



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 12:32 AM EST

PDB ID : 8FVY
EMDB ID : EMD-29495
Title : 40S subunit of the Giardia lamblia 80S ribosome
Authors : Eiler, D.R.; Wimberly, B.T.; Bilodeau, D.Y.; Rissland, O.S.; Kieft, J.S.
Deposited on : 2023-01-20
Resolution : 2.94 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

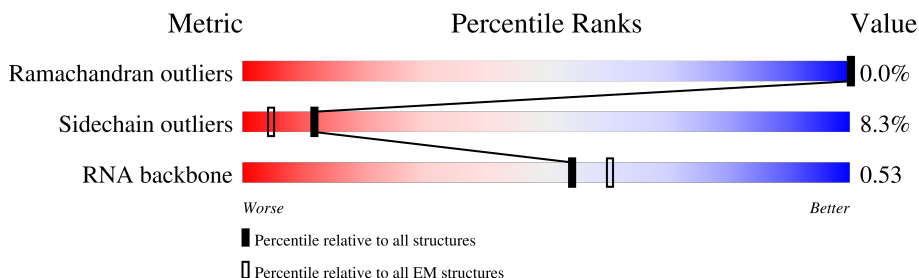
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 2.94 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) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 2 | 1451 |  |
| 2 | A | 245 |  |
| 3 | B | 248 |  |
| 4 | C | 242 |  |
| 5 | D | 217 |  |
| 6 | E | 268 |  |
| 7 | F | 190 |  |
| 8 | G | 248 |  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 9 | H | 201 | |
| 10 | I | 174 | |
| 11 | J | 189 | |
| 12 | K | 134 | |
| 13 | L | 199 | |
| 14 | N | 154 | |
| 15 | O | 145 | |
| 16 | P | 145 | |
| 17 | Q | 158 | |
| 18 | R | 137 | |
| 19 | S | 154 | |
| 20 | T | 158 | |
| 21 | U | 126 | |
| 22 | V | 89 | |
| 23 | W | 130 | |
| 24 | X | 143 | |
| 25 | Y | 132 | |
| 26 | Z | 88 | |
| 27 | a | 109 | |
| 28 | b | 124 | |
| 29 | c | 64 | |
| 30 | d | 137 | |
| 31 | f | 137 | |
| 32 | g | 74 | |
| 33 | M | 125 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 34 | e | 69 | <div><div></div><div>70%</div><div>6%</div><div>25%</div></div> |

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 119930 atoms, of which 52077 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 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|------|------|---------|-------|
| 1 | 2 | 1441 | Total | C | H | N | O | P | 0 | 0 |
| | | | 46630 | 13746 | 15711 | 5742 | 9991 | 1440 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|---------------|
| 2 | 932 | C | U | conflict | GB 2333213660 |

- Molecule 2 is a protein called 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 2 | A | 199 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3230 | 1030 | 1632 | 279 | 281 | 8 | | |

- Molecule 3 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 3 | B | 224 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3657 | 1144 | 1847 | 335 | 318 | 13 | | |

- Molecule 4 is a protein called Ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 4 | C | 209 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3267 | 1028 | 1651 | 292 | 292 | 4 | | |

- Molecule 5 is a protein called Ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 5 | D | 209 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3354 | 1044 | 1698 | 305 | 291 | 16 | | |

- Molecule 6 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6 | E | 258 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4212 | 1323 | 2144 | 378 | 354 | 13 | | |

- Molecule 7 is a protein called SSU ribosomal protein S7P (Fragment).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 7 | F | 190 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2958 | 914 | 1487 | 279 | 268 | 10 | | |

- Molecule 8 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 8 | G | 216 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3532 | 1081 | 1814 | 328 | 298 | 11 | | |

- Molecule 9 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 9 | H | 165 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2689 | 848 | 1367 | 227 | 241 | 6 | | |

- Molecule 10 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 10 | I | 167 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2659 | 820 | 1349 | 251 | 236 | 3 | | |

- Molecule 11 is a protein called Ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 11 | J | 164 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2733 | 834 | 1400 | 260 | 233 | 6 | | |

- Molecule 12 is a protein called Ribosomal protein S10B.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 12 | K | 105 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1700 | 556 | 841 | 144 | 156 | 3 | | |

- Molecule 13 is a protein called SSU ribosomal protein S17P.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 13 | L | 170 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2826 | 885 | 1427 | 275 | 232 | 7 | | |

- Molecule 14 is a protein called Ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 14 | N | 153 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2532 | 780 | 1304 | 237 | 206 | 5 | | |

- Molecule 15 is a protein called Ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 15 | O | 139 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2113 | 645 | 1058 | 210 | 196 | 4 | | |

- Molecule 16 is a protein called Ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 16 | P | 108 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1825 | 564 | 942 | 172 | 139 | 8 | | |

- Molecule 17 is a protein called Ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 17 | Q | 158 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2537 | 768 | 1302 | 244 | 219 | 4 | | |

- Molecule 18 is a protein called Ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 18 | R | 81 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1350 | 405 | 699 | 130 | 114 | 2 | | |

- Molecule 19 is a protein called Ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 19 | S | 143 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2294 | 701 | 1156 | 228 | 202 | 7 | | |

- Molecule 20 is a protein called SSU ribosomal protein S19E (Fragment).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 20 | T | 137 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2163 | 683 | 1089 | 203 | 185 | 3 | | |

- Molecule 21 is a protein called Ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 21 | U | 103 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1668 | 522 | 849 | 148 | 144 | 5 | | |

- Molecule 22 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 22 | V | 81 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1214 | 377 | 607 | 112 | 112 | 6 | | |

- Molecule 23 is a protein called SSU ribosomal protein S8P (Fragment).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 23 | W | 129 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2104 | 659 | 1074 | 192 | 176 | 3 | | |

- Molecule 24 is a protein called SSU ribosomal protein S12P.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 24 | X | 143 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2310 | 703 | 1195 | 223 | 185 | 4 | | |

- Molecule 25 is a protein called Ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 25 | Y | 122 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1988 | 613 | 1019 | 181 | 168 | 7 | | |

- Molecule 26 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 26 | Z | 73 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1183 | 366 | 605 | 104 | 102 | 6 | | |

- Molecule 27 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 27 | a | 96 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1575 | 480 | 795 | 161 | 132 | 7 | | |

- Molecule 28 is a protein called Ribosomal protein S27.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|---------|-------|
| 28 | b | 70 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1078 | 349 | 532 | 92 | 101 | 4 | | |

- Molecule 29 is a protein called Ribosomal protein S28.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 29 | c | 60 | Total | C | H | N | O | S | 0 | 0 |
| | | | 957 | 293 | 483 | 91 | 88 | 2 | | |

- Molecule 30 is a protein called Ribosomal protein S29A.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 30 | d | 85 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1336 | 425 | 654 | 129 | 121 | 7 | | |

- Molecule 31 is a protein called Ribosomal protein S27a.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 31 | f | 35 | Total | C | H | N | O | S | 0 | 0 |
| | | | 535 | 165 | 265 | 53 | 48 | 4 | | |

- Molecule 32 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 32 | g | 74 | Total | C | H | N | O | P | 0 | 0 |
| | | | 2314 | 701 | 745 | 274 | 521 | 73 | | |

- Molecule 33 is a protein called Ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 33 | M | 103 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1679 | 532 | 843 | 148 | 148 | 8 | | |

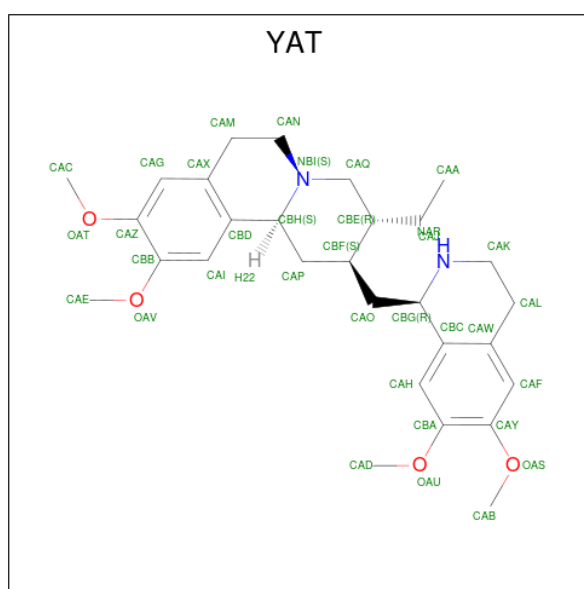
- Molecule 34 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|-------|
| 34 | e | 52 | Total | C | H | N | O | 0 | 0 |
| | | | 886 | 269 | 453 | 93 | 71 | | |

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 35 | 2 | 23 | Total | Mg | 0 |
| | | | 23 | 23 | |

- Molecule 36 is emetine (three-letter code: YAT) (formula: C₂₉H₄₀N₂O₄) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 36 | 2 | 1 | Total | C | H | N | O | 0 |
| | | | 75 | 29 | 40 | 2 | 4 | |

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 37 | a | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 38 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 38 | 2 | 591 | Total | O | 0 |
| | | | 591 | 591 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 38 | B | 1 | Total 1 | O 1 | 0 |
| 38 | C | 6 | Total 6 | O 6 | 0 |
| 38 | D | 6 | Total 6 | O 6 | 0 |
| 38 | E | 10 | Total 10 | O 10 | 0 |
| 38 | F | 12 | Total 12 | O 12 | 0 |
| 38 | G | 2 | Total 2 | O 2 | 0 |
| 38 | H | 1 | Total 1 | O 1 | 0 |
| 38 | I | 10 | Total 10 | O 10 | 0 |
| 38 | K | 7 | Total 7 | O 7 | 0 |
| 38 | L | 4 | Total 4 | O 4 | 0 |
| 38 | N | 9 | Total 9 | O 9 | 0 |
| 38 | O | 3 | Total 3 | O 3 | 0 |
| 38 | P | 2 | Total 2 | O 2 | 0 |
| 38 | Q | 12 | Total 12 | O 12 | 0 |
| 38 | R | 2 | Total 2 | O 2 | 0 |
| 38 | S | 10 | Total 10 | O 10 | 0 |
| 38 | T | 10 | Total 10 | O 10 | 0 |
| 38 | U | 6 | Total 6 | O 6 | 0 |
| 38 | W | 4 | Total 4 | O 4 | 0 |
| 38 | X | 5 | Total 5 | O 5 | 0 |
| 38 | Z | 6 | Total 6 | O 6 | 0 |

Continued on next page...

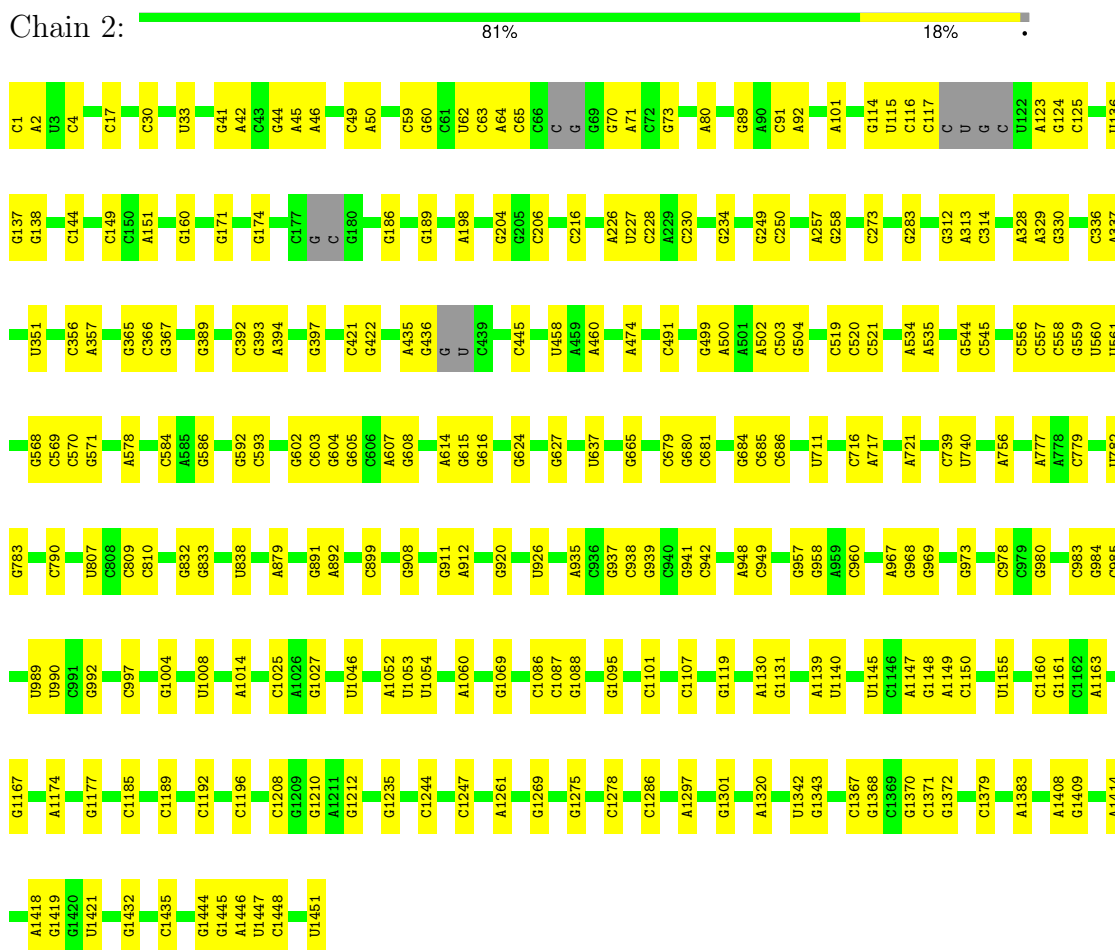
Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|--------|---------|
| 38 | a | 6 | Total 6 | O 6 | 0 |
| 38 | b | 1 | Total 1 | O 1 | 0 |
| 38 | d | 6 | Total 6 | O 6 | 0 |
| 38 | f | 1 | Total 1 | O 1 | 0 |
| 38 | g | 2 | Total 2 | O 2 | 0 |
| 38 | M | 7 | Total 7 | O 7 | 0 |
| 38 | e | 1 | Total 1 | O 1 | 0 |

