



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2025 – 10:59 AM EDT

PDB ID : 9D89
EMDB ID : EMD-46632
Title : E. coli 50S ribosomal subunit in complex with PrAMP rumicidin-2 (focused refinement)
Authors : Pichkur, E.B.; Panteleev, P.V.; Konevega, A.L.
Deposited on : 2024-08-19
Resolution : 1.95 Å(reported)
Based on initial model : 8B0X

This is a wwPDB EM Validation Summary 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
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) : 2.41.4

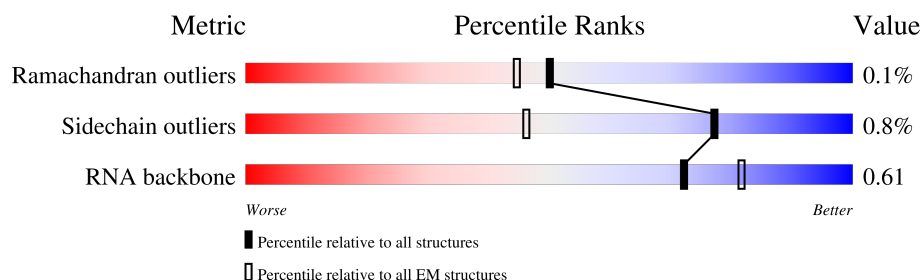
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.95 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.



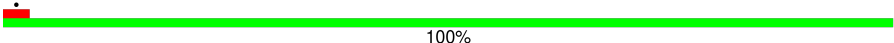
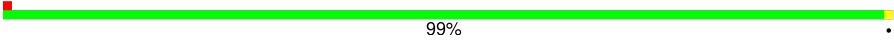
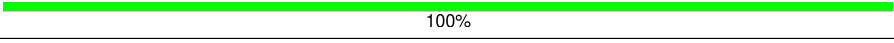
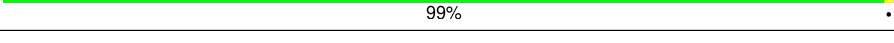
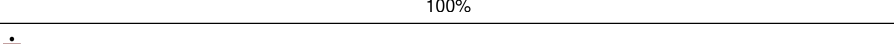
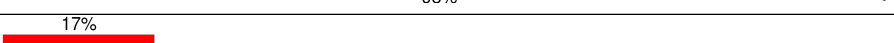


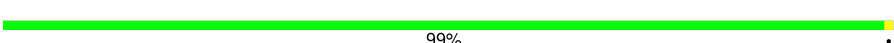
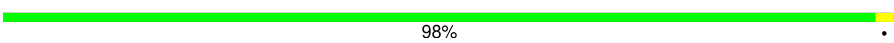
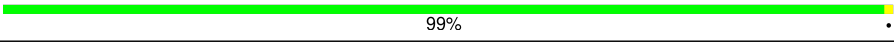
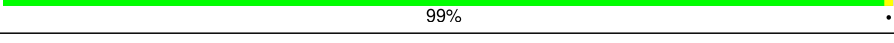
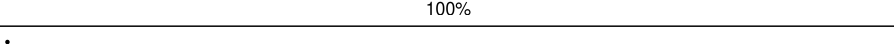
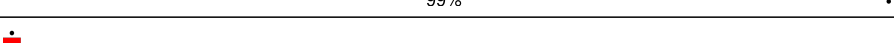


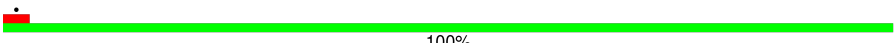
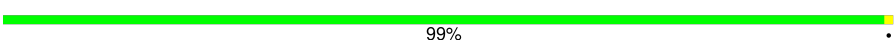

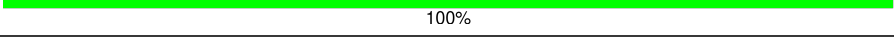
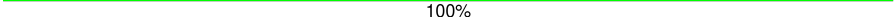


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

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 | 0 | 55 | |
| 2 | 1 | 46 | |
| 3 | B | 65 | |
| 4 | C | 38 | |
| 5 | D | 2728 | |
| 6 | E | 119 | |
| 7 | F | 273 | |
| 8 | G | 209 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 9 | H | 201 |  100% |
| 10 | I | 144 |  99% |
| 11 | J | 118 |  100% |
| 12 | K | 93 |  99% |
| 13 | L | 78 |  100% |
| 14 | M | 56 |  98% |
| 15 | f | 177 |  99% |
| 16 | g | 176 |  100% |
| 17 | h | 38 |  100% |
| 18 | i | 142 |  99% |
| 19 | j | 123 |  98% |
| 20 | l | 135 |  99% |
| 21 | n | 116 |  99% |
| 22 | o | 114 |  100% |
| 23 | p | 117 |  99% |
| 24 | q | 103 |  100% |
| 25 | r | 110 |  97% |
| 26 | t | 102 |  97% |
| 27 | u | 94 |  100% |
| 28 | w | 77 |  99% |
| 29 | x | 62 |  100% |
| 30 | y | 58 |  100% |
| 31 | T | 16 |  100% |

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 90166 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 1 | 0 | 51 | Total | C | N | O | 0 | 0 |
| | | | 417 | 269 | 76 | 72 | | |

- Molecule 2 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 2 | 1 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 3 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 3 | B | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 4 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 4 | C | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 5 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 5 | D | 2728 | Total | C | N | O | P | 0 | 0 |
| | | | 58601 | 26147 | 10802 | 18924 | 2728 | | |

- Molecule 6 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 6 | E | 119 | Total | C | N | O | P | 0 | 0 |
| | | | 2549 | 1135 | 466 | 829 | 119 | | |

- Molecule 7 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | F | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | |

- Molecule 8 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | G | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1566 | 980 | 288 | 294 | 4 | | |

- Molecule 9 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | H | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 10 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | I | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | |

- Molecule 11 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | J | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 945 | 585 | 194 | 161 | 5 | | |

- Molecule 12 is a protein called Large ribosomal subunit protein uL23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | K | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | |

- Molecule 13 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | L | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 586 | 362 | 116 | 107 | 1 | | |

- Molecule 14 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14 | M | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 15 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | f | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | |

- Molecule 16 is a protein called Large ribosomal subunit protein uL6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | g | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 17 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17 | h | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 282 | 181 | 50 | 50 | 1 | | |

- Molecule 18 is a protein called Large ribosomal subunit protein uL13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | i | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 19 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | j | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 946 | 593 | 181 | 166 | 6 | | |

- Molecule 20 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | l | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1067 | 681 | 204 | 177 | 5 | | |

- Molecule 21 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 21 | n | 116 | Total | C | N | O | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | |

- Molecule 22 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | o | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 23 is a protein called Large ribosomal subunit protein bL20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 23 | p | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 24 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24 | q | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 25 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25 | r | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 26 is a protein called Large ribosomal subunit protein uL24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 26 | t | 102 | Total | C | N | O | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | |

- Molecule 27 is a protein called Large ribosomal subunit protein bL25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | u | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 28 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | w | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

- Molecule 29 is a protein called Large ribosomal subunit protein uL29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 29 | x | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 501 | 308 | 98 | 94 | 1 | | |

- Molecule 30 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 30 | y | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 31 is a protein called Rumicidin-2 (12-27).

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 31 | T | 16 | Total | C | N | O | 0 | 0 |
| | | | 143 | 96 | 31 | 16 | | |

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 32 | C | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

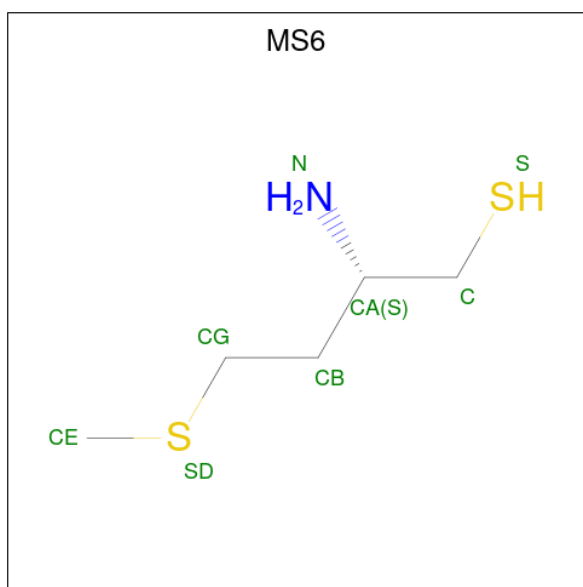
- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|-----|---------|
| 33 | D | 198 | Total | Mg | 0 |
| | | | 198 | 198 | |
| 33 | E | 3 | Total | Mg | 0 |
| | | | 3 | 3 | |
| 33 | F | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 33 | G | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 33 | M | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 34 | D | 88 | Total | K | 0 |
| | | | 88 | 88 | |
| 34 | F | 4 | Total | K | 0 |
| | | | 4 | 4 | |
| 34 | H | 1 | Total | K | 0 |
| | | | 1 | 1 | |

- Molecule 35 is (2S)-2-amino-4-(methylsulfanyl)butane-1-thiol (three-letter code: MS6) (formula: C₅H₁₃NS₂).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 35 | 1 | 1 | Total | C | N | S | 0 |
| | | | 8 | 5 | 1 | 2 | |

- Molecule 36 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|------|---------|
| 36 | 1 | 15 | Total | O | 0 |
| | | | 15 | 15 | |
| 36 | B | 19 | Total | O | 0 |
| | | | 19 | 19 | |
| 36 | C | 3 | Total | O | 0 |
| | | | 3 | 3 | |
| 36 | D | 3780 | Total | O | 0 |
| | | | 3780 | 3780 | |
| 36 | E | 48 | Total | O | 0 |
| | | | 48 | 48 | |

