



wwPDB EM Validation Summary Report ⓘ

Jan 23, 2023 – 10:06 PM EST

PDB ID : 7SYK
EMDB ID : EMD-25531
Title : Structure of the HCV IRES binding to the 40S ribosomal subunit, closed conformation. Structure 5(delta dII)
Authors : Brown, Z.P.; Abaeva, I.S.; De, S.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2021-11-25
Resolution : 4.20 Å (reported)
Based on initial models : 5FLX, 6D9J

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

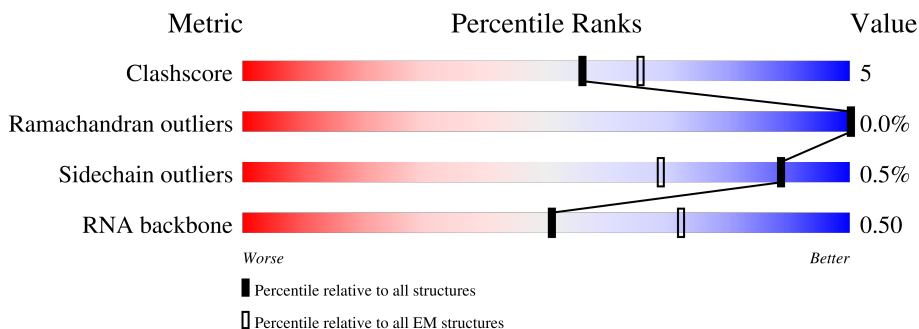
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 2 | 1870 | |
| 2 | B | 295 | |
| 3 | C | 264 | |
| 4 | D | 221 | |
| 5 | E | 281 | |
| 6 | F | 263 | |
| 7 | G | 204 | |

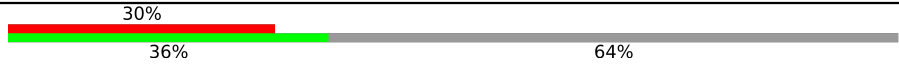
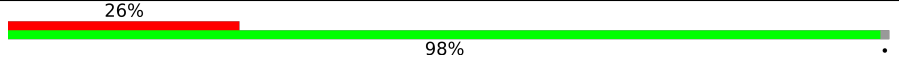
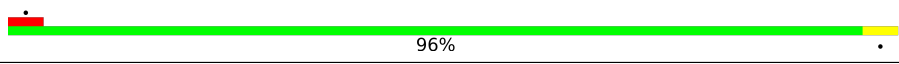

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8 | H | 249 | 84% 11% 5% |
| 9 | I | 432 | 6% 37% 6% 57% |
| 10 | J | 208 | 90% 9% |
| 11 | K | 194 | 82% 13% 5% |
| 12 | L | 149 | 18% 55% 7% 36% |
| 13 | M | 158 | 8% 74% 22% |
| 14 | N | 132 | 83% 74% 14% 11% |
| 15 | O | 151 | 81% 17% |
| 16 | P | 168 | 64% 17% 19% |
| 17 | Q | 145 | 11% 69% 10% 21% |
| 18 | R | 172 | 8% 66% 15% 17% |
| 19 | S | 135 | 21% 79% 19% |
| 20 | T | 152 | 12% 78% 17% 5% |
| 21 | U | 145 | 78% 19% |
| 22 | V | 119 | 44% 68% 16% 16% |
| 23 | W | 83 | 95% 5% |
| 24 | X | 130 | 86% 13% |
| 25 | Y | 143 | 87% 11% |
| 26 | Z | 131 | 82% 13% 5% |
| 27 | a | 124 | 25% 62% 38% |
| 28 | b | 101 | 5% 98% |
| 29 | c | 84 | 6% 98% |
| 30 | d | 69 | 19% 97% |
| 31 | e | 56 | 7% 98% |
| 32 | f | 133 | 11% 43% 57% |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 33 | g | 188 |  <p>30% 36% 64%</p> |
| 34 | h | 317 |  <p>26% 98%</p> |
| 35 | n | 25 |  <p>96%</p> |
| 36 | z | 400 |  <p>30% 10% 60%</p> |

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 78761 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| | | | Total | C | N | O | P | | |
| 1 | 2 | 1697 | 36227 | 16170 | 6504 | 11857 | 1696 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | B | 217 | 1710 | 1086 | 300 | 316 | 8 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| B | 114 | THR | ALA | conflict | UNP G1TLT8 |

- Molecule 3 is a protein called eS1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 3 | C | 213 | 1729 | 1098 | 309 | 308 | 14 | 0 | 0 |

- Molecule 4 is a protein called uS5 (S2).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 4 | D | 221 | 1716 | 1111 | 295 | 301 | 9 | 0 | 0 |

- Molecule 5 is a protein called uS3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 5 | E | 228 | 1768 | 1126 | 318 | 316 | 8 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | F | 262 | Total | C | N | O | S | 0 | 0 |
| | | | 2076 | 1324 | 386 | 358 | 8 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| F | 25 | GLY | SER | conflict | UNP G1TK17 |
| F | 51 | ARG | LYS | conflict | UNP G1TK17 |
| F | 78 | THR | ALA | conflict | UNP G1TK17 |
| F | 156 | VAL | MET | conflict | UNP G1TK17 |

- Molecule 7 is a protein called uS7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | G | 191 | Total | C | N | O | S | 0 | 0 |
| | | | 1509 | 943 | 286 | 273 | 7 | | |

- Molecule 8 is a protein called eS6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8 | H | 237 | Total | C | N | O | S | 0 | 0 |
| | | | 1923 | 1200 | 387 | 329 | 7 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | I | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1488 | 952 | 271 | 264 | 1 | | |

- Molecule 10 is a protein called eS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10 | J | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1686 | 1058 | 332 | 291 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| J | 47 | ARG | GLY | conflict | UNP G1TJW1 |

- Molecule 11 is a protein called uS4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | K | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1525 | 969 | 306 | 248 | 2 | | |

- Molecule 12 is a protein called eS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | L | 96 | Total | C | N | O | S | 0 | 0 |
| | | | 810 | 530 | 143 | 131 | 6 | | |

- Molecule 13 is a protein called uS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | M | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1233 | 785 | 231 | 211 | 6 | | |

- Molecule 14 is a protein called eS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | N | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 908 | 570 | 161 | 169 | 8 | | |

- Molecule 15 is a protein called uS15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | O | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1202 | 770 | 228 | 203 | 1 | | |

- Molecule 16 is a protein called uS11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | P | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1016 | 621 | 199 | 190 | 6 | | |

- Molecule 17 is a protein called uS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | Q | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 956 | 610 | 176 | 163 | 7 | | |

- Molecule 18 is a protein called uS9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 18 | R | 142 | 1128 | 717 | 213 | 195 | 3 | 0 | 0 |

- Molecule 19 is a protein called eS17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 19 | S | 132 | 1068 | 670 | 199 | 195 | 4 | 0 | 0 |

- Molecule 20 is a protein called uS13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 20 | T | 144 | 1190 | 746 | 241 | 202 | 1 | 0 | 0 |

- Molecule 21 is a protein called eS19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 21 | U | 141 | 1097 | 688 | 211 | 195 | 3 | 0 | 0 |

- Molecule 22 is a protein called uS10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 22 | V | 100 | 795 | 498 | 152 | 141 | 4 | 0 | 0 |

- Molecule 23 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 23 | W | 83 | 636 | 393 | 117 | 121 | 5 | 0 | 0 |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| W | 3 | ASN | SER | conflict | UNP G1TM82 |
| W | 4 | ASP | ASN | conflict | UNP G1TM82 |
| W | 33 | GLN | PRO | conflict | UNP G1TM82 |
| W | 50 | PHE | SER | conflict | UNP G1TM82 |
| W | 75 | ALA | SER | conflict | UNP G1TM82 |
| W | 76 | ASP | HIS | conflict | UNP G1TM82 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| W | 81 | LYS | GLN | conflict | UNP G1TM82 |

- Molecule 24 is a protein called uS8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 24 | X | 129 | 1034 | 659 | 193 | 176 | 6 | 0 | 0 |

- Molecule 25 is a protein called uS12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 25 | Y | 141 | 1098 | 693 | 219 | 183 | 3 | 0 | 0 |

- Molecule 26 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 26 | Z | 124 | 1011 | 640 | 198 | 168 | 5 | 0 | 0 |

- Molecule 27 is a protein called eS25 (S25).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 27 | a | 77 | 614 | 393 | 114 | 106 | 1 | 0 | 0 |

- Molecule 28 is a protein called eS26 (S26).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 28 | b | 101 | 814 | 507 | 170 | 132 | 5 | 0 | 0 |

- Molecule 29 is a protein called eS27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 29 | c | 83 | 651 | 408 | 121 | 115 | 7 | 0 | 0 |

- Molecule 30 is a protein called eS28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 30 | d | 67 | Total | C | N | O | S | 0 | 0 |
| | | | 530 | 321 | 108 | 99 | 2 | | |

- Molecule 31 is a protein called eS29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31 | e | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 459 | 286 | 94 | 74 | 5 | | |

- Molecule 32 is a protein called eS30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 32 | f | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 457 | 282 | 101 | 73 | 1 | | |

- Molecule 33 is a protein called 40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 33 | g | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 555 | 351 | 103 | 94 | 7 | | |

- Molecule 34 is a protein called RACK1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34 | h | 313 | Total | C | N | O | S | 0 | 0 |
| | | | 2436 | 1535 | 424 | 465 | 12 | | |

- Molecule 35 is a protein called 60s ribosomal protein l41.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35 | n | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 239 | 145 | 64 | 27 | 3 | | |

- Molecule 36 is a RNA chain called HCV IRES.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 36 | z | 162 | Total | C | N | O | P | 0 | 0 |
| | | | 3465 | 1542 | 621 | 1140 | 162 | | |

