



## Full wwPDB EM Validation Report ⓘ

Jun 23, 2021 – 06:27 AM BST

PDB ID : 7OF7  
EMDB ID : EMD-12872  
Title : Structure of a human mitochondrial ribosome large subunit assembly intermediate in complex with MTERF4-NSUN4 and GTPBP5 (dataset1).  
Authors : Hillen, H.S.; Lavdovskaia, E.; Nadler, F.; Hanitsch, E.; Linden, A.; Bohnsack, K.E.; Urlaub, H.; Richter-Dennerlein, R.  
Deposited on : 2021-05-04  
Resolution : 2.50 Å (reported)  
Based on initial model : 5OOL

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

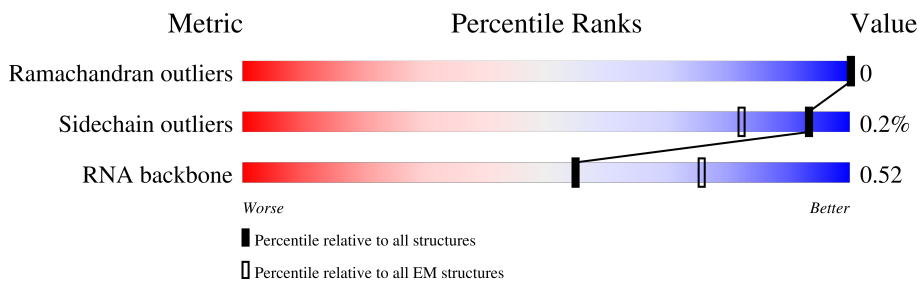
EMDB validation analysis : 0.0.0.dev75  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.20

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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.















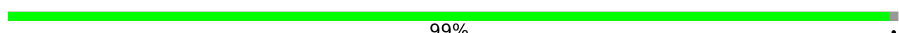

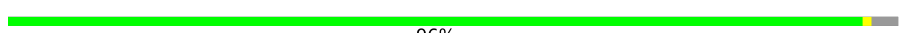







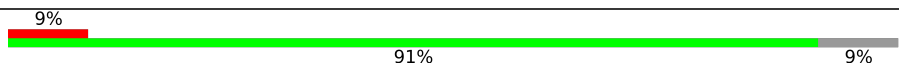


| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |
| RNA backbone          | 4643                        | 859                         |

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  $\geq 3$ , 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     | 108    | 100%             |
| 2   | 1     | 65     | 80% 20%          |
| 3   | 2     | 92     | 49% 51%          |
| 4   | 3     | 188    | 51% 49%          |
| 5   | 4     | 103    | 36% 64%          |
| 6   | 5     | 423    | 92% 7%           |
| 7   | 6     | 380    | 85% 15%          |
| 8   | 7     | 338    | 85% 15%          |

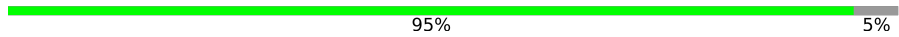








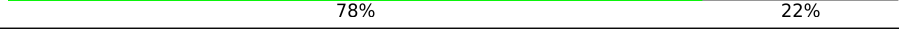
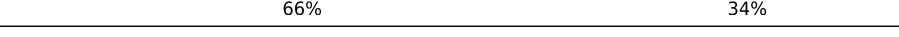

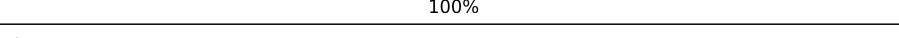
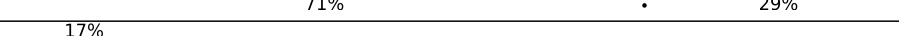
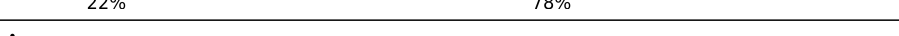


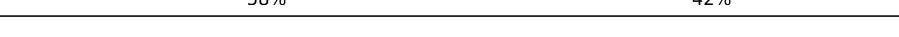
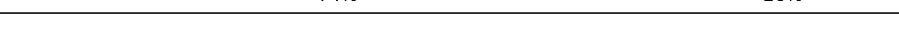

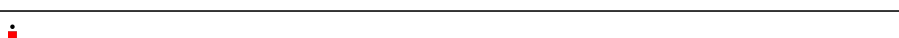

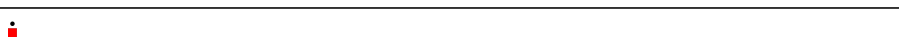
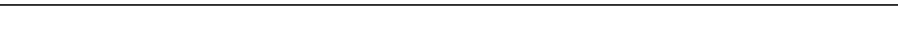
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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 9   | 8     | 206    |    |
| 10  | 9     | 137    |    |
| 11  | A     | 1559   |    |
| 12  | B     | 69     |    |
| 13  | C     | 384    |    |
| 14  | D     | 305    |    |
| 15  | E     | 348    |    |
| 16  | F     | 311    |    |
| 17  | G     | 381    |    |
| 18  | H     | 267    |    |
| 19  | I     | 261    |    |
| 20  | J     | 192    |   |
| 21  | K     | 178    |  |
| 22  | L     | 145    |  |
| 23  | M     | 296    |  |
| 24  | N     | 251    |  |
| 25  | O     | 175    |  |
| 26  | P     | 180    |  |
| 27  | Q     | 292    |  |
| 28  | R     | 149    |  |
| 29  | S     | 205    |  |
| 30  | T     | 206    |  |
| 31  | U     | 153    |  |
| 32  | V     | 216    |  |
| 33  | W     | 148    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 34  | X     | 256    |  95% 5%        |
| 35  | Y     | 250    |  70% 30%       |
| 36  | Z     | 161    |  71% 29%       |
| 37  | a     | 142    |  50% 50%       |
| 38  | b     | 215    |  69% 31%       |
| 39  | c     | 332    |  83% 17%       |
| 40  | d     | 306    |  13% 65% 35%   |
| 41  | e     | 279    |  59% 71% 29%   |
| 42  | f     | 212    |  26% 51% 49%   |
| 43  | g     | 166    |  78% 22%       |
| 44  | h     | 158    |  66% 34%       |
| 45  | i     | 128    |  76% 24%      |
| 46  | j     | 85     |  100%        |
| 47  | k     | 112    |  71% 29%     |
| 48  | m     | 128    |  17% 22% 78% |
| 49  | o     | 102    |  90% 9%      |
| 50  | p     | 206    |  62% 38%     |
| 51  | q     | 222    |  58% 42%     |
| 52  | r     | 196    |  74% 26%     |
| 53  | s     | 439    |  84% 16%     |
| 54  | u     | 234    |  47% 53%     |
| 55  | v     | 70     |  97% 2%      |
| 56  | w     | 156    |  6% 50% 49%  |
| 57  | x     | 406    |  36% 64%     |

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 101032 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 39S ribosomal protein L32, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 1   | 0     | 108      | 880   | 545 | 172 | 157 | 6 | 0       | 0     |

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 2   | 1     | 52       | 433   | 278 | 83 | 70 | 2 | 0       | 0     |

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 3   | 2     | 45       | 367   | 227 | 81 | 58 | 1 | 0       | 0     |

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 4   | 3     | 95       | 831   | 539 | 162 | 127 | 3 | 0       | 0     |

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
|     |       |          | Total | C   | N  | O  | S |         |       |
| 5   | 4     | 37       | 333   | 212 | 71 | 47 | 3 | 0       | 0     |

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 6   | 5     | 392      | 3199  | 2067 | 558 | 563 | 11 | 0       | 0     |

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 7   | 6     | 324      | 2723  | 1743 | 488 | 484 | 8 | 0       | 0     |

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 8   | 7     | 287      | 2334  | 1495 | 397 | 425 | 17 | 0       | 0     |

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 9   | 8     | 77       | 651   | 413 | 113 | 123 | 2 | 0       | 0     |

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 10  | 9     | 117      | 947   | 614 | 163 | 168 | 2 | 0       | 0     |

- Molecule 11 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|------|---------|-------|
|     |       |          | Total | C     | N    | O    | P    |         |       |
| 11  | A     | 1376     | 29222 | 13113 | 5273 | 9460 | 1376 | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference     |
|-------|---------|----------|--------|----------|---------------|
| A     | 3107    | U        | N      | conflict | GB 1025814679 |

- Molecule 12 is a RNA chain called mitochondrial tRNAVal.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O   | P  |         |       |
| 12  | B     | 56       | 1191  | 534 | 214 | 387 | 56 | 0       | 0     |

- Molecule 13 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 13  | C     | 338      | 2690  | 1715 | 470 | 489 | 16 | 1       | 0     |

- Molecule 14 is a protein called 39S ribosomal protein L2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 14  | D     | 240      | 1872  | 1165 | 378 | 320 | 9 | 0       | 0     |

- Molecule 15 is a protein called 39S ribosomal protein L3, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 15  | E     | 308      | 2427  | 1559 | 423 | 434 | 11 | 0       | 0     |

- Molecule 16 is a protein called 39S ribosomal protein L4, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |       |
| 16  | F     | 250      | 2013  | 1294 | 365 | 348 | 6 | 0       | 0     |

- Molecule 17 is a protein called Transcription termination factor 4, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |       |
| 17  | G     | 238      | 1943  | 1243 | 336 | 352 | 12 | 0       | 0     |

- Molecule 18 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 18  | H     | 95       | 784   | 498 | 152 | 134 | 0       | 0     |

- Molecule 19 is a protein called 39S ribosomal protein L10, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
|     |       |          | Total | C   | N   | O   | S  |         |       |
| 19  | I     | 158      | 1283  | 828 | 235 | 210 | 10 | 0       | 0     |

- Molecule 20 is a protein called 39S ribosomal protein L11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | J     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1061  | 680 | 192 | 187 | 2 |         |       |

- Molecule 21 is a protein called 39S ribosomal protein L13, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | K     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1451  | 934 | 259 | 251 | 7 |         |       |

- Molecule 22 is a protein called 39S ribosomal protein L14, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | L     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 889   | 559 | 171 | 154 | 5 |         |       |

- Molecule 23 is a protein called 39S ribosomal protein L15, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | M     | 287      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2305  | 1472 | 425 | 402 | 6 |         |       |

- Molecule 24 is a protein called 39S ribosomal protein L16, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | N     | 205      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1654  | 1056 | 308 | 280 | 10 |         |       |

- Molecule 25 is a protein called 39S ribosomal protein L17, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | O     | 152      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1245  | 784 | 239 | 215 | 7 |         |       |

- Molecule 26 is a protein called 39S ribosomal protein L18, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | P     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1148  | 719 | 221 | 203 | 5 |         |       |

- Molecule 27 is a protein called 39S ribosomal protein L19, mitochondrial.



