# Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 04:10 am BST

| | | |
|---|---|---|
| PDB ID | : | 7PNV / pdb_00007pnv |
| EMDB ID | : | EMD-13553 |
| Title | : | Assembly intermediate of mouse mitochondrial ribosome small subunit without mS37 in complex with RbfA and Mettl15 |
| Authors | : | Itoh, Y.; Khawaja, A.; Laptev, I.; Sergiev, P.; Rorbach, J.; Amunts, A. |
| Deposited on | : | 2021-09-08 |
| Resolution | : | 3.06 Å(reported) |
| Based on initial model | : | 6RW4 |

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.

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

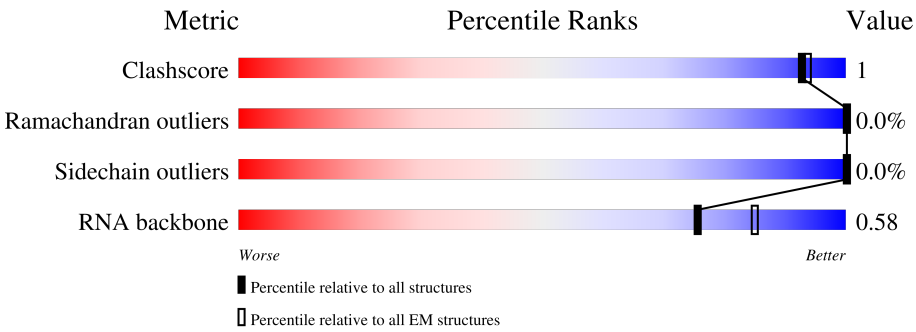
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 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) | : | 2.50 |

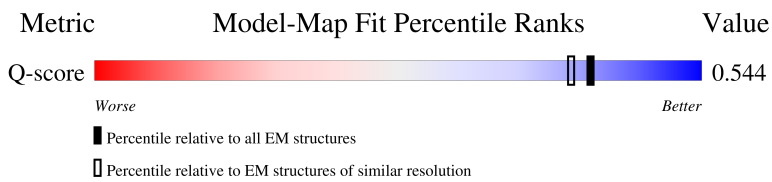
# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.06 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 | - |
| RNA backbone | 8273 | 3508 | - |
| Q-score | - | 25397 | 13976 ( 2.56 - 3.56 ) |

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 | 956 | 82% 16% |
| 2 | B | 291 | 73% 23% |
| 3 | C | 167 | 74% 5% 21% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | D | 432 | 75% 5% 21% |
| 5 | E | 125 | 90% 5% 5% |
| 6 | F | 242 | 83% 14% |
| 7 | G | 390 | 79% 17% |
| 8 | H | 160 | 79% 8% 12% |
| 9 | I | 191 | 69% 28% |
| 10 | J | 139 | 75% 22% |
| 11 | K | 128 | 71% 8% 21% |
| 12 | L | 258 | 5% 66% 32% |
| 13 | M | 135 | 7% 92% 7% |
| 14 | N | 120 | 91% 6% |
| 15 | O | 254 | 78% 22% |
| 16 | P | 143 | 64% 32% |
| 17 | Q | 86 | 97% |
| 18 | R | 359 | 80% 18% |
| 19 | S | 177 | 75% 23% |
| 20 | T | 171 | 95% |
| 21 | U | 200 | 87% 13% |
| 22 | V | 415 | 86% 12% |
| 23 | W | 186 | 52% 46% |
| 24 | X | 391 | 87% 5% 9% |
| 25 | Y | 384 | 7% 38% 61% |
| 26 | Z | 106 | 7% 94% 5% |
| 27 | 0 | 218 | 97% |
| 28 | 1 | 320 | 85% 13% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | 3 | 200 | 36% 64% |
| 30 | 4 | 685 | 17% 84% 14% |
| 31 | a | 350 | 8% 53% 45% |
| 32 | b | 406 | 57% 74% 5% 20% |

# 2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 131939 atoms, of which 60861 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 RNA chain called 12S mitochondrial rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 1 | A | 951 | 30430 | 9078 | 10223 | 3629 | 6549 | 951 | 0 | 0 |

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 2 | B | 223 | 3590 | 1142 | 1799 | 326 | 315 | 8 | 0 | 0 |

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 3 | C | 132 | 2163 | 690 | 1091 | 197 | 180 | 5 | 0 | 0 |

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 4 | D | 343 | 5527 | 1716 | 2794 | 527 | 480 | 10 | 0 | 0 |

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 5 | E | 119 | 1916 | 599 | 968 | 171 | 175 | 3 | 0 | 0 |

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 6 | F | 208 | 3472 | 1096 | 1750 | 316 | 299 | 11 | 0 | 0 |

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 7 | G | 325 | 5304 | 1689 | 2630 | 480 | 491 | 14 | 0 | 0 |

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 8 | H | 140 | 2346 | 742 | 1193 | 200 | 207 | 4 | 0 | 0 |

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 9 | I | 137 | 2047 | 629 | 1038 | 191 | 184 | 5 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| I | 181 | 5F0 | ASN | conflict | UNP Q9DCA2 |

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 10 | J | 108 | 1749 | 528 | 903 | 172 | 141 | 5 | 0 | 0 |

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 11 | K | 101 | 1743 | 534 | 888 | 175 | 140 | 6 | 0 | 0 |

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 12 | L | 176 | 3041 | 930 | 1576 | 274 | 255 | 6 | 0 | 0 |

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 13 | M | 126 | 2004 | 623 | 1009 | 194 | 172 | 6 | 0 | 0 |

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 14 | N | 113 | 1839 | 575 | 951 | 160 | 150 | 3 | 0 | 0 |

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 15 | O | 197 | 3146 | 1014 | 1548 | 289 | 286 | 9 | 0 | 0 |

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 16 | P | 97 | 1610 | 505 | 818 | 140 | 139 | 8 | 0 | 0 |

- Molecule 17 is a protein called 28S ribosomal protein S21, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 17 | Q | 86 | 1482 | 453 | 750 | 146 | 126 | 7 | 0 | 0 |

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 18 | R | 294 | 4816 | 1526 | 2416 | 418 | 449 | 7 | 0 | 0 |

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 19 | S | 136 | 2257 | 722 | 1133 | 199 | 201 | 2 | 0 | 0 |

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 20 | T | 170 | 2801 | 892 | 1413 | 238 | 246 | 12 | 0 | 0 |

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 21 | U | 174 | 2908 | 894 | 1459 | 283 | 270 | 2 | 0 | 0 |

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 22 | V | 365 | 5970 | 1911 | 2972 | 506 | 570 | 11 | 0 | 0 |

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 23 | W | 100 | 1606 | 503 | 813 | 141 | 146 | 3 | 0 | 0 |

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 24 | X | 357 | 5762 | 1834 | 2881 | 515 | 522 | 10 | 0 | 0 |

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 25 | Y | 149 | 2439 | 809 | 1193 | 201 | 233 | 3 | 0 | 0 |

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 26 | Z | 101 | 1682 | 526 | 848 | 157 | 148 | 3 | 0 | 0 |

- Molecule 27 is a protein called 28S ribosomal protein S34, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 27 | 0 | 216 | 3649 | 1139 | 1838 | 355 | 313 | 4 | 0 | 0 |

- Molecule 28 is a protein called 28S ribosomal protein S35, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 28 | 1 | 277 | 4440 | 1397 | 2228 | 380 | 423 | 12 | 0 | 0 |

- Molecule 29 is a protein called Aurora kinase A-interacting protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 29 | 3 | 72 | 1371 | 414 | 728 | 135 | 93 | 1 | 0 | 0 |

- Molecule 30 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 30 | 4 | 589 | 9558 | 3064 | 4800 | 800 | 872 | 22 | 0 | 0 |

- Molecule 31 is a protein called Putative ribosome-binding factor A, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 31 | a | 191 | 3129 | 977 | 1583 | 280 | 284 | 5 | 0 | 0 |

- Molecule 32 is a protein called 12S rRNA N4-methylcytidine methyltransferase.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 32 | b | 323 | 5114 | 1592 | 2595 | 454 | 462 | 11 | 0 | 0 |

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 33 | A | 46 | 46 | 46 | 0 |
| 33 | B | 1 | 1 | 1 | 0 |

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| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 33 | X | 1 | 1 | 1 | 0 |
| | | | Total | Mg | |
| 33 | 3 | 1 | 1 | 1 | 0 |

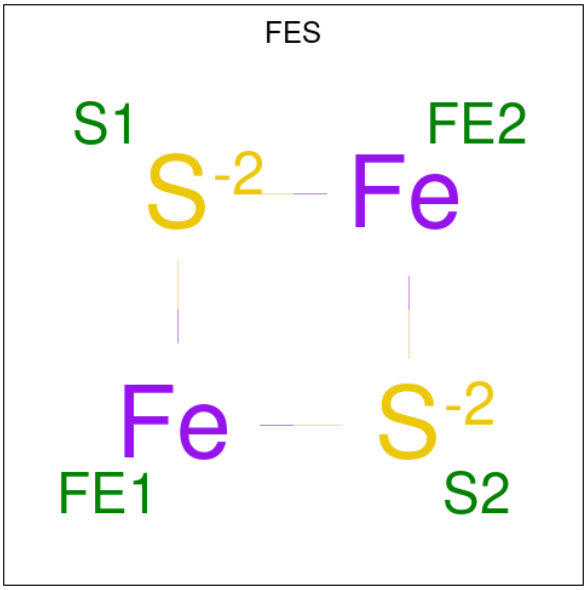
- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | K | |
| 34 | A | 13 | 13 | 13 | 0 |

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

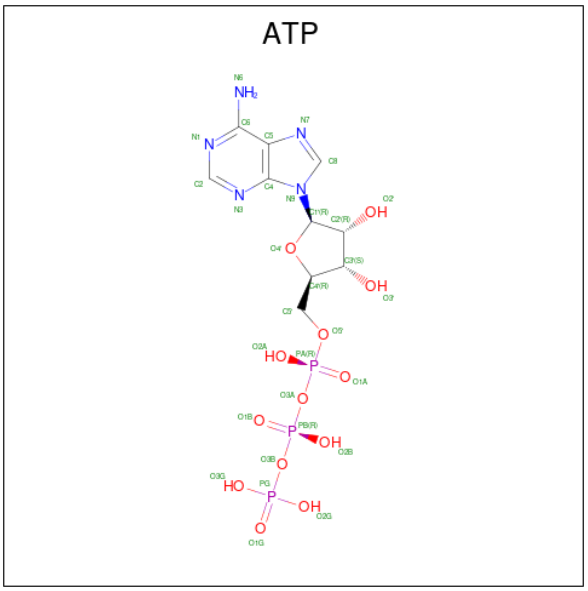
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 35 | O | 1 | 1 | 1 | 0 |

- Molecule 36 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: $Fe_2S_2$).



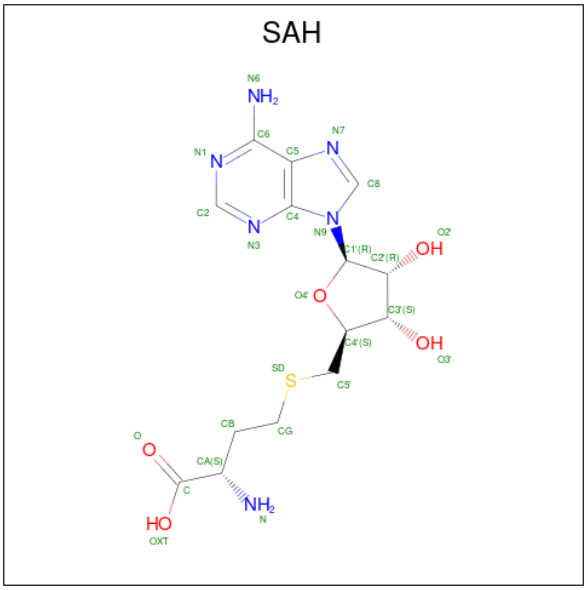

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 36 | P | 1 | 4 | 2 | 2 | 0 |
| | | | Total | Fe | S | |
| 36 | T | 1 | 4 | 2 | 2 | 0 |

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | |
| 37 | X | 1 | 43 | 10 | 12 | 5 | 13 | 3 | 0 |

- Molecule 38 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 38 | b | 1 | 46 | 14 | 20 | 6 | 5 | 1 | 0 |

- Molecule 39 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | O | |
| 39 | A | 549 | 549 | 549 | 0 |
| 39 | B | 23 | 23 | 23 | 0 |
| 39 | C | 19 | 19 | 19 | 0 |
| 39 | D | 34 | 34 | 34 | 0 |
| 39 | E | 2 | 2 | 2 | 0 |
| 39 | F | 7 | 7 | 7 | 0 |
| 39 | G | 10 | 10 | 10 | 0 |
| 39 | H | 19 | 19 | 19 | 0 |
| 39 | I | 5 | 5 | 5 | 0 |
| 39 | J | 14 | 14 | 14 | 0 |
| 39 | K | 25 | 25 | 25 | 0 |
| 39 | L | 6 | 6 | 6 | 0 |
| 39 | M | 16 | 16 | 16 | 0 |
| 39 | N | 8 | 8 | 8 | 0 |
| 39 | O | 25 | 25 | 25 | 0 |
| 39 | P | 3 | 3 | 3 | 0 |
| 39 | Q | 8 | 8 | 8 | 0 |
| 39 | R | 13 | 13 | 13 | 0 |
| 39 | S | 4 | 4 | 4 | 0 |
| 39 | T | 19 | 19 | 19 | 0 |
| 39 | U | 3 | 3 | 3 | 0 |
| 39 | W | 2 | 2 | 2 | 0 |

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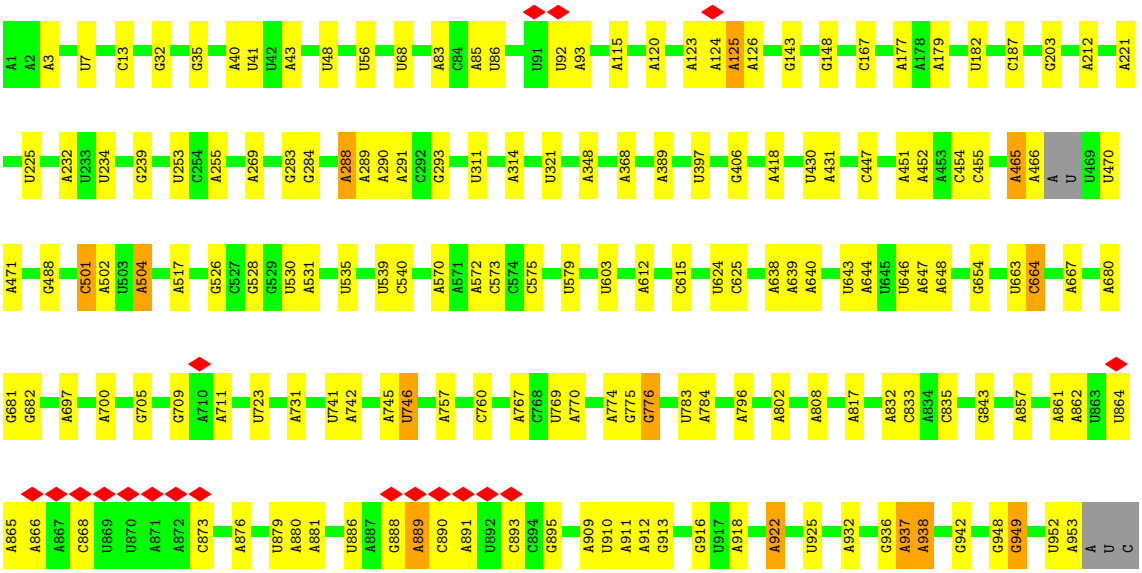
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | O | |
| 39 | X | 5 | 5 | 5 | 0 |
| | | | Total | O | |
| 39 | Y | 7 | 7 | 7 | 0 |
| | | | Total | O | |
| 39 | Z | 18 | 18 | 18 | 0 |
| | | | Total | O | |
| 39 | 0 | 7 | 7 | 7 | 0 |
| | | | Total | O | |
| 39 | 1 | 5 | 5 | 5 | 0 |
| | | | Total | O | |
| 39 | 3 | 7 | 7 | 7 | 0 |
| | | | Total | O | |
| 39 | a | 5 | 5 | 5 | 0 |