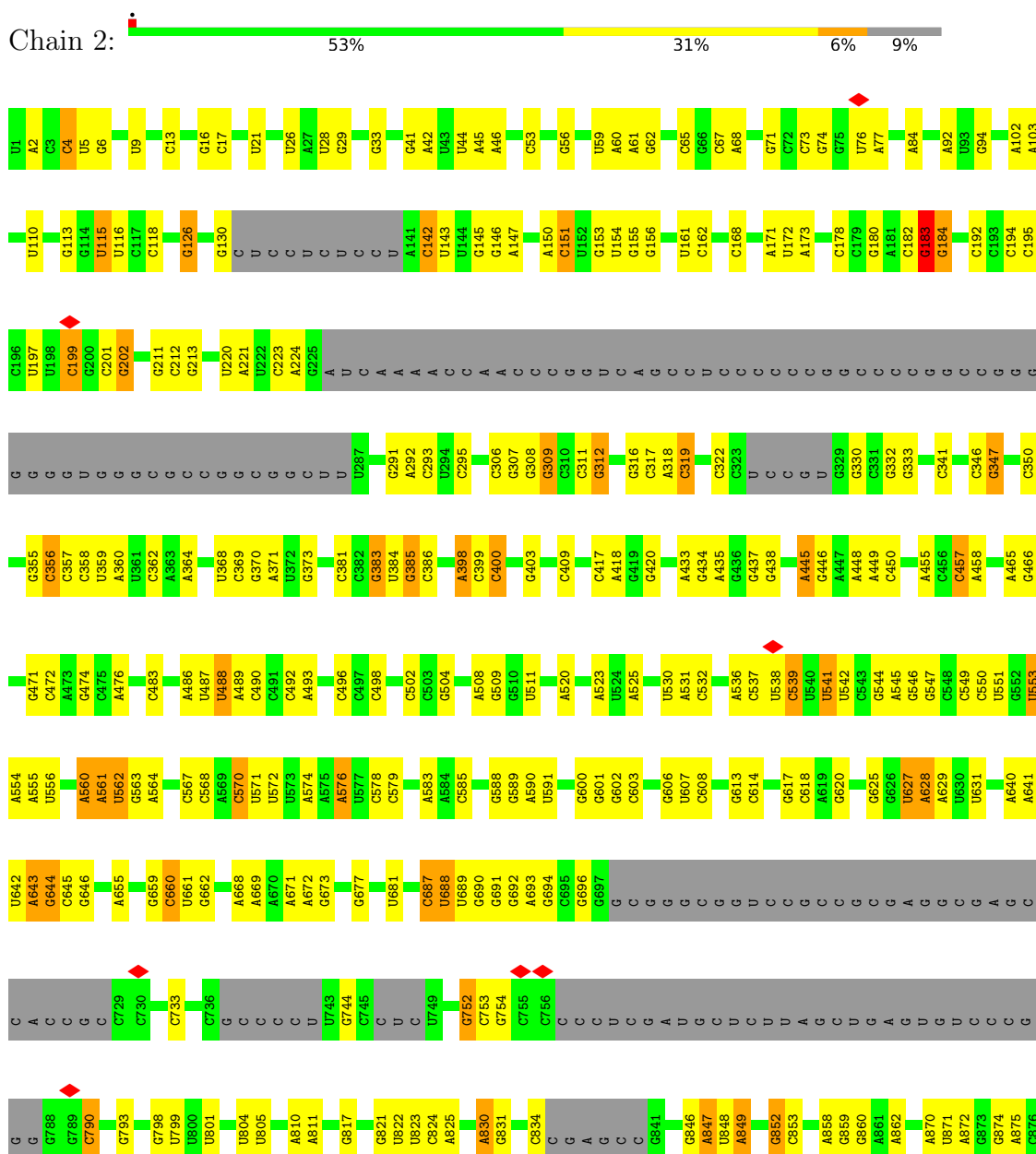
- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

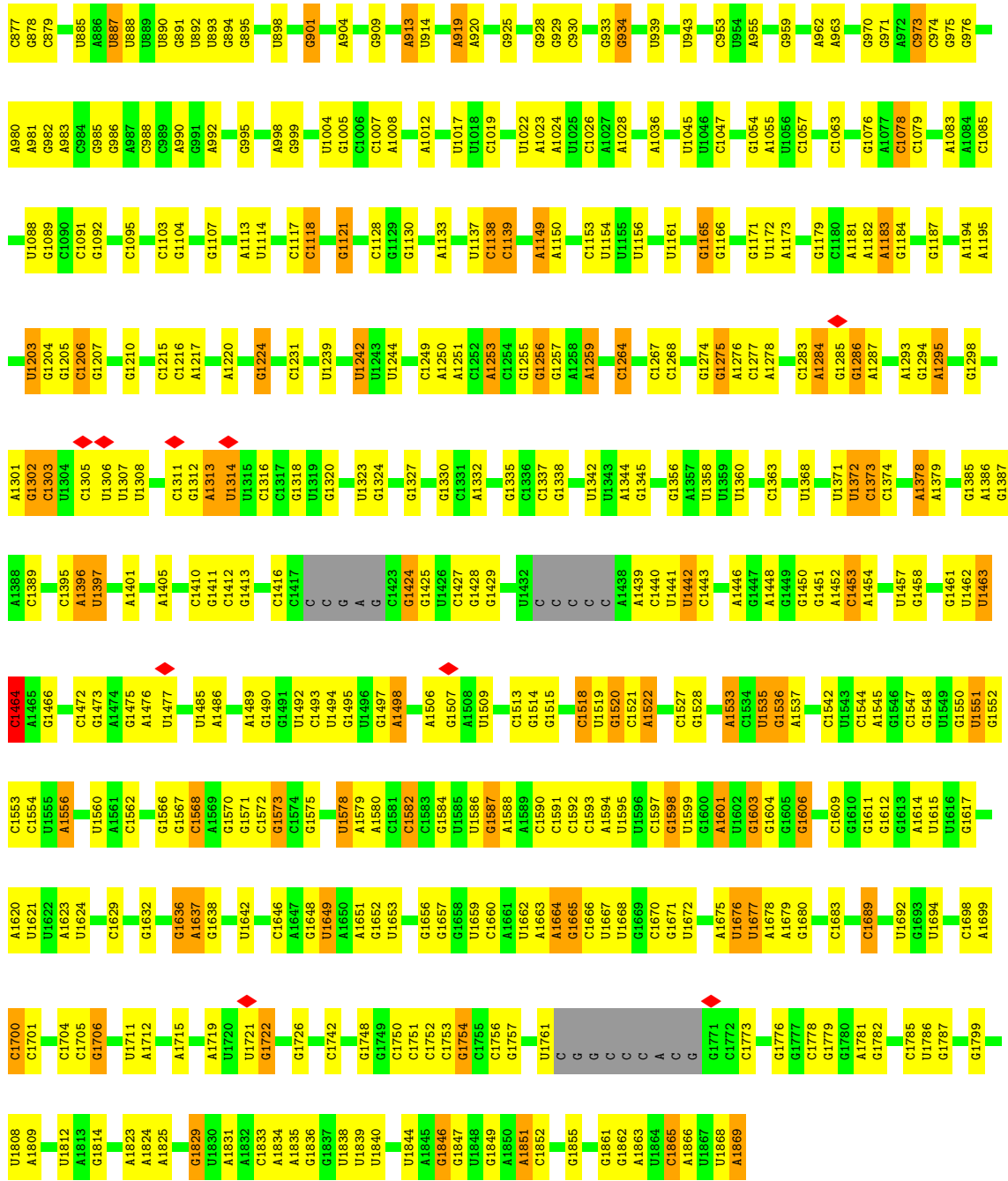
| Mol | Chain | Residues | Atoms | | AltConf |
|------------|--------------|-----------------|--------------|---------|----------------|
| 37 | b | 1 | Total 1 | Zn 1 | 0 |
| 37 | g | 1 | Total 1 | Zn 1 | 0 |

3 Residue-property plots

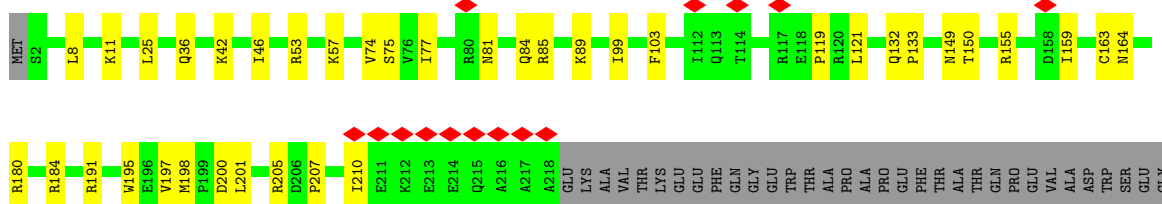
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S rRNA



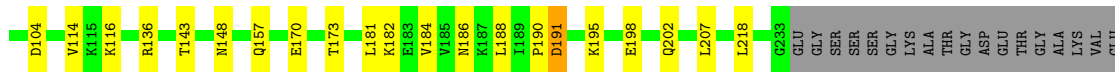
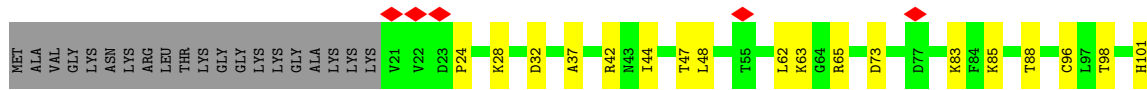


• Molecule 2: 40S ribosomal protein SA



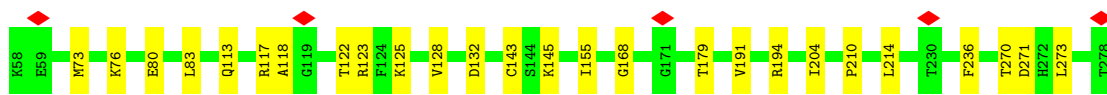
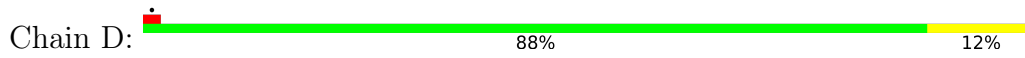
VAL GLN VAL PRO SER VAL PRO ILE GLN PHE PRO THR GLU ASP TRP SER ALA GLN PRO ALA THR TRP THR TRP SER

• Molecule 3: eS1

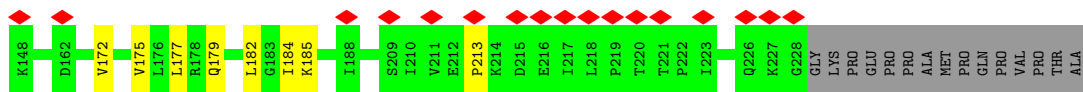
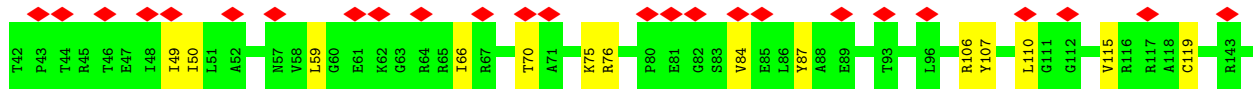
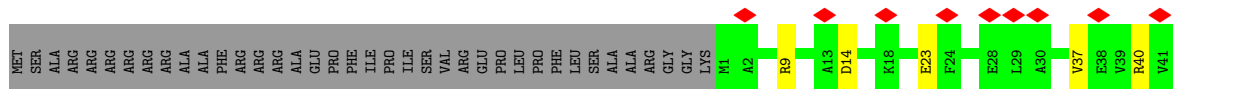


ARG ALA ASP TYR GLU PRO VAL

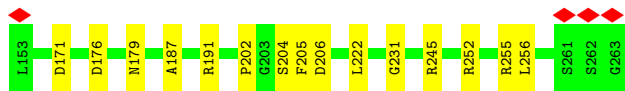
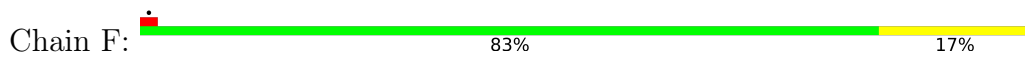
• Molecule 4: uS5 (S2)



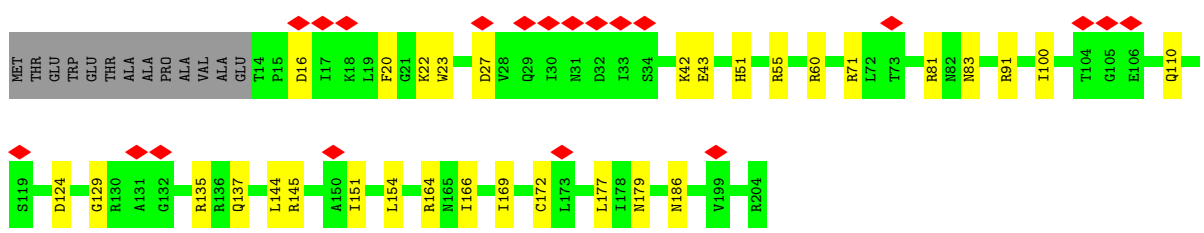
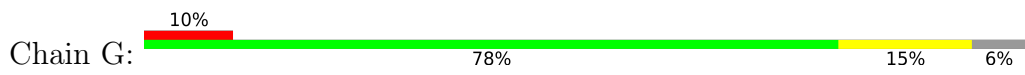
• Molecule 5: uS3



