# wwPDB EM Validation Summary Report (i)

Nov 14, 2022 – 08:49 PM EST

| | | |
|---|---|---|
| PDB ID | : | 6X6T |
| EMDB ID | : | EMD-22082 |
| Title | : | Cryo-EM structure of an Escherichia coli coupled transcription-translati on complex B1 (TTC-B1) containing an mRNA with a 24 nt long spacer, transcription factors NusA and NusG, and fMet-tRNAs at P-site and E-site |
| Authors | : | Molodtsov, V.; Ebright, R.H.; Wang, C.; Su, M. |
| Deposited on | : | 2020-05-29 |
| Resolution | : | 3.20 Å(reported) |

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

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

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

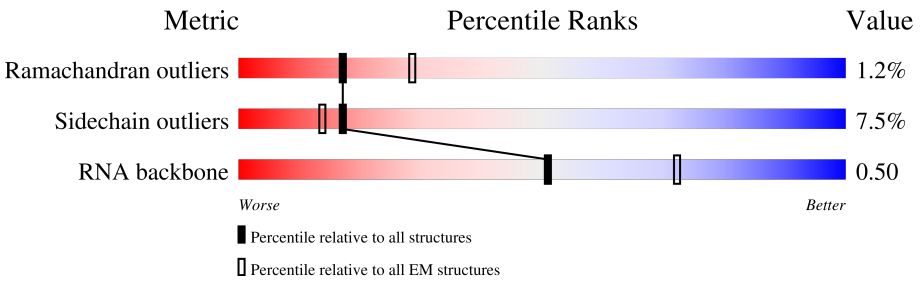
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA)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

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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




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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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 | 103 | 63%; 93%; 7% |
| 2 | 1 | 110 | 64%; 92%; 8% |
| 3 | 2 | 100 | 59%; 89%; 5%; 6% |
| 4 | 3 | 104 | 62%; 91%; 8%; • |
| 5 | 4 | 94 | 53%; 96%; • |
| 6 | 5 | 36 | 64%; 47%; 17%; 36% |
| 7 | 6 | 36 | 75%; 64%; 11%; 25% |
| 8 | 7 | 41 | 71%; 22%; 46%; 12%; 20% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 9 | 9 | 165 | 69% 54% 33% 10% |
| 10 | A | 76 | 41% 58% 38% |
| 10 | B | 76 | 43% 46% 49% 5% |
| 11 | AA | 1342 | 100% 99% |
| 12 | AB | 181 | 77% 67% 18% 10% |
| 13 | AC | 329 | 91% 90% 9% |
| 13 | AD | 329 | 91% 91% 9% |
| 14 | AE | 1407 | 95% 89% 5% 5% |
| 15 | AF | 91 | 90% 90% 10% |
| 16 | AG | 495 | 74% 69% 27% |
| 17 | C | 75 | 8% 85% 12% |
| 18 | D | 1542 | 78% 20% |
| 19 | E | 87 | 7% 93% 6% |
| 20 | F | 71 | 17% 94% |
| 21 | G | 241 | 6% 90% 7% |
| 22 | H | 557 | 46% 41% 54% |
| 23 | I | 233 | 5% 86% 11% |
| 24 | J | 206 | 96% |
| 25 | K | 167 | 88% 5% 7% |
| 26 | L | 135 | 6% 72% 23% |
| 27 | M | 179 | 9% 80% 16% |
| 28 | N | 130 | 97% |
| 29 | O | 130 | 5% 93% 5% |
| 30 | P | 103 | 17% 87% 9% |
| 31 | Q | 129 | 87% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 32 | R | 124 | 5% 92% 6% |
| 33 | S | 101 | 95% |
| 34 | T | 89 | 85% 13% |
| 35 | U | 82 | 93% 7% |
| 36 | V | 84 | 93% 5% |
| 37 | W | 92 | 53% 86% 10% |
| 38 | X | 118 | 67% 88% 10% |
| 39 | Y | 142 | 87% 68% 27% |
| 40 | Z | 121 | 25% 12% 12% 75% |
| 41 | a | 2904 | 29% 81% 18% |
| 42 | b | 85 | 52% 88% 11% |
| 43 | c | 78 | 77% 94% 5% |
| 44 | d | 120 | 12% 86% 14% |
| 45 | e | 63 | 59% 97% |
| 46 | f | 59 | 64% 95% |
| 47 | g | 70 | 63% 86% 9% 6% |
| 48 | h | 273 | 66% 93% 7% |
| 49 | i | 57 | 61% 88% 11% |
| 50 | j | 209 | 69% 97% |
| 51 | k | 55 | 53% 89% 5% 5% |
| 52 | l | 201 | 67% 93% 7% |
| 53 | m | 46 | 72% 93% 7% |
| 54 | n | 179 | 51% 89% 10% |
| 55 | o | 65 | 66% 91% 8% |
| 56 | p | 177 | 55% 97% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 57 | q | 38 | 66% 95% 5% |
| 58 | r | 149 | 72% 93% 7% |
| 59 | s | 142 | 68% 96% |
| 60 | t | 123 | 71% 95% 5% |
| 61 | u | 144 | 72% 96% |
| 62 | v | 136 | 61% 96% |
| 63 | w | 127 | 65% 87% 6% 6% |
| 64 | x | 117 | 52% 94% 5% |
| 65 | y | 115 | 64% 95% |
| 66 | z | 118 | 70% 97% |

# 2 Entry composition (i)

There are 68 unique types of molecules in this entry. The entry contains 291628 atoms, of which 109913 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 L21.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 1 | 0 | 103 | 1655 | 516 | 839 | 153 | 145 | 2 | 0 | 0 |

- Molecule 2 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 2 | 1 | 110 | 1779 | 532 | 922 | 166 | 156 | 3 | 0 | 0 |

- Molecule 3 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 3 | 2 | 94 | 1557 | 470 | 811 | 140 | 134 | 2 | 0 | 0 |

- Molecule 4 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | |
| 4 | 3 | 103 | 1632 | 498 | 844 | 148 | 142 | 0 | 0 |

- Molecule 5 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 5 | 4 | 94 | 1533 | 479 | 780 | 137 | 134 | 3 | 0 | 0 |

- Molecule 6 is a DNA chain called NT DNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 6 | 5 | 23 | 732 | 225 | 260 | 87 | 137 | 23 | 0 | 0 |

- Molecule 7 is a DNA chain called T DNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 7 | 6 | 27 | 847 | 259 | 305 | 89 | 167 | 27 | 0 | 0 |

- Molecule 8 is a RNA chain called mRNA with 24 nt long spacer.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 8 | 7 | 33 | 784 | 307 | 97 | 96 | 251 | 33 | 0 | 0 |

- Molecule 9 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | 9 | 148 | 1117 | 705 | 196 | 209 | 7 | 0 | 0 |

- Molecule 10 is a RNA chain called E-site and P-site tRNA (fMet).