# 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.

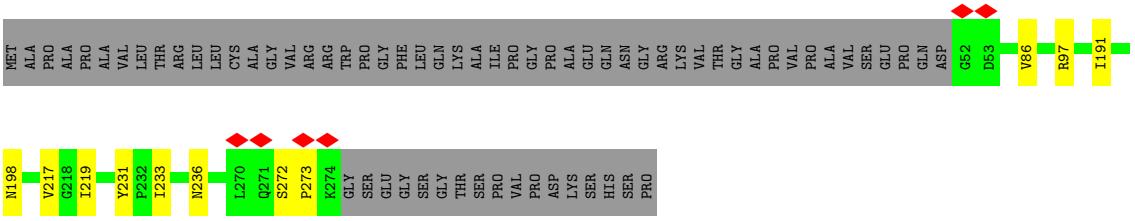
- Molecule 1: 12S mitochondrial rRNA

Chain A:




- Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:

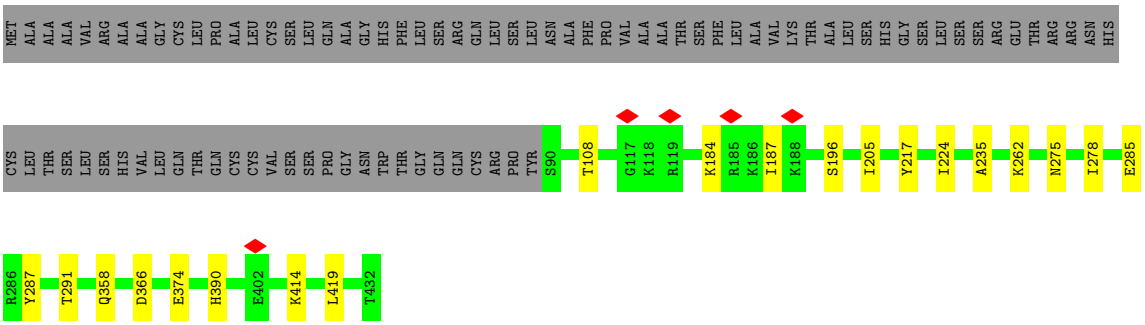



- Molecule 3: 28S ribosomal protein S24, mitochondrial

Chain C:

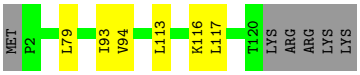
• Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain D:



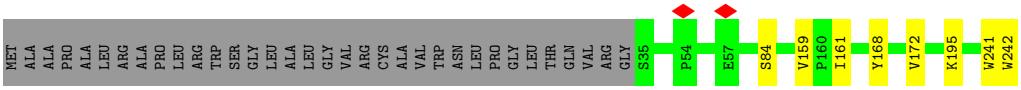

• Molecule 5: 28S ribosomal protein S6, mitochondrial

Chain E:



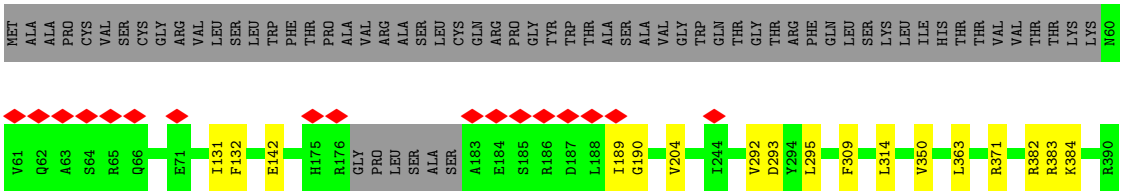

• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:



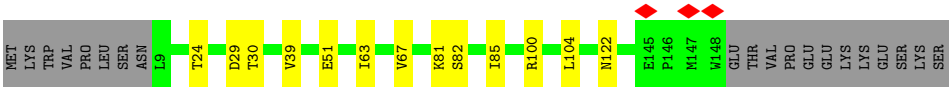

• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:



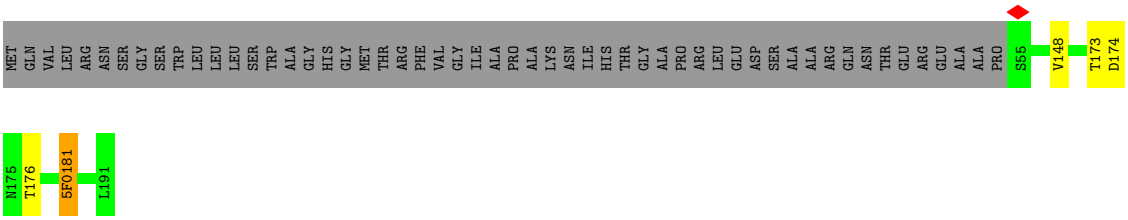

• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



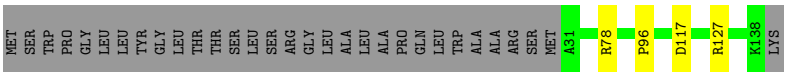

• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



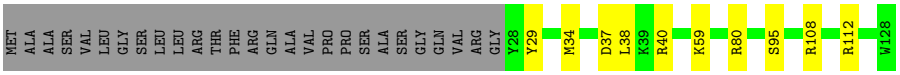

- Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



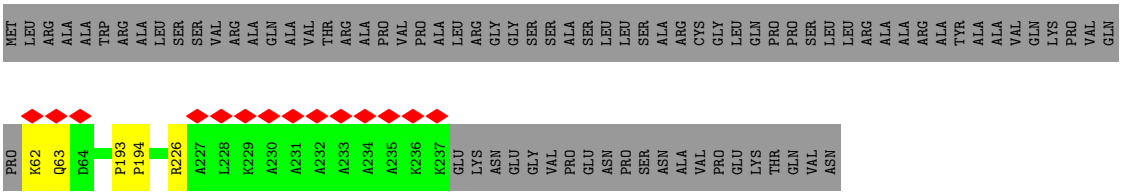

- Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:



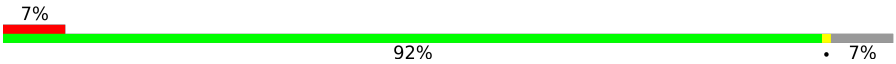

- Molecule 12: 28S ribosomal protein S15, mitochondrial

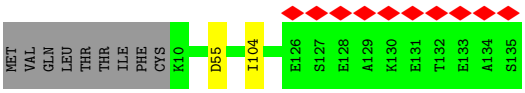
Chain L:




- Molecule 13: 28S ribosomal protein S16, mitochondrial

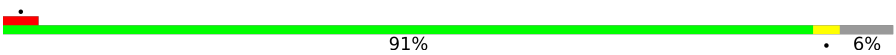
Chain M:

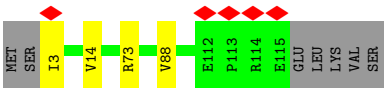



- Molecule 14: 28S ribosomal protein S17, mitochondrial

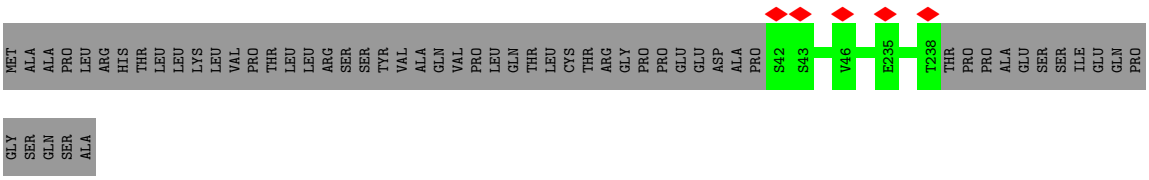
Chain N:



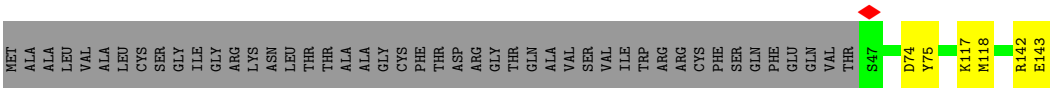

- Molecule 15: 28S ribosomal protein S18b, mitochondrial

Chain O:



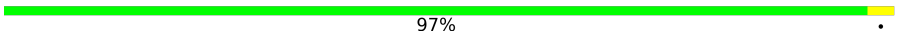

- Molecule 16: 28S ribosomal protein S18c, mitochondrial

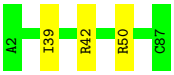
Chain P:




- Molecule 17: 28S ribosomal protein S21, mitochondrial

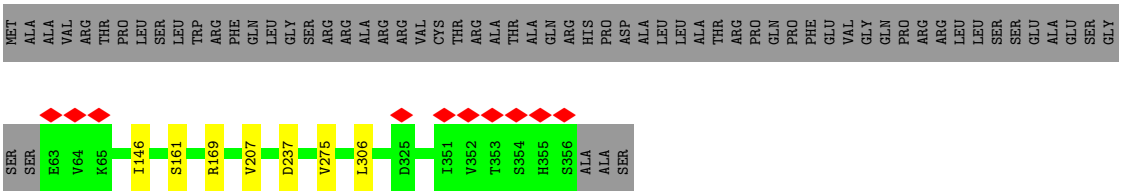
Chain Q:



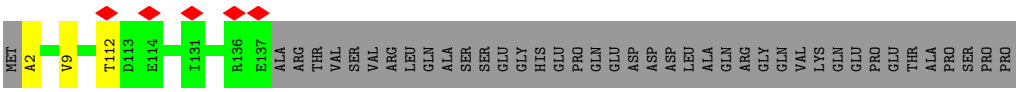

- Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:



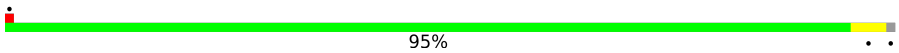

- Molecule 19: 28S ribosomal protein S23, mitochondrial

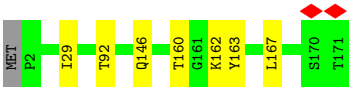
Chain S:




- Molecule 20: 28S ribosomal protein S25, mitochondrial

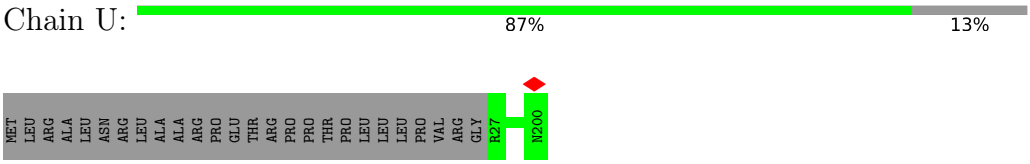
Chain T:



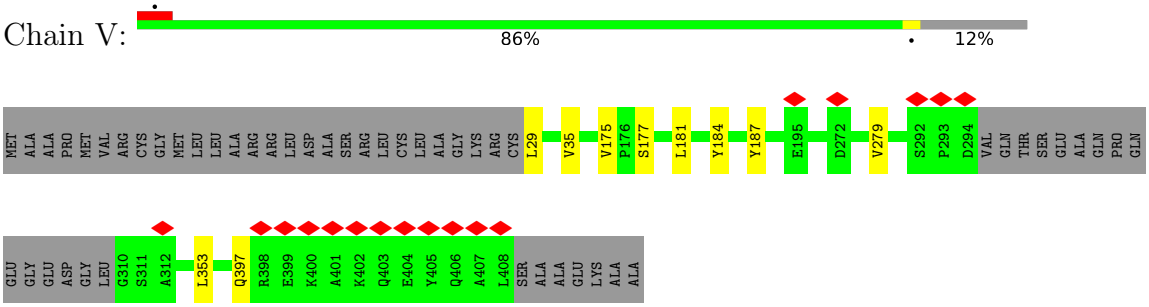

- Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U:



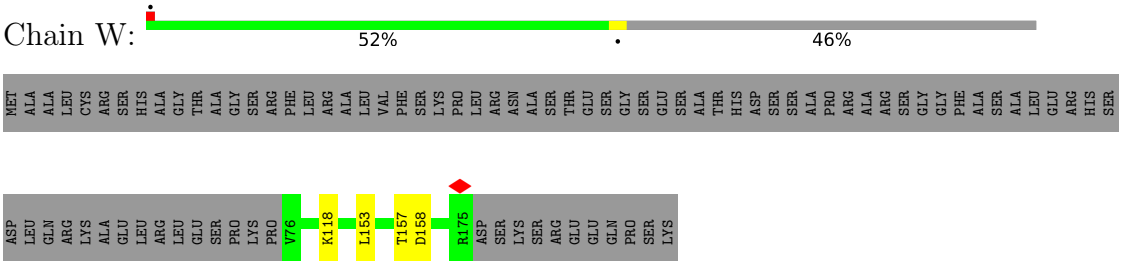

• Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V:



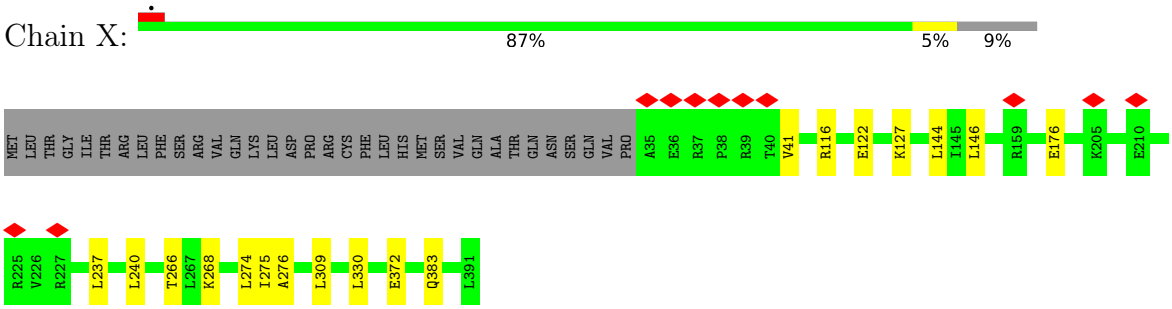

• Molecule 23: 28S ribosomal protein S28, mitochondrial

Chain W:



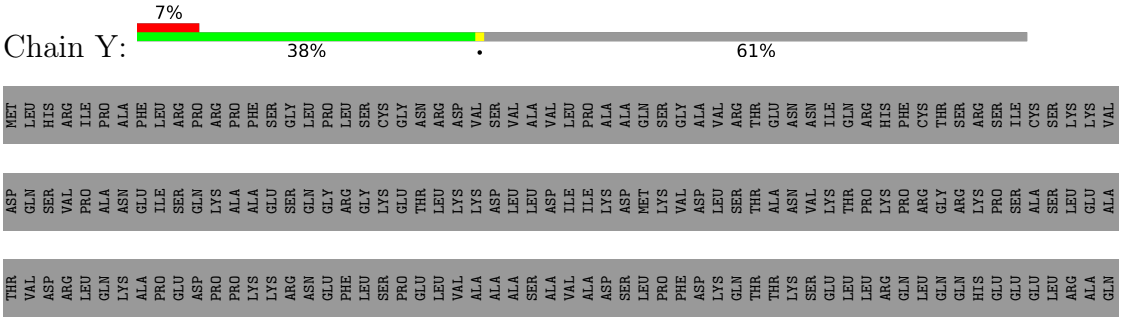

• Molecule 24: 28S ribosomal protein S29, mitochondrial

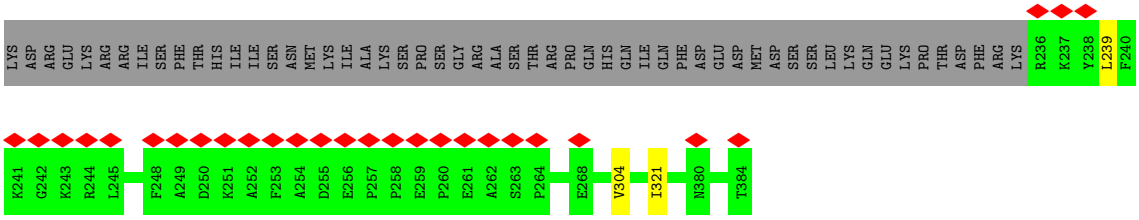
Chain X:




• Molecule 25: 28S ribosomal protein S31, mitochondrial

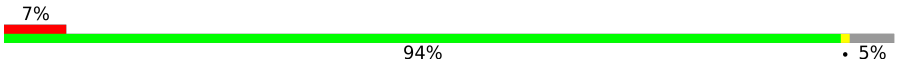
Chain Y:

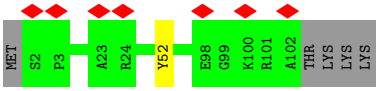





• Molecule 26: 28S ribosomal protein S33, mitochondrial

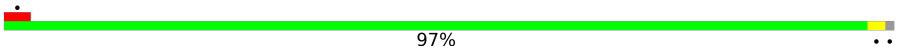
Chain Z:

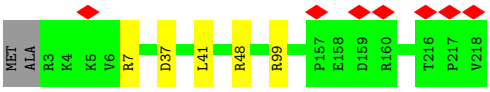



• Molecule 27: 28S ribosomal protein S34, mitochondrial

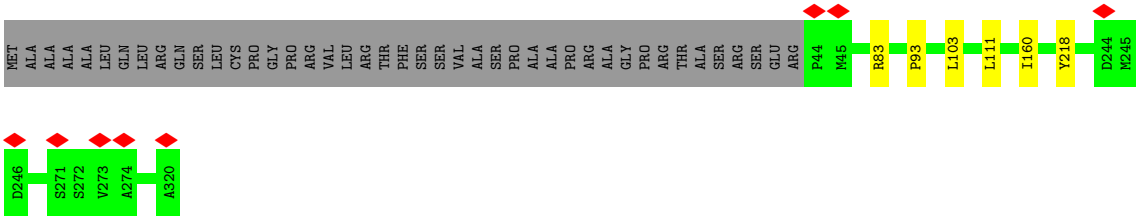
Chain 0:



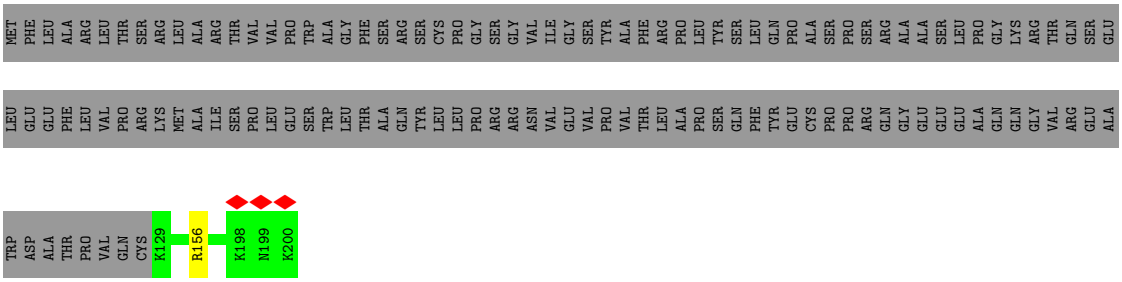

• Molecule 28: 28S ribosomal protein S35, mitochondrial

Chain 1:



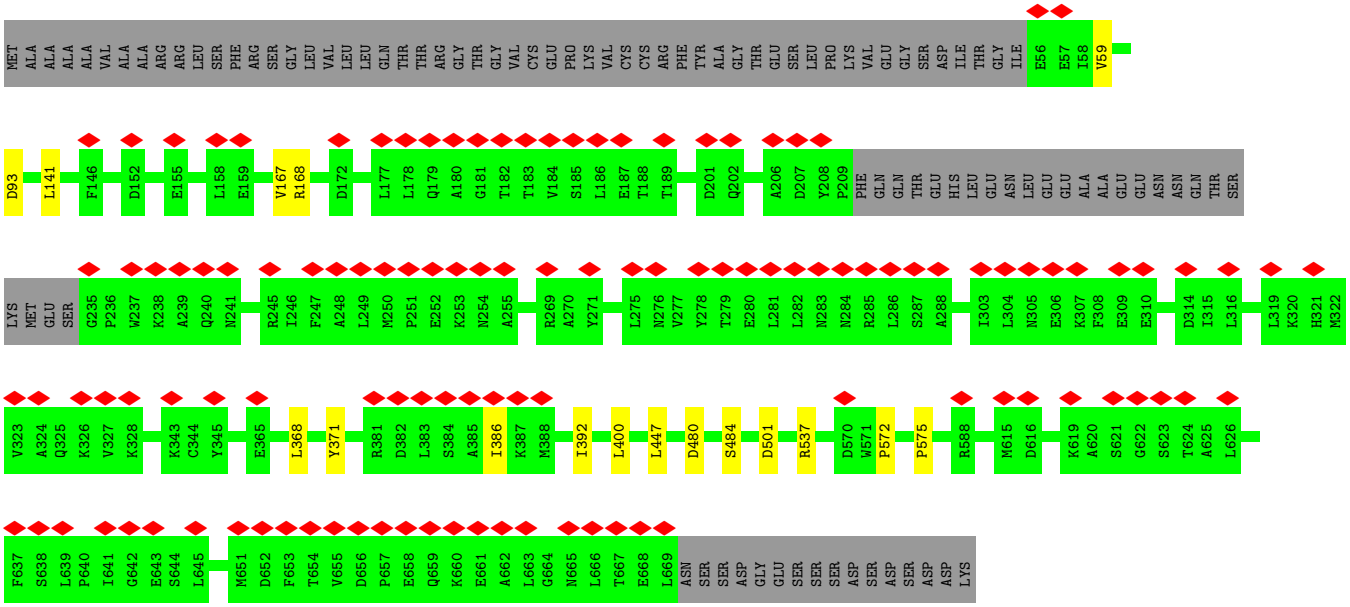

• Molecule 29: Aurora kinase A-interacting protein

Chain 3:



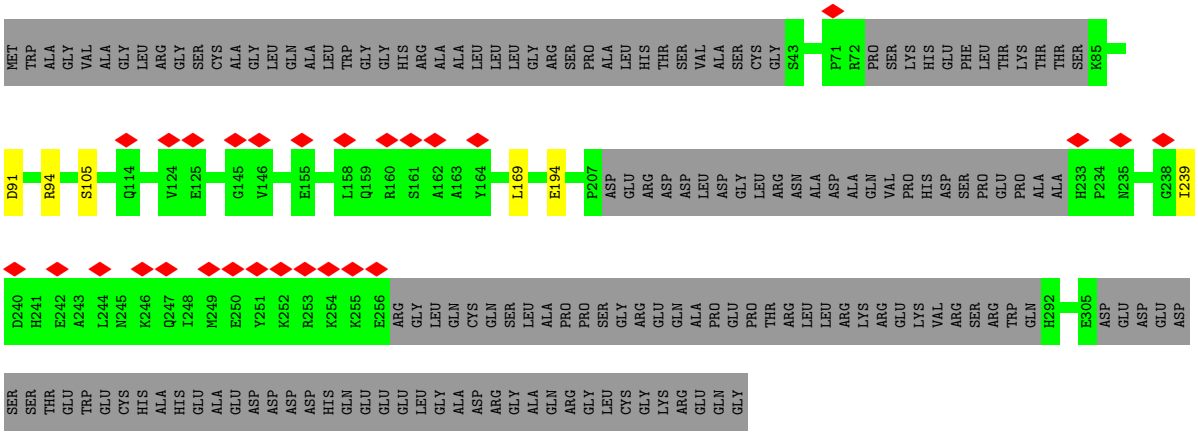

• Molecule 30: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

Chain 4:



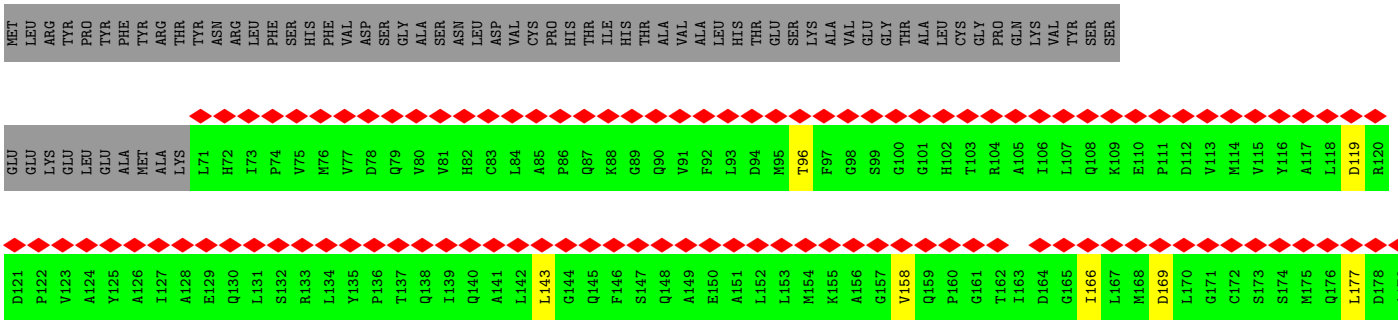

- Molecule 31: Putative ribosome-binding factor A, mitochondrial

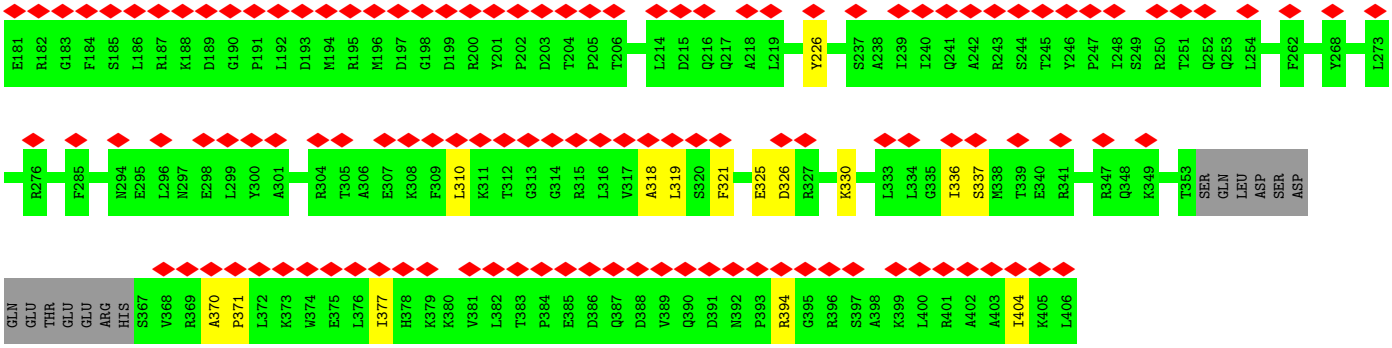
Chain a:




- Molecule 32: 12S rRNA N4-methylcytidine methyltransferase

Chain b:




E181
R182
G183
F184
S185
L186
R187
K188
D189
G190
P191
L192
D193
M194
R195
M196
D197
G198
D199
R200
Y201
P202
D203
T204
P205
T206
L214
D215
Q216
Q217
A218
L219
Y226
S237
A238
I239
I240
Q241
A242
R243
S244
T245
Y246
P247
I248
S249
R250
T251
Q252
Q253
L254
F262
Y268
L273
R276
F285
N294
E295
L296
N297
E298
L299
Y300
A301
R304
T305
A306
E307
K308
F309
L310
K311
T312
G313
G314
R315
L316
V317
A318
L319
S320
F321
E325
D326
R327
K330
L333
L334
G335
I336
S337
M338
T339
E340
R341
R347
Q348
K349
T353
SER
GLN
LEU
ASP
SER
ASP
GLN
GLU
THR
GLU
GLU
ARG
HIS
S367
V368
R369
A370
P371
L372
K373
W374
E375
L376
I377
H378
K379
K380
V381
L382
T383
P384
E385
D386
Q387
D388
V389
Q390
D391
N392
P393
R394
G395
R396
S397
A398
K399
L400
R401
A402
A403
I404
K405
L406

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 59111 | 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 ($e^-/Å^2$) | 31 | Depositor |
| Minimum defocus (nm) | 800 | Depositor |
| Maximum defocus (nm) | 3600 | Depositor |
| Magnification | 165000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 1.795 | Depositor |
| Minimum map value | -0.950 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.032 | Depositor |
| Recommended contour level | 0.1 | Depositor |
| Map size (Å) | 398.40192, 398.40192, 398.40192 | wwPDB |
| Map dimensions | 576, 576, 576 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.69167, 0.69167, 0.69167 | 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: K, 5F0, AYA, MA6, ZN, SAH, 5MC, FES, ATP, MG, B8T

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 | 0.11 | 0/22518 | 0.21 | 0/35045 |
| 2 | B | 0.13 | 0/1832 | 0.30 | 0/2479 |
| 3 | C | 0.13 | 0/1100 | 0.30 | 0/1485 |
| 4 | D | 0.13 | 0/2789 | 0.29 | 0/3739 |
| 5 | E | 0.12 | 0/966 | 0.30 | 0/1308 |
| 6 | F | 0.12 | 0/1763 | 0.29 | 0/2368 |
| 7 | G | 0.11 | 0/2734 | 0.31 | 0/3669 |
| 8 | H | 0.13 | 0/1179 | 0.28 | 0/1597 |
| 9 | I | 0.13 | 0/1018 | 0.31 | 0/1374 |
| 10 | J | 0.14 | 0/862 | 0.32 | 0/1155 |
| 11 | K | 0.15 | 0/871 | 0.34 | 0/1167 |
| 12 | L | 0.11 | 0/1485 | 0.26 | 0/1980 |
| 13 | M | 0.15 | 0/1017 | 0.32 | 0/1366 |
| 14 | N | 0.13 | 0/907 | 0.32 | 0/1228 |
| 15 | O | 0.11 | 0/1653 | 0.28 | 0/2254 |
| 16 | P | 0.12 | 0/809 | 0.30 | 0/1085 |
| 17 | Q | 0.13 | 0/735 | 0.31 | 0/980 |
| 18 | R | 0.11 | 0/2449 | 0.27 | 0/3311 |
| 19 | S | 0.12 | 0/1148 | 0.28 | 0/1541 |
| 20 | T | 0.11 | 0/1420 | 0.28 | 0/1903 |
| 21 | U | 0.12 | 0/1470 | 0.29 | 0/1976 |
| 22 | V | 0.09 | 0/3059 | 0.24 | 0/4135 |
| 23 | W | 0.12 | 0/805 | 0.30 | 0/1084 |
| 24 | X | 0.10 | 0/2952 | 0.26 | 0/3995 |
| 25 | Y | 0.10 | 0/1283 | 0.24 | 0/1730 |
| 26 | Z | 0.13 | 0/851 | 0.28 | 0/1133 |
| 27 | 0 | 0.13 | 0/1856 | 0.33 | 0/2511 |
| 28 | 1 | 0.11 | 0/2260 | 0.26 | 0/3063 |
| 29 | 3 | 0.13 | 0/654 | 0.32 | 0/860 |
| 30 | 4 | 0.09 | 0/4868 | 0.25 | 0/6597 |
| 31 | a | 0.10 | 0/1573 | 0.27 | 0/2115 |
| 32 | b | 0.10 | 0/2561 | 0.28 | 0/3457 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| All | All | 0.11 | 0/73447 | 0.26 | 0/103690 |