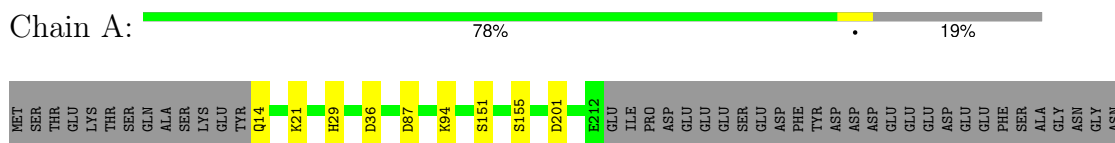
3 Residue-property plots

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

• Molecule 1: 18S rRNA




• Molecule 2: 40S ribosomal protein SA




LEU
PHE
ASP
GLU
TYR

- Molecule 3: 40S ribosomal protein S3a

Chain B:  85% 5% 10%

MET ALA ILE GLY GLY ASN LYS THR PRO GLY LYS LYS LYS ILE T14 E26 Y85 D93 M103 M125 E175 K178 K196 E199 Q202 K219 N223 T224 V237 ARG ASN LEU ALA GLY GLN SER ILE GLN

- Molecule 4: Ribosomal protein S2

Chain C:  84% 14%

MET GLN ALA GLU SER ALA PRO ARG PRO GLU ARG PRO ARG ARG GLN MET GLU E25 K67 E73 V115 A116 N117 K124 D144 Q235 ASP ILE ARG THR MET SER LEU ALA ASP

- Molecule 5: Ribosomal protein S3

Chain D:  90% 6%

MET PRO ARG I4 V5 R6 D20 E62 R71 R82 D95 R100 R130 E141 R152 K157 E176 K191 D206 A212 PHE SER ARG GLN LYS

- Molecule 6: 40S ribosomal protein S4

Chain E:  91% 6%


M1 R11 R39 T98 R108 L123 V126 L139 R148 D170 E171 S204 T220 C223 D231 K249 T253 ALA LYS ARG GLY GLY ALA TYR GLU

- Molecule 7: SSU ribosomal protein S7P (Fragment)

Chain F:  95% 5%

M1 S2 L3 K17 L23 R41 D126 K146 K172 S181 S188 R189 R190

- Molecule 8: 40S ribosomal protein S6

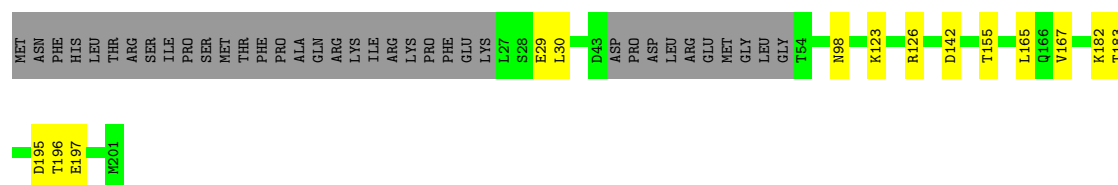
Chain G:  76% 11% 13%

MET PRO LYS G4 K8 S12 V15 L22 W23 F27 E49 Y70 Q71 S76 Q77 L81 C89 R93 S102 V118 L119 V120 G123 LEU THR ASP VAL V134 R138 F151 GLY LEU PRO THR T156 E168 L169 I170 LYS GLU LEU GLY HIS


GLU VAL THR LEU LYS ASN GLY K184 K187 Y188 W214 L218 Q219 R230 K233 Y240 LYS PRO ALA ARG THR VAL GLU

- Molecule 9: 40S ribosomal protein S7

Chain H: 




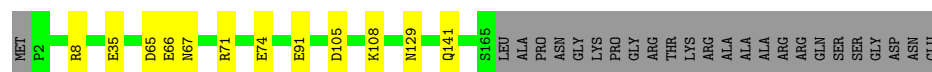
- Molecule 10: 40S ribosomal protein S8

Chain I: 



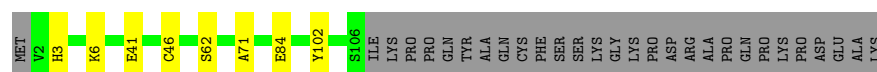
- Molecule 11: Ribosomal protein S9

Chain J: 




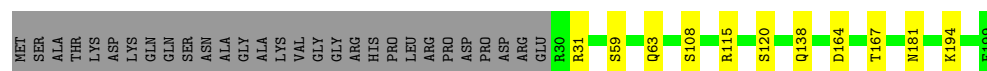
- Molecule 12: Ribosomal protein S10B

Chain K: 



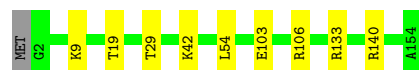
- Molecule 13: SSU ribosomal protein S17P

Chain L: 




- Molecule 14: Ribosomal protein S13

Chain N: 



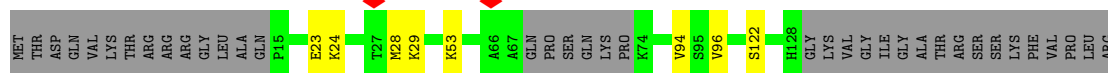
- Molecule 15: Ribosomal protein S14

Chain O: 



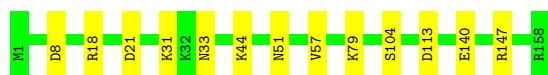
- Molecule 16: Ribosomal protein S15

Chain P:  69% 6% 26%



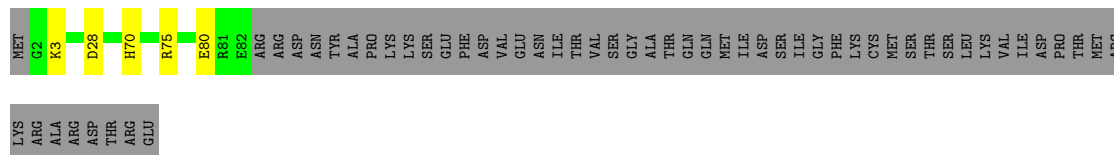
- Molecule 17: Ribosomal protein S16

Chain Q:  92% 8%




- Molecule 18: Ribosomal protein S17

Chain R:  55% 41%




- Molecule 19: Ribosomal protein S18

Chain S:  86% 6% 7%



- Molecule 20: SSU ribosomal protein S19E (Fragment)

Chain T:  78% 9% 13%




- Molecule 21: Ribosomal protein S20

Chain U:  75% 6% 18%



- Molecule 22: 40S ribosomal protein S21

Chain V:  82% 9% 9%



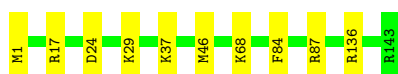
- Molecule 23: SSU ribosomal protein S8P (Fragment)

Chain W: 94% 5%



- Molecule 24: SSU ribosomal protein S12P

Chain X: 93% 7%



- Molecule 25: Ribosomal protein S24

Chain Y: 89% 8%



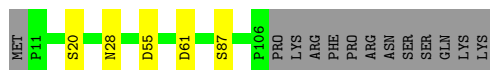
- Molecule 26: 40S ribosomal protein S25

Chain Z: 69% 14% 17%



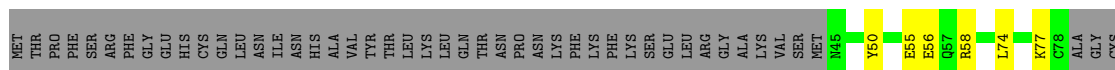
- Molecule 27: 40S ribosomal protein S26

Chain a: 83% 5% 12%




- Molecule 28: Ribosomal protein S27

Chain b: 51% 6% 44%



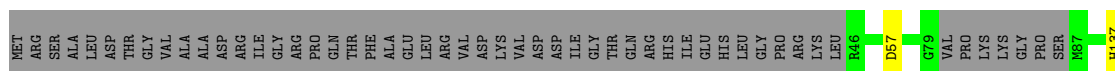
- Molecule 29: Ribosomal protein S28

Chain c:  81% 12% 6%



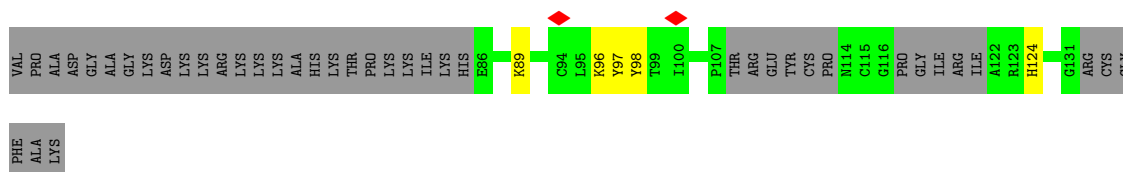
- Molecule 30: Ribosomal protein S29A

Chain d:  61% 38%




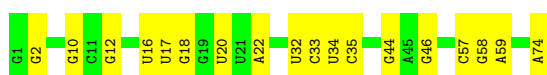
- Molecule 31: Ribosomal protein S27a

Chain f:  22% 74%




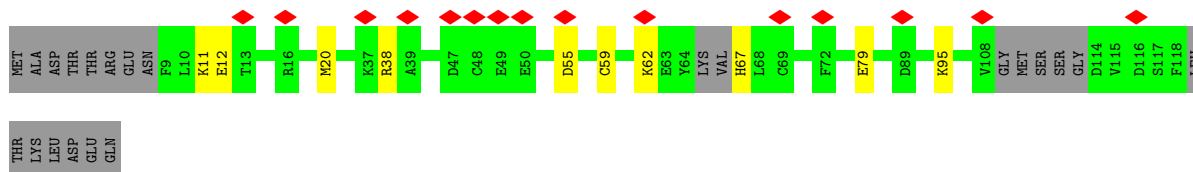
- Molecule 32: tRNA

Chain g:  76% 24%



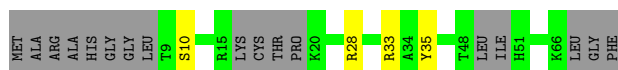
- Molecule 33: Ribosomal protein S12

Chain M:  12% 74% 8% 18%



- Molecule 34: 40S ribosomal protein S30

Chain e:  70% 6% 25%



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 289618 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 72.26 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 1900 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 3.990 | Depositor |
| Minimum map value | -1.460 | Depositor |
| Average map value | -0.001 | Depositor |
| Map value standard deviation | 0.152 | Depositor |
| Recommended contour level | 0.0895 | Depositor |
| Map size (Å) | 369.495, 369.495, 369.495 | wwPDB |
| Map dimensions | 450, 450, 450 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.8211, 0.8211, 0.8211 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, YAT, ZN

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 | 2 | 0.58 | 2/34573 (0.0%) | 0.85 | 12/53952 (0.0%) |
| 2 | A | 0.32 | 0/1633 | 0.52 | 0/2219 |
| 3 | B | 0.34 | 0/1845 | 0.57 | 0/2488 |
| 4 | C | 0.35 | 0/1649 | 0.52 | 0/2225 |
| 5 | D | 0.63 | 0/1682 | 0.63 | 0/2259 |
| 6 | E | 0.32 | 0/2114 | 0.56 | 0/2852 |
| 7 | F | 0.70 | 0/1494 | 0.61 | 0/2010 |
| 8 | G | 0.30 | 0/1739 | 0.58 | 0/2317 |
| 9 | H | 0.33 | 0/1345 | 0.53 | 0/1815 |
| 10 | I | 0.34 | 0/1330 | 0.58 | 0/1784 |
| 11 | J | 0.30 | 0/1351 | 0.57 | 0/1807 |
| 12 | K | 0.76 | 0/884 | 0.61 | 0/1204 |
| 13 | L | 0.39 | 0/1429 | 0.59 | 0/1912 |
| 14 | N | 0.36 | 0/1252 | 0.56 | 0/1681 |
| 15 | O | 0.35 | 0/1070 | 0.62 | 0/1436 |
| 16 | P | 0.61 | 0/898 | 0.64 | 0/1198 |
| 17 | Q | 0.67 | 0/1247 | 0.67 | 0/1666 |
| 18 | R | 0.54 | 0/657 | 0.65 | 0/877 |
| 19 | S | 0.61 | 0/1154 | 0.63 | 0/1549 |
| 20 | T | 0.75 | 0/1098 | 0.63 | 0/1476 |
| 21 | U | 0.65 | 0/835 | 0.62 | 0/1128 |
| 22 | V | 0.33 | 0/615 | 0.54 | 0/825 |
| 23 | W | 0.35 | 0/1047 | 0.56 | 0/1412 |
| 24 | X | 0.33 | 0/1130 | 0.61 | 0/1512 |
| 25 | Y | 0.30 | 0/983 | 0.53 | 0/1314 |
| 26 | Z | 0.68 | 0/584 | 0.69 | 0/779 |
| 27 | a | 0.39 | 0/792 | 0.58 | 0/1065 |
| 28 | b | 0.35 | 0/558 | 0.47 | 0/757 |
| 29 | c | 0.61 | 0/477 | 0.68 | 0/638 |
| 30 | d | 0.55 | 0/696 | 0.64 | 0/932 |
| 31 | f | 0.36 | 0/273 | 0.62 | 0/362 |
| 32 | g | 0.27 | 0/1751 | 0.76 | 0/2727 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | M | 0.45 | 0/848 | 0.63 | 0/1132 |
| 34 | e | 0.30 | 0/438 | 0.61 | 0/578 |
| All | All | 0.52 | 2/71471 (0.0%) | 0.74 | 12/103888 (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 |
|-----|-------|---------------------|---------------------|
| 17 | Q | 0 | 1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | 2 | 189 | G | N3-C4 | 5.77 | 1.39 | 1.35 |
| 1 | 2 | 189 | G | C5-C4 | 5.55 | 1.42 | 1.38 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | 2 | 189 | G | C6-N1-C2 | 18.29 | 136.07 | 125.10 |
| 1 | 2 | 189 | G | N1-C2-N3 | -12.29 | 116.53 | 123.90 |
| 1 | 2 | 189 | G | C5-C6-N1 | -11.83 | 105.58 | 111.50 |
| 1 | 2 | 30 | C | O5'-P-OP1 | -9.75 | 96.93 | 105.70 |
| 1 | 2 | 189 | G | C2-N3-C4 | 7.65 | 115.72 | 111.90 |
| 1 | 2 | 189 | G | N3-C4-C5 | -6.95 | 125.12 | 128.60 |
| 1 | 2 | 716 | C | C2-N1-C1' | 6.09 | 125.50 | 118.80 |
| 1 | 2 | 1161 | G | C4-N9-C1' | 5.85 | 134.10 | 126.50 |
| 1 | 2 | 1161 | G | C8-N9-C1' | -5.26 | 120.17 | 127.00 |
| 1 | 2 | 189 | G | C4-C5-N7 | -5.25 | 108.70 | 110.80 |
| 1 | 2 | 30 | C | C6-N1-C2 | -5.09 | 118.27 | 120.30 |
| 1 | 2 | 189 | G | C5-C6-O6 | 5.02 | 131.61 | 128.60 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 17 | Q | 57 | VAL | Peptide |