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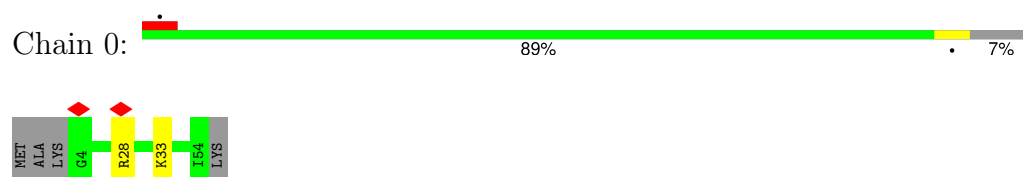
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| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------------|---------|---------|
| 36 | F | 79 | Total 79 | O 79 | 0 |
| 36 | G | 38 | Total 38 | O 38 | 0 |
| 36 | H | 36 | Total 36 | O 36 | 0 |
| 36 | I | 38 | Total 38 | O 38 | 0 |
| 36 | J | 22 | Total 22 | O 22 | 0 |
| 36 | K | 12 | Total 12 | O 12 | 0 |
| 36 | L | 14 | Total 14 | O 14 | 0 |
| 36 | M | 25 | Total 25 | O 25 | 0 |
| 36 | h | 1 | Total 1 | O 1 | 0 |
| 36 | i | 22 | Total 22 | O 22 | 0 |
| 36 | j | 12 | Total 12 | O 12 | 0 |
| 36 | l | 26 | Total 26 | O 26 | 0 |
| 36 | o | 13 | Total 13 | O 13 | 0 |
| 36 | p | 32 | Total 32 | O 32 | 0 |
| 36 | q | 19 | Total 19 | O 19 | 0 |
| 36 | r | 30 | Total 30 | O 30 | 0 |
| 36 | t | 6 | Total 6 | O 6 | 0 |
| 36 | u | 3 | Total 3 | O 3 | 0 |
| 36 | w | 9 | Total 9 | O 9 | 0 |
| 36 | x | 1 | Total 1 | O 1 | 0 |
| 36 | y | 5 | Total 5 | O 5 | 0 |

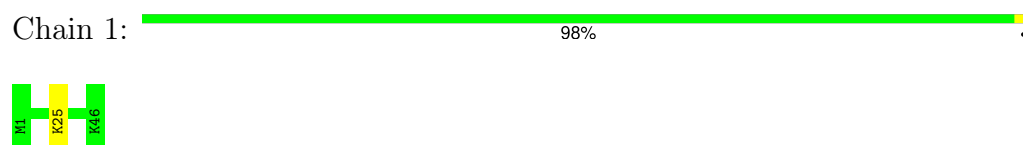
3 Residue-property plots [i](#)

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.

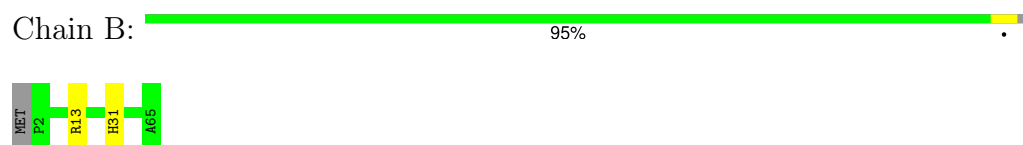
- Molecule 1: 50S ribosomal protein L33



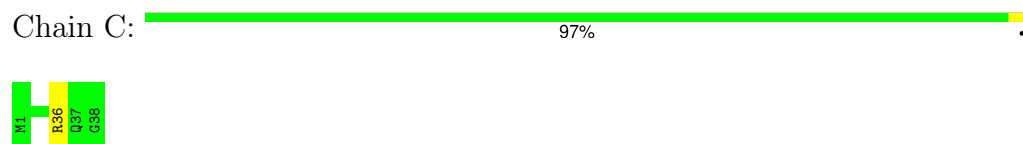
- Molecule 2: 50S ribosomal protein L34



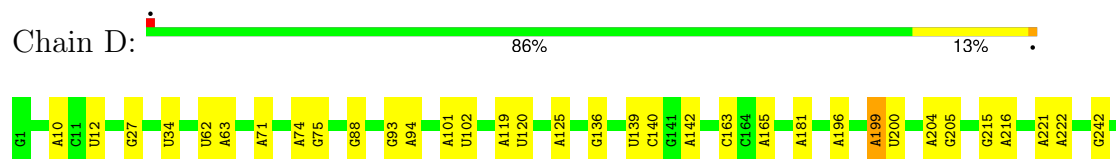
- Molecule 3: 50S ribosomal protein L35

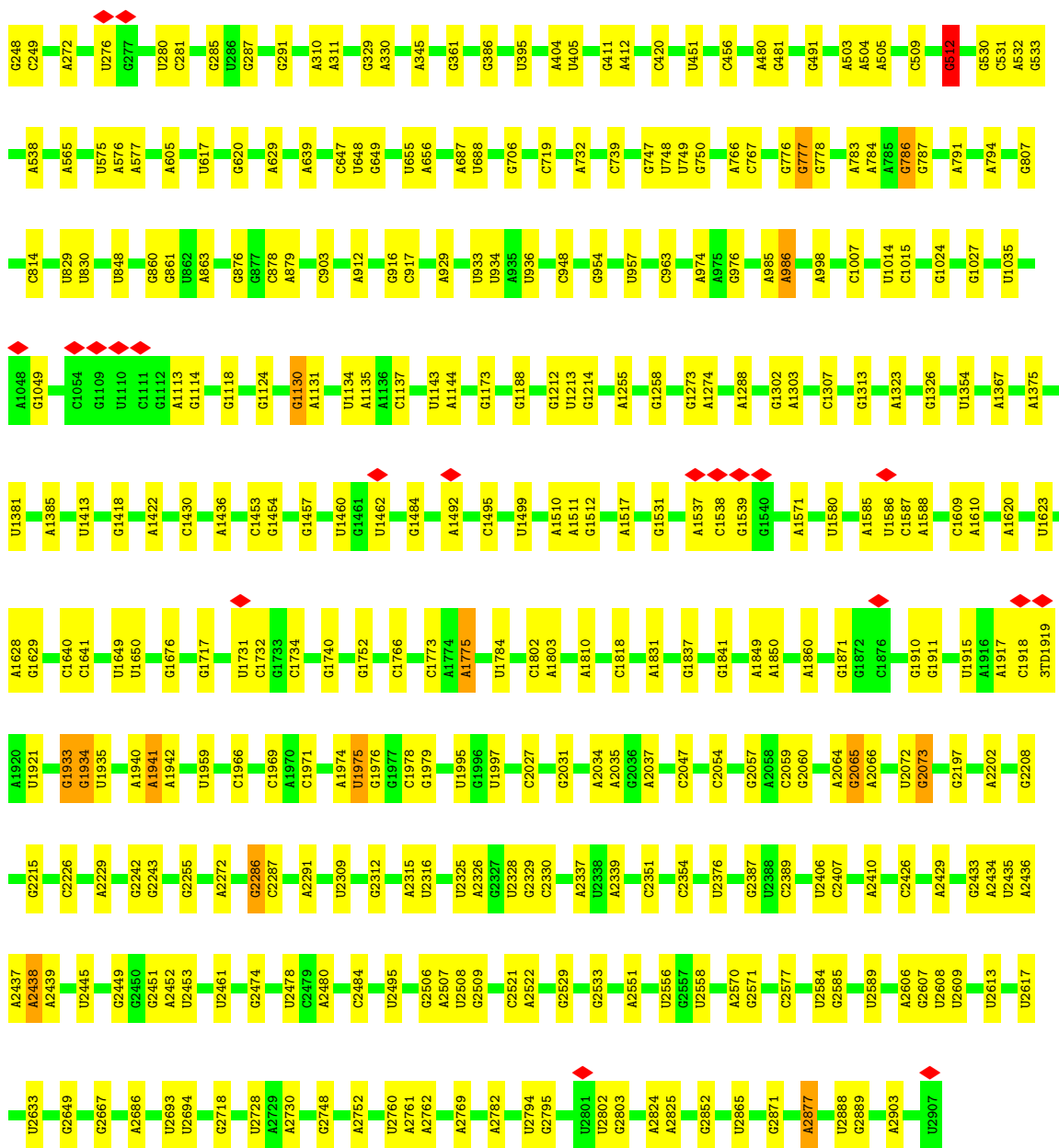


- Molecule 4: 50S ribosomal protein L36



- Molecule 5: 23S rRNA





• Molecule 6: 5S rRNA

Chain E: 88% 12%



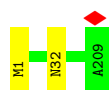
• Molecule 7: 50S ribosomal protein L2

Chain F: 99%



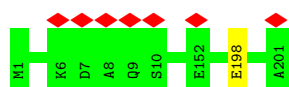
- Molecule 8: 50S ribosomal protein L3

Chain G:  99%



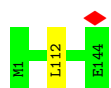
- Molecule 9: 50S ribosomal protein L4

Chain H:  100%



- Molecule 10: 50S ribosomal protein L15

Chain I:  99%



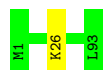
- Molecule 11: 50S ribosomal protein L17

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Large ribosomal subunit protein uL23

Chain K:  99%



- Molecule 13: 50S ribosomal protein L27

Chain L:  100%

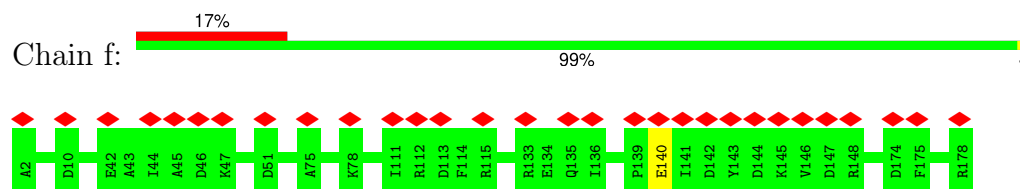


- Molecule 14: 50S ribosomal protein L32

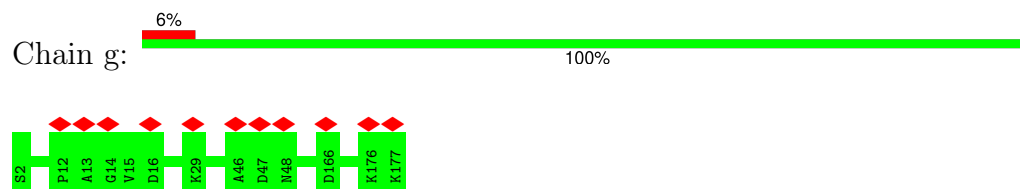
Chain M:  98%



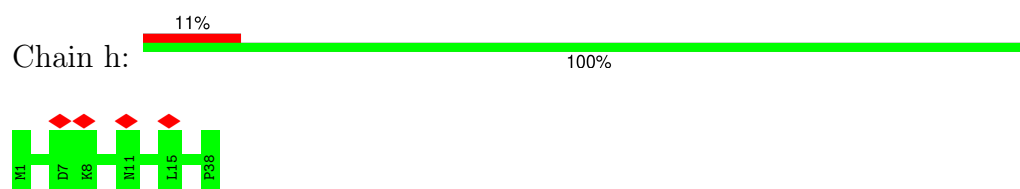
- Molecule 15: 50S ribosomal protein L5



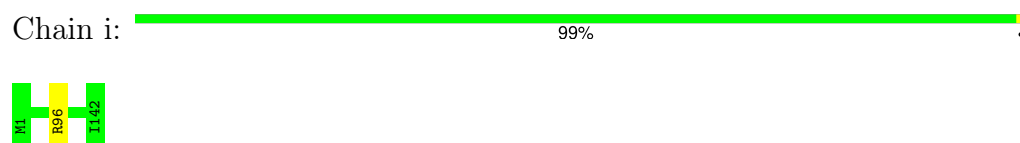
- Molecule 16: Large ribosomal subunit protein uL6