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | Q     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1805  | 1159 | 317 | 320 | 9 |         |       |

- Molecule 28 is a protein called 39S ribosomal protein L20, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | R     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 971   | 616 | 200 | 151 | 4 |         |       |

- Molecule 29 is a protein called 39S ribosomal protein L21, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | S     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1251  | 806 | 222 | 219 | 4 |         |       |

- Molecule 30 is a protein called 39S ribosomal protein L22, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | T     | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1368  | 875 | 254 | 232 | 7 |         |       |

- Molecule 31 is a protein called 39S ribosomal protein L23, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | U     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1154  | 734 | 220 | 197 | 3 |         |       |

- Molecule 32 is a protein called 39S ribosomal protein L24, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 32  | V     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 395   | 255 | 62 | 75 | 3 |         |       |

- Molecule 33 is a protein called 39S ribosomal protein L27, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | W     | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 859   | 552 | 162 | 142 | 3 |         |       |

- Molecule 34 is a protein called 39S ribosomal protein L28, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 34  | X     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2035  | 1317 | 351 | 362 | 5 |         |       |

- Molecule 35 is a protein called 39S ribosomal protein L47, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | Y     | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1517  | 970 | 291 | 252 | 4 |         |       |

- Molecule 36 is a protein called 39S ribosomal protein L30, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | Z     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 937   | 598 | 175 | 161 | 3 |         |       |

- Molecule 37 is a protein called 39S ribosomal protein L42, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | a     | 71       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 597   | 378 | 112 | 103 | 4 |         |       |

- Molecule 38 is a protein called 39S ribosomal protein L43, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | b     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1178  | 733 | 229 | 213 | 3 |         |       |

- Molecule 39 is a protein called 39S ribosomal protein L44, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | c     | 275      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2217  | 1415 | 383 | 410 | 9 |         |       |

- Molecule 40 is a protein called 39S ribosomal protein L45, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40  | d     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1653  | 1075 | 276 | 293 | 9 |         |       |

- Molecule 41 is a protein called 39S ribosomal protein L46, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 41  | e     | 197      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1599  | 1027 | 277 | 290 | 5 |         |       |

- Molecule 42 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | f     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 549 | 140 | 165 | 3 |         |       |

- Molecule 43 is a protein called 39S ribosomal protein L49, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | g     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1067  | 690 | 185 | 190 | 2 |         |       |

- Molecule 44 is a protein called 39S ribosomal protein L50, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | h     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 548 | 151 | 160 | 3 |         |       |

- Molecule 45 is a protein called 39S ribosomal protein L51, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | i     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 532 | 165 | 126 | 4 |         |       |

- Molecule 46 is a protein called 39S ribosomal protein L52, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | j     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 684   | 423 | 133 | 126 | 2 |         |       |

- Molecule 47 is a protein called 39S ribosomal protein L53, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | k     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 627   | 392 | 116 | 114 | 5 |         |       |

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48  | m     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 234   | 151 | 44 | 37 | 2 |         |       |

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | o     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 786   | 495 | 161 | 127 | 3 |         |       |

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | p     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1058  | 661 | 201 | 192 | 4 |         |       |

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | q     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1076  | 671 | 208 | 192 | 5 |         |       |

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | r     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1203  | 764 | 232 | 199 | 8 |         |       |

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | s     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3036  | 1946 | 542 | 534 | 14 |         |       |

- Molecule 54 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 54  | u     | 111      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 927   | 595 | 155 | 167 | 10 |         |       |

- Molecule 55 is a protein called MIEF1 upstream open reading frame protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
|     |       |          | Total | C   | N   | O   |         |       |
| 55  | v     | 69       | 588   | 372 | 116 | 100 | 0       | 0     |

- Molecule 56 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
|     |       |          | Total | C   | N  | O   | S |         |       |
| 56  | w     | 79       | 638   | 410 | 95 | 128 | 5 | 0       | 0     |

- Molecule 57 is a protein called Mitochondrial ribosome-associated GTPase 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |       |
| 57  | x     | 148      | 1073  | 659 | 205 | 204 | 5 | 0       | 0     |

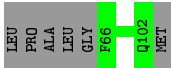
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
|     |       |          | Total | Zn |         |
| 58  | 0     | 1        | 1     | 1  | 0       |
| 58  | 4     | 1        | 1     | 1  | 0       |
| 58  | r     | 1        | 1     | 1  | 0       |

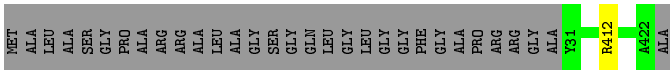
- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
|     |       |          | Total | Mg |         |
| 59  | A     | 71       | 71    | 71 | 0       |
| 59  | E     | 1        | 1     | 1  | 0       |
| 59  | W     | 1        | 1     | 1  | 0       |
| 59  | g     | 1        | 1     | 1  | 0       |

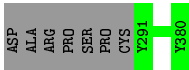
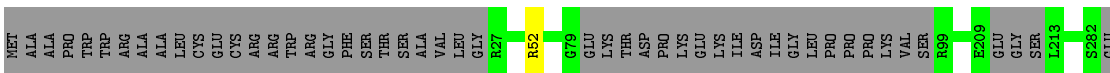
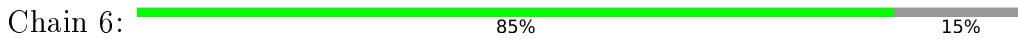




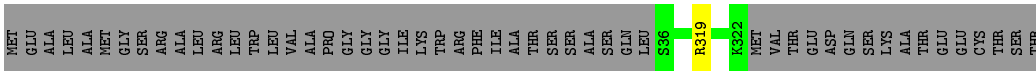
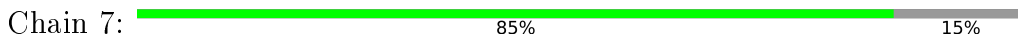
- Molecule 6: 39S ribosomal protein L37, mitochondrial



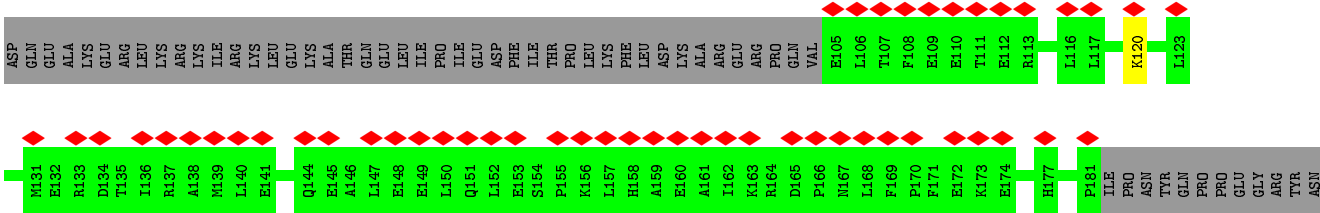
- Molecule 7: 39S ribosomal protein L38, mitochondrial



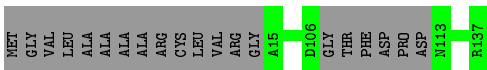
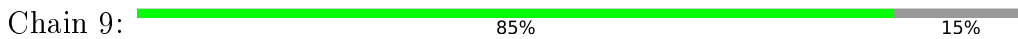
- Molecule 8: 39S ribosomal protein L39, mitochondrial



- Molecule 9: 39S ribosomal protein L40, mitochondrial



- Molecule 10: 39S ribosomal protein L41, mitochondrial

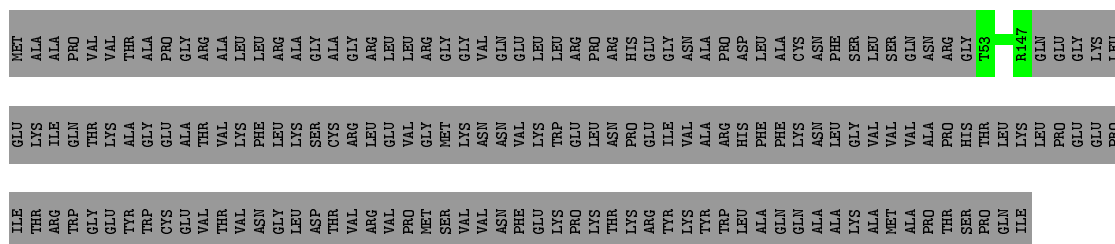






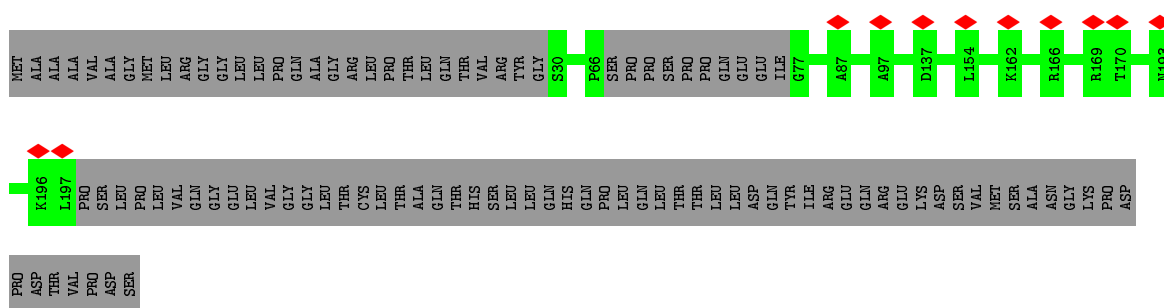


Chain H: 36% 64%



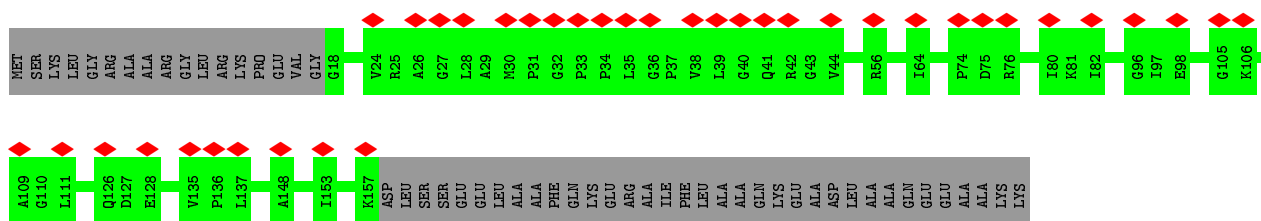
- Molecule 19: 39S ribosomal protein L10, mitochondrial

Chain I: 61% 39%



- Molecule 20: 39S ribosomal protein L11, mitochondrial

Chain J: 20% 73% 27%



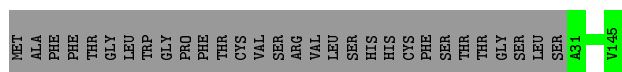
- Molecule 21: 39S ribosomal protein L13, mitochondrial

Chain K: 99%



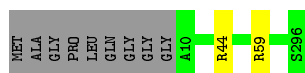
- Molecule 22: 39S ribosomal protein L14, mitochondrial

Chain L: 79% 21%




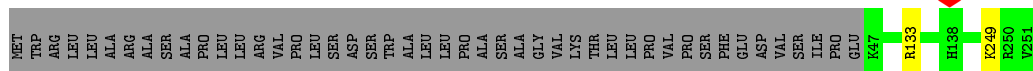
- Molecule 23: 39S ribosomal protein L15, mitochondrial

Chain M:  96%




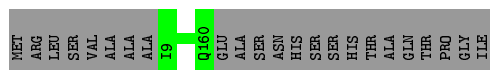
- Molecule 24: 39S ribosomal protein L16, mitochondrial

Chain N:  81% 18%




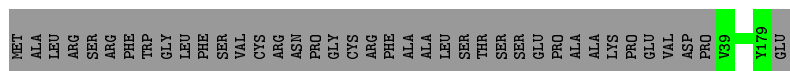
- Molecule 25: 39S ribosomal protein L17, mitochondrial

Chain O:  87% 13%



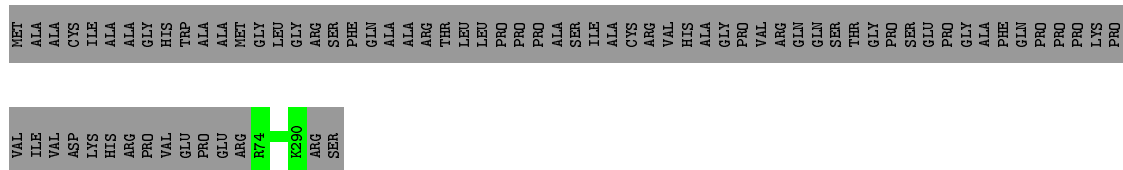
- Molecule 26: 39S ribosomal protein L18, mitochondrial

Chain P:  78% 22%



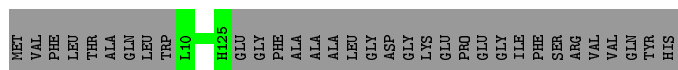
- Molecule 27: 39S ribosomal protein L19, mitochondrial

Chain Q:  74% 26%



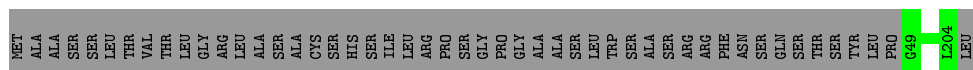
- Molecule 28: 39S ribosomal protein L20, mitochondrial

Chain R:  78% 22%



- Molecule 29: 39S ribosomal protein L21, mitochondrial

Chain S:  76% 24%









• Molecule 45: 39S ribosomal protein L51, mitochondrial

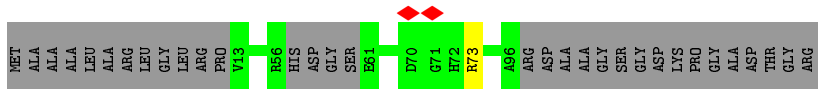


• Molecule 46: 39S ribosomal protein L52, mitochondrial

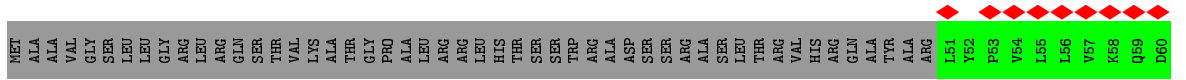


There are no outlier residues recorded for this chain.

