



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:13 PM UTC

PDB ID : 9HCF / pdb\_00009hcf  
EMDB ID : EMD-52047  
Title : Mouse mitoribosome large subunit assembly intermediate bound to NSUN4, METRF4, GTPBP7, GTPBP10 and the MALSU-L0R8F8-mtACP complex with uL16m, State B2 (SAMC knock-out)  
Authors : Singh, V.; Rorbach, J.; Freyer, C.; Amunts, A.; Wredenber, A.  
Deposited on : 2024-11-08  
Resolution : 2.85 Å(reported)

This is a wwPDB EM Validation Summary 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.

The types of validation reports are described at

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

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

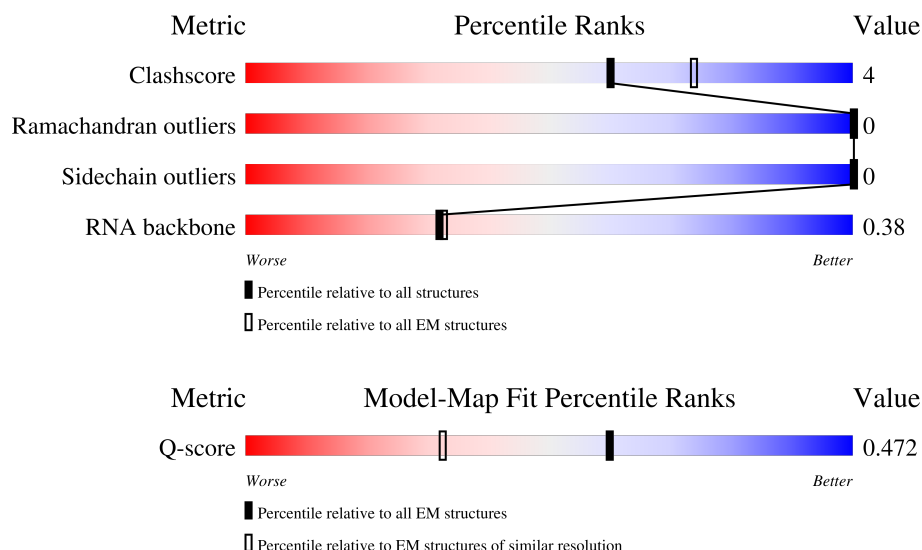
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.85 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) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 11965 ( 2.35 - 3.35 )                                    |

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   | A     | 1584   |                  |
| 2   | B     | 68     |                  |
| 3   | D     | 246    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | E     | 348    |                  |
| 5   | F     | 294    |                  |
| 6   | H     | 265    |                  |
| 7   | I     | 262    |                  |
| 8   | J     | 192    |                  |
| 9   | K     | 178    |                  |
| 10  | L     | 145    |                  |
| 11  | M     | 295    |                  |
| 12  | N     | 251    |                  |
| 13  | O     | 176    |                  |
| 14  | P     | 180    |                  |
| 15  | Q     | 292    |                  |
| 16  | R     | 149    |                  |
| 17  | S     | 209    |                  |
| 18  | T     | 206    |                  |
| 19  | U     | 146    |                  |
| 20  | V     | 216    |                  |
| 21  | W     | 148    |                  |
| 22  | X     | 294    |                  |
| 23  | Y     | 252    |                  |
| 24  | Z     | 160    |                  |
| 25  | x     | 381    |                  |
| 26  | 1     | 65     |                  |
| 27  | 2     | 92     |                  |
| 28  | 3     | 188    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | 4     | 101    |                  |
| 30  | 6     | 380    |                  |
| 31  | 7     | 336    |                  |
| 32  | b     | 159    |                  |
| 33  | f     | 211    |                  |
| 34  | h     | 159    |                  |
| 35  | i     | 128    |                  |
| 36  | j     | 121    |                  |
| 37  | o     | 102    |                  |
| 38  | q     | 222    |                  |
| 39  | r     | 196    |                  |
| 40  | s     | 442    |                  |
| 41  | u     | 228    |                  |
| 42  | v     | 70     |                  |
| 43  | 5     | 423    |                  |
| 44  | 8     | 206    |                  |
| 45  | 9     | 135    |                  |
| 46  | a     | 142    |                  |
| 47  | m     | 127    |                  |
| 48  | z     | 326    |                  |
| 49  | l     | 135    |                  |
| 50  | y     | 346    |                  |
| 51  | w     | 156    |                  |
| 52  | c     | 308    |                  |
| 53  | g     | 166    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | k     | 118    |                  |
| 55  | 0     | 187    |                  |
| 56  | d     | 306    |                  |
| 57  | e     | 283    |                  |
| 58  | p     | 206    |                  |
| 59  | t     | 366    |                  |

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 202333 atoms, of which 93796 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA (1432-MER).

| Mol | Chain | Residues | Atoms |       |       |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|------|------|---------|-------|
| 1   | A     | 1428     | Total | C     | H     | N    | O    | P    | 0       | 0     |
|     |       |          | 45695 | 13636 | 15333 | 5478 | 9820 | 1428 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| A     | 1842    | U        | C      | conflict | GB 10336604 |
| A     | 2197    | A        | U      | conflict | GB 10336604 |
| A     | 2431    | A        | G      | conflict | GB 10336604 |

- Molecule 2 is a RNA chain called RNA (63-MER).

| Mol | Chain | Residues | Atoms |     |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 2   | B     | 62       | Total | C   | H   | N   | O   | P  | 0       | 0     |
|     |       |          | 1993  | 595 | 667 | 244 | 425 | 62 |         |       |

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 3   | D     | 227      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3598  | 1105 | 1830 | 349 | 305 | 9 |         |       |

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 4   | E     | 308      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4900  | 1577 | 2441 | 432 | 442 | 8 |         |       |

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 5   | F     | 250      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4030  | 1286 | 2025 | 364 | 349 | 6 |         |       |

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

| Mol | Chain | Residues | Atoms |     |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|
| 6   | H     | 95       | Total | C   | H   | N   | O   | 0       | 0     |
|     |       |          | 1593  | 492 | 814 | 150 | 137 |         |       |

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 7   | I     | 161      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2700  | 851 | 1393 | 235 | 214 | 7 |         |       |

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

| Mol | Chain | Residues | Atoms |     |     |     |     | AltConf | Trace |   |
|-----|-------|----------|-------|-----|-----|-----|-----|---------|-------|---|
| 8   | J     | 97       | Total | C   | H   | N   | O   | S       | 0     | 0 |
|     |       |          | 1543  | 487 | 796 | 126 | 131 | 3       |       |   |

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 9   | K     | 177      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2893  | 927 | 1444 | 262 | 253 | 7 |         |       |

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 10  | L     | 115      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1837  | 560 | 944 | 174 | 155 | 4 |         |       |

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 11  | M     | 287      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4692  | 1475 | 2377 | 428 | 406 | 6 |         |       |

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

| Mol | Chain | Residues | Atoms |     |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 12  | N     | 184      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3037  | 978 | 1521 | 273 | 255 | 10 |         |       |

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 13  | O     | 153      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2541  | 795 | 1282 | 240 | 219 | 5 |         |       |

- Molecule 14 is a protein called Large ribosomal subunit protein uL18m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 14  | P     | 141      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2302  | 725 | 1148 | 221 | 203 | 5 |         |       |

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 15  | Q     | 217      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3612  | 1150 | 1822 | 309 | 322 | 9 |         |       |

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 16  | R     | 140      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2385  | 738 | 1224 | 233 | 187 | 3 |         |       |

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 17  | S     | 155      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2582  | 813 | 1323 | 222 | 222 | 2 |         |       |

- Molecule 18 is a protein called Large ribosomal subunit protein uL22m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 18  | T     | 166      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2771  | 871 | 1402 | 256 | 234 | 8 |         |       |

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 19  | U     | 127      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2109  | 675 | 1057 | 196 | 178 | 3 |         |       |

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.



| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 20  | V     | 201      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3295  | 1043 | 1643 | 305 | 298 | 6 |         |       |

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 21  | W     | 100      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1602  | 515 | 808 | 141 | 135 | 3 |         |       |

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m, Large ribosomal subunit protein bL32m.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 22  | X     | 242      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4072  | 1304 | 2051 | 358 | 355 | 4 |         |       |

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 23  | Y     | 176      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3076  | 973 | 1553 | 290 | 255 | 5 |         |       |

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 24  | Z     | 120      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2004  | 626 | 1026 | 180 | 169 | 3 |         |       |

- Molecule 25 is a protein called 5-cytosine rRNA methyltransferase NSUN4.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 25  | x     | 325      | Total | C    | H    | N   | O   | S  | 1       | 0     |
|     |       |          | 5110  | 1626 | 2546 | 448 | 473 | 17 |         |       |

- Molecule 26 is a protein called Large ribosomal subunit protein bL33m.

| Mol | Chain | Residues | Atoms |     |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|--|---------|-------|
| 26  | 1     | 52       | Total | C   | H   | N  | O  |  | 0       | 0     |
|     |       |          | 900   | 278 | 472 | 80 | 70 |  |         |       |

- Molecule 27 is a protein called Large ribosomal subunit protein bL34m.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 27  | 2     | 46       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 787   | 235 | 407 | 86 | 58 | 1 |         |       |

- Molecule 28 is a protein called Large ribosomal subunit protein bL35m.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 28  | 3     | 95       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 528 | 872 | 164 | 127 | 4 |         |       |

- Molecule 29 is a protein called Large ribosomal subunit protein bL36m.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 29  | 4     | 37       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 676   | 206 | 354 | 68 | 45 | 3 |         |       |

- Molecule 30 is a protein called Large ribosomal subunit protein mL38.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 30  | 6     | 315      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5248  | 1726 | 2559 | 487 | 470 | 6 |         |       |

- Molecule 31 is a protein called Large ribosomal subunit protein mL39.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 31  | 7     | 292      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4757  | 1517 | 2378 | 409 | 438 | 15 |         |       |

- Molecule 32 is a protein called Large ribosomal subunit protein mL43.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 32  | b     | 148      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2376  | 731 | 1195 | 234 | 214 | 2 |         |       |

- Molecule 33 is a protein called Large ribosomal subunit protein mL48.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 33  | f     | 104      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1674  | 533 | 836 | 141 | 160 | 4 |         |       |

- Molecule 34 is a protein called Large ribosomal subunit protein mL50.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 34  | h     | 110      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1739  | 552 | 867 | 156 | 160 | 4 |         |       |

- Molecule 35 is a protein called Large ribosomal subunit protein mL51.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 35  | i     | 97       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1685  | 540 | 854 | 161 | 128 | 2 |         |       |

- Molecule 36 is a protein called Large ribosomal subunit protein mL52.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 36  | j     | 93       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1512  | 467 | 768 | 145 | 130 | 2 |         |       |

- Molecule 37 is a protein called Large ribosomal subunit protein mL63.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 37  | o     | 78       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1263  | 402 | 623 | 118 | 116 | 4 |         |       |

- Molecule 38 is a protein called Large ribosomal subunit protein mL64.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 38  | q     | 135      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2253  | 703 | 1123 | 223 | 199 | 5 |         |       |

- Molecule 39 is a protein called Large ribosomal subunit protein mL66.

| Mol | Chain | Residues | Atoms |     |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 39  | r     | 157      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2606  | 812 | 1331 | 242 | 210 | 11 |         |       |

- Molecule 40 is a protein called Large ribosomal subunit protein mL65.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 40  | s     | 377      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6104  | 1938 | 3059 | 555 | 540 | 12 |         |       |

- Molecule 41 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 41  | u     | 125      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2041  | 659 | 1012 | 170 | 191 | 9 |         |       |

- Molecule 42 is a protein called Predicted gene, 55359.

| Mol | Chain | Residues | Atoms |     |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 42  | v     | 69       | Total | C   | H   | N   | O  | S | 0       | 0     |
|     |       |          | 1189  | 374 | 603 | 112 | 99 | 1 |         |       |

- Molecule 43 is a protein called Large ribosomal subunit protein mL37.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 43  | 5     | 394      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 6468  | 2081 | 3243 | 564 | 571 | 9 |         |       |

- Molecule 44 is a protein called Large ribosomal subunit protein mL40.

| Mol | Chain | Residues | Atoms |     |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|---------|-------|
| 44  | 8     | 67       | Total | C   | H   | N  | O   | S | 0       | 0     |
|     |       |          | 1121  | 354 | 557 | 97 | 111 | 2 |         |       |

- Molecule 45 is a protein called Large ribosomal subunit protein mL41.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 45  | 9     | 122      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1973  | 635 | 990 | 167 | 179 | 2 |         |       |

- Molecule 46 is a protein called Large ribosomal subunit protein mL42.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 46  | a     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1703  | 542 | 843 | 156 | 159 | 3 |         |       |

- Molecule 47 is a protein called Large ribosomal subunit protein mL55.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|---------|-------|
| 47  | m     | 45       | Total | C   | H   | N  | O  | S | 0       | 0     |
|     |       |          | 769   | 233 | 395 | 77 | 61 | 3 |         |       |

- Molecule 48 is a protein called Mitochondrial ribosome-associated GTPase 1.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 48  | z     | 311      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 5001  | 1562 | 2546 | 444 | 433 | 16 |         |       |

- Molecule 49 is a protein called Large ribosomal subunit protein mL54.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 49  | l     | 65       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 355 | 549 | 101 | 102 | 1 |         |       |

- Molecule 50 is a protein called Transcription termination factor 4, mitochondrial.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 50  | y     | 237      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3938  | 1238 | 1995 | 345 | 351 | 9 |         |       |

- Molecule 51 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|---------|-------|
| 51  | w     | 79       | Total | C   | H   | N  | O   | S | 0       | 0     |
|     |       |          | 1277  | 410 | 640 | 95 | 127 | 5 |         |       |

- Molecule 52 is a protein called Large ribosomal subunit protein mL44.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 52  | c     | 281      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 4535  | 1450 | 2273 | 392 | 412 | 8 |         |       |

- Molecule 53 is a protein called Large ribosomal subunit protein mL49.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 53  | g     | 132      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2184  | 709 | 1094 | 187 | 192 | 2 |         |       |

- Molecule 54 is a protein called Large ribosomal subunit protein mL53.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 54  | k     | 85       | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1331  | 413 | 667 | 121 | 125 | 5 |         |       |

- Molecule 55 is a protein called Large ribosomal subunit protein bL32m.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 55  | 0     | 108      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1789  | 546 | 908 | 174 | 155 | 6 |         |       |

- Molecule 56 is a protein called Large ribosomal subunit protein mL45.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 56  | d     | 238      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3901  | 1262 | 1940 | 348 | 341 | 10 |         |       |

- Molecule 57 is a protein called Large ribosomal subunit protein mL46.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 57  | e     | 193      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3174  | 1013 | 1598 | 278 | 279 | 6 |         |       |

- Molecule 58 is a protein called Large ribosomal subunit protein mL62.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 58  | p     | 144      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2374  | 735 | 1198 | 218 | 219 | 4 |         |       |

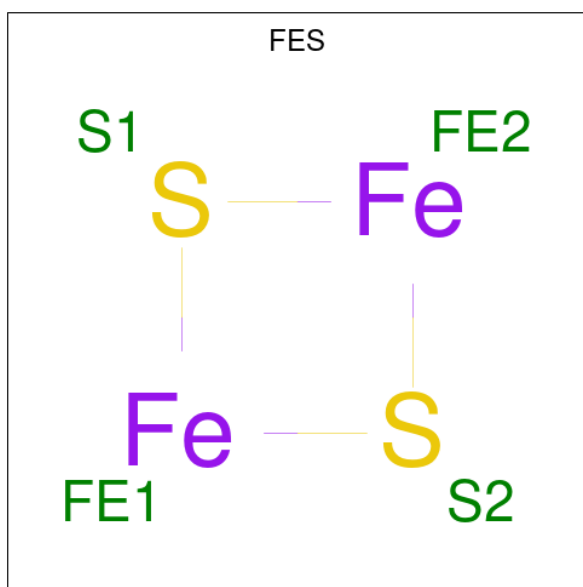
- Molecule 59 is a protein called GTP-binding protein 10.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 59  | t     | 321      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5015  | 1569 | 2551 | 431 | 455 | 9 |         |       |

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 60  | A     | 96       | Total | Mg | 0       |
|     |       |          | 96    | 96 |         |
| 60  | M     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 60  | O     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 60  | R     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 61 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

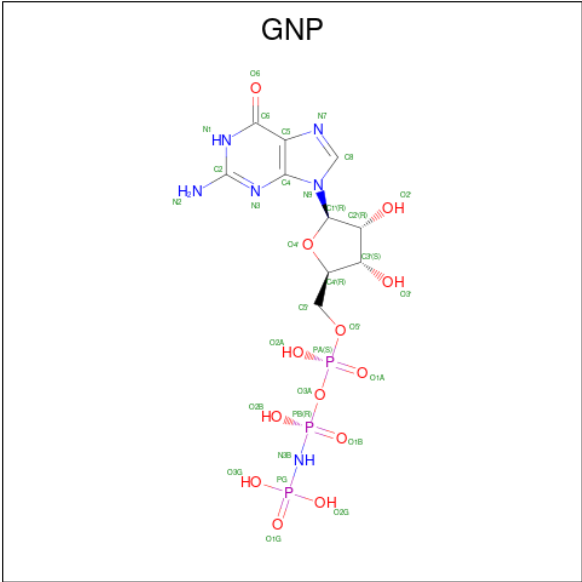


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 61  | I     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 62  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 62  | 0     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