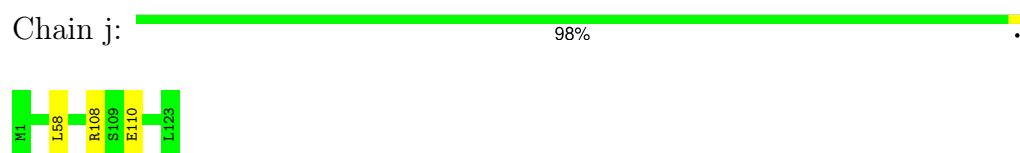
- Molecule 17: 50S ribosomal protein L9



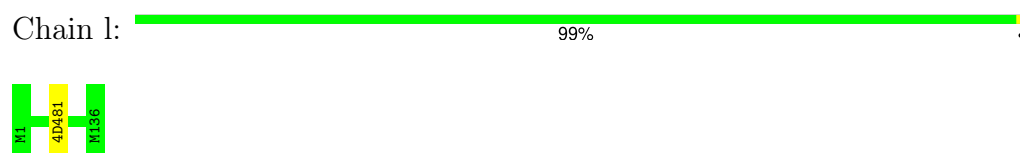
- Molecule 18: Large ribosomal subunit protein uL13



- Molecule 19: 50S ribosomal protein L14

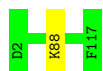


- Molecule 20: 50S ribosomal protein L16



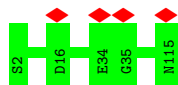
- Molecule 21: 50S ribosomal protein L18





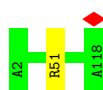
- Molecule 22: 50S ribosomal protein L19

Chain o: 100%



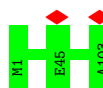
- Molecule 23: Large ribosomal subunit protein bL20

Chain p: 99%



- Molecule 24: 50S ribosomal protein L21

Chain q: 100%



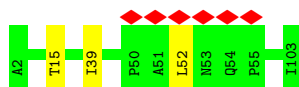
- Molecule 25: 50S ribosomal protein L22

Chain r: 97%



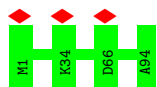
- Molecule 26: Large ribosomal subunit protein uL24

Chain t: 6%
 97%



- Molecule 27: Large ribosomal subunit protein bL25

Chain u: 100%



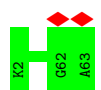
- Molecule 28: 50S ribosomal protein L28

Chain w:  99% .



- Molecule 29: Large ribosomal subunit protein uL29

Chain x:  100%



- Molecule 30: 50S ribosomal protein L30

Chain y:  100%



- Molecule 31: Rumicidin-2 (12-27)

Chain T:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 371000 | 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 ($e^-/\text{\AA}^2$) | 80 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 20000 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 6.240 | Depositor |
| Minimum map value | -0.674 | Depositor |
| Average map value | -0.006 | Depositor |
| Map value standard deviation | 0.274 | Depositor |
| Recommended contour level | 1.1 | Depositor |
| Map size (Å) | 441.856, 441.856, 441.856 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.863, 0.863, 0.863 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MC, OMU, H2U, K, 5MU, MS6, PSU, MG, ZN, G7M, 1MG, MEQ, 6MZ, 2MG, OMG, 3TD, 4D4, 2MA

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 0 | 0.31 | 0/424 | 0.57 | 0/565 |
| 2 | 1 | 0.33 | 0/380 | 0.76 | 0/498 |
| 3 | B | 0.36 | 0/513 | 0.61 | 0/676 |
| 4 | C | 0.32 | 0/303 | 0.71 | 0/397 |
| 5 | D | 0.44 | 0/65057 | 0.98 | 58/101481 (0.1%) |
| 6 | E | 0.44 | 0/2850 | 0.93 | 0/4444 |
| 7 | F | 0.31 | 0/2121 | 0.66 | 0/2852 |
| 8 | G | 0.32 | 0/1576 | 0.60 | 0/2119 |
| 9 | H | 0.30 | 0/1571 | 0.58 | 0/2113 |
| 10 | I | 0.33 | 0/1062 | 0.58 | 0/1413 |
| 11 | J | 0.31 | 0/958 | 0.63 | 0/1281 |
| 12 | K | 0.29 | 0/744 | 0.58 | 0/994 |
| 13 | L | 0.33 | 0/593 | 0.64 | 0/785 |
| 14 | M | 0.33 | 0/450 | 0.65 | 0/599 |
| 15 | f | 0.29 | 0/1434 | 0.53 | 0/1926 |
| 16 | g | 0.29 | 0/1343 | 0.55 | 0/1816 |
| 17 | h | 0.30 | 0/285 | 0.55 | 0/385 |
| 18 | i | 0.30 | 0/1152 | 0.59 | 0/1551 |
| 19 | j | 0.30 | 0/955 | 0.61 | 0/1279 |
| 20 | l | 0.30 | 0/1073 | 0.61 | 0/1433 |
| 21 | n | 0.28 | 0/902 | 0.55 | 0/1209 |
| 22 | o | 0.31 | 0/929 | 0.60 | 0/1242 |
| 23 | p | 0.31 | 0/960 | 0.66 | 0/1278 |
| 24 | q | 0.31 | 0/829 | 0.62 | 0/1107 |
| 25 | r | 0.32 | 0/864 | 0.63 | 0/1156 |
| 26 | t | 0.30 | 0/787 | 0.57 | 0/1051 |
| 27 | u | 0.30 | 0/766 | 0.55 | 0/1025 |
| 28 | w | 0.31 | 0/635 | 0.62 | 0/848 |
| 29 | x | 0.27 | 0/502 | 0.53 | 0/667 |
| 30 | y | 0.29 | 0/453 | 0.59 | 0/605 |
| 31 | T | 0.41 | 0/154 | 0.68 | 0/213 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.41 | 0/92625 | 0.90 | 58/139008 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | B | 0 | 1 |
| 5 | D | 0 | 1 |
| 7 | F | 0 | 1 |
| 28 | w | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

The worst 5 of 58 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 5 | D | 512 | G | O4'-C1'-N9 | 11.65 | 117.52 | 108.20 |
| 5 | D | 576 | A | O5'-P-OP1 | -11.52 | 95.33 | 105.70 |
| 5 | D | 576 | A | O5'-P-OP2 | 9.79 | 122.45 | 110.70 |
| 5 | D | 739 | C | O5'-P-OP2 | -8.59 | 97.97 | 105.70 |
| 5 | D | 739 | C | O5'-P-OP1 | 8.55 | 120.97 | 110.70 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | B | 13 | ARG | Sidechain |
| 5 | D | 512 | G | Sidechain |
| 7 | F | 43 | ARG | Sidechain |
| 28 | w | 16 | ASN | 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 | |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1 | 0 | 49/55 (89%) | 49 (100%) | 0 | 0 | 100 | 100 |
| 2 | 1 | 44/46 (96%) | 44 (100%) | 0 | 0 | 100 | 100 |
| 3 | B | 62/65 (95%) | 60 (97%) | 2 (3%) | 0 | 100 | 100 |
| 4 | C | 36/38 (95%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 7 | F | 269/273 (98%) | 260 (97%) | 9 (3%) | 0 | 100 | 100 |
| 8 | G | 206/209 (99%) | 200 (97%) | 6 (3%) | 0 | 100 | 100 |
| 9 | H | 199/201 (99%) | 194 (98%) | 5 (2%) | 0 | 100 | 100 |
| 10 | I | 142/144 (99%) | 138 (97%) | 4 (3%) | 0 | 100 | 100 |
| 11 | J | 116/118 (98%) | 110 (95%) | 6 (5%) | 0 | 100 | 100 |
| 12 | K | 91/93 (98%) | 89 (98%) | 2 (2%) | 0 | 100 | 100 |
| 13 | L | 76/78 (97%) | 74 (97%) | 2 (3%) | 0 | 100 | 100 |
| 14 | M | 54/56 (96%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 15 | f | 175/177 (99%) | 165 (94%) | 10 (6%) | 0 | 100 | 100 |
| 16 | g | 174/176 (99%) | 160 (92%) | 14 (8%) | 0 | 100 | 100 |
| 17 | h | 36/38 (95%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |
| 18 | i | 140/142 (99%) | 139 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | j | 121/123 (98%) | 116 (96%) | 4 (3%) | 1 (1%) | 16 | 8 |
| 20 | l | 131/135 (97%) | 128 (98%) | 3 (2%) | 0 | 100 | 100 |
| 21 | n | 114/116 (98%) | 108 (95%) | 5 (4%) | 1 (1%) | 14 | 7 |
| 22 | o | 112/114 (98%) | 110 (98%) | 2 (2%) | 0 | 100 | 100 |
| 23 | p | 115/117 (98%) | 115 (100%) | 0 | 0 | 100 | 100 |
| 24 | q | 101/103 (98%) | 100 (99%) | 1 (1%) | 0 | 100 | 100 |
| 25 | r | 108/110 (98%) | 107 (99%) | 1 (1%) | 0 | 100 | 100 |
| 26 | t | 100/102 (98%) | 96 (96%) | 3 (3%) | 1 (1%) | 13 | 5 |
| 27 | u | 92/94 (98%) | 91 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 28 | w | 75/77 (97%) | 75 (100%) | 0 | 0 | 100 | 100 |
| 29 | x | 60/62 (97%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 30 | y | 56/58 (97%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 31 | T | 14/16 (88%) | 12 (86%) | 2 (14%) | 0 | 100 | 100 |
| All | All | 3068/3136 (98%) | 2977 (97%) | 88 (3%) | 3 (0%) | 50 | 42 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | j | 108 | ARG |
| 21 | n | 88 | LYS |
| 26 | t | 39 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | 0 | 46/49 (94%) | 44 (96%) | 2 (4%) | 25 | 14 |
| 2 | 1 | 38/38 (100%) | 37 (97%) | 1 (3%) | 41 | 33 |
| 3 | B | 51/52 (98%) | 50 (98%) | 1 (2%) | 50 | 44 |
| 4 | C | 34/34 (100%) | 33 (97%) | 1 (3%) | 37 | 28 |
| 7 | F | 216/218 (99%) | 216 (100%) | 0 | 100 | 100 |
| 8 | G | 163/163 (100%) | 161 (99%) | 2 (1%) | 67 | 65 |
| 9 | H | 165/165 (100%) | 164 (99%) | 1 (1%) | 84 | 83 |
| 10 | I | 103/103 (100%) | 102 (99%) | 1 (1%) | 73 | 72 |
| 11 | J | 98/98 (100%) | 98 (100%) | 0 | 100 | 100 |
| 12 | K | 80/80 (100%) | 79 (99%) | 1 (1%) | 65 | 62 |
| 13 | L | 58/59 (98%) | 58 (100%) | 0 | 100 | 100 |
| 14 | M | 47/47 (100%) | 46 (98%) | 1 (2%) | 48 | 43 |
| 15 | f | 148/148 (100%) | 147 (99%) | 1 (1%) | 81 | 81 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 16 | g | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 17 | h | 30/30 (100%) | 30 (100%) | 0 | 100 | 100 |
| 18 | i | 116/116 (100%) | 115 (99%) | 1 (1%) | 75 | 75 |
| 19 | j | 104/104 (100%) | 102 (98%) | 2 (2%) | 52 | 47 |
| 20 | l | 107/107 (100%) | 107 (100%) | 0 | 100 | 100 |
| 21 | n | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 22 | o | 99/99 (100%) | 99 (100%) | 0 | 100 | 100 |
| 23 | p | 89/89 (100%) | 88 (99%) | 1 (1%) | 70 | 68 |
| 24 | q | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 25 | r | 93/93 (100%) | 90 (97%) | 3 (3%) | 34 | 24 |
| 26 | t | 83/83 (100%) | 81 (98%) | 2 (2%) | 44 | 37 |
| 27 | u | 78/78 (100%) | 78 (100%) | 0 | 100 | 100 |
| 28 | w | 67/67 (100%) | 67 (100%) | 0 | 100 | 100 |
| 29 | x | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |
| 30 | y | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 31 | T | 16/16 (100%) | 16 (100%) | 0 | 100 | 100 |
| All | All | 2538/2545 (100%) | 2517 (99%) | 21 (1%) | 77 | 78 |