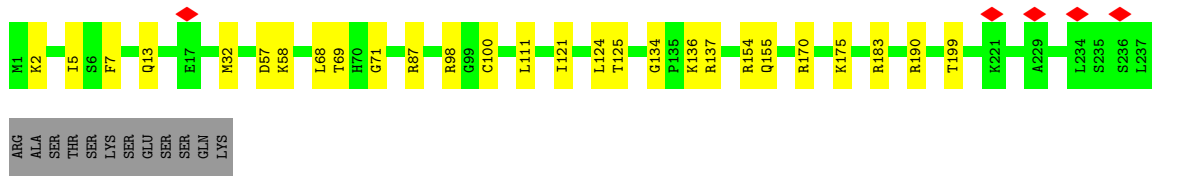
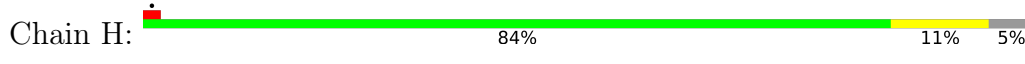
• Molecule 6: 40S ribosomal protein S4



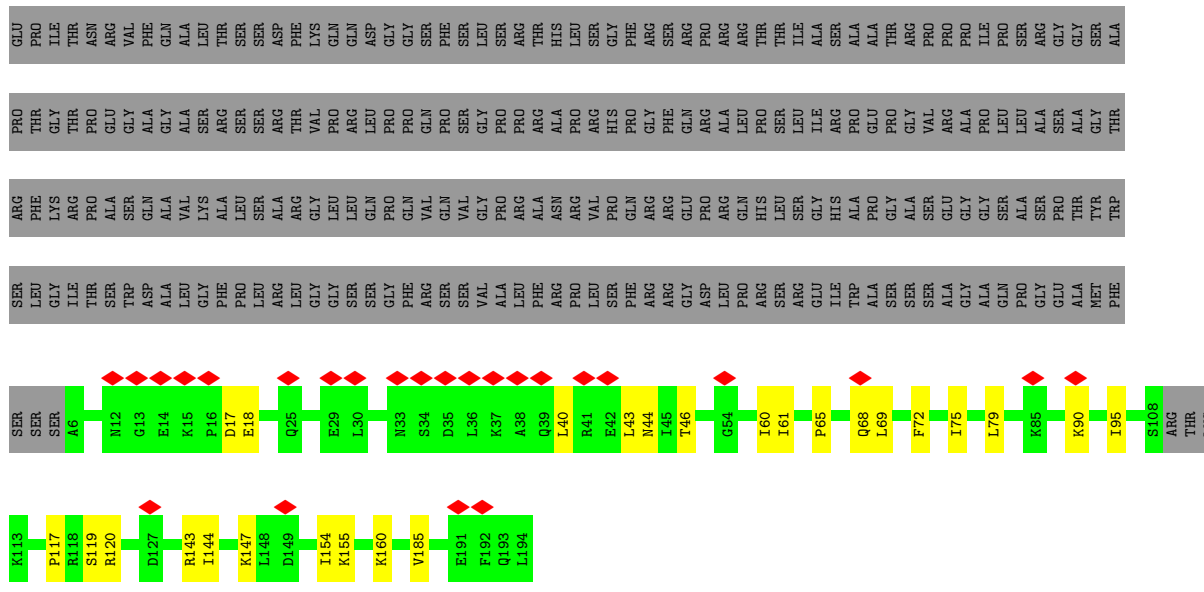
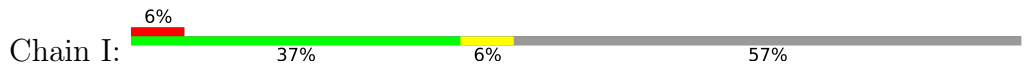
• Molecule 7: uS7



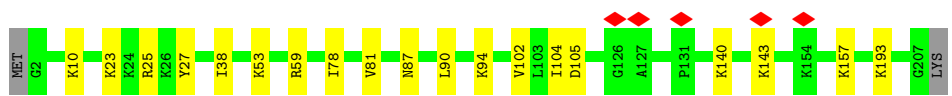
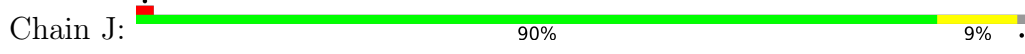
• Molecule 8: eS6



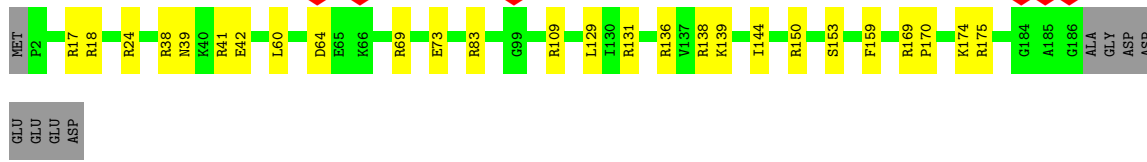
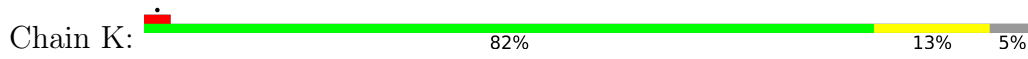
• Molecule 9: 40S ribosomal protein S7



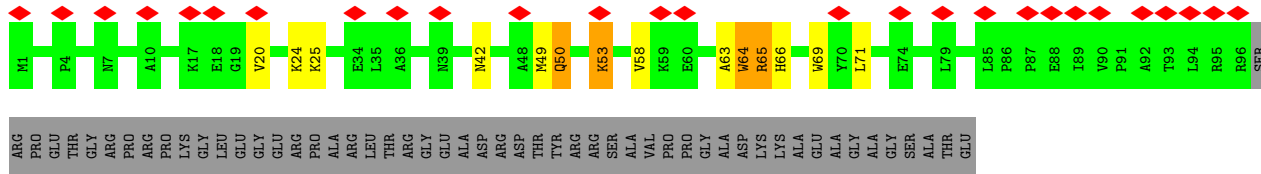
• Molecule 10: eS8



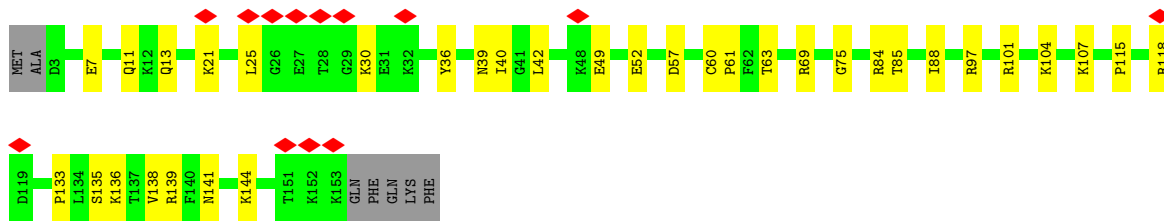
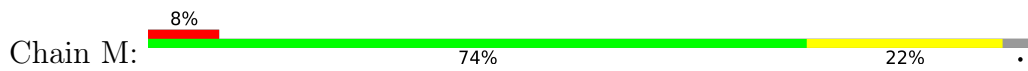
• Molecule 11: uS4



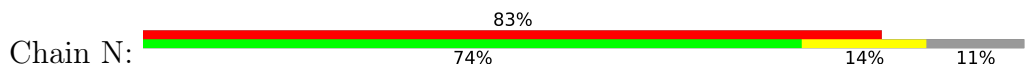
• Molecule 12: eS10



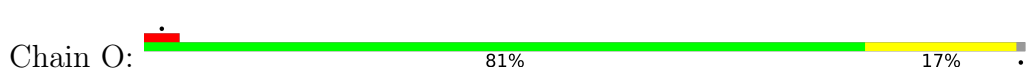
• Molecule 13: uS17

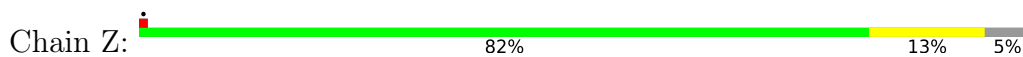


• Molecule 14: eS12

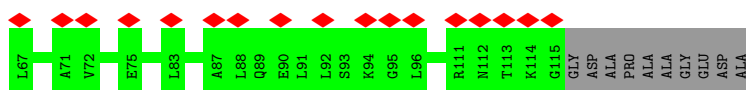
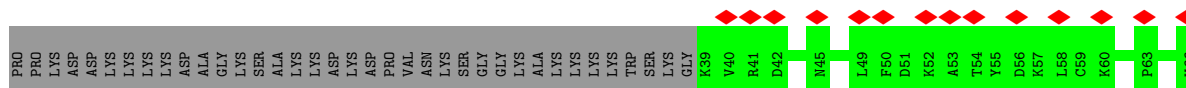


• Molecule 15: uS15

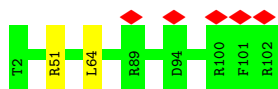




• Molecule 27: eS25 (S25)



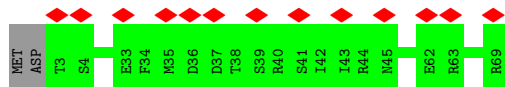
• Molecule 28: eS26 (S26)



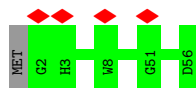
• Molecule 29: eS27



• Molecule 30: eS28



• Molecule 31: eS29



• Molecule 32: eS30



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 48757 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 70.9 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | 52000 | Depositor |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.037 | Depositor |
| Minimum map value | -0.015 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.006 | Depositor |
| Map size (Å) | 380.0, 380.0, 380.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.95, 0.95, 0.95 | Depositor |