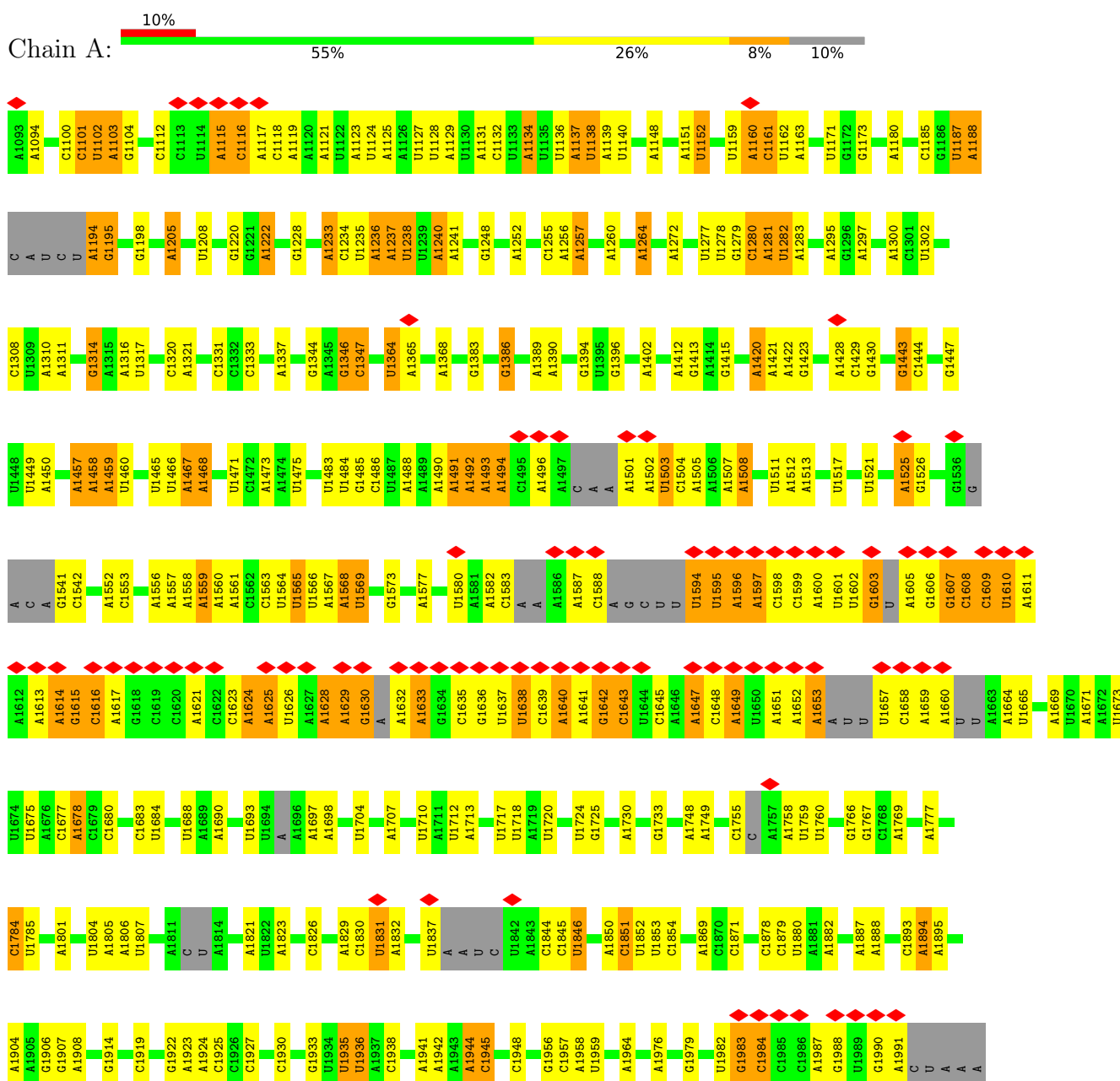
| Mol | Chain | Residues | Atoms |    |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|
| 63  | z     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 45    | 10 | 13 | 6 | 13 | 3 |         |
| 63  | t     | 1        | Total | C  | H  | N | O  | P | 0       |
|     |       |          | 45    | 10 | 13 | 6 | 13 | 3 |         |



### 3 Residue-property plots [i](#)

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

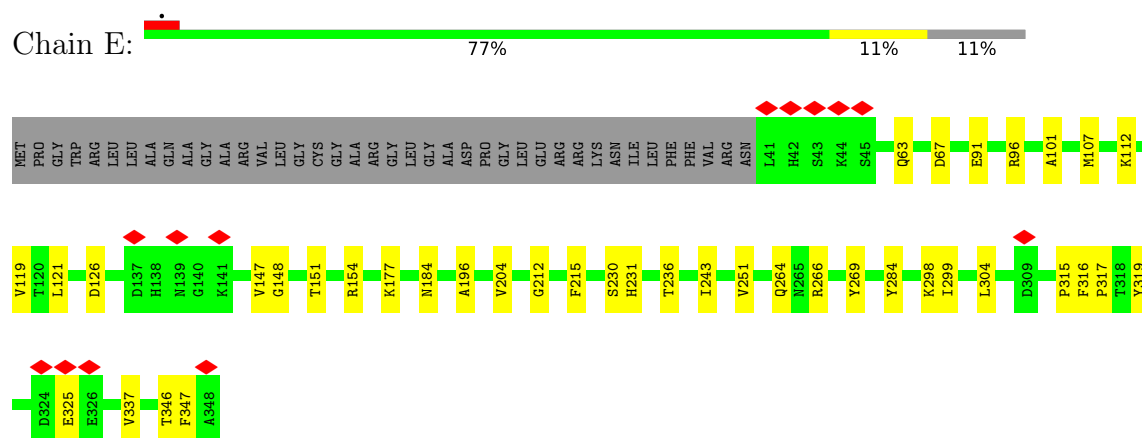
#### • Molecule 1: 16S rRNA (1432-MER)





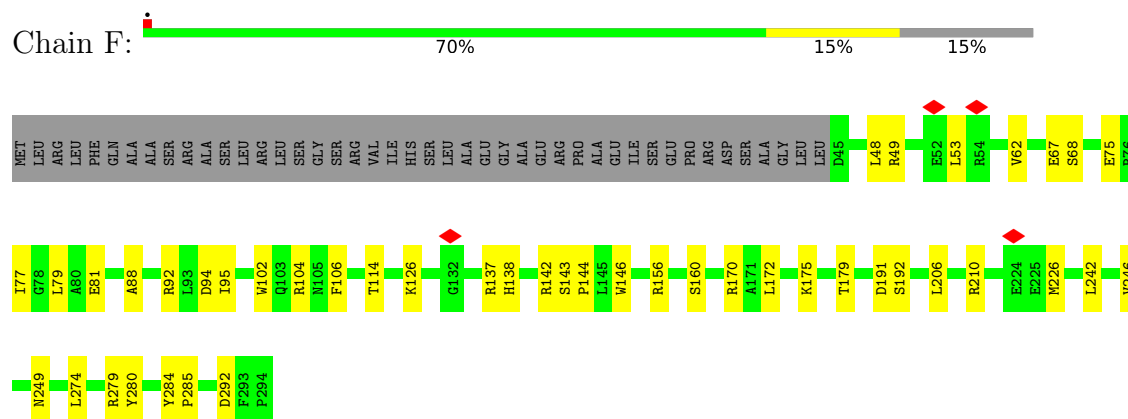
- Molecule 4: Large ribosomal subunit protein uL3m

Chain E:



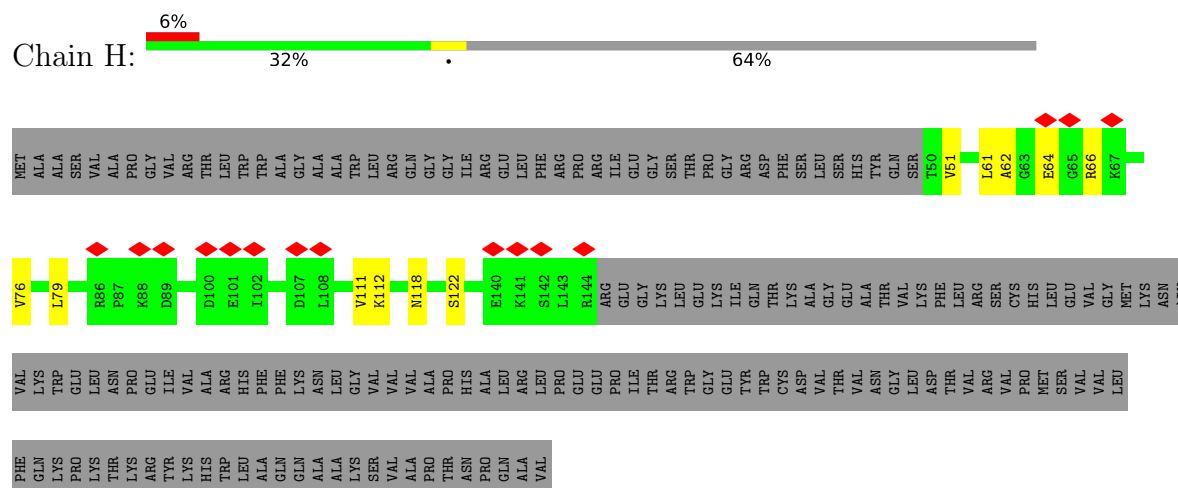
- Molecule 5: Large ribosomal subunit protein uL4m

Chain F:



- Molecule 6: Large ribosomal subunit protein bL9m

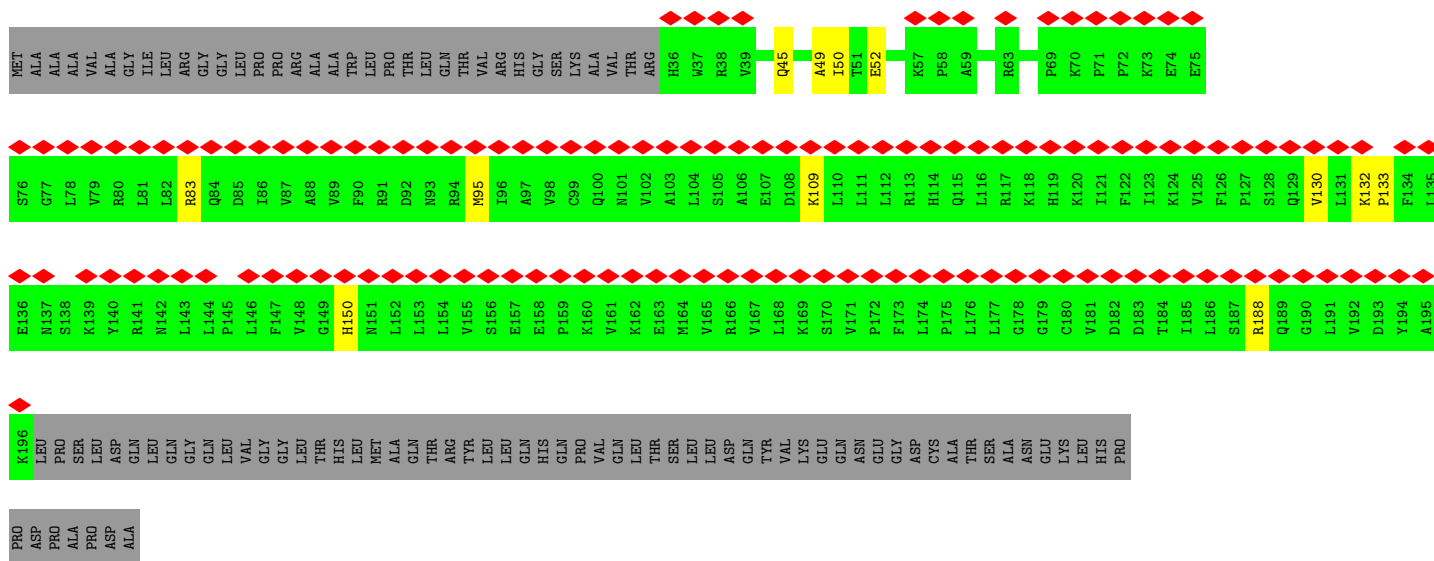
Chain H:



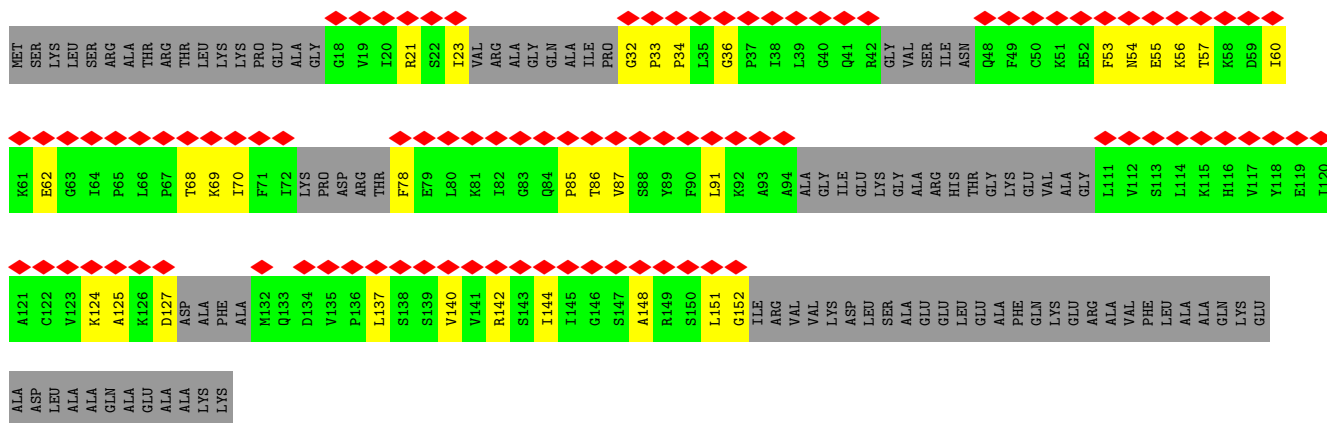
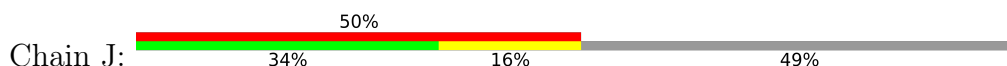
- Molecule 7: Large ribosomal subunit protein uL10m

Chain I:

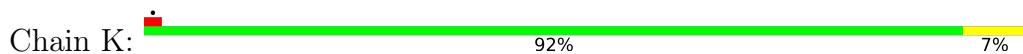




- Molecule 8: Large ribosomal subunit protein uL11m

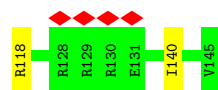


- Molecule 9: Large ribosomal subunit protein uL13m



- Molecule 10: Large ribosomal subunit protein uL14m

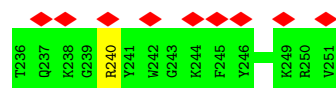
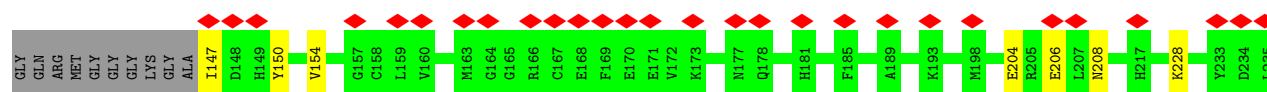
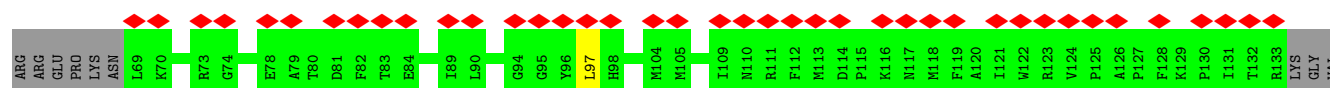
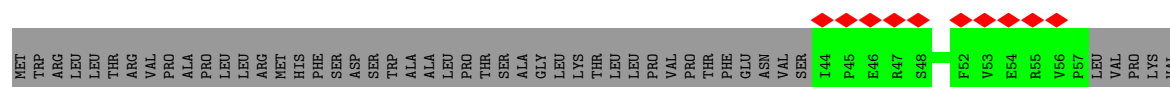




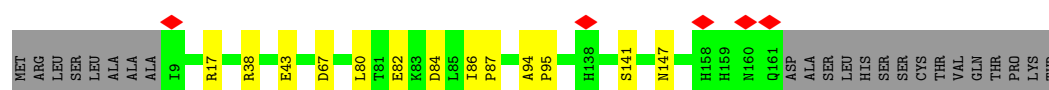
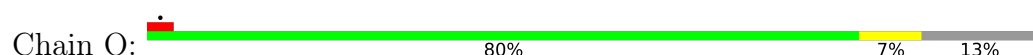
- Molecule 11: Large ribosomal subunit protein uL15m



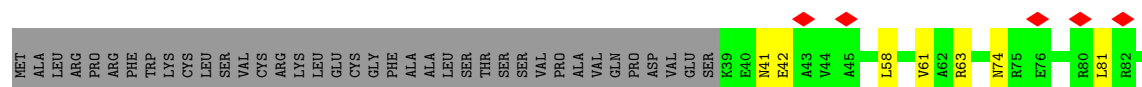
- Molecule 12: Large ribosomal subunit protein uL16m



- Molecule 13: Large ribosomal subunit protein bL17m



- Molecule 14: Large ribosomal subunit protein uL18m



- Molecule 15: Large ribosomal subunit protein bL19m

Chain Q:  70% 26%

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

VAL ILE VAL ASP ARG ARG VAL PRO GLU ASP GLU ARG R74 Y125 A126 S127 G128 R152 N153 T154 I155 E156 G157 Q158 E210 A211 C212 Q213 D246 L247 E251 E252 K262 I265 R271 E279 E284 Y290 LYS SER

- Molecule 16: Large ribosomal subunit protein bL20m

Chain R:  88% 6% 6% 5%

MET VAL PHE LEU THR ARG LEU TRP L10 R11 N12 D16 F31 R58 E78 E96 R99 L119 L132 G133 D134 G135 K136 E137 H149

- Molecule 17: Large ribosomal subunit protein bL21m

Chain S:  66% 9% 26%

MET ALA ALA ILE ALA SER ALA PRO GLY PHE GLY VAL SER VAL CYS ARG SER ILE LEU ALA SER GLN G133 D134 G135 K136 E137 H149 Y50 Q109 W110 K111 V112 E115 D116 L117 I118

N122 R131 I132 R133 K136 E161 E166 K167 T168 I174 K177 PHE ARG LYS K182 N183 F184 R185 I196 L197 R198 I199 L208 LEU

- Molecule 18: Large ribosomal subunit protein uL22m

Chain T:  75% 6% 19%

MET ALA ALA LEU LEU ARG GLU LEU GLY ALA ARG VAL PRO ASN LEU ARG ILE TRP ALA THR GLN THR LEU ARG VAL LEU LEU PRO PRO CYS ILE HIS THR SER ALA SER LEU ASP I41 Y53 G59 E60 L84 A85 I93 D94 E101 I111 N127 S139

