# wwPDB EM Validation Summary Report (i)

Nov 12, 2024 – 10:10 am GMT

| | | |
|---|---|---|
| PDB ID | : | 8P8W |
| EMDB ID | : | EMD-17145 |
| Title | : | Mycoplasma pneumoniae di-ribosome in chloramphenicol-treated cells (following 70S) |
| Authors | : | Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J. |
| Deposited on | : | 2023-06-02 |
| Resolution | : | 8.70 Å(reported) |
| Based on initial models | : | 7OOD, 7OOC |

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 (i) 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 (1)) were used in the production of this report:

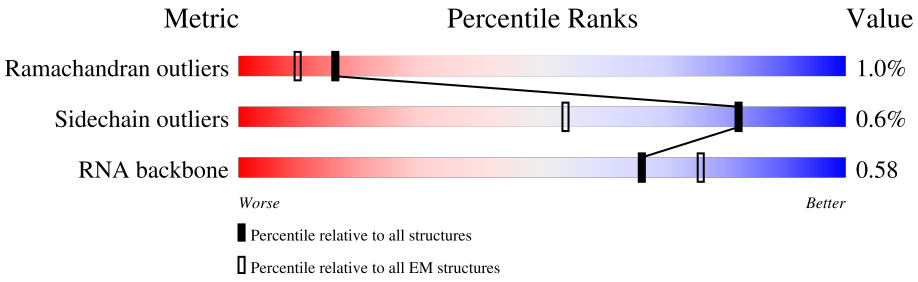
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev113 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 8.70 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0 | 48 | 12% 98% |
| 2 | 1 | 59 | 17% 100% |
| 3 | 2 | 37 | 14% 100% |
| 4 | 3 | 2907 | 81% 19% |
| 5 | 4 | 108 | 73% 27% |
| 6 | 5 | 1520 | 82% 17% |
| 7 | 6 | 76 | 68% 67% 28% 5% |
| 8 | 7 | 75 | 69% 31% |

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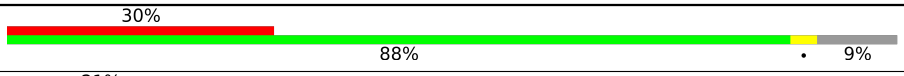
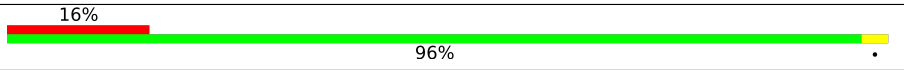
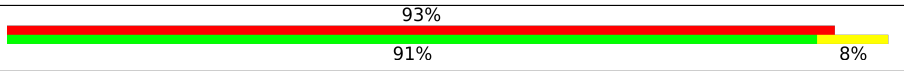
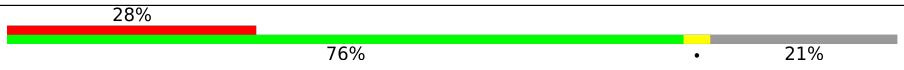
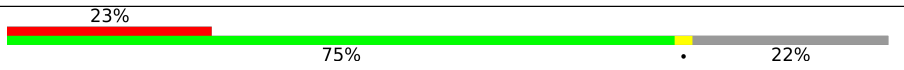
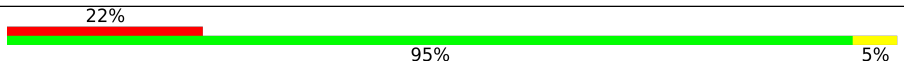
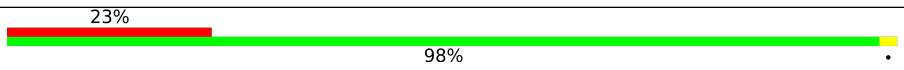
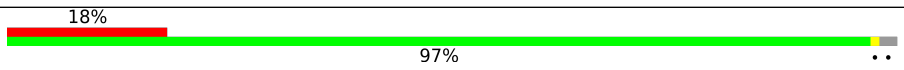
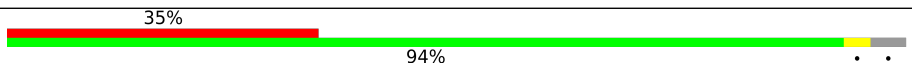
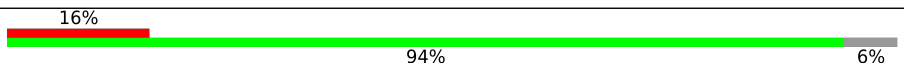
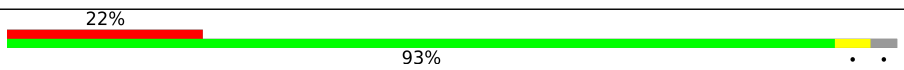
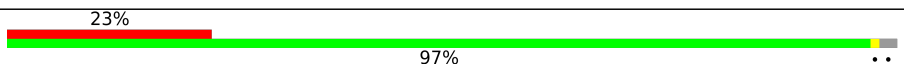
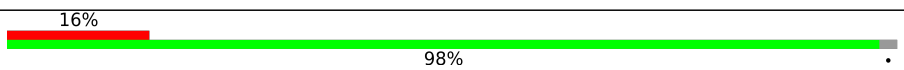
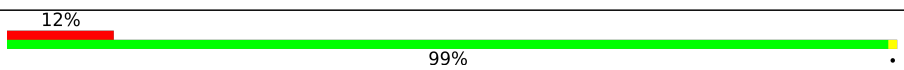
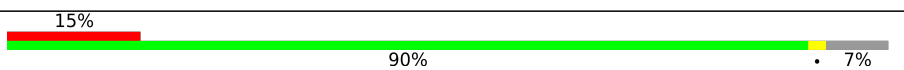
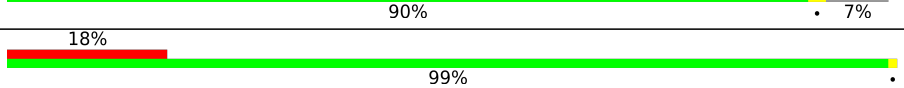
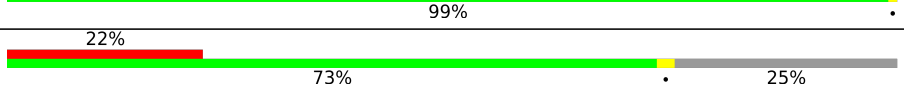
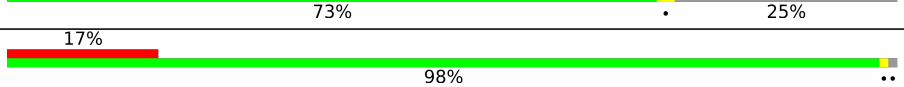
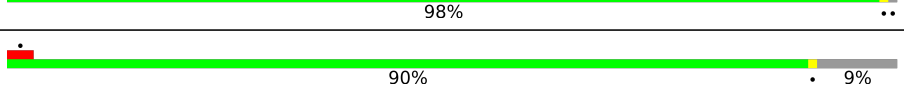
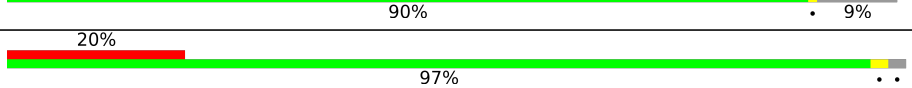
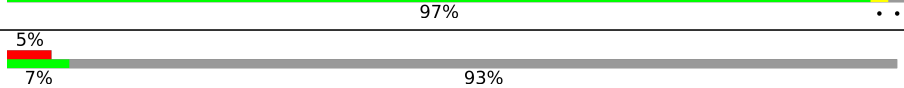
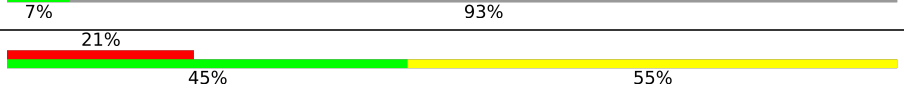
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | A | 294 |   |
| 10 | B | 273 |   |
| 11 | C | 205 |   |
| 11 | U | 205 |   |
| 12 | D | 219 |   |
| 13 | E | 215 |   |
| 14 | F | 155 |   |
| 15 | G | 142 |   |
| 16 | H | 132 |   |
| 17 | I | 108 |   |
| 18 | J | 121 |   |
| 19 | K | 139 |   |
| 20 | L | 124 |   |
| 21 | M | 61 |   |
| 22 | N | 86 |   |
| 23 | O | 94 |   |
| 24 | P | 85 |   |
| 25 | Q | 104 |   |
| 26 | R | 87 |   |
| 27 | S | 87 |   |
| 28 | T | 60 |   |
| 29 | X | 444 |   |
| 30 | Y | 29 |   |
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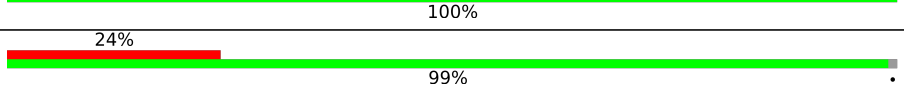
| 32 | a | 287 |   |

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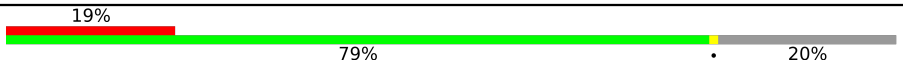
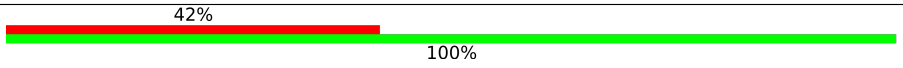
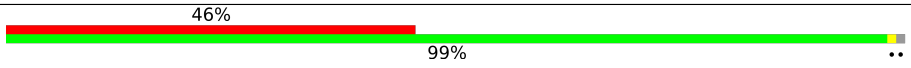
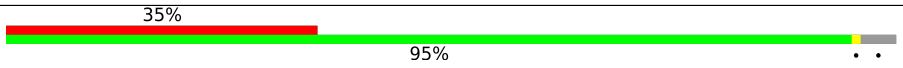
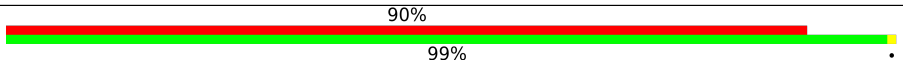
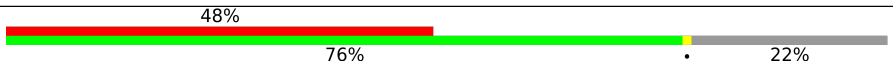
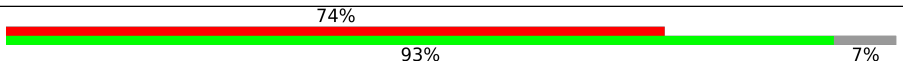
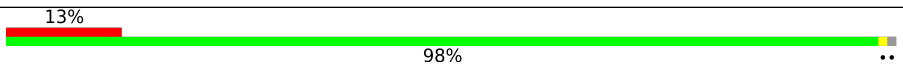
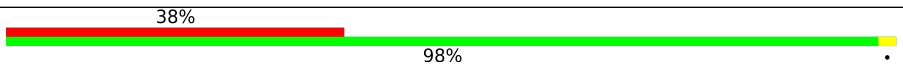
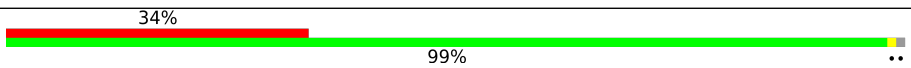
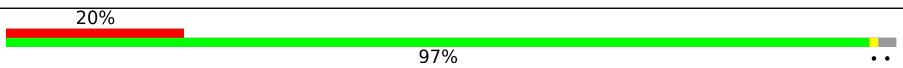
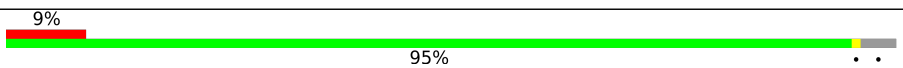
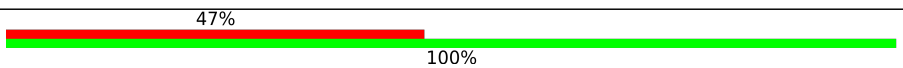
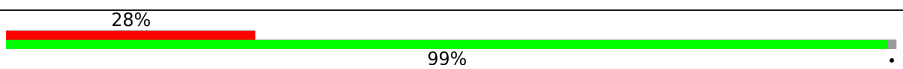
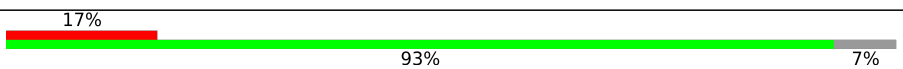
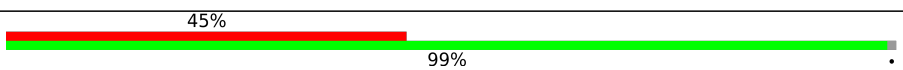
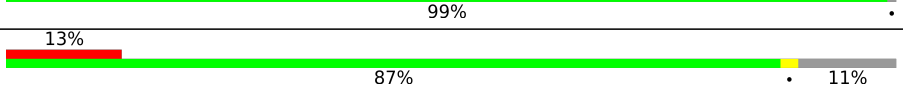
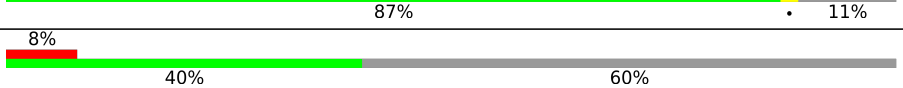
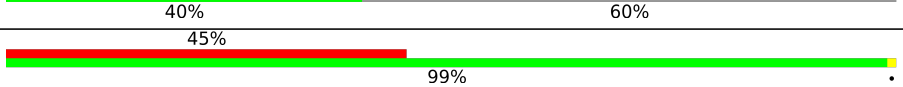
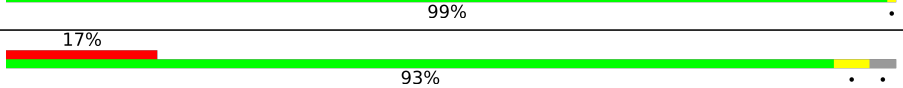
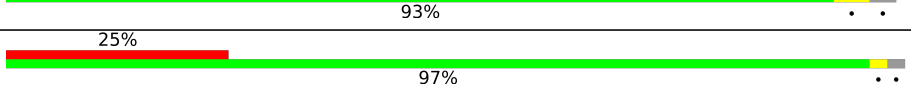
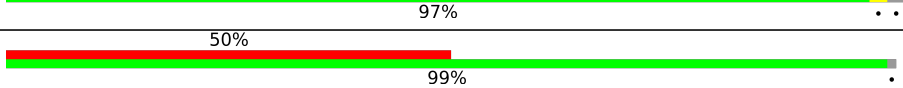
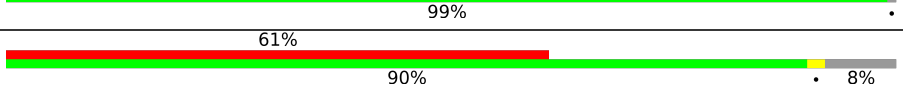
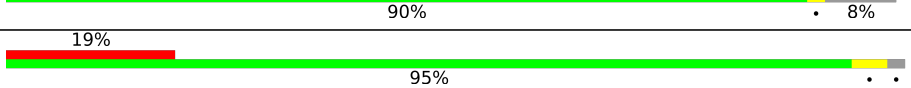
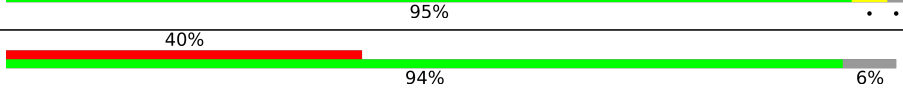
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 33 | b | 287 |   |
| 34 | c | 212 |   |
| 35 | d | 180 |   |
| 36 | e | 184 |   |
| 37 | f | 149 |   |
| 38 | g | 161 |   |
| 39 | h | 137 |   |
| 40 | i | 146 |   |
| 41 | j | 122 |   |
| 42 | k | 151 |   |
| 43 | l | 139 |   |
| 44 | m | 124 |   |
| 45 | n | 116 |   |
| 46 | o | 119 |   |
| 47 | p | 127 |   |
| 48 | q | 100 |   |
| 49 | r | 159 |   |
| 50 | s | 237 |   |
| 51 | t | 111 |   |
| 52 | u | 104 |   |
| 53 | v | 65 |   |
| 54 | w | 111 |   |
| 55 | x | 97 |   |
| 56 | y | 57 |   |
| 57 | z | 53 |   |

# 2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 151559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 0 | 47 | 380 | 236 | 81 | 61 | 2 | 0 | 0 |

- Molecule 2 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 1 | 59 | 477 | 300 | 99 | 77 | 1 | 0 | 0 |

- Molecule 3 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | 2 | 37 | 304 | 189 | 65 | 46 | 4 | 0 | 0 |

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 4 | 3 | 2893 | 61995 | 27704 | 11293 | 20105 | 2893 | 0 | 0 |

- Molecule 5 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 5 | 4 | 108 | 2305 | 1030 | 415 | 752 | 108 | 0 | 0 |

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 6 | 5 | 1507 | 32258 | 14420 | 5847 | 10484 | 1507 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 5 | 1003 | A | G | conflict | GB 26117688 |

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 6 | 76 | Total | C | N | O | P | 0 | 0 |
| | | | 1620 | 723 | 287 | 534 | 76 | | |

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | 7 | 75 | Total | C | N | O | P | 0 | 0 |
| | | | 1599 | 712 | 279 | 533 | 75 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 7 | 17 | G | - | insertion | GB 26117688 |
| 7 | 55 | C | U | conflict | GB 26117688 |

- Molecule 9 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | A | 268 | Total | C | N | O | S | 0 | 0 |
| | | | 2152 | 1368 | 379 | 396 | 9 | | |

- Molecule 10 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | B | 225 | Total | C | N | O | S | 0 | 0 |
| | | | 1773 | 1121 | 328 | 319 | 5 | | |

- Molecule 11 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | C | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1669 | 1057 | 316 | 292 | 4 | | |
| 11 | U | 204 | Total | C | N | O | S | 0 | 0 |
| | | | 1669 | 1057 | 316 | 292 | 4 | | |

- Molecule 12 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | D | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1346 | 846 | 265 | 232 | 3 | | |

- Molecule 13 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | E | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1362 | 857 | 240 | 263 | 2 | | |

- Molecule 14 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | F | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1254 | 790 | 240 | 217 | 7 | | |

- Molecule 15 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | G | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1118 | 728 | 194 | 193 | 3 | | |

- Molecule 16 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | H | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1040 | 661 | 195 | 183 | 1 | | |

- Molecule 17 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | I | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 832 | 536 | 147 | 148 | 1 | | |

- Molecule 18 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | J | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 829 | 514 | 153 | 156 | 6 | | |

- Molecule 19 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | K | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1071 | 677 | 212 | 180 | 2 | | |