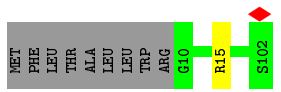
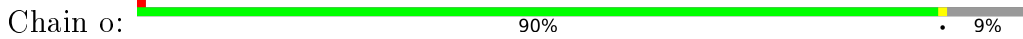
• Molecule 47: 39S ribosomal protein L53, mitochondrial



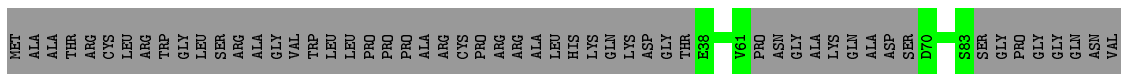
• Molecule 48: 39S ribosomal protein L55, mitochondrial



• Molecule 49: Ribosomal protein 63, mitochondrial



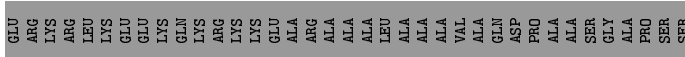
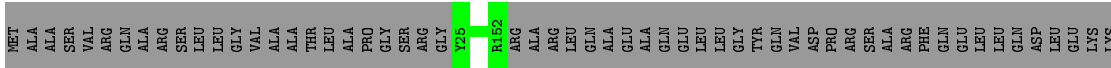
• Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial





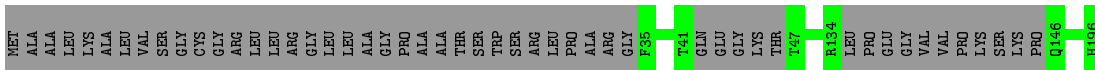
- Molecule 51: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:  58% 42%




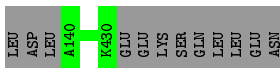
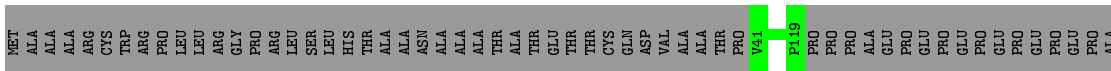
- Molecule 52: 39S ribosomal protein S18a, mitochondrial

Chain r:  74% 26%



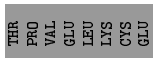
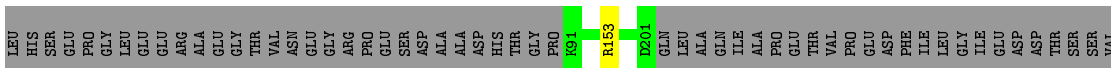
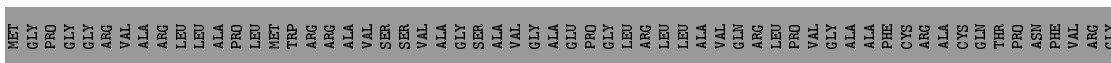
- Molecule 53: 39S ribosomal protein S30, mitochondrial

Chain s:  84% 16%



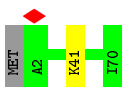
- Molecule 54: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:  47% 53%



- Molecule 55: MIEF1 upstream open reading frame protein

Chain v:  97% ..



- Molecule 56: Acyl carrier protein, mitochondrial





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 98227                                   | 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 ( $e^-/\text{\AA}^2$ ) | 36                                      | Depositor |
| Minimum defocus (nm)                 | 300                                     | Depositor |
| Maximum defocus (nm)                 | 2800                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.113                                   | Depositor |
| Minimum map value                    | -0.035                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.004                                   | Depositor |
| Recommended contour level            | 0.006                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 367.49997, 367.49997, 367.49997         | wwPDB     |
| Map dimensions                       | 350, 350, 350                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.05, 1.05, 1.05                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.36         | 0/895   | 0.54        | 0/1201         |
| 2   | 1     | 0.26         | 0/438   | 0.54        | 0/583          |
| 3   | 2     | 0.41         | 0/373   | 0.58        | 0/496          |
| 4   | 3     | 0.42         | 0/852   | 0.54        | 0/1136         |
| 5   | 4     | 0.39         | 0/341   | 0.59        | 0/451          |
| 6   | 5     | 0.33         | 0/3294  | 0.50        | 0/4488         |
| 7   | 6     | 0.34         | 0/2809  | 0.54        | 0/3818         |
| 8   | 7     | 0.32         | 0/2391  | 0.47        | 0/3234         |
| 9   | 8     | 0.25         | 0/665   | 0.51        | 0/894          |
| 10  | 9     | 0.37         | 0/972   | 0.50        | 0/1306         |
| 11  | A     | 0.78         | 0/32605 | 0.80        | 8/50720 (0.0%) |
| 12  | B     | 0.26         | 0/1328  | 0.75        | 0/2056         |
| 13  | C     | 0.27         | 0/2754  | 0.49        | 0/3734         |
| 14  | D     | 0.37         | 0/1910  | 0.58        | 0/2569         |
| 15  | E     | 0.41         | 0/2497  | 0.49        | 0/3386         |
| 16  | F     | 0.40         | 0/2071  | 0.53        | 0/2817         |
| 17  | G     | 0.28         | 0/1974  | 0.48        | 0/2652         |
| 18  | H     | 0.33         | 0/798   | 0.55        | 0/1073         |
| 19  | I     | 0.27         | 0/1308  | 0.51        | 0/1761         |
| 20  | J     | 0.25         | 0/1077  | 0.50        | 0/1452         |
| 21  | K     | 0.40         | 0/1495  | 0.49        | 0/2029         |
| 22  | L     | 0.37         | 0/904   | 0.56        | 0/1218         |
| 23  | M     | 0.41         | 0/2359  | 0.54        | 0/3185         |
| 24  | N     | 0.35         | 0/1697  | 0.54        | 0/2281         |
| 25  | O     | 0.37         | 0/1269  | 0.57        | 0/1708         |
| 26  | P     | 0.33         | 0/1173  | 0.55        | 0/1588         |
| 27  | Q     | 0.37         | 0/1846  | 0.52        | 0/2487         |
| 28  | R     | 0.42         | 0/987   | 0.57        | 0/1320         |
| 29  | S     | 0.38         | 0/1276  | 0.53        | 0/1729         |
| 30  | T     | 0.42         | 0/1402  | 0.53        | 0/1886         |
| 31  | U     | 0.38         | 0/1183  | 0.55        | 0/1600         |
| 32  | V     | 0.36         | 0/404   | 0.45        | 0/545          |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 33  | W     | 0.44         | 0/881    | 0.52        | 0/1188          |
| 34  | X     | 0.36         | 0/2090   | 0.48        | 0/2825          |
| 35  | Y     | 0.36         | 0/1552   | 0.52        | 0/2079          |
| 36  | Z     | 0.36         | 0/960    | 0.49        | 0/1295          |
| 37  | a     | 0.38         | 0/616    | 0.52        | 0/833           |
| 38  | b     | 0.38         | 0/1202   | 0.59        | 0/1626          |
| 39  | c     | 0.35         | 0/2264   | 0.49        | 0/3059          |
| 40  | d     | 0.27         | 0/1702   | 0.48        | 0/2307          |
| 41  | e     | 0.25         | 0/1633   | 0.49        | 0/2204          |
| 42  | f     | 0.28         | 0/873    | 0.47        | 0/1180          |
| 43  | g     | 0.40         | 0/1102   | 0.51        | 0/1503          |
| 44  | h     | 0.27         | 0/884    | 0.48        | 0/1203          |
| 45  | i     | 0.43         | 0/849    | 0.56        | 0/1135          |
| 46  | j     | 0.33         | 0/698    | 0.51        | 0/940           |
| 47  | k     | 0.24         | 0/635    | 0.53        | 0/855           |
| 48  | m     | 0.23         | 0/239    | 0.59        | 0/322           |
| 49  | o     | 0.37         | 0/807    | 0.58        | 0/1083          |
| 50  | p     | 0.28         | 0/1071   | 0.54        | 0/1433          |
| 51  | q     | 0.30         | 0/1107   | 0.53        | 0/1498          |
| 52  | r     | 0.35         | 0/1238   | 0.53        | 0/1676          |
| 53  | s     | 0.39         | 0/3114   | 0.53        | 0/4225          |
| 54  | u     | 0.31         | 0/949    | 0.50        | 0/1281          |
| 55  | v     | 0.26         | 0/597    | 0.61        | 0/796           |
| 56  | w     | 0.26         | 0/647    | 0.44        | 0/871           |
| 57  | x     | 0.33         | 0/1091   | 0.56        | 0/1467          |
| All | All   | 0.52         | 0/106148 | 0.63        | 8/150287 (0.0%) |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 11  | A     | 2215 | C    | C2-N1-C1'  | 8.26  | 127.88      | 118.80   |
| 11  | A     | 2186 | C    | N1-C2-O2   | 6.16  | 122.59      | 118.90   |
| 11  | A     | 2215 | C    | C6-N1-C1'  | -6.16 | 113.41      | 120.80   |
| 11  | A     | 2215 | C    | N1-C2-O2   | 5.99  | 122.49      | 118.90   |
| 11  | A     | 2163 | A    | O4'-C1'-N9 | 5.46  | 112.57      | 108.20   |
| 11  | A     | 2185 | G    | N1-C6-O6   | -5.39 | 116.67      | 119.90   |
| 11  | A     | 2523 | C    | C2-N1-C1'  | 5.36  | 124.70      | 118.80   |
| 11  | A     | 1823 | A    | P-O3'-C3'  | 5.08  | 125.80      | 119.70   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 0     | 106/108 (98%) | 105 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 2   | 1     | 50/65 (77%)   | 49 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 3   | 2     | 43/92 (47%)   | 42 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 4   | 3     | 93/188 (50%)  | 90 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 5   | 4     | 35/103 (34%)  | 34 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 6   | 5     | 390/423 (92%) | 376 (96%) | 14 (4%) | 0        | 100         | 100 |
| 7   | 6     | 316/380 (83%) | 303 (96%) | 13 (4%) | 0        | 100         | 100 |
| 8   | 7     | 285/338 (84%) | 268 (94%) | 17 (6%) | 0        | 100         | 100 |
| 9   | 8     | 75/206 (36%)  | 72 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 10  | 9     | 113/137 (82%) | 112 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 13  | C     | 335/384 (87%) | 317 (95%) | 18 (5%) | 0        | 100         | 100 |
| 14  | D     | 238/305 (78%) | 232 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 15  | E     | 306/348 (88%) | 296 (97%) | 10 (3%) | 0        | 100         | 100 |
| 16  | F     | 248/311 (80%) | 242 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 17  | G     | 236/381 (62%) | 225 (95%) | 11 (5%) | 0        | 100         | 100 |
| 18  | H     | 93/267 (35%)  | 88 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 19  | I     | 154/261 (59%) | 146 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 20  | J     | 138/192 (72%) | 126 (91%) | 12 (9%) | 0        | 100         | 100 |
| 21  | K     | 175/178 (98%) | 171 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 22  | L     | 113/145 (78%) | 109 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 23  | M     | 285/296 (96%) | 282 (99%) | 3 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 24  | N     | 203/251 (81%) | 191 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 25  | O     | 150/175 (86%) | 147 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 26  | P     | 139/180 (77%) | 134 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 27  | Q     | 215/292 (74%) | 212 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 28  | R     | 114/149 (76%) | 113 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 29  | S     | 154/205 (75%) | 151 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 30  | T     | 164/206 (80%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 31  | U     | 135/153 (88%) | 133 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 32  | V     | 45/216 (21%)  | 45 (100%)  | 0       | 0        | 100         | 100 |
| 33  | W     | 107/148 (72%) | 105 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 34  | X     | 241/256 (94%) | 236 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 35  | Y     | 174/250 (70%) | 170 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 36  | Z     | 113/161 (70%) | 110 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 37  | a     | 67/142 (47%)  | 67 (100%)  | 0       | 0        | 100         | 100 |
| 38  | b     | 146/215 (68%) | 141 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 39  | c     | 271/332 (82%) | 267 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 40  | d     | 189/306 (62%) | 183 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 41  | e     | 191/279 (68%) | 179 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 42  | f     | 102/212 (48%) | 94 (92%)   | 8 (8%)  | 0        | 100         | 100 |
| 43  | g     | 127/166 (76%) | 120 (94%)  | 7 (6%)  | 0        | 100         | 100 |
| 44  | h     | 101/158 (64%) | 99 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 45  | i     | 95/128 (74%)  | 94 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 46  | j     | 83/85 (98%)   | 83 (100%)  | 0       | 0        | 100         | 100 |
| 47  | k     | 76/112 (68%)  | 70 (92%)   | 6 (8%)  | 0        | 100         | 100 |
| 48  | m     | 26/128 (20%)  | 20 (77%)   | 6 (23%) | 0        | 100         | 100 |
| 49  | o     | 91/102 (89%)  | 89 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 50  | p     | 119/206 (58%) | 116 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 51  | q     | 126/222 (57%) | 126 (100%) | 0       | 0        | 100         | 100 |
| 52  | r     | 140/196 (71%) | 133 (95%)  | 7 (5%)  | 0        | 100         | 100 |
| 53  | s     | 366/439 (83%) | 358 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 54  | u     | 109/234 (47%) | 100 (92%)  | 9 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 55  | v     | 67/70 (96%)      | 65 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 56  | w     | 77/156 (49%)     | 73 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 57  | x     | 146/406 (36%)    | 138 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| All | All   | 8496/12044 (70%) | 8208 (97%) | 288 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | 0     | 97/97 (100%)  | 97 (100%)  | 0        | 100         | 100 |
| 2   | 1     | 49/60 (82%)   | 49 (100%)  | 0        | 100         | 100 |
| 3   | 2     | 39/72 (54%)   | 39 (100%)  | 0        | 100         | 100 |
| 4   | 3     | 88/166 (53%)  | 88 (100%)  | 0        | 100         | 100 |
| 5   | 4     | 36/89 (40%)   | 36 (100%)  | 0        | 100         | 100 |
| 6   | 5     | 353/368 (96%) | 352 (100%) | 1 (0%)   | 92          | 97  |
| 7   | 6     | 286/332 (86%) | 285 (100%) | 1 (0%)   | 92          | 97  |
| 8   | 7     | 263/303 (87%) | 262 (100%) | 1 (0%)   | 91          | 97  |
| 9   | 8     | 70/190 (37%)  | 69 (99%)   | 1 (1%)   | 67          | 86  |
| 10  | 9     | 99/112 (88%)  | 99 (100%)  | 0        | 100         | 100 |
| 13  | C     | 293/328 (89%) | 292 (100%) | 1 (0%)   | 92          | 97  |
| 14  | D     | 194/245 (79%) | 193 (100%) | 1 (0%)   | 88          | 96  |
| 15  | E     | 262/290 (90%) | 262 (100%) | 0        | 100         | 100 |
| 16  | F     | 217/262 (83%) | 217 (100%) | 0        | 100         | 100 |
| 17  | G     | 221/350 (63%) | 221 (100%) | 0        | 100         | 100 |
| 18  | H     | 86/228 (38%)  | 86 (100%)  | 0        | 100         | 100 |
| 19  | I     | 145/232 (62%) | 145 (100%) | 0        | 100         | 100 |
| 20  | J     | 113/150 (75%) | 113 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 21  | K     | 155/156 (99%) | 155 (100%) | 0        | 100         | 100 |
| 22  | L     | 98/124 (79%)  | 98 (100%)  | 0        | 100         | 100 |
| 23  | M     | 245/249 (98%) | 243 (99%)  | 2 (1%)   | 81          | 93  |
| 24  | N     | 172/211 (82%) | 170 (99%)  | 2 (1%)   | 71          | 88  |
| 25  | O     | 133/150 (89%) | 133 (100%) | 0        | 100         | 100 |
| 26  | P     | 123/155 (79%) | 123 (100%) | 0        | 100         | 100 |
| 27  | Q     | 199/256 (78%) | 199 (100%) | 0        | 100         | 100 |
| 28  | R     | 101/126 (80%) | 101 (100%) | 0        | 100         | 100 |
| 29  | S     | 141/180 (78%) | 141 (100%) | 0        | 100         | 100 |
| 30  | T     | 146/176 (83%) | 146 (100%) | 0        | 100         | 100 |
| 31  | U     | 124/135 (92%) | 124 (100%) | 0        | 100         | 100 |
| 32  | V     | 43/191 (22%)  | 43 (100%)  | 0        | 100         | 100 |
| 33  | W     | 89/119 (75%)  | 89 (100%)  | 0        | 100         | 100 |
| 34  | X     | 219/229 (96%) | 218 (100%) | 1 (0%)   | 88          | 96  |
| 35  | Y     | 159/223 (71%) | 159 (100%) | 0        | 100         | 100 |
| 36  | Z     | 106/147 (72%) | 105 (99%)  | 1 (1%)   | 78          | 92  |
| 37  | a     | 67/133 (50%)  | 67 (100%)  | 0        | 100         | 100 |
| 38  | b     | 130/186 (70%) | 130 (100%) | 0        | 100         | 100 |
| 39  | c     | 241/288 (84%) | 241 (100%) | 0        | 100         | 100 |
| 40  | d     | 184/274 (67%) | 183 (100%) | 1 (0%)   | 88          | 96  |
| 41  | e     | 171/236 (72%) | 171 (100%) | 0        | 100         | 100 |
| 42  | f     | 95/188 (50%)  | 95 (100%)  | 0        | 100         | 100 |
| 43  | g     | 119/148 (80%) | 119 (100%) | 0        | 100         | 100 |
| 44  | h     | 100/148 (68%) | 100 (100%) | 0        | 100         | 100 |
| 45  | i     | 86/110 (78%)  | 86 (100%)  | 0        | 100         | 100 |
| 46  | j     | 68/68 (100%)  | 68 (100%)  | 0        | 100         | 100 |
| 47  | k     | 71/90 (79%)   | 70 (99%)   | 1 (1%)   | 67          | 86  |
| 48  | m     | 26/113 (23%)  | 26 (100%)  | 0        | 100         | 100 |
| 49  | o     | 79/87 (91%)   | 78 (99%)   | 1 (1%)   | 69          | 87  |
| 50  | p     | 117/181 (65%) | 117 (100%) | 0        | 100         | 100 |
| 51  | q     | 110/178 (62%) | 110 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 52  | r     | 133/169 (79%)    | 133 (100%)  | 0        | 100         | 100 |
| 53  | s     | 326/381 (86%)    | 326 (100%)  | 0        | 100         | 100 |
| 54  | u     | 105/200 (52%)    | 104 (99%)   | 1 (1%)   | 76          | 90  |
| 55  | v     | 59/60 (98%)      | 58 (98%)    | 1 (2%)   | 60          | 82  |
| 56  | w     | 73/136 (54%)     | 72 (99%)    | 1 (1%)   | 67          | 86  |
| 57  | x     | 109/320 (34%)    | 109 (100%)  | 0        | 100         | 100 |
| All | All   | 7633/10395 (73%) | 7615 (100%) | 18 (0%)  | 93          | 98  |