5 of 21 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | j | 110 | GLU |
| 25 | r | 83 | LYS |
| 26 | t | 52 | LEU |
| 25 | r | 92 | ARG |
| 25 | r | 82 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | H | 9 | GLN |
| 10 | I | 104 | GLN |
| 14 | M | 42 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 5 | D | 2717/2728 (99%) | 302 (11%) | 47 (1%) |
| 6 | E | 118/119 (99%) | 14 (11%) | 1 (0%) |
| All | All | 2835/2847 (99%) | 316 (11%) | 48 (1%) |

5 of 316 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | D | 10 | A |
| 5 | D | 12 | U |
| 5 | D | 34 | U |
| 5 | D | 63 | A |
| 5 | D | 71 | A |

5 of 48 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 5 | D | 1585 | A |
| 5 | D | 2315 | A |
| 5 | D | 1628 | A |
| 5 | D | 1917 | A |
| 5 | D | 2406 | U |

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

26 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 | $\# Z > 2$ |
| 8 | MEQ | G | 150 | 8 | 8,9,10 | 0.49 | 0 | 5,10,12 | 0.65 | 0 |
| 5 | G7M | D | 2073 | 5,34 | 20,26,27 | 1.20 | 3 (15%) | 16,39,42 | 0.35 | 0 |
| 5 | PSU | D | 2584 | 5 | 18,21,22 | 0.94 | 1 (5%) | 21,30,33 | 0.81 | 0 |
| 5 | 1MG | D | 747 | 5 | 19,26,27 | 1.16 | 2 (10%) | 18,39,42 | 0.68 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | PSU | D | 2609 | 5 | 18,21,22 | 0.96 | 1 (5%) | 21,30,33 | 0.90 | 1 (4%) |
| 5 | 5MU | D | 749 | 5 | 19,22,23 | 0.28 | 0 | 27,32,35 | 0.51 | 0 |
| 5 | PSU | D | 1915 | 5 | 18,21,22 | 0.96 | 1 (5%) | 21,30,33 | 0.62 | 0 |
| 5 | 6MZ | D | 2034 | 5 | 17,25,26 | 1.12 | 2 (11%) | 15,36,39 | 0.95 | 1 (6%) |
| 5 | PSU | D | 748 | 33,5 | 18,21,22 | 0.97 | 1 (5%) | 21,30,33 | 0.66 | 0 |
| 5 | 2MG | D | 2449 | 5 | 18,26,27 | 1.11 | 3 (16%) | 16,38,41 | 0.85 | 1 (6%) |
| 5 | 2MA | D | 2507 | 33,5,34 | 18,25,26 | 1.04 | 1 (5%) | 20,37,40 | 1.58 | 5 (25%) |
| 5 | PSU | D | 2608 | 5 | 18,21,22 | 0.99 | 1 (5%) | 21,30,33 | 0.87 | 1 (4%) |
| 5 | H2U | D | 2453 | 5 | 18,21,22 | 0.62 | 0 | 19,30,33 | 0.97 | 2 (10%) |
| 5 | 5MC | D | 1966 | 5,34 | 19,22,23 | 0.64 | 1 (5%) | 26,32,35 | 0.47 | 0 |
| 5 | PSU | D | 2508 | 5,34 | 18,21,22 | 0.94 | 1 (5%) | 21,30,33 | 0.93 | 0 |
| 5 | PSU | D | 1921 | 5 | 18,21,22 | 0.97 | 1 (5%) | 21,30,33 | 0.63 | 0 |
| 5 | 5MU | D | 1943 | 5,34 | 19,22,23 | 0.33 | 0 | 27,32,35 | 0.53 | 0 |
| 5 | OMG | D | 2255 | 5,34 | 19,26,27 | 1.05 | 1 (5%) | 21,38,41 | 0.73 | 1 (4%) |
| 5 | OMU | D | 2556 | 5 | 19,22,23 | 0.26 | 0 | 25,31,34 | 0.58 | 1 (4%) |
| 5 | 3TD | D | 1919 | 5 | 19,22,23 | 1.26 | 2 (10%) | 23,32,35 | 0.76 | 0 |
| 5 | 6MZ | D | 1620 | 5 | 17,25,26 | 1.04 | 2 (11%) | 15,36,39 | 0.82 | 1 (6%) |
| 5 | 2MG | D | 1837 | 5 | 18,26,27 | 1.09 | 1 (5%) | 16,38,41 | 0.83 | 1 (6%) |
| 5 | PSU | D | 957 | 5 | 18,21,22 | 0.91 | 1 (5%) | 21,30,33 | 0.74 | 0 |
| 20 | 4D4 | l | 81 | 20 | 9,11,12 | 0.53 | 0 | 7,13,15 | 1.06 | 1 (14%) |
| 5 | OMC | D | 2502 | 33,5 | 19,22,23 | 0.29 | 0 | 25,31,34 | 0.59 | 0 |
| 5 | PSU | D | 2461 | 5 | 18,21,22 | 0.96 | 1 (5%) | 21,30,33 | 0.71 | 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 |
|-----|------|-------|------|------|---------|-----------|---------|
| 8 | MEQ | G | 150 | 8 | - | 3/8/9/11 | - |
| 5 | G7M | D | 2073 | 5,34 | - | 1/3/25/26 | 0/3/3/3 |
| 5 | PSU | D | 2584 | 5 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | 1MG | D | 747 | 5 | - | 0/3/25/26 | 0/3/3/3 |
| 5 | PSU | D | 2609 | 5 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | 5MU | D | 749 | 5 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | PSU | D | 1915 | 5 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | 6MZ | D | 2034 | 5 | - | 2/5/27/28 | 0/3/3/3 |
| 5 | PSU | D | 748 | 33,5 | - | 2/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|------------|---------|
| 5 | 2MG | D | 2449 | 5 | - | 0/5/27/28 | 0/3/3/3 |
| 5 | 2MA | D | 2507 | 33,5,34 | - | 1/3/25/26 | 0/3/3/3 |
| 5 | PSU | D | 2608 | 5 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | H2U | D | 2453 | 5 | - | 0/7/38/39 | 0/2/2/2 |
| 5 | 5MC | D | 1966 | 5,34 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | PSU | D | 2508 | 5,34 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | PSU | D | 1921 | 5 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | 5MU | D | 1943 | 5,34 | - | 0/7/25/26 | 0/2/2/2 |
| 5 | OMG | D | 2255 | 5,34 | - | 0/5/27/28 | 0/3/3/3 |
| 5 | OMU | D | 2556 | 5 | - | 0/9/27/28 | 0/2/2/2 |
| 5 | 3TD | D | 1919 | 5 | - | 2/7/25/26 | 0/2/2/2 |
| 5 | 6MZ | D | 1620 | 5 | - | 0/5/27/28 | 0/3/3/3 |
| 5 | 2MG | D | 1837 | 5 | - | 0/5/27/28 | 0/3/3/3 |
| 5 | PSU | D | 957 | 5 | - | 0/7/25/26 | 0/2/2/2 |
| 20 | 4D4 | l | 81 | 20 | - | 1/11/12/14 | - |
| 5 | OMC | D | 2502 | 33,5 | - | 0/9/27/28 | 0/2/2/2 |
| 5 | PSU | D | 2461 | 5 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 27 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 5 | D | 1919 | 3TD | C6-C5 | 3.89 | 1.39 | 1.35 |
| 5 | D | 1921 | PSU | C6-C5 | 3.81 | 1.39 | 1.35 |
| 5 | D | 1915 | PSU | C6-C5 | 3.81 | 1.39 | 1.35 |
| 5 | D | 2608 | PSU | C6-C5 | 3.80 | 1.39 | 1.35 |
| 5 | D | 748 | PSU | C6-C5 | 3.79 | 1.39 | 1.35 |

The worst 5 of 16 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5 | D | 2507 | 2MA | C5-C6-N6 | 3.75 | 126.03 | 120.31 |
| 5 | D | 2507 | 2MA | CM2-C2-N1 | 3.46 | 122.31 | 117.13 |
| 5 | D | 2453 | H2U | O2-C2-N1 | -2.99 | 119.51 | 123.10 |
| 5 | D | 2507 | 2MA | C5-C6-N1 | -2.82 | 117.50 | 120.84 |
| 20 | l | 81 | 4D4 | O-C-CA | -2.62 | 118.04 | 124.77 |

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 5 | D | 1919 | 3TD | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 8 | G | 150 | MEQ | NE2-CD-CG-CB |
| 8 | G | 150 | MEQ | OE1-CD-CG-CB |
| 5 | D | 1919 | 3TD | C3'-C4'-C5'-O5' |
| 5 | D | 2034 | 6MZ | O4'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 299 ligands modelled in this entry, 298 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 | $\# Z > 2$ |
| 35 | MS6 | 1 | 201 | - | 7,7,7 | 0.57 | 0 | 7,7,7 | 0.62 | 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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 35 | MS6 | 1 | 201 | - | - | 1/4/6/6 | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 35 | 1 | 201 | MS6 | CB-CG-SD-CE |

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 5 | D | 6 |
| 20 | 1 | 1 |

The worst 5 of 7 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | D | 880:A | O3' | 901:A | P | 17.61 |
| 1 | D | 544:G | O3' | 551:C | P | 17.04 |
| 1 | D | 1054:C | O3' | 1109:G | P | 17.03 |
| 1 | D | 2102:U | O3' | 2195:A | P | 16.99 |
| 1 | D | 1174:C | O3' | 1179:G | P | 15.94 |

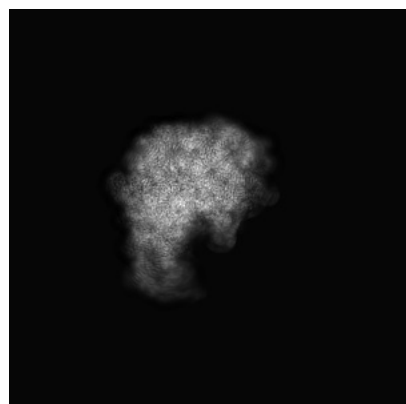
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46632. These allow visual inspection of the internal detail of the map and identification of artifacts.