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 10 | A | 76 | 2446 | 723 | 826 | 295 | 527 | 75 | 0 | 0 |
| | | | Total | C | H | N | O | P | | |
| 10 | B | 76 | 2433 | 723 | 813 | 295 | 527 | 75 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | ? | - | U | deletion | GB 1837817527 |
| B | ? | - | U | deletion | GB 1837817527 |

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | AA | 1340 | 10567 | 6631 | 1841 | 2052 | 43 | 0 | 0 |

- Molecule 12 is a protein called Transcription termination/antitermination protein NusG.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 12 | AB | 162 | 1283 | 816 | 1 | 222 | 237 | 7 | 0 | 0 |

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | AC | 301 | 2094 | 1296 | 379 | 413 | 6 | 0 | 0 |
| 13 | AD | 299 | 2078 | 1287 | 378 | 407 | 6 | 0 | 0 |

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 14 | AE | 1335 | 21000 | 6526 | 10612 | 1854 | 1958 | 50 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| AE | 1384 | VAL | MET | variant | UNP A0A4S1NBU2 |

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | AF | 82 | 650 | 396 | 122 | 131 | 1 | 0 | 0 |

- Molecule 16 is a protein called Transcription termination/antitermination protein NusA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | AG | 495 | 3852 | 2396 | 669 | 774 | 13 | 0 | 0 |

- Molecule 17 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 17 | C | 66 | 1103 | 344 | 559 | 102 | 97 | 1 | 0 | 0 |

- Molecule 18 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 18 | D | 1524 | 49126 | 14585 | 16423 | 6003 | 10591 | 1524 | 0 | 0 |

- Molecule 19 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 19 | E | 86 | 1388 | 414 | 719 | 138 | 114 | 3 | 0 | 0 |

- Molecule 20 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 20 | F | 70 | 1218 | 366 | 629 | 125 | 97 | 1 | 0 | 0 |

- Molecule 21 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 21 | G | 225 | 3545 | 1113 | 1785 | 316 | 323 | 8 | 0 | 0 |

- Molecule 22 is a protein called 30S ribosomal protein S1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 22 | H | 259 | 3184 | 1073 | 1454 | 305 | 349 | 3 | 0 | 0 |

- Molecule 23 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 23 | I | 208 | 3346 | 1036 | 1710 | 307 | 290 | 3 | 0 | 0 |

- Molecule 24 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 24 | J | 205 | 3350 | 1026 | 1707 | 315 | 298 | 4 | 0 | 0 |

- Molecule 25 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 25 | K | 156 | 2348 | 717 | 1196 | 217 | 212 | 6 | 0 | 0 |

- Molecule 26 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 26 | L | 104 | 1694 | 536 | 846 | 153 | 152 | 7 | 0 | 0 |

- Molecule 27 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 27 | M | 151 | 2416 | 735 | 1235 | 227 | 215 | 4 | 0 | 0 |

- Molecule 28 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 28 | N | 129 | 2010 | 616 | 1031 | 173 | 184 | 6 | 0 | 0 |

- Molecule 29 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 29 | O | 127 | 2092 | 634 | 1070 | 206 | 179 | 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 30 | P | 99 | 1621 | 495 | 831 | 151 | 143 | 1 | 0 | 0 |

- Molecule 31 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 31 | Q | 117 | 1764 | 540 | 887 | 174 | 160 | 3 | 0 | 0 |

- Molecule 32 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 32 | R | 121 | 1940 | 580 | 1001 | 194 | 161 | 4 | 0 | 0 |

- Molecule 33 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 33 | S | 100 | 1649 | 499 | 844 | 164 | 139 | 3 | 0 | 0 |

- Molecule 34 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 34 | T | 88 | 1448 | 439 | 734 | 144 | 130 | 1 | 0 | 0 |

- Molecule 35 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 35 | U | 82 | 1315 | 406 | 666 | 128 | 114 | 1 | 0 | 0 |

- Molecule 36 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 36 | V | 80 | 1339 | 411 | 691 | 121 | 113 | 3 | 0 | 0 |

- Molecule 37 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 37 | W | 83 | 1351 | 424 | 688 | 126 | 111 | 2 | 0 | 0 |

- Molecule 38 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 38 | X | 116 | 1864 | 558 | 964 | 181 | 158 | 3 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 39 | Y | 141 | 1032 | 651 | 179 | 196 | 6 | 0 | 0 |

- Molecule 40 is a protein called 50S ribosomal protein L7/L12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | Z | 30 | 227 | 144 | 33 | 47 | 3 | 0 | 0 |

- Molecule 41 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 41 | a | 2880 | 92918 | 27587 | 31077 | 11398 | 19976 | 2880 | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| a | 887 | A | U | variant | GB 937521852 |

- Molecule 42 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 42 | b | 76 | 1181 | 360 | 599 | 117 | 104 | 1 | 0 | 0 |

- Molecule 43 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 43 | c | 77 | 1277 | 388 | 652 | 129 | 106 | 2 | 0 | 0 |

- Molecule 44 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | | |
| 44 | d | 120 | 3870 | 1144 | 1301 | 468 | 837 | 120 | 0 | 0 |

- Molecule 45 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 45 | e | 62 | 1032 | 308 | 531 | 98 | 94 | 1 | 0 | 0 |

- Molecule 46 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 46 | f | 58 | 936 | 281 | 488 | 87 | 78 | 2 | 0 | 0 |

- Molecule 47 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 47 | g | 66 | 1042 | 323 | 520 | 99 | 94 | 6 | 0 | 0 |

- Molecule 48 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 48 | h | 271 | 4236 | 1288 | 2154 | 423 | 364 | 7 | 0 | 0 |

- Molecule 49 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 49 | i | 56 | 903 | 269 | 459 | 94 | 80 | 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 50 | j | 209 | 3182 | 979 | 1617 | 288 | 294 | 4 | 0 | 0 |

- Molecule 51 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | |
| 51 | k | 52 | 890 | 275 | 464 | 78 | 73 | 0 | 0 |

- Molecule 52 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 52 | l | 201 | 3171 | 974 | 1619 | 283 | 290 | 5 | 0 | 0 |

- Molecule 53 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 53 | m | 46 | 795 | 228 | 418 | 90 | 57 | 2 | 0 | 0 |

- Molecule 54 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 54 | n | 177 | 2853 | 899 | 1443 | 249 | 256 | 6 | 0 | 0 |

- Molecule 55 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 55 | o | 64 | 1076 | 323 | 572 | 105 | 74 | 2 | 0 | 0 |

- Molecule 56 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 56 | p | 175 | 2671 | 826 | 1358 | 241 | 244 | 2 | 0 | 0 |

- Molecule 57 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 57 | q | 38 | 645 | 185 | 343 | 65 | 48 | 4 | 0 | 0 |

- Molecule 58 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 58 | r | 149 | 2259 | 699 | 1148 | 197 | 214 | 1 | 0 | 0 |

- Molecule 59 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 59 | s | 142 | 2291 | 714 | 1162 | 212 | 199 | 4 | 0 | 0 |

- Molecule 60 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 60 | t | 123 | 1969 | 593 | 1023 | 181 | 166 | 6 | 0 | 0 |

- Molecule 61 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 61 | u | 144 | 2182 | 654 | 1129 | 207 | 190 | 2 | 0 | 0 |

- Molecule 62 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 62 | v | 136 | 2231 | 686 | 1157 | 205 | 177 | 6 | 0 | 0 |

- Molecule 63 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 63 | w | 119 | 1945 | 588 | 994 | 195 | 163 | 5 | 0 | 0 |

- Molecule 64 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | |
| 64 | x | 116 | 1815 | 552 | 923 | 178 | 162 | 0 | 0 |

- Molecule 65 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | |
| 65 | y | 114 | 1879 | 574 | 962 | 179 | 163 | 1 | 0 | 0 |

- Molecule 66 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | |
| 66 | z | 117 | 1967 | 604 | 1020 | 192 | 151 | 0 | 0 |

- Molecule 67 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 67 | 7 | 1 | 1 | 1 | 0 |

- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

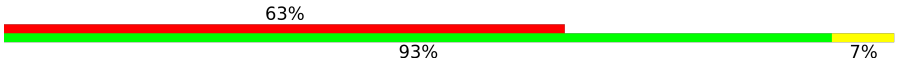
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 68 | AA | 2 | 2 | 2 | 0 |