All (18) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 5     | 412 | ARG  |
| 7   | 6     | 52  | ARG  |
| 8   | 7     | 319 | ARG  |
| 9   | 8     | 120 | LYS  |
| 13  | C     | 346 | ARG  |
| 14  | D     | 285 | LYS  |
| 23  | M     | 44  | ARG  |
| 23  | M     | 59  | ARG  |
| 24  | N     | 133 | ARG  |
| 24  | N     | 249 | LYS  |
| 34  | X     | 23  | ARG  |
| 36  | Z     | 44  | LYS  |
| 40  | d     | 198 | ARG  |
| 47  | k     | 73  | ARG  |
| 49  | o     | 15  | ARG  |
| 54  | u     | 153 | ARG  |
| 55  | v     | 41  | LYS  |
| 56  | w     | 106 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | C     | 46  | GLN  |
| 22  | L     | 33  | GLN  |
| 23  | M     | 26  | ASN  |
| 29  | S     | 118 | ASN  |
| 47  | k     | 19  | GLN  |
| 51  | q     | 130 | GLN  |

5.3.3 RNA 

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11  | A     | 1359/1559 (87%) | 294 (21%)         | 21 (1%)         |
| 12  | B     | 51/69 (73%)     | 16 (31%)          | 1 (1%)          |
| All | All   | 1410/1628 (86%) | 310 (21%)         | 22 (1%)         |