5 Model quality i

5.1 Standard geometry i

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | 2 | 0.29 | 1/40506 (0.0%) | 1.03 | 196/63123 (0.3%) |
| 2 | B | 0.27 | 0/1747 | 0.62 | 0/2374 |
| 3 | C | 0.27 | 0/1756 | 0.60 | 1/2350 (0.0%) |
| 4 | D | 0.28 | 0/1753 | 0.65 | 1/2369 (0.0%) |
| 5 | E | 0.29 | 0/1796 | 0.67 | 0/2417 |
| 6 | F | 0.27 | 0/2118 | 0.64 | 1/2849 (0.0%) |
| 7 | G | 0.26 | 0/1531 | 0.62 | 0/2059 |
| 8 | H | 0.26 | 0/1946 | 0.63 | 1/2590 (0.0%) |
| 9 | I | 0.27 | 0/1510 | 0.61 | 0/2022 |
| 10 | J | 0.27 | 0/1715 | 0.61 | 0/2287 |
| 11 | K | 0.28 | 0/1550 | 0.65 | 0/2069 |
| 12 | L | 0.30 | 0/834 | 0.69 | 1/1125 (0.1%) |
| 13 | M | 0.29 | 0/1254 | 0.68 | 1/1677 (0.1%) |
| 14 | N | 0.27 | 0/918 | 0.60 | 0/1233 |
| 15 | O | 0.29 | 0/1226 | 0.64 | 1/1649 (0.1%) |
| 16 | P | 0.27 | 0/1029 | 0.63 | 0/1380 |
| 17 | Q | 0.28 | 0/974 | 0.71 | 0/1301 |
| 18 | R | 0.29 | 0/1146 | 0.68 | 2/1534 (0.1%) |
| 19 | S | 0.32 | 0/1082 | 0.71 | 0/1452 |
| 20 | T | 0.27 | 0/1208 | 0.66 | 1/1618 (0.1%) |
| 21 | U | 0.27 | 0/1115 | 0.63 | 0/1493 |
| 22 | V | 0.26 | 0/805 | 0.62 | 0/1081 |
| 23 | W | 0.30 | 0/643 | 0.63 | 0/860 |
| 24 | X | 0.31 | 0/1051 | 0.69 | 0/1406 |
| 25 | Y | 0.28 | 0/1116 | 0.67 | 1/1490 (0.1%) |
| 26 | Z | 0.26 | 0/1028 | 0.60 | 0/1366 |
| 27 | a | 0.26 | 0/620 | 0.60 | 0/831 |
| 28 | b | 0.28 | 0/828 | 0.64 | 1/1109 (0.1%) |
| 29 | c | 0.29 | 0/665 | 0.62 | 0/891 |
| 30 | d | 0.24 | 0/532 | 0.67 | 0/712 |
| 31 | e | 0.29 | 0/470 | 0.63 | 0/623 |
| 32 | f | 0.27 | 0/462 | 0.63 | 0/607 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 33 | g | 0.25 | 0/567 | 0.57 | 0/753 |
| 34 | h | 0.26 | 0/2493 | 0.61 | 0/3394 |
| 35 | n | 0.27 | 0/240 | 0.75 | 0/305 |
| 36 | z | 0.31 | 0/3871 | 0.99 | 7/6034 (0.1%) |
| All | All | 0.28 | 1/84105 (0.0%) | 0.88 | 215/122433 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3 | C | 0 | 1 |
| 6 | F | 0 | 1 |
| 12 | L | 0 | 1 |
| 29 | c | 0 | 1 |
| 35 | n | 0 | 1 |
| All | All | 0 | 5 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1 | 2 | 1556 | A | N9-C4 | 5.04 | 1.40 | 1.37 |

The worst 5 of 215 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | 2 | 1022 | U | C2-N1-C1' | 11.80 | 131.86 | 117.70 |
| 1 | 2 | 1078 | C | N3-C2-O2 | -10.94 | 114.24 | 121.90 |
| 1 | 2 | 1078 | C | N1-C2-O2 | 10.79 | 125.37 | 118.90 |
| 1 | 2 | 1700 | C | C6-N1-C2 | -10.40 | 116.14 | 120.30 |
| 1 | 2 | 1022 | U | N1-C2-O2 | 10.38 | 130.07 | 122.80 |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 3 | C | 191 | ASP | Peptide |
| 6 | F | 18 | TRP | Peptide |
| 12 | L | 64 | TRP | Peptide |
| 29 | c | 41 | TYR | Peptide |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 35 | n | 1 | MET | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 2 | 36227 | 0 | 18299 | 279 | 0 |
| 2 | B | 1710 | 0 | 1708 | 23 | 0 |
| 3 | C | 1729 | 0 | 1803 | 24 | 0 |
| 4 | D | 1716 | 0 | 1806 | 17 | 0 |
| 5 | E | 1768 | 0 | 1866 | 18 | 0 |
| 6 | F | 2076 | 0 | 2177 | 29 | 0 |
| 7 | G | 1509 | 0 | 1563 | 21 | 0 |
| 8 | H | 1923 | 0 | 2089 | 18 | 0 |
| 9 | I | 1488 | 0 | 1582 | 16 | 0 |
| 10 | J | 1686 | 0 | 1772 | 13 | 0 |
| 11 | K | 1525 | 0 | 1640 | 19 | 0 |
| 12 | L | 810 | 0 | 836 | 10 | 0 |
| 13 | M | 1233 | 0 | 1310 | 21 | 0 |
| 14 | N | 908 | 0 | 939 | 12 | 0 |
| 15 | O | 1202 | 0 | 1289 | 17 | 0 |
| 16 | P | 1016 | 0 | 1039 | 19 | 0 |
| 17 | Q | 956 | 0 | 1002 | 9 | 0 |
| 18 | R | 1128 | 0 | 1195 | 22 | 0 |
| 19 | S | 1068 | 0 | 1121 | 18 | 0 |
| 20 | T | 1190 | 0 | 1249 | 17 | 0 |
| 21 | U | 1097 | 0 | 1130 | 19 | 0 |
| 22 | V | 795 | 0 | 862 | 13 | 0 |
| 23 | W | 636 | 0 | 637 | 2 | 0 |
| 24 | X | 1034 | 0 | 1080 | 13 | 0 |
| 25 | Y | 1098 | 0 | 1167 | 11 | 0 |
| 26 | Z | 1011 | 0 | 1083 | 11 | 0 |
| 27 | a | 614 | 0 | 678 | 0 | 0 |
| 28 | b | 814 | 0 | 863 | 0 | 0 |
| 29 | c | 651 | 0 | 672 | 0 | 0 |
| 30 | d | 530 | 0 | 561 | 0 | 0 |
| 31 | e | 459 | 0 | 452 | 0 | 0 |
| 32 | f | 457 | 0 | 502 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33 | g | 555 | 0 | 563 | 0 | 0 |
| 34 | h | 2436 | 0 | 2393 | 0 | 0 |
| 35 | n | 239 | 0 | 289 | 0 | 0 |
| 36 | z | 3465 | 0 | 1751 | 0 | 0 |
| 37 | b | 1 | 0 | 0 | 0 | 0 |
| 37 | g | 1 | 0 | 0 | 0 | 0 |
| All | All | 78761 | 0 | 60968 | 568 | 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 5.

The worst 5 of 568 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:2:1332:A:H62 | 1:2:1493:C:N4 | 1.61 | 0.99 |
| 1:2:1472:C:H42 | 1:2:1476:A:H62 | 1.09 | 0.97 |
| 1:2:1656:G:H1 | 1:2:1668:U:H3 | 1.10 | 0.95 |
| 1:2:318:A:C2 | 1:2:333:G:N1 | 2.37 | 0.92 |
| 1:2:1332:A:N6 | 1:2:1493:C:H42 | 1.67 | 0.91 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 2 | B | 215/295 (73%) | 203 (94%) | 12 (6%) | 0 | 100 | 100 |
| 3 | C | 211/264 (80%) | 196 (93%) | 14 (7%) | 1 (0%) | 29 | 68 |
| 4 | D | 219/221 (99%) | 207 (94%) | 12 (6%) | 0 | 100 | 100 |
| 5 | E | 226/281 (80%) | 217 (96%) | 9 (4%) | 0 | 100 | 100 |
| 6 | F | 260/263 (99%) | 240 (92%) | 20 (8%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 7 | G | 189/204 (93%) | 180 (95%) | 9 (5%) | 0 | 100 | 100 |
| 8 | H | 235/249 (94%) | 225 (96%) | 10 (4%) | 0 | 100 | 100 |
| 9 | I | 181/432 (42%) | 174 (96%) | 7 (4%) | 0 | 100 | 100 |
| 10 | J | 204/208 (98%) | 191 (94%) | 13 (6%) | 0 | 100 | 100 |
| 11 | K | 183/194 (94%) | 175 (96%) | 8 (4%) | 0 | 100 | 100 |
| 12 | L | 94/149 (63%) | 91 (97%) | 3 (3%) | 0 | 100 | 100 |
| 13 | M | 149/158 (94%) | 138 (93%) | 11 (7%) | 0 | 100 | 100 |
| 14 | N | 115/132 (87%) | 106 (92%) | 9 (8%) | 0 | 100 | 100 |
| 15 | O | 147/151 (97%) | 143 (97%) | 4 (3%) | 0 | 100 | 100 |
| 16 | P | 134/168 (80%) | 124 (92%) | 10 (8%) | 0 | 100 | 100 |
| 17 | Q | 113/145 (78%) | 100 (88%) | 13 (12%) | 0 | 100 | 100 |
| 18 | R | 140/172 (81%) | 133 (95%) | 7 (5%) | 0 | 100 | 100 |
| 19 | S | 130/135 (96%) | 113 (87%) | 17 (13%) | 0 | 100 | 100 |
| 20 | T | 142/152 (93%) | 133 (94%) | 9 (6%) | 0 | 100 | 100 |
| 21 | U | 139/145 (96%) | 136 (98%) | 3 (2%) | 0 | 100 | 100 |
| 22 | V | 98/119 (82%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 23 | W | 81/83 (98%) | 76 (94%) | 5 (6%) | 0 | 100 | 100 |
| 24 | X | 127/130 (98%) | 124 (98%) | 3 (2%) | 0 | 100 | 100 |
| 25 | Y | 139/143 (97%) | 131 (94%) | 8 (6%) | 0 | 100 | 100 |
| 26 | Z | 122/131 (93%) | 116 (95%) | 6 (5%) | 0 | 100 | 100 |
| 27 | a | 75/124 (60%) | 69 (92%) | 6 (8%) | 0 | 100 | 100 |
| 28 | b | 99/101 (98%) | 95 (96%) | 4 (4%) | 0 | 100 | 100 |
| 29 | c | 81/84 (96%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 30 | d | 65/69 (94%) | 60 (92%) | 5 (8%) | 0 | 100 | 100 |
| 31 | e | 53/56 (95%) | 51 (96%) | 2 (4%) | 0 | 100 | 100 |
| 32 | f | 55/133 (41%) | 51 (93%) | 4 (7%) | 0 | 100 | 100 |
| 33 | g | 66/188 (35%) | 63 (96%) | 3 (4%) | 0 | 100 | 100 |
| 34 | h | 311/317 (98%) | 279 (90%) | 32 (10%) | 0 | 100 | 100 |
| 35 | n | 23/25 (92%) | 23 (100%) | 0 | 0 | 100 | 100 |
| All | All | 4821/5821 (83%) | 4534 (94%) | 286 (6%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 190 | PRO |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2 | B | 180/245 (74%) | 180 (100%) | 0 | 100 | 100 |
| 3 | C | 194/231 (84%) | 194 (100%) | 0 | 100 | 100 |
| 4 | D | 187/187 (100%) | 187 (100%) | 0 | 100 | 100 |
| 5 | E | 190/232 (82%) | 189 (100%) | 1 (0%) | 88 | 93 |
| 6 | F | 224/225 (100%) | 224 (100%) | 0 | 100 | 100 |
| 7 | G | 161/170 (95%) | 160 (99%) | 1 (1%) | 86 | 92 |
| 8 | H | 207/218 (95%) | 205 (99%) | 2 (1%) | 76 | 86 |
| 9 | I | 165/360 (46%) | 165 (100%) | 0 | 100 | 100 |
| 10 | J | 178/180 (99%) | 176 (99%) | 2 (1%) | 73 | 84 |
| 11 | K | 161/168 (96%) | 160 (99%) | 1 (1%) | 86 | 92 |
| 12 | L | 87/125 (70%) | 85 (98%) | 2 (2%) | 50 | 70 |
| 13 | M | 136/142 (96%) | 133 (98%) | 3 (2%) | 52 | 70 |
| 14 | N | 99/108 (92%) | 98 (99%) | 1 (1%) | 76 | 86 |
| 15 | O | 130/131 (99%) | 129 (99%) | 1 (1%) | 81 | 89 |
| 16 | P | 106/130 (82%) | 105 (99%) | 1 (1%) | 78 | 87 |
| 17 | Q | 105/130 (81%) | 105 (100%) | 0 | 100 | 100 |
| 18 | R | 117/140 (84%) | 117 (100%) | 0 | 100 | 100 |
| 19 | S | 119/121 (98%) | 117 (98%) | 2 (2%) | 60 | 78 |
| 20 | T | 125/132 (95%) | 125 (100%) | 0 | 100 | 100 |
| 21 | U | 111/116 (96%) | 111 (100%) | 0 | 100 | 100 |
| 22 | V | 92/107 (86%) | 92 (100%) | 0 | 100 | 100 |
| 23 | W | 67/67 (100%) | 67 (100%) | 0 | 100 | 100 |
| 24 | X | 112/113 (99%) | 112 (100%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 25 | Y | 113/115 (98%) | 113 (100%) | 0 | 100 | 100 |
| 26 | Z | 107/113 (95%) | 107 (100%) | 0 | 100 | 100 |
| 27 | a | 68/102 (67%) | 68 (100%) | 0 | 100 | 100 |
| 28 | b | 88/88 (100%) | 87 (99%) | 1 (1%) | 73 | 84 |
| 29 | c | 75/76 (99%) | 75 (100%) | 0 | 100 | 100 |
| 30 | d | 60/62 (97%) | 60 (100%) | 0 | 100 | 100 |
| 31 | e | 48/49 (98%) | 48 (100%) | 0 | 100 | 100 |
| 32 | f | 47/106 (44%) | 47 (100%) | 0 | 100 | 100 |
| 33 | g | 61/154 (40%) | 61 (100%) | 0 | 100 | 100 |
| 34 | h | 272/275 (99%) | 271 (100%) | 1 (0%) | 91 | 94 |
| 35 | n | 24/24 (100%) | 24 (100%) | 0 | 100 | 100 |
| All | All | 4216/4942 (85%) | 4197 (100%) | 19 (0%) | 89 | 93 |