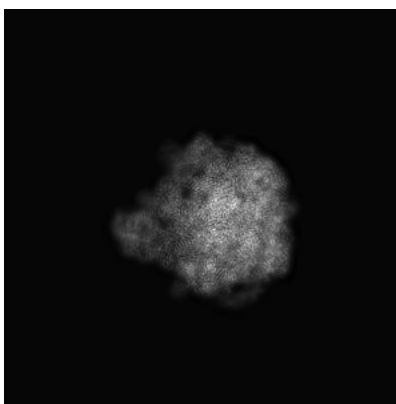
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

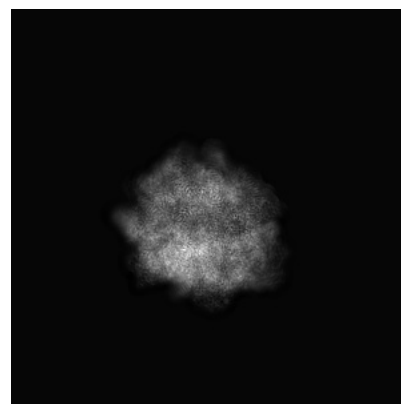
6.1.1 Primary map



X

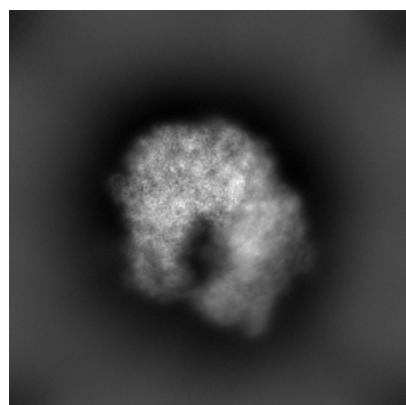


Y

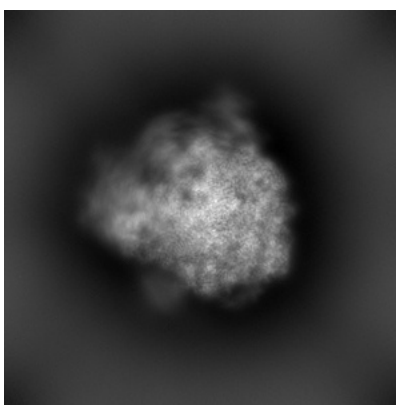


Z

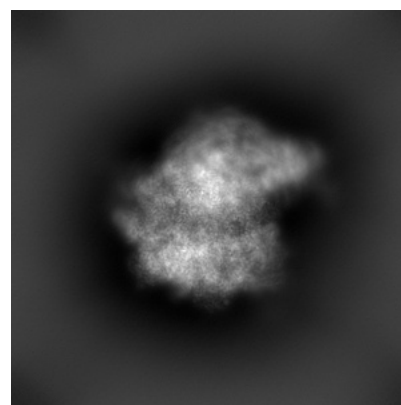
6.1.2 Raw map



X



Y

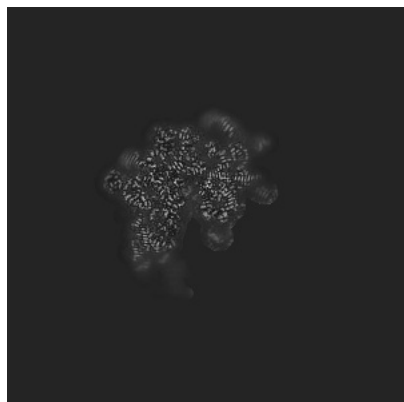


Z

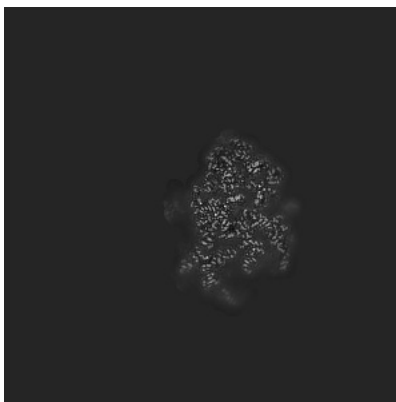
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

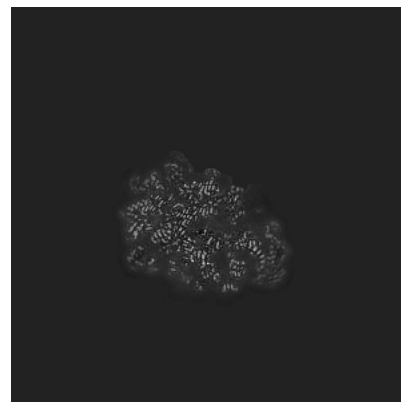
6.2.1 Primary map



X Index: 256

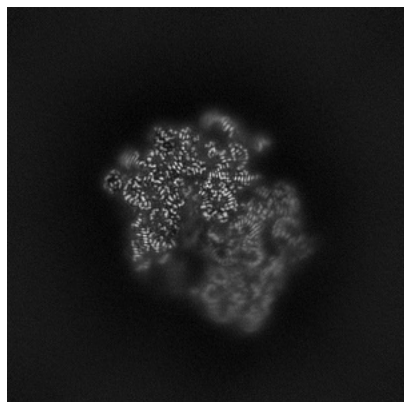


Y Index: 256

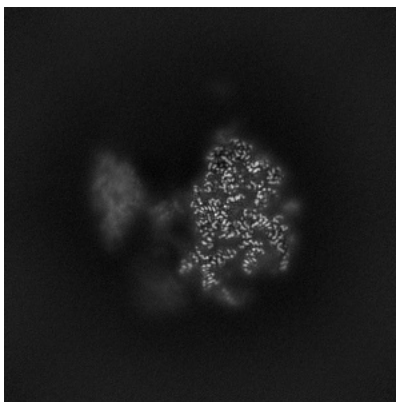


Z Index: 256

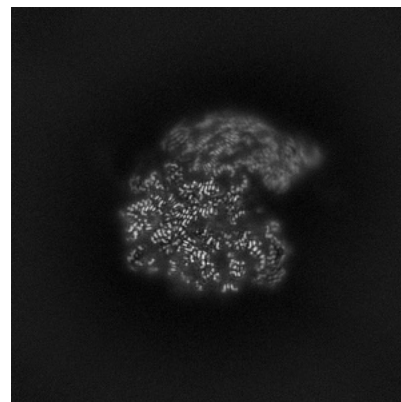
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

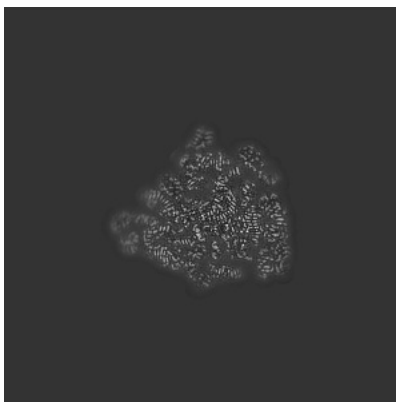
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

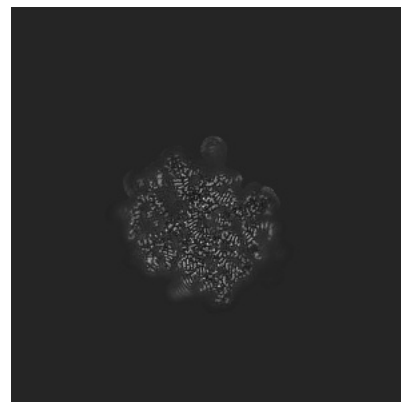
6.3.1 Primary map



X Index: 225

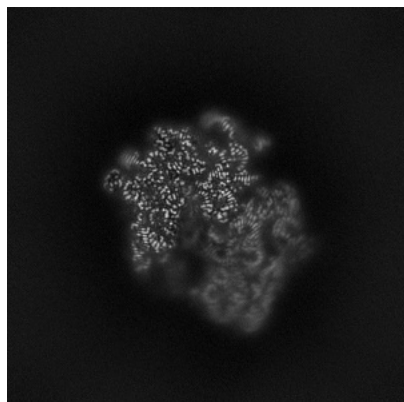


Y Index: 199

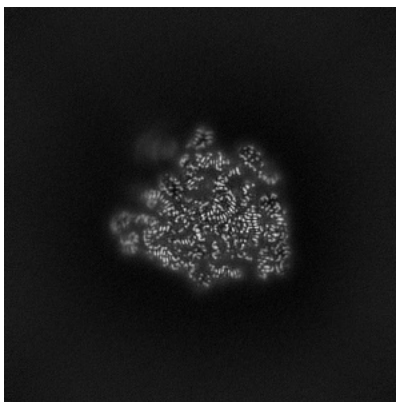


Z Index: 270

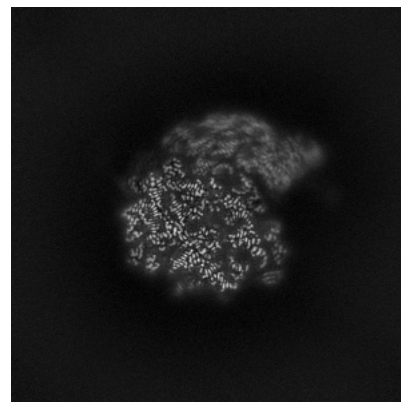
6.3.2 Raw map



X Index: 255



Y Index: 199

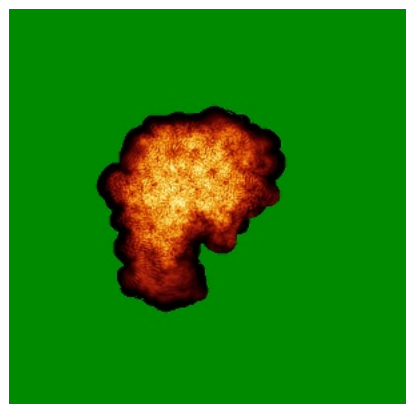


Z Index: 261

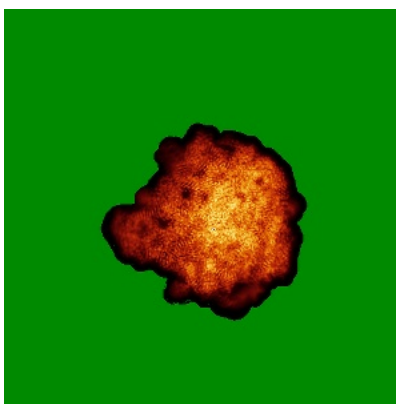
The images above show the largest variance slices of the map in three orthogonal directions.