- Molecule 20 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 20 | L | 121 | Total | C | N | O | 0 | 0 |
| | | | 975 | 609 | 197 | 169 | | |

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | M | 60 | Total | C | N | O | S | 0 | 0 |
| | | | 474 | 302 | 96 | 72 | 4 | | |

- Molecule 22 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | N | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 697 | 441 | 131 | 124 | 1 | | |

- Molecule 23 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | O | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 705 | 453 | 130 | 118 | 4 | | |

- Molecule 24 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | P | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 693 | 436 | 138 | 118 | 1 | | |

- Molecule 25 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Q | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 651 | 417 | 129 | 100 | 5 | | |

- Molecule 26 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | R | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 700 | 444 | 132 | 122 | 2 | | |

- Molecule 27 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 27 | S | 79 | Total | C | N | O | 0 | 0 |
| | | | 643 | 391 | 138 | 114 | | |

- Molecule 28 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | T | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 519 | 326 | 111 | 80 | 2 | | |

- Molecule 29 is a protein called Trigger factor.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | X | 30 | Total | C | N | O | S | 0 | 0 |
| | | | 242 | 155 | 43 | 43 | 1 | | |

- Molecule 30 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | Y | 29 | Total | C | N | O | P | 0 | 0 |
| | | | 623 | 280 | 120 | 194 | 29 | | |

- Molecule 31 is a protein called Nascent chain.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 31 | Z | 36 | Total | C | N | O | 0 | 0 |
| | | | 187 | 112 | 37 | 38 | | |

- Molecule 32 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | a | 285 | Total | C | N | O | S | 0 | 0 |
| | | | 2225 | 1385 | 437 | 397 | 6 | | |

- Molecule 33 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | b | 231 | Total | C | N | O | S | 0 | 0 |
| | | | 1778 | 1129 | 320 | 322 | 7 | | |

- Molecule 34 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | c | 211 | Total | C | N | O | S | 0 | 0 |
| | | | 1654 | 1053 | 299 | 299 | 3 | | |

- Molecule 35 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | d | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1416 | 910 | 251 | 251 | 4 | | |

- Molecule 36 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 36 | e | 176 | Total | C | N | O | 0 | 0 |
| | | | 1396 | 899 | 247 | 250 | | |

- Molecule 37 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | f | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 780 | 212 | 215 | 3 | | |

- Molecule 38 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | g | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 951 | 606 | 165 | 177 | 3 | | |

- Molecule 39 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | h | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 959 | 616 | 160 | 177 | 6 | | |

- Molecule 40 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | i | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1164 | 737 | 213 | 209 | 5 | | |

- Molecule 41 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | j | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 944 | 595 | 178 | 167 | 4 | | |

- Molecule 42 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | k | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1170 | 741 | 228 | 200 | 1 | | |

- Molecule 43 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | l | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1079 | 694 | 196 | 182 | 7 | | |

- Molecule 44 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | m | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 958 | 609 | 175 | 171 | 3 | | |

- Molecule 45 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | n | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 918 | 573 | 181 | 162 | 2 | | |

- Molecule 46 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | o | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 966 | 609 | 186 | 170 | 1 | | |

- Molecule 47 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | p | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 981 | 624 | 194 | 161 | 2 | | |

- Molecule 48 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | q | 99 | Total | C | N | O | S | 0 | 0 |
| | | | 811 | 525 | 148 | 134 | 4 | | |

- Molecule 49 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | r | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1091 | 677 | 212 | 195 | 7 | | |

- Molecule 50 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | s | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 740 | 486 | 125 | 128 | 1 | | |

- Molecule 51 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | t | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 871 | 550 | 166 | 152 | 3 | | |

- Molecule 52 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | u | 101 | Total | C | N | O | S | 0 | 0 |
| | | | 786 | 498 | 148 | 139 | 1 | | |

- Molecule 53 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | v | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 520 | 320 | 109 | 90 | 1 | | |

- Molecule 54 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 54 | w | 110 | Total<br>906 | C<br>576 | N<br>168 | O<br>162 | 0 | 0 |

- Molecule 55 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | x | 89 | Total<br>708 | C<br>449 | N<br>124 | O<br>131 | S<br>4 | 0 | 0 |

- Molecule 56 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | y | 56 | Total<br>452 | C<br>274 | N<br>98 | O<br>75 | S<br>5 | 0 | 0 |

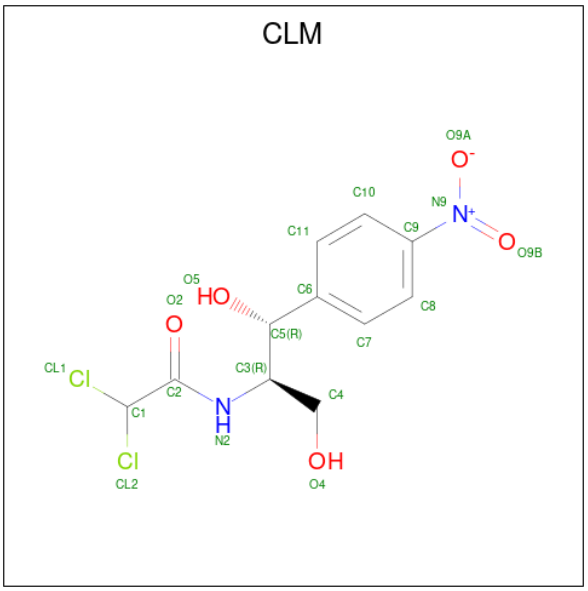
- Molecule 57 is a protein called 50S ribosomal protein L33 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | z | 50 | Total<br>408 | C<br>255 | N<br>81 | O<br>68 | S<br>4 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 58 | 2 | 1 | Total<br>1 | Zn<br>1 | 0 |
| 58 | M | 1 | Total<br>1 | Zn<br>1 | 0 |
| 58 | Q | 1 | Total<br>1 | Zn<br>1 | 0 |
| 58 | x | 1 | Total<br>1 | Zn<br>1 | 0 |
| 58 | y | 1 | Total<br>1 | Zn<br>1 | 0 |
| 58 | z | 1 | Total<br>1 | Zn<br>1 | 0 |

- Molecule 59 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 59 | 3 | 1 | Total | C | Cl | N | O | 0 |
| | | | 20 | 11 | 2 | 2 | 5 | |

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 60 | 3 | 1 | Total | K | 0 |
| | | | 1 | 1 | |

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 61 | 3 | 206 | Total | Mg | 0 |
| | | | 206 | 206 | |
| 61 | 4 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 61 | 5 | 90 | Total | Mg | 0 |
| | | | 90 | 90 | |
| 61 | 6 | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 61 | K | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 61 | P | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 61 | Y | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

*Continued on next page...*

*Continued from previous page...*

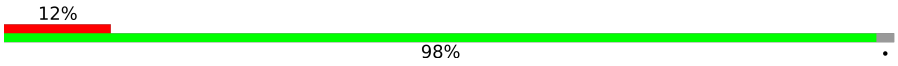
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 61 | b | 2 | Total Mg<br>2 2 | 0 |
| 61 | i | 1 | Total Mg<br>1 1 | 0 |
| 61 | k | 2 | Total Mg<br>2 2 | 0 |
| 61 | y | 2 | Total Mg<br>2 2 | 0 |

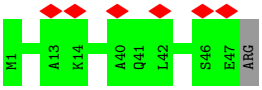
# 3 Residue-property plots (i)

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

• Molecule 1: 50S ribosomal protein L34

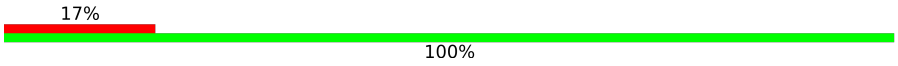
Chain 0:

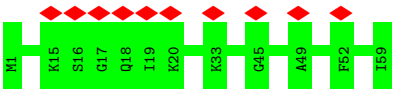



• Molecule 2: 50S ribosomal protein L35

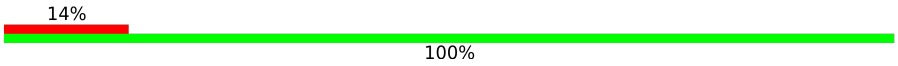
Chain 1:

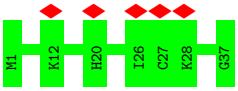



• Molecule 3: 50S ribosomal protein L36

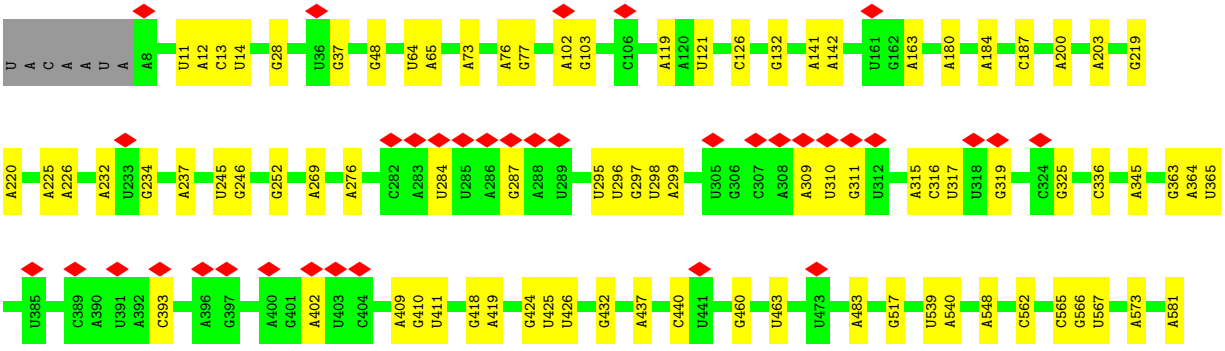
Chain 2:

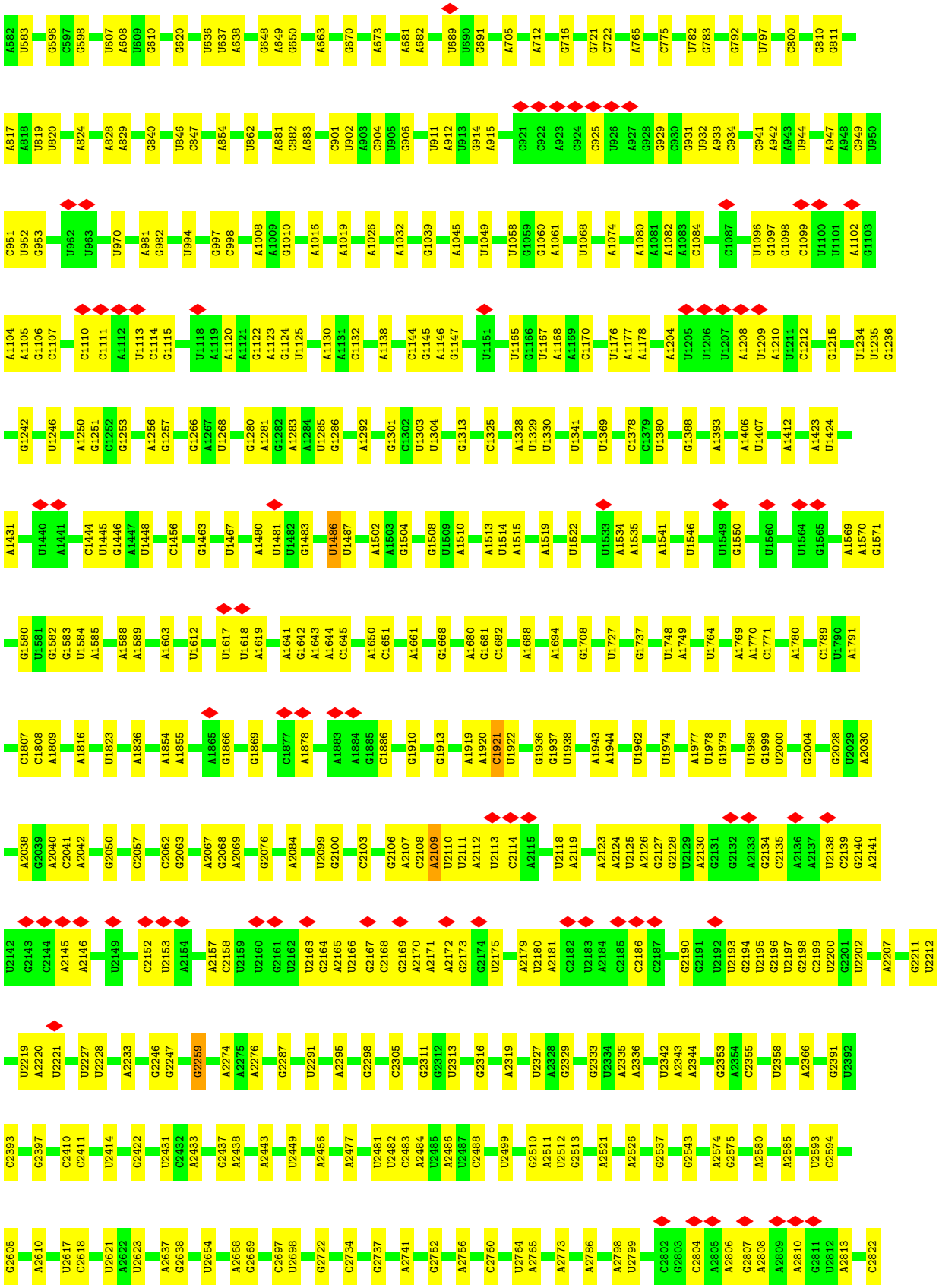


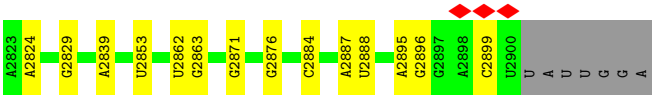




• Molecule 4: 23S ribosomal RNA

Chain 3:

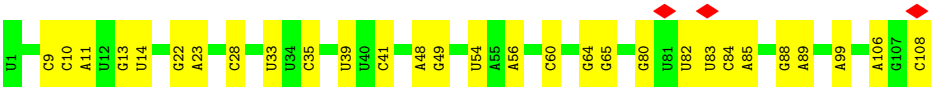







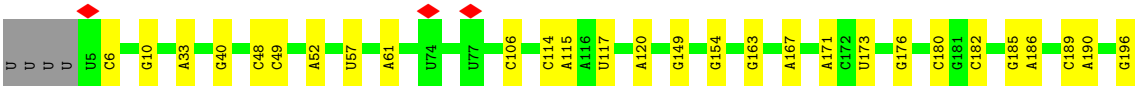

• Molecule 5: 5S ribosomal RNA

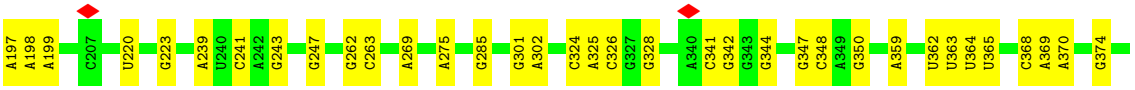
Chain 4:

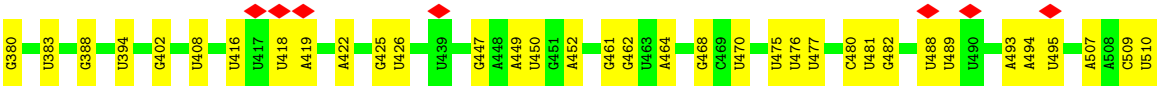




• Molecule 6: 16S ribosomal RNA

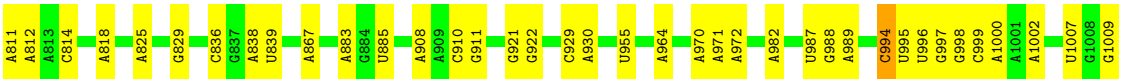
Chain 5:

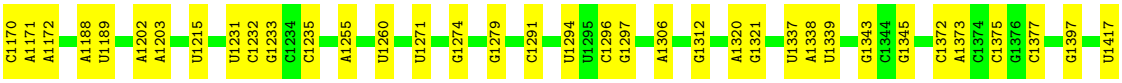



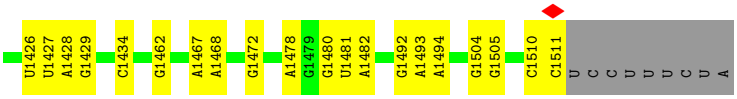







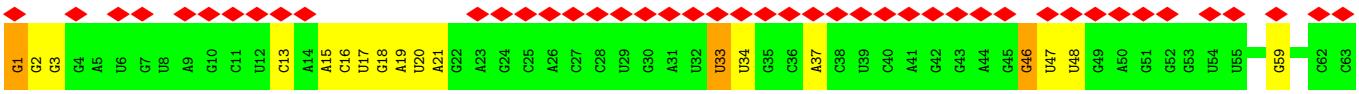


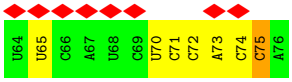



• Molecule 7: tRNA-Ala (E-site)

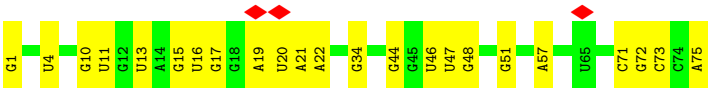
Chain 6:



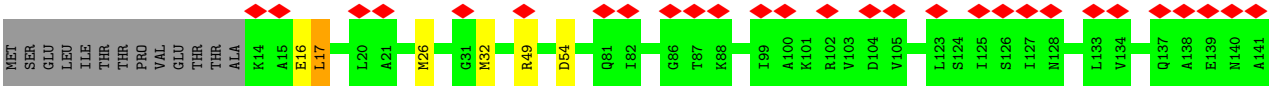

• Molecule 8: tRNA-Asp (P-site)

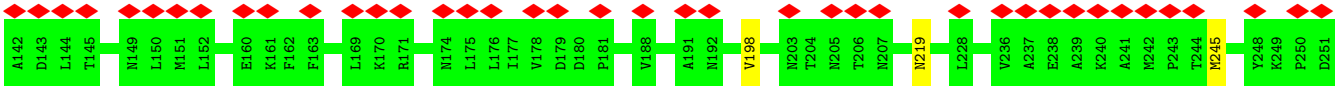
Chain 7:

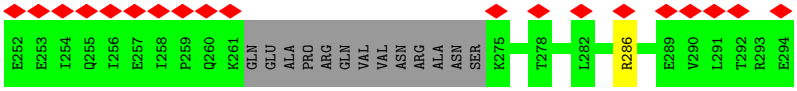




• Molecule 9: 30S ribosomal protein S2

Chain A:

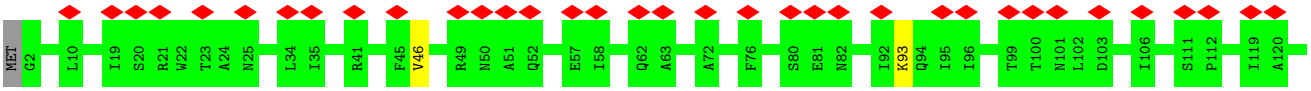



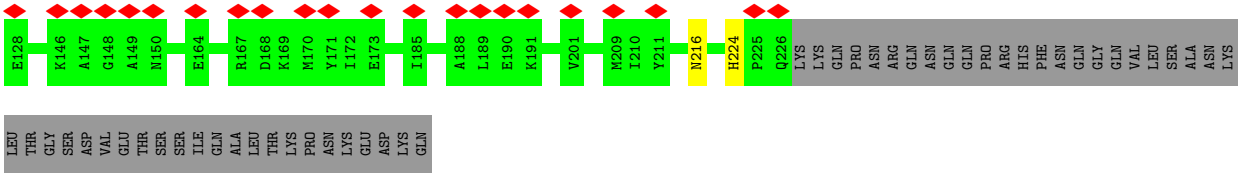




• Molecule 10: 30S ribosomal protein S3

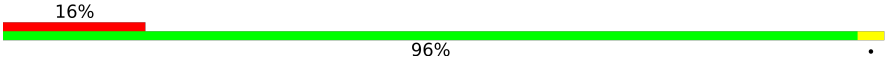
Chain B:

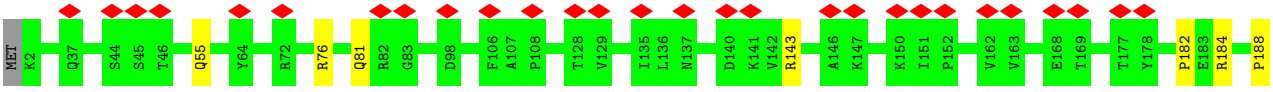



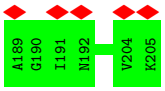




• Molecule 11: 30S ribosomal protein S4

Chain C:

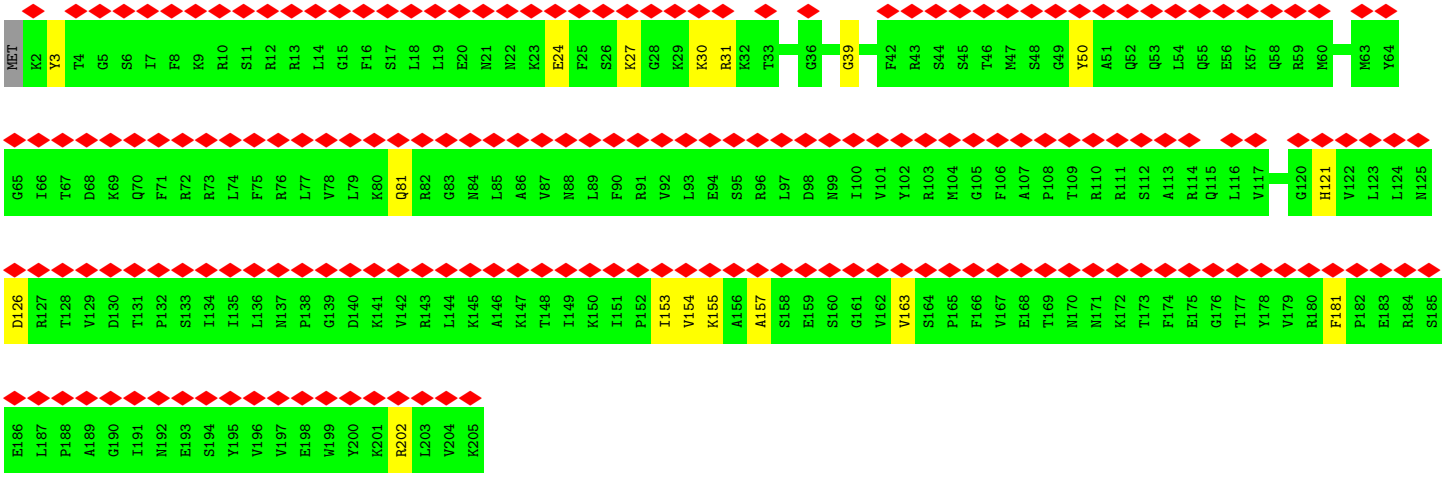


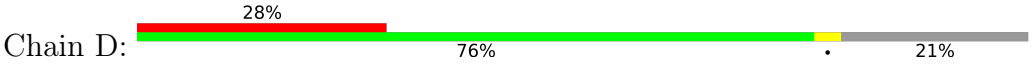
• Molecule 11: 30S ribosomal protein S4

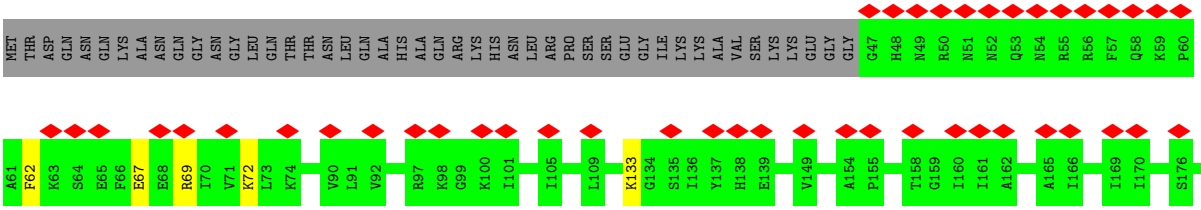
Chain U:


• Molecule 12: 30S ribosomal protein S5

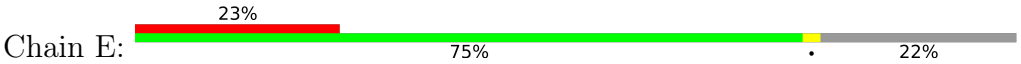
Chain D:

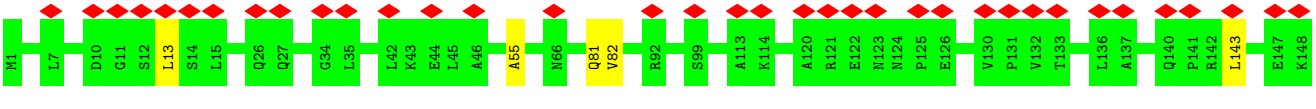



• Molecule 13: 30S ribosomal protein S6

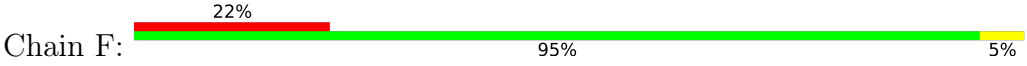
Chain E:

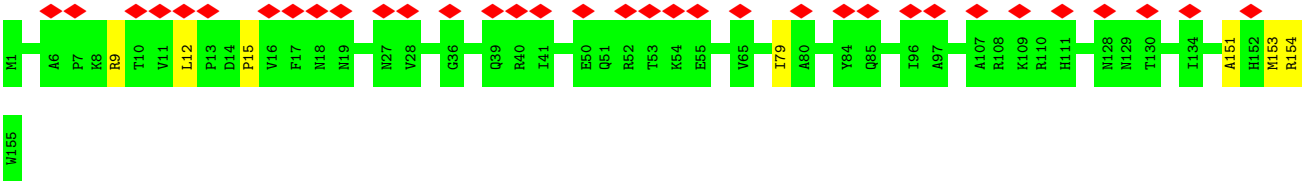



• Molecule 14: 30S ribosomal protein S7

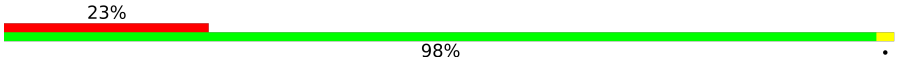
Chain F:

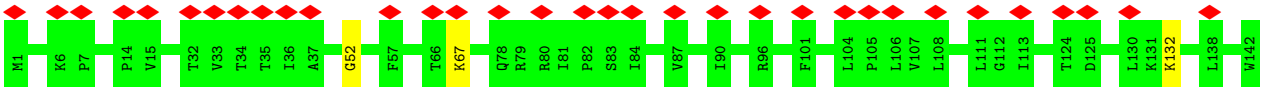





• Molecule 15: 30S ribosomal protein S8

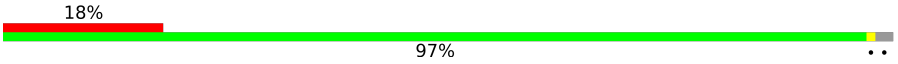
Chain G:

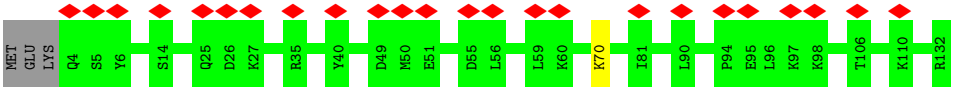



• Molecule 16: 30S ribosomal protein S9

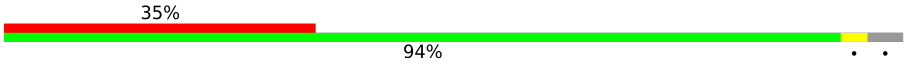
Chain H:

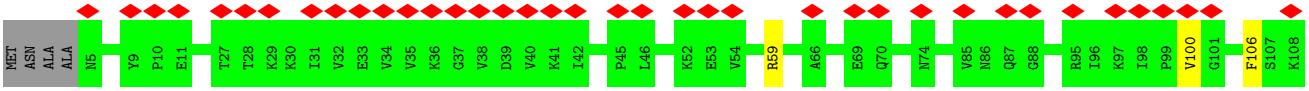



• Molecule 17: 30S ribosomal protein S10

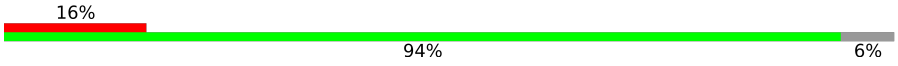
Chain I:

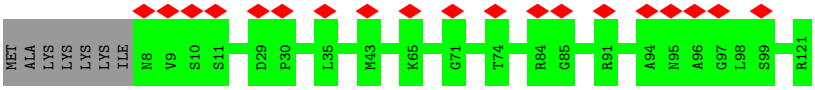



• Molecule 18: 30S ribosomal protein S11

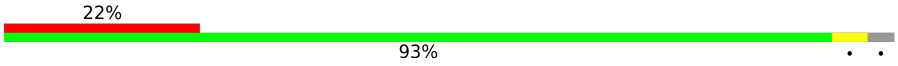
Chain J:

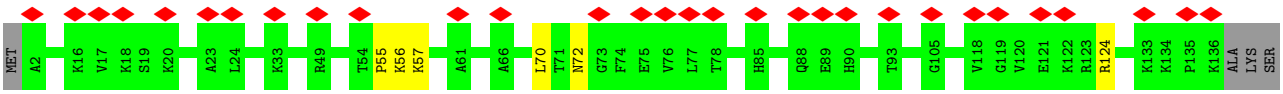



• Molecule 19: 30S ribosomal protein S12

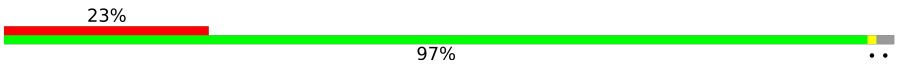
Chain K:

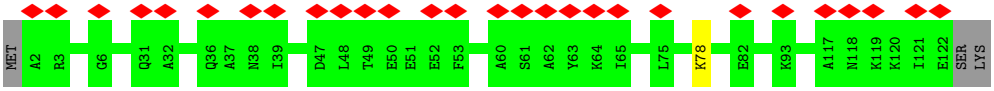


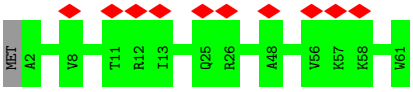

• Molecule 20: 30S ribosomal protein S13

Chain L:

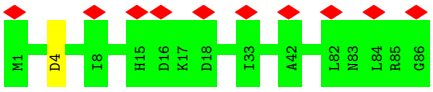




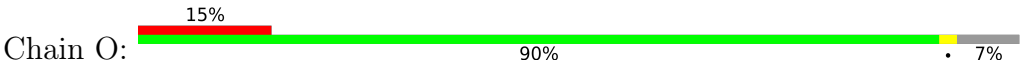

• Molecule 21: 30S ribosomal protein S14 type Z

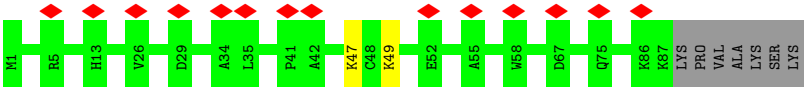




• Molecule 22: 30S ribosomal protein S15

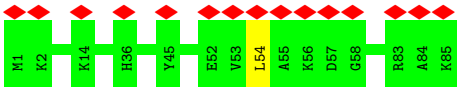




• Molecule 23: 30S ribosomal protein S16

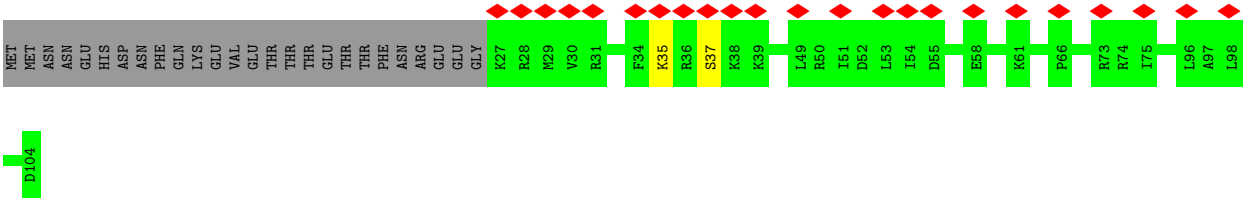


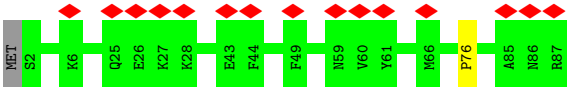

• Molecule 24: 30S ribosomal protein S17


• Molecule 25: 30S ribosomal protein S18

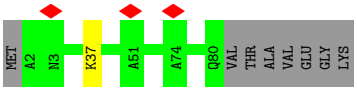




• Molecule 26: 30S ribosomal protein S19



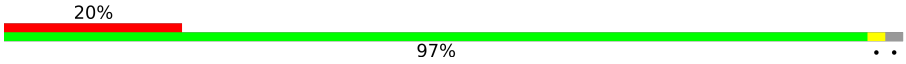

• Molecule 27: 30S ribosomal protein S20

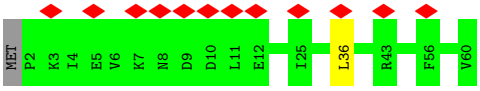
Chain S:


• Molecule 28: 30S ribosomal protein S21

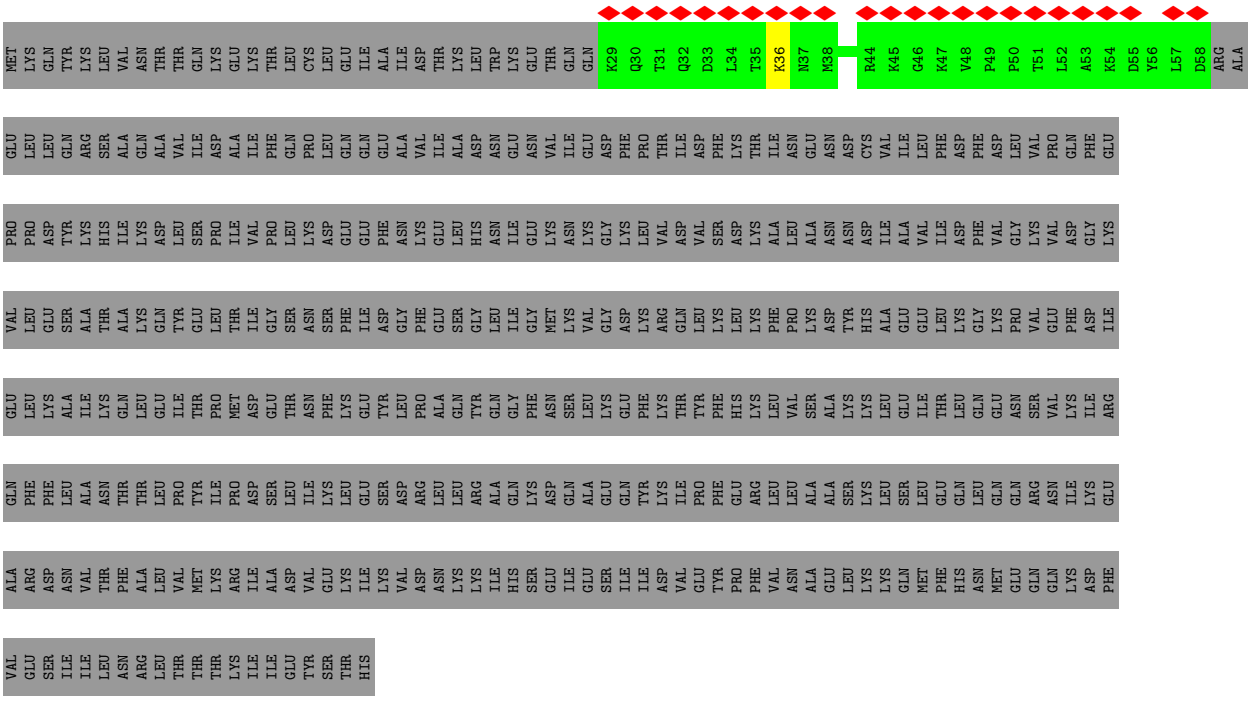
Chain T:



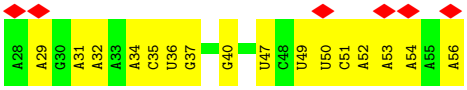

• Molecule 29: Trigger factor

Chain X:

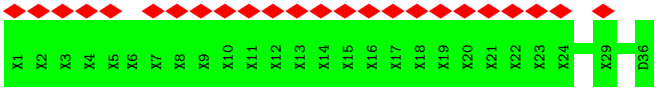

• Molecule 30: mRNA

Chain Y:

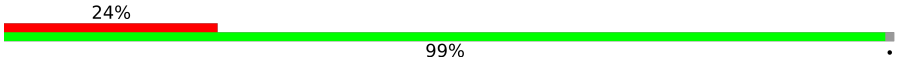
• Molecule 31: Nascent chain

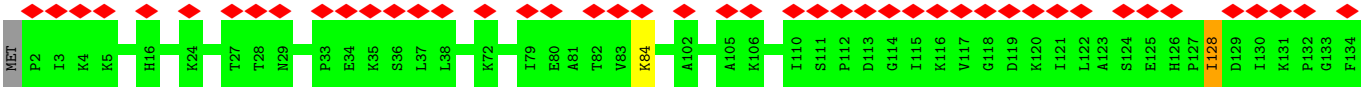
Chain Z:

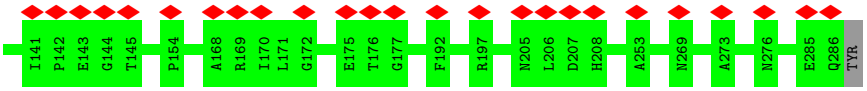




• Molecule 32: 50S ribosomal protein L2

Chain a:

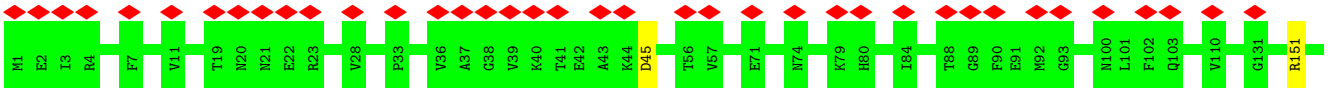


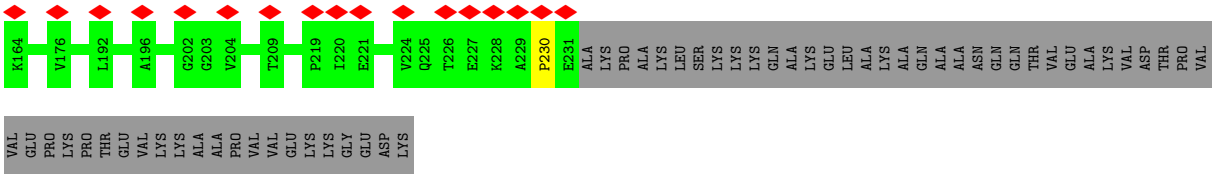




• Molecule 33: 50S ribosomal protein L3

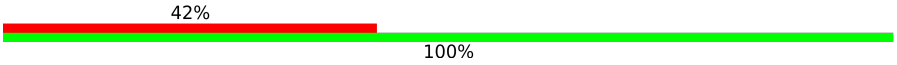
Chain b:

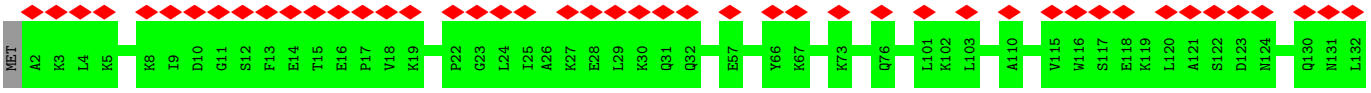



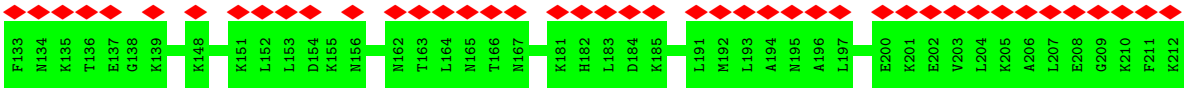




• Molecule 34: 50S ribosomal protein L4

Chain c:

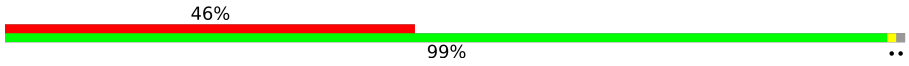


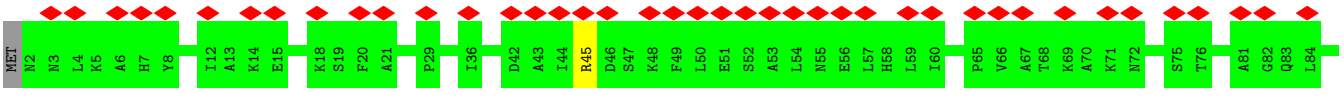



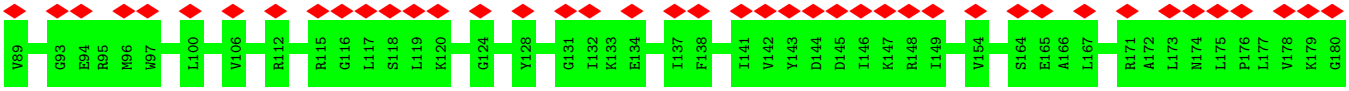




• Molecule 35: 50S ribosomal protein L5

Chain d:

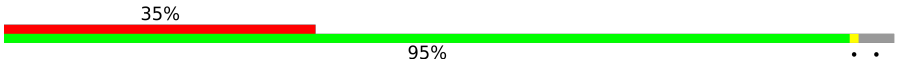


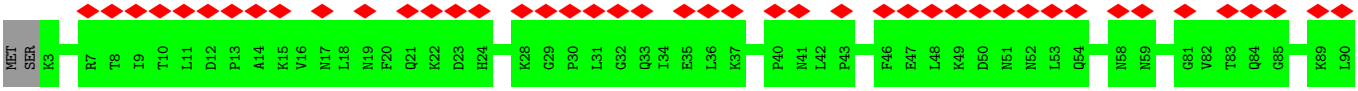



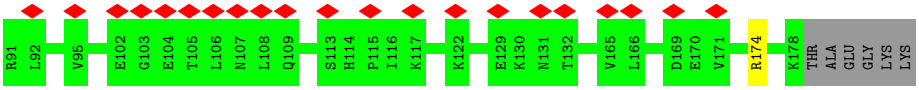



• Molecule 36: 50S ribosomal protein L6

Chain e:

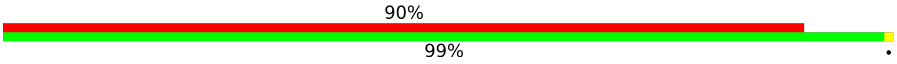


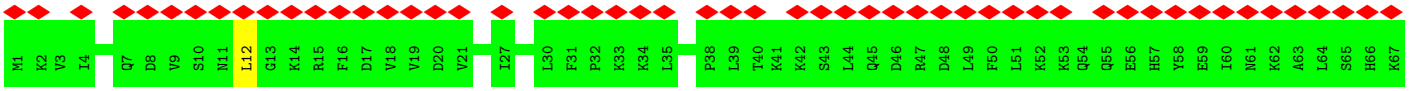



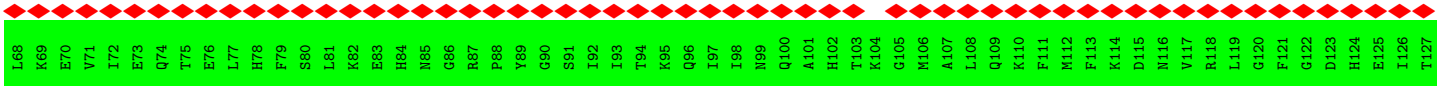



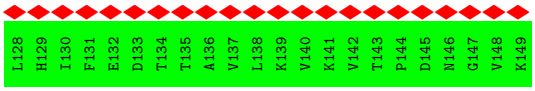

• Molecule 37: 50S ribosomal protein L9

Chain f:



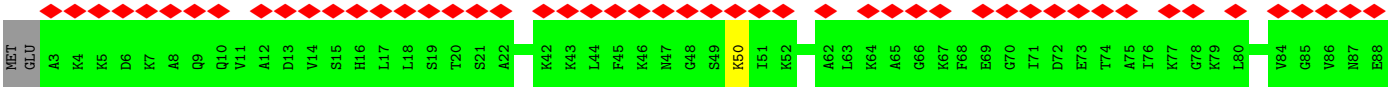



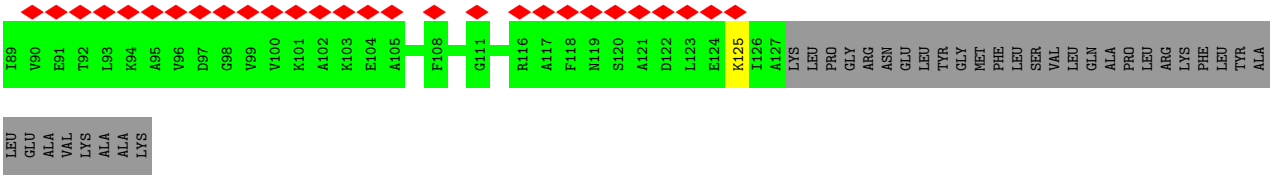




• Molecule 38: 50S ribosomal protein L10

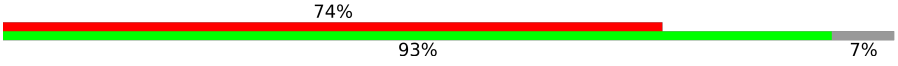
Chain g:

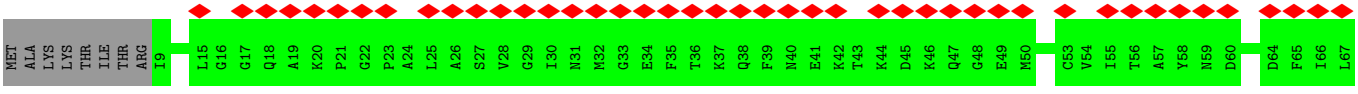



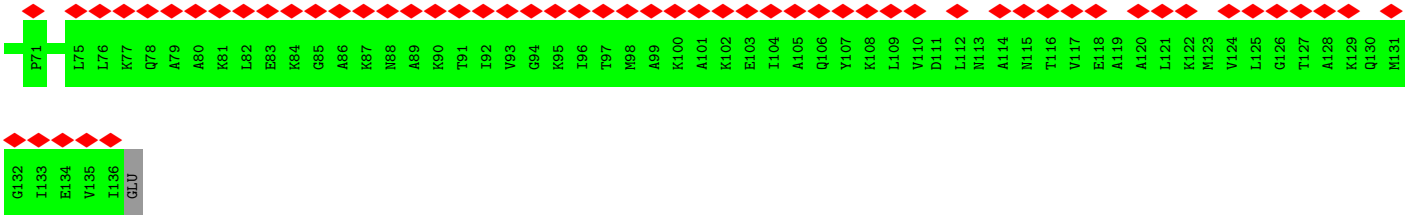




• Molecule 39: 50S ribosomal protein L11

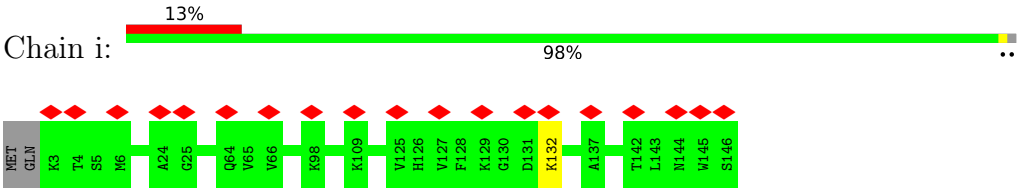
Chain h:



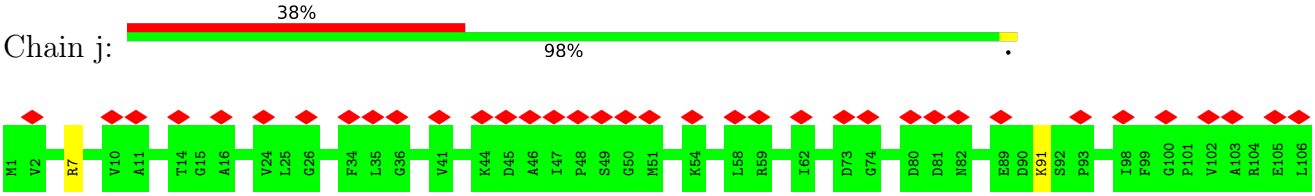





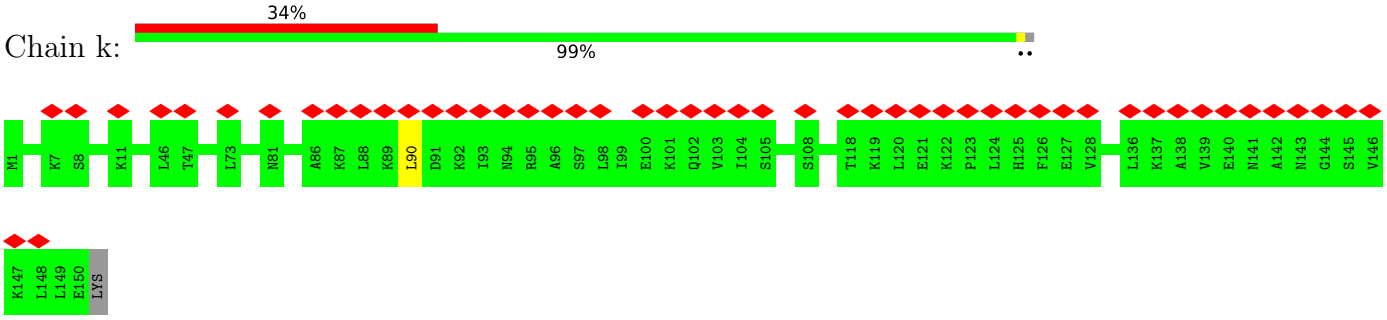

• Molecule 40: 50S ribosomal protein L13



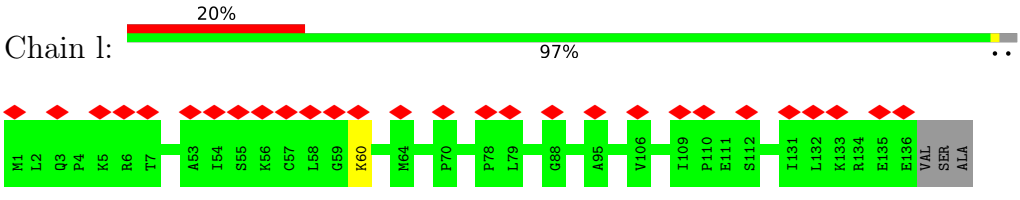

• Molecule 41: 50S ribosomal protein L14



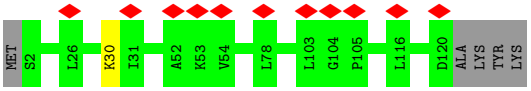

• Molecule 42: 50S ribosomal protein L15



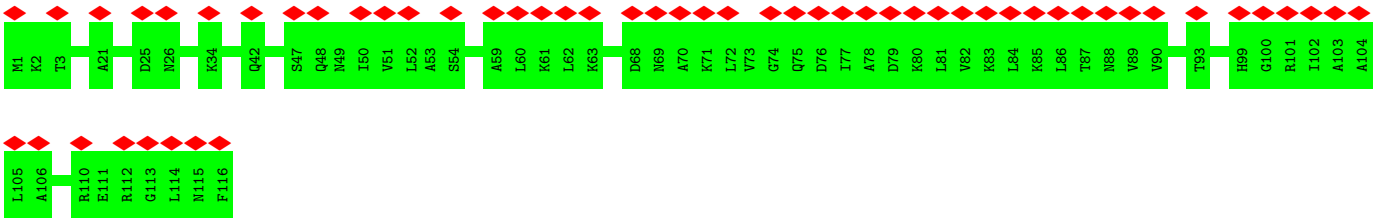

• Molecule 43: 50S ribosomal protein L16



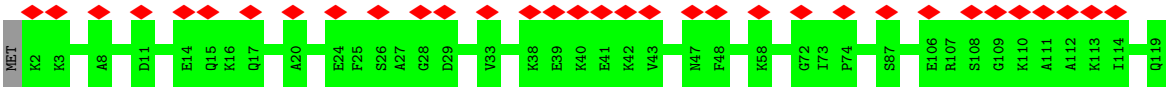

• Molecule 44: 50S ribosomal protein L17



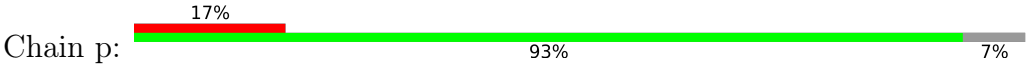

• Molecule 45: 50S ribosomal protein L18

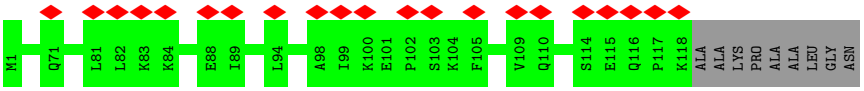




• Molecule 46: 50S ribosomal protein L19

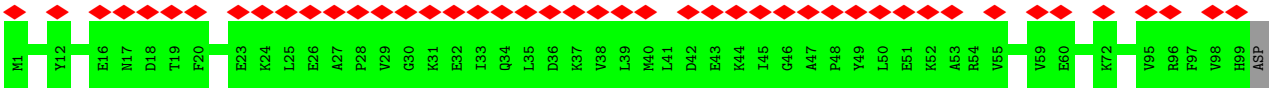




• Molecule 47: 50S ribosomal protein L20

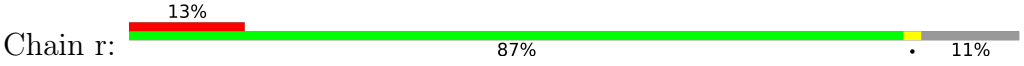


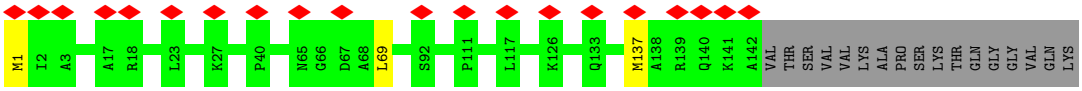




• Molecule 48: 50S ribosomal protein L21

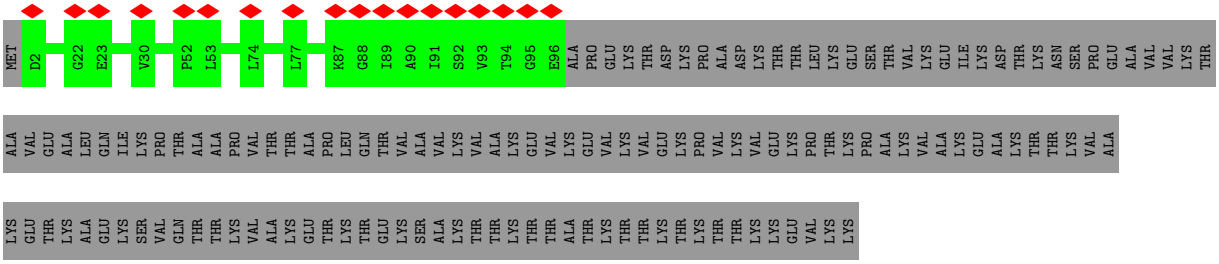




• Molecule 49: 50S ribosomal protein L22



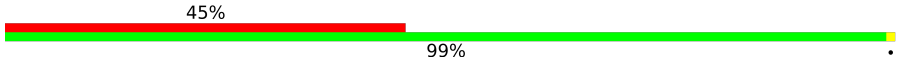



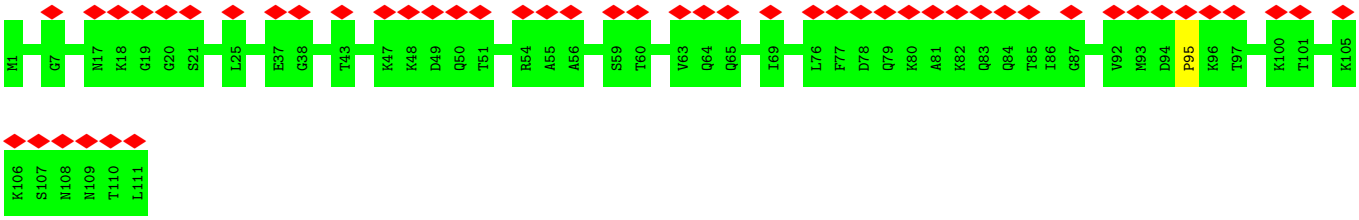

• Molecule 50: 50S ribosomal protein L23




• Molecule 51: 50S ribosomal protein L24

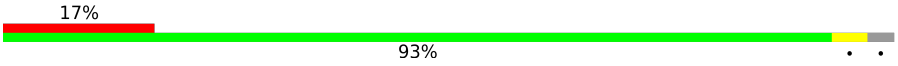
Chain t:

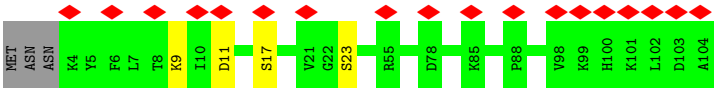



• Molecule 52: 50S ribosomal protein L27

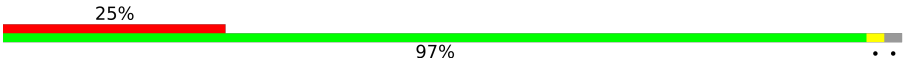
Chain u:

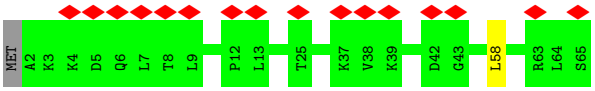



• Molecule 53: 50S ribosomal protein L28

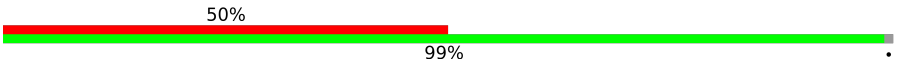
Chain v:

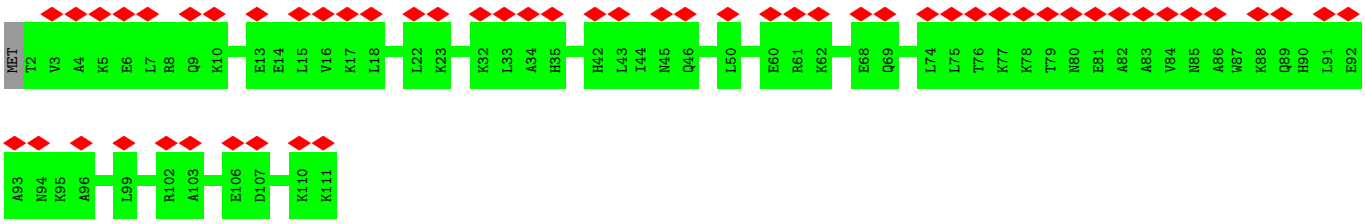



• Molecule 54: 50S ribosomal protein L29

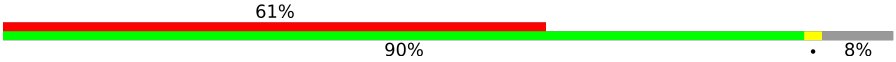
Chain w:

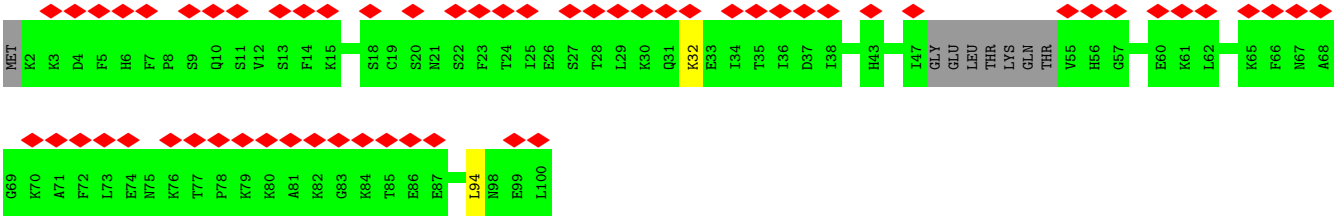


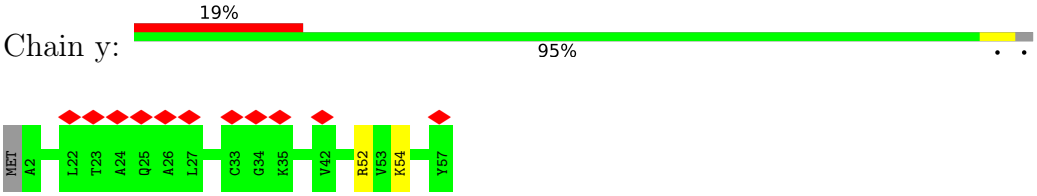

• Molecule 55: 50S ribosomal protein L31

Chain x:

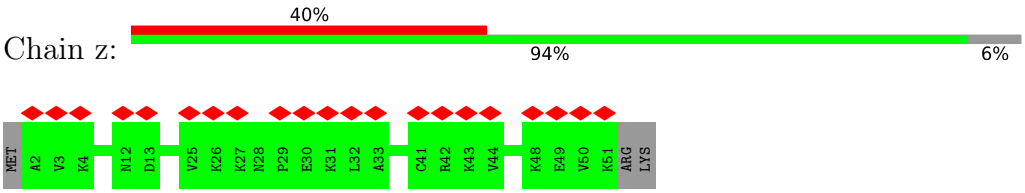





• Molecule 56: 50S ribosomal protein L32




• Molecule 57: 50S ribosomal protein L33 1



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of subtomograms used | 963 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 137 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3250 | Depositor |
| Magnification | 64000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 5.477 | Depositor |
| Minimum map value | -2.425 | Depositor |
| Average map value | 0.022 | Depositor |
| Map value standard deviation | 0.237 | Depositor |
| Recommended contour level | 1.2 | Depositor |
| Map size (Å) | 793.6, 793.6, 793.6 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 3.1, 3.1, 3.1 | 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, 7MG, K, B8T, OMG, MG, 5MC, CLM, 2MA, MA6, 1MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 0 | 0.25 | 0/383 | 0.61 | 0/504 |
| 2 | 1 | 0.25 | 0/484 | 0.53 | 0/637 |
| 3 | 2 | 0.27 | 0/306 | 0.68 | 0/401 |
| 4 | 3 | 0.18 | 0/69363 | 0.73 | 9/108161 (0.0%) |
| 5 | 4 | 0.15 | 0/2578 | 0.72 | 0/4016 |
| 6 | 5 | 0.18 | 0/35992 | 0.72 | 5/56111 (0.0%) |
| 7 | 6 | 0.34 | 1/1810 (0.1%) | 0.86 | 3/2817 (0.1%) |
| 8 | 7 | 0.40 | 2/1785 (0.1%) | 0.77 | 0/2779 |
| 9 | A | 0.31 | 0/2186 | 0.67 | 4/2952 (0.1%) |
| 10 | B | 0.28 | 0/1800 | 0.62 | 1/2433 (0.0%) |
| 11 | C | 0.34 | 0/1700 | 0.72 | 0/2278 |
| 11 | U | 0.34 | 0/1700 | 0.78 | 0/2278 |
| 12 | D | 0.30 | 0/1365 | 0.66 | 0/1827 |
| 13 | E | 0.28 | 0/1384 | 0.71 | 2/1867 (0.1%) |
| 14 | F | 0.29 | 0/1274 | 0.66 | 0/1710 |
| 15 | G | 0.31 | 0/1134 | 0.69 | 1/1527 (0.1%) |
| 16 | H | 0.28 | 0/1056 | 0.65 | 0/1409 |
| 17 | I | 0.30 | 0/843 | 0.69 | 2/1132 (0.2%) |
| 18 | J | 0.27 | 0/844 | 0.57 | 0/1136 |
| 19 | K | 0.26 | 0/1089 | 0.63 | 0/1461 |
| 20 | L | 0.28 | 0/986 | 0.67 | 0/1321 |
| 21 | M | 0.35 | 0/483 | 0.69 | 0/643 |
| 22 | N | 0.24 | 0/703 | 0.61 | 0/936 |
| 23 | O | 0.32 | 0/718 | 0.76 | 0/962 |
| 24 | P | 0.25 | 0/702 | 0.62 | 0/934 |
| 25 | Q | 0.27 | 0/663 | 0.69 | 0/883 |
| 26 | R | 0.30 | 0/716 | 0.61 | 1/958 (0.1%) |
| 27 | S | 0.26 | 0/645 | 0.55 | 0/857 |
| 28 | T | 0.30 | 0/524 | 0.79 | 1/685 (0.1%) |
| 29 | X | 0.28 | 0/245 | 0.72 | 0/325 |
| 30 | Y | 0.29 | 0/699 | 0.90 | 0/1087 |
| 31 | Z | 0.74 | 0/26 | 1.33 | 0/33 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 32 | a | 0.26 | 0/2267 | 0.61 | 1/3044 (0.0%) |
| 33 | b | 0.29 | 0/1812 | 0.63 | 1/2436 (0.0%) |
| 34 | c | 0.27 | 0/1681 | 0.57 | 0/2257 |
| 35 | d | 0.27 | 0/1437 | 0.61 | 0/1931 |
| 36 | e | 0.30 | 0/1420 | 0.60 | 0/1912 |
| 37 | f | 0.27 | 0/1233 | 0.59 | 0/1653 |
| 38 | g | 0.28 | 0/960 | 0.56 | 0/1284 |
| 39 | h | 0.25 | 0/968 | 0.54 | 0/1298 |
| 40 | i | 0.26 | 0/1186 | 0.58 | 0/1592 |
| 41 | j | 0.29 | 0/953 | 0.68 | 0/1275 |
| 42 | k | 0.26 | 0/1187 | 0.62 | 1/1581 (0.1%) |
| 43 | l | 0.30 | 0/1104 | 0.61 | 0/1481 |
| 44 | m | 0.27 | 0/973 | 0.58 | 0/1309 |
| 45 | n | 0.25 | 0/927 | 0.61 | 0/1239 |
| 46 | o | 0.29 | 0/976 | 0.65 | 0/1296 |
| 47 | p | 0.25 | 0/996 | 0.55 | 0/1325 |
| 48 | q | 0.30 | 0/828 | 0.64 | 0/1111 |
| 49 | r | 0.27 | 0/1100 | 0.67 | 3/1471 (0.2%) |
| 50 | s | 0.26 | 0/752 | 0.53 | 0/1015 |
| 51 | t | 0.30 | 0/878 | 0.69 | 1/1165 (0.1%) |
| 52 | u | 0.25 | 0/798 | 0.58 | 0/1063 |
| 53 | v | 0.30 | 0/526 | 0.82 | 1/703 (0.1%) |
| 54 | w | 0.23 | 0/916 | 0.50 | 0/1222 |
| 55 | x | 0.30 | 0/722 | 0.71 | 2/959 (0.2%) |
| 56 | y | 0.27 | 0/457 | 0.74 | 1/601 (0.2%) |
| 57 | z | 0.26 | 0/412 | 0.59 | 0/547 |
| All | All | 0.22 | 3/163655 (0.0%) | 0.71 | 40/243830 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 11 | U | 0 | 2 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | 6 | 1 | G | OP3-P | -10.58 | 1.48 | 1.61 |
| 8 | 7 | 1 | G | OP3-P | -10.54 | 1.48 | 1.61 |
| 8 | 7 | 72 | G | O3'-P | -8.01 | 1.51 | 1.61 |

The worst 5 of 40 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | 3 | 2109 | A | O5'-P-OP2 | -10.18 | 96.54 | 105.70 |
| 6 | 5 | 1434 | C | P-O3'-C3' | -9.93 | 107.79 | 119.70 |
| 53 | v | 58 | LEU | CA-CB-CG | 8.88 | 135.72 | 115.30 |
| 55 | x | 94 | LEU | CA-CB-CG | 7.74 | 133.10 | 115.30 |
| 4 | 3 | 393 | C | C6-N1-C2 | -7.29 | 117.38 | 120.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 11 | U | 121 | HIS | Peptide |
| 11 | U | 153 | ILE | Peptide |

## 5.2 Too-close contacts (i)

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

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | 0 | 45/48 (94%) | 45 (100%) | 0 | 0 | 100 100 |
| 2 | 1 | 57/59 (97%) | 57 (100%) | 0 | 0 | 100 100 |
| 3 | 2 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 100 |
| 9 | A | 264/294 (90%) | 233 (88%) | 25 (10%) | 6 (2%) | 5 28 |
| 10 | B | 223/273 (82%) | 197 (88%) | 24 (11%) | 2 (1%) | 14 52 |
| 11 | C | 202/205 (98%) | 166 (82%) | 33 (16%) | 3 (2%) | 8 40 |
| 11 | U | 202/205 (98%) | 148 (73%) | 41 (20%) | 13 (6%) | 1 13 |
| 12 | D | 171/219 (78%) | 141 (82%) | 25 (15%) | 5 (3%) | 3 23 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 13 | E | 165/215 (77%) | 142 (86%) | 18 (11%) | 5 (3%) | 3 23 |
| 14 | F | 153/155 (99%) | 132 (86%) | 15 (10%) | 6 (4%) | 2 19 |
| 15 | G | 140/142 (99%) | 132 (94%) | 8 (6%) | 0 | 100 100 |
| 16 | H | 127/132 (96%) | 115 (91%) | 12 (9%) | 0 | 100 100 |
| 17 | I | 102/108 (94%) | 88 (86%) | 13 (13%) | 1 (1%) | 13 49 |
| 18 | J | 112/121 (93%) | 105 (94%) | 7 (6%) | 0 | 100 100 |
| 19 | K | 133/139 (96%) | 113 (85%) | 15 (11%) | 5 (4%) | 2 19 |
| 20 | L | 119/124 (96%) | 112 (94%) | 7 (6%) | 0 | 100 100 |
| 21 | M | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 100 |
| 22 | N | 84/86 (98%) | 77 (92%) | 6 (7%) | 1 (1%) | 11 44 |
| 23 | O | 85/94 (90%) | 78 (92%) | 5 (6%) | 2 (2%) | 5 27 |
| 24 | P | 83/85 (98%) | 71 (86%) | 11 (13%) | 1 (1%) | 11 44 |
| 25 | Q | 76/104 (73%) | 65 (86%) | 9 (12%) | 2 (3%) | 4 26 |
| 26 | R | 84/87 (97%) | 79 (94%) | 5 (6%) | 0 | 100 100 |
| 27 | S | 77/87 (88%) | 74 (96%) | 2 (3%) | 1 (1%) | 10 43 |
| 28 | T | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 100 |
| 29 | X | 28/444 (6%) | 24 (86%) | 4 (14%) | 0 | 100 100 |
| 31 | Z | 3/36 (8%) | 3 (100%) | 0 | 0 | 100 100 |
| 32 | a | 283/287 (99%) | 267 (94%) | 15 (5%) | 1 (0%) | 30 68 |
| 33 | b | 229/287 (80%) | 219 (96%) | 9 (4%) | 1 (0%) | 30 68 |
| 34 | c | 209/212 (99%) | 198 (95%) | 11 (5%) | 0 | 100 100 |
| 35 | d | 177/180 (98%) | 169 (96%) | 8 (4%) | 0 | 100 100 |
| 36 | e | 174/184 (95%) | 162 (93%) | 12 (7%) | 0 | 100 100 |
| 37 | f | 147/149 (99%) | 131 (89%) | 15 (10%) | 1 (1%) | 19 57 |
| 38 | g | 123/161 (76%) | 117 (95%) | 6 (5%) | 0 | 100 100 |
| 39 | h | 126/137 (92%) | 121 (96%) | 5 (4%) | 0 | 100 100 |
| 40 | i | 142/146 (97%) | 133 (94%) | 9 (6%) | 0 | 100 100 |
| 41 | j | 120/122 (98%) | 115 (96%) | 5 (4%) | 0 | 100 100 |
| 42 | k | 148/151 (98%) | 138 (93%) | 10 (7%) | 0 | 100 100 |
| 43 | l | 134/139 (96%) | 132 (98%) | 2 (2%) | 0 | 100 100 |
| 44 | m | 117/124 (94%) | 112 (96%) | 5 (4%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 45 | n | 114/116 (98%) | 109 (96%) | 5 (4%) | 0 | 100 100 |
| 46 | o | 116/119 (98%) | 108 (93%) | 8 (7%) | 0 | 100 100 |
| 47 | p | 116/127 (91%) | 114 (98%) | 2 (2%) | 0 | 100 100 |
| 48 | q | 97/100 (97%) | 92 (95%) | 5 (5%) | 0 | 100 100 |
| 49 | r | 140/159 (88%) | 137 (98%) | 3 (2%) | 0 | 100 100 |
| 50 | s | 93/237 (39%) | 89 (96%) | 4 (4%) | 0 | 100 100 |
| 51 | t | 109/111 (98%) | 102 (94%) | 7 (6%) | 0 | 100 100 |
| 52 | u | 99/104 (95%) | 86 (87%) | 9 (9%) | 4 (4%) | 2 18 |
| 53 | v | 62/65 (95%) | 57 (92%) | 5 (8%) | 0 | 100 100 |
| 54 | w | 108/111 (97%) | 102 (94%) | 6 (6%) | 0 | 100 100 |
| 55 | x | 85/97 (88%) | 64 (75%) | 21 (25%) | 0 | 100 100 |
| 56 | y | 54/57 (95%) | 53 (98%) | 1 (2%) | 0 | 100 100 |
| 57 | z | 48/53 (91%) | 47 (98%) | 1 (2%) | 0 | 100 100 |
| All | All | 6255/7355 (85%) | 5717 (91%) | 478 (8%) | 60 (1%) | 16 49 |