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 |
|---|---|---|---|
| 9 | I | 0 | 1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 9 | I | 181 | 5F0 | 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 | A | 20207 | 10223 | 10209 | 43 | 0 |
| 2 | B | 1791 | 1799 | 1797 | 8 | 0 |
| 3 | C | 1072 | 1091 | 1087 | 7 | 0 |
| 4 | D | 2733 | 2794 | 2790 | 13 | 0 |
| 5 | E | 948 | 968 | 968 | 5 | 0 |
| 6 | F | 1722 | 1750 | 1748 | 8 | 0 |
| 7 | G | 2674 | 2630 | 2626 | 11 | 0 |
| 8 | H | 1153 | 1193 | 1190 | 10 | 0 |
| 9 | I | 1009 | 1038 | 1029 | 3 | 0 |
| 10 | J | 846 | 903 | 901 | 2 | 0 |
| 11 | K | 855 | 888 | 887 | 8 | 0 |
| 12 | L | 1465 | 1576 | 1574 | 3 | 0 |
| 13 | M | 995 | 1009 | 1006 | 2 | 0 |
| 14 | N | 888 | 951 | 947 | 4 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 15 | O | 1598 | 1548 | 1547 | 0 | 0 |
| 16 | P | 792 | 818 | 817 | 5 | 0 |
| 17 | Q | 732 | 750 | 750 | 4 | 0 |
| 18 | R | 2400 | 2416 | 2415 | 6 | 0 |
| 19 | S | 1124 | 1133 | 1132 | 3 | 0 |
| 20 | T | 1388 | 1413 | 1413 | 5 | 0 |
| 21 | U | 1449 | 1459 | 1456 | 0 | 0 |
| 22 | V | 2998 | 2972 | 2967 | 8 | 0 |
| 23 | W | 793 | 813 | 811 | 3 | 0 |
| 24 | X | 2881 | 2881 | 2879 | 12 | 0 |
| 25 | Y | 1246 | 1193 | 1191 | 3 | 0 |
| 26 | Z | 834 | 848 | 847 | 1 | 0 |
| 27 | 0 | 1811 | 1838 | 1834 | 3 | 0 |
| 28 | 1 | 2212 | 2228 | 2226 | 5 | 0 |
| 29 | 3 | 643 | 728 | 726 | 1 | 0 |
| 30 | 4 | 4758 | 4800 | 4793 | 11 | 0 |
| 31 | a | 1546 | 1583 | 1579 | 4 | 0 |
| 32 | b | 2519 | 2595 | 2593 | 13 | 0 |
| 33 | 3 | 1 | 0 | 0 | 0 | 0 |
| 33 | A | 46 | 0 | 0 | 0 | 0 |
| 33 | B | 1 | 0 | 0 | 0 | 0 |
| 33 | X | 1 | 0 | 0 | 0 | 0 |
| 34 | A | 13 | 0 | 0 | 0 | 0 |
| 35 | O | 1 | 0 | 0 | 0 | 0 |
| 36 | P | 4 | 0 | 0 | 0 | 0 |
| 36 | T | 4 | 0 | 0 | 0 | 0 |
| 37 | X | 31 | 12 | 12 | 0 | 0 |
| 38 | b | 26 | 20 | 19 | 0 | 0 |
| 39 | 0 | 7 | 0 | 0 | 0 | 0 |
| 39 | 1 | 5 | 0 | 0 | 0 | 0 |
| 39 | 3 | 7 | 0 | 0 | 0 | 0 |
| 39 | A | 549 | 0 | 0 | 8 | 0 |
| 39 | B | 23 | 0 | 0 | 0 | 0 |
| 39 | C | 19 | 0 | 0 | 1 | 0 |
| 39 | D | 34 | 0 | 0 | 1 | 0 |
| 39 | E | 2 | 0 | 0 | 0 | 0 |
| 39 | F | 7 | 0 | 0 | 0 | 0 |
| 39 | G | 10 | 0 | 0 | 0 | 0 |
| 39 | H | 19 | 0 | 0 | 0 | 0 |
| 39 | I | 5 | 0 | 0 | 0 | 0 |
| 39 | J | 14 | 0 | 0 | 0 | 0 |
| 39 | K | 25 | 0 | 0 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 39 | L | 6 | 0 | 0 | 0 | 0 |
| 39 | M | 16 | 0 | 0 | 0 | 0 |
| 39 | N | 8 | 0 | 0 | 0 | 0 |
| 39 | O | 25 | 0 | 0 | 0 | 0 |
| 39 | P | 3 | 0 | 0 | 0 | 0 |
| 39 | Q | 8 | 0 | 0 | 0 | 0 |
| 39 | R | 13 | 0 | 0 | 0 | 0 |
| 39 | S | 4 | 0 | 0 | 0 | 0 |
| 39 | T | 19 | 0 | 0 | 0 | 0 |
| 39 | U | 3 | 0 | 0 | 0 | 0 |
| 39 | W | 2 | 0 | 0 | 0 | 0 |
| 39 | X | 5 | 0 | 0 | 0 | 0 |
| 39 | Y | 7 | 0 | 0 | 0 | 0 |
| 39 | Z | 18 | 0 | 0 | 0 | 0 |
| 39 | a | 5 | 0 | 0 | 0 | 0 |
| All | All | 71078 | 60861 | 60766 | 174 | 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 1.

All (174) 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:A:465:A:OP1 | 2:B:97:ARG:NH1 | 2.23 | 0.72 |
| 1:A:705:G:N7 | 39:A:1112:HOH:O | 2.27 | 0.67 |
| 4:D:196:SER:O | 39:D:501:HOH:O | 2.13 | 0.65 |
| 1:A:942:G:O6 | 39:A:1102:HOH:O | 2.12 | 0.64 |
| 13:M:55:ASP:OD2 | 20:T:146:GLN:NE2 | 2.31 | 0.64 |
| 32:b:158:VAL:HG12 | 32:b:158:VAL:O | 1.99 | 0.63 |
| 4:D:287:TYR:OH | 4:D:374:GLU:OE2 | 2.17 | 0.63 |
| 20:T:92:THR:HG22 | 20:T:92:THR:O | 1.99 | 0.62 |
| 5:E:94:VAL:CG1 | 16:P:118:MET:HE1 | 2.29 | 0.62 |
| 14:N:3:ILE:HG22 | 14:N:3:ILE:O | 1.99 | 0.61 |
| 6:F:84:SER:OG | 24:X:372:GLU:OE2 | 2.15 | 0.61 |
| 1:A:647:A:OP1 | 2:B:198:ASN:ND2 | 2.34 | 0.60 |
| 1:A:817:A:O2' | 6:F:242:TRP:OXT | 2.14 | 0.60 |
| 1:A:123:A:OP2 | 14:N:73:ARG:NH2 | 2.32 | 0.59 |
| 5:E:94:VAL:HG11 | 16:P:118:MET:HE1 | 1.84 | 0.59 |
| 11:K:40:ARG:NH1 | 39:K:202:HOH:O | 2.35 | 0.59 |
| 22:V:279:VAL:HG23 | 22:V:353:LEU:HD11 | 1.85 | 0.59 |
| 32:b:321:PHE:N | 32:b:325:GLU:OE1 | 2.32 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:783:U:OP1 | 7:G:382:ARG:NH1 | 2.33 | 0.58 |
| 7:G:204:VAL:HG12 | 7:G:204:VAL:O | 2.03 | 0.57 |
| 11:K:59:LYS:NZ | 39:K:203:HOH:O | 2.36 | 0.57 |
| 4:D:414:LYS:HG3 | 4:D:419:LEU:HD12 | 1.85 | 0.57 |
| 22:V:29:LEU:HD12 | 22:V:181:LEU:HD23 | 1.86 | 0.57 |
| 5:E:79:LEU:HG | 5:E:93:ILE:HD12 | 1.87 | 0.57 |
| 11:K:80:ARG:NH1 | 39:K:204:HOH:O | 2.38 | 0.57 |
| 6:F:159:VAL:HG23 | 6:F:172:VAL:HG21 | 1.85 | 0.56 |
| 1:A:35:G:OP2 | 39:A:1105:HOH:O | 2.18 | 0.56 |
| 24:X:268:LYS:HG2 | 24:X:274:LEU:HD23 | 1.89 | 0.55 |
| 8:H:82:SER:O | 11:K:108:ARG:NH2 | 2.40 | 0.55 |
| 1:A:43:A:N7 | 1:A:68:U:O2' | 2.39 | 0.55 |
| 22:V:35:VAL:HG12 | 22:V:35:VAL:O | 2.07 | 0.54 |
| 28:1:83:ARG:NH1 | 28:1:93:PRO:O | 2.40 | 0.54 |
| 9:I:148:VAL:HG13 | 9:I:148:VAL:O | 2.05 | 0.54 |
| 4:D:184:LYS:HA | 4:D:187:ILE:HD12 | 1.89 | 0.54 |
| 11:K:37:ASP:OD2 | 26:Z:52:TYR:OH | 2.22 | 0.54 |
| 22:V:279:VAL:CG2 | 22:V:353:LEU:HD11 | 2.37 | 0.54 |
| 24:X:176:GLU:N | 24:X:176:GLU:OE2 | 2.41 | 0.54 |
| 3:C:157:THR:OG1 | 30:4:93:ASP:OD2 | 2.12 | 0.53 |
| 1:A:808:A:OP2 | 7:G:371:ARG:NH2 | 2.40 | 0.53 |
| 4:D:217:TYR:HH | 19:S:2:ALA:N | 2.06 | 0.53 |
| 1:A:451:A:OP1 | 39:A:1104:HOH:O | 2.18 | 0.53 |
| 24:X:275:ILE:HG22 | 24:X:276:ALA:N | 2.24 | 0.53 |
| 3:C:72:HIS:O | 39:C:201:HOH:O | 2.19 | 0.53 |
| 3:C:119:ILE:HB | 3:C:153:LEU:HD12 | 1.90 | 0.53 |
| 5:E:117:LEU:HD12 | 23:W:153:LEU:HD11 | 1.92 | 0.52 |
| 1:A:876:A:OP2 | 22:V:397:GLN:NE2 | 2.42 | 0.52 |
| 32:b:166:ILE:HD12 | 32:b:310:LEU:HD13 | 1.92 | 0.52 |
| 8:H:81:LYS:O | 11:K:112:ARG:NH1 | 2.43 | 0.52 |
| 5:E:113:LEU:HD23 | 5:E:116:LYS:HD2 | 1.92 | 0.51 |
| 1:A:949:G:O6 | 17:Q:50:ARG:NH2 | 2.42 | 0.51 |
| 1:A:447:C:O2' | 1:A:501:C:O2' | 2.24 | 0.51 |
| 7:G:314:LEU:HD13 | 7:G:350:VAL:HG11 | 1.93 | 0.51 |
| 4:D:205:ILE:HG21 | 4:D:224:ILE:HD11 | 1.93 | 0.51 |
| 30:4:501:ASP:OD1 | 30:4:537:ARG:NH2 | 2.44 | 0.51 |
| 1:A:888:G:O2' | 1:A:889:A:O4' | 2.29 | 0.51 |
| 1:A:125:A:N7 | 12:L:226:ARG:NH2 | 2.60 | 0.50 |
| 2:B:86:VAL:HG12 | 2:B:86:VAL:O | 2.11 | 0.50 |
| 6:F:161:ILE:HD12 | 6:F:241:TRP:CH2 | 2.46 | 0.50 |
| 1:A:321:U:O2 | 16:P:117:LYS:NZ | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:833:C:OP1 | 39:A:1106:HOH:O | 2.20 | 0.49 |
| 31:a:239:ILE:HD11 | 32:b:226:TYR:CZ | 2.47 | 0.49 |
| 1:A:881:A:OP1 | 27:0:99:ARG:NH1 | 2.46 | 0.49 |
| 24:X:41:VAL:HG12 | 24:X:41:VAL:O | 2.11 | 0.49 |
| 30:4:386:ILE:HG22 | 30:4:386:ILE:O | 2.13 | 0.49 |
| 1:A:865:A:OP2 | 27:0:7:ARG:NH2 | 2.45 | 0.49 |
| 8:H:51:GLU:OE1 | 8:H:100:ARG:NH1 | 2.45 | 0.49 |
| 4:D:108:THR:HG22 | 4:D:108:THR:O | 2.12 | 0.49 |
| 18:R:161:SER:O | 18:R:169:ARG:NH2 | 2.41 | 0.49 |
| 7:G:142:GLU:OE1 | 7:G:142:GLU:N | 2.39 | 0.49 |
| 1:A:13:C:O2' | 1:A:288:A:N1 | 2.42 | 0.48 |
| 1:A:528:G:O2' | 1:A:530:U:OP2 | 2.29 | 0.48 |
| 24:X:122:GLU:O | 24:X:127:LYS:NZ | 2.46 | 0.48 |
| 1:A:579:U:O2' | 1:A:796:A:O4' | 2.30 | 0.48 |
| 6:F:159:VAL:CG2 | 6:F:172:VAL:HG21 | 2.44 | 0.48 |
| 2:B:272:SER:HB3 | 2:B:273:PRO:HD3 | 1.95 | 0.48 |
| 1:A:68:U:OP1 | 39:A:1107:HOH:O | 2.20 | 0.47 |
| 3:C:148:LYS:NZ | 30:4:141:LEU:O | 2.38 | 0.47 |
| 8:H:39:VAL:HG22 | 8:H:100:ARG:O | 2.15 | 0.47 |
| 30:4:59:VAL:O | 30:4:59:VAL:HG23 | 2.15 | 0.47 |
| 24:X:116:ARG:NH2 | 24:X:330:LEU:O | 2.48 | 0.47 |
| 1:A:700:A:N7 | 39:A:1125:HOH:O | 2.36 | 0.47 |
| 7:G:292:VAL:HG12 | 7:G:293:ASP:N | 2.30 | 0.47 |
| 1:A:504:A:OP2 | 29:3:156:ARG:NH2 | 2.48 | 0.47 |
| 1:A:746:U:O2' | 1:A:802:A:N6 | 2.48 | 0.47 |
| 3:C:87:LEU:HD13 | 3:C:87:LEU:O | 2.16 | 0.46 |
| 8:H:122:ASN:HB3 | 28:1:111:LEU:HD11 | 1.97 | 0.46 |
| 20:T:160:THR:HG22 | 20:T:162:LYS:H | 1.81 | 0.46 |
| 24:X:146:LEU:HD21 | 24:X:237:LEU:HD22 | 1.97 | 0.46 |
| 1:A:177:A:O2' | 1:A:179:A:N7 | 2.41 | 0.46 |
| 31:a:105:SER:HB3 | 31:a:169:LEU:HD22 | 1.98 | 0.46 |
| 3:C:120:CYS:HB3 | 28:1:103:LEU:HD21 | 1.98 | 0.46 |
| 14:N:88:VAL:HG13 | 14:N:88:VAL:O | 2.16 | 0.46 |
| 17:Q:42:ARG:O | 17:Q:42:ARG:HG3 | 2.15 | 0.46 |
| 25:Y:304:VAL:HG13 | 28:1:160:ILE:HD11 | 1.97 | 0.46 |
| 32:b:96:THR:HG21 | 32:b:169:ASP:O | 2.16 | 0.46 |
| 16:P:74:ASP:OD1 | 16:P:75:TYR:N | 2.49 | 0.46 |
| 1:A:406:G:H4' | 1:A:932:A:H4' | 1.98 | 0.45 |
| 31:a:91:ASP:OD1 | 31:a:94:ARG:NH2 | 2.49 | 0.45 |
| 7:G:383:ARG:NH2 | 7:G:384:LYS:O | 2.50 | 0.45 |
| 20:T:163:TYR:CE2 | 20:T:167:LEU:HD11 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:191:ILE:HA | 2:B:217:VAL:O | 2.17 | 0.45 |
| 12:L:62:LYS:HG2 | 12:L:63:GLN:H | 1.81 | 0.45 |
| 30:4:368:LEU:HD12 | 30:4:447:LEU:HD13 | 1.99 | 0.45 |
| 1:A:526:G:OP1 | 4:D:235:ALA:HB2 | 2.17 | 0.45 |
| 25:Y:321:ILE:HD13 | 28:1:218:TYR:CD1 | 2.51 | 0.45 |
| 10:J:96:PRO:O | 10:J:127:ARG:NH1 | 2.48 | 0.45 |
| 11:K:29:TYR:CZ | 11:K:38:LEU:HD22 | 2.51 | 0.45 |
| 1:A:640:A:OP2 | 4:D:262:LYS:NZ | 2.45 | 0.45 |
| 7:G:309:PHE:CD2 | 7:G:363:LEU:HD21 | 2.51 | 0.45 |
| 8:H:104:LEU:HD12 | 8:H:104:LEU:N | 2.32 | 0.45 |
| 32:b:370:ALA:HB1 | 32:b:371:PRO:HD2 | 1.99 | 0.45 |
| 19:S:9:VAL:O | 19:S:9:VAL:HG13 | 2.17 | 0.44 |
| 1:A:530:U:O2' | 1:A:922:A:N7 | 2.38 | 0.44 |
| 1:A:723:U:OP1 | 6:F:195:LYS:NZ | 2.43 | 0.44 |
| 4:D:275:ASN:O | 4:D:278:ILE:HG22 | 2.17 | 0.44 |
| 4:D:285:GLU:O | 4:D:358:GLN:NE2 | 2.50 | 0.44 |
| 22:V:175:VAL:HG12 | 22:V:177:SER:H | 1.83 | 0.44 |
| 1:A:775:G:H5" | 1:A:776:G:OP1 | 2.17 | 0.44 |
| 22:V:29:LEU:HD11 | 22:V:184:TYR:CD2 | 2.52 | 0.44 |
| 24:X:144:LEU:CD2 | 24:X:240:LEU:HD22 | 2.48 | 0.44 |
| 1:A:284:G:O2' | 1:A:290:A:N1 | 2.44 | 0.44 |
| 13:M:104:ILE:HG23 | 18:R:146:ILE:HG12 | 2.00 | 0.44 |
| 30:4:371:TYR:CE2 | 30:4:400:LEU:HD21 | 2.53 | 0.44 |
| 23:W:157:THR:HG22 | 23:W:158:ASP:N | 2.33 | 0.44 |
| 8:H:24:THR:O | 8:H:24:THR:HG23 | 2.18 | 0.43 |
| 8:H:51:GLU:OE2 | 8:H:67:VAL:HG11 | 2.17 | 0.43 |
| 22:V:187:TYR:CE1 | 22:V:353:LEU:HD13 | 2.53 | 0.43 |
| 4:D:366:ASP:OD2 | 4:D:390:HIS:ND1 | 2.51 | 0.43 |
| 9:I:176:THR:HG21 | 17:Q:39:ILE:HD13 | 2.01 | 0.43 |
| 2:B:217:VAL:HG22 | 2:B:231:TYR:HB2 | 2.01 | 0.43 |
| 12:L:193:PRO:HA | 12:L:194:PRO:HD3 | 1.95 | 0.43 |
| 1:A:225:U:O2' | 1:A:232:A:N1 | 2.49 | 0.43 |
| 1:A:817:A:N6 | 31:a:194:GLU:OE2 | 2.52 | 0.43 |
| 6:F:161:ILE:HG23 | 6:F:241:TRP:CH2 | 2.54 | 0.43 |
| 24:X:266:THR:HG23 | 24:X:309:LEU:HD13 | 2.01 | 0.43 |
| 32:b:326:ASP:O | 32:b:330:LYS:N | 2.39 | 0.43 |
| 24:X:275:ILE:HG22 | 24:X:276:ALA:H | 1.84 | 0.43 |
| 18:R:207:VAL:O | 18:R:207:VAL:HG12 | 2.19 | 0.42 |
| 27:0:37:ASP:O | 27:0:41:LEU:N | 2.52 | 0.42 |
| 32:b:119:ASP:O | 32:b:143:LEU:HD12 | 2.19 | 0.42 |
| 6:F:161:ILE:N | 6:F:168:TYR:O | 2.46 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 30:4:572:PRO:HB2 | 30:4:575:PRO:HD2 | 2.01 | 0.42 |
| 1:A:916:G:O2' | 1:A:937:MA6:N1 | 2.52 | 0.42 |
| 4:D:287:TYR:N | 4:D:291:THR:O | 2.44 | 0.42 |
| 10:J:78:ARG:NE | 10:J:117:ASP:OD2 | 2.51 | 0.42 |
| 32:b:318:ALA:C | 32:b:319:LEU:HD12 | 2.44 | 0.42 |
| 18:R:275:VAL:HG11 | 18:R:306:LEU:HD12 | 2.02 | 0.42 |
| 7:G:189:ILE:HG22 | 7:G:190:GLY:N | 2.35 | 0.42 |
| 32:b:336:ILE:HG22 | 32:b:337:SER:N | 2.35 | 0.42 |
| 19:S:112:THR:HG22 | 19:S:112:THR:O | 2.20 | 0.42 |
| 30:4:480:ASP:O | 30:4:484:SER:OG | 2.38 | 0.42 |
| 30:4:167:VAL:HG23 | 30:4:168:ARG:N | 2.35 | 0.41 |
| 1:A:949:G:O6 | 17:Q:50:ARG:NH1 | 2.52 | 0.41 |
| 14:N:14:VAL:HG23 | 20:T:29:ILE:HD13 | 2.01 | 0.41 |
| 3:C:136:VAL:HG22 | 3:C:153:LEU:HD23 | 2.01 | 0.41 |
| 7:G:295:LEU:HD11 | 24:X:383:GLN:HG3 | 2.03 | 0.41 |
| 25:Y:239:LEU:HD21 | 30:4:392:ILE:HG23 | 2.02 | 0.41 |
| 2:B:236:ASN:OD1 | 23:W:118:LYS:NZ | 2.54 | 0.41 |
| 32:b:377:ILE:HD11 | 32:b:404:ILE:HD11 | 2.03 | 0.41 |
| 7:G:131:ILE:HG13 | 7:G:132:PHE:N | 2.36 | 0.41 |
| 18:R:237:ASP:OD1 | 18:R:237:ASP:N | 2.53 | 0.41 |
| 1:A:239:G:N1 | 1:A:255:A:OP1 | 2.40 | 0.41 |
| 1:A:663:U:H3' | 1:A:664:C:H5' | 2.02 | 0.41 |
| 11:K:34:MET:HE3 | 11:K:95:SER:HB2 | 2.02 | 0.41 |
| 16:P:142:ARG:O | 16:P:143:GLU:C | 2.63 | 0.41 |
| 9:I:173:THR:HG22 | 9:I:174:ASP:N | 2.36 | 0.41 |
| 1:A:909:A:H2' | 1:A:910:U:O4' | 2.21 | 0.40 |
| 8:H:63:ILE:HG21 | 8:H:104:LEU:HD23 | 2.03 | 0.40 |
| 18:R:207:VAL:O | 18:R:207:VAL:CG1 | 2.69 | 0.40 |
| 32:b:177:LEU:HD23 | 32:b:394:ARG:CZ | 2.52 | 0.40 |
| 32:b:158:VAL:O | 32:b:158:VAL:CG1 | 2.68 | 0.40 |
| 8:H:29:ASP:OD1 | 8:H:30:THR:N | 2.54 | 0.40 |
| 1:A:682:G:OP2 | 39:A:1109:HOH:O | 2.22 | 0.40 |
| 2:B:219:ILE:HD13 | 2:B:233:ILE:HB | 2.02 | 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 | |
|---|---|---|---|---|---|---|---|
| 2 | B | 221/291 (76%) | 217 (98%) | 4 (2%) | 0 | 100 | 100 |
| 3 | C | 130/167 (78%) | 124 (95%) | 6 (5%) | 0 | 100 | 100 |
| 4 | D | 341/432 (79%) | 336 (98%) | 5 (2%) | 0 | 100 | 100 |
| 5 | E | 117/125 (94%) | 115 (98%) | 2 (2%) | 0 | 100 | 100 |
| 6 | F | 206/242 (85%) | 202 (98%) | 4 (2%) | 0 | 100 | 100 |
| 7 | G | 321/390 (82%) | 317 (99%) | 4 (1%) | 0 | 100 | 100 |
| 8 | H | 138/160 (86%) | 135 (98%) | 2 (1%) | 1 (1%) | 18 | 45 |
| 9 | I | 134/191 (70%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |
| 10 | J | 106/139 (76%) | 105 (99%) | 1 (1%) | 0 | 100 | 100 |
| 11 | K | 99/128 (77%) | 99 (100%) | 0 | 0 | 100 | 100 |
| 12 | L | 174/258 (67%) | 173 (99%) | 1 (1%) | 0 | 100 | 100 |
| 13 | M | 124/135 (92%) | 124 (100%) | 0 | 0 | 100 | 100 |
| 14 | N | 111/120 (92%) | 108 (97%) | 3 (3%) | 0 | 100 | 100 |
| 15 | O | 195/254 (77%) | 193 (99%) | 2 (1%) | 0 | 100 | 100 |
| 16 | P | 95/143 (66%) | 95 (100%) | 0 | 0 | 100 | 100 |
| 17 | Q | 84/86 (98%) | 83 (99%) | 1 (1%) | 0 | 100 | 100 |
| 18 | R | 292/359 (81%) | 283 (97%) | 9 (3%) | 0 | 100 | 100 |
| 19 | S | 134/177 (76%) | 132 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | T | 168/171 (98%) | 167 (99%) | 1 (1%) | 0 | 100 | 100 |
| 21 | U | 172/200 (86%) | 171 (99%) | 1 (1%) | 0 | 100 | 100 |
| 22 | V | 361/415 (87%) | 356 (99%) | 5 (1%) | 0 | 100 | 100 |
| 23 | W | 98/186 (53%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 24 | X | 355/391 (91%) | 349 (98%) | 6 (2%) | 0 | 100 | 100 |
| 25 | Y | 147/384 (38%) | 145 (99%) | 2 (1%) | 0 | 100 | 100 |
| 26 | Z | 99/106 (93%) | 98 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 27 | 0 | 214/218 (98%) | 209 (98%) | 5 (2%) | 0 | 100 | 100 |
| 28 | 1 | 275/320 (86%) | 273 (99%) | 2 (1%) | 0 | 100 | 100 |
| 29 | 3 | 70/200 (35%) | 70 (100%) | 0 | 0 | 100 | 100 |
| 30 | 4 | 585/685 (85%) | 580 (99%) | 5 (1%) | 0 | 100 | 100 |
| 31 | a | 183/350 (52%) | 180 (98%) | 3 (2%) | 0 | 100 | 100 |
| 32 | b | 319/406 (79%) | 310 (97%) | 9 (3%) | 0 | 100 | 100 |
| All | All | 6068/7829 (78%) | 5973 (98%) | 94 (2%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | H | 85 | ILE |