G154 Y168 F169 V170 E181 L206

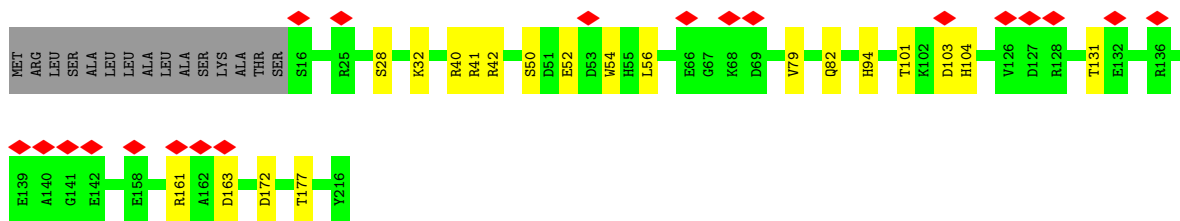
- Molecule 19: Large ribosomal subunit protein uL23m

Chain U:  81% 6% 13%

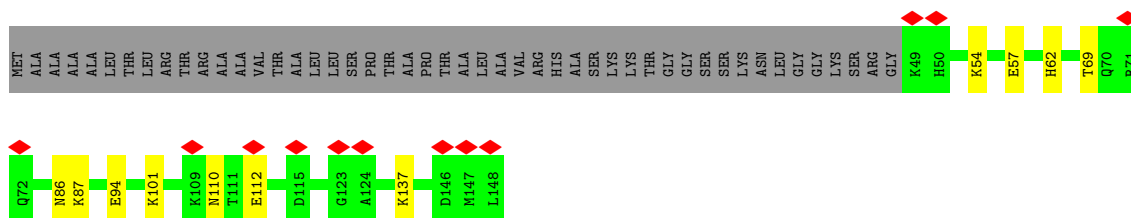
MET A2 T22 N23 F24 V29 E37 R43 Q59 E113 K114 ASP PRO ARG SER PRO GLU PRO PRO LEU GLU GLU LEU LEU PRO PRO GLN ARG GLN SER S133 D134 L135 R136 I140 L146

- Molecule 20: Large ribosomal subunit protein uL24m

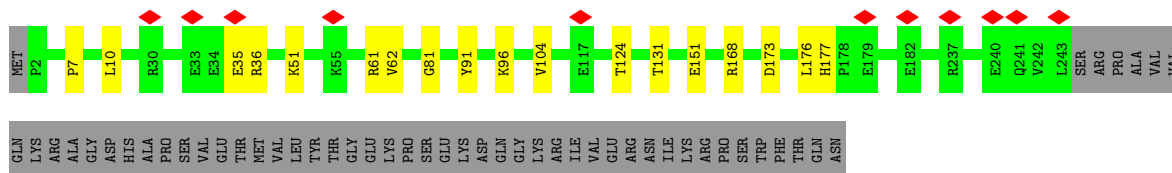
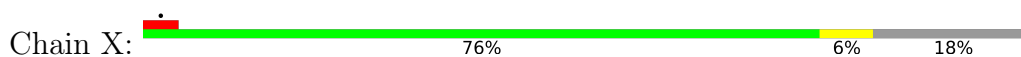
Chain V:  84% 9% 7% 9%



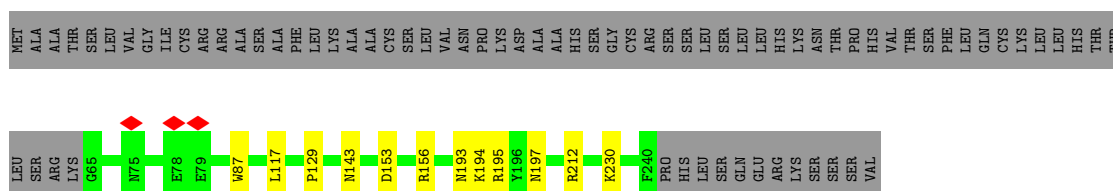
- Molecule 21: Large ribosomal subunit protein bL27m



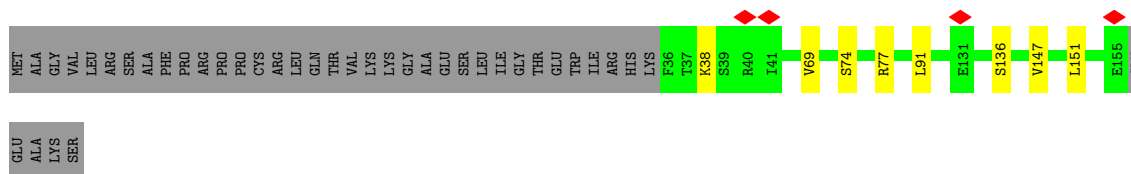
- Molecule 22: Large ribosomal subunit protein bL28m, Large ribosomal subunit protein bL32m



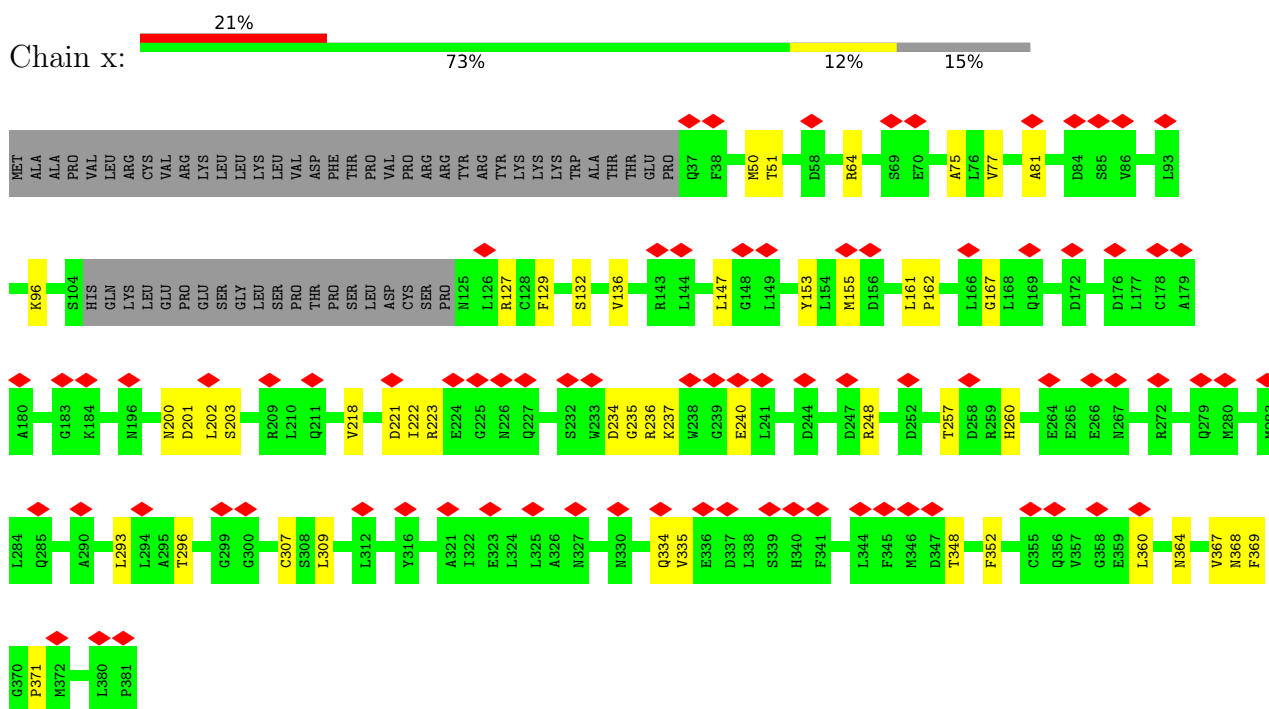
- Molecule 23: Large ribosomal subunit protein uL29m



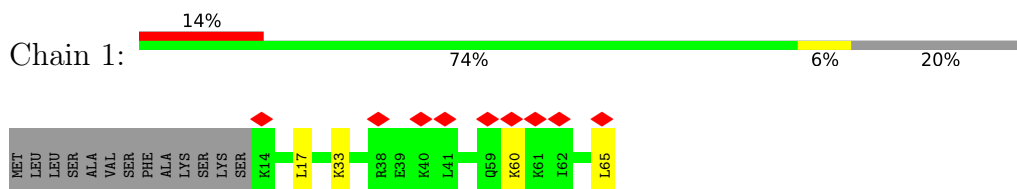
- Molecule 24: Large ribosomal subunit protein uL30m



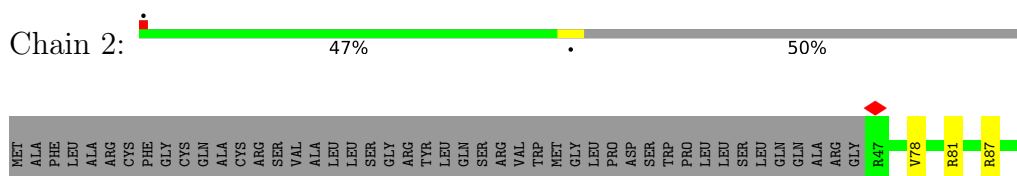
- Molecule 25: 5-cytosine rRNA methyltransferase NSUN4



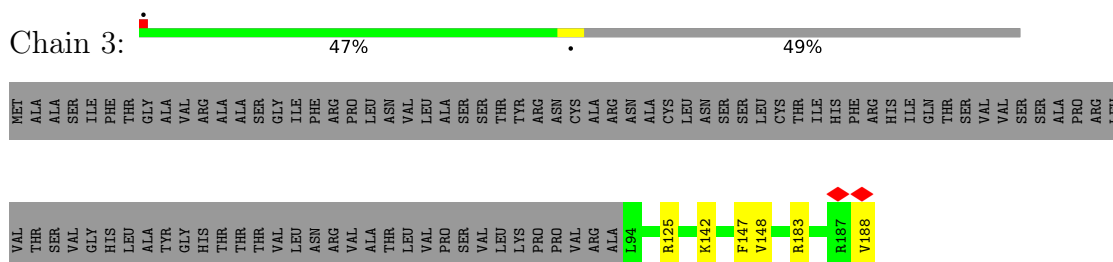
- Molecule 26: Large ribosomal subunit protein bL33m



- Molecule 27: Large ribosomal subunit protein bL34m



- Molecule 28: Large ribosomal subunit protein bL35m



- Molecule 29: Large ribosomal subunit protein bL36m





MET ALA ALA LEU VAL ARG SER VAL VAL ALA SER VAL VAL ASP PRO PHE LEU HIS LEU SER LEU ARG LEU VAL VAL LYS PRO PHE ARG VAL PHE SER SER PHE LEU LEU LEU THR THR LEU PRO ARG ALA LYS PRO CYS ALA GLU VAL ARG SER VAL VAL CYS GLY ARG ARG PRO PRO THR PRO THR LEU

PRO SER LEU GLY F65 F66 F67 K73 K76 D77 C78 V81 K82 R83 T93 H97 K98 Q99 R100 Q101

• Molecule 30: Large ribosomal subunit protein mL38

Chain 6: 17% 67% 16% 17%

MET ALA ALA PRO TRP ARG ALA ALA PHE PHE GLY ILE GLY ARG CYS ARG GLY PHE SER THR ALA LEU SER ARG THR PRO PRO LEU SER ARG THR PRO PRO MET ASN GLU ASP ILE ASP VAL SER ASN LEU E46 R47 L48 E49 K50 Y51 R52 E55 R56 Y57 R60 A61 E64 E70 W71 W72 F78 VAL LYS THR ASP PRO LYS LYS ILE ASP ILE GLY THR PRO PRO ARG VAL SER L104 H108 F109 L110 R111 E112 L113 R114 A115 E118 E119 E120 R121 A122 A123 R124 L125 R126 T127 A128 S129 I130 A137 E138 W139 E140 R141 G144 P145 R159 D160 A165 P169 W170 L173 H174 V175 A176 G180 E181 E182 D183 L184 Y188 H189 E192 A198 S199 R200 E203 Y206 E207 A208 D209 K210 D211 T215 L216 L217 F218 L219 N220 L221 D222 G223 H224 L225 L226 E227 V233 L236 S242 N243 R244 V245 A246 E247 T251 Y254 R267 F270 L271 L272 F273 K274 Q275 D276 K277 V280 E283 D284 Q292 L293 R296 R299 D302 F303 Y304 Q308 G315 L316 A317 L334 L335 R338 F344 Y345 R346 K355 E360 T380

• Molecule 31: Large ribosomal subunit protein mL39

Chain 7: 11% 78% 9% 13%

MET ALA THR ALA VAL GLY ARG LEU VAL LEU ARG ARG PRO GLY ALA GLY GLY ALA ARG TRP ARG PHE ILE ALA THR SER PRO ALA ALA GLU LEU S33 E39 M40 R41 R47 Q42 T56 P57 R58 E63 V67 V77 W95 V105 D106 D111 C120 D131 A144 L147 I151 F155 K156 D157 D158 V164 R165 L182 D183 K184 E188 P191 E214 D217 E225 L226 F227 Q228 D235 F236 L237 E238 A241 S242 Q243 N244 P245 E246 R247 R253 D256 D259 V260 S261 E262 F273 V280 L283 N284 F285 S286 Q287 P288 R289 R292 R293 T301 Q306 V321 T322 E323 D324 VAL ARG GLN THR GLU ASN THR GLU THR THR GLU

• Molecule 32: Large ribosomal subunit protein mL43

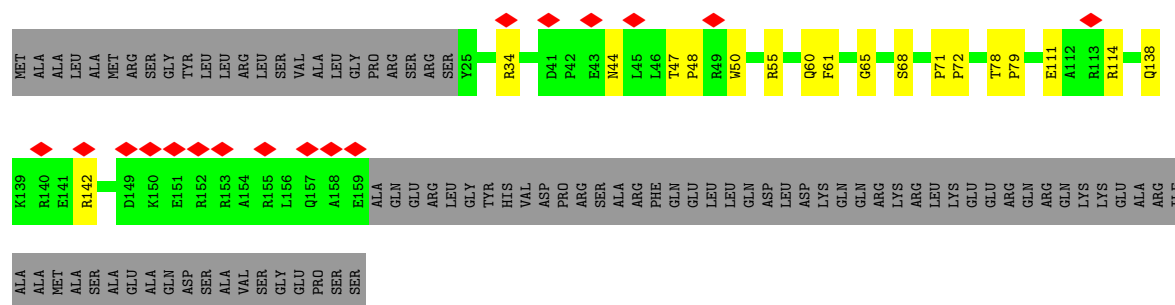
Chain b: 81% 12% 7%

MET T2 T6 S7 T12 S13 R21 D36 E45 F46 V47 V51 V65 N66 P67 V69 V94 Q107 H131 T134 N135 K136 R137 R149 ASP SER ALA PRO ALA SER MET GLN ALA GLN

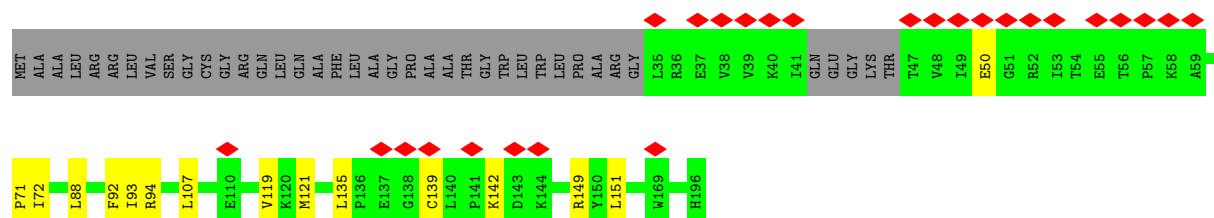
• Molecule 33: Large ribosomal subunit protein mL48

Chain f: 46% 36% 13% 51%

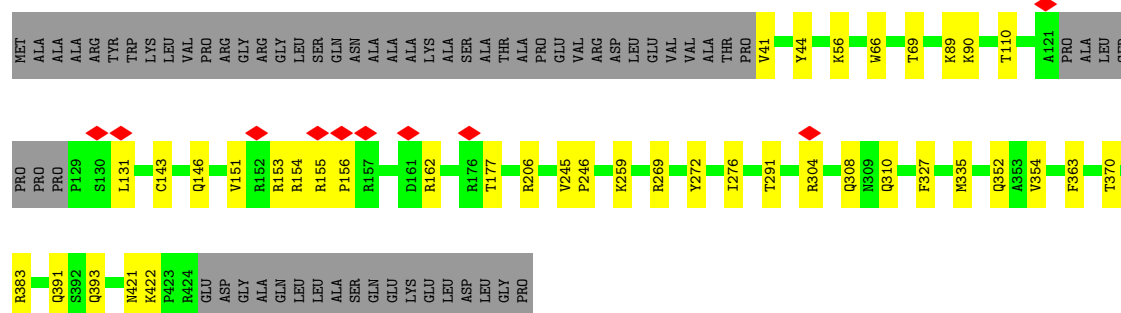
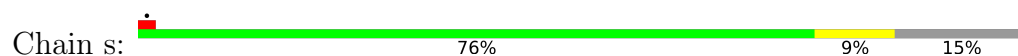




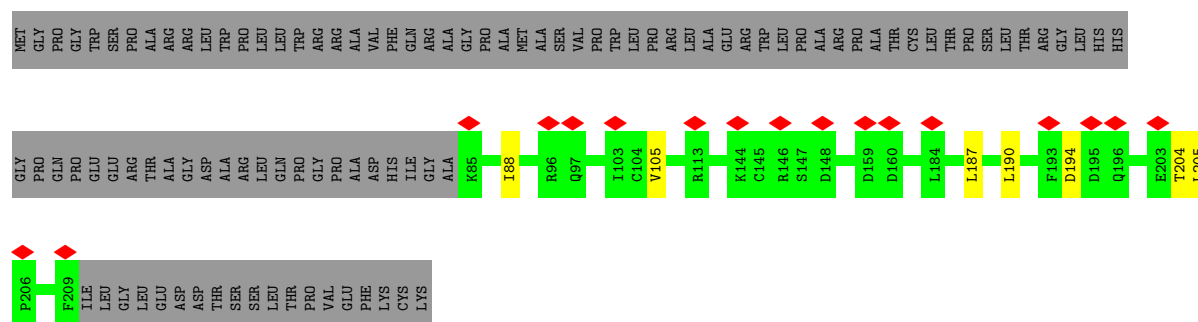
- Molecule 39: Large ribosomal subunit protein mL66