All (310) RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1672 | C    |
| 11  | A     | 1676 | A    |
| 11  | A     | 1677 | C    |
| 11  | A     | 1679 | U    |
| 11  | A     | 1680 | A    |
| 11  | A     | 1681 | G    |
| 11  | A     | 1689 | C    |
| 11  | A     | 1690 | C    |
| 11  | A     | 1699 | C    |
| 11  | A     | 1700 | U    |
| 11  | A     | 1704 | U    |
| 11  | A     | 1708 | A    |
| 11  | A     | 1714 | C    |
| 11  | A     | 1715 | C    |
| 11  | A     | 1724 | A    |
| 11  | A     | 1727 | A    |
| 11  | A     | 1728 | U    |
| 11  | A     | 1731 | A    |
| 11  | A     | 1732 | C    |
| 11  | A     | 1748 | G    |
| 11  | A     | 1750 | G    |
| 11  | A     | 1751 | A    |
| 11  | A     | 1767 | G    |
| 11  | A     | 1770 | G    |
| 11  | A     | 1777 | A    |
| 11  | A     | 1794 | A    |
| 11  | A     | 1817 | C    |
| 11  | A     | 1819 | U    |
| 11  | A     | 1821 | A    |
| 11  | A     | 1823 | A    |
| 11  | A     | 1824 | U    |
| 11  | A     | 1827 | C    |
| 11  | A     | 1828 | A    |
| 11  | A     | 1829 | A    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 11         | A            | 1832       | A           |
| 11         | A            | 1836       | A           |
| 11         | A            | 1844       | A           |
| 11         | A            | 1849       | C           |
| 11         | A            | 1853       | A           |
| 11         | A            | 1854       | U           |
| 11         | A            | 1855       | A           |
| 11         | A            | 1856       | A           |
| 11         | A            | 1869       | A           |
| 11         | A            | 1878       | U           |
| 11         | A            | 1882       | A           |
| 11         | A            | 1883       | G           |
| 11         | A            | 1887       | A           |
| 11         | A            | 1888       | G           |
| 11         | A            | 1892       | A           |
| 11         | A            | 1893       | A           |
| 11         | A            | 1902       | C           |
| 11         | A            | 1903       | C           |
| 11         | A            | 1918       | G           |
| 11         | A            | 1938       | A           |
| 11         | A            | 1940       | A           |
| 11         | A            | 1958       | G           |
| 11         | A            | 1972       | A           |
| 11         | A            | 1974       | A           |
| 11         | A            | 1985       | G           |
| 11         | A            | 1987       | G           |
| 11         | A            | 1992       | C           |
| 11         | A            | 1994       | A           |
| 11         | A            | 1995       | A           |
| 11         | A            | 2001       | C           |
| 11         | A            | 2002       | G           |
| 11         | A            | 2015       | G           |
| 11         | A            | 2021       | U           |
| 11         | A            | 2022       | G           |
| 11         | A            | 2029       | A           |
| 11         | A            | 2030       | U           |
| 11         | A            | 2036       | C           |
| 11         | A            | 2037       | U           |
| 11         | A            | 2039       | A           |
| 11         | A            | 2054       | U           |
| 11         | A            | 2055       | U           |
| 11         | A            | 2060       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 11         | A            | 2065       | A           |
| 11         | A            | 2074       | A           |
| 11         | A            | 2079       | C           |
| 11         | A            | 2083       | U           |
| 11         | A            | 2085       | A           |
| 11         | A            | 2093       | U           |
| 11         | A            | 2097       | A           |
| 11         | A            | 2098       | G           |
| 11         | A            | 2113       | G           |
| 11         | A            | 2114       | C           |
| 11         | A            | 2124       | A           |
| 11         | A            | 2126       | U           |
| 11         | A            | 2132       | A           |
| 11         | A            | 2141       | U           |
| 11         | A            | 2147       | G           |
| 11         | A            | 2154       | A           |
| 11         | A            | 2155       | A           |
| 11         | A            | 2157       | U           |
| 11         | A            | 2159       | U           |
| 11         | A            | 2163       | A           |
| 11         | A            | 2164       | C           |
| 11         | A            | 2165       | C           |
| 11         | A            | 2166       | C           |
| 11         | A            | 2172       | A           |
| 11         | A            | 2173       | G           |
| 11         | A            | 2177       | U           |
| 11         | A            | 2180       | A           |
| 11         | A            | 2182       | G           |
| 11         | A            | 2183       | C           |
| 11         | A            | 2184       | A           |
| 11         | A            | 2187       | C           |
| 11         | A            | 2193       | U           |
| 11         | A            | 2194       | U           |
| 11         | A            | 2197       | G           |
| 11         | A            | 2198       | A           |
| 11         | A            | 2199       | A           |
| 11         | A            | 2200       | A           |
| 11         | A            | 2210       | C           |
| 11         | A            | 2212       | C           |
| 11         | A            | 2213       | A           |
| 11         | A            | 2215       | C           |
| 11         | A            | 2216       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 11         | A            | 2233       | U           |
| 11         | A            | 2237       | A           |
| 11         | A            | 2239       | A           |
| 11         | A            | 2241       | A           |
| 11         | A            | 2242       | U           |
| 11         | A            | 2243       | A           |
| 11         | A            | 2246       | A           |
| 11         | A            | 2262       | C           |
| 11         | A            | 2263       | C           |
| 11         | A            | 2282       | C           |
| 11         | A            | 2285       | U           |
| 11         | A            | 2297       | A           |
| 11         | A            | 2300       | G           |
| 11         | A            | 2316       | U           |
| 11         | A            | 2322       | C           |
| 11         | A            | 2331       | C           |
| 11         | A            | 2332       | C           |
| 11         | A            | 2335       | A           |
| 11         | A            | 2345       | G           |
| 11         | A            | 2349       | G           |
| 11         | A            | 2369       | A           |
| 11         | A            | 2371       | U           |
| 11         | A            | 2374       | A           |
| 11         | A            | 2381       | A           |
| 11         | A            | 2384       | A           |
| 11         | A            | 2386       | C           |
| 11         | A            | 2387       | U           |
| 11         | A            | 2390       | A           |
| 11         | A            | 2393       | C           |
| 11         | A            | 2399       | A           |
| 11         | A            | 2404       | U           |
| 11         | A            | 2408       | U           |
| 11         | A            | 2415       | C           |
| 11         | A            | 2427       | C           |
| 11         | A            | 2432       | A           |
| 11         | A            | 2434       | A           |
| 11         | A            | 2444       | A           |
| 11         | A            | 2446       | A           |
| 11         | A            | 2451       | A           |
| 11         | A            | 2458       | A           |
| 11         | A            | 2478       | G           |
| 11         | A            | 2485       | U           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 11         | A            | 2493       | C           |
| 11         | A            | 2496       | G           |
| 11         | A            | 2500       | A           |
| 11         | A            | 2502       | C           |
| 11         | A            | 2507       | A           |
| 11         | A            | 2508       | C           |
| 11         | A            | 2511       | C           |
| 11         | A            | 2520       | C           |
| 11         | A            | 2521       | A           |
| 11         | A            | 2527       | A           |
| 11         | A            | 2528       | G           |
| 11         | A            | 2531       | U           |
| 11         | A            | 2540       | C           |
| 11         | A            | 2618       | U           |
| 11         | A            | 2635       | G           |
| 11         | A            | 2636       | G           |
| 11         | A            | 2637       | C           |
| 11         | A            | 2639       | C           |
| 11         | A            | 2645       | G           |
| 11         | A            | 2654       | U           |
| 11         | A            | 2656       | U           |
| 11         | A            | 2660       | U           |
| 11         | A            | 2683       | C           |
| 11         | A            | 2684       | C           |
| 11         | A            | 2686       | G           |
| 11         | A            | 2694       | A           |
| 11         | A            | 2696       | A           |
| 11         | A            | 2706       | A           |
| 11         | A            | 2709       | A           |
| 11         | A            | 2718       | C           |
| 11         | A            | 2719       | G           |
| 11         | A            | 2721       | G           |
| 11         | A            | 2722       | A           |
| 11         | A            | 2724       | G           |
| 11         | A            | 2732       | G           |
| 11         | A            | 2739       | U           |
| 11         | A            | 2748       | A           |
| 11         | A            | 2750       | U           |
| 11         | A            | 2756       | C           |
| 11         | A            | 2804       | A           |
| 11         | A            | 2810       | G           |
| 11         | A            | 2815       | OMG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 11         | A            | 2819       | G           |
| 11         | A            | 2831       | G           |
| 11         | A            | 2832       | A           |
| 11         | A            | 2833       | A           |
| 11         | A            | 2836       | C           |
| 11         | A            | 2837       | A           |
| 11         | A            | 2838       | A           |
| 11         | A            | 2839       | C           |
| 11         | A            | 2846       | G           |
| 11         | A            | 2847       | C           |
| 11         | A            | 2853       | A           |
| 11         | A            | 2854       | U           |
| 11         | A            | 2855       | G           |
| 11         | A            | 2857       | U           |
| 11         | A            | 2859       | A           |
| 11         | A            | 2864       | U           |
| 11         | A            | 2865       | C           |
| 11         | A            | 2871       | U           |
| 11         | A            | 2890       | U           |
| 11         | A            | 2895       | U           |
| 11         | A            | 2896       | G           |
| 11         | A            | 2906       | C           |
| 11         | A            | 2911       | C           |
| 11         | A            | 2912       | C           |
| 11         | A            | 2913       | A           |
| 11         | A            | 2917       | G           |
| 11         | A            | 2918       | A           |
| 11         | A            | 2919       | A           |
| 11         | A            | 2922       | A           |
| 11         | A            | 2926       | A           |
| 11         | A            | 2928       | C           |
| 11         | A            | 2932       | G           |
| 11         | A            | 2935       | A           |
| 11         | A            | 2936       | U           |
| 11         | A            | 2943       | G           |
| 11         | A            | 2955       | U           |
| 11         | A            | 2956       | A           |
| 11         | A            | 2958       | A           |
| 11         | A            | 2962       | C           |
| 11         | A            | 2963       | A           |
| 11         | A            | 2965       | A           |
| 11         | A            | 2971       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 11         | A            | 2989       | G           |
| 11         | A            | 2990       | A           |
| 11         | A            | 2991       | U           |
| 11         | A            | 3005       | A           |
| 11         | A            | 3016       | G           |
| 11         | A            | 3022       | G           |
| 11         | A            | 3041       | U           |
| 11         | A            | 3042       | U           |
| 11         | A            | 3043       | C           |
| 11         | A            | 3051       | A           |
| 11         | A            | 3053       | A           |
| 11         | A            | 3054       | G           |
| 11         | A            | 3060       | C           |
| 11         | A            | 3063       | G           |
| 11         | A            | 3068       | G           |
| 11         | A            | 3073       | C           |
| 11         | A            | 3089       | A           |
| 11         | A            | 3093       | C           |
| 11         | A            | 3096       | U           |
| 11         | A            | 3097       | U           |
| 11         | A            | 3100       | U           |
| 11         | A            | 3102       | U           |
| 11         | A            | 3108       | U           |
| 11         | A            | 3109       | U           |
| 11         | A            | 3113       | A           |
| 11         | A            | 3123       | G           |
| 11         | A            | 3124       | U           |
| 11         | A            | 3129       | A           |
| 11         | A            | 3134       | C           |
| 11         | A            | 3141       | A           |
| 11         | A            | 3150       | U           |
| 11         | A            | 3155       | C           |
| 11         | A            | 3157       | C           |
| 11         | A            | 3158       | A           |
| 11         | A            | 3162       | C           |
| 11         | A            | 3168       | C           |
| 11         | A            | 3169       | C           |
| 11         | A            | 3172       | C           |
| 11         | A            | 3173       | G           |
| 11         | A            | 3180       | A           |
| 11         | A            | 3189       | C           |
| 11         | A            | 3190       | A           |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 11         | A            | 3197       | U           |
| 11         | A            | 3198       | A           |
| 11         | A            | 3200       | U           |
| 11         | A            | 3202       | U           |
| 11         | A            | 3207       | A           |
| 11         | A            | 3217       | A           |
| 11         | A            | 3218       | A           |
| 11         | A            | 3220       | A           |
| 12         | B            | 1607       | U           |
| 12         | B            | 1608       | G           |
| 12         | B            | 1609       | U           |
| 12         | B            | 1611       | G           |
| 12         | B            | 1614       | U           |
| 12         | B            | 1615       | A           |
| 12         | B            | 1625       | A           |
| 12         | B            | 1631       | C           |
| 12         | B            | 1632       | U           |
| 12         | B            | 1633       | U           |
| 12         | B            | 1641       | G           |
| 12         | B            | 1644       | G           |
| 12         | B            | 1645       | A           |
| 12         | B            | 1649       | C           |
| 12         | B            | 1651       | A           |
| 12         | B            | 1669       | G           |

All (22) RNA pucker outliers are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 11         | A            | 1707       | C           |
| 11         | A            | 1713       | A           |
| 11         | A            | 1766       | U           |
| 11         | A            | 1823       | A           |
| 11         | A            | 1986       | A           |
| 11         | A            | 2164       | C           |
| 11         | A            | 2182       | G           |
| 11         | A            | 2186       | C           |
| 11         | A            | 2209       | G           |
| 11         | A            | 2284       | C           |
| 11         | A            | 2457       | A           |
| 11         | A            | 2507       | A           |
| 11         | A            | 2530       | A           |
| 11         | A            | 2635       | G           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 2695 | G    |
| 11  | A     | 2836 | C    |
| 11  | A     | 2837 | A    |
| 11  | A     | 2905 | A    |
| 11  | A     | 3092 | U    |
| 11  | A     | 3122 | U    |
| 11  | A     | 3196 | G    |
| 12  | B     | 1607 | U    |

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

3 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 |
| 11  | OMG  | A     | 2815 | 11   | 18,26,27     | 1.26 | 2 (11%)  | 20,38,41    | 2.28 | 6 (30%)  |
| 11  | OMG  | A     | 3040 | 11   | 18,26,27     | 1.16 | 2 (11%)  | 20,38,41    | 2.16 | 6 (30%)  |
| 11  | OMU  | A     | 3039 | 11   | 14,22,23     | 0.94 | 1 (7%)   | 14,31,34    | 0.99 | 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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 11  | OMG  | A     | 2815 | 11   | -       | 2/5/27/28 | 0/3/3/3 |
| 11  | OMG  | A     | 3040 | 11   | -       | 0/5/27/28 | 0/3/3/3 |
| 11  | OMU  | A     | 3039 | 11   | -       | 0/7/27/28 | 0/2/2/2 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 11  | A     | 2815 | OMG  | C6-C5 | 4.12 | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A     | 3040 | OMG  | C6-C5 | 3.71  | 1.47        | 1.41     |
| 11  | A     | 3039 | OMU  | C2-N3 | -2.53 | 1.33        | 1.38     |
| 11  | A     | 2815 | OMG  | C5-C4 | 2.20  | 1.46        | 1.40     |
| 11  | A     | 3040 | OMG  | C5-C4 | 2.01  | 1.46        | 1.40     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | A     | 3040 | OMG  | C2-N3-C4 | 4.98  | 121.05      | 115.36   |
| 11  | A     | 2815 | OMG  | C2-N3-C4 | 4.93  | 120.98      | 115.36   |
| 11  | A     | 2815 | OMG  | C6-C5-C4 | -4.24 | 116.75      | 120.80   |
| 11  | A     | 3040 | OMG  | C6-C5-C4 | -4.07 | 116.91      | 120.80   |
| 11  | A     | 2815 | OMG  | C6-N1-C2 | 4.03  | 122.34      | 115.93   |
| 11  | A     | 3040 | OMG  | C6-N1-C2 | 3.86  | 122.07      | 115.93   |
| 11  | A     | 2815 | OMG  | C5-C6-N1 | -3.86 | 118.15      | 123.43   |
| 11  | A     | 3040 | OMG  | C5-C6-N1 | -3.72 | 118.34      | 123.43   |
| 11  | A     | 2815 | OMG  | N3-C2-N1 | -3.47 | 122.60      | 127.22   |
| 11  | A     | 3040 | OMG  | N3-C2-N1 | -3.30 | 122.82      | 127.22   |
| 11  | A     | 2815 | OMG  | C4-C5-N7 | -2.73 | 106.55      | 109.40   |
| 11  | A     | 3040 | OMG  | C4-C5-N7 | -2.59 | 106.69      | 109.40   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | A     | 2815 | OMG  | O4'-C4'-C5'-O5' |
| 11  | A     | 2815 | OMG  | C3'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 77 ligands modelled in this entry, 77 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

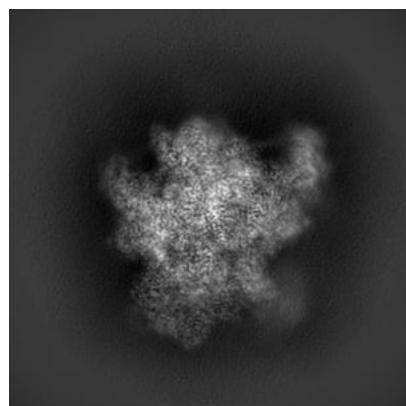
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12872. These allow visual inspection of the internal detail of the map and identification of artifacts.