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

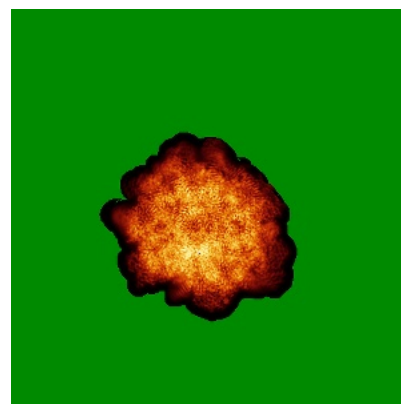
6.4.1 Primary map



X

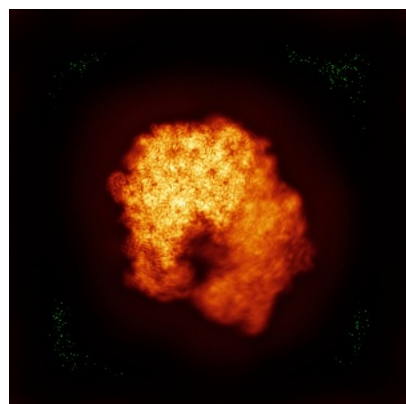


Y

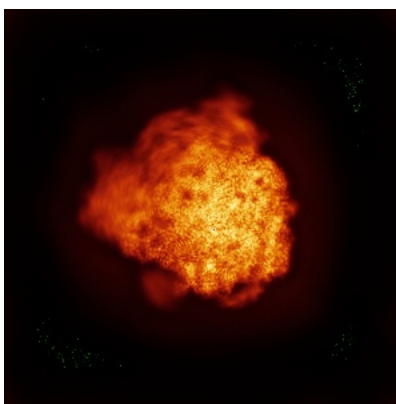


Z

6.4.2 Raw map



X



Y

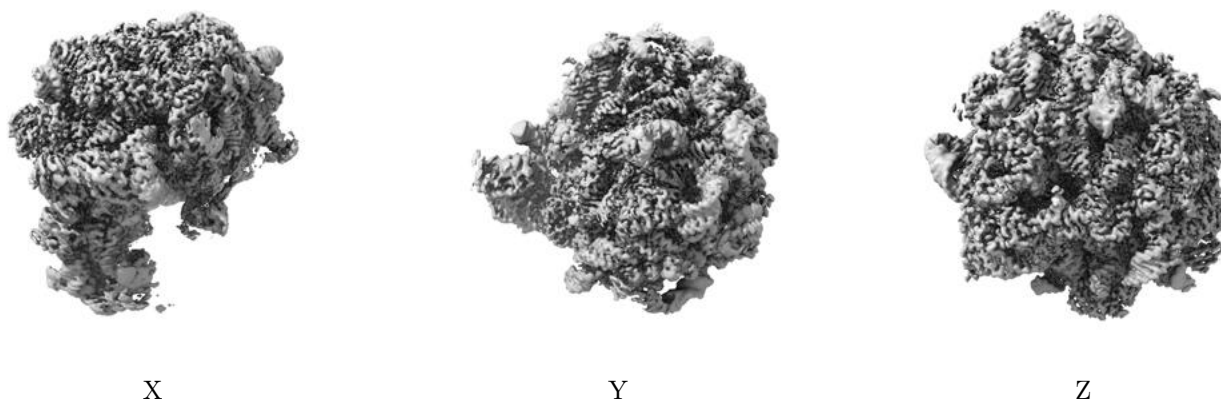


Z

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 1.1. 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



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.

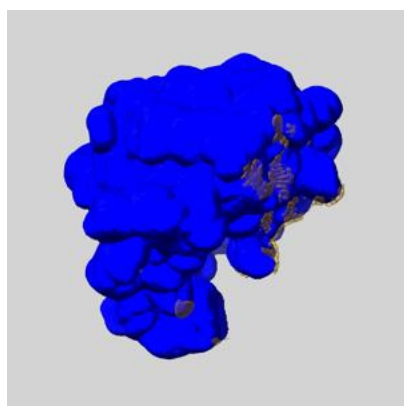
6.6 Mask visualisation [i](#)

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

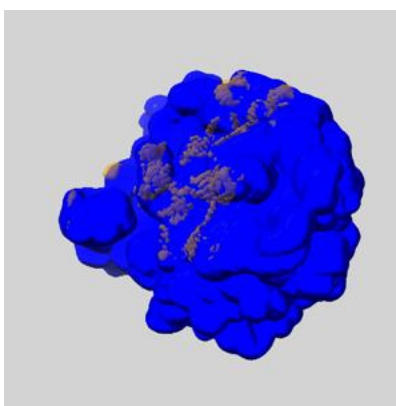
A mask typically either:

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

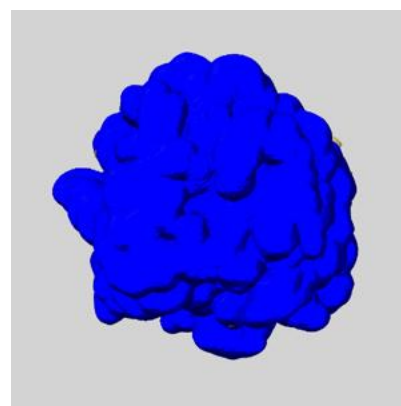
6.6.1 emd_46632_msk_1.map [i](#)