### 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 | |
|---|---|---|---|---|---|---|
| 2 | B | 195/247 (79%) | 195 (100%) | 0 | 100 | 100 |
| 3 | C | 113/139 (81%) | 113 (100%) | 0 | 100 | 100 |
| 4 | D | 282/354 (80%) | 282 (100%) | 0 | 100 | 100 |
| 5 | E | 104/110 (94%) | 104 (100%) | 0 | 100 | 100 |
| 6 | F | 180/204 (88%) | 180 (100%) | 0 | 100 | 100 |
| 7 | G | 282/335 (84%) | 282 (100%) | 0 | 100 | 100 |
| 8 | H | 130/150 (87%) | 130 (100%) | 0 | 100 | 100 |
| 9 | I | 102/143 (71%) | 102 (100%) | 0 | 100 | 100 |
| 10 | J | 93/117 (80%) | 93 (100%) | 0 | 100 | 100 |
| 11 | K | 90/110 (82%) | 90 (100%) | 0 | 100 | 100 |
| 12 | L | 161/224 (72%) | 161 (100%) | 0 | 100 | 100 |
| 13 | M | 103/112 (92%) | 103 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 14 | N | 97/104 (93%) | 97 (100%) | 0 | 100 | 100 |
| 15 | O | 176/225 (78%) | 176 (100%) | 0 | 100 | 100 |
| 16 | P | 89/125 (71%) | 89 (100%) | 0 | 100 | 100 |
| 17 | Q | 77/77 (100%) | 77 (100%) | 0 | 100 | 100 |
| 18 | R | 261/313 (83%) | 261 (100%) | 0 | 100 | 100 |
| 19 | S | 117/152 (77%) | 117 (100%) | 0 | 100 | 100 |
| 20 | T | 153/154 (99%) | 153 (100%) | 0 | 100 | 100 |
| 21 | U | 149/171 (87%) | 149 (100%) | 0 | 100 | 100 |
| 22 | V | 326/362 (90%) | 326 (100%) | 0 | 100 | 100 |
| 23 | W | 87/156 (56%) | 87 (100%) | 0 | 100 | 100 |
| 24 | X | 314/346 (91%) | 314 (100%) | 0 | 100 | 100 |
| 25 | Y | 133/341 (39%) | 133 (100%) | 0 | 100 | 100 |
| 26 | Z | 88/93 (95%) | 88 (100%) | 0 | 100 | 100 |
| 27 | 0 | 190/191 (100%) | 189 (100%) | 1 (0%) | 81 | 82 |
| 28 | 1 | 247/279 (88%) | 247 (100%) | 0 | 100 | 100 |
| 29 | 3 | 68/176 (39%) | 68 (100%) | 0 | 100 | 100 |
| 30 | 4 | 519/599 (87%) | 519 (100%) | 0 | 100 | 100 |
| 31 | a | 174/299 (58%) | 174 (100%) | 0 | 100 | 100 |
| 32 | b | 270/343 (79%) | 270 (100%) | 0 | 100 | 100 |
| All | All | 5370/6751 (80%) | 5369 (100%) | 1 (0%) | 100 | 100 |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 27 | 0 | 48 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 131 | HIS |
| 2 | B | 164 | HIS |
| 3 | C | 81 | HIS |
| 3 | C | 116 | GLN |
| 4 | D | 198 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 279 | HIS |
| 6 | F | 113 | GLN |
| 6 | F | 224 | HIS |
| 7 | G | 87 | HIS |
| 7 | G | 139 | GLN |
| 7 | G | 288 | HIS |
| 7 | G | 306 | GLN |
| 8 | H | 84 | HIS |
| 8 | H | 89 | HIS |
| 9 | I | 84 | HIS |
| 10 | J | 105 | HIS |
| 10 | J | 134 | HIS |
| 12 | L | 119 | ASN |
| 12 | L | 196 | HIS |
| 12 | L | 198 | GLN |
| 12 | L | 219 | GLN |
| 13 | M | 61 | HIS |
| 14 | N | 57 | GLN |
| 16 | P | 96 | HIS |
| 17 | Q | 53 | GLN |
| 18 | R | 247 | GLN |
| 18 | R | 304 | HIS |
| 19 | S | 91 | ASN |
| 22 | V | 39 | GLN |
| 22 | V | 145 | ASN |
| 23 | W | 120 | HIS |
| 24 | X | 136 | HIS |
| 24 | X | 228 | ASN |
| 24 | X | 319 | HIS |
| 25 | Y | 370 | ASN |
| 25 | Y | 379 | ASN |
| 26 | Z | 82 | GLN |
| 27 | 0 | 45 | HIS |
| 27 | 0 | 111 | HIS |
| 27 | 0 | 207 | GLN |
| 28 | 1 | 143 | HIS |
| 28 | 1 | 182 | HIS |
| 29 | 3 | 141 | HIS |
| 30 | 4 | 372 | HIS |
| 31 | a | 114 | GLN |
| 31 | a | 172 | GLN |
| 31 | a | 185 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 32 | b | 212 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A | 949/956 (99%) | 124 (13%) | 0 |

All (124) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3 | A |
| 1 | A | 7 | U |
| 1 | A | 32 | G |
| 1 | A | 40 | A |
| 1 | A | 41 | U |
| 1 | A | 48 | U |
| 1 | A | 56 | U |
| 1 | A | 83 | A |
| 1 | A | 85 | A |
| 1 | A | 86 | U |
| 1 | A | 92 | U |
| 1 | A | 93 | A |
| 1 | A | 115 | A |
| 1 | A | 120 | A |
| 1 | A | 124 | A |
| 1 | A | 125 | A |
| 1 | A | 126 | A |
| 1 | A | 143 | G |
| 1 | A | 148 | G |
| 1 | A | 167 | C |
| 1 | A | 182 | U |
| 1 | A | 187 | C |
| 1 | A | 203 | G |
| 1 | A | 212 | A |
| 1 | A | 221 | A |
| 1 | A | 234 | U |
| 1 | A | 253 | U |
| 1 | A | 269 | A |
| 1 | A | 283 | G |
| 1 | A | 288 | A |
| 1 | A | 289 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 291 | A |
| 1 | A | 293 | G |
| 1 | A | 311 | U |
| 1 | A | 314 | A |
| 1 | A | 348 | A |
| 1 | A | 368 | A |
| 1 | A | 389 | A |
| 1 | A | 397 | U |
| 1 | A | 418 | A |
| 1 | A | 430 | U |
| 1 | A | 431 | A |
| 1 | A | 452 | A |
| 1 | A | 454 | C |
| 1 | A | 455 | C |
| 1 | A | 465 | A |
| 1 | A | 466 | A |
| 1 | A | 470 | U |
| 1 | A | 471 | A |
| 1 | A | 488 | G |
| 1 | A | 501 | C |
| 1 | A | 502 | A |
| 1 | A | 504 | A |
| 1 | A | 517 | A |
| 1 | A | 531 | A |
| 1 | A | 535 | U |
| 1 | A | 539 | U |
| 1 | A | 540 | C |
| 1 | A | 570 | A |
| 1 | A | 572 | A |
| 1 | A | 573 | C |
| 1 | A | 575 | C |
| 1 | A | 603 | U |
| 1 | A | 612 | A |
| 1 | A | 615 | C |
| 1 | A | 624 | U |
| 1 | A | 625 | C |
| 1 | A | 638 | A |
| 1 | A | 639 | A |
| 1 | A | 643 | U |
| 1 | A | 644 | A |
| 1 | A | 646 | U |
| 1 | A | 648 | A |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 654 | G |
| 1 | A | 664 | C |
| 1 | A | 667 | A |
| 1 | A | 680 | A |
| 1 | A | 681 | G |
| 1 | A | 697 | A |
| 1 | A | 709 | G |
| 1 | A | 711 | A |
| 1 | A | 731 | A |
| 1 | A | 741 | U |
| 1 | A | 742 | A |
| 1 | A | 745 | A |
| 1 | A | 746 | U |
| 1 | A | 757 | A |
| 1 | A | 760 | C |
| 1 | A | 767 | A |
| 1 | A | 769 | U |
| 1 | A | 770 | A |
| 1 | A | 774 | A |
| 1 | A | 776 | G |
| 1 | A | 784 | A |
| 1 | A | 832 | A |
| 1 | A | 835 | C |
| 1 | A | 843 | G |
| 1 | A | 857 | A |
| 1 | A | 861 | A |
| 1 | A | 862 | A |
| 1 | A | 864 | U |
| 1 | A | 866 | A |
| 1 | A | 868 | C |
| 1 | A | 873 | C |
| 1 | A | 879 | U |
| 1 | A | 880 | A |
| 1 | A | 886 | U |
| 1 | A | 889 | A |
| 1 | A | 890 | C |
| 1 | A | 891 | A |
| 1 | A | 893 | C |
| 1 | A | 895 | G |
| 1 | A | 911 | A |
| 1 | A | 912 | A |
| 1 | A | 913 | G |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 918 | A |
| 1 | A | 922 | A |
| 1 | A | 925 | U |
| 1 | A | 936 | G |
| 1 | A | 938 | MA6 |
| 1 | A | 948 | G |
| 1 | A | 949 | G |
| 1 | A | 952 | U |
| 1 | A | 953 | A |

There are no RNA pucker outliers to report.