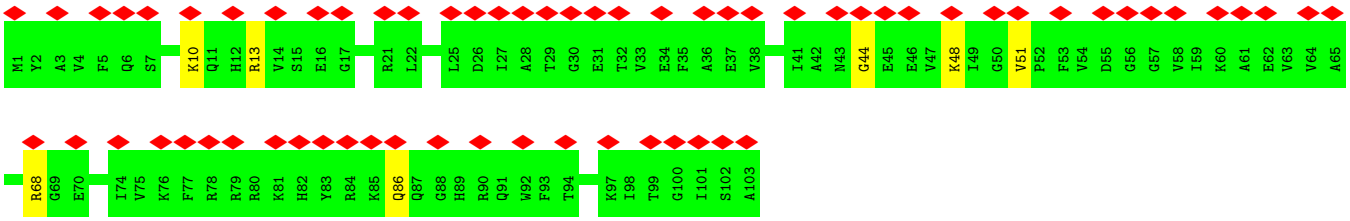
# 3 Residue-property plots (i)

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 L21

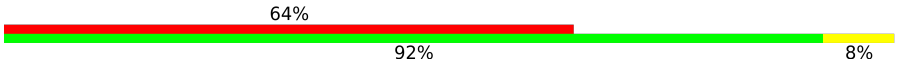
Chain 0:

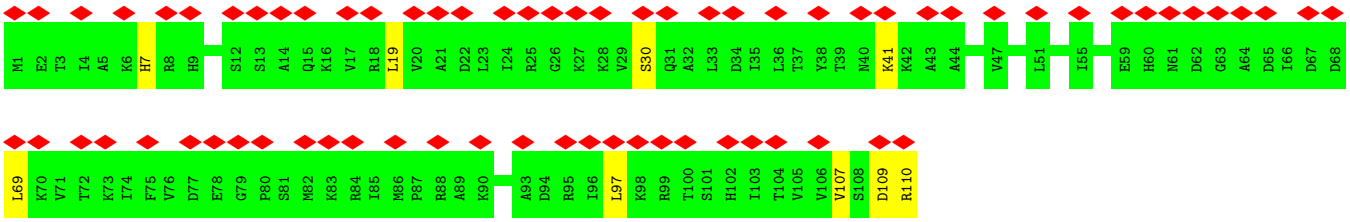



- Molecule 2: 50S ribosomal protein L22

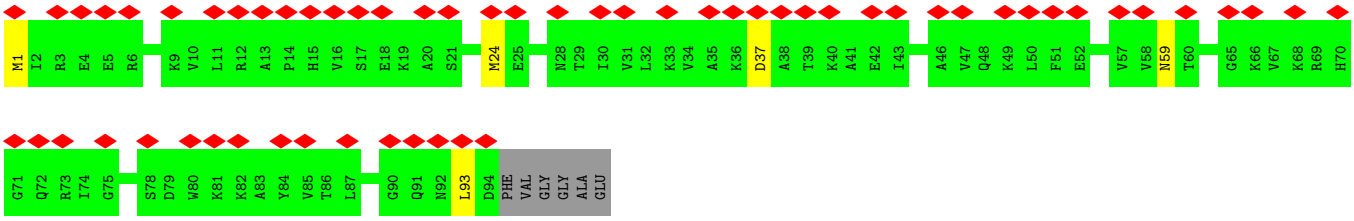
Chain 1:



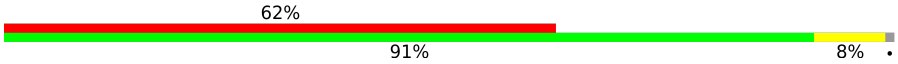

- Molecule 3: 50S ribosomal protein L23

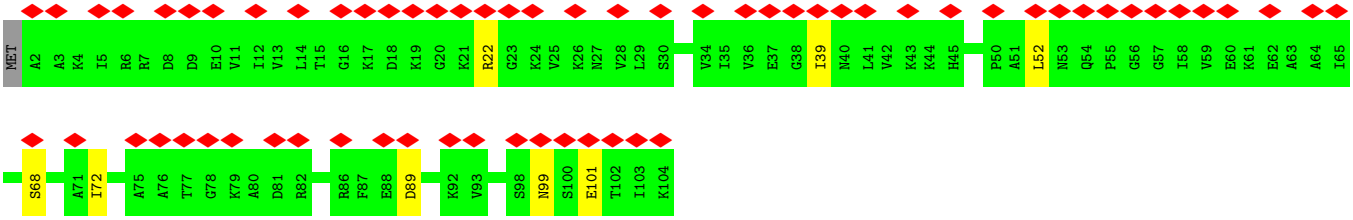
Chain 2:




- Molecule 4: 50S ribosomal protein L24

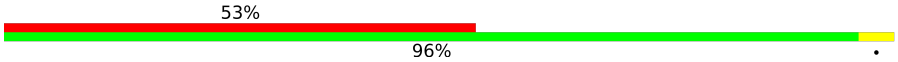
Chain 3:

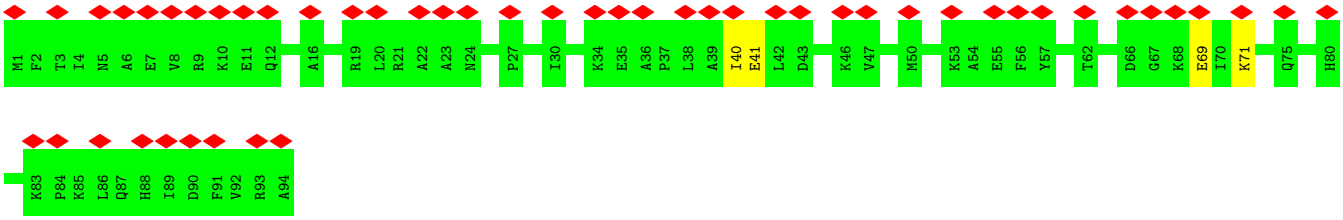





- Molecule 5: 50S ribosomal protein L25

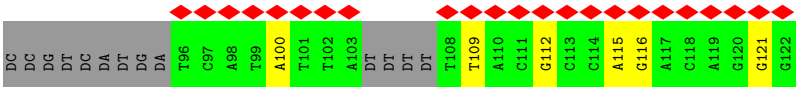
Chain 4:



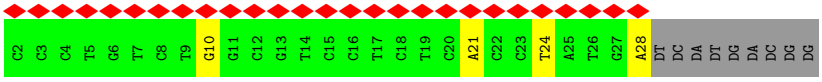

- Molecule 6: NT DNA

Chain 5:



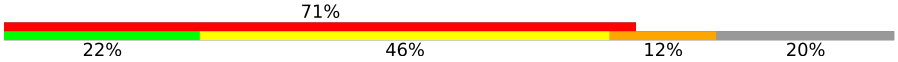

- Molecule 7: T DNA

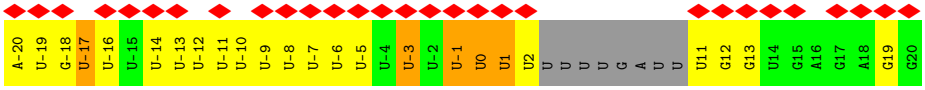
Chain 6:




- Molecule 8: mRNA with 24 nt long spacer

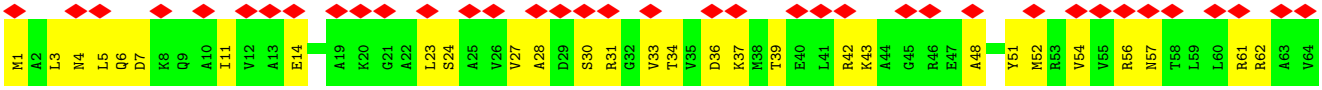
Chain 7:

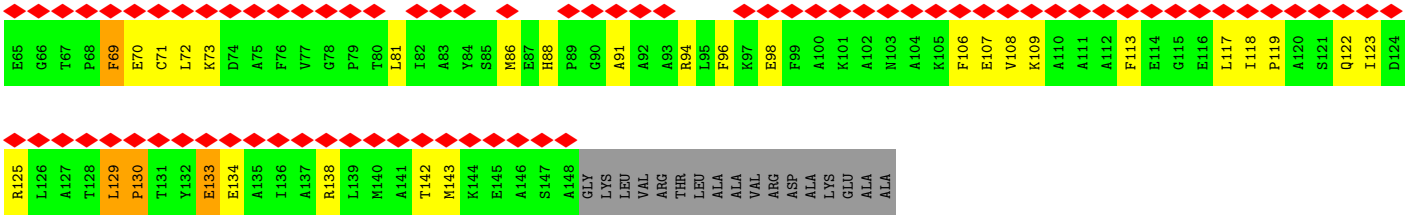



- Molecule 9: 50S ribosomal protein L10

Chain 9:



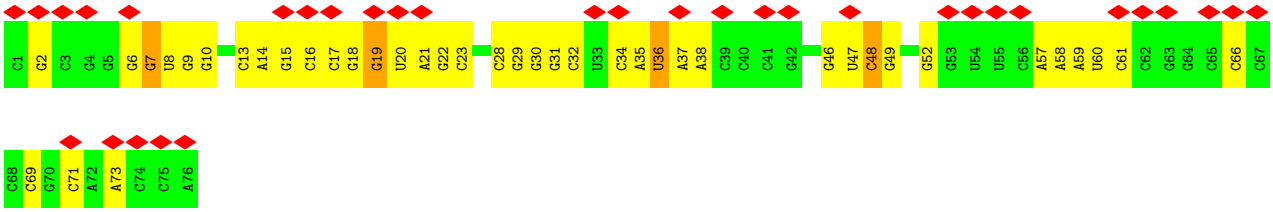



- Molecule 10: E-site and P-site tRNA (fMet)

Chain A:

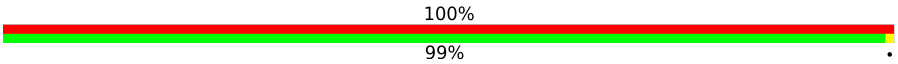
- Molecule 10: E-site and P-site tRNA (fMet)

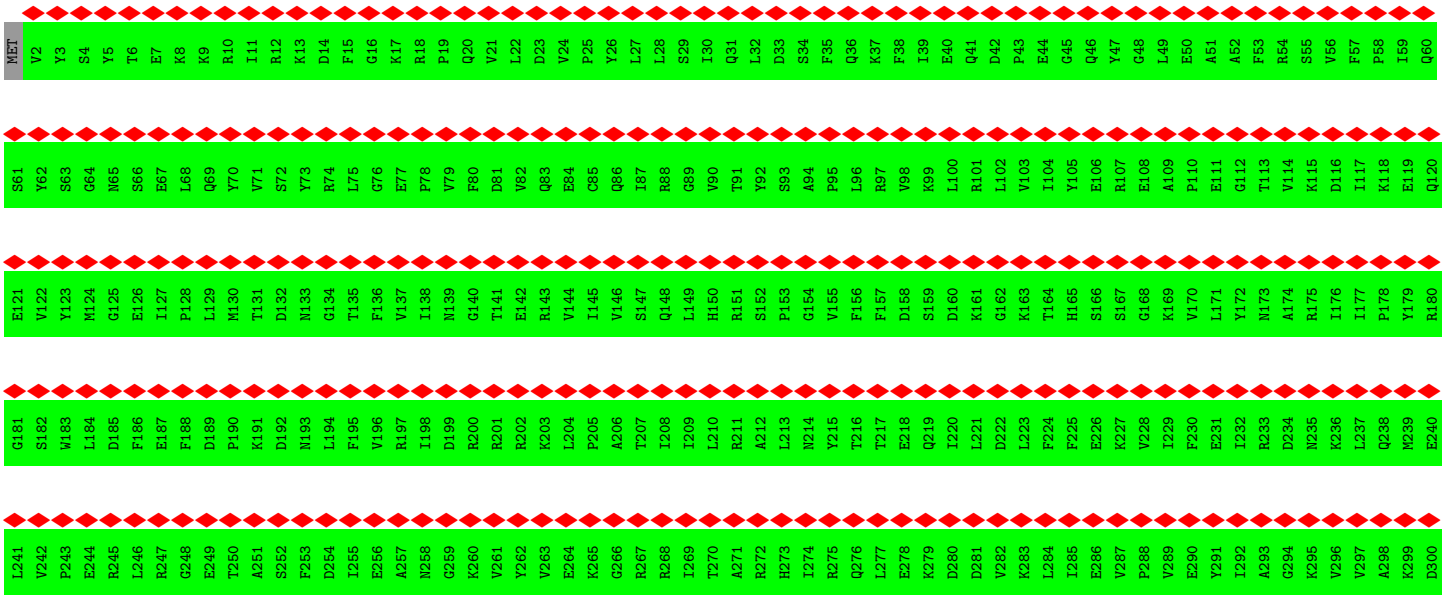
Chain B:




- Molecule 11: DNA-directed RNA polymerase subunit beta

Chain AA:



Y301 I302 D303 E304 S305 T306 G307 E308 L309 I310 C311 A312 A313 N314 M315 E316 L317 S318 L319 D320 L321 L322 A323 K324 L325 S326 Q327 S328 G329 H330 K331 R332 I333 E334 T335 L336 F337 T338 N339 D340 L341 D342 H343 G344 P345 Y346 I347 S348 E349 T350 L351 R352 V353 D354 P355 T356 N357 D358 R359 L360

S361 A362 L363 V364 E365 I366 Y367 R368 M369 M370 R371 P372 G373 E374 P375 P376 T377 R378 E379 A380 A381 E382 S383 L384 F385 E386 N387 L388 F389 F390 S391 E392 D393 R394 Y395 D396 L397 S398 A399 V400 G401 R402 M403 K404 F405 N406 R407 S408 L409 L410 R411 E412 E413 I414 E415 G416 S417 G418 I419 L420

S421 K422 D423 D424 I425 I426 D427 V428 M429 K430 K431 L432 I433 D434 I435 R436 M437 G438 K439 G440 E441 V442 D443 D444 I445 D446 H447 L448 G449 N450 R451 R452 I453 R454 S455 V456 G457 E458 M459 A460 E461 N462 Q463 F464 R465 V466 G467 L468 V469 R470 V471 E472 R473 A474 V475 K476 E477 R478 L479 S480

L481 G482 D483 L484 D485 T486 L487 M488 P489 Q490 D491 M492 I493 N494 A495 K496 P497 I498 S499 A500 A501 V502 K503 E504 F505 F506 G507 S508 S509 Q510 L511 S512 Q513 F514 M515 D516 Q517 N518 N519 P520 L521 S522 E523 I524 T525 H526 K527 R528 R529 I530 S531 A532 L533 G534 P535 G536 G537 L538 T539 R540

