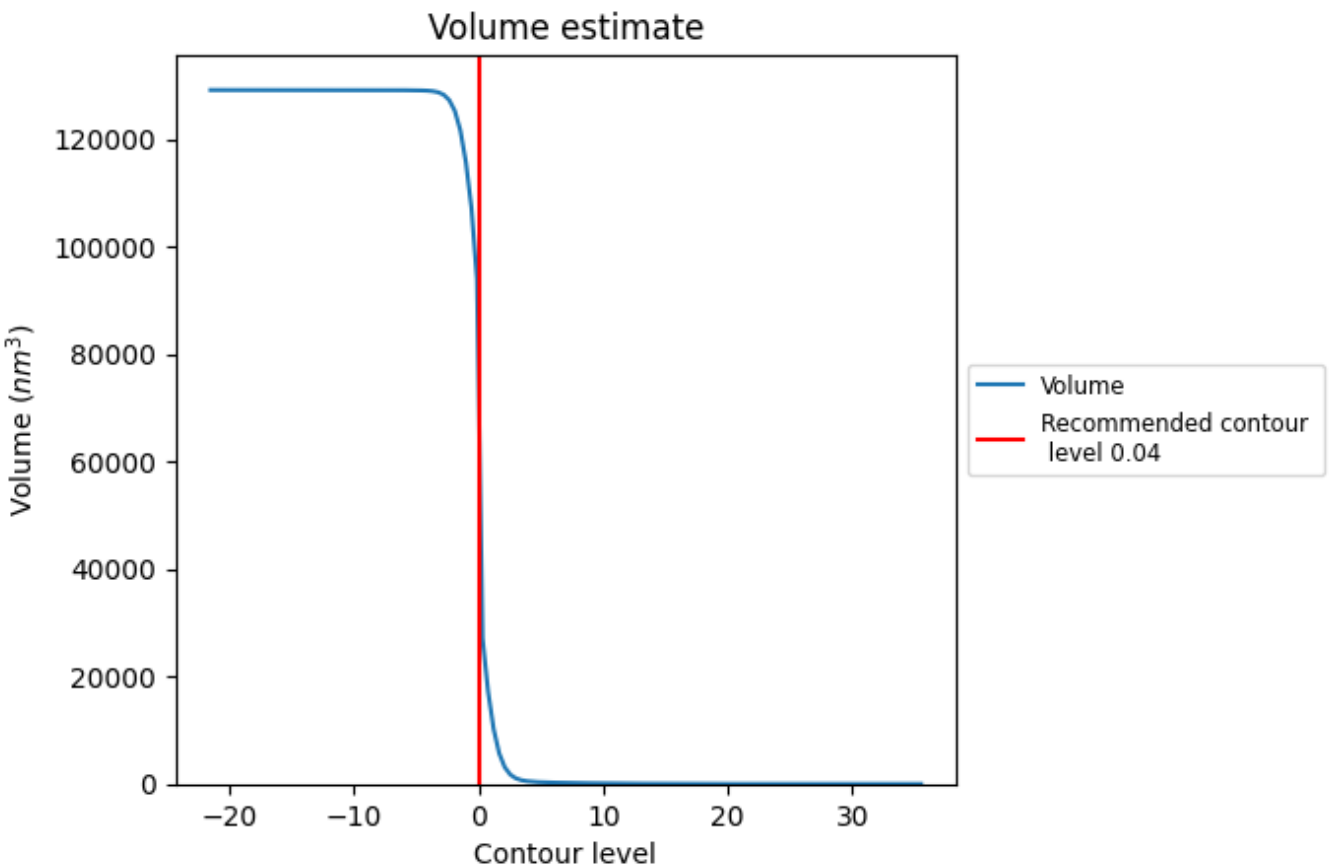
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