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

6 non-standard protein/DNA/RNA residues 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 | $\#\|Z\| > 2$ |
| 1 | 5MC | A | 842 | 1 | 18,22,23 | 0.32 | 0 | 26,32,35 | 0.40 | 0 |
| 9 | 5F0 | I | 181 | 9 | 8,8,9 | 0.55 | 0 | 7,9,11 | 1.05 | 1 (14%) |
| 1 | MA6 | A | 937 | 1 | 23,26,27 | 0.30 | 0 | 34,38,41 | 0.58 | 1 (2%) |
| 17 | AYA | Q | 2 | 17 | 6,7,8 | 0.77 | 0 | 5,8,10 | 0.57 | 0 |
| 1 | MA6 | A | 938 | 1 | 23,26,27 | 0.30 | 0 | 34,38,41 | 0.57 | 1 (2%) |
| 1 | B8T | A | 840 | 1 | 19,22,23 | 0.30 | 0 | 26,31,34 | 0.32 | 0 |

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 |
|---|---|---|---|---|---|---|---|
| 1 | 5MC | A | 842 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 9 | 5F0 | I | 181 | 9 | - | 0/9/9/10 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | MA6 | A | 937 | 1 | - | 0/11/29/30 | 0/3/3/3 |
| 17 | AYA | Q | 2 | 17 | - | 0/4/6/8 | - |
| 1 | MA6 | A | 938 | 1 | - | 1/11/29/30 | 0/3/3/3 |
| 1 | B8T | A | 840 | 1 | - | 0/7/27/28 | 0/2/2/2 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | I | 181 | 5F0 | O-C-CB | -2.44 | 118.31 | 125.43 |
| 1 | A | 937 | MA6 | C2-N1-C6 | 2.37 | 117.34 | 111.75 |
| 1 | A | 938 | MA6 | C2-N1-C6 | 2.36 | 117.34 | 111.75 |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | A | 938 | MA6 | C4'-C5'-O5'-P |
| 1 | A | 842 | 5MC | O4'-C4'-C5'-O5' |
| 1 | A | 842 | 5MC | C3'-C4'-C5'-O5' |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | A | 937 | MA6 | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 63 are monoatomic - leaving 4 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 | $\#\|Z\| > 2$ |
| 36 | FES | P | 201 | 16,5 | 0,4,4 | - | - | - | | |
| 38 | SAH | b | 501 | - | 27,28,28 | 0.40 | 0 | 38,40,40 | 0.44 | 0 |
| 37 | ATP | X | 401 | 33 | 29,33,33 | 0.49 | 0 | 44,52,52 | 0.51 | 0 |
| 36 | FES | T | 201 | 13,20 | 0,4,4 | - | - | - | | |

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 |
|---|---|---|---|---|---|---|---|
| 36 | FES | P | 201 | 16,5 | - | - | 0/1/1/1 |
| 38 | SAH | b | 501 | - | - | 3/15/31/31 | 0/3/3/3 |
| 37 | ATP | X | 401 | 33 | - | 0/22/38/38 | 0/3/3/3 |
| 36 | FES | T | 201 | 13,20 | - | - | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 38 | b | 501 | SAH | C4'-C5'-SD-CG |
| 38 | b | 501 | SAH | C2'-C1'-N9-C8 |
| 38 | b | 501 | SAH | CA-CB-CG-SD |

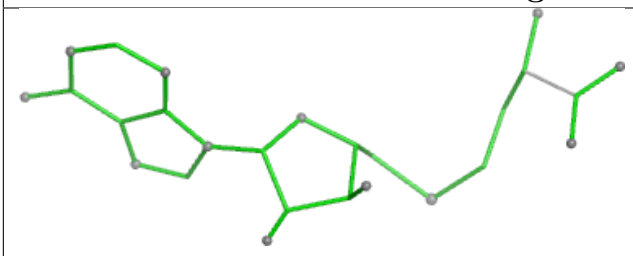
There are no ring outliers.

No monomer is involved in short contacts.

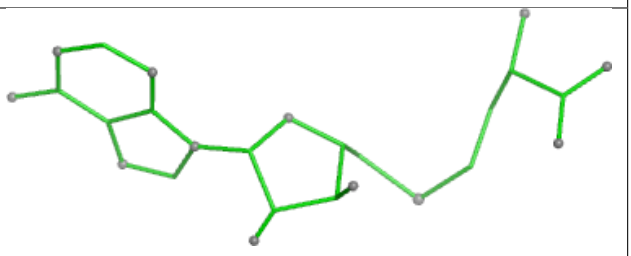
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

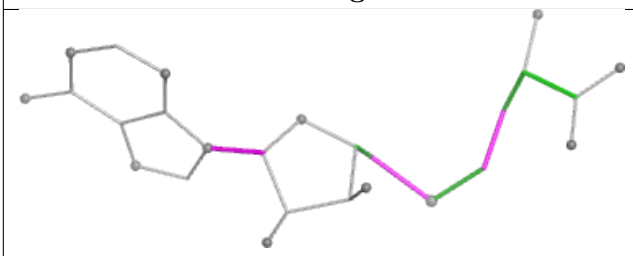
**Ligand SAH b 501**



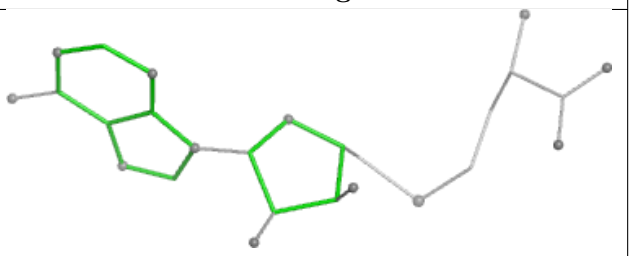
**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

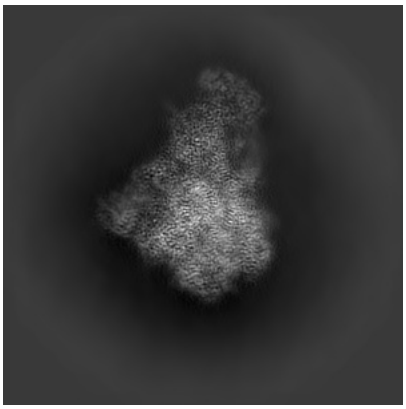
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13553. These allow visual inspection of the internal detail of the map and identification of artifacts.

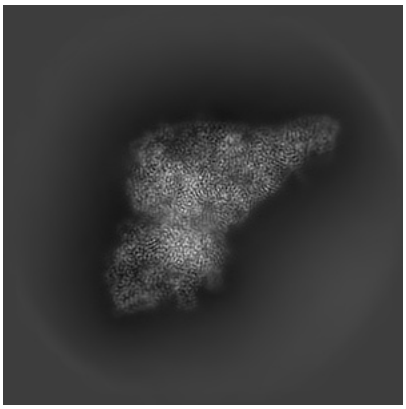
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

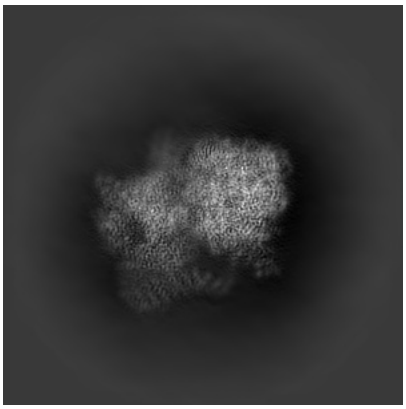
### 6.1.1 Primary map



X

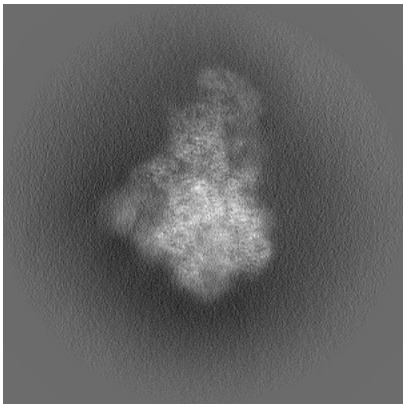


Y

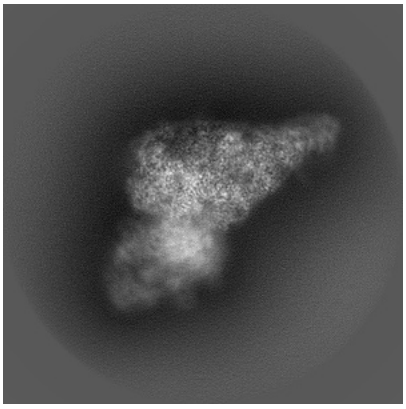


Z

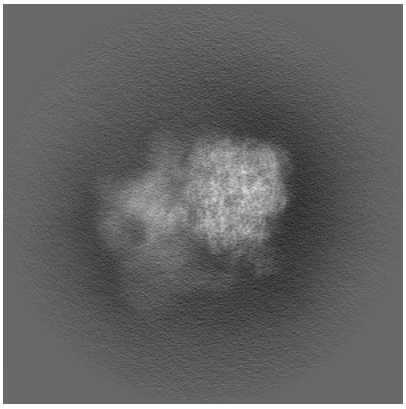
### 6.1.2 Raw map



X



Y



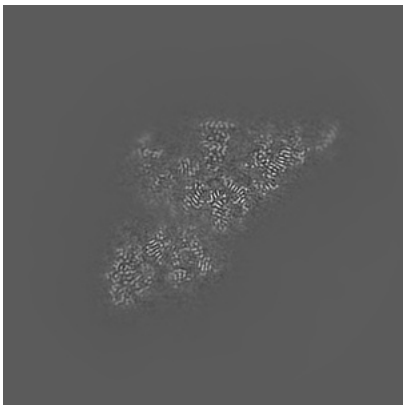
Z

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

## 6.2 Central slices (i)

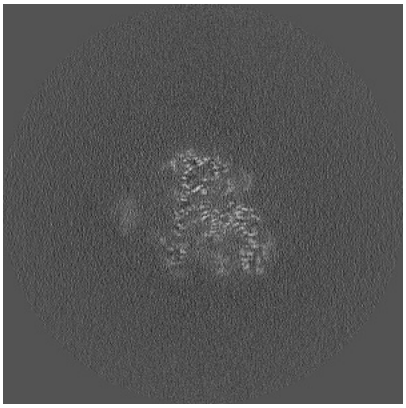
### 6.2.1 Primary map

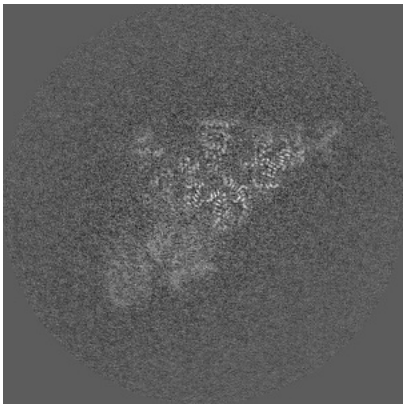
X Index: 288

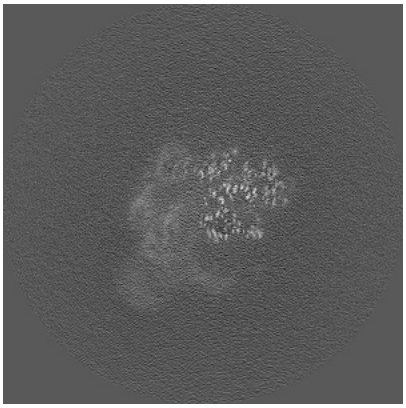

Y Index: 288

Z Index: 288

### 6.2.2 Raw map


X Index: 240

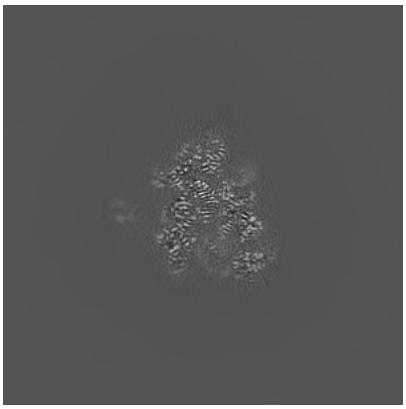

Y Index: 240

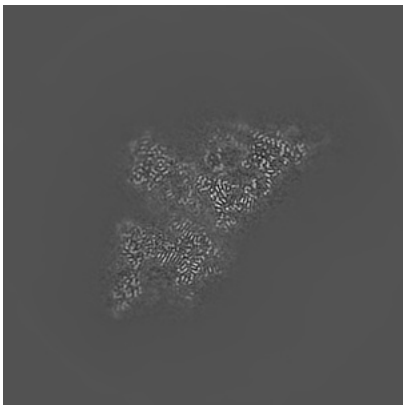

Z Index: 240

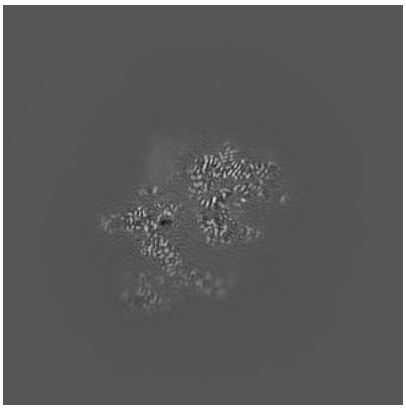
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

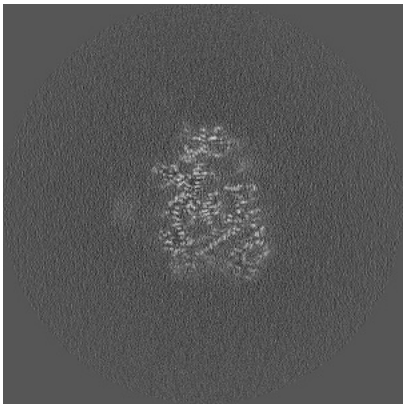
### 6.3.1 Primary map

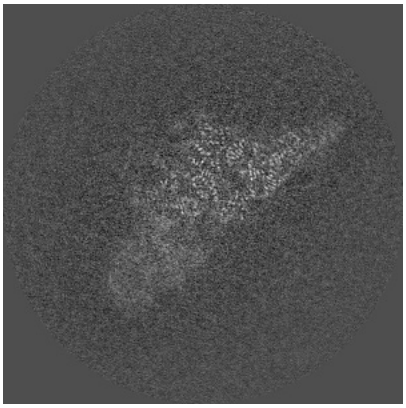

X Index: 301

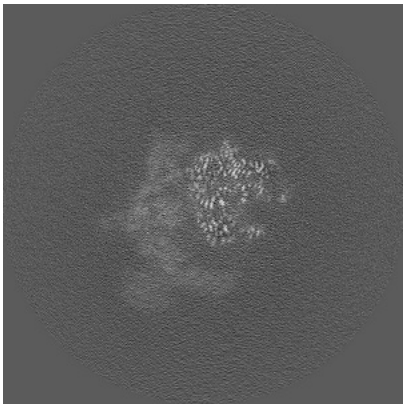

Y Index: 277


Z Index: 276

### 6.3.2 Raw map


X Index: 262

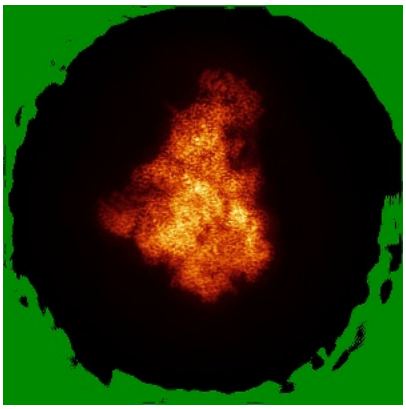

Y Index: 256

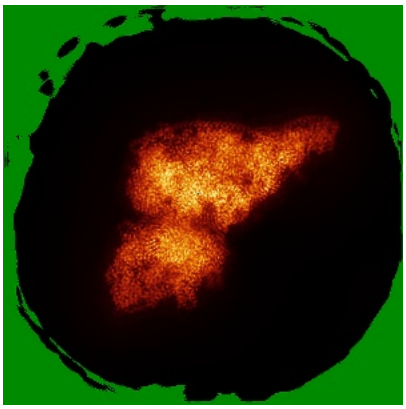

Z Index: 231

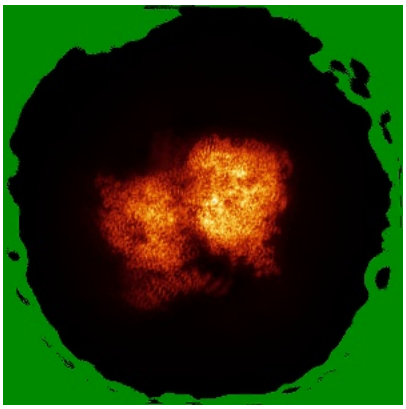
The images above show the largest variance slices of the map in three orthogonal directions.