5 of 60 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | D | 67 | GLU |
| 12 | D | 69 | ARG |
| 12 | D | 212 | ARG |
| 12 | D | 216 | LEU |
| 13 | E | 81 | GLN |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 0 | 40/41 (98%) | 40 (100%) | 0 | 100 100 |
| 2 | 1 | 51/51 (100%) | 51 (100%) | 0 | 100 100 |
| 3 | 2 | 35/35 (100%) | 35 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 9 | A | 239/262 (91%) | 238 (100%) | 1 (0%) | 89 91 |
| 10 | B | 188/232 (81%) | 187 (100%) | 1 (0%) | 86 89 |
| 11 | C | 182/183 (100%) | 178 (98%) | 4 (2%) | 47 65 |
| 11 | U | 182/183 (100%) | 180 (99%) | 2 (1%) | 70 80 |
| 12 | D | 141/178 (79%) | 139 (99%) | 2 (1%) | 62 75 |
| 13 | E | 150/196 (76%) | 150 (100%) | 0 | 100 100 |
| 14 | F | 132/132 (100%) | 131 (99%) | 1 (1%) | 79 85 |
| 15 | G | 124/124 (100%) | 122 (98%) | 2 (2%) | 58 73 |
| 16 | H | 112/115 (97%) | 111 (99%) | 1 (1%) | 75 83 |
| 17 | I | 97/99 (98%) | 96 (99%) | 1 (1%) | 73 82 |
| 18 | J | 91/97 (94%) | 91 (100%) | 0 | 100 100 |
| 19 | K | 117/120 (98%) | 116 (99%) | 1 (1%) | 75 83 |
| 20 | L | 102/105 (97%) | 101 (99%) | 1 (1%) | 73 82 |
| 21 | M | 47/48 (98%) | 47 (100%) | 0 | 100 100 |
| 22 | N | 78/78 (100%) | 78 (100%) | 0 | 100 100 |
| 23 | O | 76/82 (93%) | 76 (100%) | 0 | 100 100 |
| 24 | P | 75/75 (100%) | 75 (100%) | 0 | 100 100 |
| 25 | Q | 69/94 (73%) | 69 (100%) | 0 | 100 100 |
| 26 | R | 76/77 (99%) | 76 (100%) | 0 | 100 100 |
| 27 | S | 71/77 (92%) | 71 (100%) | 0 | 100 100 |
| 28 | T | 55/56 (98%) | 55 (100%) | 0 | 100 100 |
| 29 | X | 27/406 (7%) | 26 (96%) | 1 (4%) | 29 49 |
| 31 | Z | 2/2 (100%) | 2 (100%) | 0 | 100 100 |
| 32 | a | 241/243 (99%) | 240 (100%) | 1 (0%) | 89 91 |
| 33 | b | 188/233 (81%) | 187 (100%) | 1 (0%) | 86 89 |
| 34 | c | 183/184 (100%) | 183 (100%) | 0 | 100 100 |
| 35 | d | 153/154 (99%) | 152 (99%) | 1 (1%) | 81 87 |
| 36 | e | 153/159 (96%) | 152 (99%) | 1 (1%) | 81 87 |
| 37 | f | 134/134 (100%) | 134 (100%) | 0 | 100 100 |
| 38 | g | 100/129 (78%) | 98 (98%) | 2 (2%) | 50 68 |
| 39 | h | 102/110 (93%) | 102 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 40 | i | 126/128 (98%) | 125 (99%) | 1 (1%) | 79 85 |
| 41 | j | 103/103 (100%) | 101 (98%) | 2 (2%) | 52 69 |
| 42 | k | 125/126 (99%) | 125 (100%) | 0 | 100 100 |
| 43 | l | 113/115 (98%) | 112 (99%) | 1 (1%) | 75 83 |
| 44 | m | 105/109 (96%) | 104 (99%) | 1 (1%) | 73 82 |
| 45 | n | 99/99 (100%) | 99 (100%) | 0 | 100 100 |
| 46 | o | 104/105 (99%) | 104 (100%) | 0 | 100 100 |
| 47 | p | 104/108 (96%) | 104 (100%) | 0 | 100 100 |
| 48 | q | 90/91 (99%) | 90 (100%) | 0 | 100 100 |
| 49 | r | 118/132 (89%) | 118 (100%) | 0 | 100 100 |
| 50 | s | 84/208 (40%) | 84 (100%) | 0 | 100 100 |
| 51 | t | 96/96 (100%) | 96 (100%) | 0 | 100 100 |
| 52 | u | 82/85 (96%) | 82 (100%) | 0 | 100 100 |
| 53 | v | 59/60 (98%) | 59 (100%) | 0 | 100 100 |
| 54 | w | 97/98 (99%) | 97 (100%) | 0 | 100 100 |
| 55 | x | 79/86 (92%) | 78 (99%) | 1 (1%) | 65 77 |
| 56 | y | 48/49 (98%) | 47 (98%) | 1 (2%) | 48 66 |
| 57 | z | 47/50 (94%) | 47 (100%) | 0 | 100 100 |
| All | All | 5492/6342 (87%) | 5461 (99%) | 31 (1%) | 82 88 |

5 of 31 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | L | 78 | LYS |
| 43 | l | 60 | LYS |
| 29 | X | 36 | LYS |
| 55 | x | 32 | LYS |
| 40 | i | 132 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | d | 63 | GLN |
| 43 | l | 99 | GLN |
| 36 | e | 33 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | j | 18 | GLN |
| 45 | n | 49 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 30 | Y | 28/29 (96%) | 16 (57%) | 4 (14%) |
| 4 | 3 | 2891/2907 (99%) | 537 (18%) | 18 (0%) |
| 5 | 4 | 107/108 (99%) | 29 (27%) | 0 |
| 6 | 5 | 1503/1520 (98%) | 257 (17%) | 10 (0%) |
| 7 | 6 | 76/76 (100%) | 23 (30%) | 5 (6%) |
| 8 | 7 | 74/75 (98%) | 20 (27%) | 2 (2%) |
| All | All | 4679/4715 (99%) | 882 (18%) | 39 (0%) |

5 of 882 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | 3 | 11 | U |
| 4 | 3 | 12 | A |
| 4 | 3 | 13 | C |
| 4 | 3 | 14 | U |
| 4 | 3 | 28 | G |

5 of 39 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 6 | 1 | G |
| 30 | Y | 34 | A |
| 7 | 6 | 15 | A |
| 7 | 6 | 74 | C |
| 30 | Y | 49 | U |

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 4 | 1MG | 3 | 783 | 4 | 18,26,27 | 0.94 | 1 (5%) | 19,39,42 | 0.81 | 0 |
| 6 | 5MC | 5 | 1375 | 6 | 18,22,23 | 0.34 | 0 | 26,32,35 | 0.69 | 2 (7%) |
| 6 | B8T | 5 | 1377 | 6 | 19,22,23 | 4.71 | 13 (68%) | 26,31,34 | 0.97 | 1 (3%) |
| 6 | MA6 | 5 | 1494 | 6 | 18,26,27 | 1.06 | 2 (11%) | 19,38,41 | 3.37 | 3 (15%) |
| 4 | 2MA | 3 | 2511 | 61,4 | 17,25,26 | 6.17 | 10 (58%) | 17,37,40 | 1.54 | 3 (17%) |
| 6 | 7MG | 5 | 525 | 6 | 22,26,27 | 3.89 | 10 (45%) | 29,39,42 | 2.03 | 9 (31%) |
| 4 | OMG | 3 | 2259 | 8,4 | 18,26,27 | 0.99 | 2 (11%) | 19,38,41 | 0.71 | 0 |
| 6 | MA6 | 5 | 1493 | 6 | 18,26,27 | 1.06 | 2 (11%) | 19,38,41 | 3.31 | 3 (15%) |

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 |
|---|---|---|---|---|---|---|---|
| 4 | 1MG | 3 | 783 | 4 | - | 0/3/25/26 | 0/3/3/3 |
| 6 | 5MC | 5 | 1375 | 6 | - | 0/7/25/26 | 0/2/2/2 |
| 6 | B8T | 5 | 1377 | 6 | - | 0/7/27/28 | 0/2/2/2 |
| 6 | MA6 | 5 | 1494 | 6 | - | 2/7/29/30 | 0/3/3/3 |
| 4 | 2MA | 3 | 2511 | 61,4 | - | 2/3/25/26 | 0/3/3/3 |
| 6 | 7MG | 5 | 525 | 6 | - | 2/7/37/38 | 0/3/3/3 |
| 4 | OMG | 3 | 2259 | 8,4 | - | 3/5/27/28 | 0/3/3/3 |
| 6 | MA6 | 5 | 1493 | 6 | - | 0/7/29/30 | 0/3/3/3 |

The worst 5 of 40 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | 3 | 2511 | 2MA | C2'-C1' | -15.49 | 1.30 | 1.53 |
| 4 | 3 | 2511 | 2MA | O4'-C1' | 15.36 | 1.62 | 1.41 |
| 6 | 5 | 525 | 7MG | C8-N9 | 9.90 | 1.51 | 1.46 |
| 6 | 5 | 1377 | B8T | O4'-C1' | 8.89 | 1.63 | 1.42 |
| 4 | 3 | 2511 | 2MA | C2-N3 | 7.94 | 1.48 | 1.31 |

The worst 5 of 21 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | 5 | 1494 | MA6 | N1-C6-N6 | -12.24 | 104.18 | 117.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | 5 | 1493 | MA6 | N1-C6-N6 | -11.86 | 104.57 | 117.06 |
| 6 | 5 | 1494 | MA6 | N3-C2-N1 | -5.64 | 119.86 | 128.68 |
| 6 | 5 | 1493 | MA6 | C1'-N9-C4 | 5.54 | 136.38 | 126.64 |
| 6 | 5 | 1493 | MA6 | N3-C2-N1 | -5.54 | 120.02 | 128.68 |

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | 3 | 2259 | OMG | C1'-C2'-O2'-CM2 |
| 6 | 5 | 525 | 7MG | O4'-C4'-C5'-O5' |
| 6 | 5 | 525 | 7MG | C3'-C4'-C5'-O5' |
| 6 | 5 | 1494 | MA6 | O4'-C4'-C5'-O5' |
| 6 | 5 | 1494 | MA6 | C3'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 316 ligands modelled in this entry, 315 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 59 | CLM | 3 | 3001 | - | 19,20,20 | 2.08 | 2 (10%) | 23,27,27 | 0.84 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 59 | CLM | 3 | 3001 | - | - | 2/20/22/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 59 | 3 | 3001 | CLM | C2-N2 | 7.25 | 1.50 | 1.34 |
| 59 | 3 | 3001 | CLM | O9B-N9 | -2.65 | 1.18 | 1.22 |

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

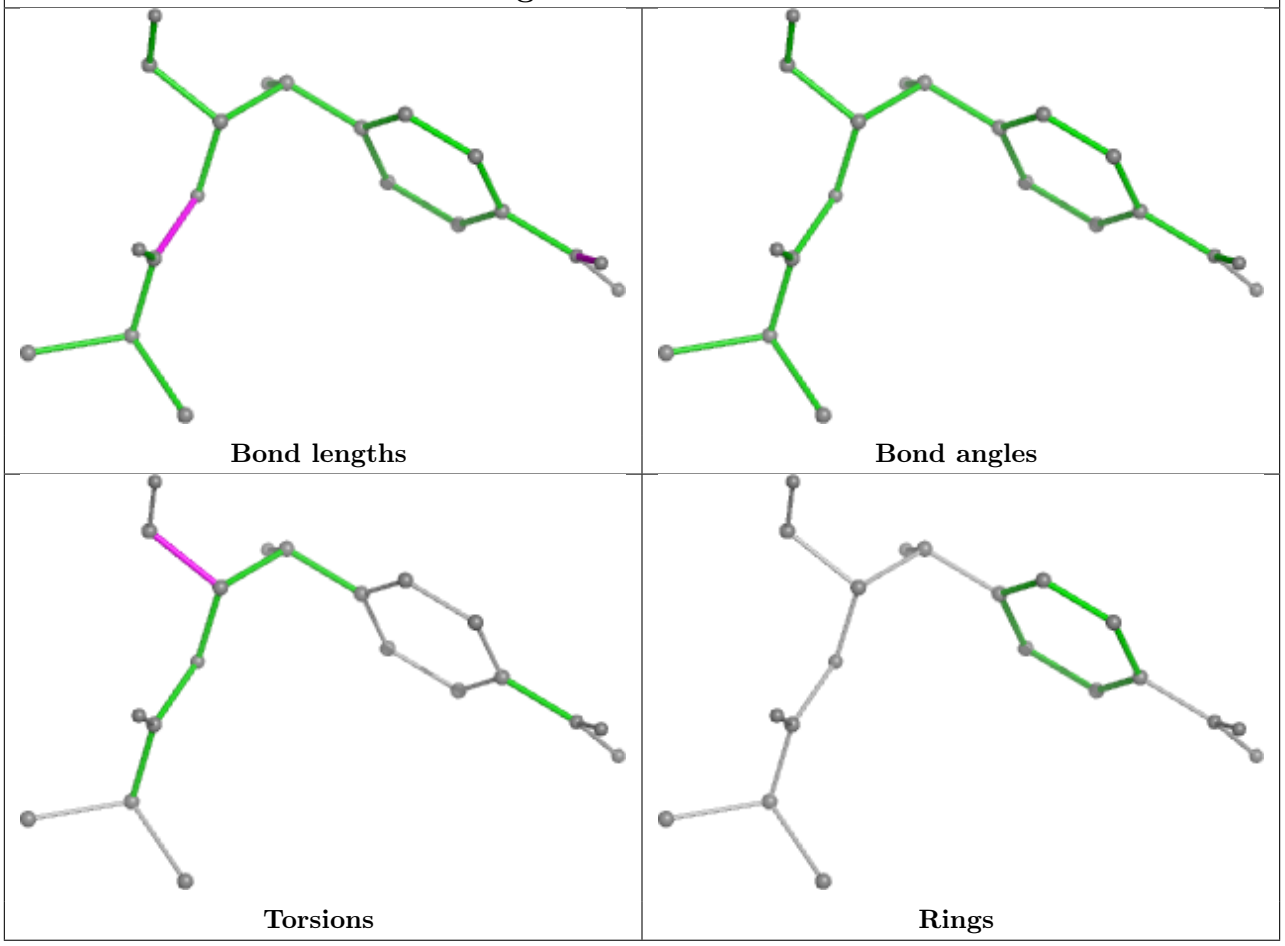
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | 3 | 3001 | CLM | C5-C3-C4-O4 |
| 59 | 3 | 3001 | CLM | N2-C3-C4-O4 |

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 CLM 3 3001**




## 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.

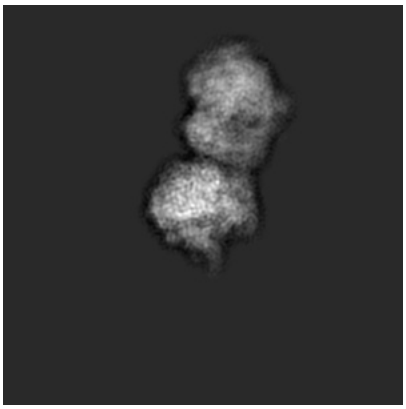
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17145. These allow visual inspection of the internal detail of the map and identification of artifacts.

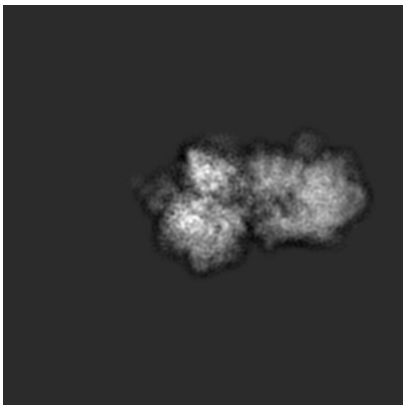
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

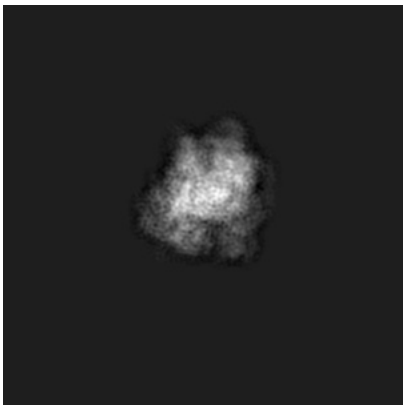
### 6.1.1 Primary map



X

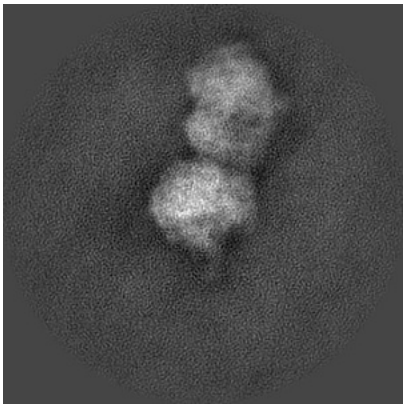


Y

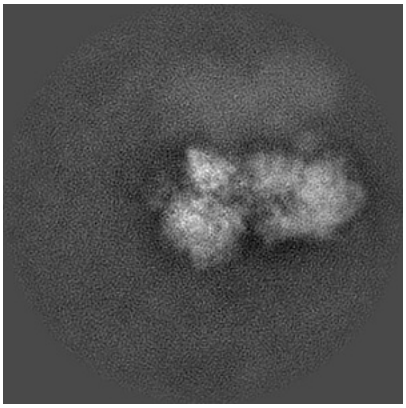


Z

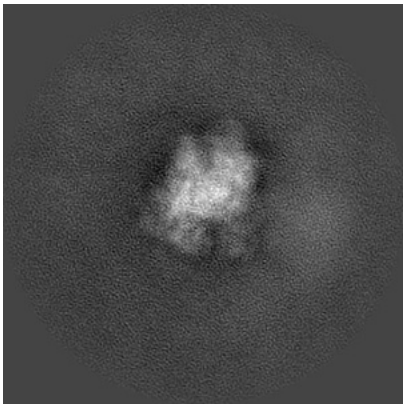
### 6.1.2 Raw map



X



Y

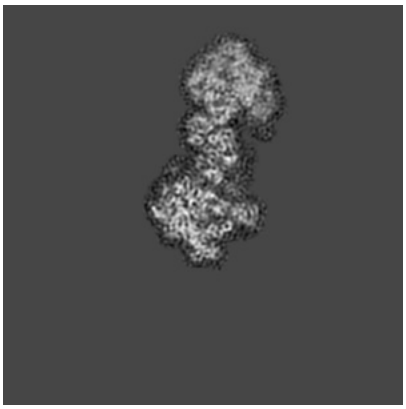


Z

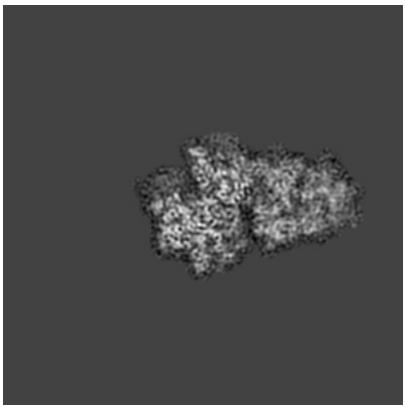
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