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | A | 197/245 (80%) | 192 (98%) | 5 (2%) | 0 | 100 | 100 |
| 3 | B | 222/248 (90%) | 216 (97%) | 6 (3%) | 0 | 100 | 100 |
| 4 | C | 207/242 (86%) | 202 (98%) | 5 (2%) | 0 | 100 | 100 |
| 5 | D | 207/217 (95%) | 190 (92%) | 17 (8%) | 0 | 100 | 100 |
| 6 | E | 256/268 (96%) | 246 (96%) | 10 (4%) | 0 | 100 | 100 |
| 7 | F | 188/190 (99%) | 173 (92%) | 15 (8%) | 0 | 100 | 100 |
| 8 | G | 208/248 (84%) | 198 (95%) | 10 (5%) | 0 | 100 | 100 |
| 9 | H | 161/201 (80%) | 155 (96%) | 6 (4%) | 0 | 100 | 100 |
| 10 | I | 163/174 (94%) | 159 (98%) | 4 (2%) | 0 | 100 | 100 |
| 11 | J | 162/189 (86%) | 158 (98%) | 4 (2%) | 0 | 100 | 100 |
| 12 | K | 103/134 (77%) | 93 (90%) | 9 (9%) | 1 (1%) | 13 | 32 |
| 13 | L | 168/199 (84%) | 163 (97%) | 5 (3%) | 0 | 100 | 100 |
| 14 | N | 151/154 (98%) | 149 (99%) | 2 (1%) | 0 | 100 | 100 |
| 15 | O | 137/145 (94%) | 134 (98%) | 3 (2%) | 0 | 100 | 100 |
| 16 | P | 104/145 (72%) | 99 (95%) | 5 (5%) | 0 | 100 | 100 |
| 17 | Q | 156/158 (99%) | 142 (91%) | 14 (9%) | 0 | 100 | 100 |
| 18 | R | 79/137 (58%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | S | 141/154 (92%) | 122 (86%) | 19 (14%) | 0 | 100 | 100 |
| 20 | T | 135/158 (85%) | 127 (94%) | 8 (6%) | 0 | 100 | 100 |
| 21 | U | 101/126 (80%) | 94 (93%) | 7 (7%) | 0 | 100 | 100 |
| 22 | V | 79/89 (89%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 23 | W | 127/130 (98%) | 115 (91%) | 12 (9%) | 0 | 100 | 100 |
| 24 | X | 141/143 (99%) | 133 (94%) | 8 (6%) | 0 | 100 | 100 |
| 25 | Y | 118/132 (89%) | 110 (93%) | 8 (7%) | 0 | 100 | 100 |
| 26 | Z | 71/88 (81%) | 63 (89%) | 8 (11%) | 0 | 100 | 100 |
| 27 | a | 94/109 (86%) | 93 (99%) | 1 (1%) | 0 | 100 | 100 |
| 28 | b | 66/124 (53%) | 63 (96%) | 3 (4%) | 0 | 100 | 100 |
| 29 | c | 58/64 (91%) | 53 (91%) | 5 (9%) | 0 | 100 | 100 |
| 30 | d | 81/137 (59%) | 66 (82%) | 15 (18%) | 0 | 100 | 100 |
| 31 | f | 29/137 (21%) | 21 (72%) | 7 (24%) | 1 (3%) | 3 | 7 |
| 33 | M | 97/125 (78%) | 81 (84%) | 16 (16%) | 0 | 100 | 100 |
| 34 | e | 46/69 (67%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| All | All | 4253/5079 (84%) | 4011 (94%) | 240 (6%) | 2 (0%) | 100 | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | K | 71 | ALA |
| 31 | f | 124 | HIS |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2 | A | 175/217 (81%) | 166 (95%) | 9 (5%) | 20 | 42 |
| 3 | B | 202/220 (92%) | 189 (94%) | 13 (6%) | 14 | 33 |
| 4 | C | 173/201 (86%) | 167 (96%) | 6 (4%) | 31 | 55 |
| 5 | D | 174/182 (96%) | 160 (92%) | 14 (8%) | 10 | 23 |
| 6 | E | 227/232 (98%) | 212 (93%) | 15 (7%) | 14 | 31 |
| 7 | F | 156/157 (99%) | 146 (94%) | 10 (6%) | 14 | 33 |
| 8 | G | 185/213 (87%) | 158 (85%) | 27 (15%) | 2 | 7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 9 | H | 148/181 (82%) | 134 (90%) | 14 (10%) | 7 | 18 |
| 10 | I | 141/148 (95%) | 129 (92%) | 12 (8%) | 8 | 22 |
| 11 | J | 146/164 (89%) | 134 (92%) | 12 (8%) | 9 | 23 |
| 12 | K | 94/119 (79%) | 87 (93%) | 7 (7%) | 11 | 27 |
| 13 | L | 146/171 (85%) | 135 (92%) | 11 (8%) | 11 | 26 |
| 14 | N | 129/130 (99%) | 120 (93%) | 9 (7%) | 12 | 29 |
| 15 | O | 107/113 (95%) | 96 (90%) | 11 (10%) | 6 | 16 |
| 16 | P | 97/128 (76%) | 89 (92%) | 8 (8%) | 9 | 23 |
| 17 | Q | 130/130 (100%) | 118 (91%) | 12 (9%) | 7 | 19 |
| 18 | R | 72/123 (58%) | 67 (93%) | 5 (7%) | 13 | 30 |
| 19 | S | 122/131 (93%) | 112 (92%) | 10 (8%) | 9 | 23 |
| 20 | T | 113/133 (85%) | 99 (88%) | 14 (12%) | 4 | 10 |
| 21 | U | 92/110 (84%) | 84 (91%) | 8 (9%) | 8 | 21 |
| 22 | V | 64/72 (89%) | 56 (88%) | 8 (12%) | 3 | 10 |
| 23 | W | 114/115 (99%) | 107 (94%) | 7 (6%) | 15 | 35 |
| 24 | X | 114/114 (100%) | 104 (91%) | 10 (9%) | 8 | 21 |
| 25 | Y | 106/113 (94%) | 101 (95%) | 5 (5%) | 22 | 45 |
| 26 | Z | 65/79 (82%) | 53 (82%) | 12 (18%) | 1 | 3 |
| 27 | a | 90/103 (87%) | 85 (94%) | 5 (6%) | 17 | 39 |
| 28 | b | 64/112 (57%) | 57 (89%) | 7 (11%) | 5 | 14 |
| 29 | c | 53/57 (93%) | 45 (85%) | 8 (15%) | 2 | 6 |
| 30 | d | 73/116 (63%) | 71 (97%) | 2 (3%) | 40 | 64 |
| 31 | f | 28/112 (25%) | 24 (86%) | 4 (14%) | 2 | 7 |
| 33 | M | 93/112 (83%) | 83 (89%) | 10 (11%) | 5 | 14 |
| 34 | e | 46/58 (79%) | 42 (91%) | 4 (9%) | 8 | 21 |
| All | All | 3739/4366 (86%) | 3430 (92%) | 309 (8%) | 12 | 22 |