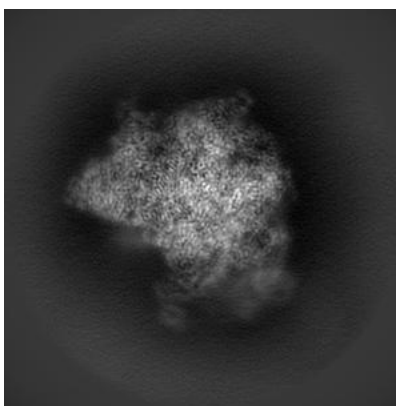
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

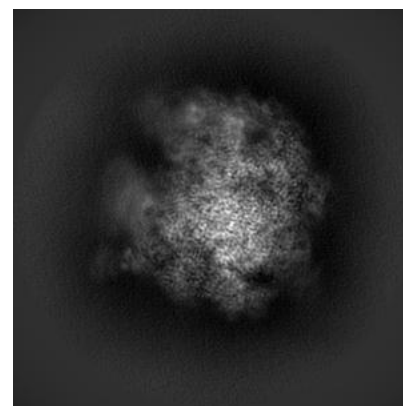
#### 6.1.1 Primary map



X

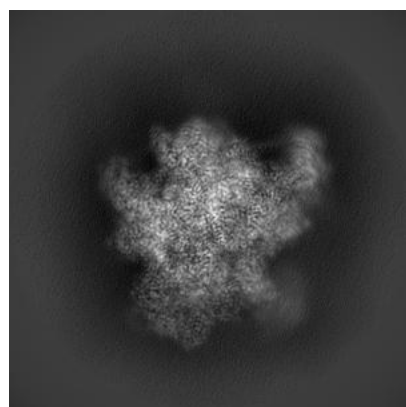


Y

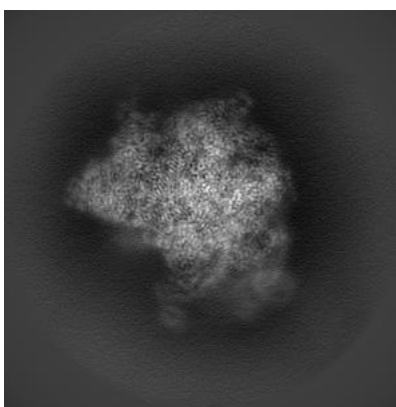


Z

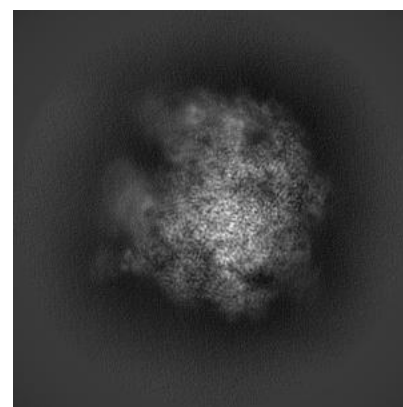
#### 6.1.2 Raw map



X



Y

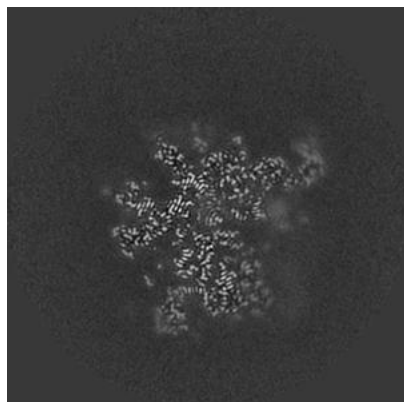


Z

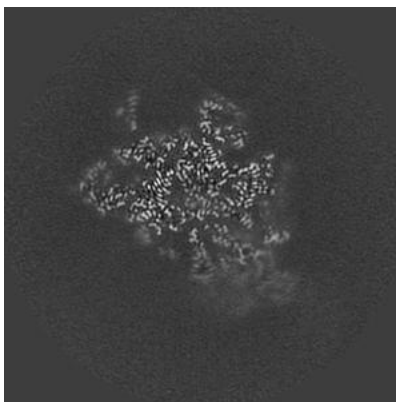
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

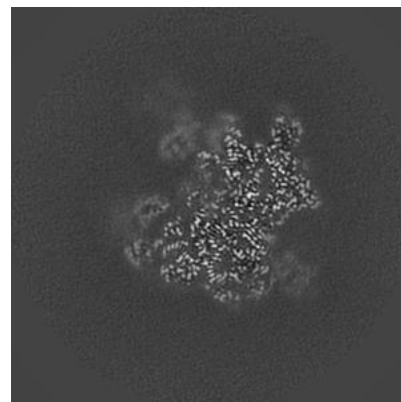
### 6.2.1 Primary map



X Index: 175

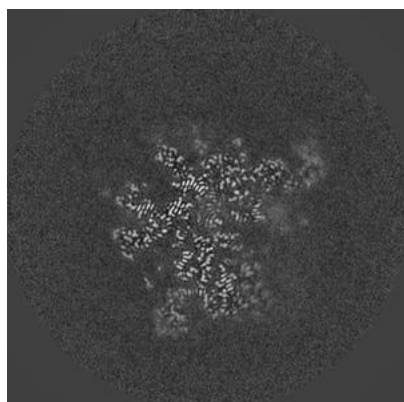


Y Index: 175

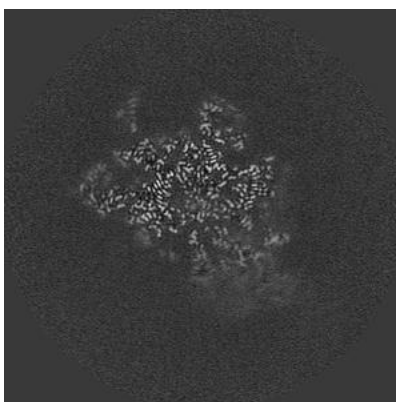


Z Index: 175

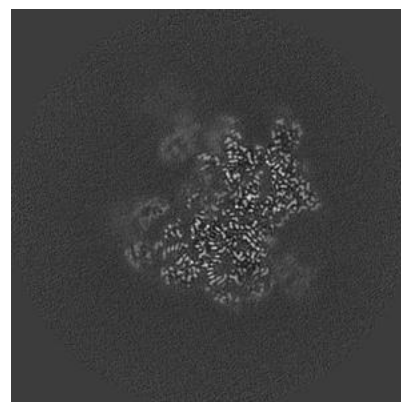
### 6.2.2 Raw map



X Index: 175



Y Index: 175

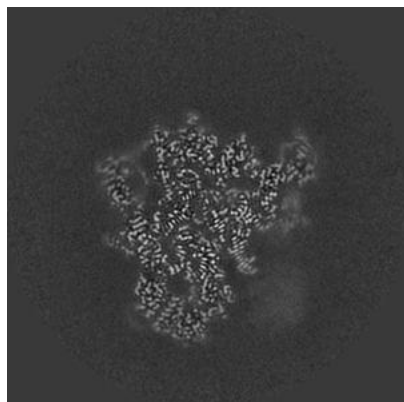


Z Index: 175

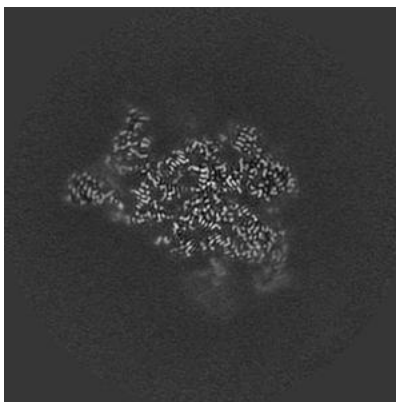
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

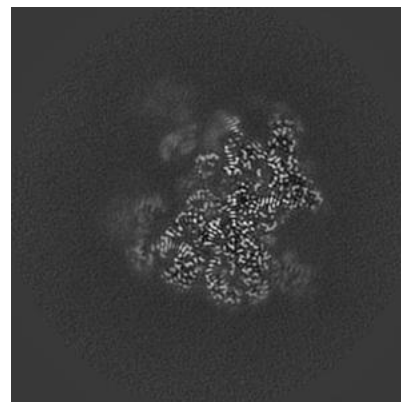
### 6.3.1 Primary map



X Index: 188

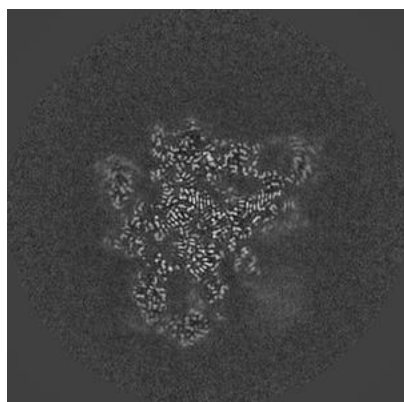


Y Index: 159

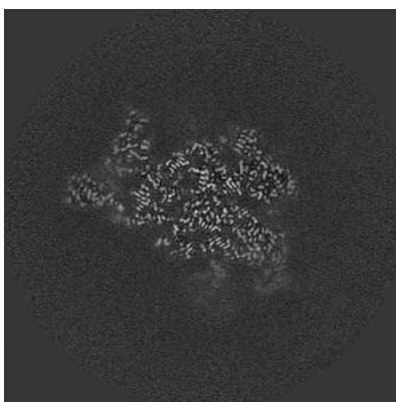


Z Index: 178

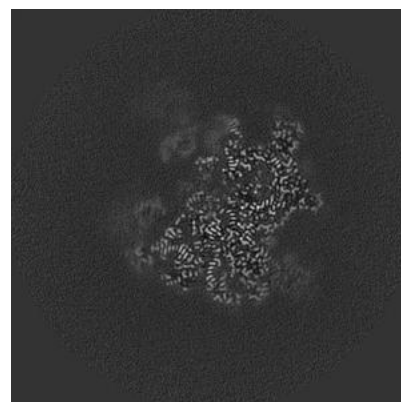
### 6.3.2 Raw map



X Index: 192



Y Index: 159

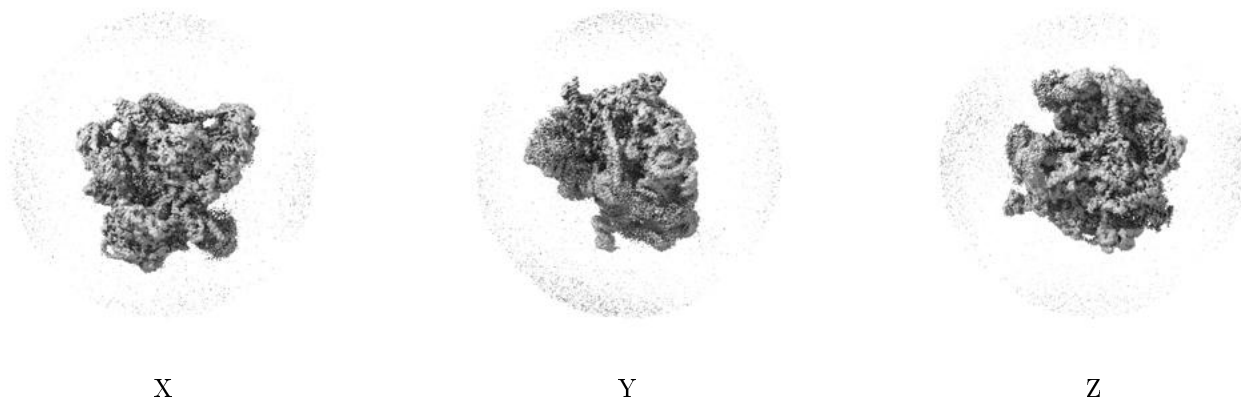


Z Index: 177

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

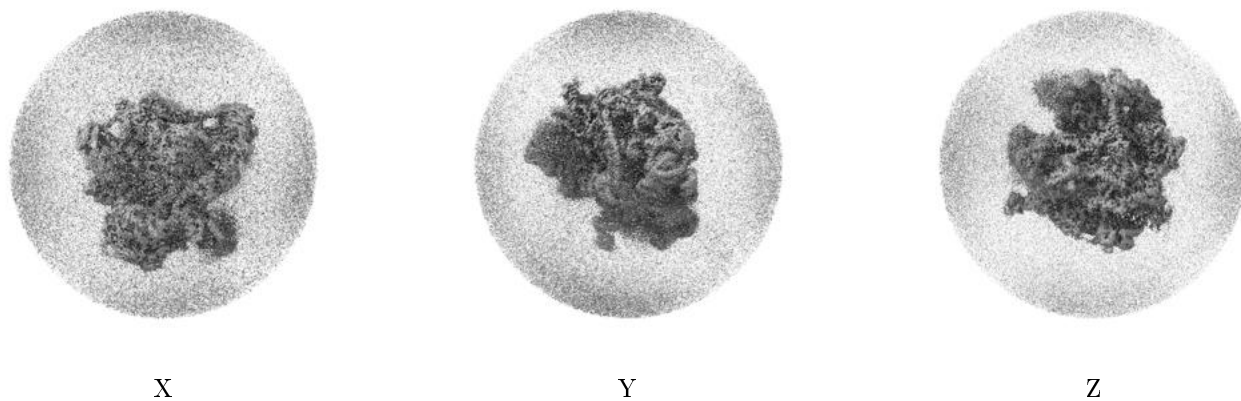
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.