- Molecule 40: Large ribosomal subunit protein mL65

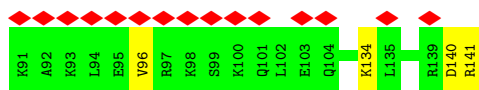


- Molecule 41: Mitochondrial assembly of ribosomal large subunit protein 1

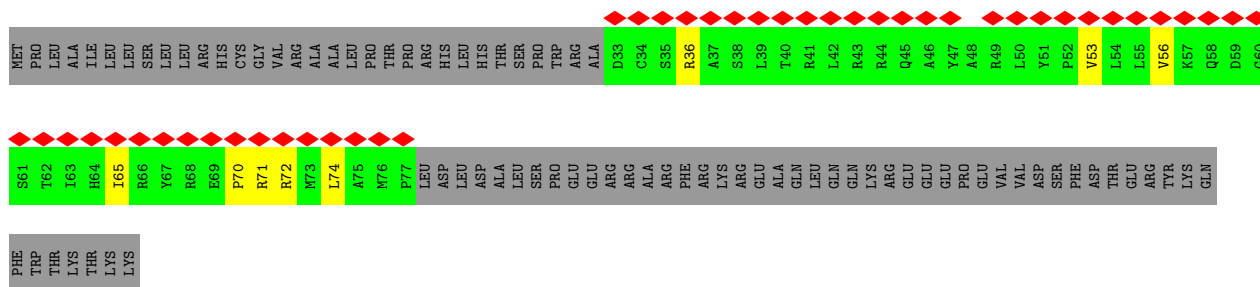


- Molecule 42: Predicted gene, 55359

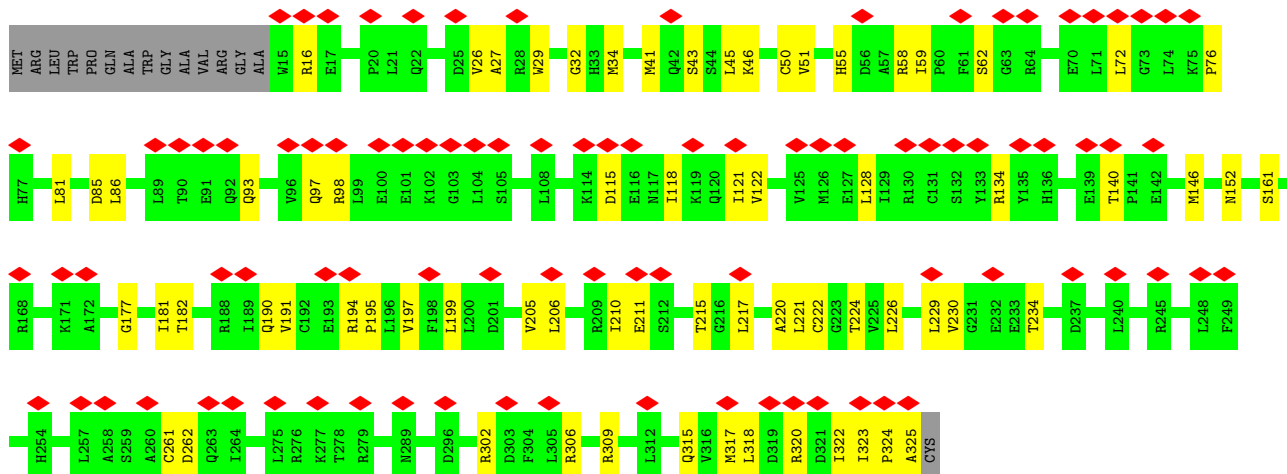




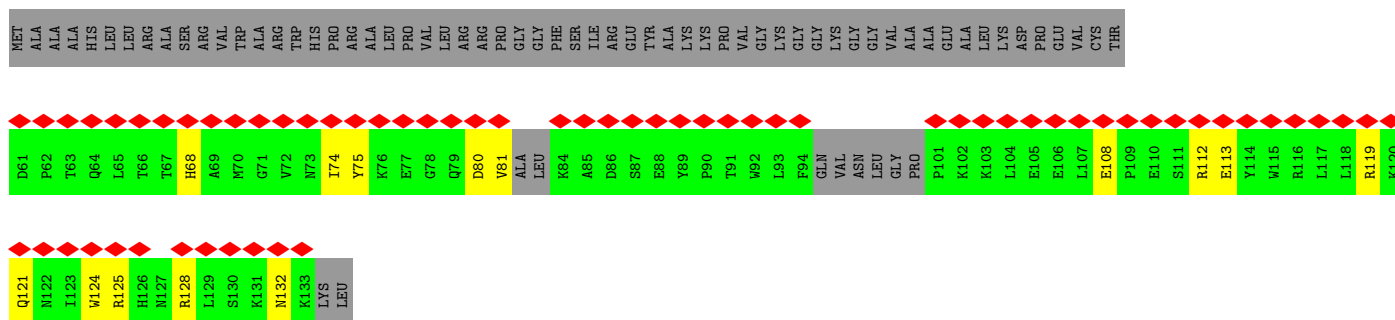
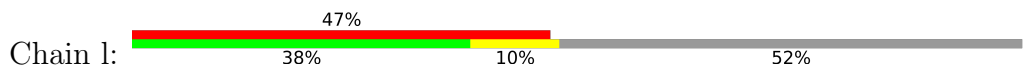
- Molecule 47: Large ribosomal subunit protein mL55



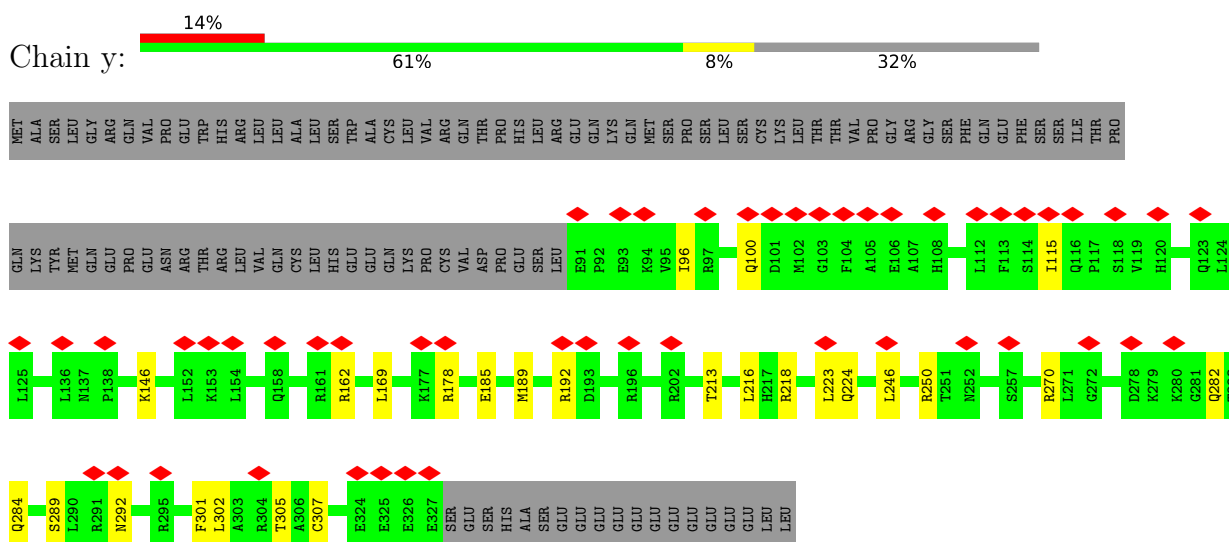
- Molecule 48: Mitochondrial ribosome-associated GTPase 1



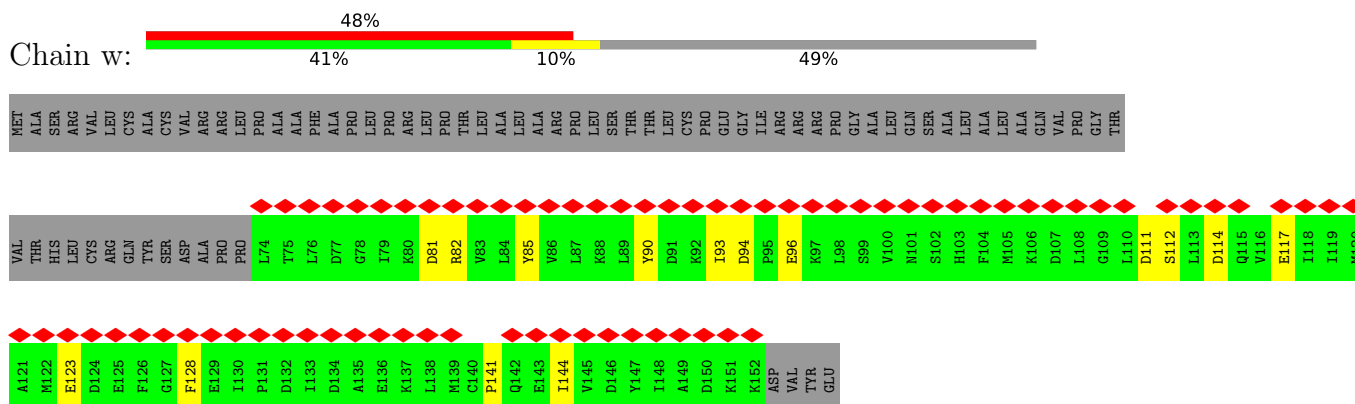
- Molecule 49: Large ribosomal subunit protein mL54



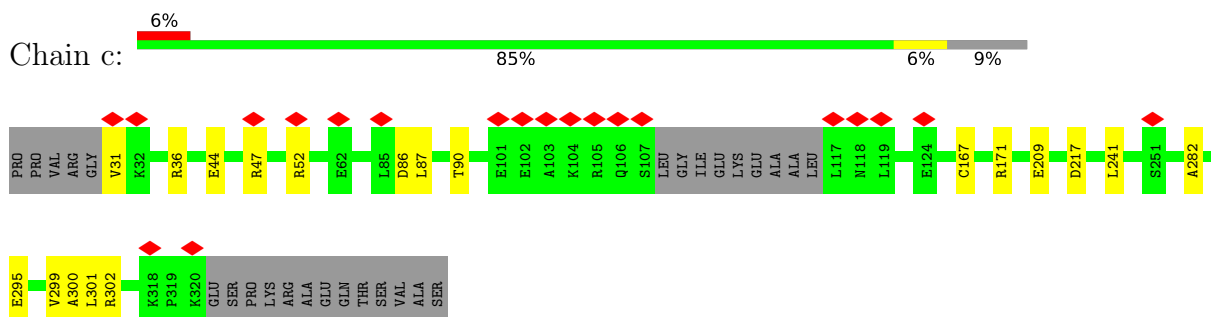
- Molecule 50: Transcription termination factor 4, mitochondrial



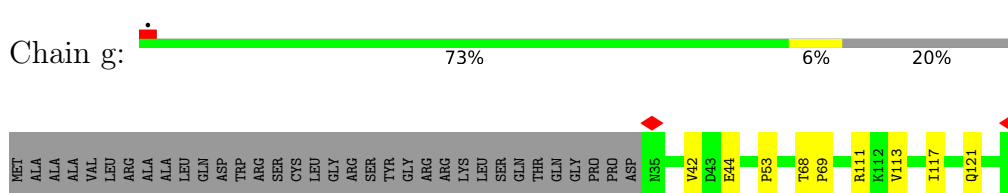
- Molecule 51: Acyl carrier protein, mitochondrial



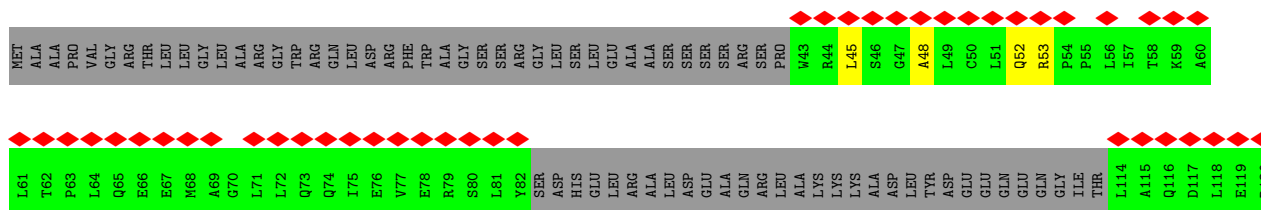
- Molecule 52: Large ribosomal subunit protein mL44

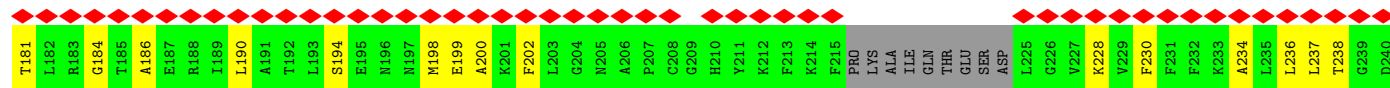


- Molecule 53: Large ribosomal subunit protein mL49

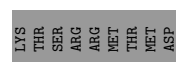
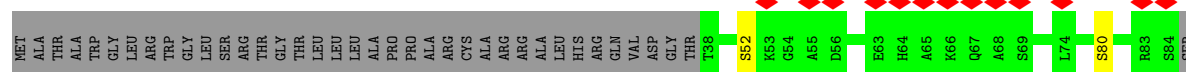


- Molecule 54: Large ribosomal subunit protein mL53

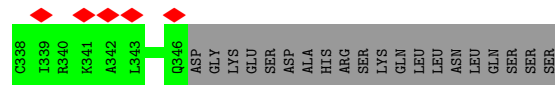
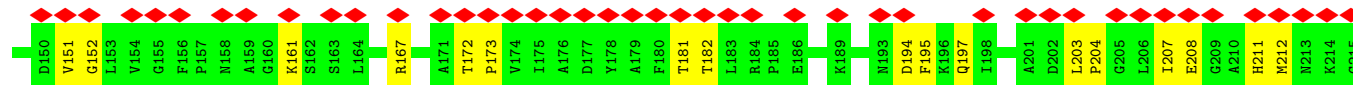
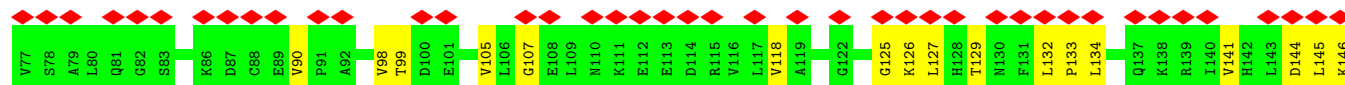
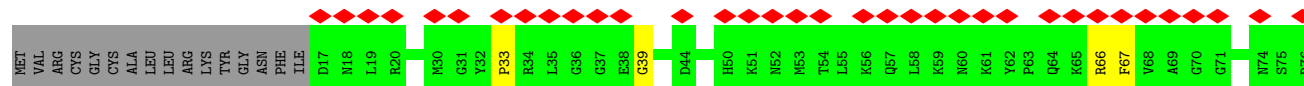