All (309) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 14 | GLN |
| 2 | A | 21 | LYS |
| 2 | A | 29 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 36 | ASP |
| 2 | A | 87 | ASP |
| 2 | A | 94 | LYS |
| 2 | A | 151 | SER |
| 2 | A | 155 | SER |
| 2 | A | 201 | ASP |
| 3 | B | 26 | GLU |
| 3 | B | 85 | TYR |
| 3 | B | 93 | ASP |
| 3 | B | 103 | MET |
| 3 | B | 125 | MET |
| 3 | B | 175 | GLU |
| 3 | B | 178 | LYS |
| 3 | B | 196 | LYS |
| 3 | B | 199 | GLU |
| 3 | B | 202 | GLN |
| 3 | B | 219 | LYS |
| 3 | B | 223 | ASN |
| 3 | B | 224 | THR |
| 4 | C | 67 | LYS |
| 4 | C | 73 | GLU |
| 4 | C | 115 | VAL |
| 4 | C | 117 | ASN |
| 4 | C | 124 | LYS |
| 4 | C | 144 | ASP |
| 5 | D | 6 | ARG |
| 5 | D | 20 | ASP |
| 5 | D | 62 | GLU |
| 5 | D | 71 | ARG |
| 5 | D | 82 | ARG |
| 5 | D | 95 | ASP |
| 5 | D | 100 | ARG |
| 5 | D | 130 | ARG |
| 5 | D | 141 | GLU |
| 5 | D | 152 | ARG |
| 5 | D | 157 | LYS |
| 5 | D | 176 | GLU |
| 5 | D | 191 | LYS |
| 5 | D | 206 | ASP |
| 6 | E | 11 | ARG |
| 6 | E | 39 | ARG |
| 6 | E | 98 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | E | 108 | ARG |
| 6 | E | 123 | LEU |
| 6 | E | 126 | VAL |
| 6 | E | 139 | LEU |
| 6 | E | 148 | ARG |
| 6 | E | 170 | ASP |
| 6 | E | 171 | GLU |
| 6 | E | 204 | SER |
| 6 | E | 220 | THR |
| 6 | E | 223 | CYS |
| 6 | E | 231 | ASP |
| 6 | E | 249 | LYS |
| 7 | F | 3 | LEU |
| 7 | F | 17 | LYS |
| 7 | F | 23 | LEU |
| 7 | F | 41 | ARG |
| 7 | F | 126 | ASP |
| 7 | F | 146 | LYS |
| 7 | F | 172 | LYS |
| 7 | F | 181 | SER |
| 7 | F | 188 | SER |
| 7 | F | 190 | ARG |
| 8 | G | 8 | LYS |
| 8 | G | 12 | SER |
| 8 | G | 15 | VAL |
| 8 | G | 22 | LEU |
| 8 | G | 23 | MET |
| 8 | G | 27 | PHE |
| 8 | G | 49 | GLU |
| 8 | G | 70 | TYR |
| 8 | G | 71 | GLN |
| 8 | G | 76 | SER |
| 8 | G | 77 | GLN |
| 8 | G | 81 | LEU |
| 8 | G | 89 | CYS |
| 8 | G | 93 | ARG |
| 8 | G | 102 | SER |
| 8 | G | 118 | VAL |
| 8 | G | 120 | VAL |
| 8 | G | 138 | ARG |
| 8 | G | 168 | GLU |
| 8 | G | 187 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | G | 188 | TYR |
| 8 | G | 214 | MET |
| 8 | G | 218 | LEU |
| 8 | G | 219 | GLN |
| 8 | G | 230 | ARG |
| 8 | G | 233 | LYS |
| 8 | G | 240 | TYR |
| 9 | H | 29 | GLU |
| 9 | H | 30 | LEU |
| 9 | H | 98 | ASN |
| 9 | H | 123 | LYS |
| 9 | H | 126 | ARG |
| 9 | H | 142 | ASP |
| 9 | H | 155 | THR |
| 9 | H | 165 | LEU |
| 9 | H | 167 | VAL |
| 9 | H | 182 | LYS |
| 9 | H | 183 | THR |
| 9 | H | 195 | ASP |
| 9 | H | 196 | THR |
| 9 | H | 197 | GLU |
| 10 | I | 27 | TYR |
| 10 | I | 37 | LYS |
| 10 | I | 53 | SER |
| 10 | I | 54 | THR |
| 10 | I | 65 | ARG |
| 10 | I | 97 | ASN |
| 10 | I | 101 | ARG |
| 10 | I | 128 | ASP |
| 10 | I | 129 | LYS |
| 10 | I | 136 | ARG |
| 10 | I | 169 | LYS |
| 10 | I | 170 | LYS |
| 11 | J | 8 | ARG |
| 11 | J | 35 | GLU |
| 11 | J | 65 | ASP |
| 11 | J | 66 | GLU |
| 11 | J | 67 | ASN |
| 11 | J | 71 | ARG |
| 11 | J | 74 | GLU |
| 11 | J | 91 | GLU |
| 11 | J | 105 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | J | 108 | LYS |
| 11 | J | 129 | ASN |
| 11 | J | 141 | GLN |
| 12 | K | 3 | HIS |
| 12 | K | 6 | LYS |
| 12 | K | 41 | GLU |
| 12 | K | 46 | CYS |
| 12 | K | 62 | SER |
| 12 | K | 84 | GLU |
| 12 | K | 102 | TYR |
| 13 | L | 31 | ARG |
| 13 | L | 59 | SER |
| 13 | L | 63 | GLN |
| 13 | L | 108 | SER |
| 13 | L | 115 | ARG |
| 13 | L | 120 | SER |
| 13 | L | 138 | GLN |
| 13 | L | 164 | ASP |
| 13 | L | 167 | THR |
| 13 | L | 181 | ASN |
| 13 | L | 194 | LYS |
| 14 | N | 9 | LYS |
| 14 | N | 19 | THR |
| 14 | N | 29 | THR |
| 14 | N | 42 | LYS |
| 14 | N | 54 | LEU |
| 14 | N | 103 | GLU |
| 14 | N | 106 | ARG |
| 14 | N | 133 | ARG |
| 14 | N | 140 | ARG |
| 15 | O | 15 | LYS |
| 15 | O | 24 | VAL |
| 15 | O | 28 | TYR |
| 15 | O | 31 | LYS |
| 15 | O | 51 | SER |
| 15 | O | 58 | ARG |
| 15 | O | 61 | ASP |
| 15 | O | 74 | ASP |
| 15 | O | 80 | THR |
| 15 | O | 82 | ARG |
| 15 | O | 124 | GLU |
| 16 | P | 23 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | P | 24 | LYS |
| 16 | P | 28 | MET |
| 16 | P | 29 | LYS |
| 16 | P | 53 | LYS |
| 16 | P | 94 | VAL |
| 16 | P | 96 | VAL |
| 16 | P | 122 | SER |
| 17 | Q | 8 | ASP |
| 17 | Q | 18 | ARG |
| 17 | Q | 21 | ASP |
| 17 | Q | 31 | LYS |
| 17 | Q | 33 | ASN |
| 17 | Q | 44 | LYS |
| 17 | Q | 51 | ASN |
| 17 | Q | 79 | LYS |
| 17 | Q | 104 | SER |
| 17 | Q | 113 | ASP |
| 17 | Q | 140 | GLU |
| 17 | Q | 147 | ARG |
| 18 | R | 3 | LYS |
| 18 | R | 28 | ASP |
| 18 | R | 70 | HIS |
| 18 | R | 75 | ARG |
| 18 | R | 80 | GLU |
| 19 | S | 12 | ASP |
| 19 | S | 54 | HIS |
| 19 | S | 59 | GLU |
| 19 | S | 69 | MET |
| 19 | S | 92 | GLU |
| 19 | S | 97 | MET |
| 19 | S | 102 | ASN |
| 19 | S | 117 | LYS |
| 19 | S | 127 | HIS |
| 19 | S | 137 | THR |
| 20 | T | 23 | VAL |
| 20 | T | 46 | LYS |
| 20 | T | 53 | TYR |
| 20 | T | 60 | ARG |
| 20 | T | 66 | ASP |
| 20 | T | 68 | ASP |
| 20 | T | 84 | SER |
| 20 | T | 86 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | T | 124 | SER |
| 20 | T | 126 | PHE |
| 20 | T | 132 | LEU |
| 20 | T | 139 | ARG |
| 20 | T | 156 | LEU |
| 20 | T | 158 | LYS |
| 21 | U | 22 | HIS |
| 21 | U | 29 | VAL |
| 21 | U | 36 | LEU |
| 21 | U | 63 | ARG |
| 21 | U | 77 | THR |
| 21 | U | 90 | ARG |
| 21 | U | 100 | ASP |
| 21 | U | 102 | SER |
| 22 | V | 9 | LYS |
| 22 | V | 17 | ASP |
| 22 | V | 51 | LYS |
| 22 | V | 52 | MET |
| 22 | V | 69 | ARG |
| 22 | V | 73 | ASP |
| 22 | V | 76 | PHE |
| 22 | V | 85 | LEU |
| 23 | W | 25 | VAL |
| 23 | W | 43 | LYS |
| 23 | W | 54 | ASP |
| 23 | W | 57 | ARG |
| 23 | W | 70 | ASN |
| 23 | W | 85 | ASP |
| 23 | W | 112 | ASP |
| 24 | X | 1 | MET |
| 24 | X | 17 | ARG |
| 24 | X | 24 | ASP |
| 24 | X | 29 | LYS |
| 24 | X | 37 | LYS |
| 24 | X | 46 | MET |
| 24 | X | 68 | LYS |
| 24 | X | 84 | PHE |
| 24 | X | 87 | ARG |
| 24 | X | 136 | ARG |
| 25 | Y | 47 | LEU |
| 25 | Y | 73 | CYS |
| 25 | Y | 83 | MET |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25 | Y | 104 | SER |
| 25 | Y | 112 | LYS |
| 26 | Z | 14 | LYS |
| 26 | Z | 21 | PHE |
| 26 | Z | 27 | MET |
| 26 | Z | 29 | GLU |
| 26 | Z | 31 | LEU |
| 26 | Z | 33 | PHE |
| 26 | Z | 39 | CYS |
| 26 | Z | 49 | LEU |
| 26 | Z | 50 | ARG |
| 26 | Z | 74 | LYS |
| 26 | Z | 77 | ARG |
| 26 | Z | 78 | MET |
| 27 | a | 20 | SER |
| 27 | a | 28 | ASN |
| 27 | a | 55 | ASP |
| 27 | a | 61 | ASP |
| 27 | a | 87 | SER |
| 28 | b | 50 | TYR |
| 28 | b | 55 | GLU |
| 28 | b | 56 | GLU |
| 28 | b | 58 | ARG |
| 28 | b | 74 | LEU |
| 28 | b | 77 | LYS |
| 28 | b | 96 | PHE |
| 29 | c | 3 | GLU |
| 29 | c | 13 | LEU |
| 29 | c | 19 | ARG |
| 29 | c | 23 | THR |
| 29 | c | 27 | VAL |
| 29 | c | 30 | MET |
| 29 | c | 39 | ARG |
| 29 | c | 58 | ARG |
| 30 | d | 57 | ASP |
| 30 | d | 137 | HIS |
| 31 | f | 89 | LYS |
| 31 | f | 96 | LYS |
| 31 | f | 97 | TYR |
| 31 | f | 98 | TYR |
| 33 | M | 11 | LYS |
| 33 | M | 12 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33 | M | 20 | MET |
| 33 | M | 38 | ARG |
| 33 | M | 55 | ASP |
| 33 | M | 59 | CYS |
| 33 | M | 62 | LYS |
| 33 | M | 67 | HIS |
| 33 | M | 79 | GLU |
| 33 | M | 95 | LYS |
| 34 | e | 10 | SER |
| 34 | e | 28 | ARG |
| 34 | e | 33 | ARG |
| 34 | e | 35 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | G | 19 | ASN |
| 9 | H | 98 | ASN |
| 12 | K | 74 | HIS |
| 14 | N | 62 | GLN |
| 19 | S | 128 | HIS |
| 24 | X | 97 | ASN |
| 33 | M | 67 | HIS |
| 33 | M | 105 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 2 | 1437/1451 (99%) | 249 (17%) | 12 (0%) |
| 32 | g | 73/74 (98%) | 18 (24%) | 0 |
| All | All | 1510/1525 (99%) | 267 (17%) | 12 (0%) |

All (267) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 2 | A |
| 1 | 2 | 4 | C |
| 1 | 2 | 17 | C |
| 1 | 2 | 33 | U |
| 1 | 2 | 41 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 42 | A |
| 1 | 2 | 44 | G |
| 1 | 2 | 45 | A |
| 1 | 2 | 46 | A |
| 1 | 2 | 49 | C |
| 1 | 2 | 50 | A |
| 1 | 2 | 59 | C |
| 1 | 2 | 60 | G |
| 1 | 2 | 62 | U |
| 1 | 2 | 63 | C |
| 1 | 2 | 64 | A |
| 1 | 2 | 65 | C |
| 1 | 2 | 70 | G |
| 1 | 2 | 71 | A |
| 1 | 2 | 73 | G |
| 1 | 2 | 80 | A |
| 1 | 2 | 89 | G |
| 1 | 2 | 91 | C |
| 1 | 2 | 92 | A |
| 1 | 2 | 101 | A |
| 1 | 2 | 114 | G |
| 1 | 2 | 116 | C |
| 1 | 2 | 117 | C |
| 1 | 2 | 124 | G |
| 1 | 2 | 125 | C |
| 1 | 2 | 136 | U |
| 1 | 2 | 137 | G |
| 1 | 2 | 138 | G |
| 1 | 2 | 144 | C |
| 1 | 2 | 149 | C |
| 1 | 2 | 151 | A |
| 1 | 2 | 160 | G |
| 1 | 2 | 171 | G |
| 1 | 2 | 174 | G |
| 1 | 2 | 186 | G |
| 1 | 2 | 198 | A |
| 1 | 2 | 204 | G |
| 1 | 2 | 206 | C |
| 1 | 2 | 216 | C |
| 1 | 2 | 226 | A |
| 1 | 2 | 227 | U |
| 1 | 2 | 228 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 230 | C |
| 1 | 2 | 234 | G |
| 1 | 2 | 249 | G |
| 1 | 2 | 250 | C |
| 1 | 2 | 257 | A |
| 1 | 2 | 258 | G |
| 1 | 2 | 273 | C |
| 1 | 2 | 283 | G |
| 1 | 2 | 313 | A |
| 1 | 2 | 314 | C |
| 1 | 2 | 328 | A |
| 1 | 2 | 329 | A |
| 1 | 2 | 330 | G |
| 1 | 2 | 336 | C |
| 1 | 2 | 337 | A |
| 1 | 2 | 351 | U |
| 1 | 2 | 356 | C |
| 1 | 2 | 357 | A |
| 1 | 2 | 365 | G |
| 1 | 2 | 366 | C |
| 1 | 2 | 367 | G |
| 1 | 2 | 389 | G |
| 1 | 2 | 393 | G |
| 1 | 2 | 394 | A |
| 1 | 2 | 397 | G |
| 1 | 2 | 421 | C |
| 1 | 2 | 422 | G |
| 1 | 2 | 435 | A |
| 1 | 2 | 436 | G |
| 1 | 2 | 445 | C |
| 1 | 2 | 458 | U |
| 1 | 2 | 460 | A |
| 1 | 2 | 474 | A |
| 1 | 2 | 491 | C |
| 1 | 2 | 499 | G |
| 1 | 2 | 500 | A |
| 1 | 2 | 502 | A |
| 1 | 2 | 503 | C |
| 1 | 2 | 504 | G |
| 1 | 2 | 519 | C |
| 1 | 2 | 520 | C |
| 1 | 2 | 521 | C |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 534 | A |
| 1 | 2 | 535 | A |
| 1 | 2 | 544 | G |
| 1 | 2 | 545 | C |
| 1 | 2 | 556 | C |
| 1 | 2 | 557 | C |
| 1 | 2 | 558 | C |
| 1 | 2 | 559 | G |
| 1 | 2 | 560 | U |
| 1 | 2 | 561 | U |
| 1 | 2 | 568 | G |
| 1 | 2 | 569 | C |
| 1 | 2 | 570 | C |
| 1 | 2 | 571 | G |
| 1 | 2 | 578 | A |
| 1 | 2 | 584 | C |
| 1 | 2 | 586 | G |
| 1 | 2 | 592 | G |
| 1 | 2 | 593 | C |
| 1 | 2 | 602 | G |
| 1 | 2 | 603 | C |
| 1 | 2 | 604 | G |
| 1 | 2 | 605 | G |
| 1 | 2 | 607 | A |
| 1 | 2 | 608 | G |
| 1 | 2 | 614 | A |
| 1 | 2 | 615 | G |
| 1 | 2 | 616 | G |
| 1 | 2 | 624 | G |
| 1 | 2 | 627 | G |
| 1 | 2 | 637 | U |
| 1 | 2 | 665 | G |
| 1 | 2 | 680 | G |
| 1 | 2 | 681 | C |
| 1 | 2 | 684 | G |
| 1 | 2 | 685 | C |
| 1 | 2 | 686 | C |
| 1 | 2 | 711 | U |
| 1 | 2 | 717 | A |
| 1 | 2 | 721 | A |
| 1 | 2 | 739 | C |
| 1 | 2 | 740 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 756 | A |
| 1 | 2 | 777 | A |
| 1 | 2 | 779 | C |
| 1 | 2 | 782 | U |
| 1 | 2 | 783 | G |
| 1 | 2 | 790 | C |
| 1 | 2 | 807 | U |
| 1 | 2 | 809 | C |
| 1 | 2 | 810 | C |
| 1 | 2 | 832 | G |
| 1 | 2 | 833 | G |
| 1 | 2 | 838 | U |
| 1 | 2 | 879 | A |
| 1 | 2 | 891 | G |
| 1 | 2 | 892 | A |
| 1 | 2 | 899 | C |
| 1 | 2 | 908 | G |
| 1 | 2 | 911 | G |
| 1 | 2 | 912 | A |
| 1 | 2 | 920 | G |
| 1 | 2 | 926 | U |
| 1 | 2 | 935 | A |
| 1 | 2 | 937 | G |
| 1 | 2 | 938 | C |
| 1 | 2 | 939 | G |
| 1 | 2 | 941 | G |
| 1 | 2 | 942 | C |
| 1 | 2 | 948 | A |
| 1 | 2 | 949 | C |
| 1 | 2 | 957 | G |
| 1 | 2 | 958 | G |
| 1 | 2 | 960 | C |
| 1 | 2 | 967 | A |
| 1 | 2 | 968 | G |
| 1 | 2 | 969 | G |
| 1 | 2 | 973 | G |
| 1 | 2 | 978 | C |
| 1 | 2 | 980 | G |
| 1 | 2 | 983 | C |
| 1 | 2 | 984 | G |
| 1 | 2 | 985 | C |
| 1 | 2 | 990 | U |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 992 | G |
| 1 | 2 | 997 | C |
| 1 | 2 | 1004 | G |
| 1 | 2 | 1008 | U |
| 1 | 2 | 1014 | A |
| 1 | 2 | 1025 | C |
| 1 | 2 | 1027 | G |
| 1 | 2 | 1046 | U |
| 1 | 2 | 1052 | A |
| 1 | 2 | 1053 | U |
| 1 | 2 | 1054 | U |
| 1 | 2 | 1060 | A |
| 1 | 2 | 1069 | G |
| 1 | 2 | 1086 | C |
| 1 | 2 | 1087 | C |
| 1 | 2 | 1088 | G |
| 1 | 2 | 1095 | G |
| 1 | 2 | 1101 | C |
| 1 | 2 | 1107 | C |
| 1 | 2 | 1119 | G |
| 1 | 2 | 1130 | A |
| 1 | 2 | 1131 | G |
| 1 | 2 | 1139 | A |
| 1 | 2 | 1140 | U |
| 1 | 2 | 1145 | U |
| 1 | 2 | 1147 | A |
| 1 | 2 | 1148 | G |
| 1 | 2 | 1149 | A |
| 1 | 2 | 1150 | C |
| 1 | 2 | 1155 | U |
| 1 | 2 | 1160 | C |
| 1 | 2 | 1163 | A |
| 1 | 2 | 1167 | G |
| 1 | 2 | 1174 | A |
| 1 | 2 | 1177 | G |
| 1 | 2 | 1185 | C |
| 1 | 2 | 1189 | C |
| 1 | 2 | 1192 | C |
| 1 | 2 | 1196 | C |
| 1 | 2 | 1208 | C |
| 1 | 2 | 1210 | G |
| 1 | 2 | 1212 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 1235 | G |
| 1 | 2 | 1244 | C |
| 1 | 2 | 1247 | C |
| 1 | 2 | 1261 | A |
| 1 | 2 | 1269 | G |
| 1 | 2 | 1275 | G |
| 1 | 2 | 1278 | C |
| 1 | 2 | 1286 | C |
| 1 | 2 | 1297 | A |
| 1 | 2 | 1301 | G |
| 1 | 2 | 1320 | A |
| 1 | 2 | 1342 | U |
| 1 | 2 | 1343 | G |
| 1 | 2 | 1367 | C |
| 1 | 2 | 1368 | G |
| 1 | 2 | 1370 | G |
| 1 | 2 | 1371 | C |
| 1 | 2 | 1372 | G |
| 1 | 2 | 1379 | C |
| 1 | 2 | 1383 | A |
| 1 | 2 | 1408 | A |
| 1 | 2 | 1409 | G |
| 1 | 2 | 1414 | A |
| 1 | 2 | 1418 | A |
| 1 | 2 | 1419 | G |
| 1 | 2 | 1421 | U |
| 1 | 2 | 1432 | G |
| 1 | 2 | 1435 | C |
| 1 | 2 | 1444 | G |
| 1 | 2 | 1445 | G |
| 1 | 2 | 1446 | A |
| 1 | 2 | 1447 | U |
| 1 | 2 | 1448 | C |
| 1 | 2 | 1451 | U |
| 32 | g | 2 | G |
| 32 | g | 10 | G |
| 32 | g | 12 | G |
| 32 | g | 16 | U |
| 32 | g | 17 | U |
| 32 | g | 18 | G |
| 32 | g | 20 | U |
| 32 | g | 22 | A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | g | 32 | U |
| 32 | g | 33 | C |
| 32 | g | 34 | U |
| 32 | g | 35 | C |
| 32 | g | 44 | G |
| 32 | g | 46 | G |
| 32 | g | 57 | C |
| 32 | g | 58 | G |
| 32 | g | 59 | A |
| 32 | g | 74 | A |