5 of 19 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16 | P | 150 | ARG |
| 28 | b | 51 | ARG |
| 34 | h | 185 | LYS |
| 19 | S | 107 | LYS |
| 12 | L | 53 | LYS |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 148 | ASN |
| 19 | S | 127 | ASN |
| 35 | n | 22 | GLN |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 2 | 1685/1870 (90%) | 389 (23%) | 10 (0%) |
| 36 | z | 160/400 (40%) | 40 (25%) | 0 |
| All | All | 1845/2270 (81%) | 429 (23%) | 10 (0%) |

5 of 429 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2 | 2 | A |
| 1 | 2 | 4 | C |
| 1 | 2 | 9 | U |
| 1 | 2 | 26 | U |
| 1 | 2 | 33 | G |

5 of 10 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2 | 1137 | U |
| 1 | 2 | 1204 | G |
| 1 | 2 | 1395 | C |
| 1 | 2 | 561 | A |
| 1 | 2 | 627 | U |

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

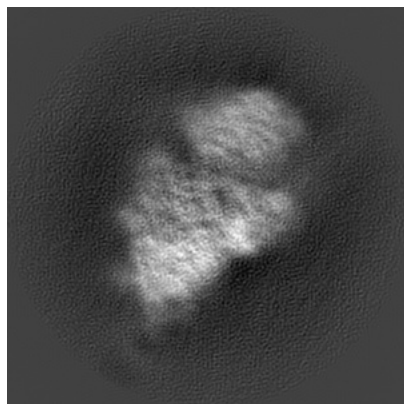
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25531. These allow visual inspection of the internal detail of the map and identification of artifacts.

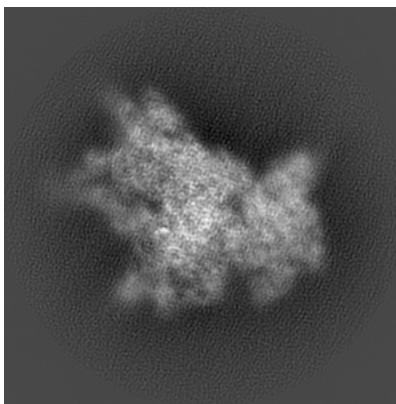
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

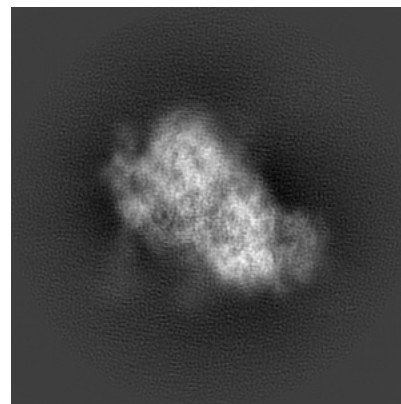
6.1.1 Primary map



X

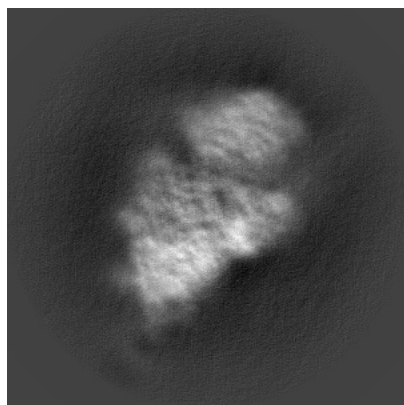


Y

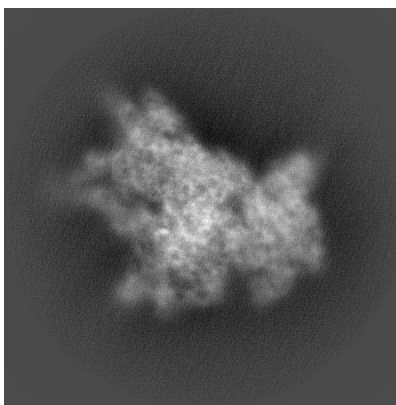


Z

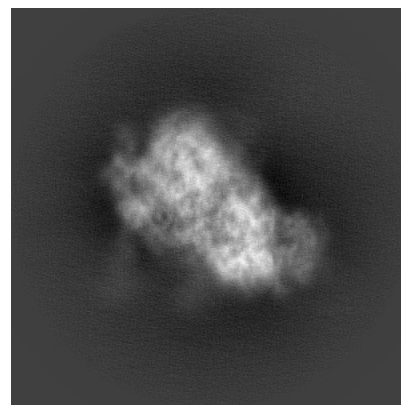
6.1.2 Raw map



X



Y

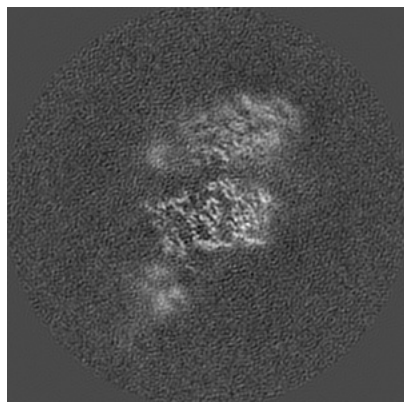


Z

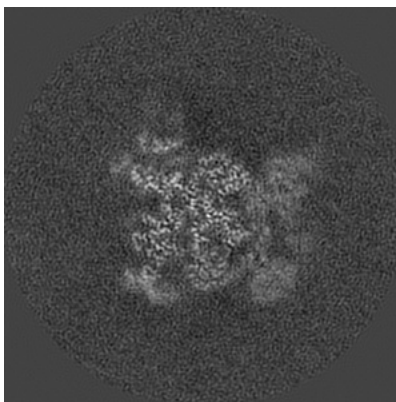
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

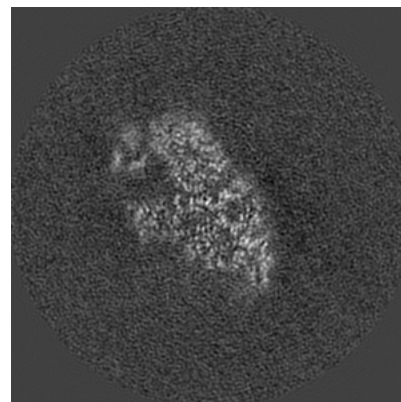
6.2.1 Primary map



X Index: 200

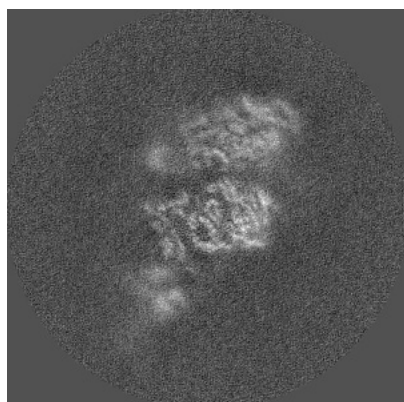


Y Index: 200

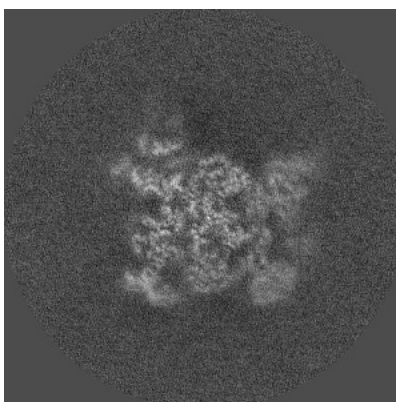


Z Index: 200

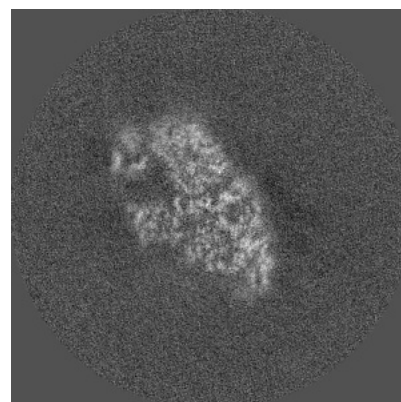
6.2.2 Raw map



X Index: 200



Y Index: 200

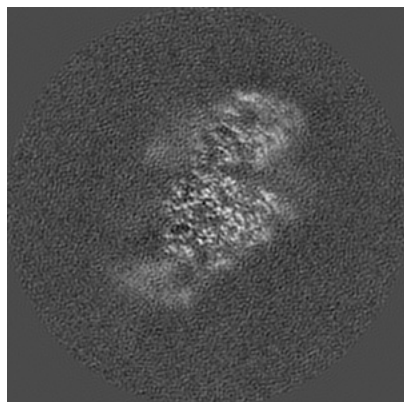


Z Index: 200

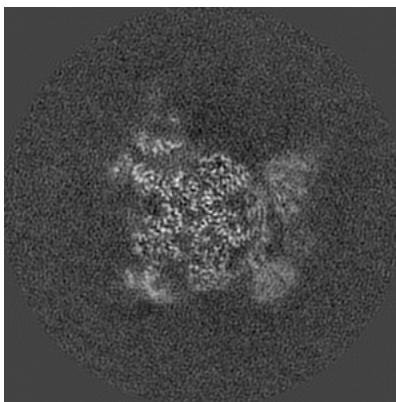
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