• Molecule 58: Large ribosomal subunit protein mL62



• Molecule 59: GTP-binding protein 10





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 55461                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | 400                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.060                                   | Depositor |
| Minimum map value                    | -0.022                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.002                                   | Depositor |
| Recommended contour level            | 0.01                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 457.2925, 457.2925, 457.2925            | wwPDB     |
| Map dimensions                       | 540, 540, 540                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.846838, 0.846838, 0.846838            | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.16         | 0/33973     | 0.29        | 0/52824     |
| 2   | B     | 0.10         | 0/1483      | 0.24        | 0/2299      |
| 3   | D     | 0.12         | 0/1802      | 0.29        | 0/2424      |
| 4   | E     | 0.14         | 0/2535      | 0.31        | 0/3443      |
| 5   | F     | 0.15         | 0/2061      | 0.31        | 0/2805      |
| 6   | H     | 0.10         | 0/793       | 0.24        | 0/1066      |
| 7   | I     | 0.10         | 0/1339      | 0.25        | 0/1813      |
| 8   | J     | 0.11         | 0/756       | 0.31        | 0/1010      |
| 9   | K     | 0.13         | 0/1491      | 0.26        | 0/2022      |
| 10  | L     | 0.13         | 0/908       | 0.30        | 0/1224      |
| 11  | M     | 0.13         | 0/2369      | 0.28        | 0/3197      |
| 12  | N     | 0.08         | 0/1558      | 0.21        | 0/2097      |
| 13  | O     | 0.12         | 0/1285      | 0.27        | 0/1732      |
| 14  | P     | 0.08         | 0/1181      | 0.24        | 0/1600      |
| 15  | Q     | 0.12         | 0/1832      | 0.28        | 0/2471      |
| 16  | R     | 0.14         | 0/1182      | 0.27        | 0/1585      |
| 17  | S     | 0.14         | 0/1284      | 0.29        | 0/1740      |
| 18  | T     | 0.14         | 0/1402      | 0.28        | 0/1885      |
| 19  | U     | 0.13         | 0/1080      | 0.27        | 0/1464      |
| 20  | V     | 0.11         | 0/1695      | 0.26        | 0/2295      |
| 21  | W     | 0.10         | 0/816       | 0.25        | 0/1105      |
| 22  | X     | 0.12         | 0/2075      | 0.25        | 0/2806      |
| 23  | Y     | 0.12         | 0/1561      | 0.23        | 0/2093      |
| 24  | Z     | 0.11         | 0/1004      | 0.27        | 0/1357      |
| 25  | x     | 0.08         | 0/2620      | 0.24        | 0/3549      |
| 26  | 1     | 0.09         | 0/434       | 0.24        | 0/578       |
| 27  | 2     | 0.16         | 0/387       | 0.29        | 0/514       |
| 28  | 3     | 0.15         | 0/843       | 0.28        | 0/1122      |
| 29  | 4     | 0.10         | 0/328       | 0.27        | 0/430       |
| 30  | 6     | 0.10         | 0/2783      | 0.26        | 0/3781      |
| 31  | 7     | 0.10         | 0/2436      | 0.24        | 0/3300      |
| 32  | b     | 0.13         | 0/1203      | 0.31        | 0/1625      |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 33  | f     | 0.08         | 0/851    | 0.25        | 0/1149   |
| 34  | h     | 0.09         | 0/894    | 0.22        | 0/1216   |
| 35  | i     | 0.15         | 0/855    | 0.30        | 0/1147   |
| 36  | j     | 0.12         | 0/759    | 0.27        | 0/1019   |
| 37  | o     | 0.11         | 0/655    | 0.25        | 0/880    |
| 38  | q     | 0.10         | 0/1161   | 0.26        | 0/1571   |
| 39  | r     | 0.12         | 0/1309   | 0.31        | 0/1767   |
| 40  | s     | 0.13         | 0/3118   | 0.30        | 0/4232   |
| 41  | u     | 0.09         | 0/1053   | 0.24        | 0/1425   |
| 42  | v     | 0.08         | 0/596    | 0.23        | 0/795    |
| 43  | 5     | 0.11         | 0/3317   | 0.27        | 0/4519   |
| 44  | 8     | 0.08         | 0/572    | 0.21        | 0/763    |
| 45  | 9     | 0.12         | 0/1009   | 0.27        | 0/1358   |
| 46  | a     | 0.12         | 0/884    | 0.27        | 0/1197   |
| 47  | m     | 0.08         | 0/380    | 0.21        | 0/510    |
| 48  | z     | 0.11         | 0/2500   | 0.29        | 0/3380   |
| 49  | l     | 0.10         | 0/572    | 0.28        | 0/768    |
| 50  | y     | 0.08         | 0/1980   | 0.21        | 0/2667   |
| 51  | w     | 0.10         | 0/646    | 0.26        | 0/869    |
| 52  | c     | 0.11         | 0/2313   | 0.25        | 0/3128   |
| 53  | g     | 0.12         | 0/1126   | 0.27        | 0/1533   |
| 54  | k     | 0.09         | 0/674    | 0.25        | 0/910    |
| 55  | 0     | 0.13         | 0/896    | 0.28        | 0/1200   |
| 56  | d     | 0.11         | 0/2017   | 0.29        | 0/2735   |
| 57  | e     | 0.08         | 0/1608   | 0.24        | 0/2165   |
| 58  | p     | 0.08         | 0/1195   | 0.23        | 0/1603   |
| 59  | t     | 0.10         | 0/2504   | 0.27        | 0/3369   |
| All | All   | 0.13         | 0/113943 | 0.27        | 0/161131 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 30362 | 15333    | 15360    | 222     | 0            |
| 2   | B     | 1326  | 667      | 670      | 12      | 0            |
| 3   | D     | 1768  | 1830     | 1830     | 19      | 0            |
| 4   | E     | 2459  | 2441     | 2441     | 26      | 0            |
| 5   | F     | 2005  | 2025     | 2024     | 31      | 0            |
| 6   | H     | 779   | 814      | 814      | 8       | 0            |
| 7   | I     | 1307  | 1393     | 1393     | 11      | 0            |
| 8   | J     | 747   | 796      | 796      | 29      | 0            |
| 9   | K     | 1449  | 1444     | 1444     | 9       | 0            |
| 10  | L     | 893   | 944      | 944      | 14      | 0            |
| 11  | M     | 2315  | 2377     | 2377     | 15      | 0            |
| 12  | N     | 1516  | 1521     | 1521     | 7       | 0            |
| 13  | O     | 1259  | 1282     | 1282     | 11      | 0            |
| 14  | P     | 1154  | 1148     | 1148     | 19      | 0            |
| 15  | Q     | 1790  | 1822     | 1822     | 9       | 0            |
| 16  | R     | 1161  | 1224     | 1224     | 9       | 0            |
| 17  | S     | 1259  | 1323     | 1323     | 14      | 0            |
| 18  | T     | 1369  | 1402     | 1402     | 8       | 0            |
| 19  | U     | 1052  | 1057     | 1057     | 8       | 0            |
| 20  | V     | 1652  | 1643     | 1643     | 20      | 0            |
| 21  | W     | 794   | 808      | 808      | 8       | 0            |
| 22  | X     | 2021  | 2051     | 2051     | 12      | 0            |
| 23  | Y     | 1523  | 1553     | 1553     | 10      | 0            |
| 24  | Z     | 978   | 1026     | 1026     | 7       | 0            |
| 25  | x     | 2564  | 2546     | 2546     | 33      | 0            |
| 26  | 1     | 428   | 472      | 472      | 3       | 0            |
| 27  | 2     | 380   | 407      | 407      | 3       | 0            |
| 28  | 3     | 823   | 872      | 872      | 5       | 0            |
| 29  | 4     | 322   | 354      | 354      | 5       | 0            |
| 30  | 6     | 2689  | 2559     | 2559     | 40      | 0            |
| 31  | 7     | 2379  | 2378     | 2378     | 22      | 0            |
| 32  | b     | 1181  | 1195     | 1195     | 19      | 0            |
| 33  | f     | 838   | 836      | 836      | 23      | 0            |
| 34  | h     | 872   | 867      | 867      | 6       | 0            |
| 35  | i     | 831   | 854      | 854      | 4       | 0            |
| 36  | j     | 744   | 768      | 768      | 7       | 0            |
| 37  | o     | 640   | 623      | 623      | 3       | 0            |
| 38  | q     | 1130  | 1123     | 1123     | 10      | 0            |
| 39  | r     | 1275  | 1331     | 1329     | 13      | 0            |
| 40  | s     | 3045  | 3059     | 3057     | 29      | 0            |
| 41  | u     | 1029  | 1012     | 1012     | 6       | 0            |
| 42  | v     | 586   | 603      | 603      | 6       | 0            |
| 43  | 5     | 3225  | 3243     | 3243     | 17      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 44  | 8     | 564    | 557      | 557      | 3       | 0            |
| 45  | 9     | 983    | 990      | 990      | 6       | 0            |
| 46  | a     | 860    | 843      | 843      | 8       | 0            |
| 47  | m     | 374    | 395      | 395      | 5       | 0            |
| 48  | z     | 2455   | 2546     | 2546     | 48      | 0            |
| 49  | l     | 559    | 549      | 549      | 12      | 0            |
| 50  | y     | 1943   | 1995     | 1995     | 17      | 0            |
| 51  | w     | 637    | 640      | 640      | 8       | 0            |
| 52  | c     | 2262   | 2273     | 2273     | 16      | 0            |
| 53  | g     | 1090   | 1094     | 1094     | 8       | 0            |
| 54  | k     | 664    | 667      | 667      | 5       | 0            |
| 55  | 0     | 881    | 908      | 908      | 9       | 0            |
| 56  | d     | 1961   | 1940     | 1940     | 25      | 0            |
| 57  | e     | 1576   | 1598     | 1598     | 26      | 0            |
| 58  | p     | 1176   | 1198     | 1198     | 8       | 0            |
| 59  | t     | 2464   | 2551     | 2551     | 46      | 0            |
| 60  | A     | 96     | 0        | 0        | 0       | 0            |
| 60  | M     | 1      | 0        | 0        | 0       | 0            |
| 60  | O     | 1      | 0        | 0        | 0       | 0            |
| 60  | R     | 1      | 0        | 0        | 0       | 0            |
| 61  | I     | 4      | 0        | 0        | 0       | 0            |
| 62  | 0     | 1      | 0        | 0        | 0       | 0            |
| 62  | 4     | 1      | 0        | 0        | 0       | 0            |
| 63  | t     | 32     | 13       | 13       | 2       | 0            |
| 63  | z     | 32     | 13       | 13       | 1       | 0            |
| All | All   | 108537 | 93796    | 93821    | 871     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 871 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:Q:155:ILE:HG22 | 15:Q:156:GLU:OE1 | 1.74                     | 0.88              |
| 1:A:1648:C:O2'    | 1:A:1649:A:O4'   | 1.92                     | 0.86              |
| 1:A:2080:G:O2'    | 1:A:2082:G:OP2   | 1.94                     | 0.86              |
| 1:A:1494:A:OP1    | 21:W:101:LYS:NZ  | 2.10                     | 0.85              |
| 20:V:101:THR:OG1  | 20:V:103:ASP:OD1 | 1.96                     | 0.83              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 3   | D     | 223/246 (91%) | 217 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 4   | E     | 306/348 (88%) | 292 (95%)  | 14 (5%) | 0        | 100         | 100 |
| 5   | F     | 248/294 (84%) | 244 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 6   | H     | 93/265 (35%)  | 92 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 7   | I     | 159/262 (61%) | 152 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 8   | J     | 85/192 (44%)  | 76 (89%)   | 9 (11%) | 0        | 100         | 100 |
| 9   | K     | 175/178 (98%) | 174 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 10  | L     | 113/145 (78%) | 109 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 11  | M     | 285/295 (97%) | 276 (97%)  | 9 (3%)  | 0        | 100         | 100 |
| 12  | N     | 178/251 (71%) | 175 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 13  | O     | 151/176 (86%) | 148 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 14  | P     | 139/180 (77%) | 139 (100%) | 0       | 0        | 100         | 100 |
| 15  | Q     | 215/292 (74%) | 211 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 16  | R     | 138/149 (93%) | 138 (100%) | 0       | 0        | 100         | 100 |
| 17  | S     | 151/209 (72%) | 147 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 18  | T     | 164/206 (80%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 19  | U     | 123/146 (84%) | 123 (100%) | 0       | 0        | 100         | 100 |
| 20  | V     | 199/216 (92%) | 194 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 21  | W     | 98/148 (66%)  | 95 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 22  | X     | 240/294 (82%) | 239 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 23  | Y     | 174/252 (69%) | 173 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 24  | Z     | 118/160 (74%) | 116 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 25  | x     | 322/381 (84%) | 309 (96%)  | 13 (4%) | 0        | 100         | 100 |
| 26  | 1     | 50/65 (77%)   | 50 (100%)  | 0       | 0        | 100         | 100 |
| 27  | 2     | 44/92 (48%)   | 43 (98%)   | 1 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 28  | 3     | 93/188 (50%)  | 93 (100%)  | 0        | 0        | 100         | 100 |
| 29  | 4     | 35/101 (35%)  | 35 (100%)  | 0        | 0        | 100         | 100 |
| 30  | 6     | 311/380 (82%) | 287 (92%)  | 24 (8%)  | 0        | 100         | 100 |
| 31  | 7     | 290/336 (86%) | 284 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 32  | b     | 146/159 (92%) | 141 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 33  | f     | 98/211 (46%)  | 92 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 34  | h     | 108/159 (68%) | 104 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 35  | i     | 95/128 (74%)  | 92 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 36  | j     | 91/121 (75%)  | 88 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 37  | o     | 76/102 (74%)  | 75 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 38  | q     | 133/222 (60%) | 132 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 39  | r     | 153/196 (78%) | 148 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 40  | s     | 373/442 (84%) | 367 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 41  | u     | 123/228 (54%) | 119 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 42  | v     | 67/70 (96%)   | 64 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 43  | 5     | 392/423 (93%) | 386 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 44  | 8     | 65/206 (32%)  | 64 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 45  | 9     | 120/135 (89%) | 119 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 46  | a     | 99/142 (70%)  | 96 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 47  | m     | 43/127 (34%)  | 42 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 48  | z     | 309/326 (95%) | 290 (94%)  | 19 (6%)  | 0        | 100         | 100 |
| 49  | l     | 59/135 (44%)  | 54 (92%)   | 5 (8%)   | 0        | 100         | 100 |
| 50  | y     | 235/346 (68%) | 230 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 51  | w     | 77/156 (49%)  | 65 (84%)   | 12 (16%) | 0        | 100         | 100 |
| 52  | c     | 277/308 (90%) | 269 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 53  | g     | 130/166 (78%) | 127 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 54  | k     | 83/118 (70%)  | 80 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 55  | 0     | 106/187 (57%) | 106 (100%) | 0        | 0        | 100         | 100 |
| 56  | d     | 230/306 (75%) | 216 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 57  | e     | 187/283 (66%) | 177 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 58  | p     | 140/206 (68%) | 135 (96%)  | 5 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 59  | t     | 317/366 (87%)    | 291 (92%)  | 26 (8%)  | 0        | 100         | 100 |
| All | All   | 9252/12421 (74%) | 8961 (97%) | 291 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 3   | D     | 186/197 (94%) | 186 (100%) | 0        | 100         | 100 |
| 4   | E     | 270/298 (91%) | 270 (100%) | 0        | 100         | 100 |
| 5   | F     | 216/250 (86%) | 216 (100%) | 0        | 100         | 100 |
| 6   | H     | 86/228 (38%)  | 86 (100%)  | 0        | 100         | 100 |
| 7   | I     | 149/230 (65%) | 149 (100%) | 0        | 100         | 100 |
| 8   | J     | 84/152 (55%)  | 84 (100%)  | 0        | 100         | 100 |
| 9   | K     | 157/158 (99%) | 157 (100%) | 0        | 100         | 100 |
| 10  | L     | 99/122 (81%)  | 99 (100%)  | 0        | 100         | 100 |
| 11  | M     | 248/252 (98%) | 248 (100%) | 0        | 100         | 100 |
| 12  | N     | 161/216 (74%) | 161 (100%) | 0        | 100         | 100 |
| 13  | O     | 133/152 (88%) | 133 (100%) | 0        | 100         | 100 |
| 14  | P     | 123/157 (78%) | 123 (100%) | 0        | 100         | 100 |
| 15  | Q     | 197/258 (76%) | 197 (100%) | 0        | 100         | 100 |
| 16  | R     | 119/128 (93%) | 119 (100%) | 0        | 100         | 100 |
| 17  | S     | 141/180 (78%) | 141 (100%) | 0        | 100         | 100 |
| 18  | T     | 147/180 (82%) | 147 (100%) | 0        | 100         | 100 |
| 19  | U     | 114/133 (86%) | 114 (100%) | 0        | 100         | 100 |
| 20  | V     | 179/190 (94%) | 179 (100%) | 0        | 100         | 100 |
| 21  | W     | 84/116 (72%)  | 84 (100%)  | 0        | 100         | 100 |
| 22  | X     | 219/265 (83%) | 219 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 23  | Y     | 162/228 (71%) | 162 (100%) | 0        | 100         | 100 |
| 24  | Z     | 113/146 (77%) | 113 (100%) | 0        | 100         | 100 |
| 25  | x     | 283/334 (85%) | 283 (100%) | 0        | 100         | 100 |
| 26  | 1     | 49/60 (82%)   | 49 (100%)  | 0        | 100         | 100 |
| 27  | 2     | 40/77 (52%)   | 40 (100%)  | 0        | 100         | 100 |
| 28  | 3     | 88/165 (53%)  | 88 (100%)  | 0        | 100         | 100 |
| 29  | 4     | 35/90 (39%)   | 35 (100%)  | 0        | 100         | 100 |
| 30  | 6     | 280/335 (84%) | 280 (100%) | 0        | 100         | 100 |
| 31  | 7     | 269/301 (89%) | 269 (100%) | 0        | 100         | 100 |
| 32  | b     | 130/138 (94%) | 130 (100%) | 0        | 100         | 100 |
| 33  | f     | 93/185 (50%)  | 93 (100%)  | 0        | 100         | 100 |
| 34  | h     | 100/143 (70%) | 100 (100%) | 0        | 100         | 100 |
| 35  | i     | 87/111 (78%)  | 87 (100%)  | 0        | 100         | 100 |
| 36  | j     | 75/99 (76%)   | 75 (100%)  | 0        | 100         | 100 |
| 37  | o     | 65/85 (76%)   | 65 (100%)  | 0        | 100         | 100 |
| 38  | q     | 117/187 (63%) | 117 (100%) | 0        | 100         | 100 |
| 39  | r     | 142/168 (84%) | 142 (100%) | 0        | 100         | 100 |
| 40  | s     | 329/378 (87%) | 329 (100%) | 0        | 100         | 100 |
| 41  | u     | 115/197 (58%) | 115 (100%) | 0        | 100         | 100 |
| 42  | v     | 60/61 (98%)   | 60 (100%)  | 0        | 100         | 100 |
| 43  | 5     | 356/372 (96%) | 356 (100%) | 0        | 100         | 100 |
| 44  | 8     | 59/182 (32%)  | 59 (100%)  | 0        | 100         | 100 |
| 45  | 9     | 104/114 (91%) | 104 (100%) | 0        | 100         | 100 |
| 46  | a     | 97/129 (75%)  | 97 (100%)  | 0        | 100         | 100 |
| 47  | m     | 40/114 (35%)  | 40 (100%)  | 0        | 100         | 100 |
| 48  | z     | 270/280 (96%) | 270 (100%) | 0        | 100         | 100 |
| 49  | l     | 61/112 (54%)  | 61 (100%)  | 0        | 100         | 100 |
| 50  | y     | 220/322 (68%) | 220 (100%) | 0        | 100         | 100 |
| 51  | w     | 73/135 (54%)  | 73 (100%)  | 0        | 100         | 100 |
| 52  | c     | 245/266 (92%) | 245 (100%) | 0        | 100         | 100 |
| 53  | g     | 122/148 (82%) | 122 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 54  | k     | 76/95 (80%)      | 76 (100%)   | 0        | 100         | 100 |
| 55  | o     | 97/170 (57%)     | 97 (100%)   | 0        | 100         | 100 |
| 56  | d     | 210/272 (77%)    | 210 (100%)  | 0        | 100         | 100 |
| 57  | e     | 166/238 (70%)    | 166 (100%)  | 0        | 100         | 100 |
| 58  | p     | 129/177 (73%)    | 129 (100%)  | 0        | 100         | 100 |
| 59  | t     | 266/306 (87%)    | 266 (100%)  | 0        | 100         | 100 |
| All | All   | 8335/10782 (77%) | 8335 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | h     | 86  | ASN  |
| 40  | s     | 228 | ASN  |
| 34  | h     | 96  | HIS  |
| 39  | r     | 131 | HIS  |
| 43  | 5     | 88  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1405/1584 (88%) | 427 (30%)         | 29 (2%)         |
| 2   | B     | 58/68 (85%)     | 24 (41%)          | 2 (3%)          |
| All | All   | 1463/1652 (88%) | 451 (30%)         | 31 (2%)         |