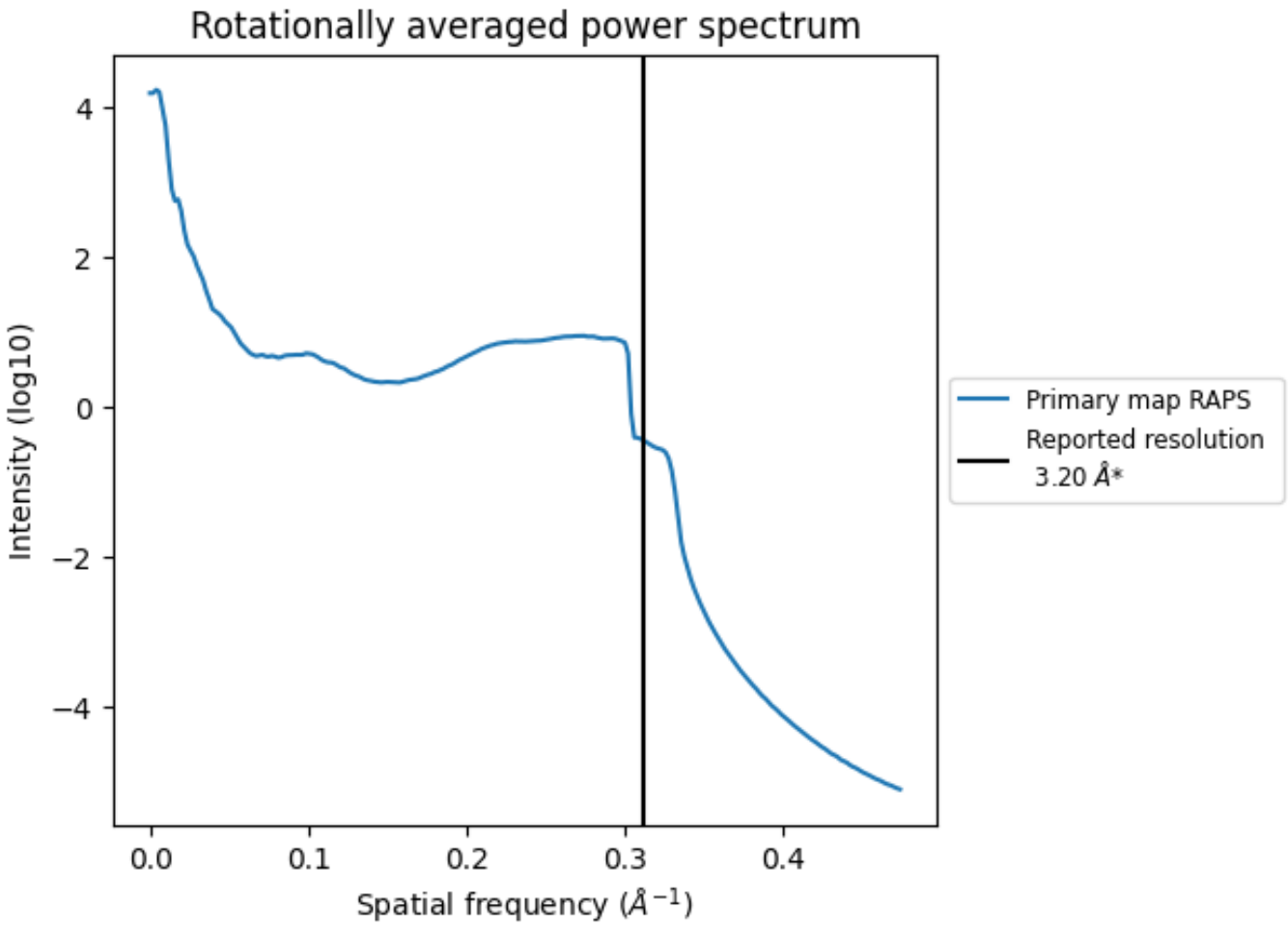
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 67252 $nm^3$; this corresponds to an approximate mass of 60750 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 0.312 Å$^{-1}$

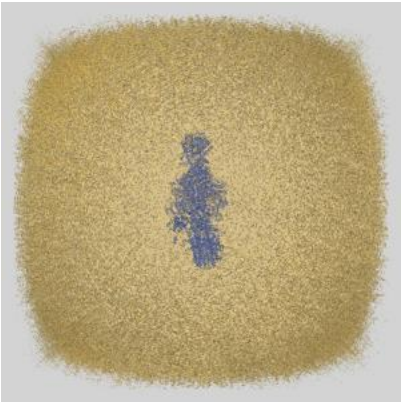
# 8 Fourier-Shell correlation (i)

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

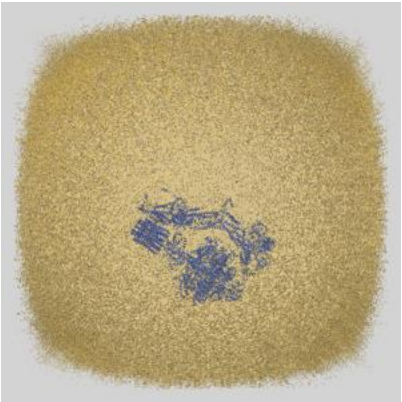
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4848 and PDB model 6REB. Per-residue inclusion information can be found in section 3 on page 10.