All (12) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 1 | C |
| 1 | 2 | 115 | U |
| 1 | 2 | 123 | A |
| 1 | 2 | 312 | G |
| 1 | 2 | 392 | C |
| 1 | 2 | 393 | G |
| 1 | 2 | 421 | C |
| 1 | 2 | 558 | C |
| 1 | 2 | 604 | G |
| 1 | 2 | 679 | C |
| 1 | 2 | 891 | G |
| 1 | 2 | 989 | U |

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 24 are monoatomic - leaving 1 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 | YAT | 2 | 1524 | - | 39,39,39 | 3.17 | 18 (46%) | 51,56,56 | 2.50 | 17 (33%) |

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 | YAT | 2 | 1524 | - | - | 8/14/49/49 | 0/5/5/5 |

All (18) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 36 | 2 | 1524 | YAT | CAN-CAM | -10.81 | 1.31 | 1.51 |
| 36 | 2 | 1524 | YAT | CAN-NBI | 10.20 | 1.66 | 1.47 |
| 36 | 2 | 1524 | YAT | CAQ-NBI | 4.20 | 1.54 | 1.47 |
| 36 | 2 | 1524 | YAT | OAT-CAZ | 3.94 | 1.43 | 1.37 |
| 36 | 2 | 1524 | YAT | CBC-CBG | 3.80 | 1.55 | 1.52 |
| 36 | 2 | 1524 | YAT | CAI-CBB | 3.63 | 1.45 | 1.38 |
| 36 | 2 | 1524 | YAT | CAF-CAW | 3.56 | 1.45 | 1.39 |
| 36 | 2 | 1524 | YAT | CAW-CBC | -3.33 | 1.34 | 1.40 |
| 36 | 2 | 1524 | YAT | CAX-CBD | 3.29 | 1.45 | 1.40 |
| 36 | 2 | 1524 | YAT | CAH-CBC | 2.96 | 1.44 | 1.39 |
| 36 | 2 | 1524 | YAT | CAG-CAX | 2.84 | 1.44 | 1.39 |
| 36 | 2 | 1524 | YAT | CAG-CAZ | 2.79 | 1.43 | 1.38 |
| 36 | 2 | 1524 | YAT | OAS-CAY | 2.70 | 1.41 | 1.37 |
| 36 | 2 | 1524 | YAT | OAV-CBB | 2.59 | 1.41 | 1.37 |
| 36 | 2 | 1524 | YAT | OAU-CBA | 2.50 | 1.41 | 1.37 |
| 36 | 2 | 1524 | YAT | CBG-NAR | 2.49 | 1.49 | 1.47 |
| 36 | 2 | 1524 | YAT | CAI-CBD | 2.13 | 1.43 | 1.39 |
| 36 | 2 | 1524 | YAT | CAO-CBF | 2.06 | 1.57 | 1.53 |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | 2 | 1524 | YAT | CAN-NBI-CAQ | 11.60 | 132.61 | 110.32 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 36 | 2 | 1524 | YAT | CAQ-CBE-CBF | 4.63 | 117.15 | 108.12 |
| 36 | 2 | 1524 | YAT | CAP-CBH-CBD | -4.35 | 106.88 | 113.07 |
| 36 | 2 | 1524 | YAT | CBE-CAQ-NBI | 3.84 | 117.25 | 112.17 |
| 36 | 2 | 1524 | YAT | CAL-CAK-NAR | 3.47 | 113.73 | 109.02 |
| 36 | 2 | 1524 | YAT | OAT-CAZ-CBB | 3.39 | 120.00 | 115.40 |
| 36 | 2 | 1524 | YAT | OAS-CAY-CBA | 3.19 | 119.72 | 115.40 |
| 36 | 2 | 1524 | YAT | OAU-CBA-CAY | 2.98 | 119.45 | 115.40 |
| 36 | 2 | 1524 | YAT | CAK-CAL-CAW | 2.95 | 115.88 | 110.66 |
| 36 | 2 | 1524 | YAT | CAJ-CBE-CAQ | -2.92 | 104.94 | 111.77 |
| 36 | 2 | 1524 | YAT | CAB-OAS-CAY | -2.77 | 113.45 | 117.51 |
| 36 | 2 | 1524 | YAT | CAP-CBF-CBE | 2.68 | 114.97 | 110.57 |
| 36 | 2 | 1524 | YAT | OAV-CBB-CAZ | 2.67 | 119.02 | 115.40 |
| 36 | 2 | 1524 | YAT | CAC-OAT-CAZ | -2.66 | 113.61 | 117.51 |
| 36 | 2 | 1524 | YAT | OAT-CAZ-CAG | -2.49 | 119.78 | 124.08 |
| 36 | 2 | 1524 | YAT | OAS-CAY-CAF | -2.22 | 120.25 | 124.08 |
| 36 | 2 | 1524 | YAT | CAJ-CBE-CBF | -2.19 | 108.96 | 114.56 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

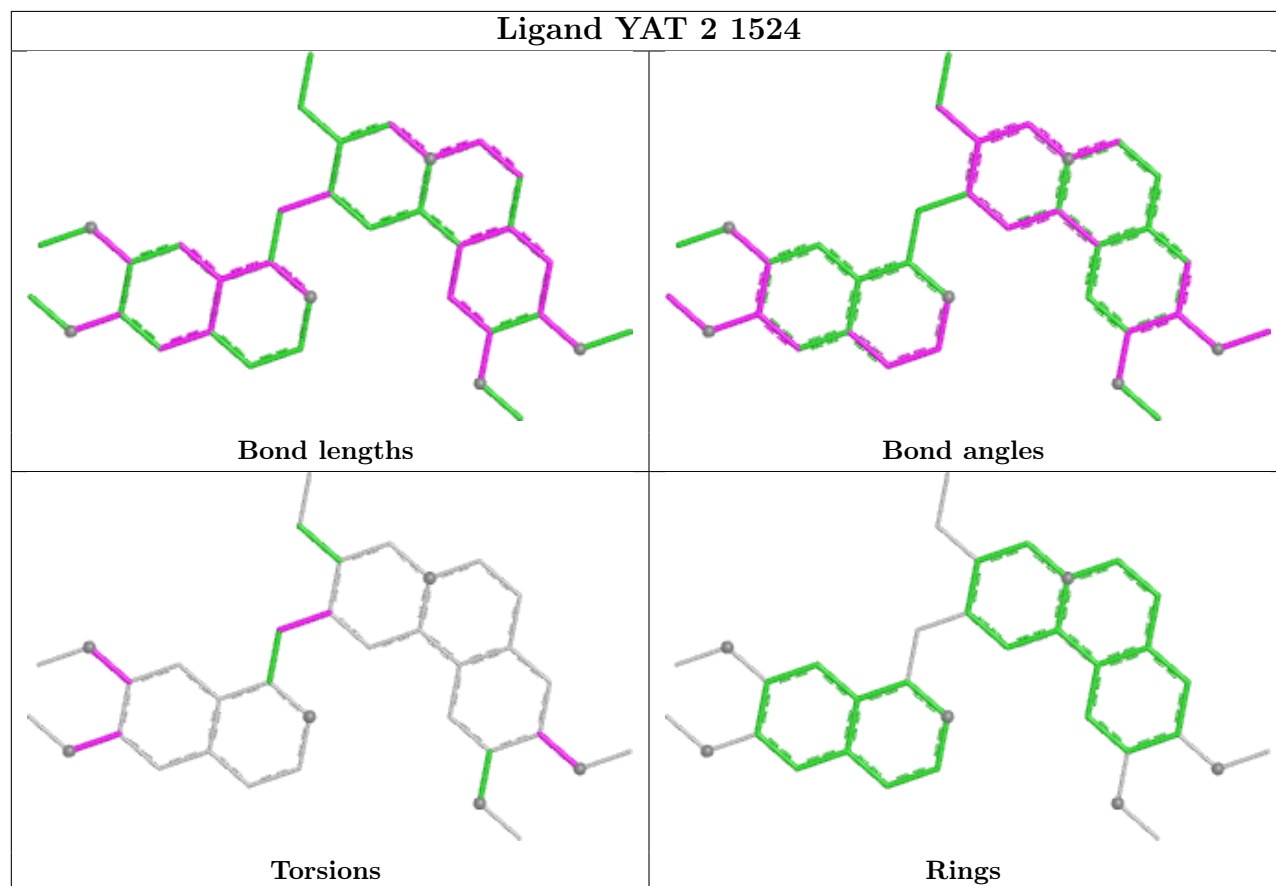
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 36 | 2 | 1524 | YAT | CAY-CBA-OAU-CAD |
| 36 | 2 | 1524 | YAT | CAG-CAZ-OAT-CAC |
| 36 | 2 | 1524 | YAT | CAF-CAY-OAS-CAB |
| 36 | 2 | 1524 | YAT | CBB-CAZ-OAT-CAC |
| 36 | 2 | 1524 | YAT | CAH-CBA-OAU-CAD |
| 36 | 2 | 1524 | YAT | CBA-CAY-OAS-CAB |
| 36 | 2 | 1524 | YAT | CBG-CAO-CBF-CBE |
| 36 | 2 | 1524 | YAT | CBG-CAO-CBF-CAP |

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

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



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.

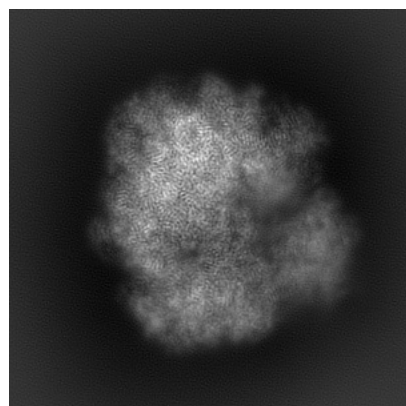
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29495. These allow visual inspection of the internal detail of the map and identification of artifacts.