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

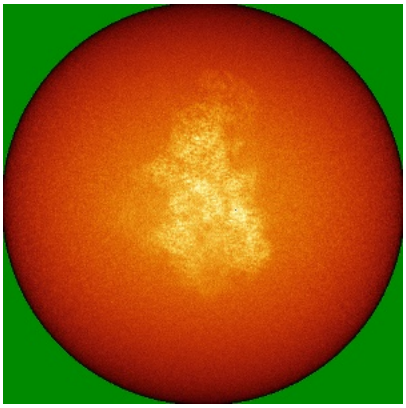
### 6.4.1 Primary map

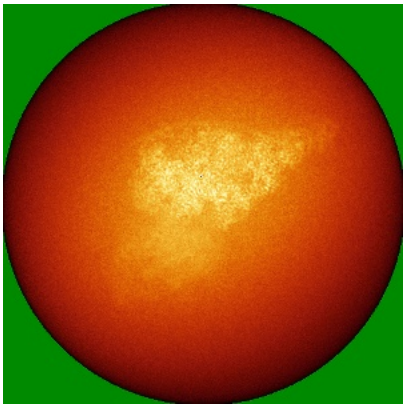

X

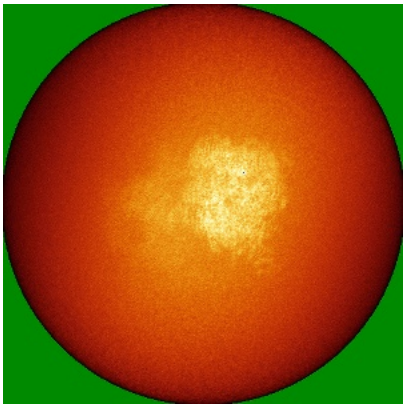

Y


Z

### 6.4.2 Raw 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.

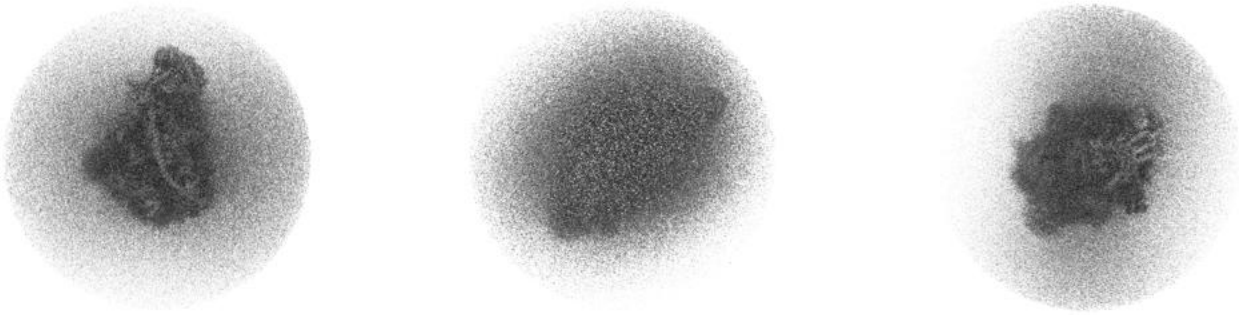
## 6.5 Orthogonal surface views (i)

### 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.

### 6.5.2 Raw map



X Y Z

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

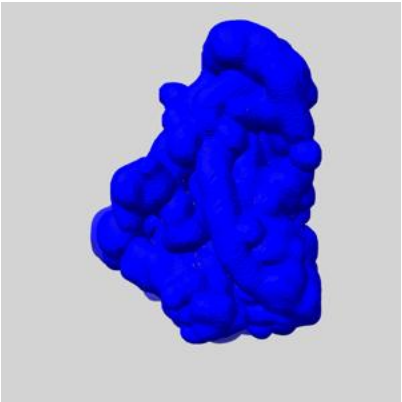
## 6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

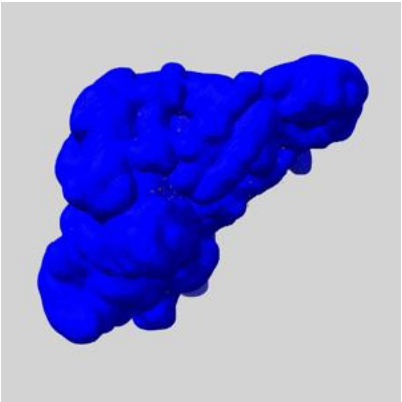
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

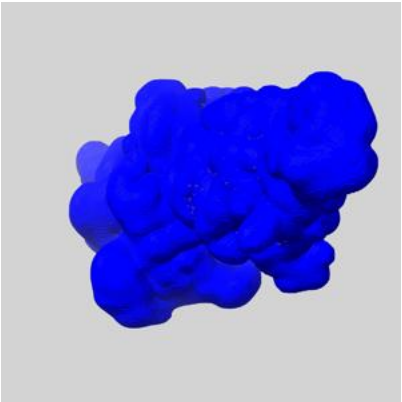
### 6.6.1 emd_13553_msk_1.map (i)



X



Y

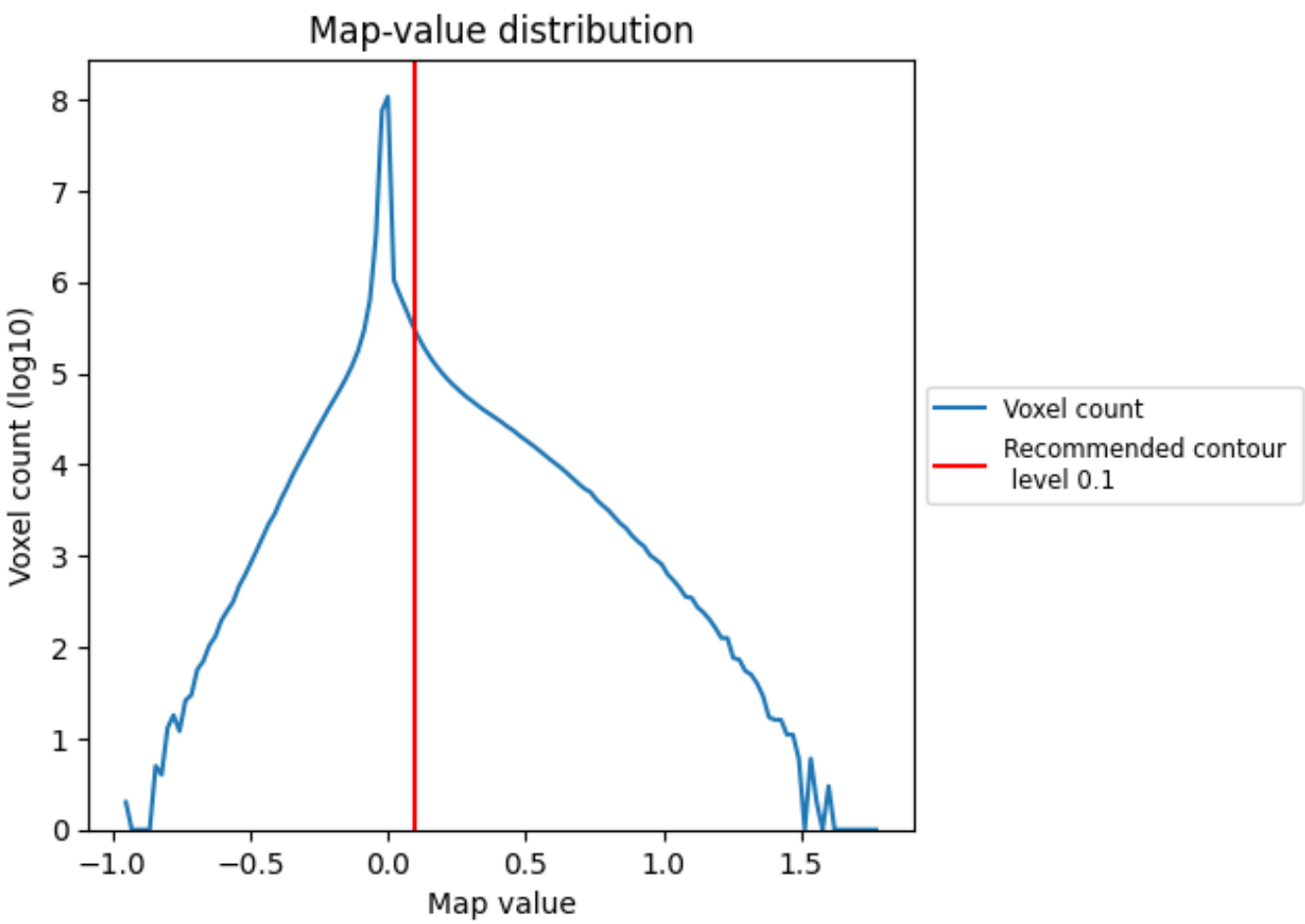


Z

# 7 Map analysis (i)

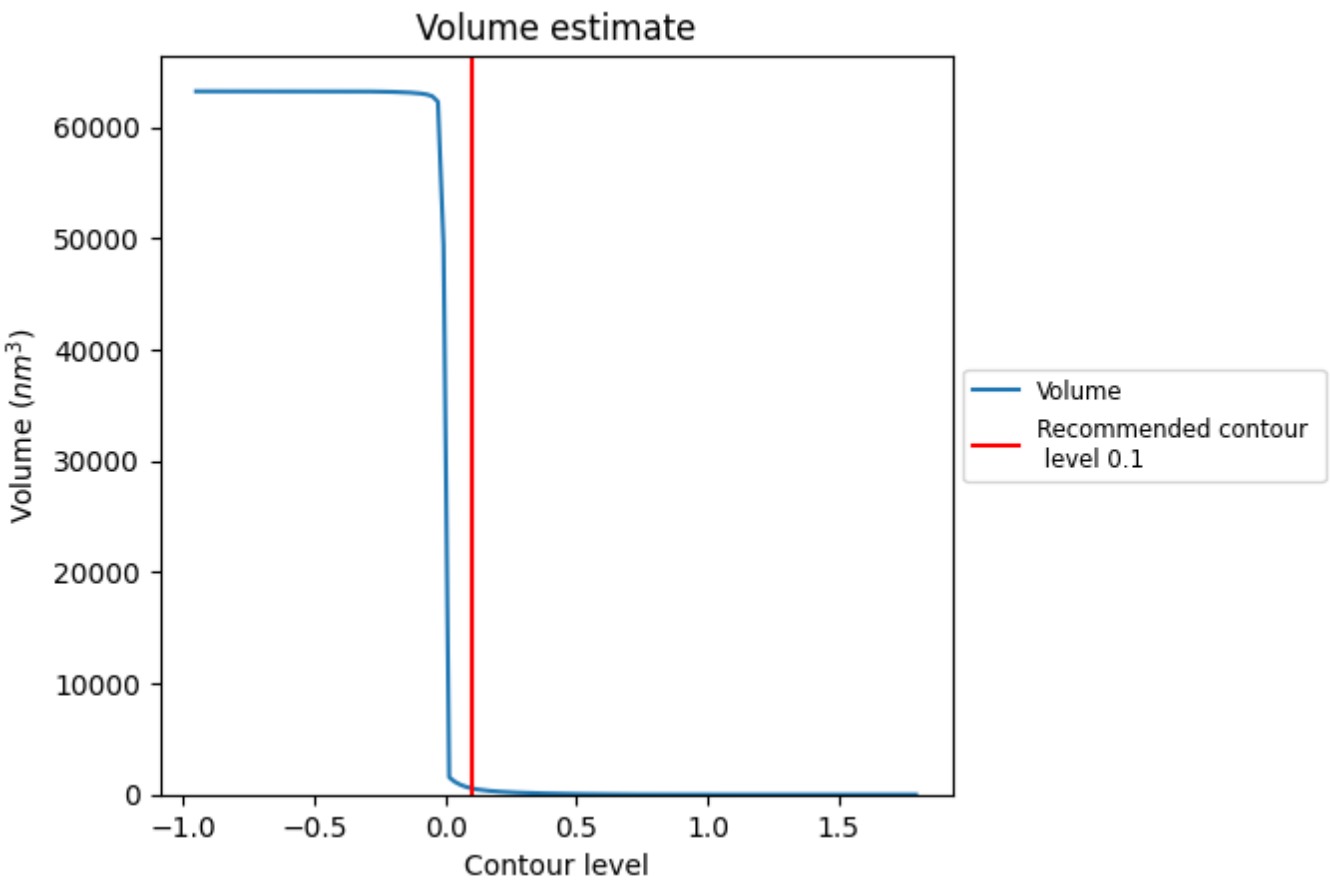
This section contains the results of statistical analysis of the map.