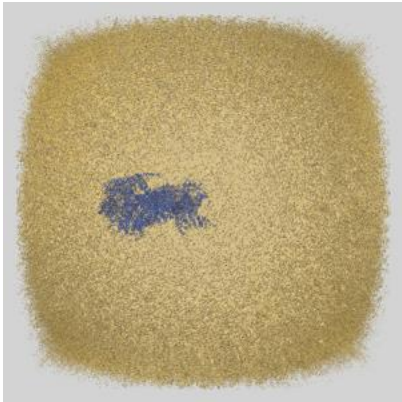
## 9.1 Map-model overlay (i)



X



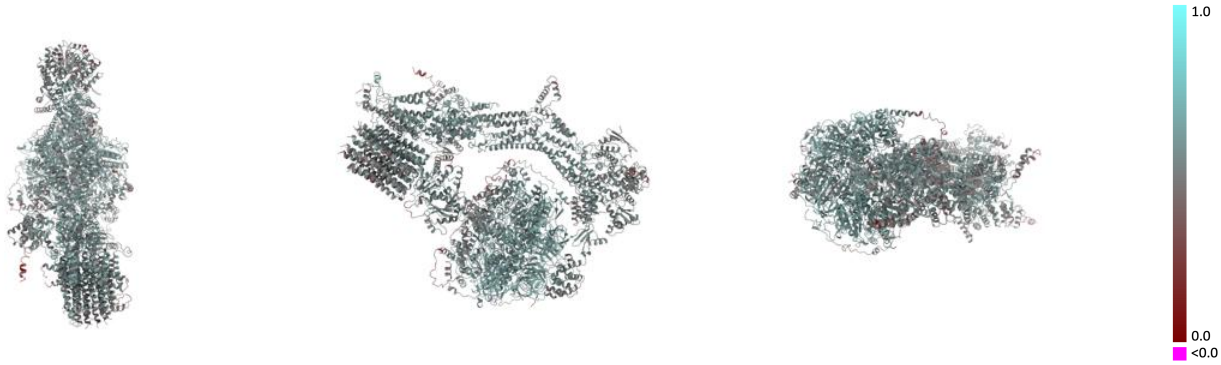
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

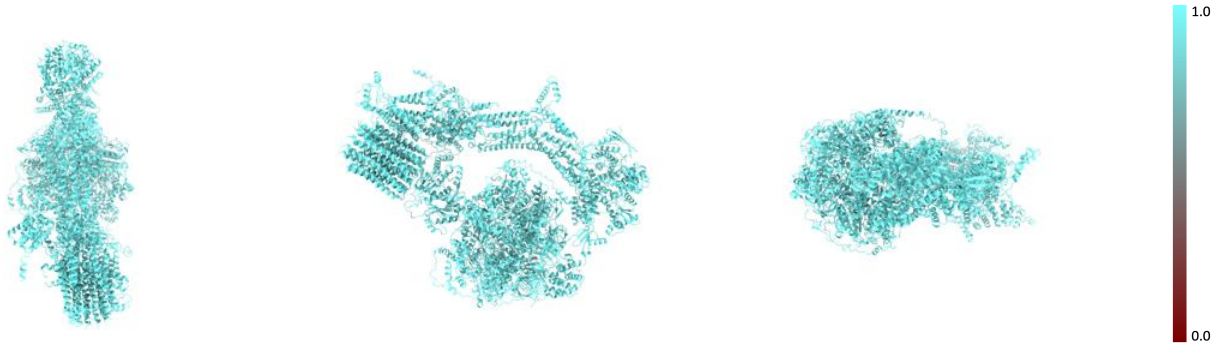
## 9.2 Q-score mapped to coordinate model (i)




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.