5 of 451 RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1094 | A    |
| 1   | A     | 1100 | C    |
| 1   | A     | 1101 | C    |
| 1   | A     | 1102 | U    |
| 1   | A     | 1103 | A    |

5 of 31 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1608 | C    |
| 1   | A     | 2627 | U    |
| 1   | A     | 1659 | A    |
| 2   | B     | 31   | C    |
| 1   | A     | 2275 | A    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 104 ligands modelled in this entry, 101 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 63  | GNP  | t     | 501 | -    | 34,34,34     | 1.14 | 5 (14%)     | 47,54,54    | 0.70 | 1 (2%)      |
| 63  | GNP  | z     | 401 | -    | 34,34,34     | 1.17 | 5 (14%)     | 47,54,54    | 0.64 | 0           |
| 61  | FES  | I     | 301 | 7,39 | 0,4,4        | -    | -           | -           |      |             |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 63  | GNP  | t     | 501 | -    | -       | 8/18/38/38 | 0/3/3/3 |
| 63  | GNP  | z     | 401 | -    | -       | 4/18/38/38 | 0/3/3/3 |
| 61  | FES  | I     | 301 | 7,39 | -       | -          | 0/1/1/1 |

The worst 5 of 10 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 63  | z     | 401 | GNP  | PB-O2B | -3.36 | 1.47        | 1.56     |
| 63  | t     | 501 | GNP  | PG-O1G | 3.32  | 1.51        | 1.46     |
| 63  | t     | 501 | GNP  | PB-O2B | -3.23 | 1.48        | 1.56     |
| 63  | z     | 401 | GNP  | PG-O1G | 3.17  | 1.51        | 1.46     |
| 63  | z     | 401 | GNP  | C6-N1  | -2.87 | 1.33        | 1.38     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 63  | t     | 501 | GNP  | C4'-O4'-C1' | -2.08 | 104.88      | 109.47   |

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 63  | z     | 401 | GNP  | PB-N3B-PG-O1G  |
| 63  | z     | 401 | GNP  | PG-N3B-PB-O1B  |
| 63  | z     | 401 | GNP  | C5'-O5'-PA-O1A |
| 63  | t     | 501 | GNP  | PB-N3B-PG-O1G  |
| 63  | t     | 501 | GNP  | PG-N3B-PB-O1B  |

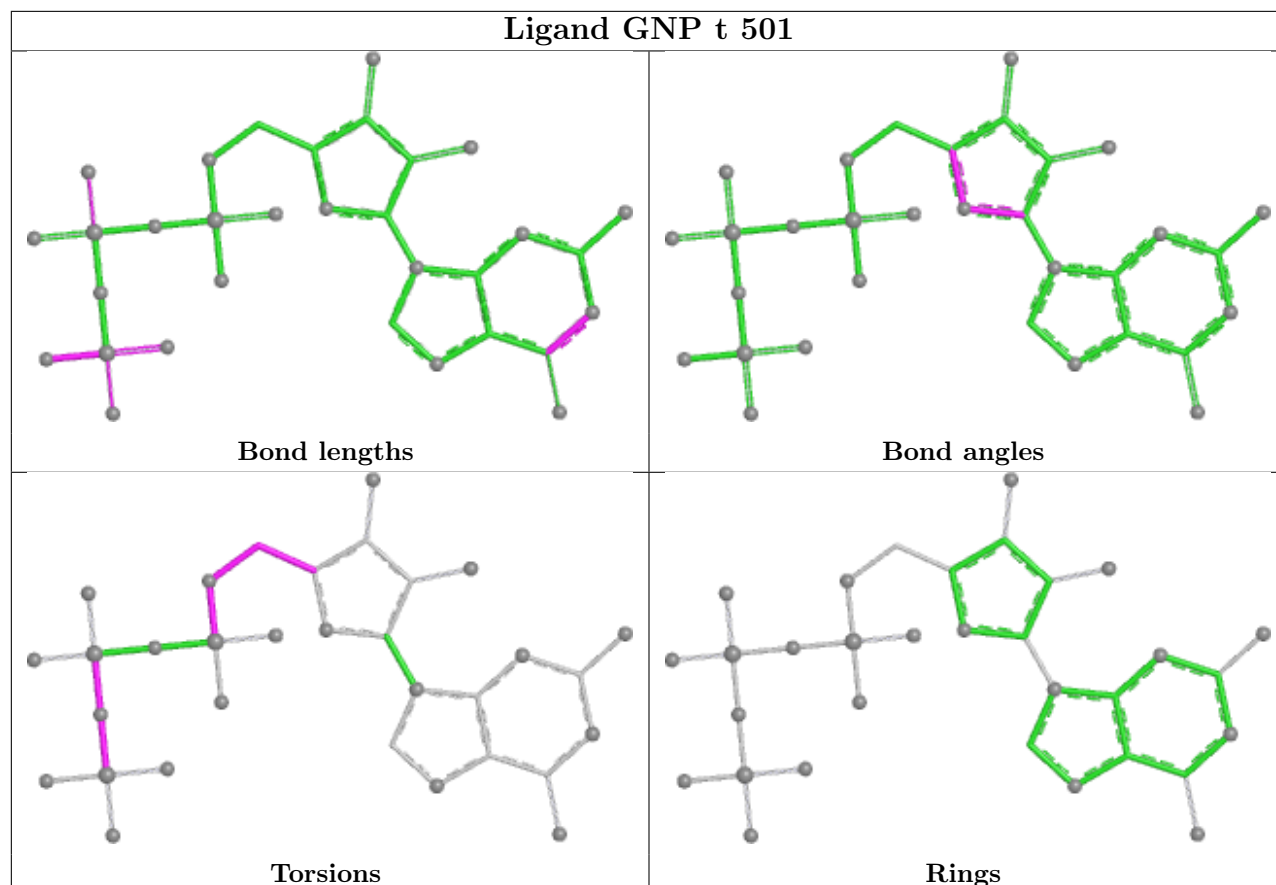
There are no ring outliers.

2 monomers are involved in 3 short contacts:

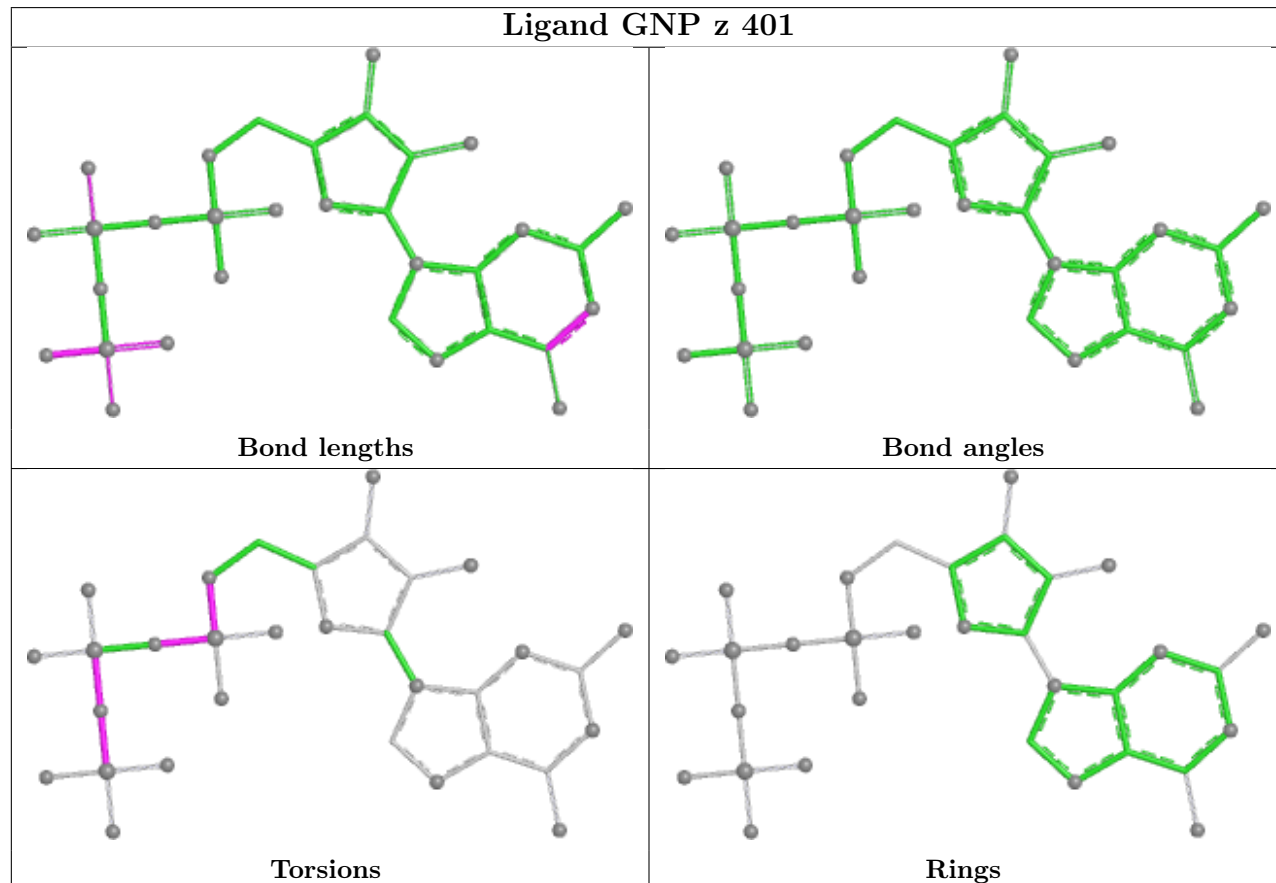
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 63  | t     | 501 | GNP  | 2       | 0            |
| 63  | z     | 401 | GNP  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand GNP t 501



## Ligand GNP z 401



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

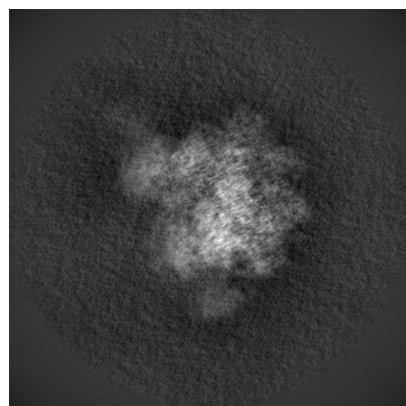
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52047. These allow visual inspection of the internal detail of the map and identification of artifacts.

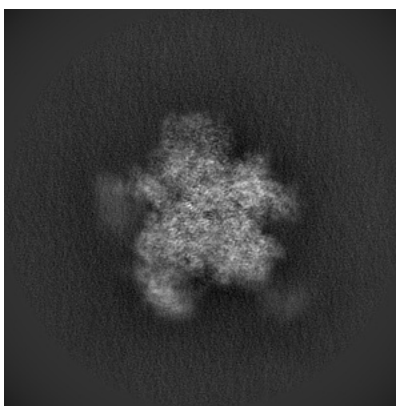
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