X



Y

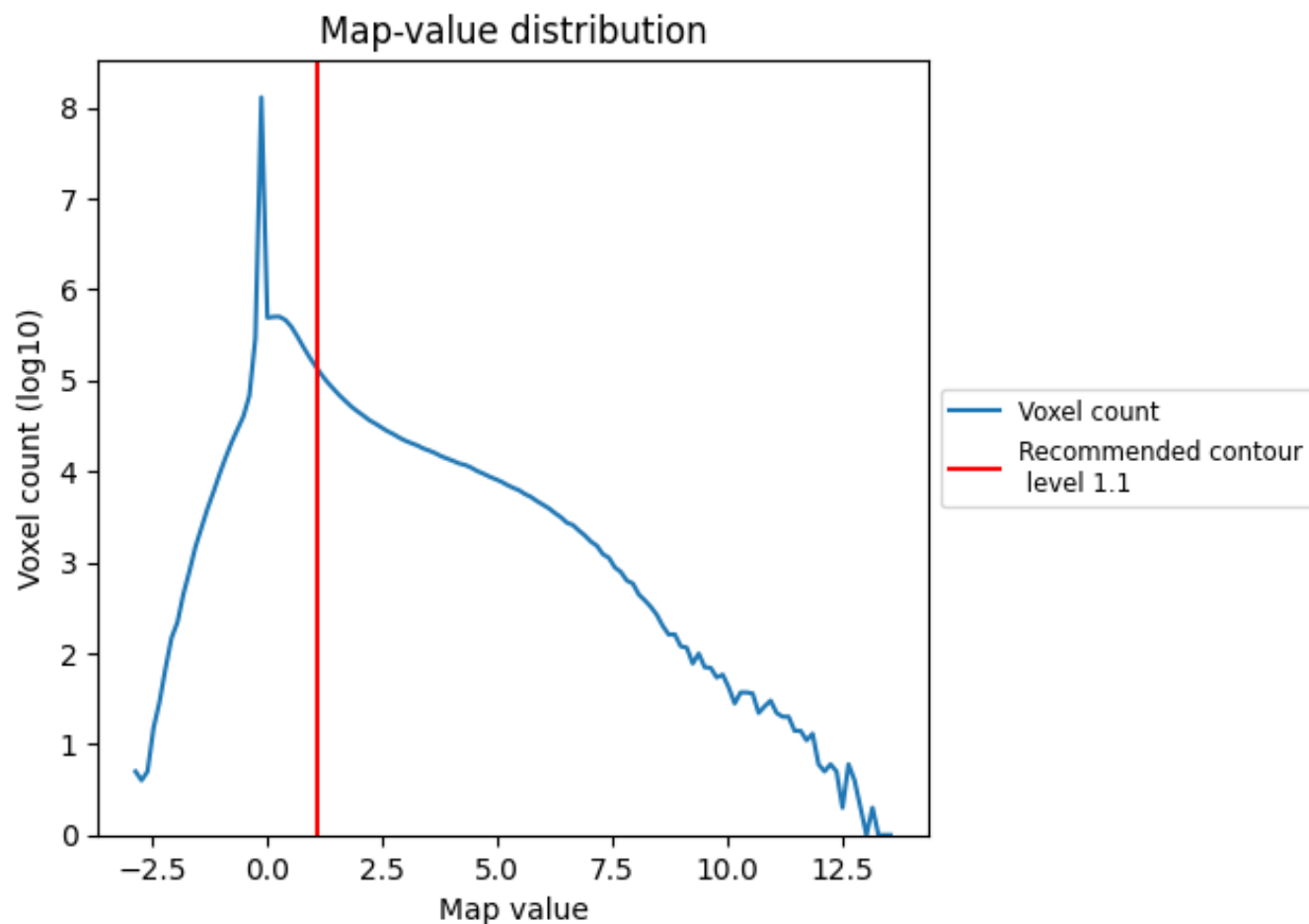


Z

7 Map analysis [i](#)

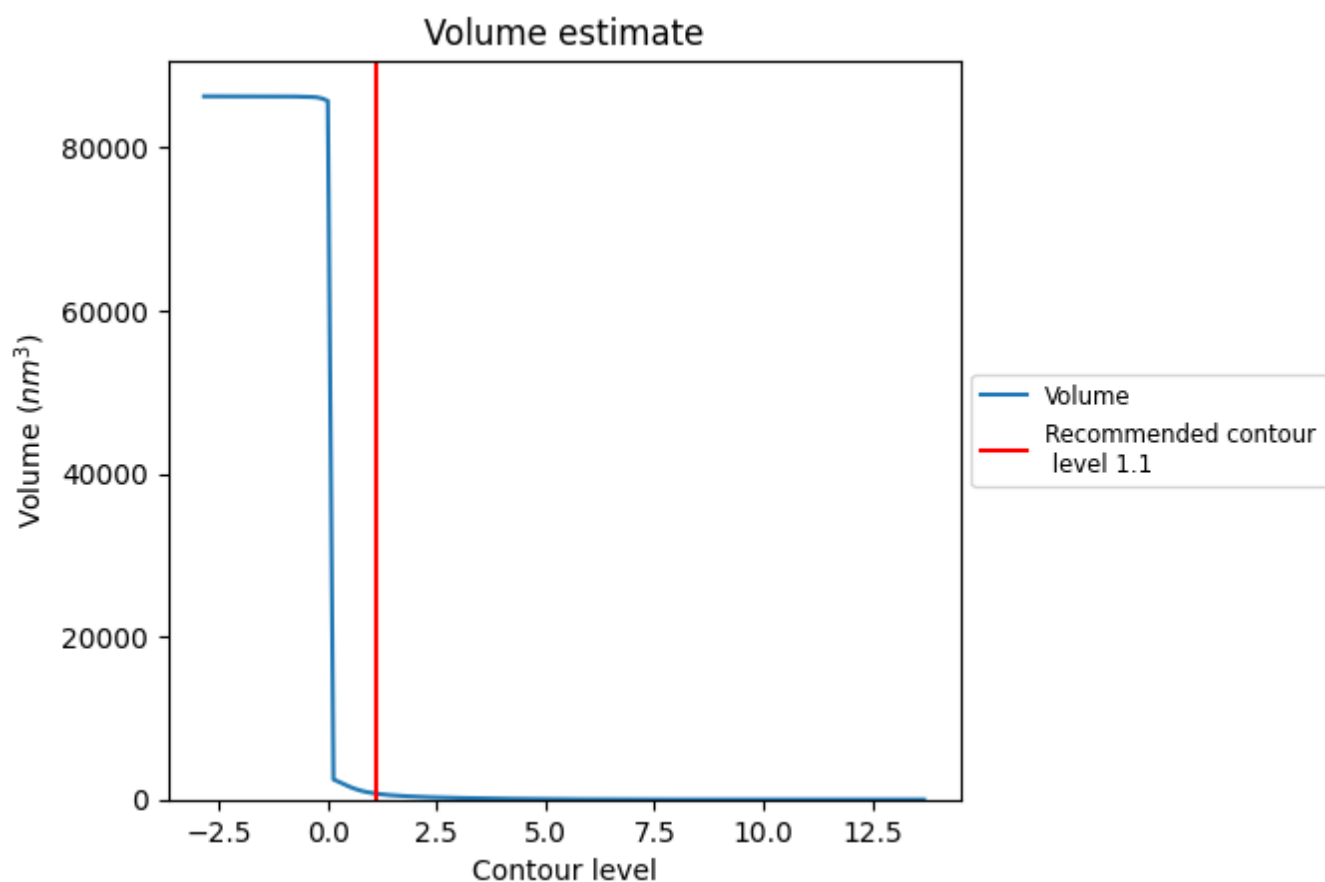
This section contains the results of statistical analysis of the map.

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.

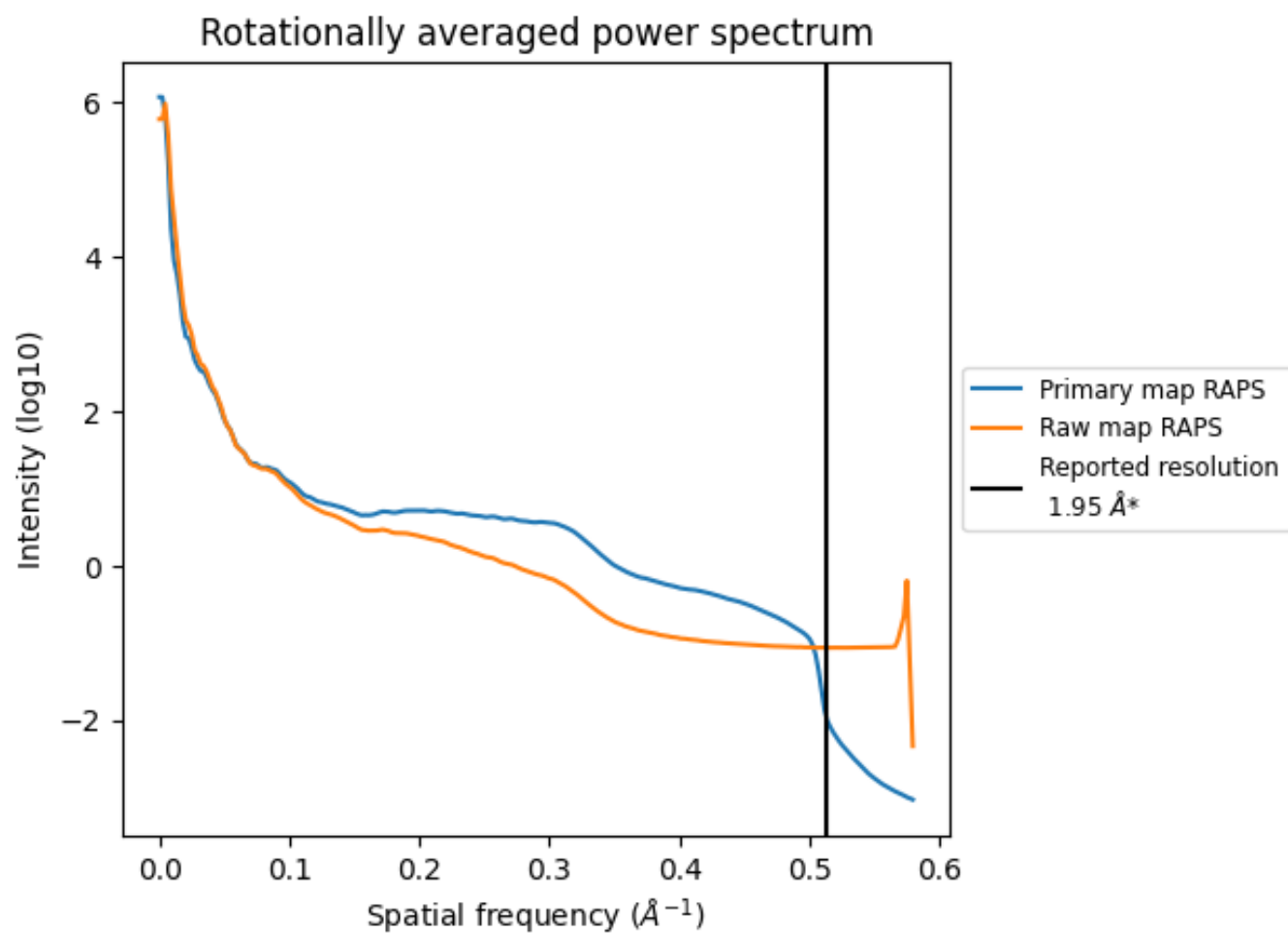
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 734 nm³; this corresponds to an approximate mass of 663 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 ⓘ

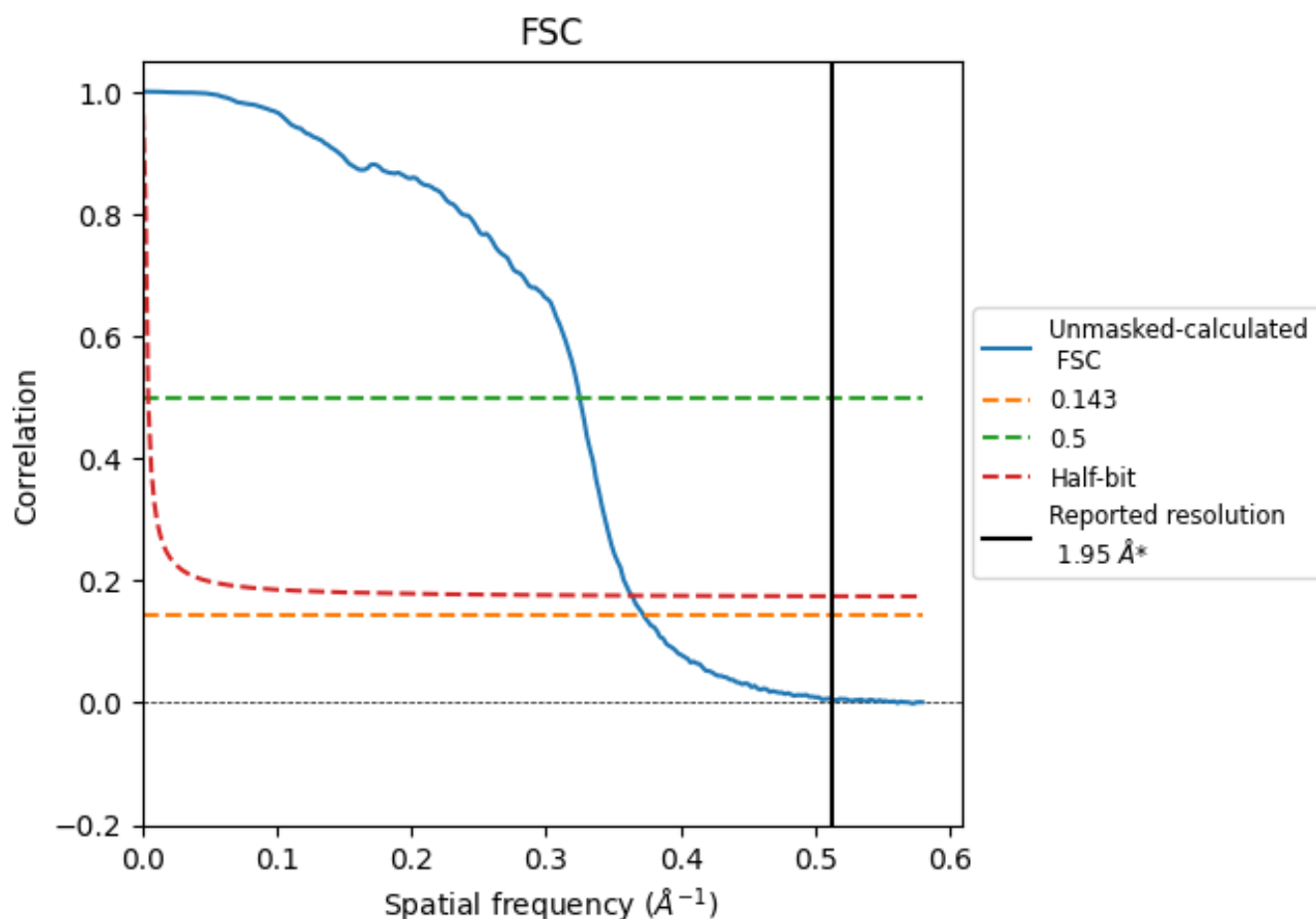


*Reported resolution corresponds to spatial frequency of 0.513 Å⁻¹

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 0.513 Å⁻¹

8.2 Resolution estimates [i](#)

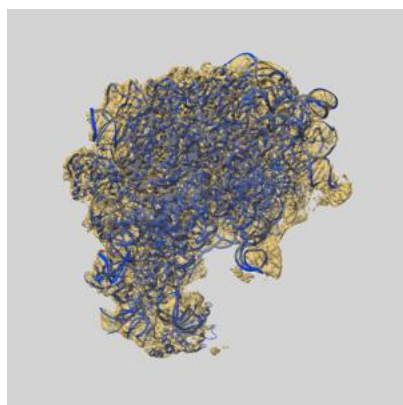
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 1.95 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 2.69 | 3.08 | 2.75 |