E541 R542 A543 G544 F545 E546 V547 R548 D549 V550 H551 P552 T553 H554 Y555 G556 R557 V558 C559 P560 I561 E562 T563 P564 E565 G566 P567 N568 I569 G570 L571 I572 N573 S574 L575 S576 V577 Y578 A579 Q580 T581 N582 E583 Y584 G585 F586 L587 E588 T589 P590 Y591 R592 K593 V594 T595 D596 G597 V598 V599 T600

D601 E602 I603 H604 Y605 L606 S607 A608 I609 E610 E611 G612 N613 Y614 V615 I616 A617 Q618 A619 N620 S621 N622 L623 D624 E625 E626 G627 H628 F629 V630 E631 D632 L633 V634 T635 C636 R637 S638 K639 G640 E641 S642 S643 L644 F645 S646 R647 D648 Q649 V650 D651 Y652 M653 D654 V655 S656 T657 Q658 Q659 V660

V661 S662 V663 G664 A665 S666 L667 I668 P669 F670 L671 E672 H673 D674 D675 A676 N677 R678 A679 L680 M681 G682 A683 N684 M685 Q686 R687 Q688 A689 V690 P691 T692 L693 R694 A695 D696 K697 P698 L699 V700 G701 T702 G703 M704 E705 R706 A707 V708 A709 V710 D711 S712 G713 V714 T715 A716 V717 A718 K719 R720

G721 G722 V723 V724 Q725 Y726 V727 D728 A729 S730 R731 I732 V733 I734 K735 V736 N737 E738 D739 E740 M741 Y742 P743 G744 E745 A746 G747 I748 D749 I750 Y751 N752 L753 T754 K755 Y756 T757 R758 S759 N760 Q761 N762 T763 C764 I765 N766 Q767 M768 P769 C770 V771 S772 G773 V774 E775 P776 V777 E778 R779 G780

D781 V782 L783 A784 D785 G786 P787 S788 T789 D790 L791 G792 E793 L794 A795 L796 G797 Q798 N799 M800 R801 V802 A803 F804 M805 P806 W807 N808 G809 Y810 N811 F812 E813 D814 S815 I816 L817 V818 S819 E820 R821 V822 V823 Q824 E825 D826 R827 F828 T829 T830 I831 H832 I833 Q834 E835 L836 A837 C838 V839 S840

R841 D842 T843 K844 L845 G846 P847 E848 E849 I850 T851 A852 D853 I854 P855 N856 V857 G858 E859 A860 A861 L862 S863 K864 L865 D866 E867 S868 G869 I870 V871 V872 I873 G874 A875 E876 V877 T878 G879 G880 D881 I882 L883 V884 G885 K886 V887 T888 P889 K890 G891 E892 T893 Q894 L895 T896 P897 E898 E899 K900

L901 L902 R903 A904 I905 F906 G907 E908 K909 A910 S911 D912 V913 K914 D915 S916 S917 L918 R919 V920 P921 N922 G923 V924 S925 G926 T927 V928 I929 D930 V931 Q932 V933 F934 T935 R936 D937 G938 V939 E940 K941 D942 K943 R944 A945 L946 E947 I948 E949 E950 M951 Q952 L953 K954 Q955 A956 K957 K958 D959 L960

S961 E962 E963 L964 Q965 I966 L967 E968 A969 G970 L971 F972 S973 R974 I975 R976 A977 V978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988 L989 D990 K991 L992 P993 R994 D995 R996 W997 L998 E999 L1000 G1001 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012 Q1013 L1014 A1015 E1016 Q1017 Y1018 D1019 E1020

L1021 K1022 H1023 E1024 F1025 E1026 K1027 K1028 L1029 E1030 A1031 K1032 R1033 R1034 K1035 I1036 T1037 Q1038 G1039 D1040 D1041 L1042 A1043 P1044 G1045 V1046 L1047 K1048 I1049 V1050 K1051 V1052 Y1053 L1054 A1055 V1056 K1057 R1058 R1059 I1060 Q1061 P1062 G1063 D1064 K1065 M1066 A1067 G1068 R1069 H1070 G1071 N1072 K1073 G1074 V1075 I1076 S1077 K1078 I1079 N1080

P1081 I1082 E1083 D1084 M1085 P1086 Y1087 D1088 E1089 N1090 G1091 T1092 P1093 V1094 D1095 I1096 V1097 L1098 N1099 P1100 L1101 G1102 V1103 P1104 S1105 R1106 M1107 N1108 I1109 G1110 Q1111 I1112 L1113 E1114 T1115 H1116 L1117 G1118 M1119 A1120 A1121 K1122 G1123 I1124 G1125 D1126 K1127 I1128 N1129 A1130 M1131 L1132 K1133 Q1134 Q1135 Q1136 E1137 V1138 A1139 K1140

L1141 R1142 E1143 F1144 I1145 Q1146 R1147 A1148 Y1149 D1150 L1151 G1152 A1153 D1154 V1155 R1156 Q1157 K1158 V1159 D1160 L1161 S1162 T1163 F1164 S1165 D1166 E1167 E1168 V1169 M1170 R1171 L1172 A1173 E1174 N1175 L1176 R1177 K1178 G1179 M1180 P1181 I1182 A1183 T1184 P1185 V1186 F1187 D1188 G1189 A1190 K1191 E1192 A1193 E1194 I1195 K1196 E1197 L1198 L1199 K1200

L1201 G1202 D1203 L1204 P1205 T1206 S1207 G1208 Q1209 I1210 R1211 L1212 Y1213 D1214 G1215 R1216 T1217 G1218 E1219 Q1220 F1221 E1222 R1223 P1224 V1225 T1226 V1227 G1228 Y1229 M1230 Y1231 M1232 L1233 K1234 L1235 N1236 H1237 L1238 V1239 D1240 D1241 K1242 M1243 H1244 A1245 R1246 S1247 T1248 G1249 S1250 Y1251 S1252 L1253 V1254 T1255 Q1256 Q1257 P1258 L1259 G1260

G1261 K1262 A1263 Q1264 F1265 G1266 G1267 Q1268 R1269 F1270 G1271 E1272 M1273 E1274 V1275 W1276 A1277 L1278 E1279 A1280 Y1281 G1282 A1283 A1284 Y1285 T1286 L1287 Q1288 E1289 M1290 L1291 T1292 V1293 K1294 S1295 D1296 D1297 V1298 N1299 G1300 R1301 T1302 K1303 M1304 Y1305 K1306 N1307 I1308 V1309 D1310 G1311 N1312 H1313 Q1314 M1315 E1316 P1317 G1318 M1319 P1320

E1321 S1322 F1323 N1324 V1325 L1326 L1327 K1328 E1329 I1330 R1331 S1332 L1333 G1334 I1335 N1336 I1337 E1338 L1339 E1340 D1341 GLU

- Molecule 12: Transcription termination/antitermination protein NusG

Chain AB: 77% 67% 18% 10%

MET SER GLU ALA PRO K6 K7 R8 W9 Y10 V11 V12 Q13 A14 F15 S16 G17 F18 E19 G20 R21 V22 A23 T24 S25 L26 R27 E28 H29 I30 K31 L32 H33 N34 M35 E36 D37 L38 F39 G40 E41 V42 M43 V44 P45 T46 E47 E48 VAL VAL GLU ILE ARG GLY GLY GLN ARG ARG LYS SER

GLU ARG K63 F64 F65 P66 G67 Y68 V69 L70 V71 Q72 M73 V74 M75 N76 D77 A78 S79 W80 H81 L82 V83 R84 S85 V86 P87 R88 V89 M90 G91 F92 I93 G94 G95 T96 S97 D98 R99 P100 A101 P102 I103 S104 D105 K106 E107 V108 D109 A110 I111 M112 N113 R114 L115 Q116 Q117 V118 G119 D120