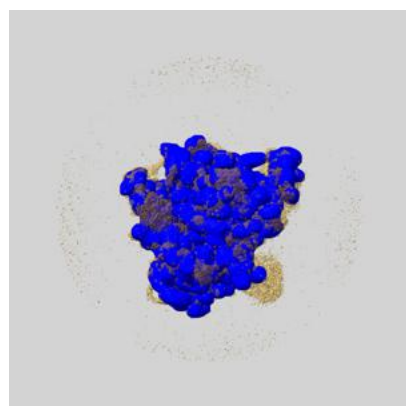
## 6.5 Mask visualisation [i](#)

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

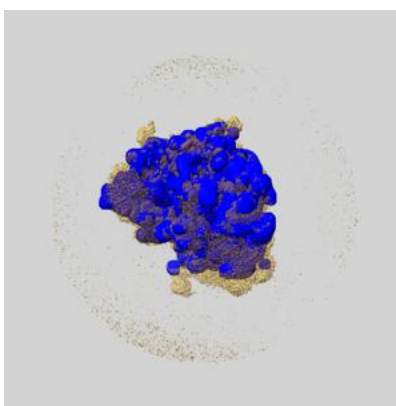
A mask typically either:

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

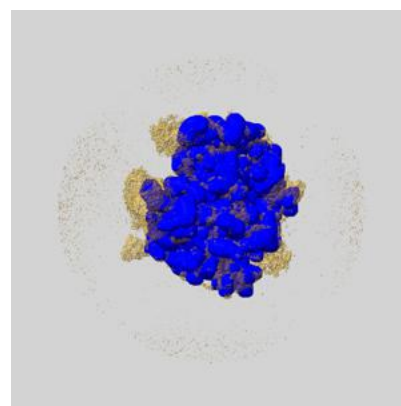
### 6.5.1 emd\_12872\_msk\_1.map [i](#)



X



Y

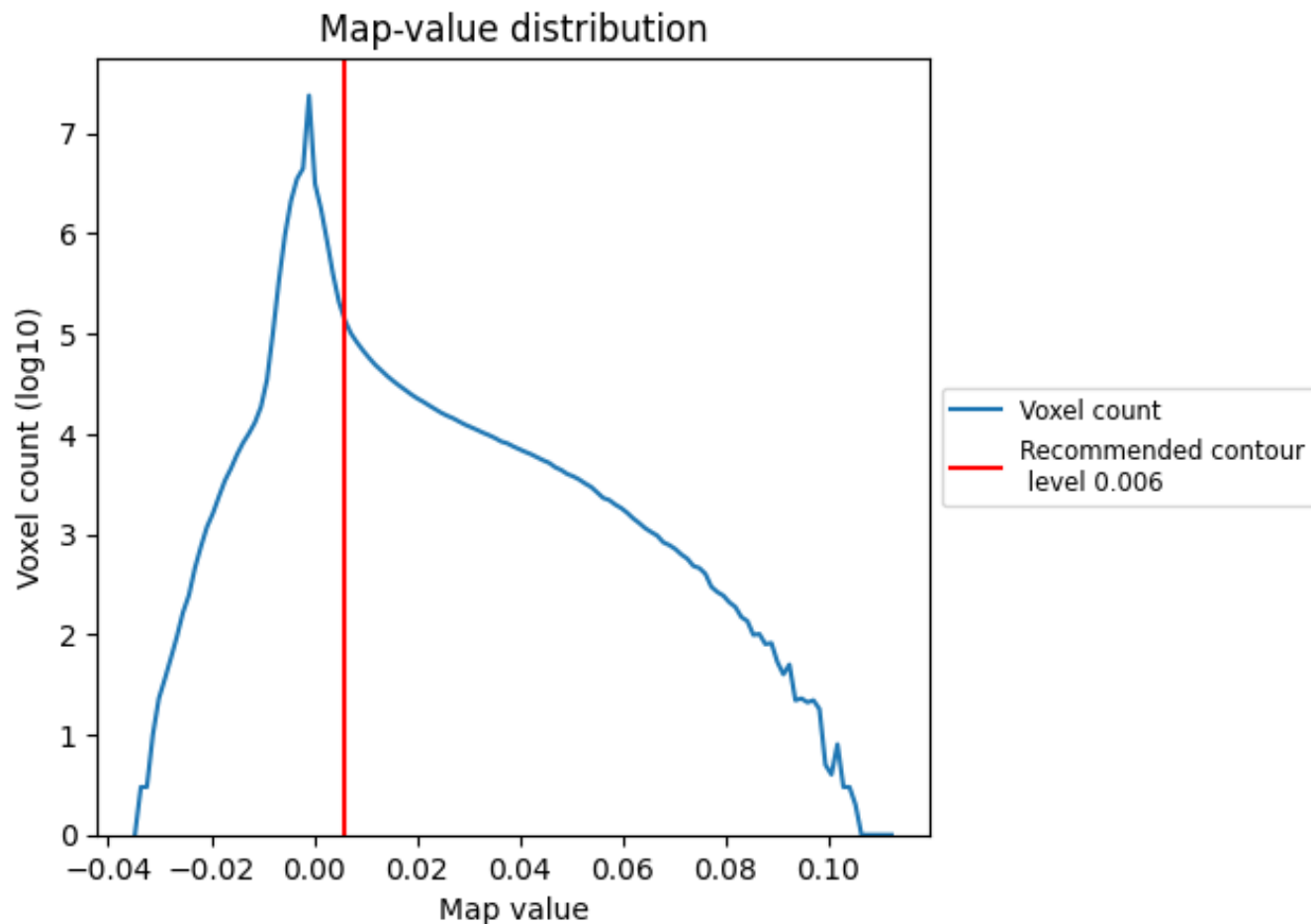


Z

## 7 Map analysis [i](#)

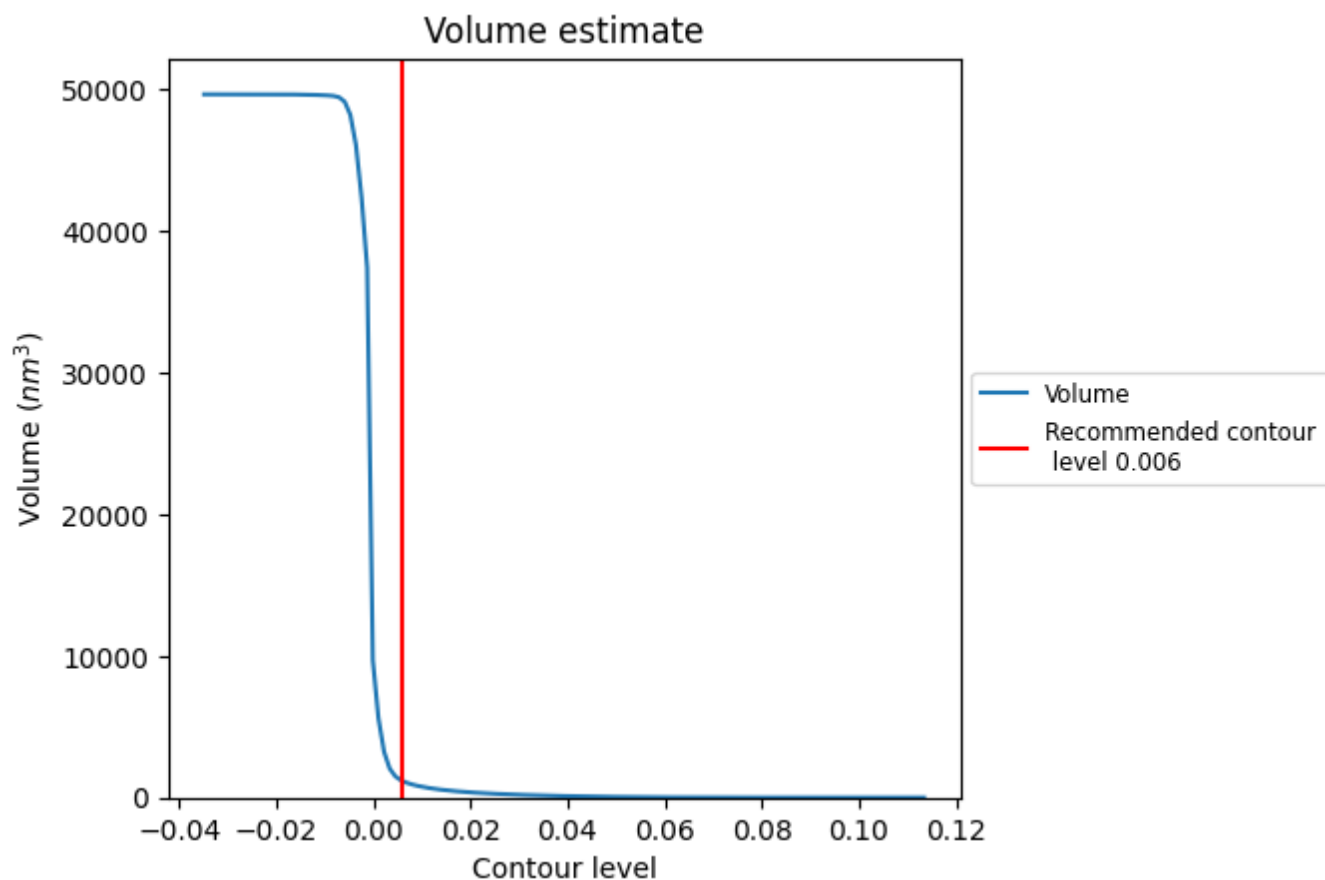
This section contains the results of statistical analysis of the map.