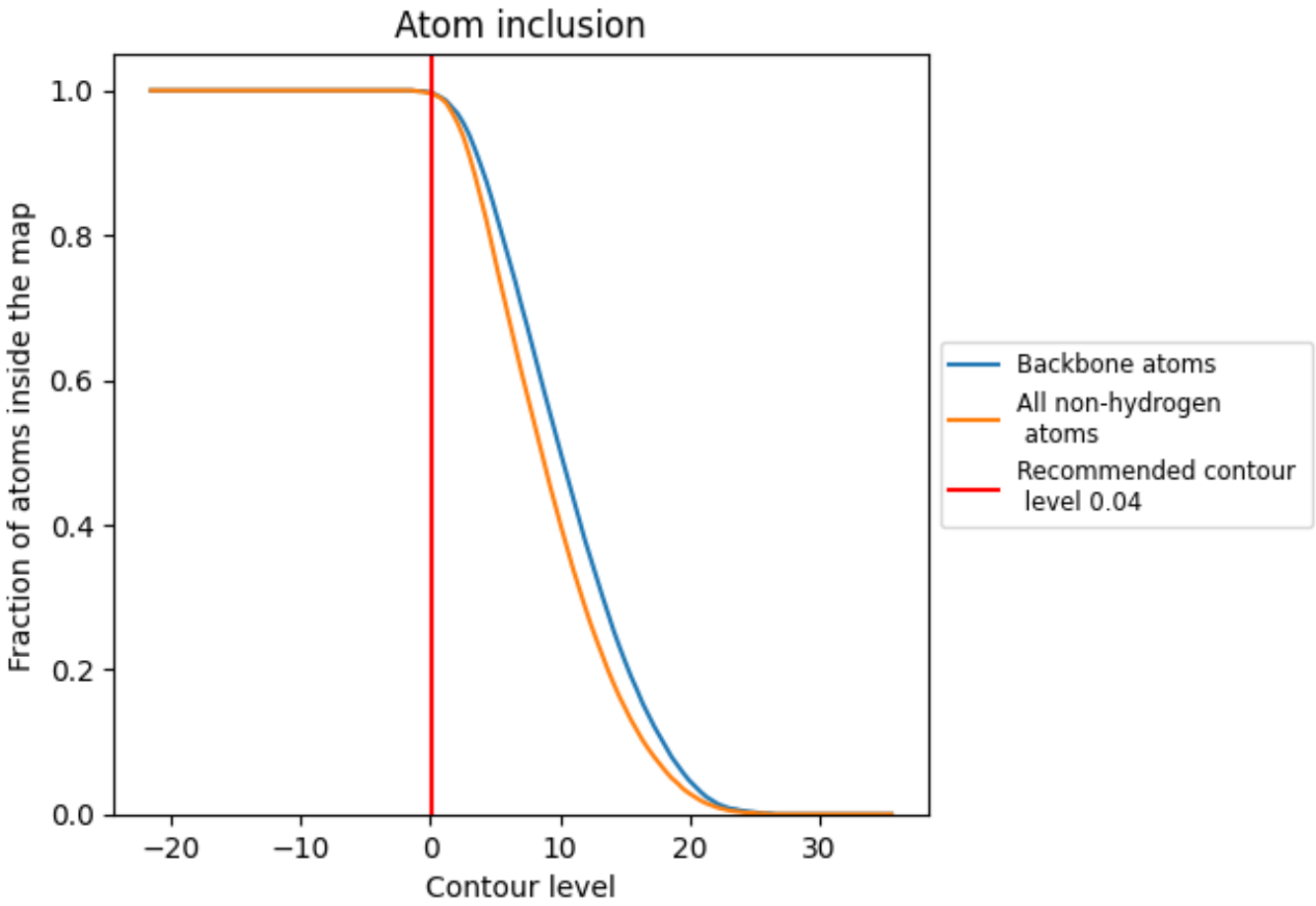
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.04).

## 9.4 Atom inclusion (i)




At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9960 | 0.5410 |
| 0 | 0.9970 | 0.5340 |
| 1 | 0.9960 | 0.5400 |
| 2 | 0.9950 | 0.4940 |
| 3 | 0.9950 | 0.4990 |
| 4 | 0.9960 | 0.5130 |
| 5 | 0.9930 | 0.5630 |
| 6 | 0.9930 | 0.5470 |
| 7 | 0.9960 | 0.5390 |
| 8 | 0.9970 | 0.5580 |
| 9 | 0.9960 | 0.4800 |
| A | 0.9980 | 0.4840 |
| B | 0.9960 | 0.4920 |
| C | 0.9940 | 0.5200 |
| D | 0.9880 | 0.5360 |
| E | 0.9960 | 0.5430 |
| F | 0.9900 | 0.5320 |
| G | 0.9980 | 0.5010 |
| H | 0.9960 | 0.4950 |
| I | 1.0000 | 0.4770 |
| J | 0.9940 | 0.4750 |
| M | 0.9940 | 0.5400 |
| P | 0.9990 | 0.5220 |
| Q | 0.9960 | 0.5240 |
| R | 0.9920 | 0.5040 |
| S | 0.9970 | 0.5370 |
| T | 0.9940 | 0.5690 |
| U | 0.9980 | 0.5620 |
| V | 0.9990 | 0.5690 |
| X | 0.9980 | 0.5620 |
| Y | 0.9960 | 0.5650 |
| Z | 0.9980 | 0.5690 |