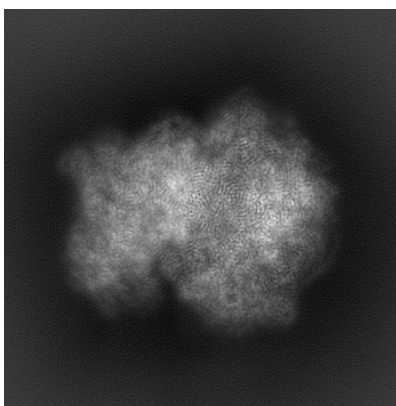
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

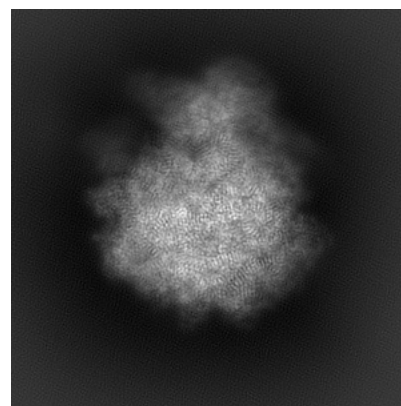
6.1.1 Primary map



X

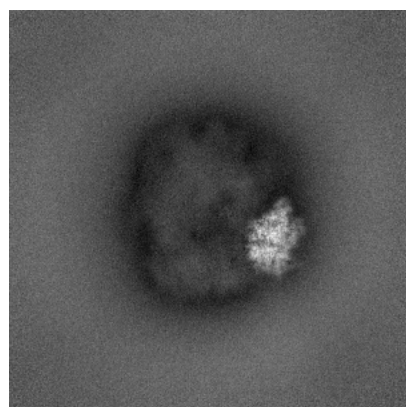


Y

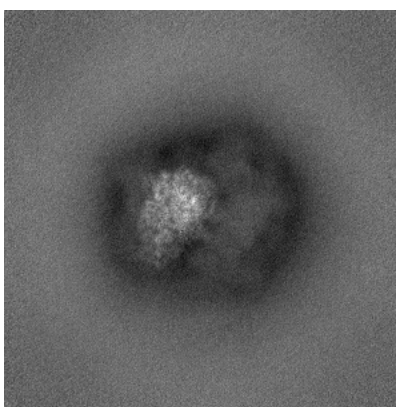


Z

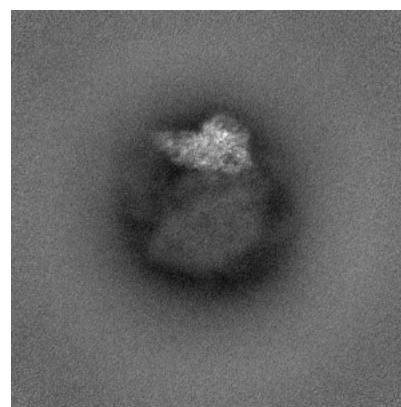
6.1.2 Raw map



X



Y

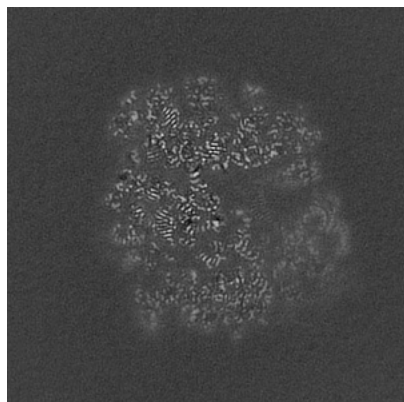


Z

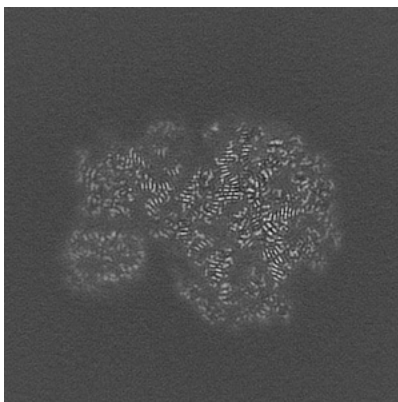
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

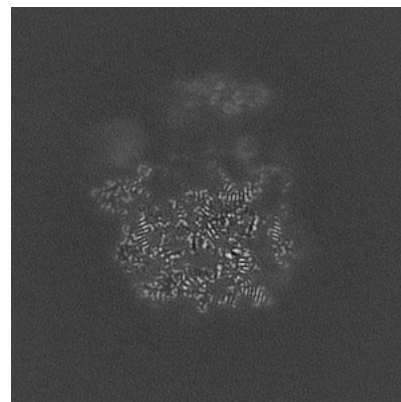
6.2.1 Primary map



X Index: 225

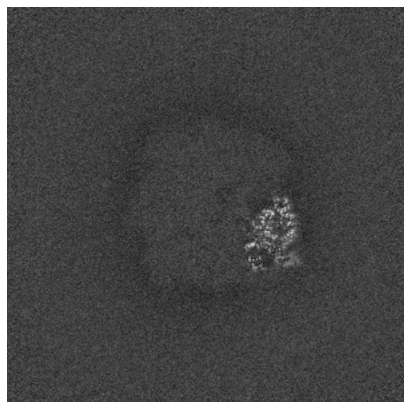


Y Index: 225

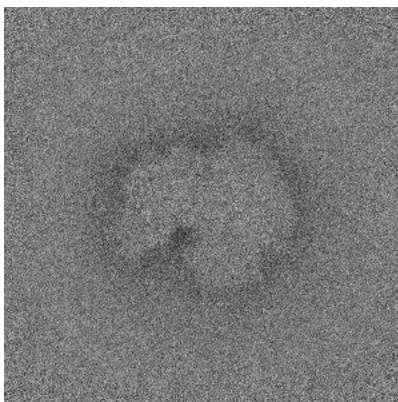


Z Index: 225

6.2.2 Raw map



X Index: 351



Y Index: 351

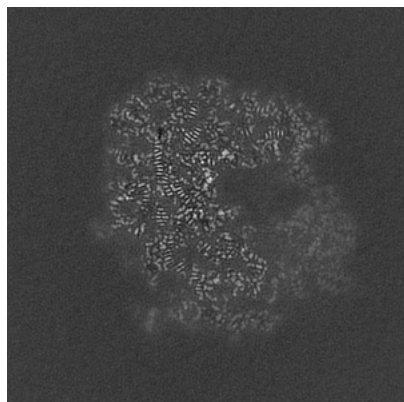


Z Index: 351

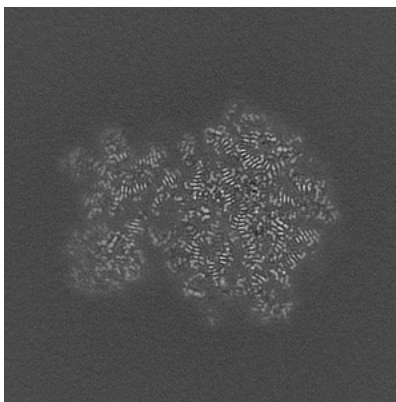
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

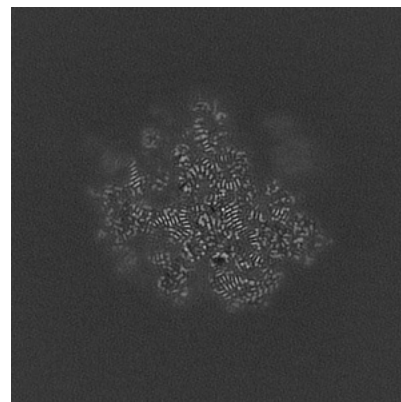
6.3.1 Primary map



X Index: 239

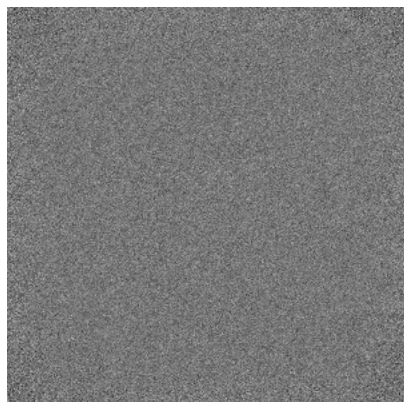


Y Index: 217

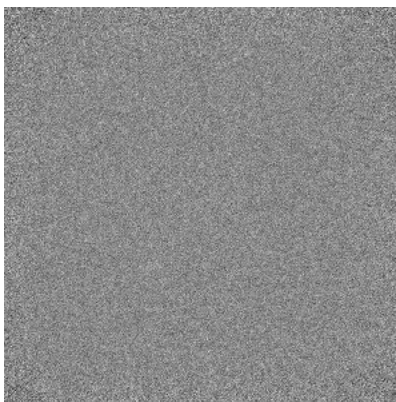


Z Index: 280

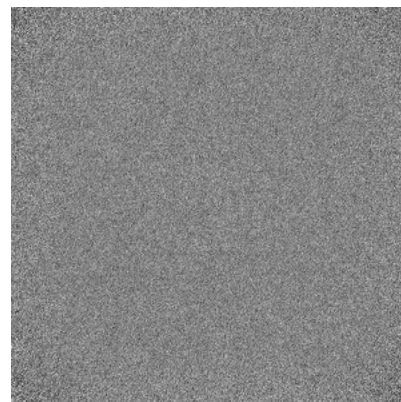
6.3.2 Raw map



X Index: 0



Y Index: 0

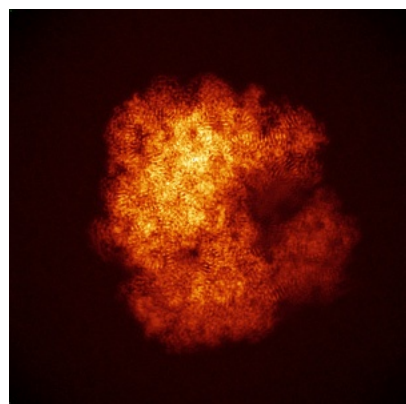


Z Index: 0

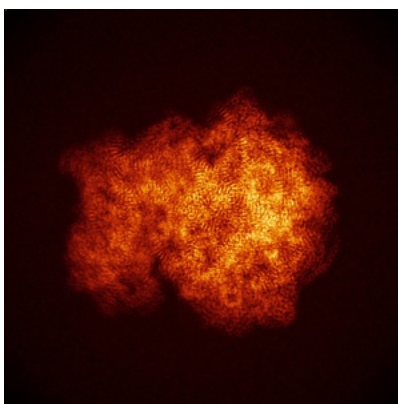
The images above show the largest variance slices of the map in three orthogonal directions.

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

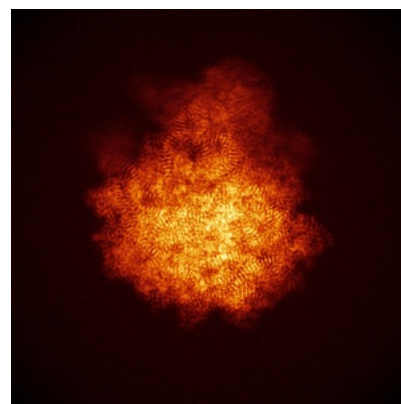
6.4.1 Primary map



X

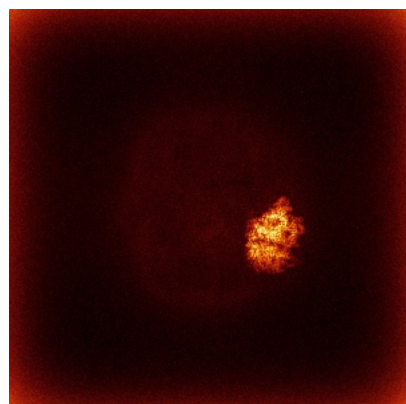


Y

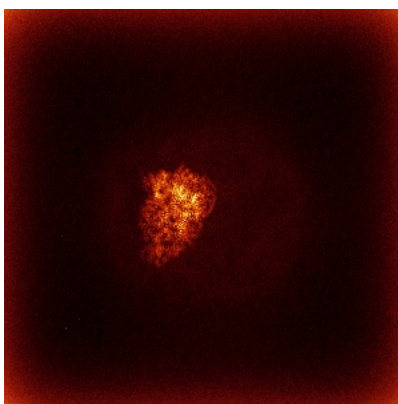


Z

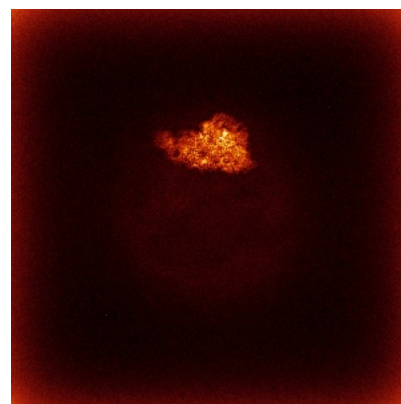
6.4.2 Raw map



X



Y

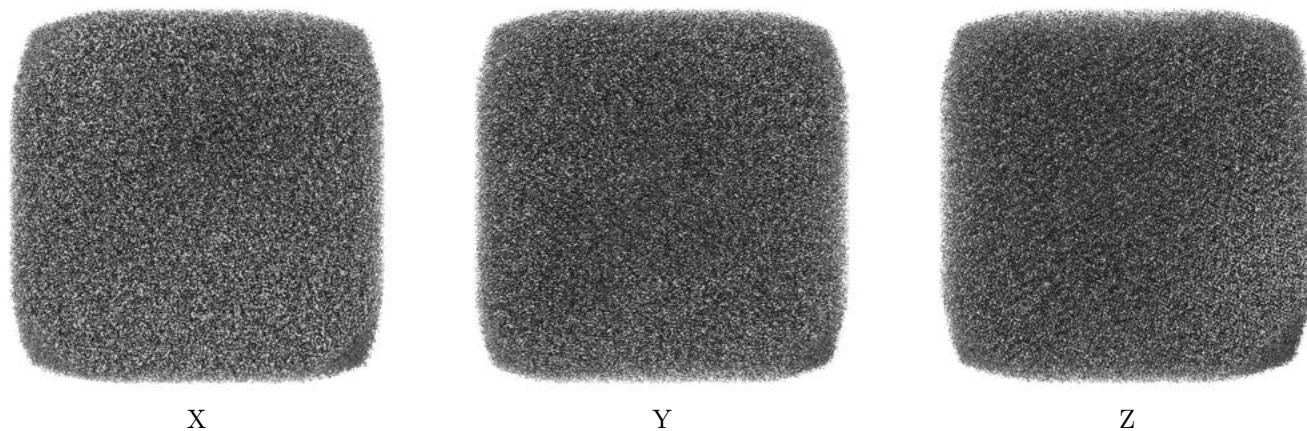


Z

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.