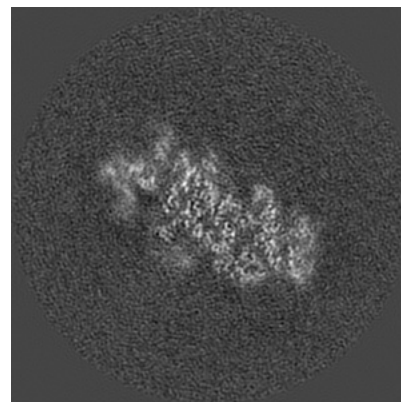
6.3.1 Primary map



X Index: 192

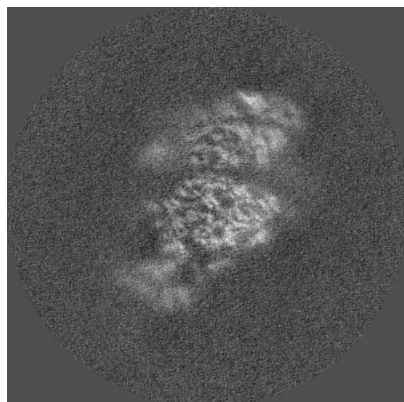


Y Index: 198

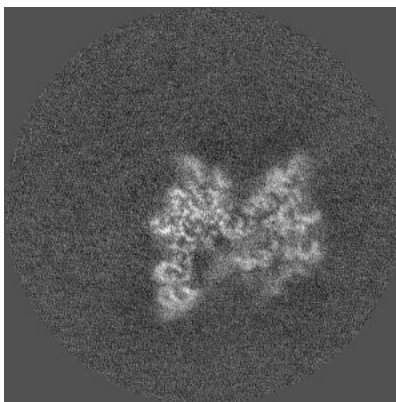


Z Index: 162

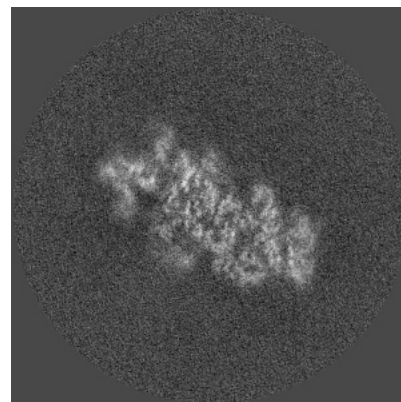
6.3.2 Raw map



X Index: 195



Y Index: 230

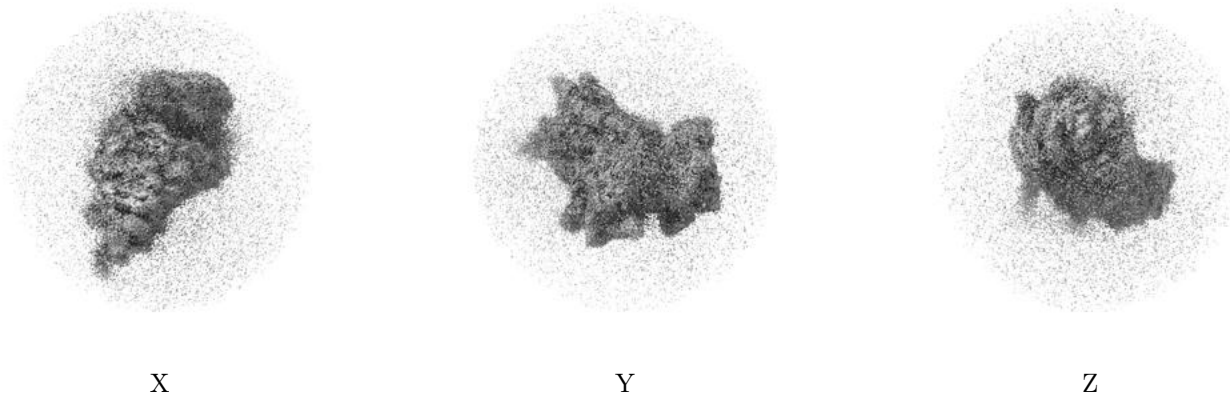


Z Index: 162

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

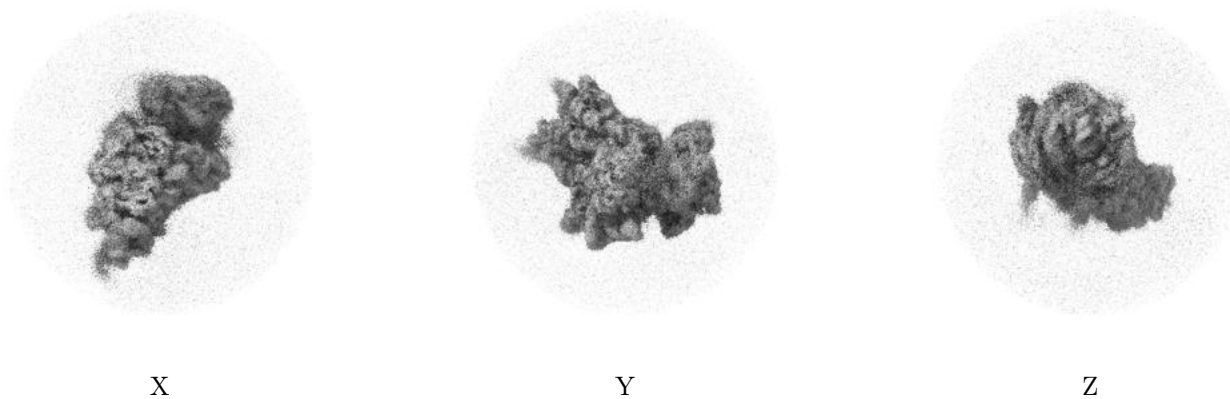
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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

6.4.2 Raw map



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

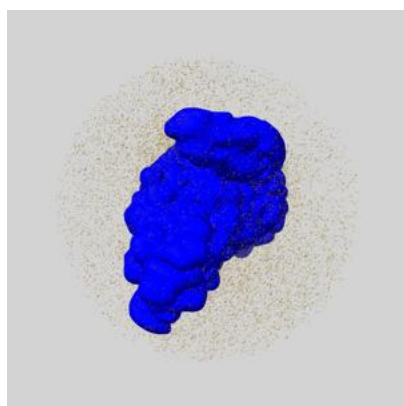
6.5 Mask visualisation [i](#)

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

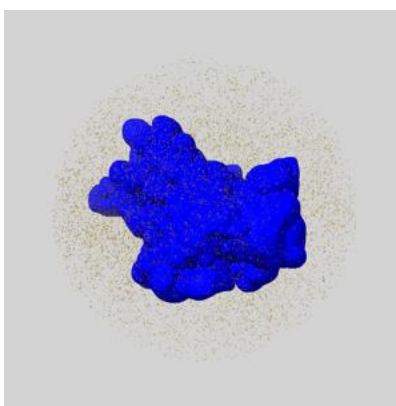
A mask typically either:

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

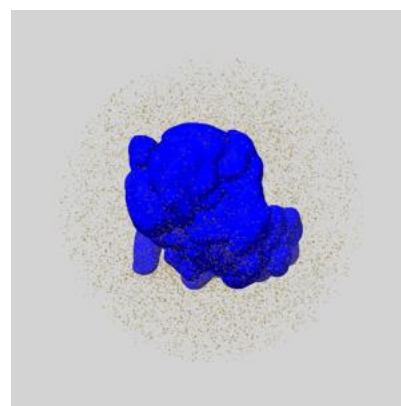
6.5.1 emd_25531_msk_1.map [i](#)