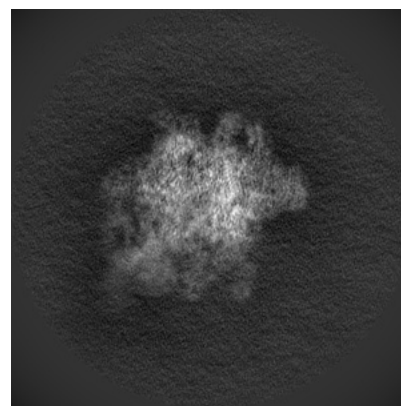
#### 6.1.1 Primary map



X

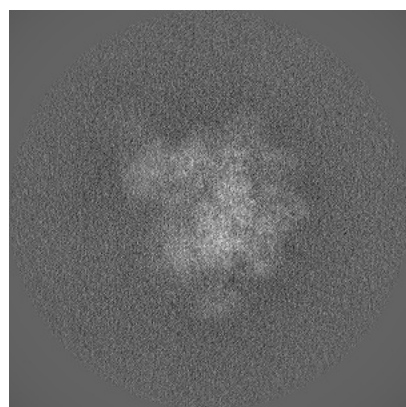


Y

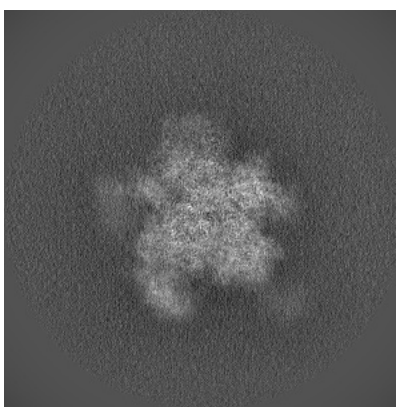


Z

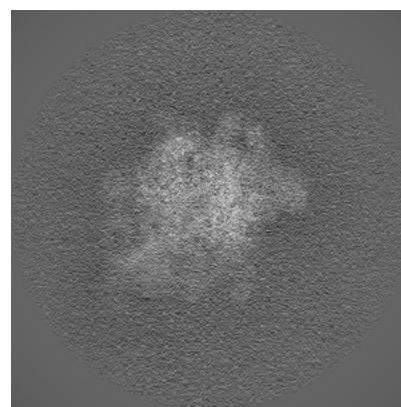
#### 6.1.2 Raw map



X



Y



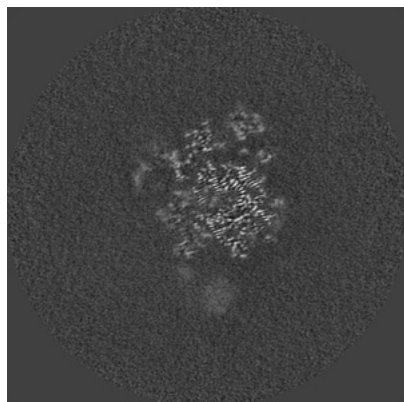
Z

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

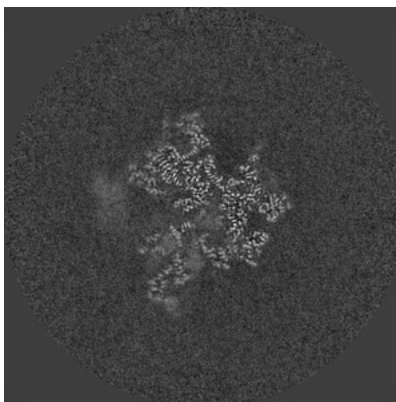


## 6.2 Central slices [i](#)

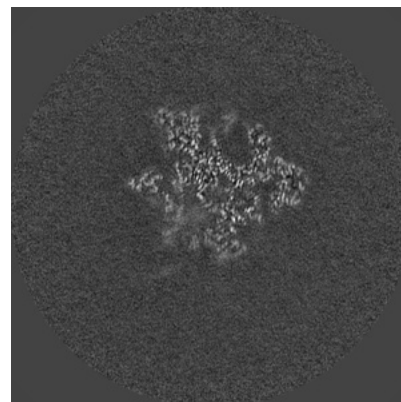
### 6.2.1 Primary map



X Index: 270

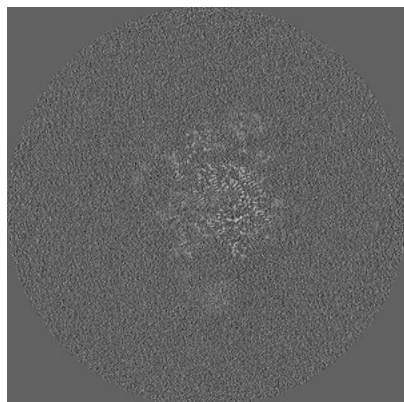


Y Index: 270

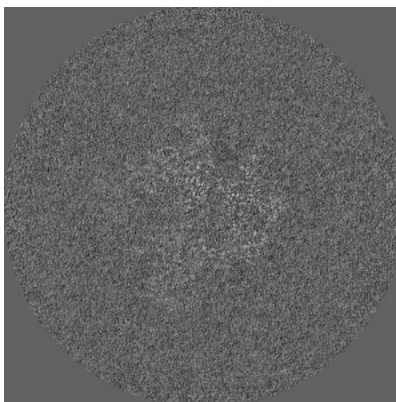


Z Index: 270

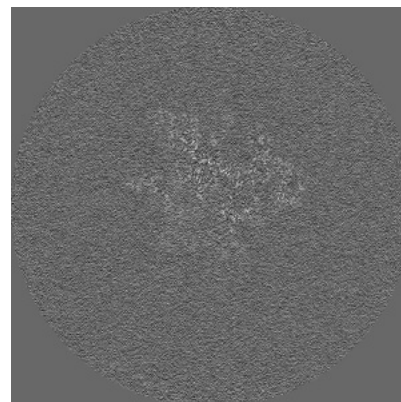
### 6.2.2 Raw map



X Index: 270



Y Index: 270



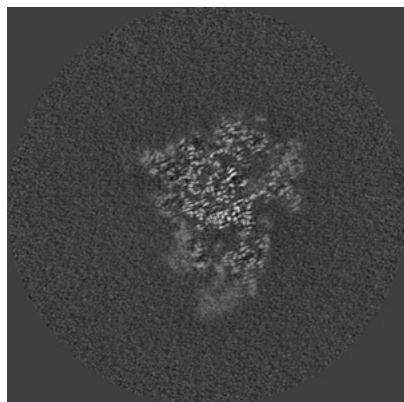
Z Index: 270

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

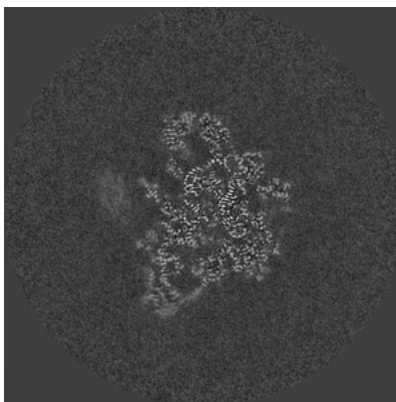


## 6.3 Largest variance slices [i](#)

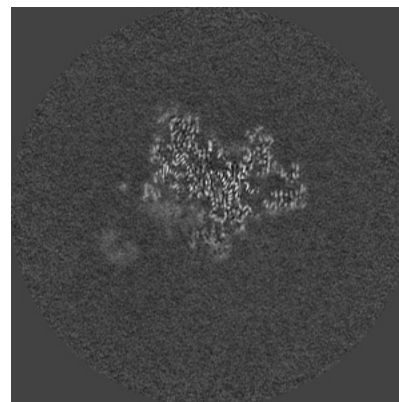
### 6.3.1 Primary map



X Index: 296

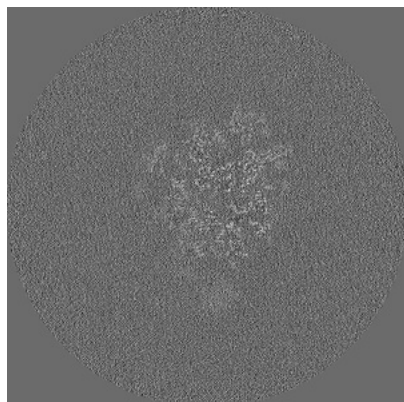


Y Index: 297

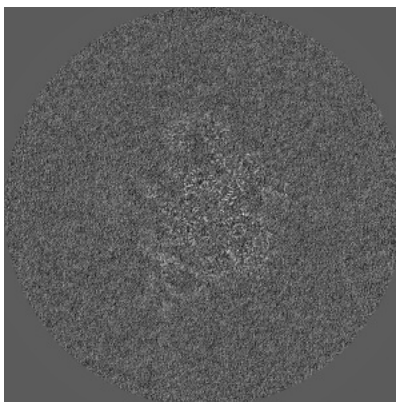


Z Index: 256

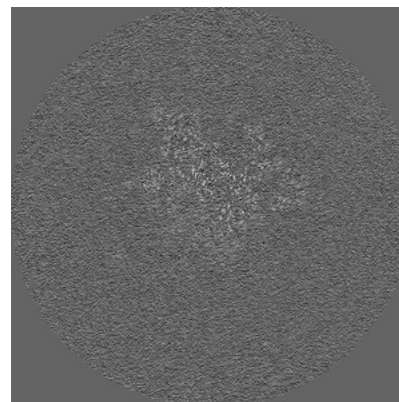
### 6.3.2 Raw map



X Index: 277



Y Index: 296

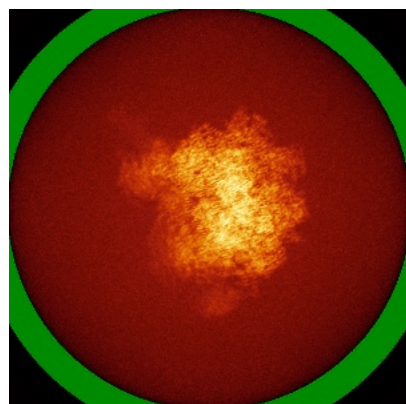


Z Index: 265

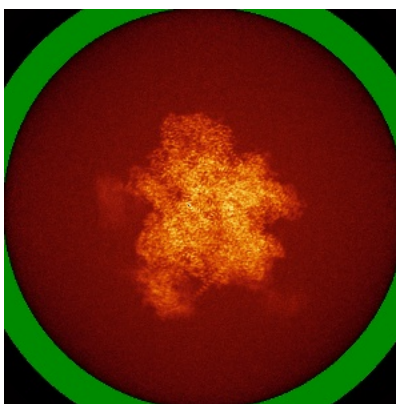
The images above show the largest variance slices of the map in three orthogonal directions.

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

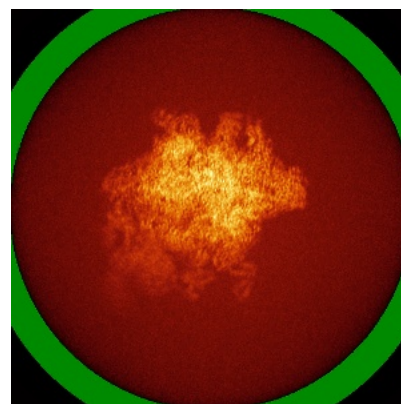
### 6.4.1 Primary map



X

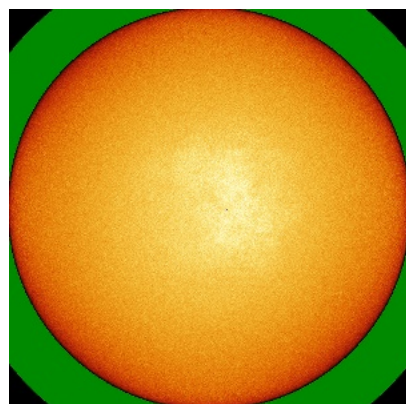


Y

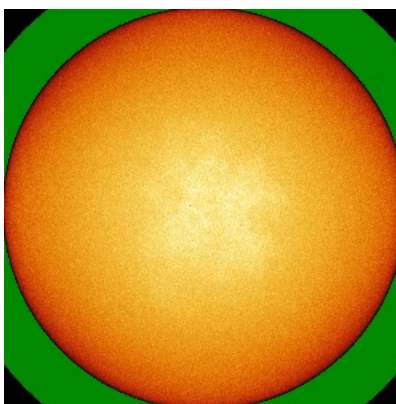


Z

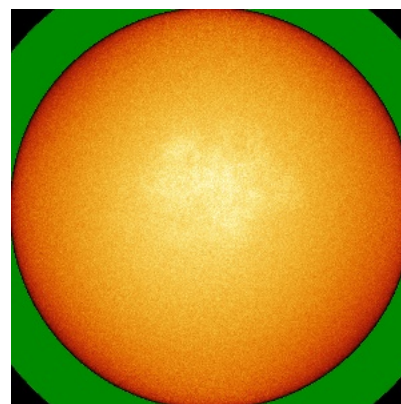
### 6.4.2 Raw map



X



Y

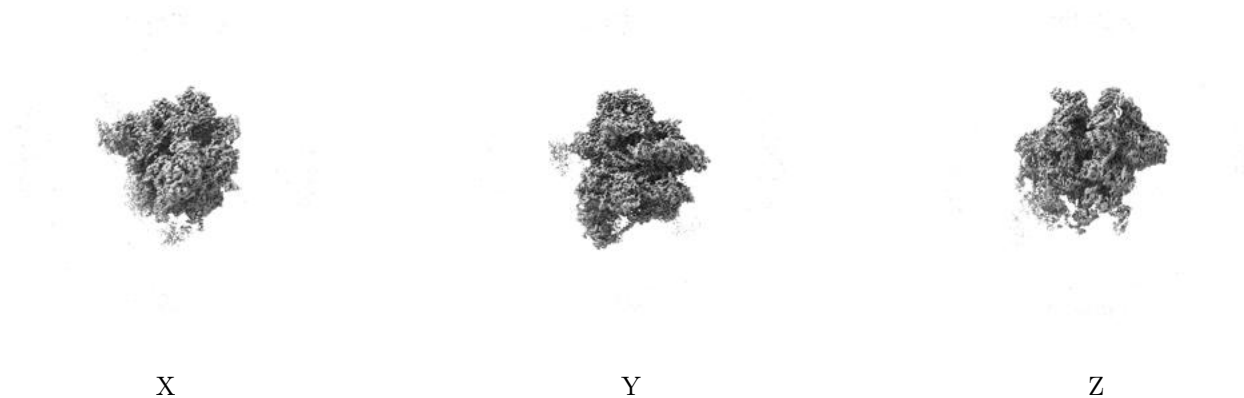


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

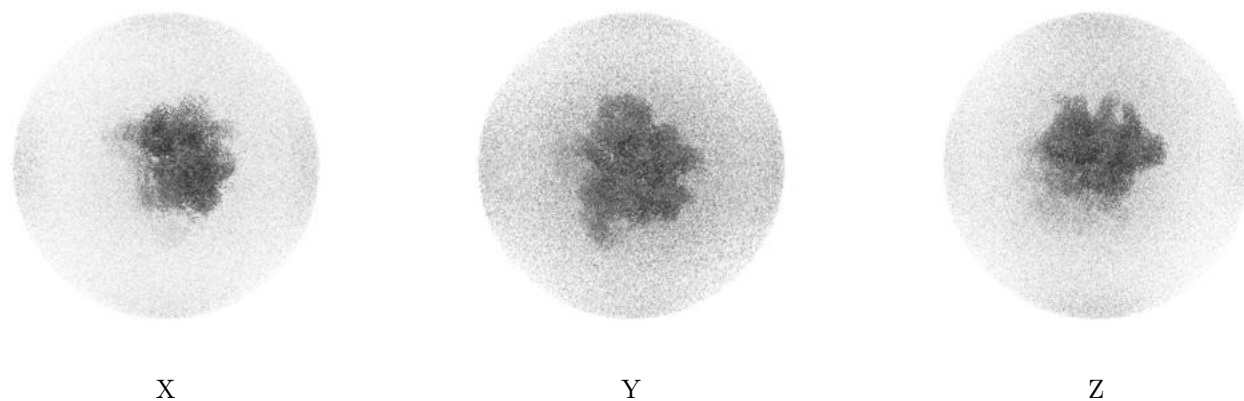
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

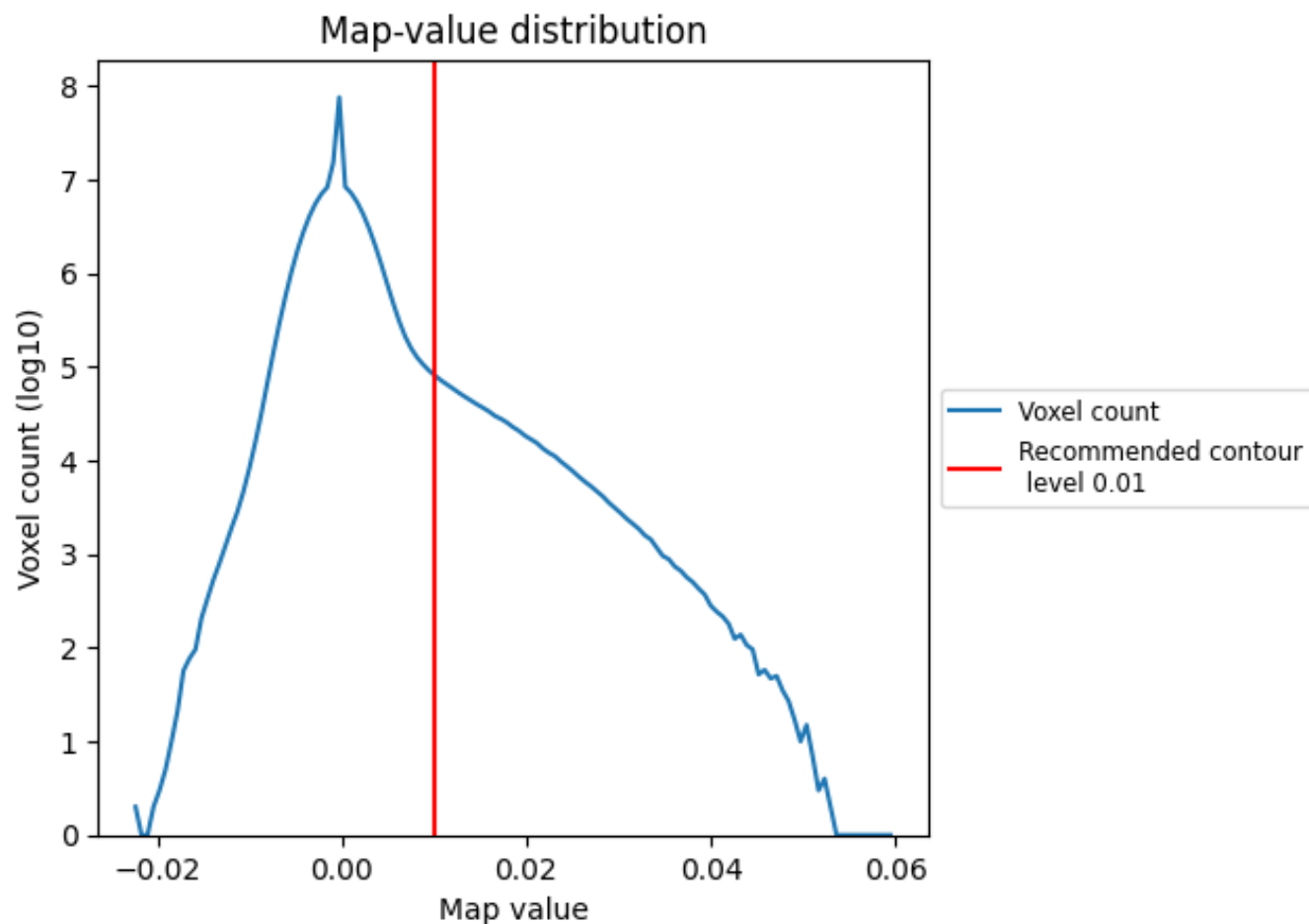
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

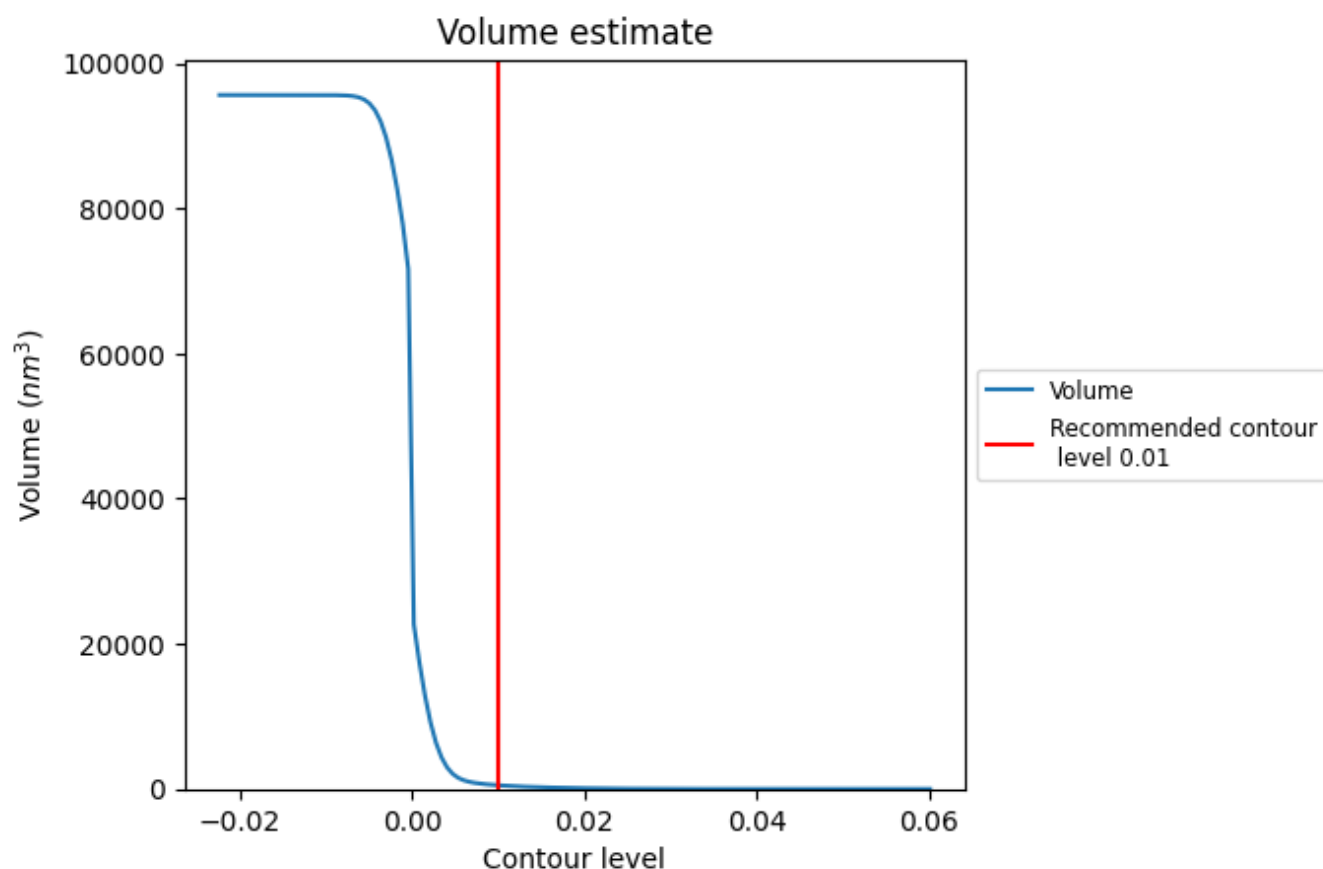
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