## 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.

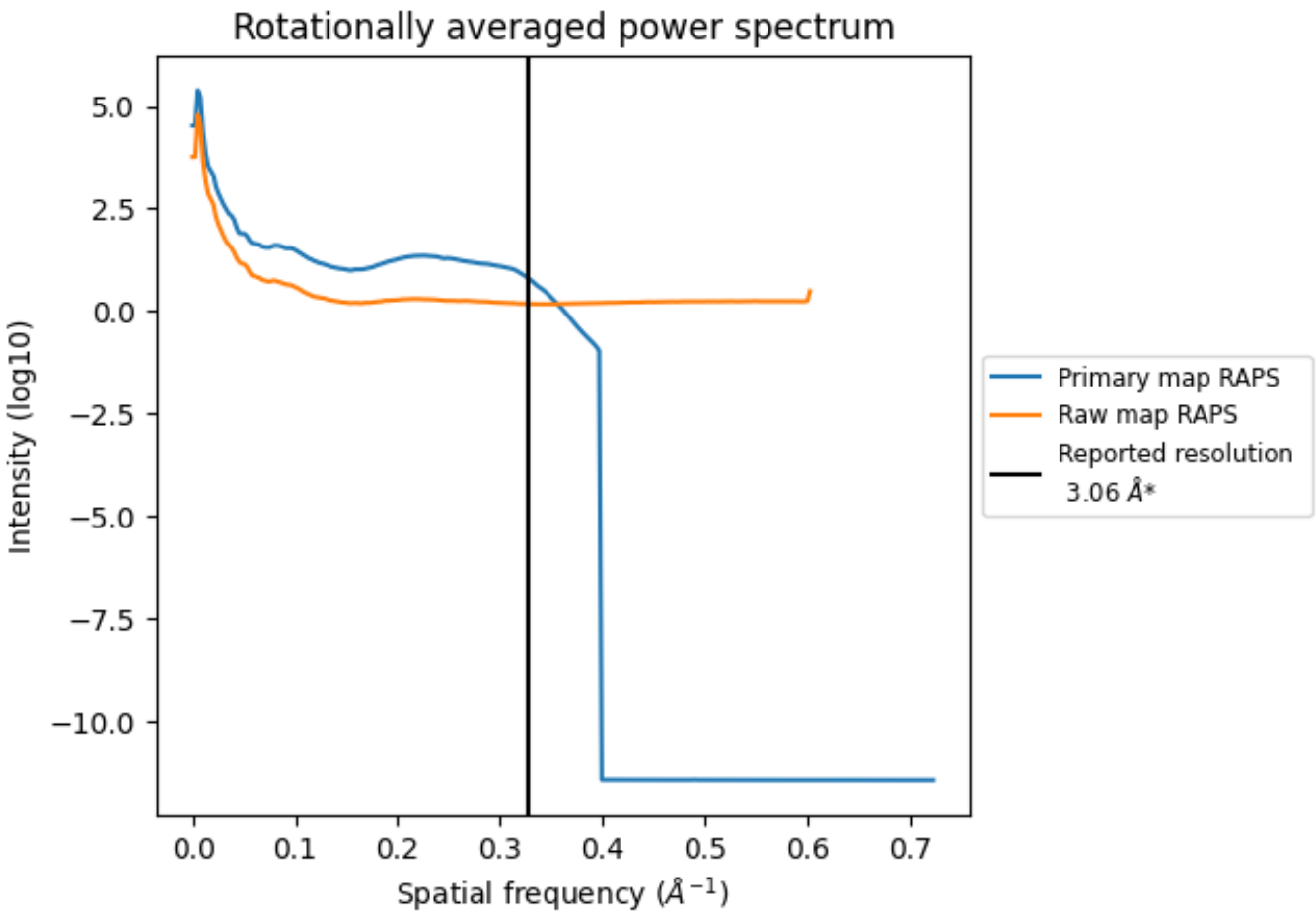
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 564 $nm^3$; this corresponds to an approximate mass of 509 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)

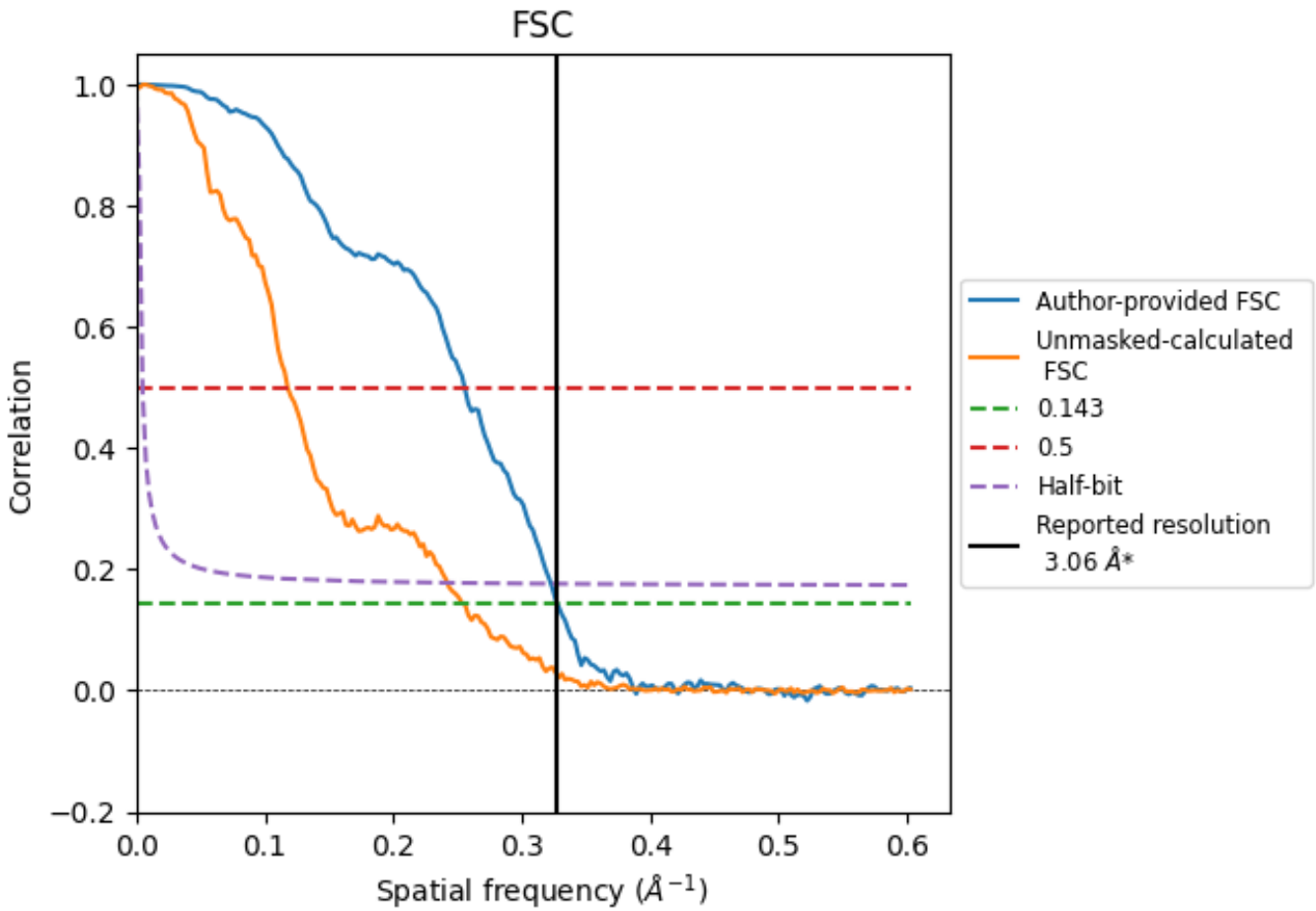



*Reported resolution corresponds to spatial frequency of 0.327 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.327 Å$^{-1}$

## 8.2 Resolution estimates (i)

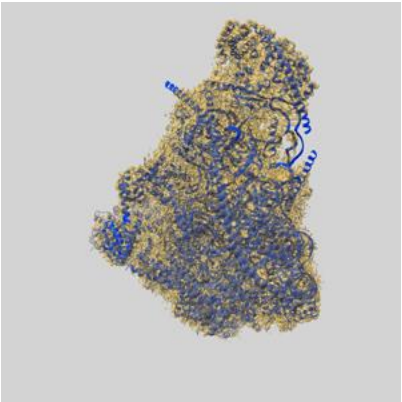
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.06 | - | - |
| Author-provided FSC curve | 3.05 | 3.91 | 3.10 |
| Unmasked-calculated* | 3.93 | 8.48 | 4.13 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.06 by more than 10 %

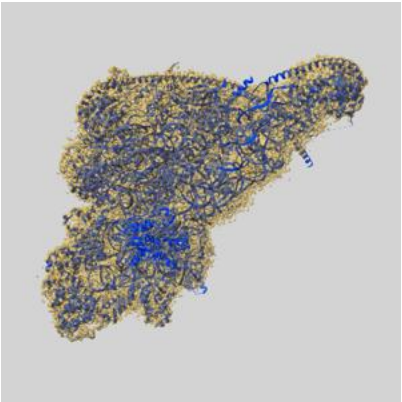
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13553 and PDB model 7PNV. Per-residue inclusion information can be found in section 3 on page 14.

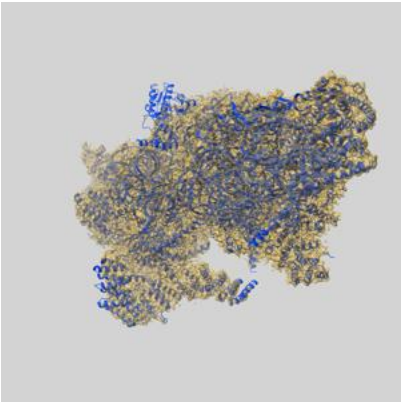
## 9.1 Map-model overlay (i)



X



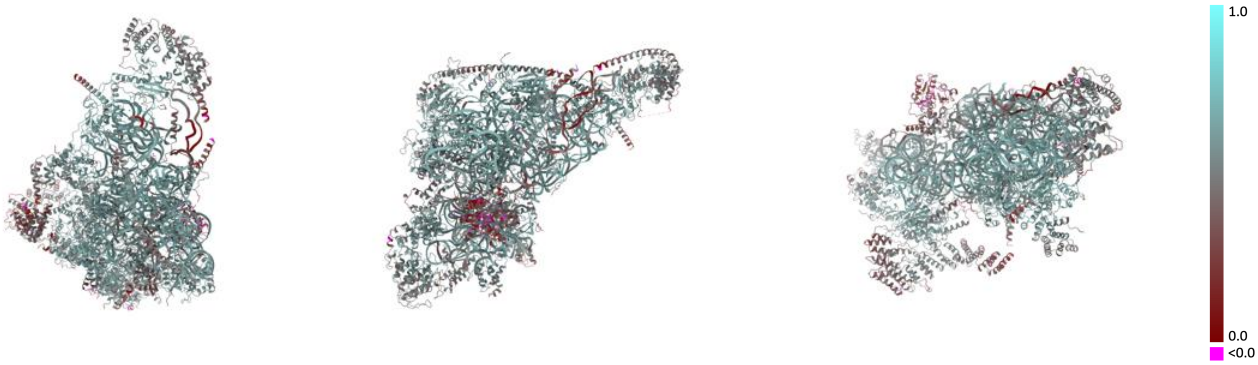
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

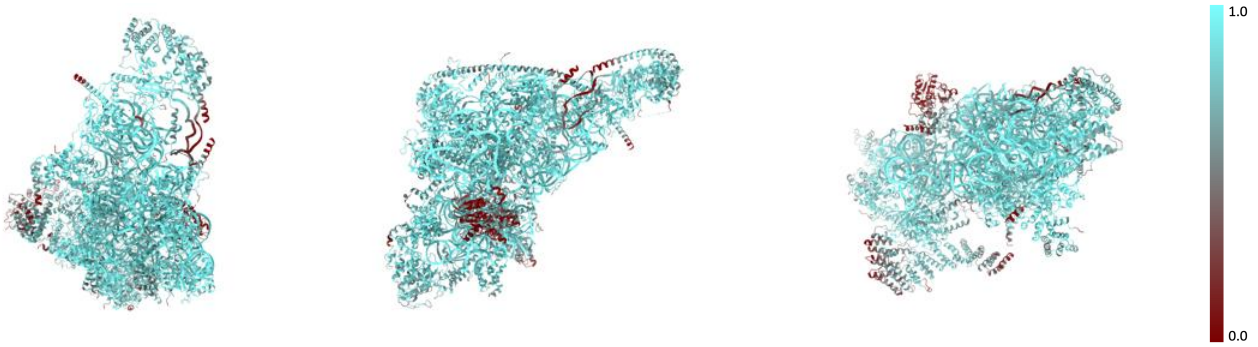
## 9.2 Q-score mapped to coordinate model (i)




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.

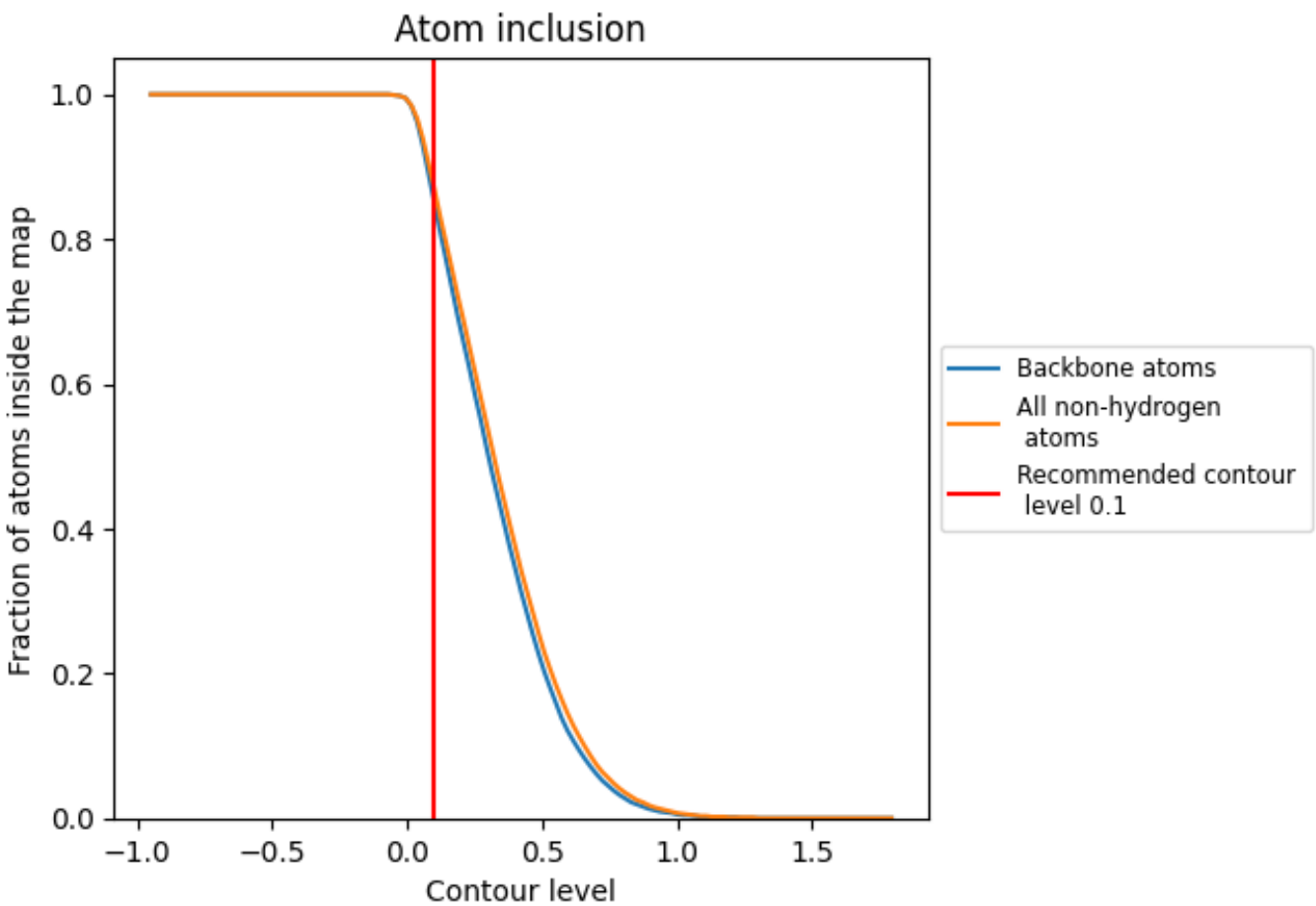
## 9.3 Atom inclusion mapped to coordinate model (i)




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, 85% of all backbone atoms, 87% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8700 | 0.5440 |
| 0 | 0.8980 | 0.5550 |
| 1 | 0.8530 | 0.5440 |
| 3 | 0.8640 | 0.5440 |
| 4 | 0.6620 | 0.4290 |
| A | 0.9580 | 0.5940 |
| B | 0.9470 | 0.6110 |
| C | 0.9740 | 0.6360 |
| D | 0.9070 | 0.5720 |
| E | 0.9240 | 0.5700 |
| F | 0.9000 | 0.5420 |
| G | 0.8570 | 0.5340 |
| H | 0.9090 | 0.5860 |
| I | 0.9480 | 0.5800 |
| J | 0.9500 | 0.5900 |
| K | 0.9590 | 0.6300 |
| L | 0.8420 | 0.5400 |
| M | 0.9000 | 0.6030 |
| N | 0.9200 | 0.5940 |
| O | 0.9360 | 0.5950 |
| P | 0.9360 | 0.5840 |
| Q | 0.9700 | 0.6090 |
| R | 0.8850 | 0.5620 |
| S | 0.8390 | 0.5160 |
| T | 0.9200 | 0.5780 |
| U | 0.8310 | 0.5230 |
| V | 0.7750 | 0.4790 |
| W | 0.9260 | 0.5870 |
| X | 0.8480 | 0.5230 |
| Y | 0.7040 | 0.4890 |
| Z | 0.8660 | 0.5490 |
| a | 0.6750 | 0.4090 |
| b | 0.2530 | 0.2420 |