X



Y

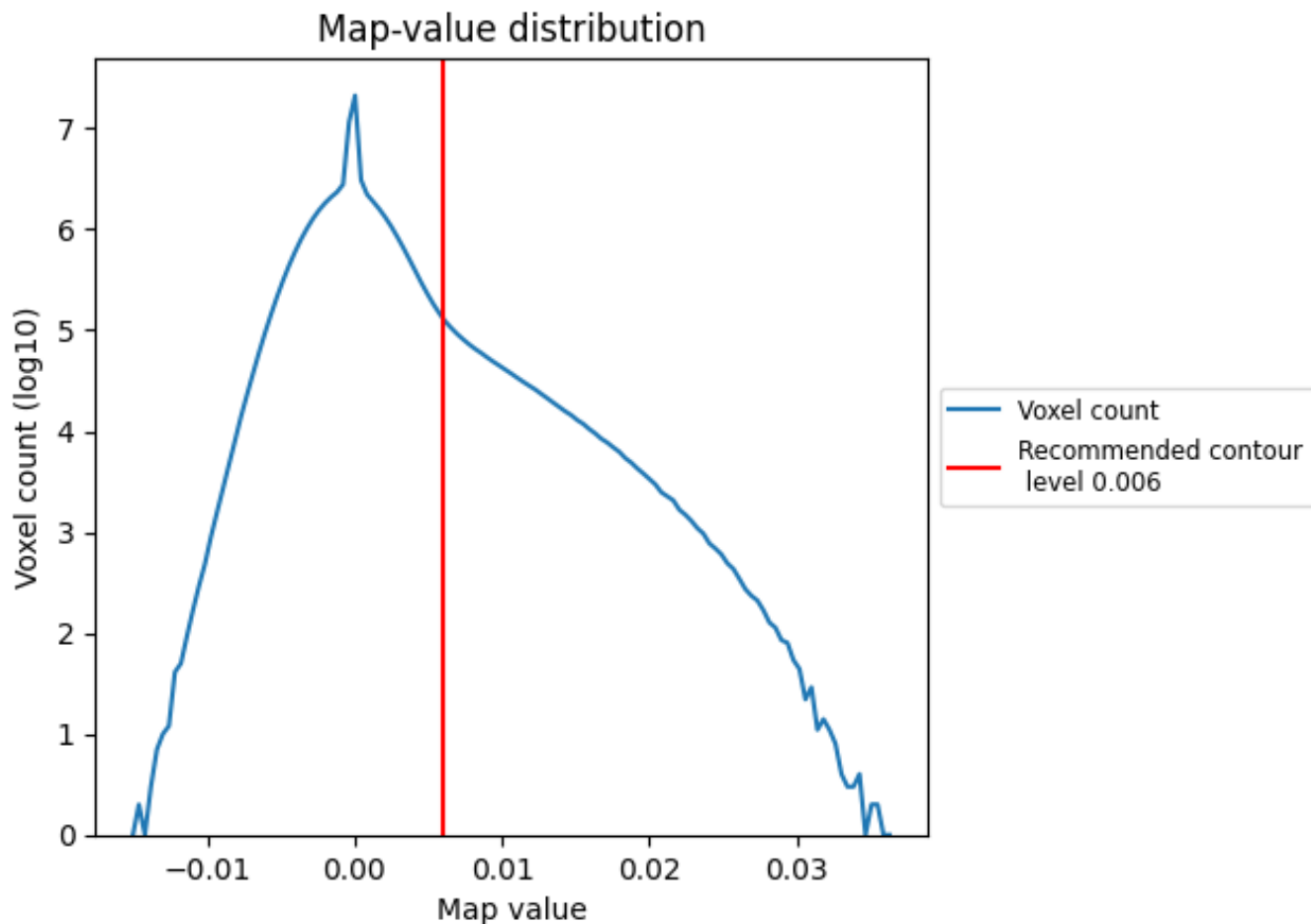


Z

7 Map analysis [i](#)

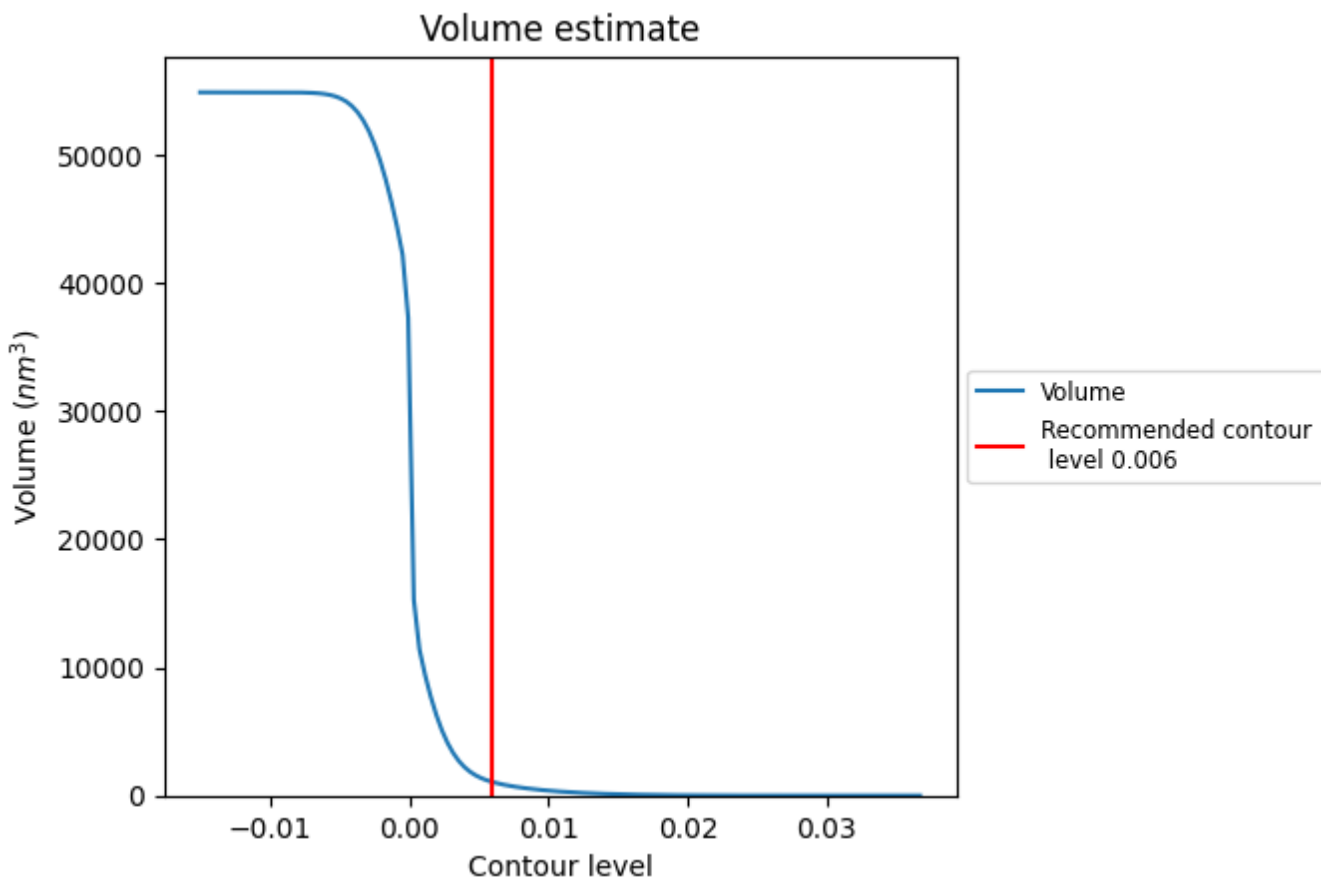
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

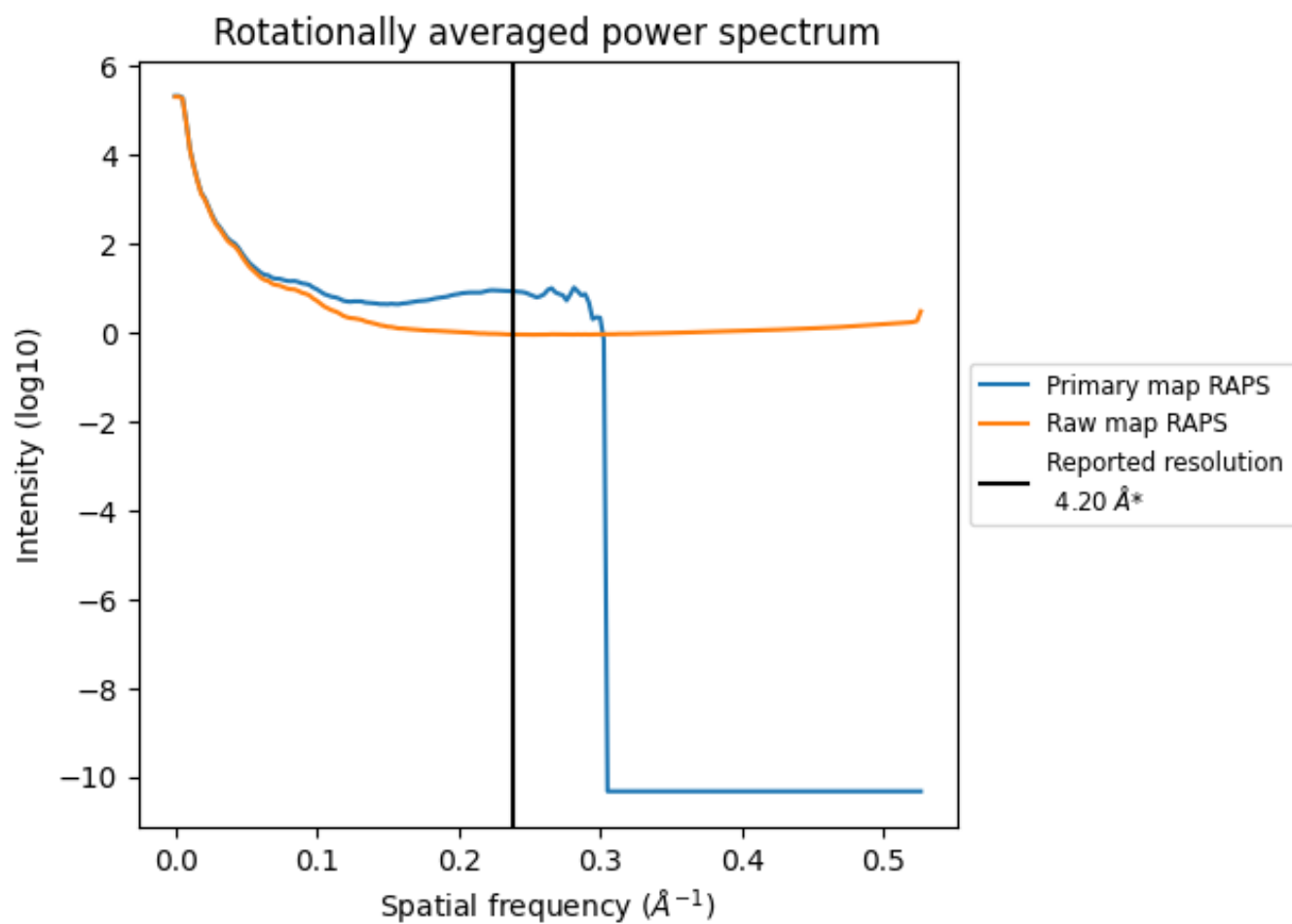
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1049 nm³; this corresponds to an approximate mass of 947 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