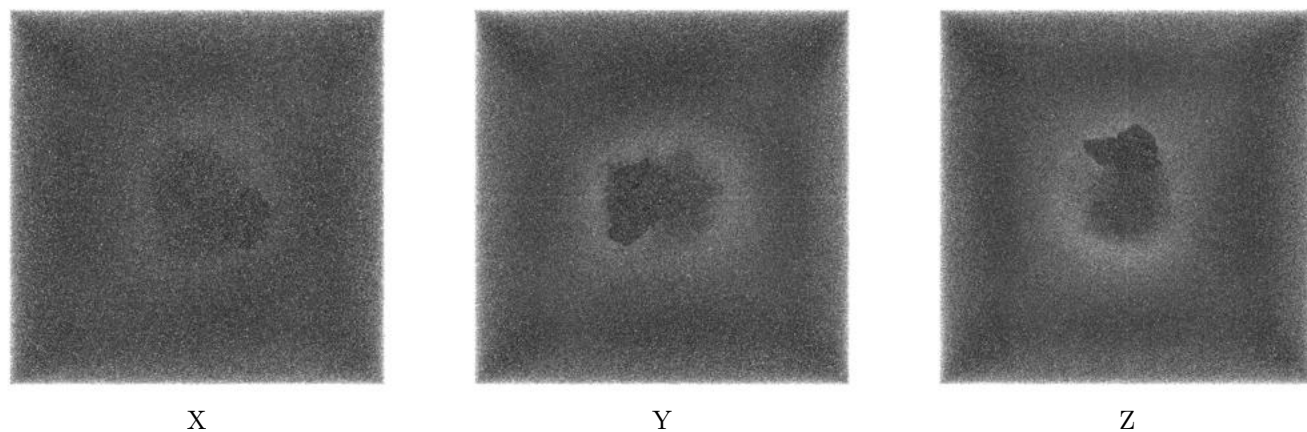
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0895. 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



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.

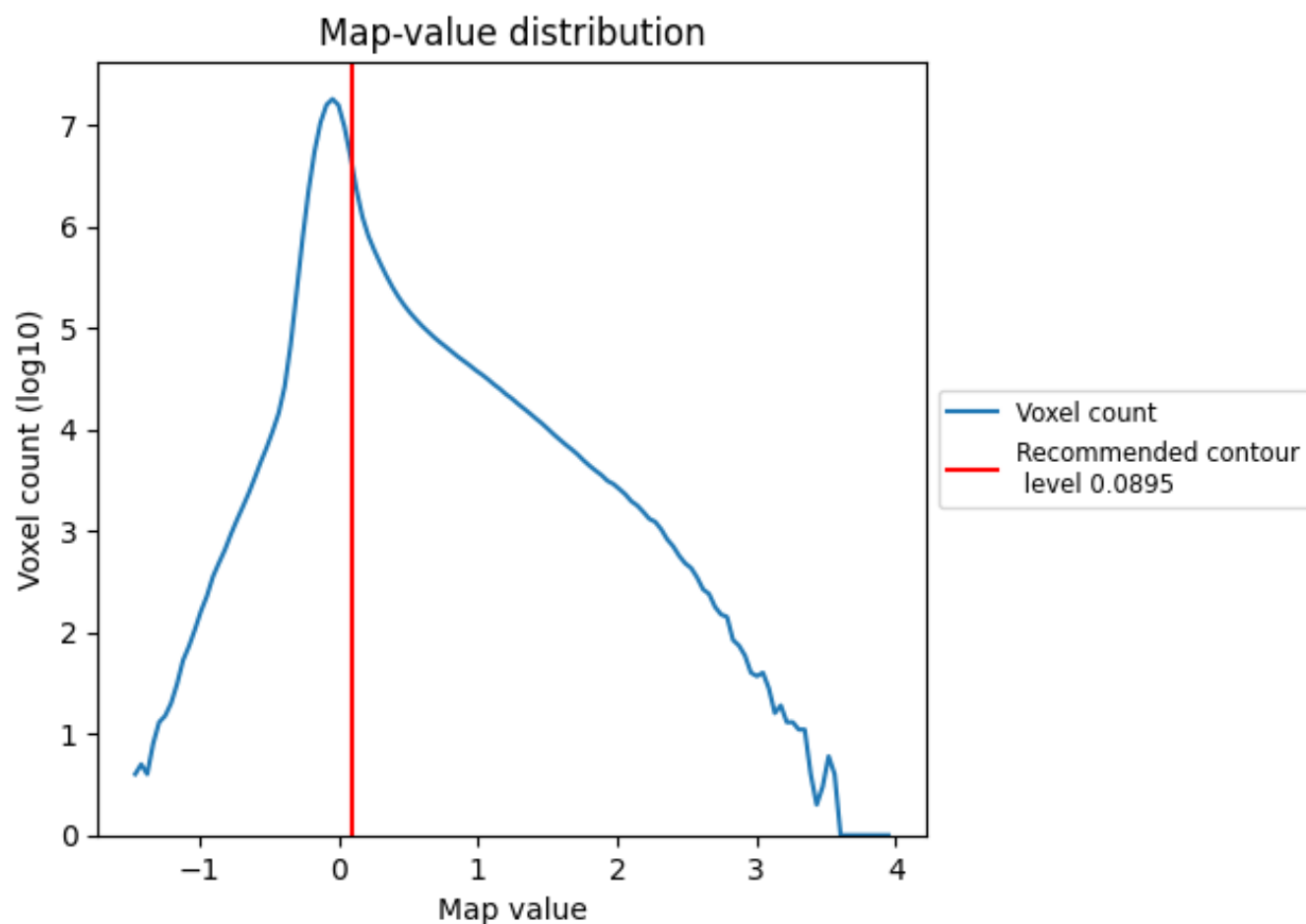
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

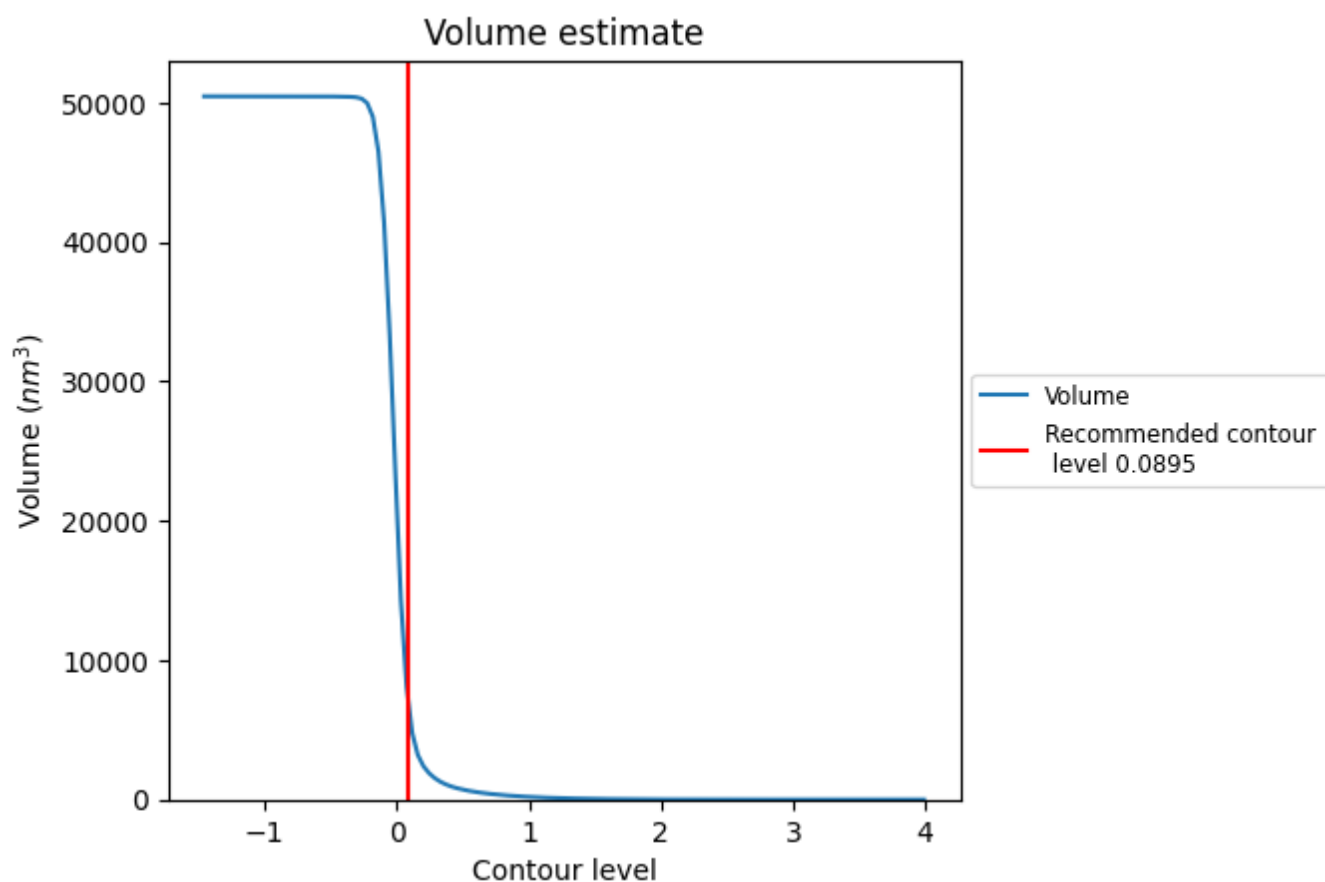
This section contains the results of statistical analysis of the map.

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.

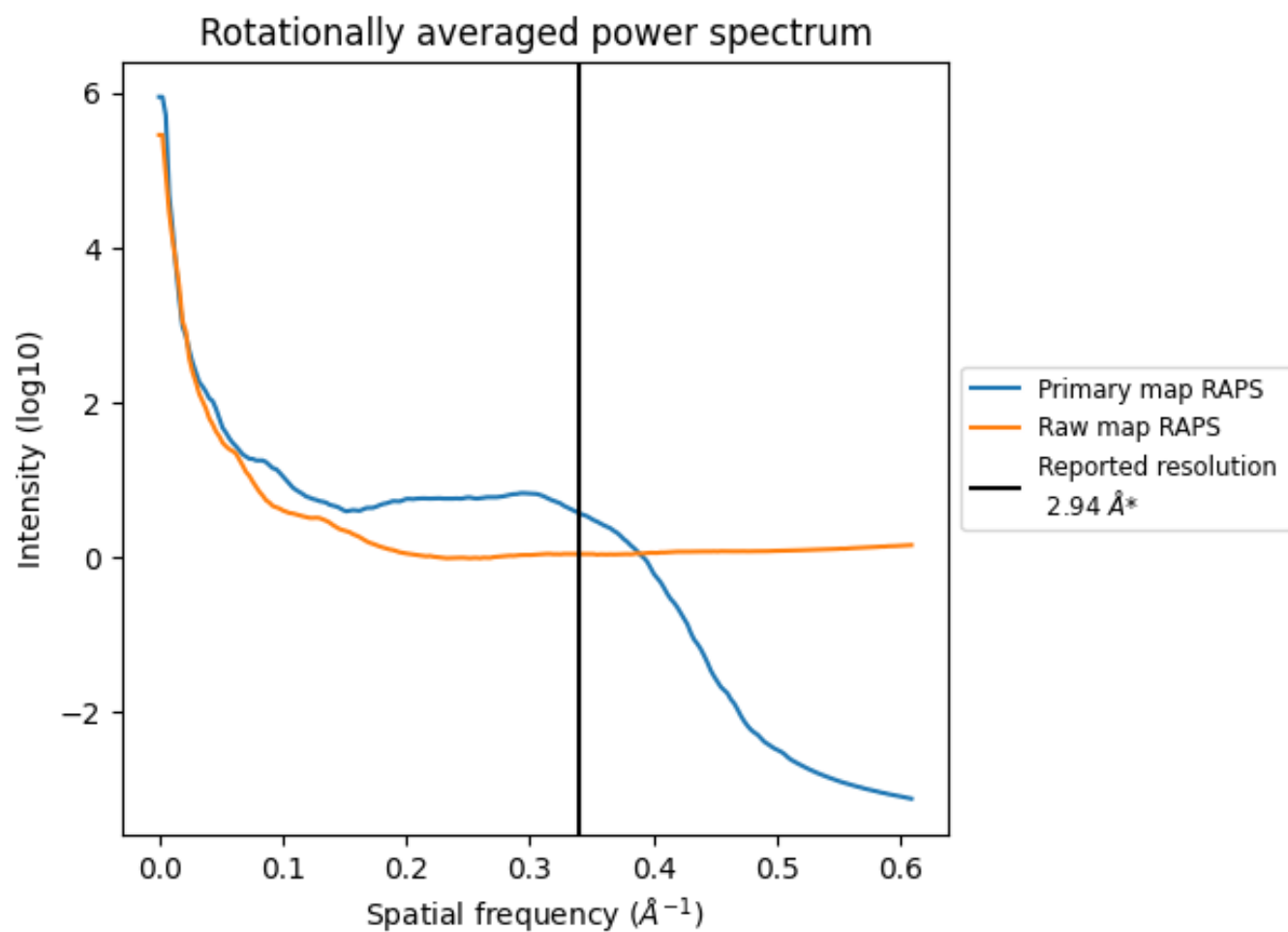
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6823 nm³; this corresponds to an approximate mass of 6164 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