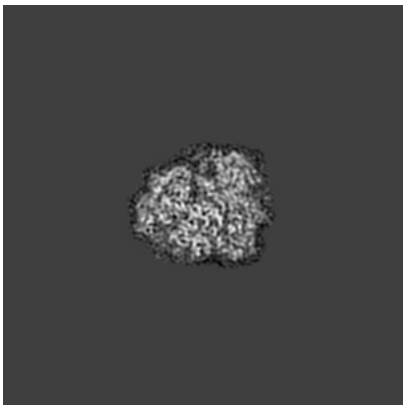
### 6.2.1 Primary map



X Index: 128

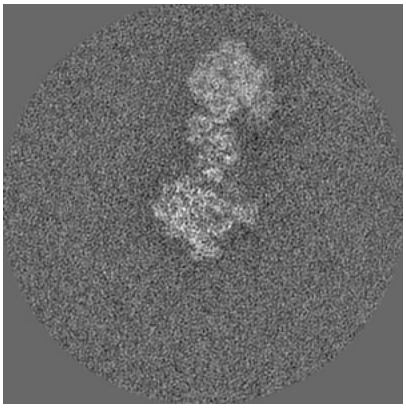


Y Index: 128

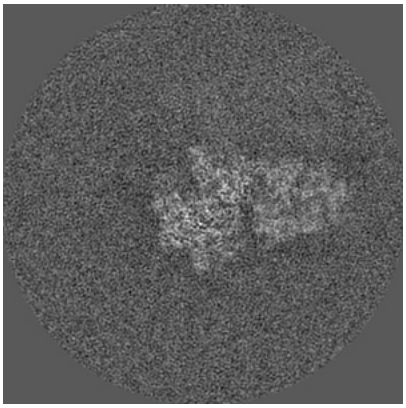


Z Index: 128

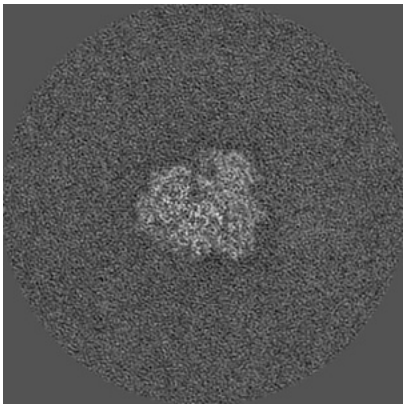
### 6.2.2 Raw map



X Index: 128



Y Index: 128

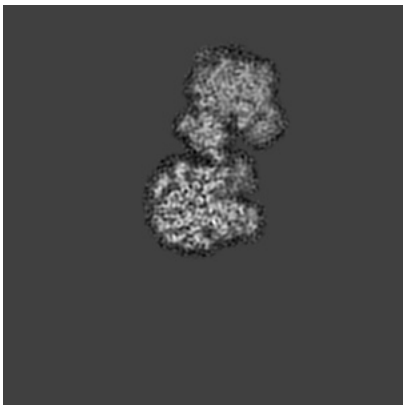


Z Index: 128

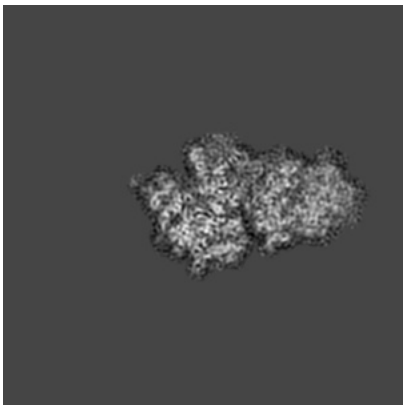
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

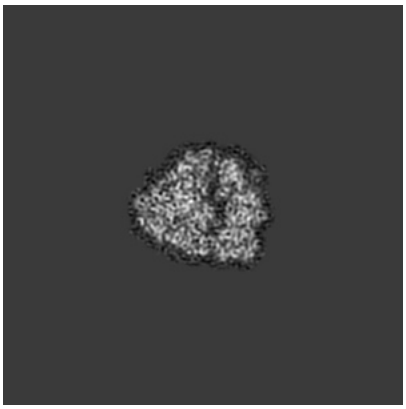
### 6.3.1 Primary map



X Index: 117

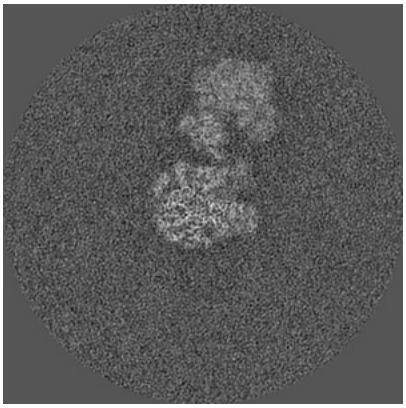


Y Index: 131

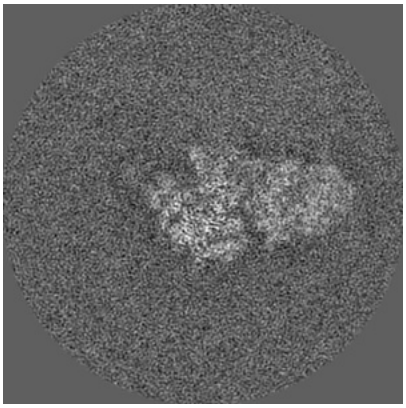


Z Index: 124

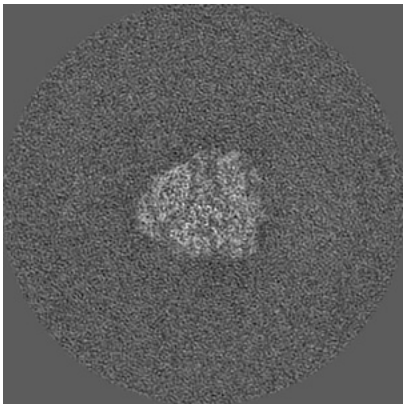
### 6.3.2 Raw map



X Index: 117



Y Index: 131

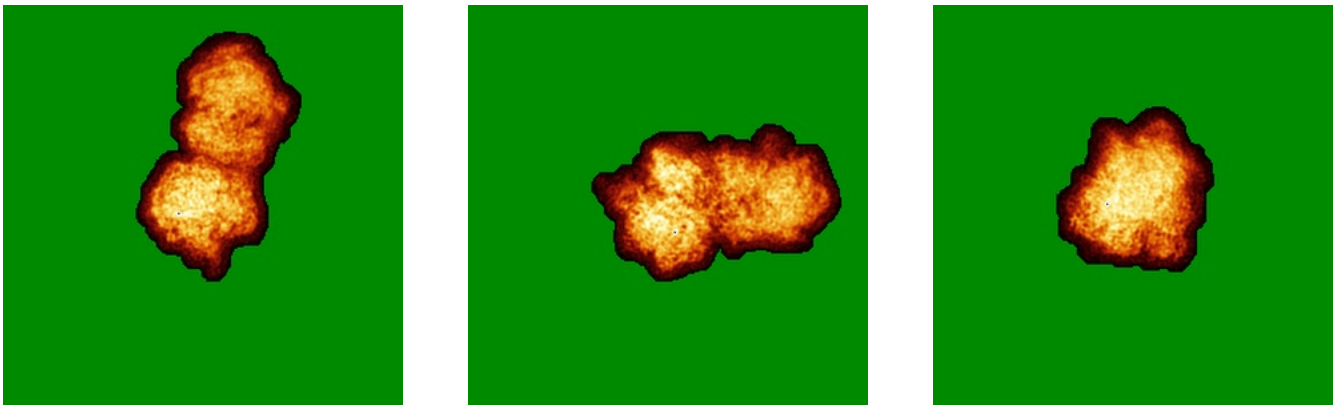


Z Index: 127

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

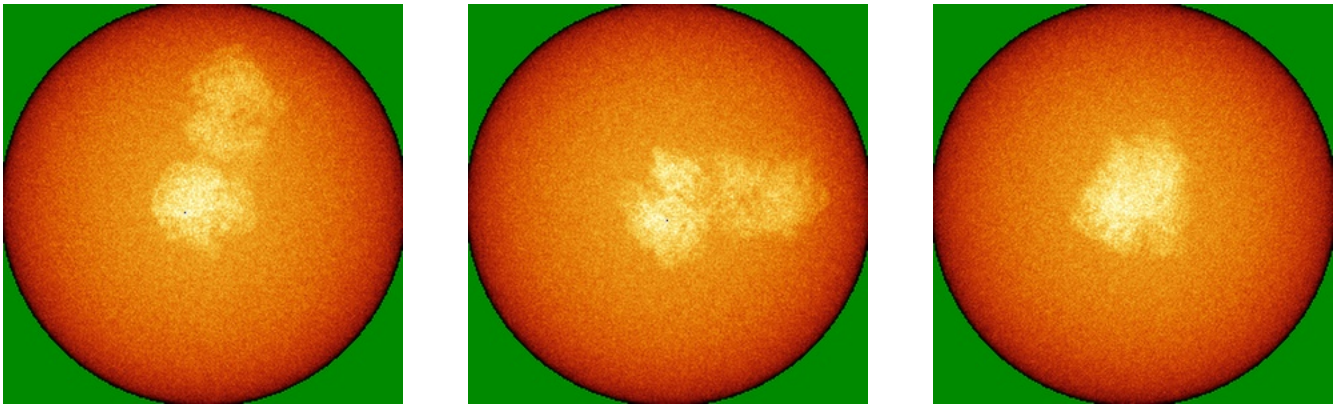
## 6.4 Orthogonal standard-deviation projections (False-color) (i)

### 6.4.1 Primary map



X Y Z

### 6.4.2 Raw map

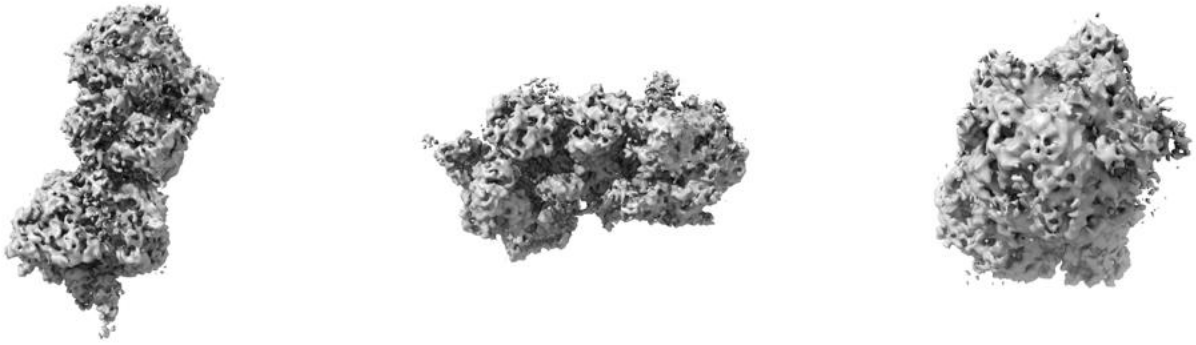


X Y Z

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)

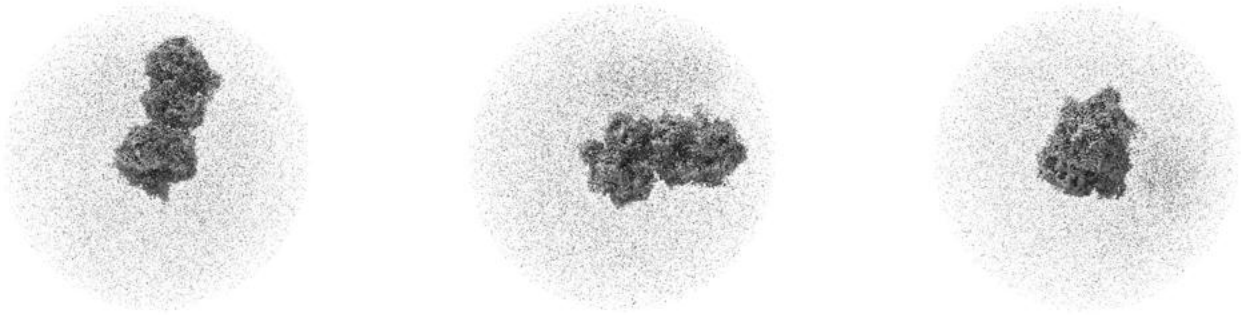
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.2. 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



X Y Z

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

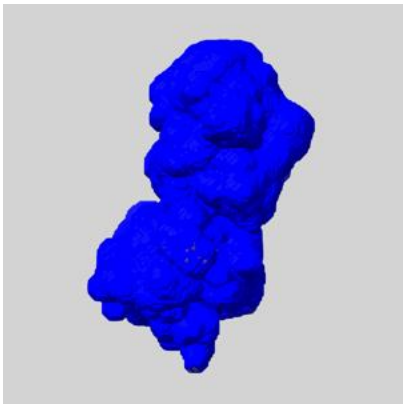
## 6.6 Mask visualisation (i)

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

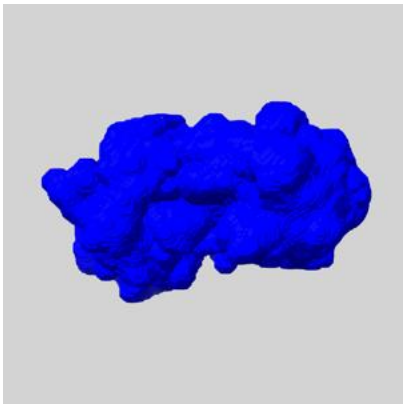
A mask typically either:

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

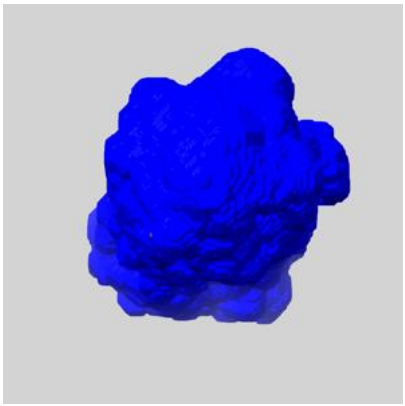
### 6.6.1 emd_17145_msk_1.map (i)



X



Y

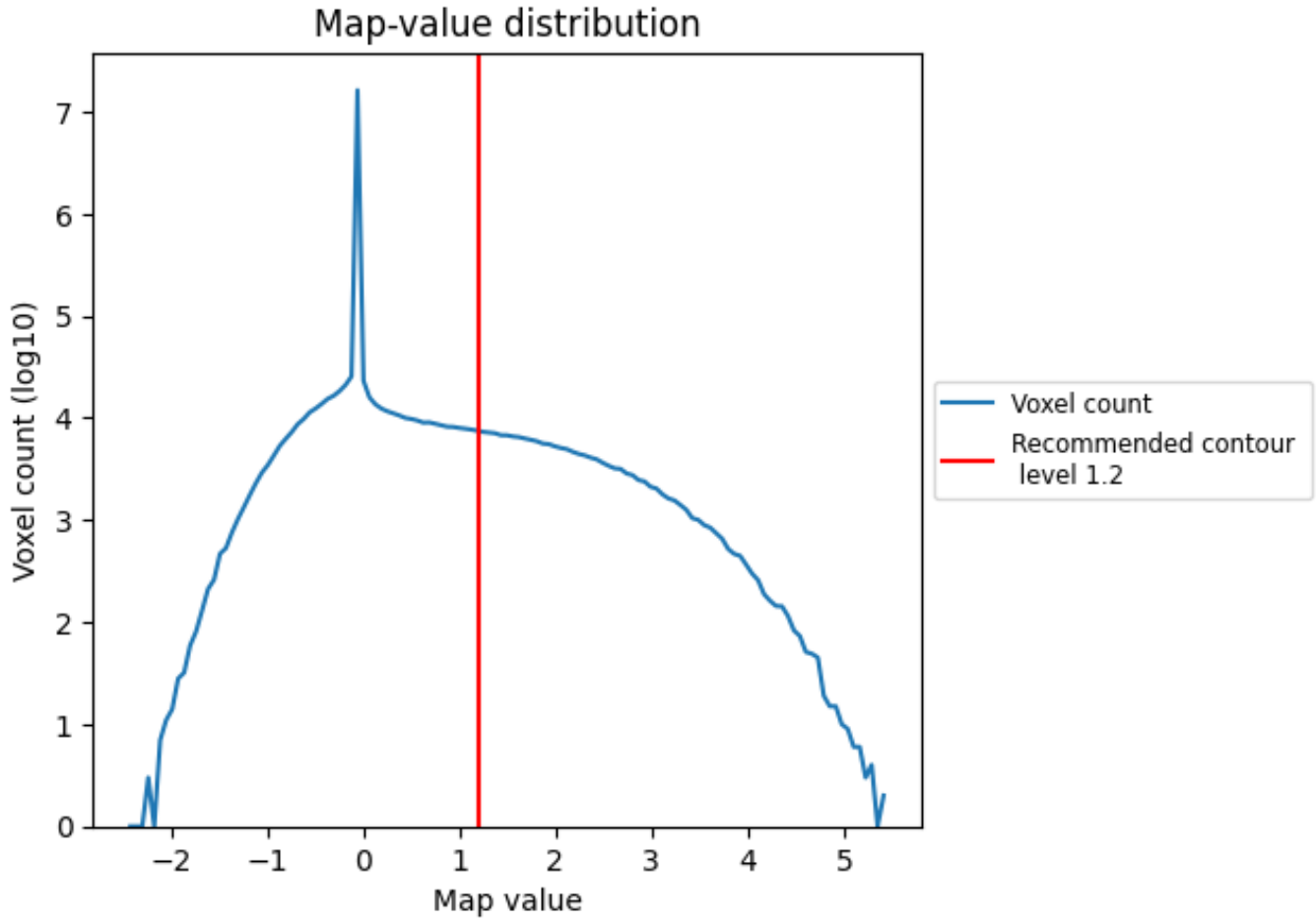


Z

# 7 Map analysis

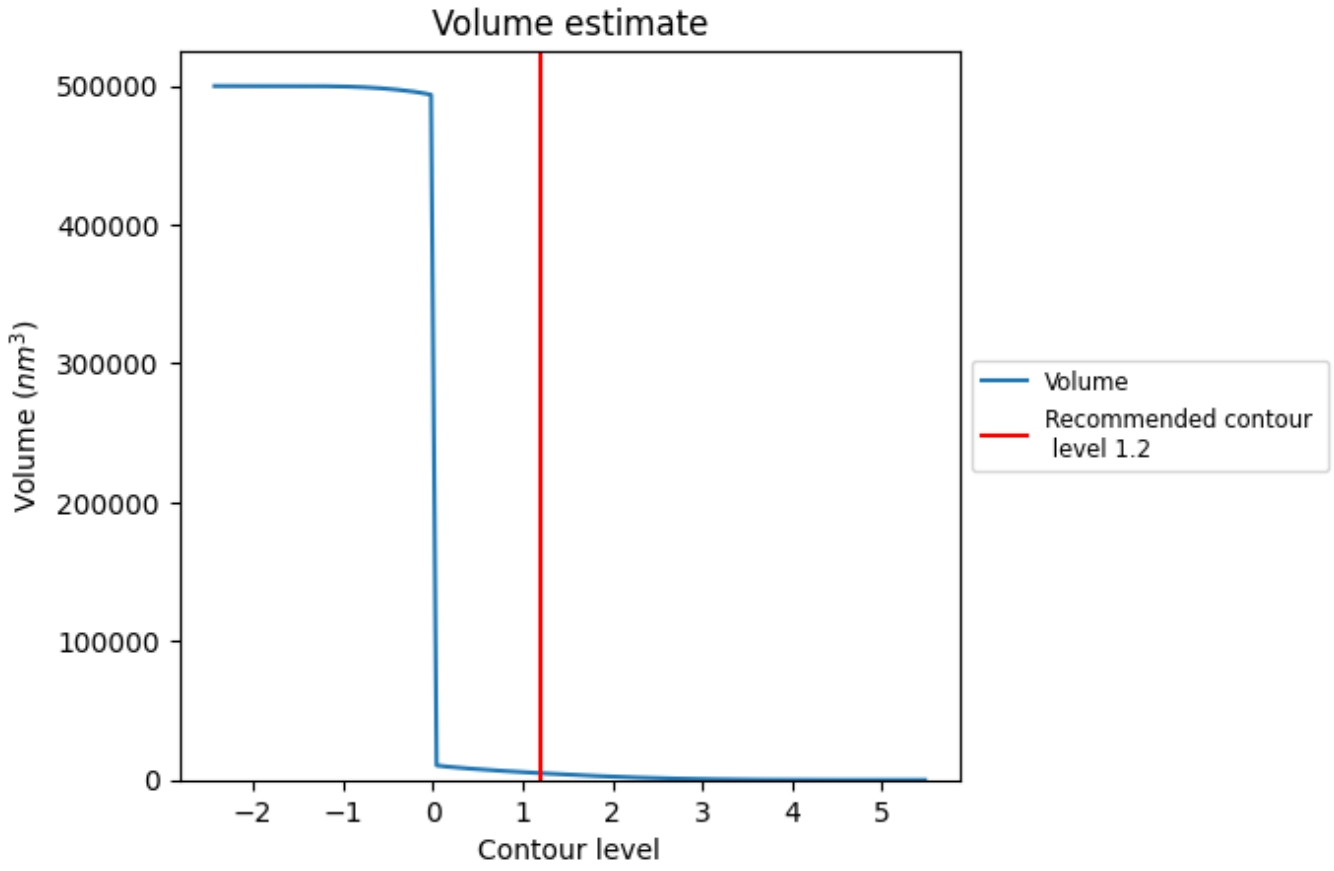
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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.