K121 P122 R123 P124 K125 T126 L127 F128 E129 P130 G131 E132 R135 V136 N137 D138 G139 P140 F141 A142 D143 F144 N145 G146 V147 V148 E149 E150 V151 D152 Y153 E154 K155 S156 R157 L158 K159 V160 S161 V162 S163 I164 F165 G166 R167 A168 T169 P170 V171 E172 L173 D174 F175 S176 Q177 V178 E179 K180 A181

- Molecule 13: DNA-directed RNA polymerase subunit alpha

Chain AC: 91% 90% 9%

MET GLN GLY SER VAL THR E7 F8 L9 K10 P11 R12 L13 V14 D15 I16 E17 Q18 V19 S20 S21 T22 H23 A24 K25 V26 T27 L28 E29 P30 L31 E32 R33 G34 F35 G36 H37 T38 L39 G40 N41 A42 L43 R44 R45 I46 L47 L48 S49 S50 M51 P52 G53 C54 A55 V56 T57 E58 V59 E60

I61 D62 G63 V64 L65 H66 E67 Y68 S69 T70 K71 E72 G73 V74 Q75 E76 D77 I78 L79 E80 I81 L82 L83 N84 L85 K86 G87 L88 A89 V90 R91 V92 Q93 G94 K95 D96 E97 V98 I99 L100 T101 L102 N103 K104 S105 G106 I107 G108 P109 V110 T111 A112 A113 D114 I115 T116 H117 D118 G119 D120

V121 E122 I123 V124 K125 P126 Q127 H128 V129 I130 C131 H132 L133 T134 D135 E136 N137 A138 S139 I140 S141 M142 R143 I144 K145 V146 Q147 R148 G149 R150 G151 Y152 V153 P154 A155 S156 T157 R158 ILE HIS SER GLU GLU ASP E165 R166 P167 I168 G169 R170 L171 L172 V173 D174 A175 C176 Y177 S178 P179 V180

E181 R182 I183 A184 Y185 N186 V187 E188 A189 A190 R191 V192 E193 Q194 R195 T196 D197 L198 D199 K200 L201 V202 I203 E204 M205 E206 T207 N208 G209 T210 I211 D212 P213 E214 E215 A216 I217 R218 R219 A220 A221 T222 I223 L224 A225 E226 Q227 L228 E229 A230 F231 V232 D233 LEU ARG ASP VAL ARG GLN PRO

GLU VAL LYS GLU GLU LYS PRO GLU PHE D250 P251 I252 L253 L254 R255 P256 V257 D258 D259 L260 E261 L262 T263 V264 R265 S266 A267 N268 C269 L270 K271 A272 E273 A274 I275 H276 Y277 I278 G279 D280 L281 V282 Q283 R284 T285 E286 V287 E288 L289 L290 K291 T292 P293 N294 L295 G296 K297 K298 S299 L300

T301 E302 I303 K304 D305 V306 L307 A308 S309 R310 G311 L312 S313 L314 G315 M316 R317 L318 E319 N320 W321 P322 P323 A324 S325 I326 A327 D328 E329

- Molecule 13: DNA-directed RNA polymerase subunit alpha

Chain AD: 91% 91% 9%

MET GLN GLY SER V5 T6 E7 F8 L9 K10 P11 R12 L13 V14 D15 I16 E17 Q18 V19 S20 S21 T22 H23 A24 K25 V26 T27 L28 E29 P30 L31 E32 R33 G34 F35 G36 H37 T38 L39 G40 N41 A42 L43 R44 R45 I46 L47 L48 S49 S50 M51 P52 G53 C54 A55 V56 T57 E58 V59 E60

I61 D62 G63 V64 L65 H66 E67 Y68 S69 T70 K71 E72 G73 V74 Q75 E76 D77 I78 L79 E80 I81 L82 L83 N84 L85 K86 G87 L88 A89 V90 R91 V92 Q93 G94 K95 D96 E97 V98 I99 L100 T101 L102 N103 K104 S105 G106 I107 G108 P109 V110 T111 A112 A113 D114 I115 T116 H117 D118 G119 D120

V121 E122 I123 V124 K125 P126 Q127 H128 V129 I130 C131 H132 L133 T134 D135 E136 N137 A138 S139 I140 S141 M142 R143 I144 K145 V146 Q147 R148 G149 R150 G151 Y152 V153 P154 A155 S156 T157 R158 ILE HIS SER GLU GLU ASP GLU ARG PRO ILE G169 R170 L171 L172 V173 D174 A175 C176 Y177 S178 P179 V180

E181 R182 I183 A184 Y185 N186 V187 E188 A189 A190 R191 V192 E193 Q194 R195 T196 D197 L198 D199 K200 L201 V202 I203 E204 M205 E206 T207 N208 G209 T210 I211 D212 P213 E214 E215 A216 I217 R218 R219 A220 A221 T222 I223 L224 A225 E226 Q227 L228 E229 A230 F231 V232 ASP LEU ARG ASP VAL ARG GLN PRO

GLU VAL LYS GLU GLU LYS PRO GLU F249 D250 P251 I252 L253 L254 R255 P256 V257 D258 D259 L260 E261 L262 T263 V264 R265 S266 A267 N268 C269 L270 K271 A272 E273 A274 I275 H276 Y277 I278 G279 D280 L281 V282 Q283 R284 T285 E286 V287 E288 L289 L290 K291 T292 P293 N294 L295 G296 K297 K298 S299 L300

T301 E302 I303 K304 D305 V306 L307 A308 S309 R310 G311 L312 S313 L314 G315 M316 R317 L318 E319 N320 W321 P322 P323 A324 S325 I326 A327 D328 E329

- Molecule 14: DNA-directed RNA polymerase subunit beta'

Chain AE: 95% 89% 5% • 5%

MET LYS ASP LEU LEU LYS PHE LEU LYS ALA GLN THR LYS THR GLU E16 F17 D18 A19 I20 K21 I22 A23 L24 A25 S26 P27 D28 M29 I30 R31 S32 W33 S34 F35 G36 E37 V38 K39 K40 P41 E42 T43 I44 M45 Y46 R47 T48 F49 K50 P51 E52 R53 D54 G55 L56 F57 C58 A59 R60

I61 P64 V65 K66 D67 Y68 E69 C70 L71 C72 G73 K74 Y75 K76 R77 L78 K79 H80 R81 G82 V83 I84 C85 E86 K87 C88 G89 V90 E91 V92 T93 Q94 T95 K96 V97 R98 R99 E100 R101 M102 G103 H104 I105 E106 L107 A108 S109 P110 T111 A112 H113 I114 W115 F116 L117 K118 S119 L120 P121

S122 R123 I124 G125 L126 L127 L128 D129 M130 P131 L132 R133 D134 I135 E136 R137 V138 L139 Y140 F141 E142 S143 Y144 V145 V146 I147 E148 G149 G150 M151 T152 N153 L154 E155 R156 Q157 Q158 I159 L160 T161 E162 E163 Q164 Y165 L166 D167 A168 L169 E170 E171 F172 G173 D174 E175 F176 D177 A178 K179 M180 G181

A182 E183 A184 I185 Q186 A187 L188 L189 K190 S191 M192 D193 L194 E195 Q196 E197 C198 E199 Q200 L201 R202 E203 E204 L205 N206 E207 T208 N209 S210 E211 T212 K213 R214 K215 K216 L217 T218 K219 R220 I221 K222 L223 L224 E225 A226 F227 V228 Q229 S230 G231 N232 K233 P234 E235 W236 M237 I238 L239 T240 V241