*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 2.69 differs from the reported value 1.95 by more than 10 %

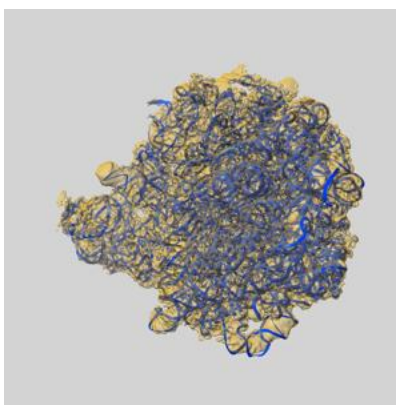
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46632 and PDB model 9D89. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

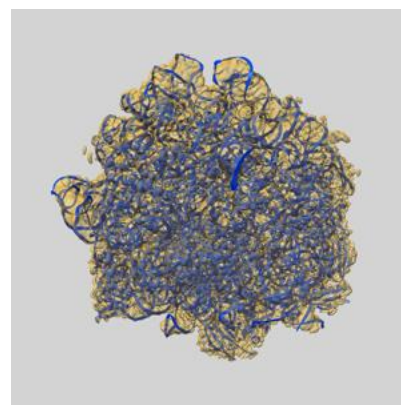
9.1 Map-model overlay [i](#)



X



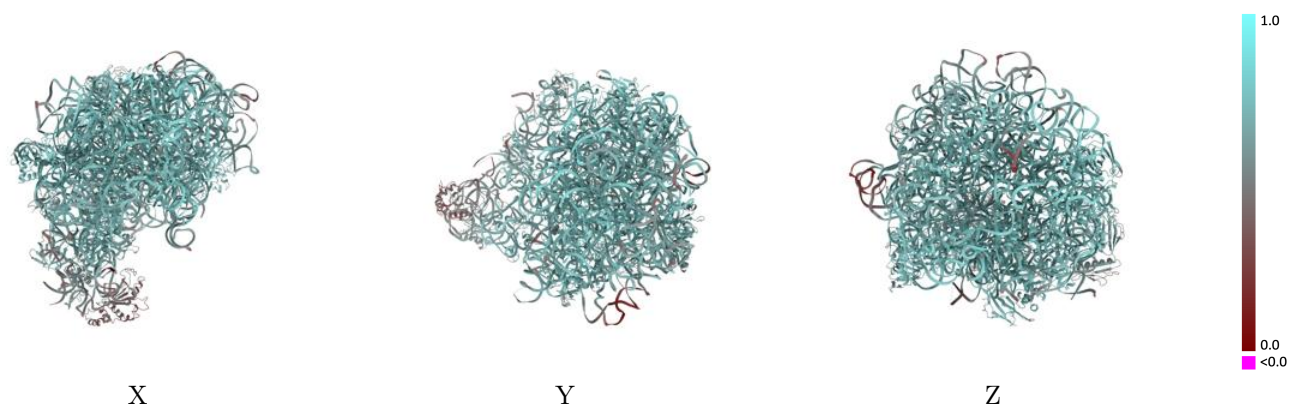
Y



Z

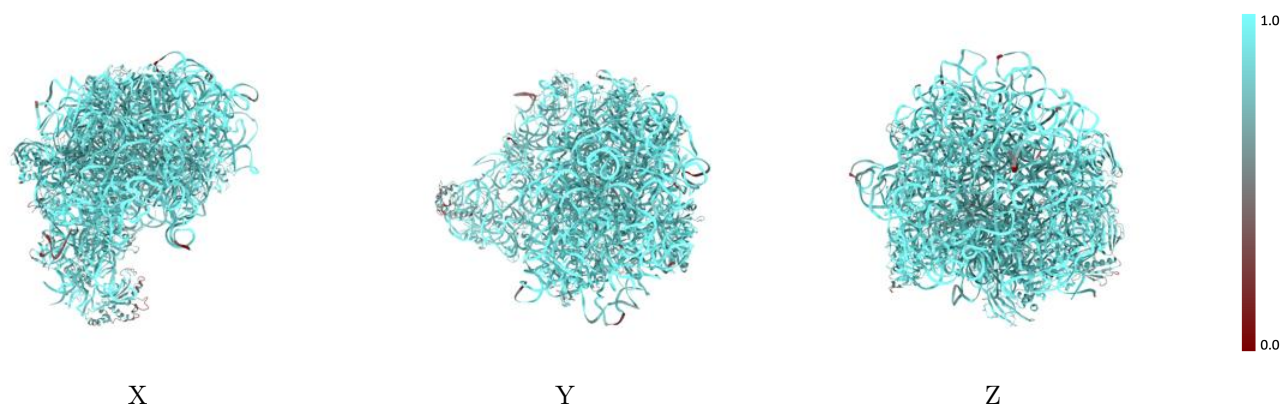
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



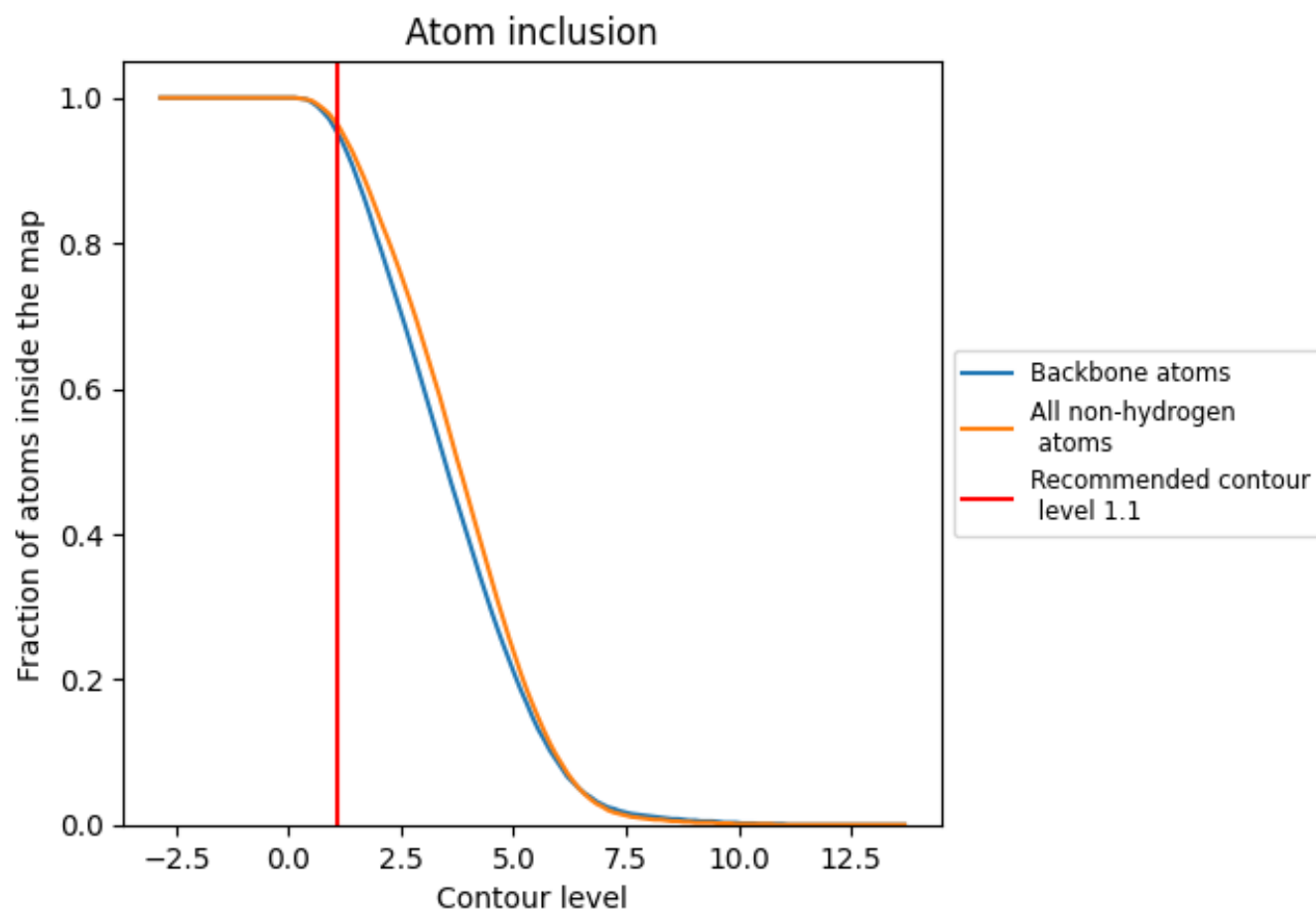
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (1.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9620 |  0.6920 |
| 0 |  0.8700 |  0.6750 |
| 1 |  0.9830 |  0.7710 |
| B |  0.9800 |  0.7500 |
| C |  0.9490 |  0.6780 |
| D |  0.9820 |  0.7030 |
| E |  0.9720 |  0.5670 |
| F |  0.9700 |  0.7390 |
| G |  0.9550 |  0.7310 |
| H |  0.9060 |  0.6970 |
| I |  0.9500 |  0.7180 |
| J |  0.9870 |  0.7540 |
| K |  0.9320 |  0.6860 |
| L |  0.9340 |  0.7110 |
| M |  0.9300 |  0.7110 |
| T |  0.9480 |  0.6340 |
| f |  0.6500 |  0.3860 |
| g |  0.8100 |  0.5610 |
| h |  0.7600 |  0.6050 |
| i |  0.9590 |  0.7320 |
| j |  0.9510 |  0.7200 |
| l |  0.9520 |  0.7160 |
| n |  0.8880 |  0.5800 |
| o |  0.9050 |  0.6980 |
| p |  0.9810 |  0.7630 |
| q |  0.9250 |  0.6980 |
| r |  0.9460 |  0.7250 |
| t |  0.8890 |  0.6570 |
| u |  0.8650 |  0.6340 |
| w |  0.9430 |  0.7000 |
| x |  0.8920 |  0.6470 |
| y |  0.9180 |  0.7170 |