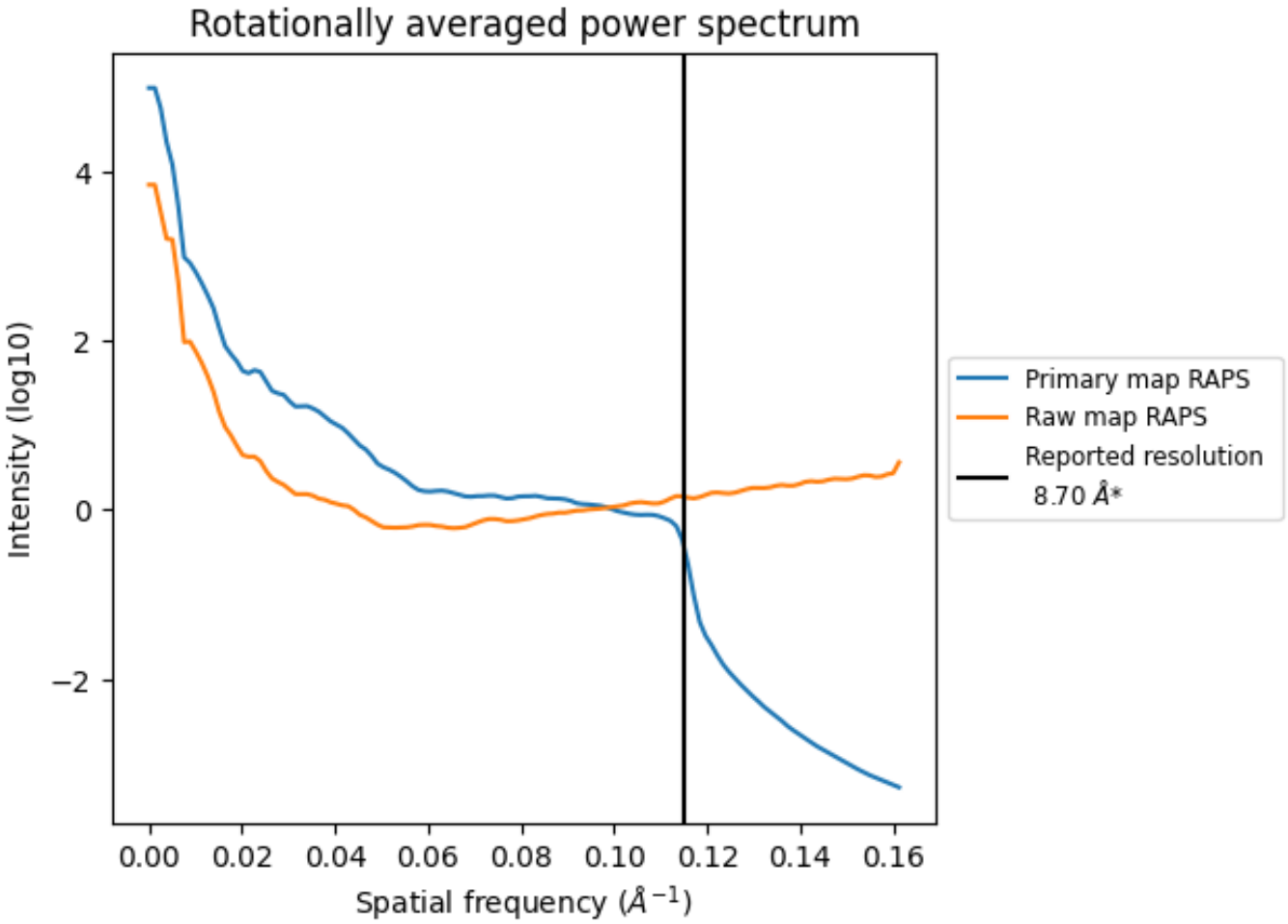
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 4893 $nm^3$; this corresponds to an approximate mass of 4420 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)

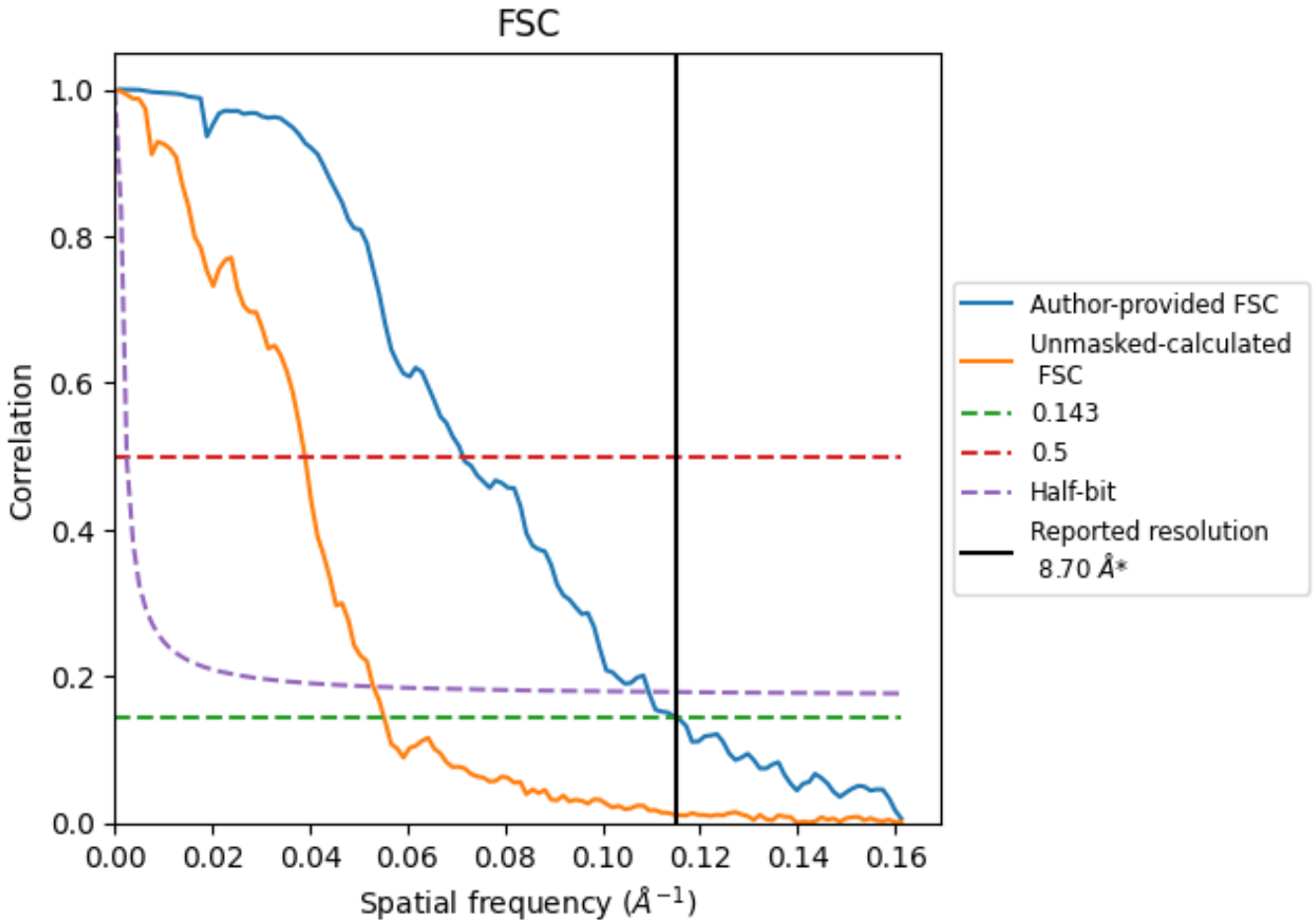



*Reported resolution corresponds to spatial frequency of 0.115 Å$^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.115 Å$^{-1}$

## 8.2 Resolution estimates (i)

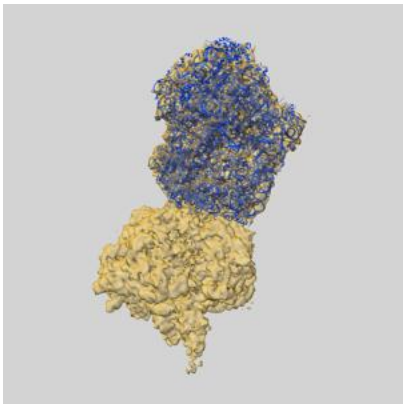
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 8.70 | - | - |
| Author-provided FSC curve | 8.68 | 14.01 | 9.13 |
| Unmasked-calculated* | 18.08 | 25.71 | 18.83 |

*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 18.08 differs from the reported value 8.7 by more than 10 %

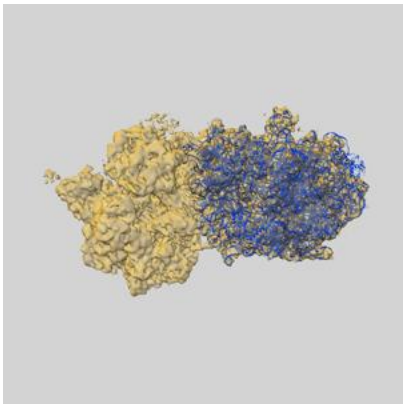
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17145 and PDB model 8P8W. Per-residue inclusion information can be found in section 3 on page 16.

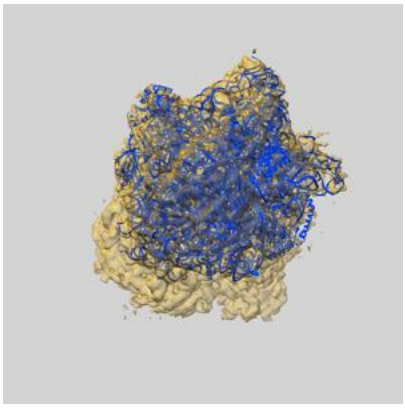
## 9.1 Map-model overlay



X



Y



Z

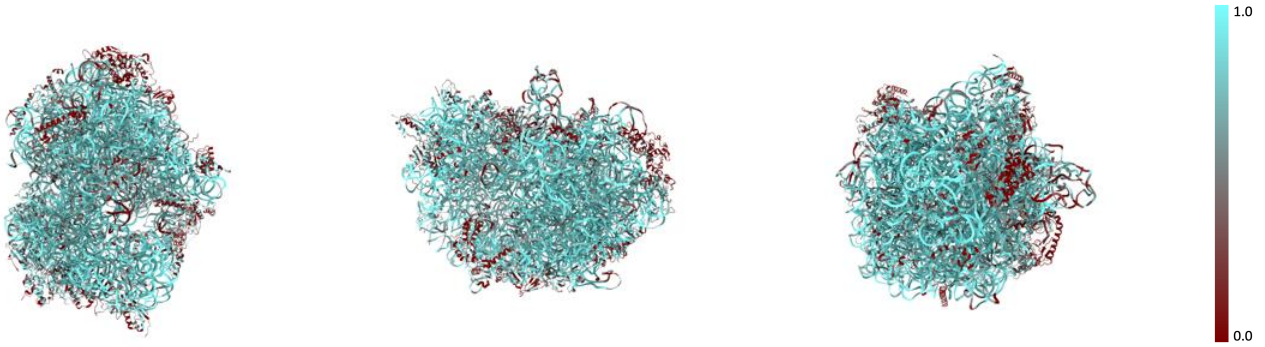
The images above show the 3D surface view of the map at the recommended contour level 1.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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


X Y Z

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.

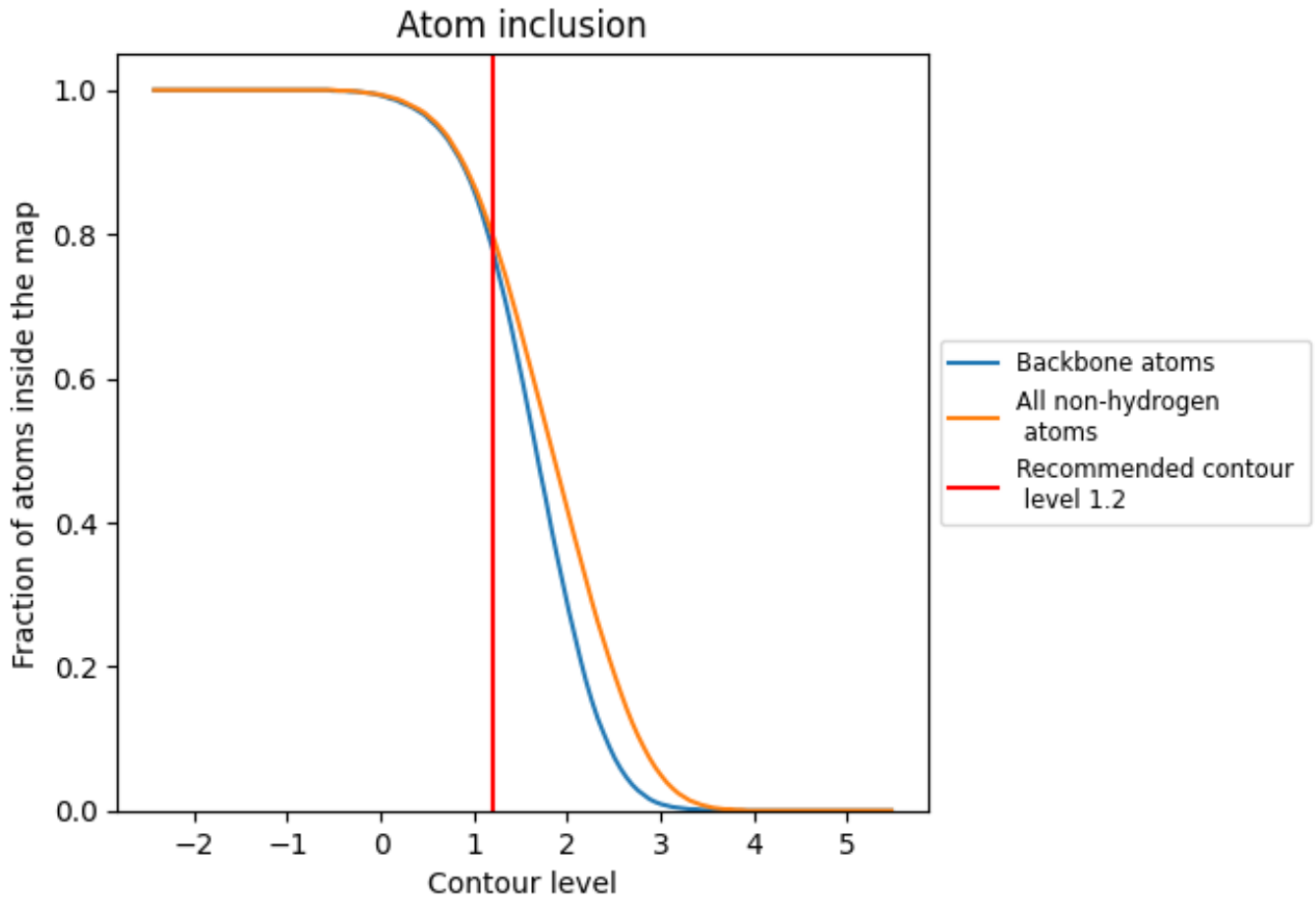
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.2).

## 9.4 Atom inclusion (i)




At the recommended contour level, 78% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8000 | 0.1070 |
| 0 | 0.7730 | 0.0600 |
| 1 | 0.7720 | 0.0250 |
| 2 | 0.8280 | 0.0470 |
| 3 | 0.9090 | 0.1110 |
| 4 | 0.8440 | 0.0940 |
| 5 | 0.9450 | 0.1390 |
| 6 | 0.3120 | 0.0370 |
| 7 | 0.8440 | 0.1400 |
| A | 0.5340 | 0.1330 |
| B | 0.5980 | 0.1260 |
| C | 0.6970 | 0.1340 |
| D | 0.5490 | 0.1380 |
| E | 0.5910 | 0.1420 |
| F | 0.6460 | 0.1170 |
| G | 0.6170 | 0.1040 |
| H | 0.6700 | 0.0840 |
| I | 0.5560 | 0.0880 |
| J | 0.7060 | 0.1090 |
| K | 0.6840 | 0.1020 |
| L | 0.6610 | 0.0890 |
| M | 0.7590 | 0.0890 |
| N | 0.7240 | 0.1390 |
| O | 0.7320 | 0.0820 |
| P | 0.6770 | 0.1220 |
| Q | 0.6270 | 0.1190 |
| R | 0.6910 | 0.0810 |
| S | 0.8540 | 0.1100 |
| T | 0.6430 | 0.1400 |
| U | 0.0650 | 0.0250 |
| X | 0.2090 | 0.0830 |
| Y | 0.6830 | 0.1210 |
| Z | 0.3740 | 0.0170 |
| a | 0.6680 | 0.0610 |
| b | 0.6670 | 0.0530 |


*Continued on next page...*

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| c | 0.5230 | 0.0460 |
| d | 0.4860 | 0.0750 |
| e | 0.5300 | 0.0720 |
| f | 0.0820 | 0.0390 |
| g | 0.3180 | 0.0540 |
| h | 0.1740 | 0.0270 |
| i | 0.7780 | 0.0780 |
| j | 0.5340 | 0.0690 |
| k | 0.5770 | 0.0380 |
| l | 0.7390 | 0.0670 |
| m | 0.8010 | 0.0970 |
| n | 0.4970 | 0.0520 |
| o | 0.6210 | 0.1010 |
| p | 0.7690 | 0.0620 |
| q | 0.5270 | 0.0470 |
| r | 0.7510 | 0.1020 |
| s | 0.7340 | 0.0600 |
| t | 0.5020 | 0.0800 |
| u | 0.7590 | 0.0310 |
| v | 0.6990 | 0.0830 |
| w | 0.3980 | 0.0770 |
| x | 0.3170 | 0.0920 |
| y | 0.8010 | 0.0860 |
| z | 0.5130 | 0.0190 |