L242 P243 V244 L245 P246 P247 D248 L249 R250 P251 L252 V253 P254 L255 D256 G257 G258 R259 F260 A261 T262 S263 D264 L265 N266 D267 L268 Y269 R270 R271 V272 I273 N274 R275 N276 N277 R278 L279 K280 R281 L282 L283 D284 L285 A286 A287 P288 D289 I290 I291 V292 R293 N294 E295 K296 R297 M298 L299 Q300 E301

A302 V303 D304 A305 L306 L307 D308 N309 G310 R311 R312 G313 R314 A315 I316 T317 G318 S319 N320 K321 R322 P323 L324 K325 S326 L327 A328 D329 M330 I331 K332 G333 K334 Q335 G336 R337 F338 R339 Q340 N341 L342 L343 G344 K345 R346 V347 D348 Y349 S350 G351 R352 S353 V354 I355 T356 V357 G358 P359 Y360 L361

R362 L363 H364 Q365 C366 G367 L368 P369 K370 K371 M372 A373 L374 E375 L376 F377 K378 P379 F380 I381 Y382 G383 K384 L385 E386 L387 R388 G389 L390 A391 T392 T393 I394 K395 A396 A397 K398 K399 M400 V401 E402 R403 E404 E405 A406 V407 V408 W409 D410 I411 L412 D413 E414 V415 I416 R417 E418 H419 P420 V421

L422 L423 N424 R425 A426 P427 T428 L429 H430 R431 L432 G433 I434 Q435 A436 F437 E438 P439 V440 L441 I442 E443 G444 K445 A446 I447 Q448 L449 H450 P451 L452 V453 C454 A455 A456 Y457 M458 A459 D460 F461 D462 G463 D464 Q465 M466 A467 V468 H469 V470 P471 L472 T473 L474 E475 A476 Q477 L478 E479 A480 R481

A482 L483 M484 M485 S486 T487 N488 N489 I490 L491 S492 P493 A494 N495 G496 E497 P498 I499 I500 V501 P502 S503 Q504 D505 V506 V507 L508 G509 L510 V511 Y512 M513 T514 R515 D516 C517 V518 N519 A520 K521 G522 E523 G524 M525 V526 L527 T528 G529 P530 K531 E532 A533 E534 R535 L536 Y537 R538 S539 G540 L541

A542 S543 L544 H545 A546 R547 V548 K549 V550 R551 I552 T553 E554 Y555 E556 K557 D558 A559 N560 G561 E562 L563 V564 A565 K566 T567 S568 L569 K570 D571 T572 T573 V574 G575 R576 A577 I578 L579 W580 M581 I582 V583 P584 K585 G586 L587 P588 Y589 S590 I591 V592 N593 Q594 A595 L596 G597 K598 K599 A600 I601

S602 K603 M604 L605 N606 T607 C608 Y609 R610 I611 L612 G613 L614 K615 P616 T617 V618 I619 F620 A621 D622 Q623 I624 M625 Y626 T627 G628 F629 A630 Y631 A632 A633 R634 S635 G636 A637 S638 V639 G640 I641 D642 D643 M644 V645 I646 P647 E648 K649 K650 H651 E652 I653 I654 S655 E656 A657 E658 A659 E660 V661

A662 E663 I664 Q665 E666 Q667 F668 Q669 S670 G671 L672 V673 T674 A675 G676 E677 R678 Y679 N680 K681 V682 I683 D684 I685 W686 A687 A688 A689 N690 D691 R692 V693 S694 K695 A696 M697 M698 D699 N700 L701 Q702 T703 E704 T705 V706 I707 N708 R709 D710 G711 Q712 E713 E714 K715 Q716 V717 S718 F719 N720 S721

I722 Y723 M724 M725 A726 D727 S728 G729 A730 R731 G732 S733 A734 A735 Q736 I737 R738 Q739 L740 A741 G742 M743 R744 G745 L746 M747 A748 K749 P750 D751 G752 S753 I754 I755 E756 T757 P758 I759 T760 A761 N762 F763 R764 E765 G766 L767 N768 V769 L770 Q771 Y772 F773 I774 S775 T776 H777 G778 A779 R780 K781

G782 L783 A784 D785 T786 A787 L788 K789 T790 A791 N792 S793 G794 Y795 L796 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 L807 V808 V809 T810 E811 D812 D813 C814 G815 T816 H817 E818 G819 I820 M821 M822 T823 P824 V825 I826 E827 G828 G829 D830 V831 K832 E833 P834 L835 R836 D837 R838 V839 L840 G841

R842 V843 T844 A845 E846 D847 V848 L849 K850 P851 G852 T853 A854 D855 I856 L857 V858 P859 R860 N861 T862 L863 L864 H865 E866 Q867 W868 C869 D870 L871 L872 E873 E874 N875 S876 V877 D878 A879 V880 K881 V882 R883 S884 V885 V886 S887 C888 D889 T890 D891 F892 G893 V894 C895 A896 H897 C898 Y899 G900 R901

D902 L903 A904 R905 G906 H907 I908 I909 N910 K911 G912 E913 A914 I915 G916 V917 I918 A919 A920 Q921 S922 I923 G924 E925 P926 G927 T928 Q929 L930 T931 M932 R933 THR PHE HIS ILE GLY GLY ALA ALA SER ARG ALA ALA ALA GLU S948 S949 I950 Q951 V952 K953 N954 K955 G956 S957 I958 K959 L960 S961

N962 V963 K964 S965 V966 V967 N968 S969 S970 G971 K972 L973 V974 I975 T976 S977 R978 N979 T980 E981 L982 K983 L984 I985 D986 E987 F988 G989 R990 T991 K992 E993 S994 Y995 K996 V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 Q1010 V1011 A1012 G1013 G1014 E1015 T1016 V1017 A1018 N1019 W1020 D1021

P1022 H1023 T1024 M1025 P1026 V1027 I1028 T1029 E1030 V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042 G1043 Q1044 T1045 I1046 T1047 R1048 Q1049 T1050 D1051 E1052 L1053 T1054 G1055 L1056 S1057 S1058 L1059 V1060 V1061 L1062 D1063 S1064 A1065 E1066 R1067 T1068 A1069 G1070 G1071 K1072 D1073 L1074 R1075 P1076 A1077 L1078 K1079 I1080 V1081

D1082 A1083 Q1084 G1085 N1086 D1087 V1088 L1089 I1090 P1091 G1092 T1093 D1094 M1095 P1096 A1097 Q1098 Y1099 F1100 L1101 P1102 G1103 K1104 A1105 I1106 V1107 Q1108 L1109 E1110 D1111 G1112 V1113 Q1114 I1115 S1116 S1117 G1118 D1119 T1120 L1121 A1122 R1123 I1124 P1125 Q1126 GLU SER GLY GLY THR LYS ASP ILE THR G1136 G1137 L1138 P1139 R1140 V1141

A1142 D1143 L1144 F1145 E1146 A1147 R1148 R1149 P1150 K1151 E1152 P1153 A1154 I1155 L1156 A1157 E1158 I1159 S1160 G1161 I1162 V1163 S1164 F1165 G1166 K1167 E1168 T1169 K1170 G1171 K1172 R1173 R1174 L1175 V1176 I1177 T1178 P1179 V1180 D1181 G1182 S1183 D1184 P1185 Y1186 E1187 E1188 M1189 I1190 P1191 K1192 W1193 R1194 Q1195 L1196 N1197 V1198 F1199 E1200 G1201