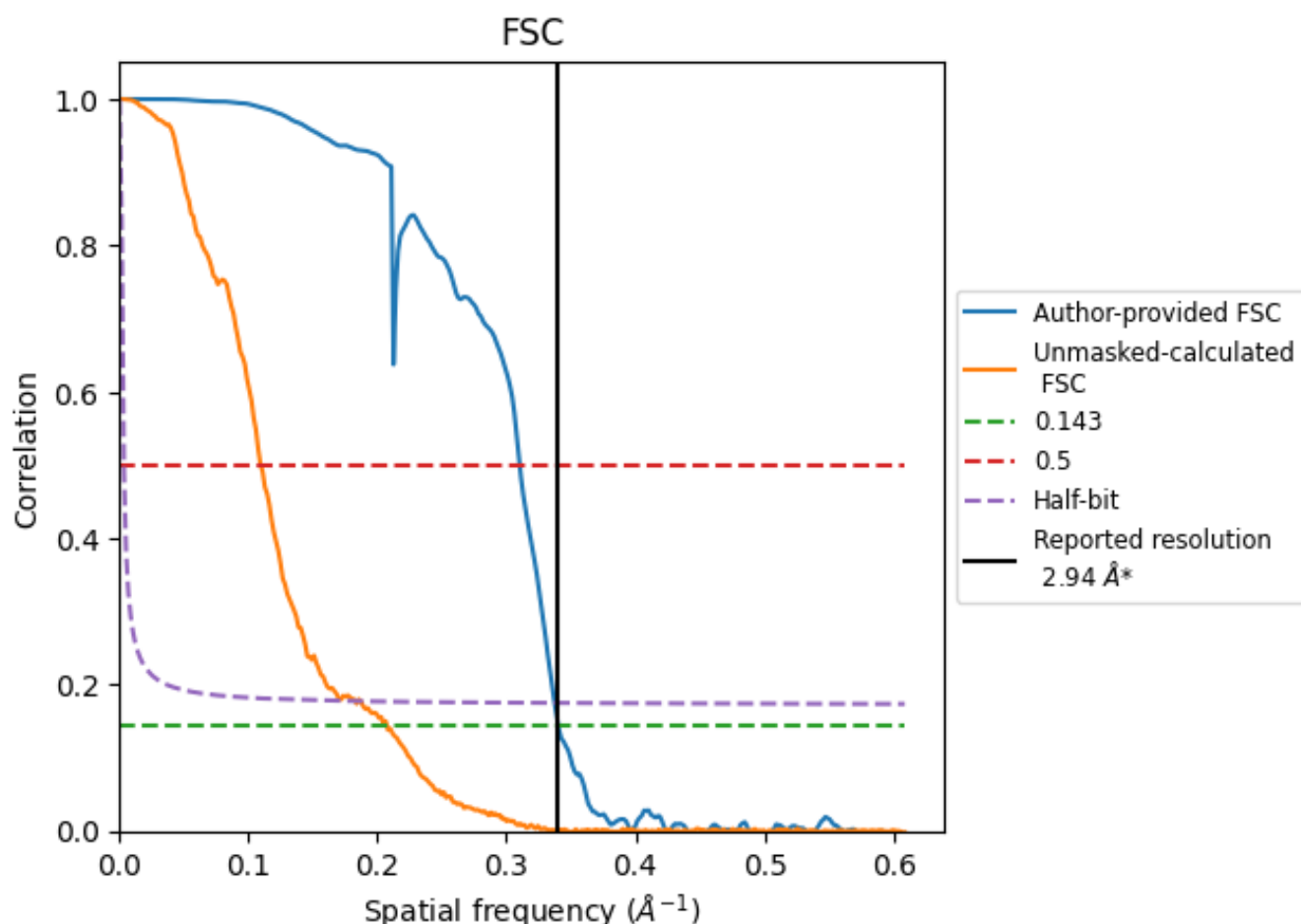


*Reported resolution corresponds to spatial frequency of 0.340 \AA^{-1}

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 0.340 Å⁻¹

8.2 Resolution estimates [i](#)

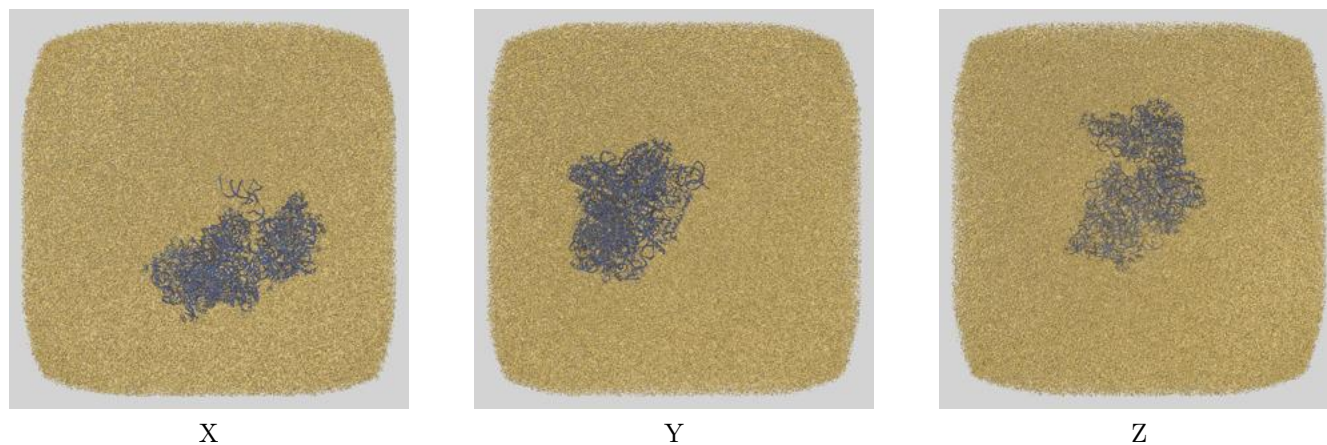
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.94 | - | - |
| Author-provided FSC curve | 2.94 | 3.22 | 2.96 |
| Unmasked-calculated* | 4.82 | 9.13 | 5.47 |

*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 4.82 differs from the reported value 2.94 by more than 10 %

9 Map-model fit [i](#)

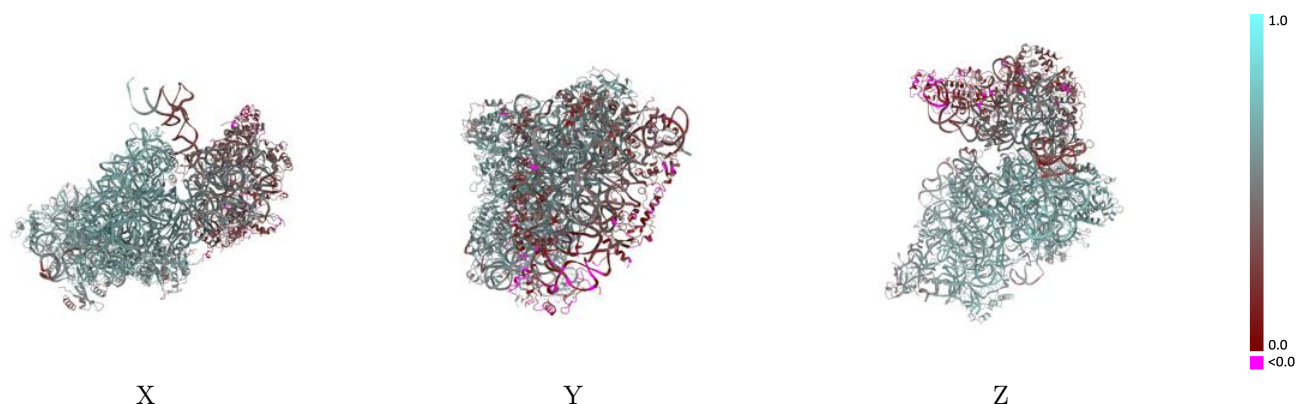
This section contains information regarding the fit between EMDB map EMD-29495 and PDB model 8FVY. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



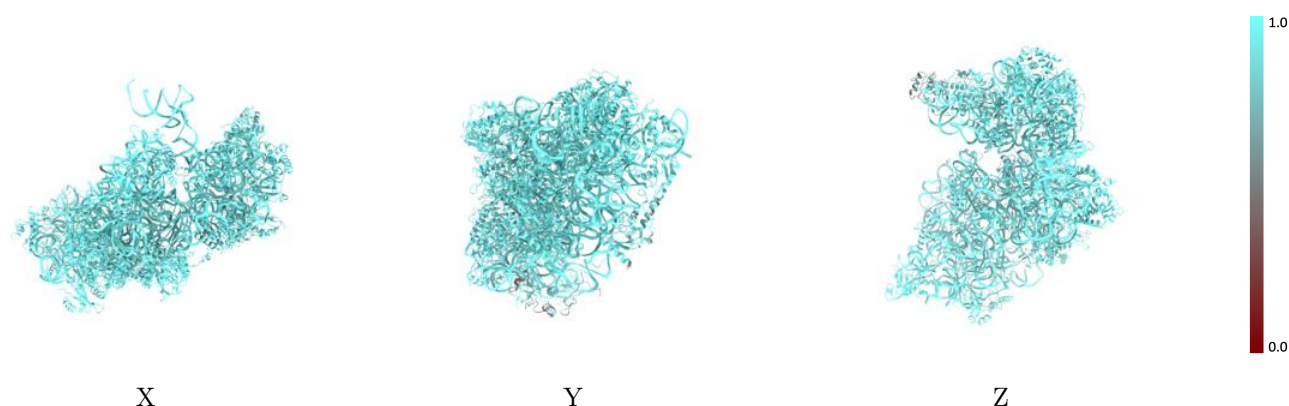
The images above show the 3D surface view of the map at the recommended contour level 0.0895 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



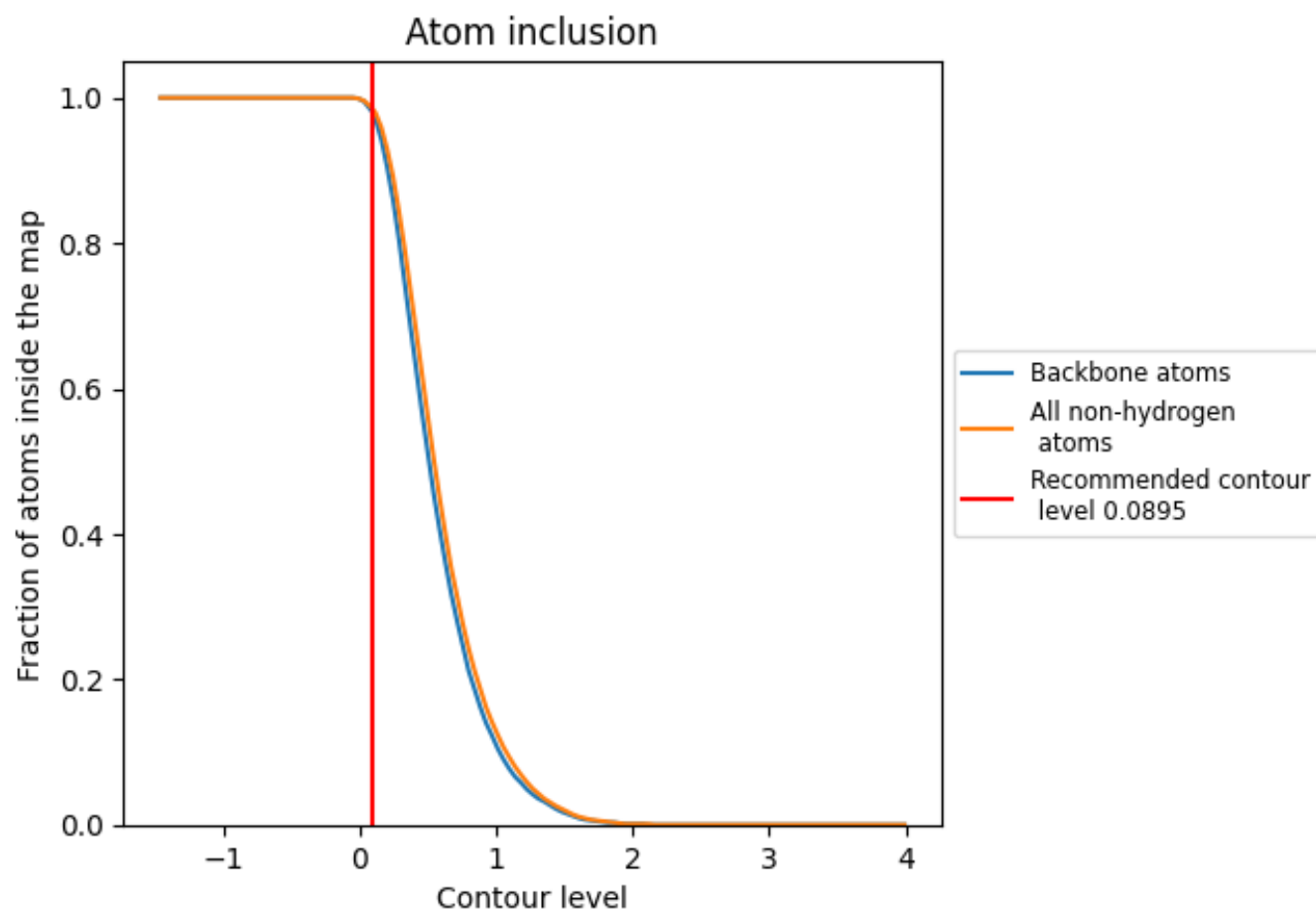
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0895).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0895) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9860 |  0.5100 |
| 2 |  0.9980 |  0.5630 |
| A |  0.9970 |  0.5450 |
| B |  0.9960 |  0.5910 |
| C |  0.9980 |  0.5950 |
| D |  0.9580 |  0.3470 |
| E |  1.0000 |  0.5950 |
| F |  0.9860 |  0.4100 |
| G |  0.9900 |  0.5010 |
| H |  0.9950 |  0.5190 |
| I |  0.9960 |  0.6120 |
| J |  0.9980 |  0.5700 |
| K |  0.9250 |  0.2060 |
| L |  0.9960 |  0.6260 |
| M |  0.6630 |  0.0740 |
| N |  0.9990 |  0.5970 |
| O |  0.9980 |  0.6060 |
| P |  0.9350 |  0.2040 |
| Q |  0.9850 |  0.3720 |
| R |  0.9750 |  0.3270 |
| S |  0.9370 |  0.1920 |
| T |  0.9910 |  0.3780 |
| U |  0.9540 |  0.3480 |
| V |  0.9920 |  0.5600 |
| W |  0.9980 |  0.6180 |
| X |  0.9920 |  0.5800 |
| Y |  0.9940 |  0.5060 |
| Z |  0.9580 |  0.2960 |
| a |  1.0000 |  0.6300 |
| b |  0.9940 |  0.5620 |
| c |  0.9760 |  0.4110 |
| d |  0.9560 |  0.2930 |
| e |  0.9300 |  0.3190 |
| f |  0.6720 |  0.0420 |
| g |  0.9640 |  0.3130 |