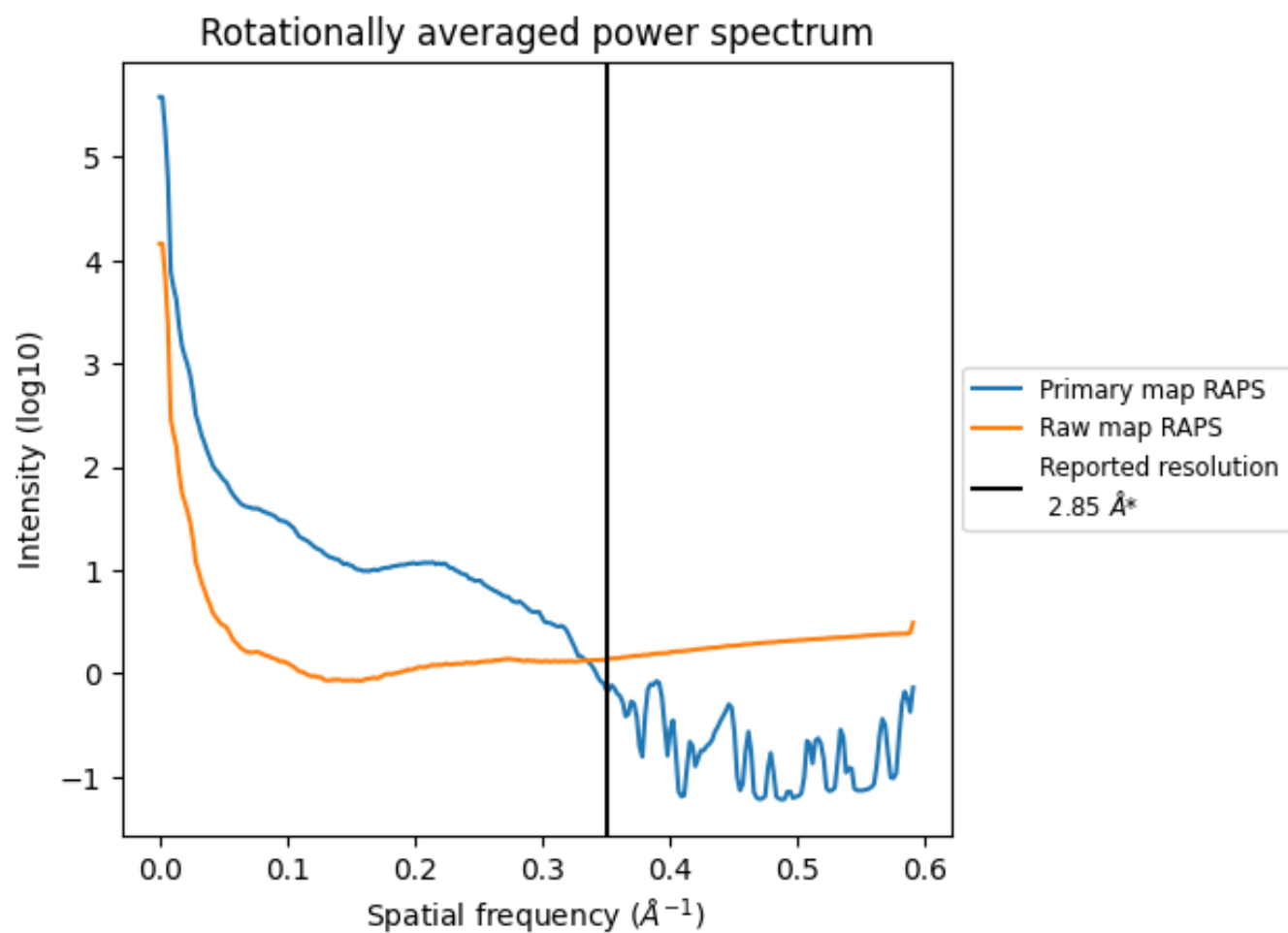
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 511 nm<sup>3</sup>; this corresponds to an approximate mass of 461 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



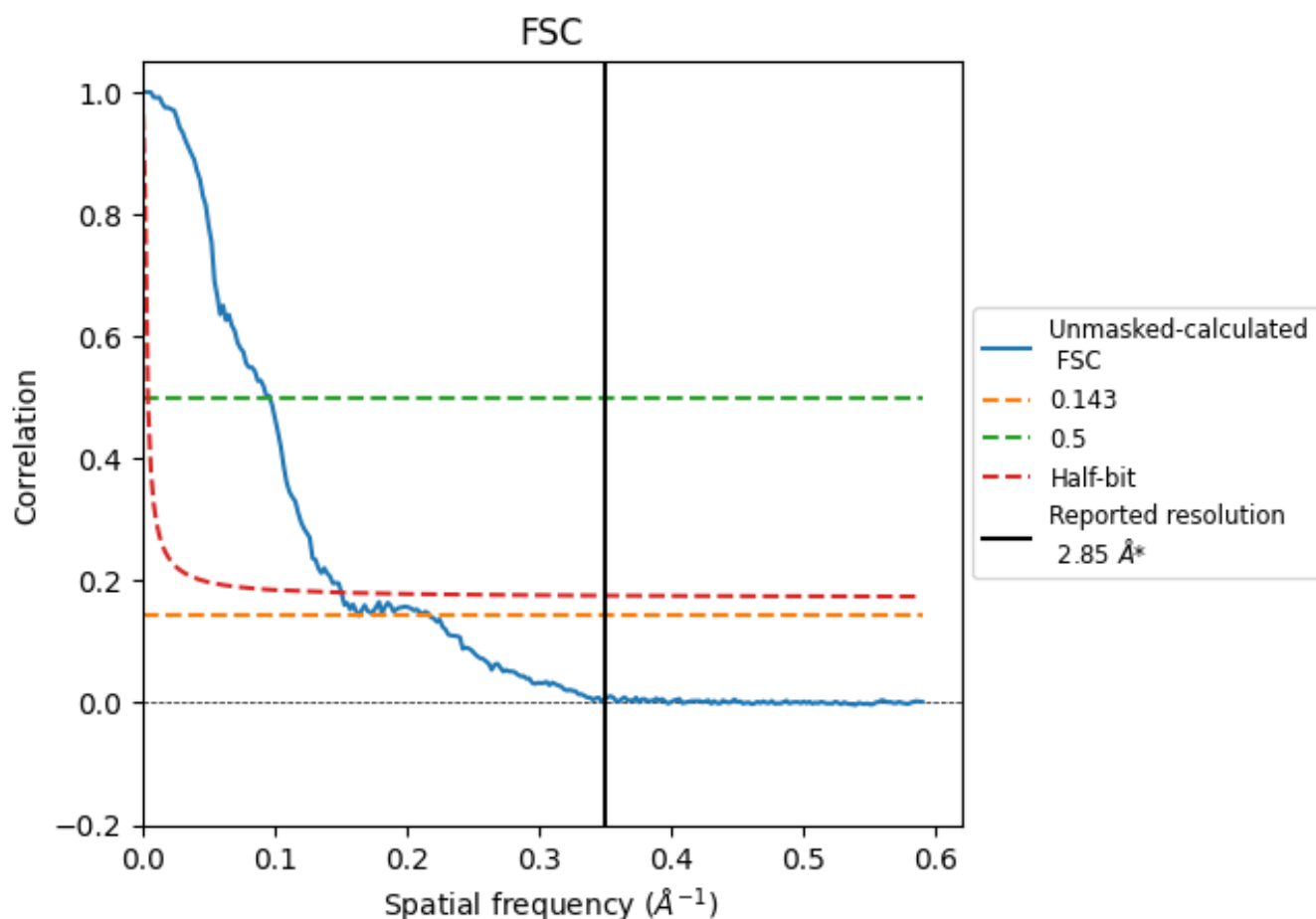
\*Reported resolution corresponds to spatial frequency of 0.351 Å<sup>-1</sup>



## 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 0.351 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        | 2.85                               | -     | -        |
| Author-provided FSC curve | -                                  | -     | -        |
| Unmasked-calculated*      | 6.11                               | 10.36 | 6.64     |

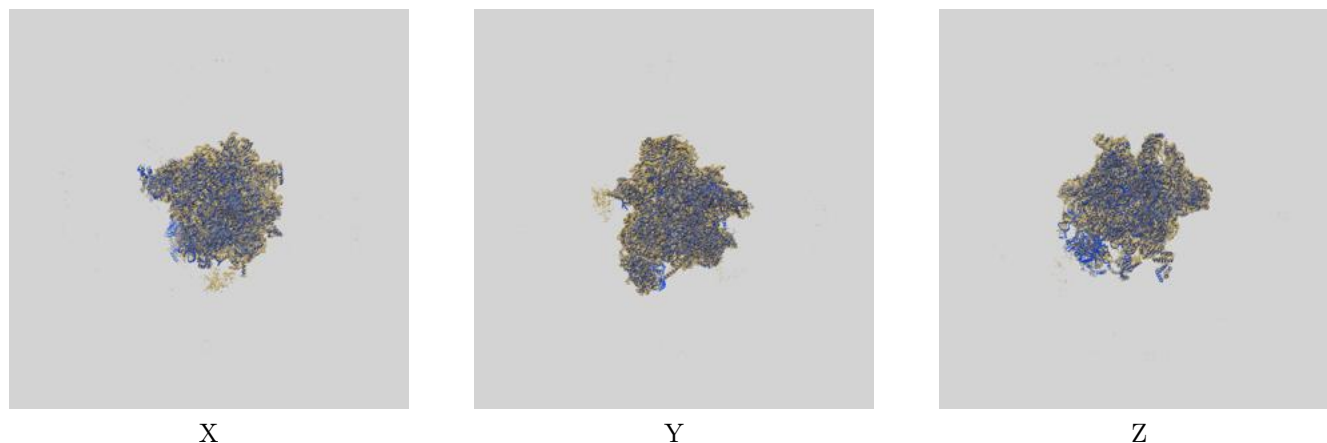
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.11 differs from the reported value 2.85 by more than 10 %



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

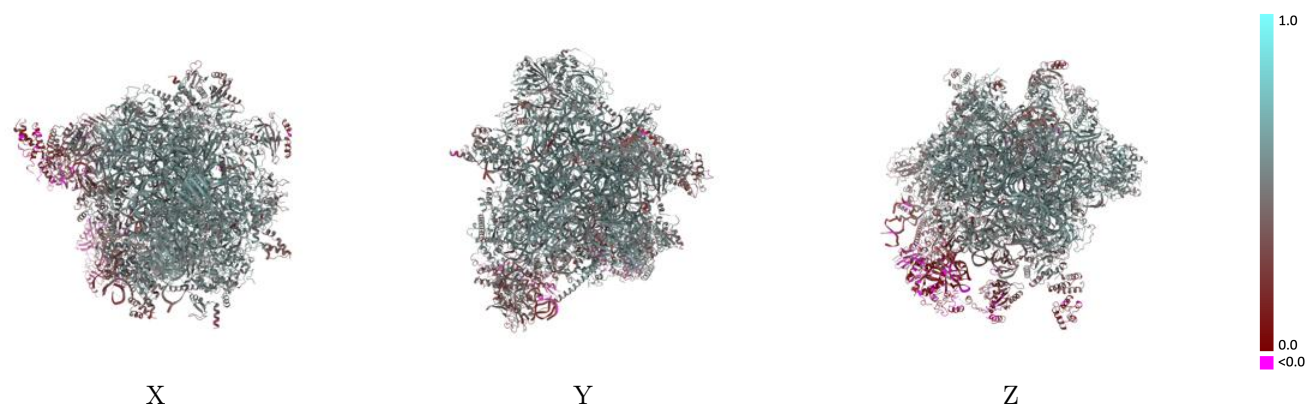
This section contains information regarding the fit between EMDB map EMD-52047 and PDB model 9HCF. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



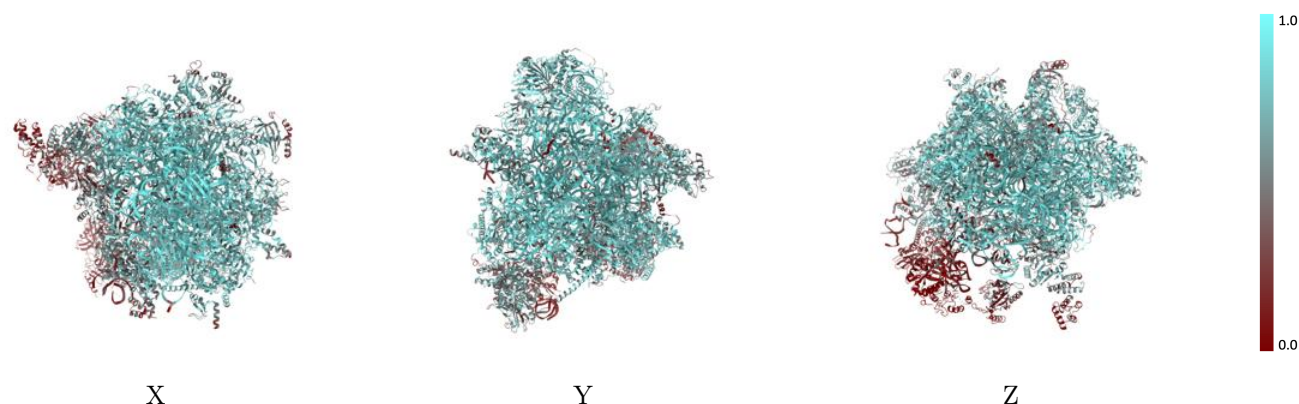
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



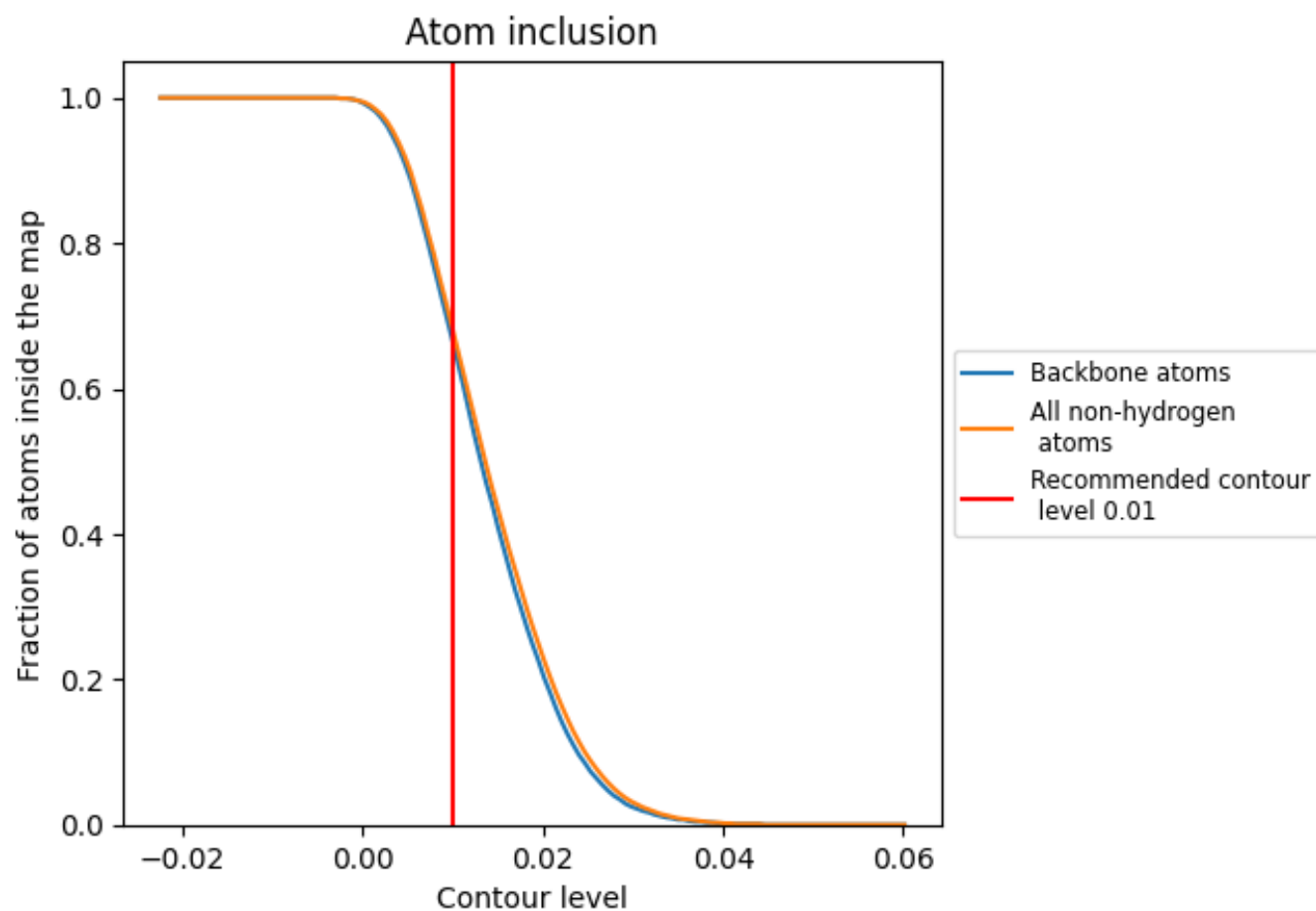
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6830   |  0.4720   |
| 0     |  0.7380   |  0.5220   |
| 1     |  0.6400   |  0.4980   |
| 2     |  0.8890   |  0.6070   |
| 3     |  0.8500   |  0.5900   |
| 4     |  0.6490   |  0.5120   |
| 5     |  0.7460   |  0.5240   |
| 6     |  0.5920   |  0.4000   |
| 7     |  0.6300   |  0.4520   |
| 8     |  0.1780   |  0.1740   |
| 9     |  0.7020   |  0.5080   |
| A     |  0.8150   |  0.5180   |
| B     |  0.3930   |  0.1940   |
| D     |  0.7610   |  0.5480   |
| E     |  0.7910  |  0.5470  |
| F     |  0.7960 |  0.5590 |
| H     |  0.6480 |  0.4910 |
| I     |  0.1680 |  0.2080 |
| J     |  0.0520 |  0.0830 |
| K     |  0.8000 |  0.5580 |
| L     |  0.6970 |  0.5260 |
| M     |  0.7960 |  0.5540 |
| N     |  0.4100 |  0.3650 |
| O     |  0.8010 |  0.5500 |
| P     |  0.6080 |  0.4340 |
| Q     |  0.7430 |  0.5240 |
| R     |  0.8050 |  0.5740 |
| S     |  0.7300 |  0.5320 |
| T     |  0.8040 |  0.5740 |
| U     |  0.8010 |  0.5590 |
| V     |  0.6780 |  0.4970 |
| W     |  0.6690 |  0.4950 |
| X     |  0.7600 |  0.5300 |
| Y     |  0.7820 |  0.5390 |
| Z     |  0.7360 |  0.5360 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| a     |  0.6350   |  0.5130   |
| b     |  0.8040   |  0.5530   |
| c     |  0.7060   |  0.4990   |
| d     |  0.5140   |  0.4190   |
| e     |  0.0410   |  0.1020   |
| f     |  0.1390   |  0.1870   |
| g     |  0.7790   |  0.5300   |
| h     |  0.6470   |  0.4610   |
| i     |  0.8480   |  0.5930   |
| j     |  0.7010   |  0.4930   |
| k     |  0.1860   |  0.2070   |
| l     |  0.0660   |  0.0770   |
| m     |  0.0820   |  0.1440   |
| o     |  0.7430   |  0.5220   |
| p     |  0.5700   |  0.4170   |
| q     |  0.6730   |  0.4390   |
| r     |  0.6890   |  0.4900   |
| s     |  0.7740  |  0.5420  |
| t     |  0.2770 |  0.2280 |
| u     |  0.6070 |  0.4460 |
| v     |  0.4610 |  0.3100 |
| w     |  0.1360 |  0.1530 |
| x     |  0.5420 |  0.4270 |
| y     |  0.5580 |  0.4490 |
| z     |  0.5210 |  0.4480 |