### 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.

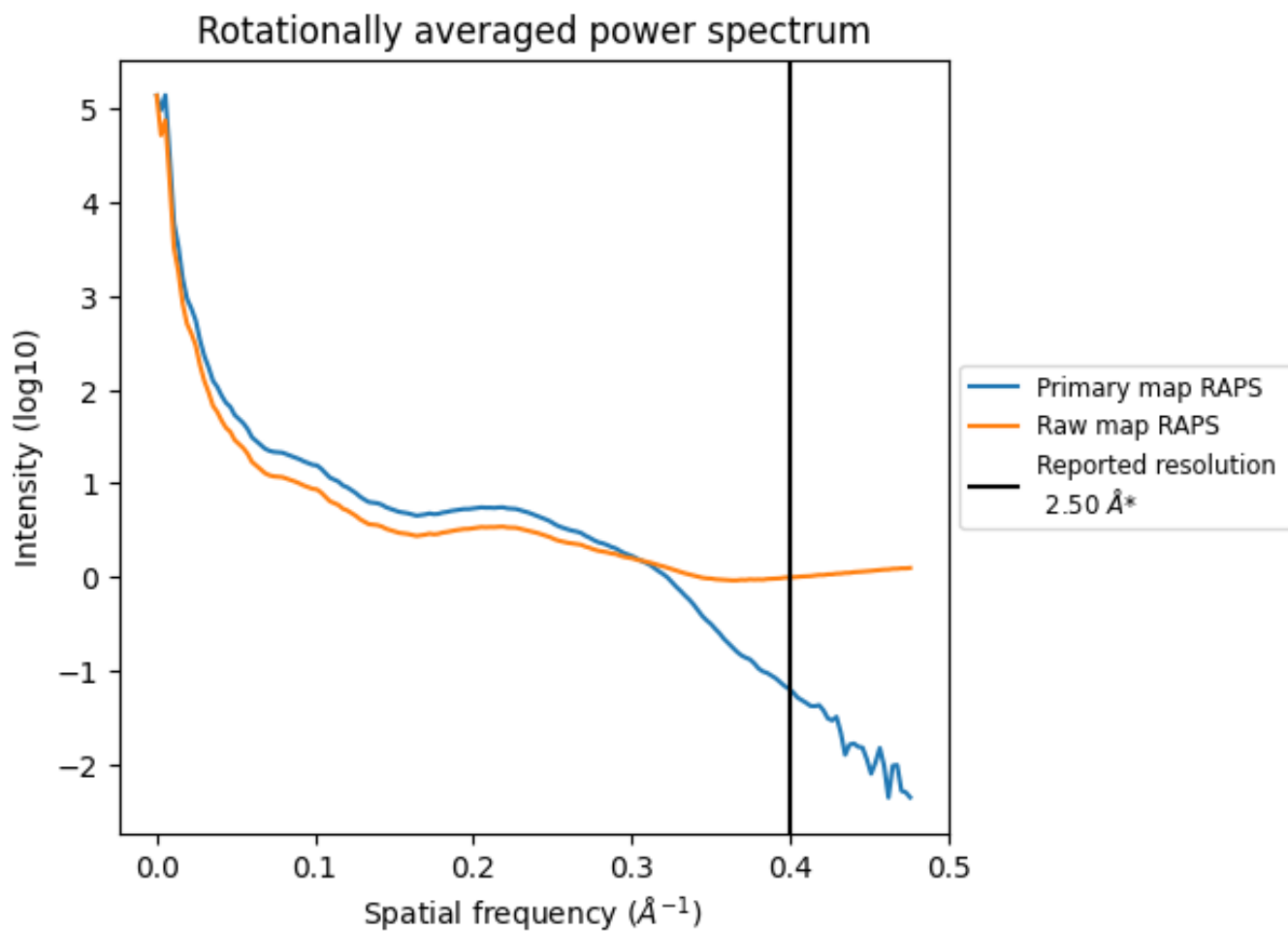
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1175 nm<sup>3</sup>; this corresponds to an approximate mass of 1062 kDa.

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

### 7.3 Rotationally averaged power spectrum i

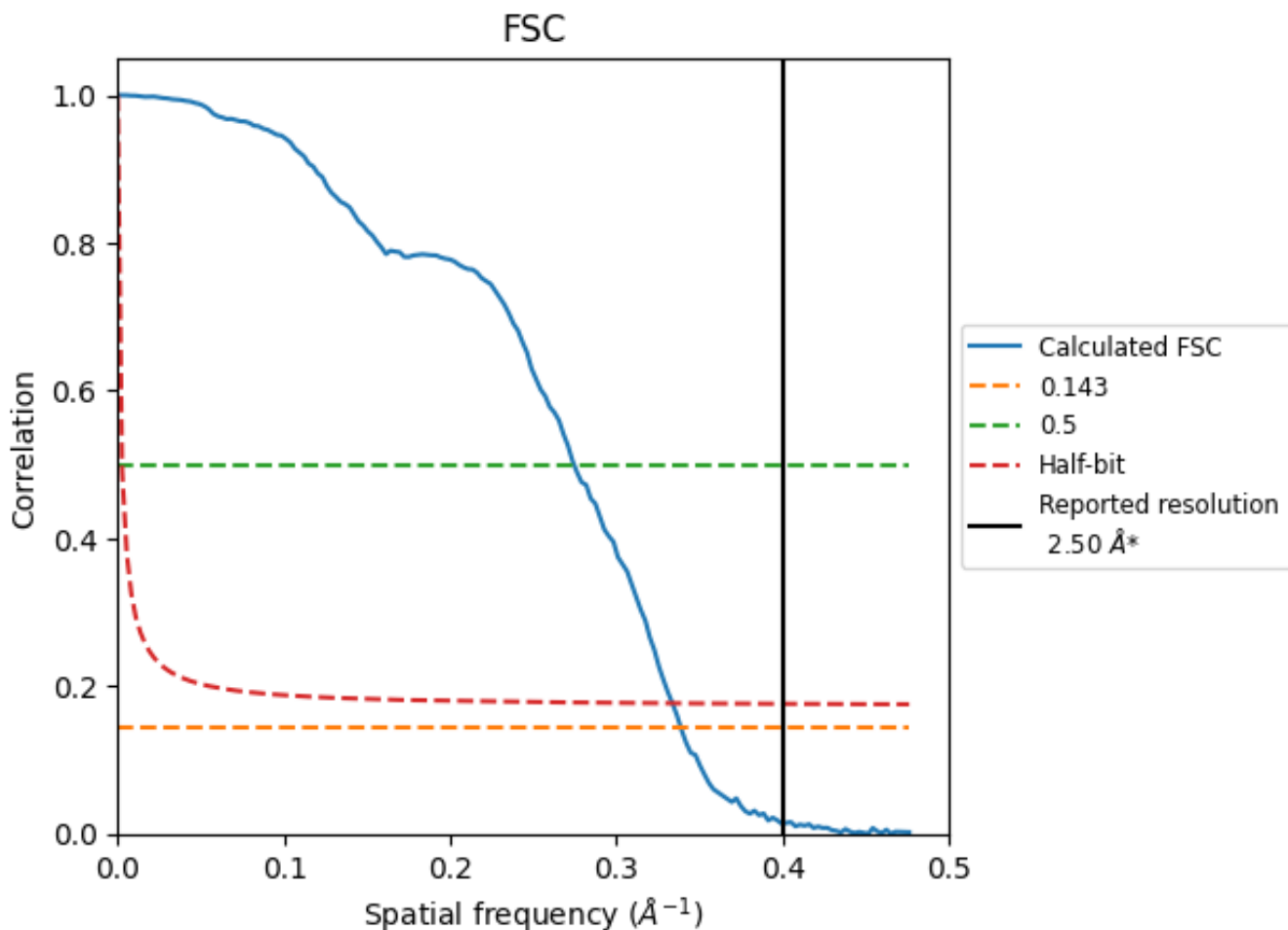


\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 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 0.400 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

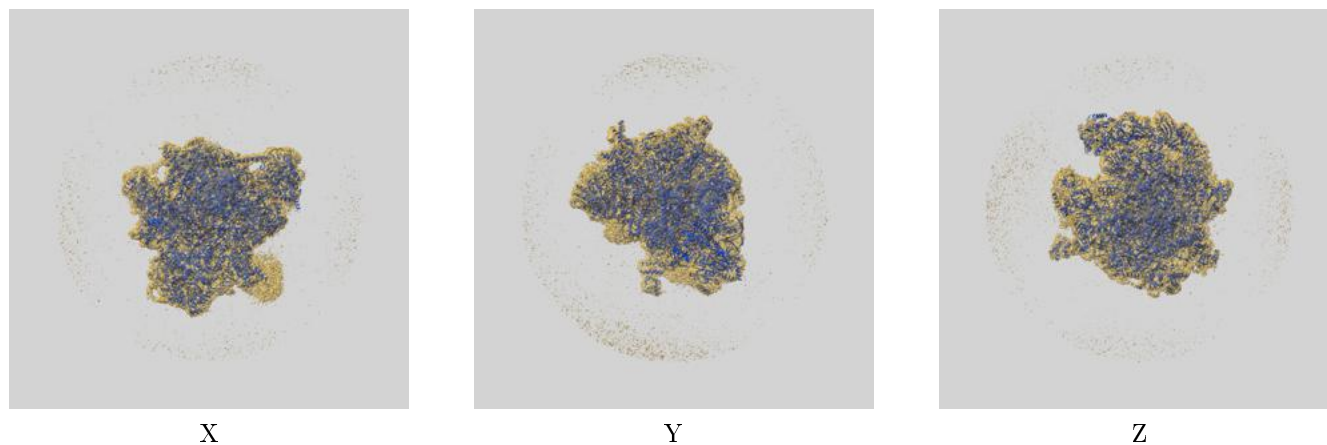
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.50                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Calculated*               | 2.95                               | 3.64 | 3.00     |

\*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 2.95 differs from the reported value 2.5 by more than 10 %

## 9 Map-model fit [i](#)

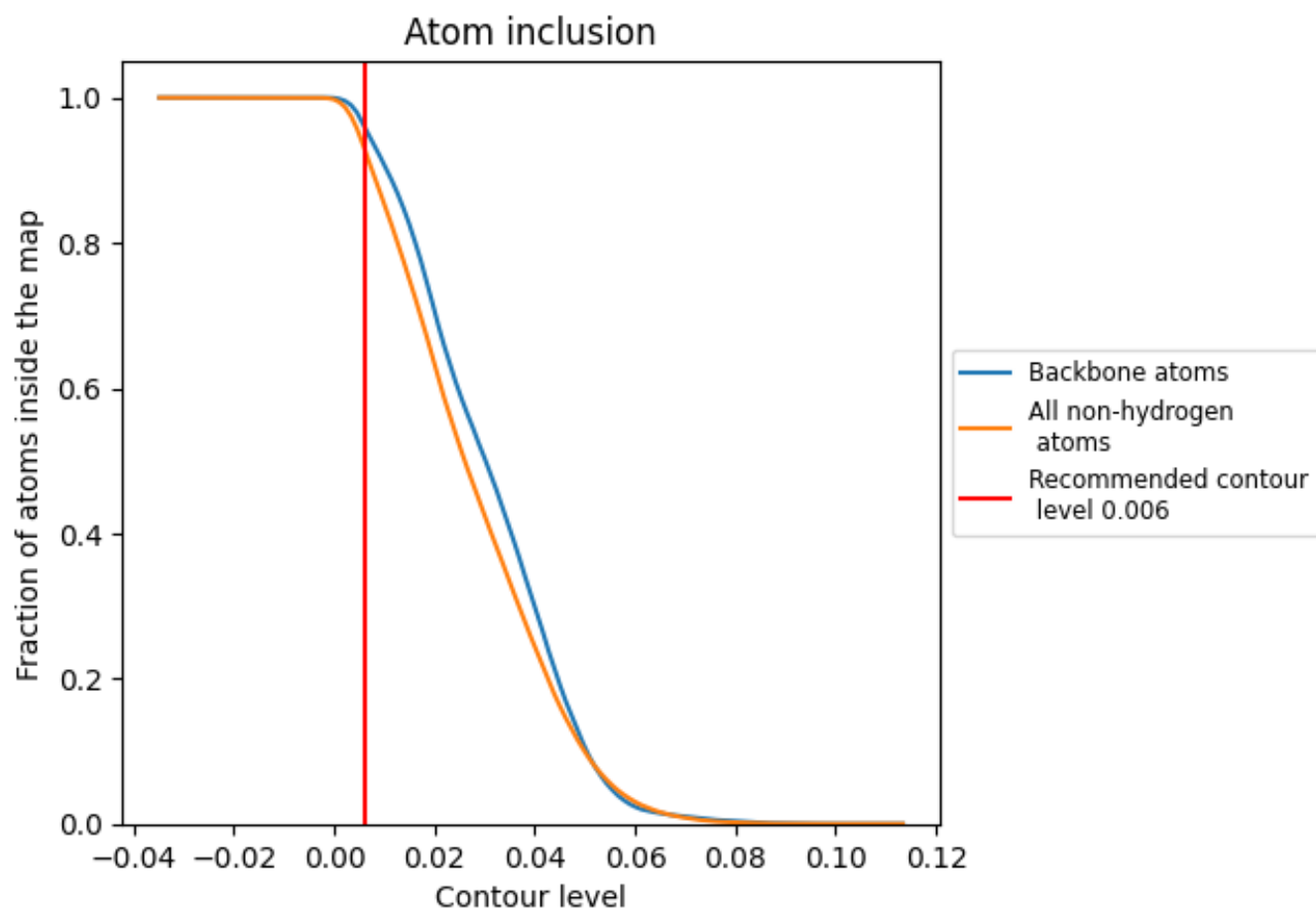
This section contains information regarding the fit between EMDB map EMD-12872 and PDB model 7OF7. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.006 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 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.