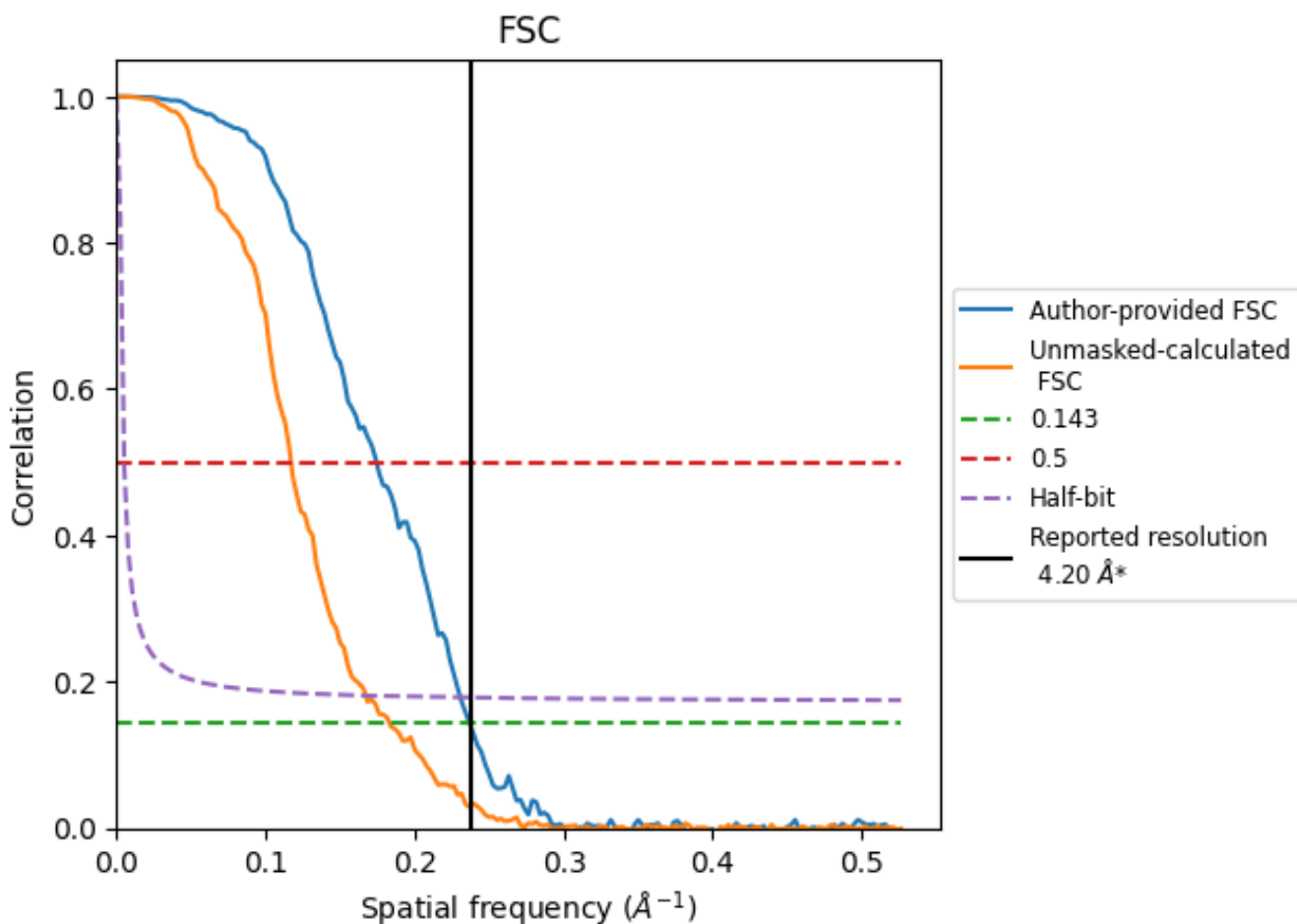


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238\AA^{-1}

8.2 Resolution estimates [i](#)

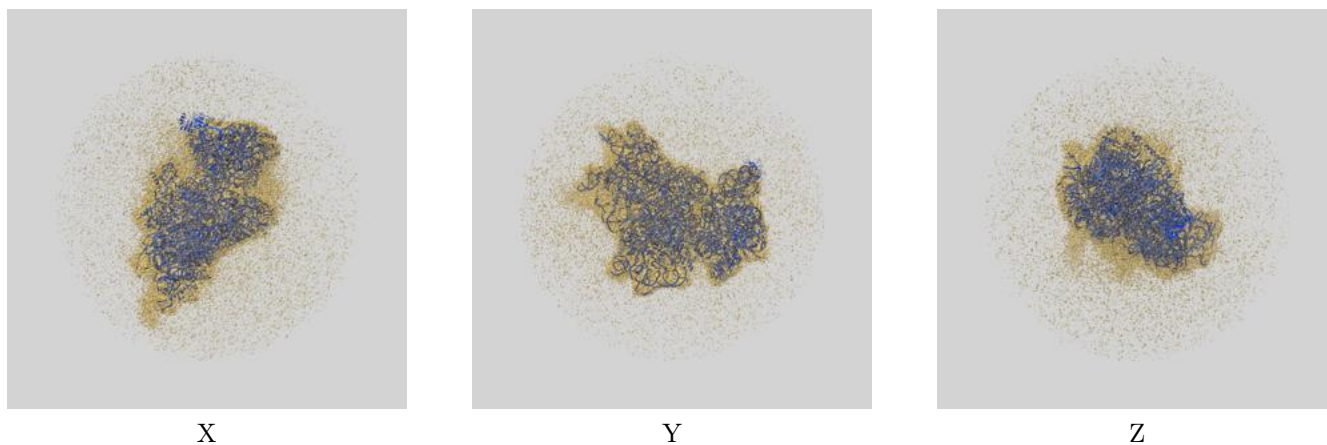
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.20 | - | - |
| Author-provided FSC curve | 4.22 | 5.73 | 4.33 |
| Unmasked-calculated* | 5.46 | 8.54 | 5.98 |

*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 5.46 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

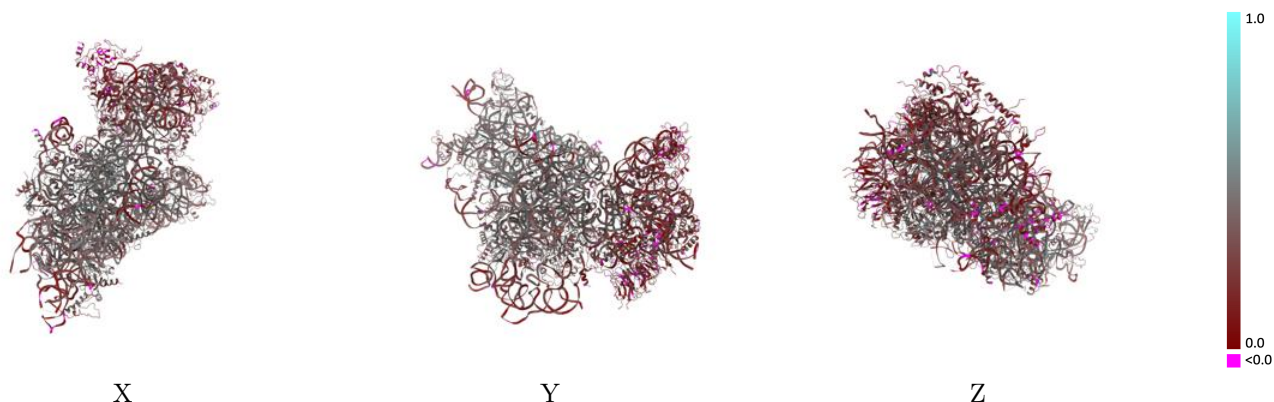
This section contains information regarding the fit between EMDB map EMD-25531 and PDB model 7SYK. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



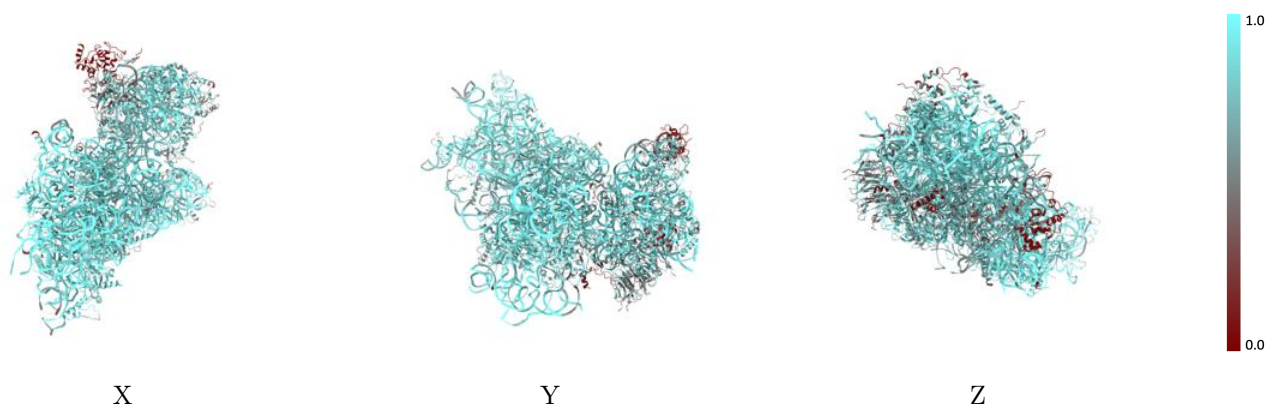
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



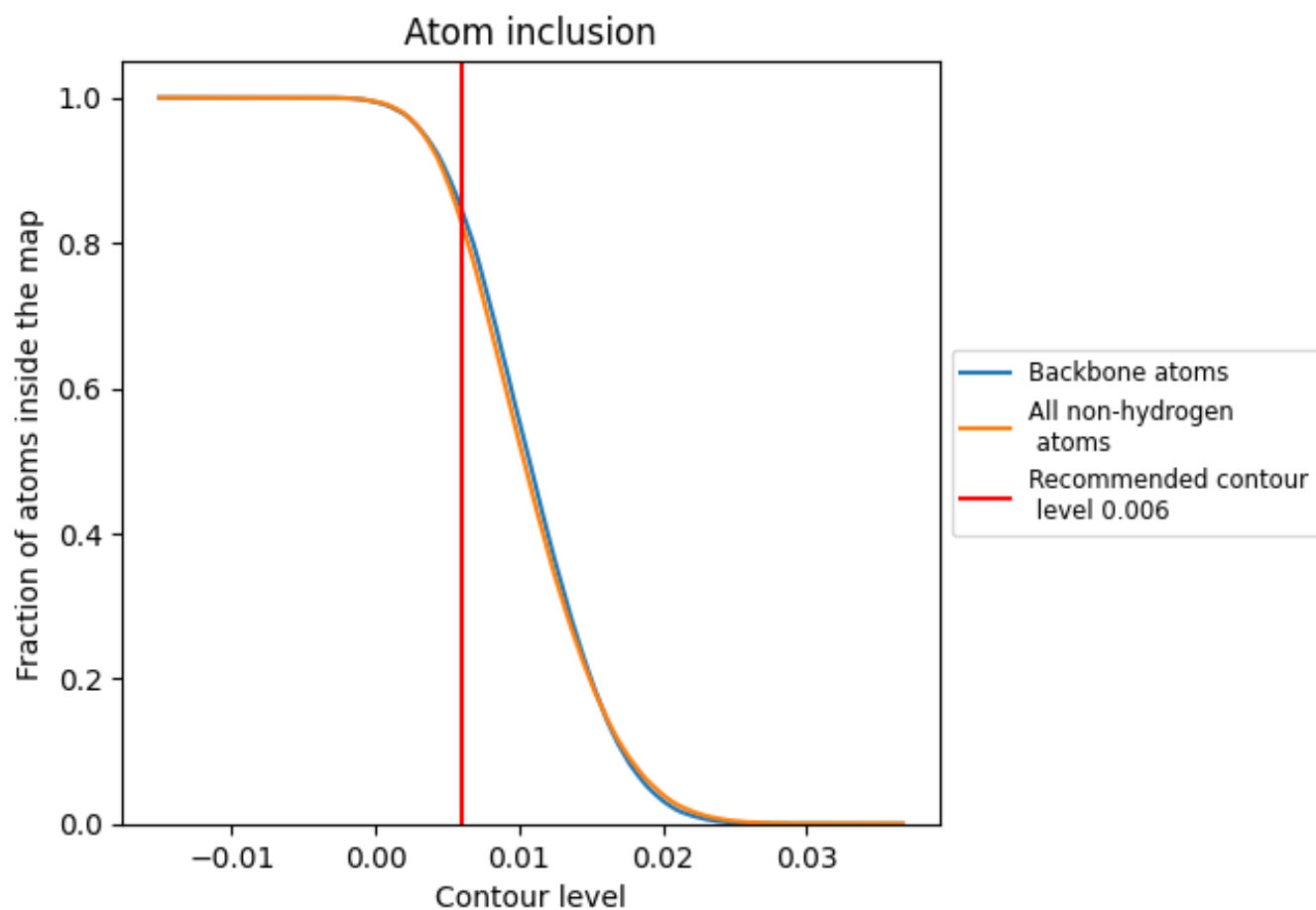
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.006).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.006) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8277 |  0.3360 |
| 2 |  0.9191 |  0.3530 |
| B |  0.7897 |  0.3880 |
| C |  0.8605 |  0.3700 |
| D |  0.7892 |  0.4020 |
| E |  0.6012 |  0.2660 |
| F |  0.8864 |  0.4310 |
| G |  0.7221 |  0.2370 |
| H |  0.8566 |  0.3670 |
| I |  0.7139 |  0.3730 |
| J |  0.8924 |  0.3990 |
| K |  0.8676 |  0.4080 |
| L |  0.5810 |  0.2100 |
| M |  0.8122 |  0.4230 |
| N |  0.0850 |  0.1010 |
| O |  0.8593 |  0.4120 |
| P |  0.9129 |  0.3740 |
| Q |  0.6890 |  0.2070 |
| R |  0.7381 |  0.2880 |
| S |  0.5848 |  0.2860 |
| T |  0.6908 |  0.2120 |
| U |  0.8238 |  0.2550 |
| V |  0.4251 |  0.2510 |
| W |  0.8167 |  0.4070 |
| X |  0.7990 |  0.4450 |
| Y |  0.8749 |  0.4400 |
| Z |  0.9307 |  0.4070 |
| a |  0.5326 |  0.1980 |
| b |  0.8517 |  0.4060 |
| c |  0.8091 |  0.4090 |
| d |  0.6102 |  0.2830 |
| e |  0.6961 |  0.2850 |
| f |  0.6386 |  0.2660 |
| g |  0.1590 |  0.1550 |
| h |  0.5788 |  0.1890 |



Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| n |  0.8211 |  0.3830 |
| z |  0.8597 |  0.2310 |