E1202 R1203 V1204 E1205 R1206 G1207 D1208 V1209 I1210 S1211 D1212 G1213 P1214 E1215 A1216 P1217 H1218 D1219 I1220 L1221 R1222 L1223 R1224 G1225 V1226 H1227 A1228 V1229 T1230 R1231 Y1232 I1233 V1234 N1235 E1236 V1237 Q1238 D1239 V1240 Y1241 R1242 L1243 Q1244 G1245 V1246 K1247 I1248 N1249 D1250 K1251 H1252 I1253 E1254 V1255 I1256 V1257 R1258 Q1259 M1260 L1261

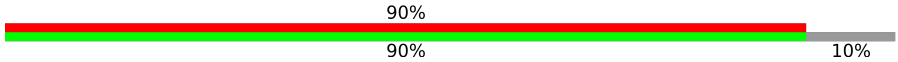
R1262 K1263 A1264 T1265 I1266 V1267 N1268 A1269 G1270 S1271 S1272 D1273 F1274 L1275 E1276 G1277 E1278 Q1279 V1280 E1281 Y1282 S1283 R1284 V1285 K1286 I1287 A1288 N1289 R1290 E1291 L1292 E1293 A1294 N1295 G1296 K1297 V1298 G1299 A1300 T1301 Y1302 S1303 R1304 D1305 L1306 L1307 G1308 I1309 T1310 K1311 A1312 S1313 L1314 A1315 T1316 E1317 S1318 F1319 I1320 S1321

A1322 A1323 S1324 F1325 Q1326 E1327 T1328 T1329 R1330 V1331 L1332 T1333 E1334 A1335 A1336 V1337 A1338 G1339 K1340 R1341 D1342 E1343 L1344 R1345 G1346 L1347 K1348 E1349 N1350 V1351 I1352 V1353 G1354 R1355 L1356 I1357 P1358 A1359 G1360 T1361 G1362 Y1363 A1364 Y1365 H1366 Q1367 D1368 R1369 M1370 R1371 R1372 R1373 ALA ALA GLY GLU ALA PRO ALA ALA

PRO GLN VAL THR ALA GLU ASP ALA SER ALA SER LEU ALA GLU LEU LEU ASN ALA GLY LEU GLY GLY SER ASP ASN GLU

- Molecule 15: DNA-directed RNA polymerase subunit omega

Chain AF:




MET ALA R3 V4 T5 V6 Q7 D8 A9 V10 E11 K12 I13 G14 N15 R16 F17 D18 L19 V20 L21 V22 A23 A24 R25 R26 A27 R28 Q29 M30 Q31 V32 G33 G34 K35 D36 P37 L38 V39 P40 E41 E42 N43 D44 K45 T46 T47 V48 I49 A50 L51 R52 E53 I54 E55 E56 G57 L58 I59 N60

N61 Q62 I63 L64 D65 V66 R67 E68 R69 Q70 E71 Q72 Q73 E74 Q75 E76 A77 A78 E79 L80 Q81 A82 V83 T84 ALA ILE ALA GLU GLY ARG ARG

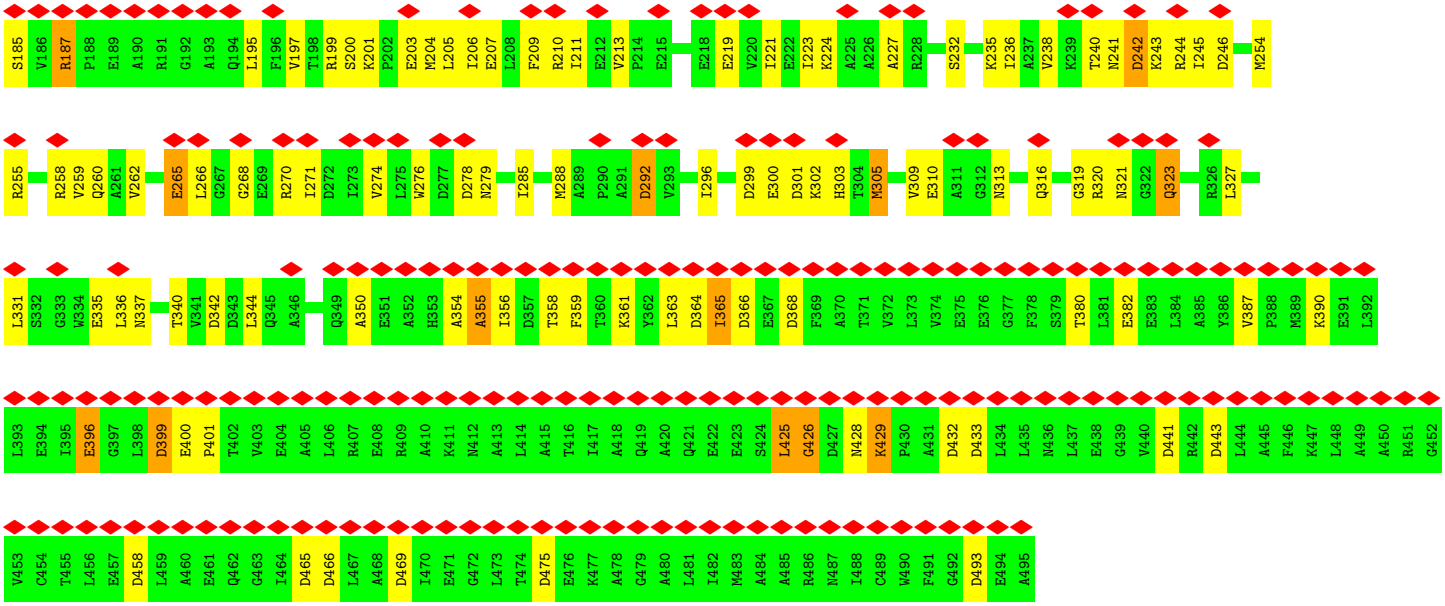
- Molecule 16: Transcription termination/antitermination protein NusA

Chain AG:

M1 N2 K3 E4 I5 L6 A7 V8 V9 E10 A11 V12 S13 N14 E15 K16 A17 L18 P19 R20 E21 K22 I23 F24 E25 A26 L27 E28 S29 A30 L31 A32 T33 A34 T35 K36 K37 K38 Y39 E40 Q41 E42 I43 D44 V45 R46 V47 Q48 I49 D50 R51 K52 S53 G54 D55 F56 D57 T58 F59 R60

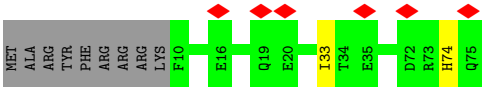
R61 W62 L63 V64 V65 D66 E67 V68 T69 Q70 P71 T72 K73 E74 I75 T76 L77 E78 A79 A80 R81 Y82 E83 D84 E85 S86 L87 N88 L89 G90 D91 Y92 V93 E94 D95 Q96 I97 E98 S99 V100 T101 F102 D103 R104 I105 T106 T107 Q108 T109 A110 K111 Q112 V113 I114 V115 Q116 K117 V118 R119 E120

A121 E122 R123 A124 M125 V126 V127 D128 Q129 F130 R131 E132 H133 E134 I138 T139 G140 V141 V142 K143 K144 V145 N146 R147 D148 N149 I150 D153 L154 G155 N156 N157 A158 E159 I162 L163 R164 E165 D166 M167 L168 P169 R170 E171 N172 F173 R174 P175 G176 D177 R178 V179 R180 G181 V182 L183 Y184



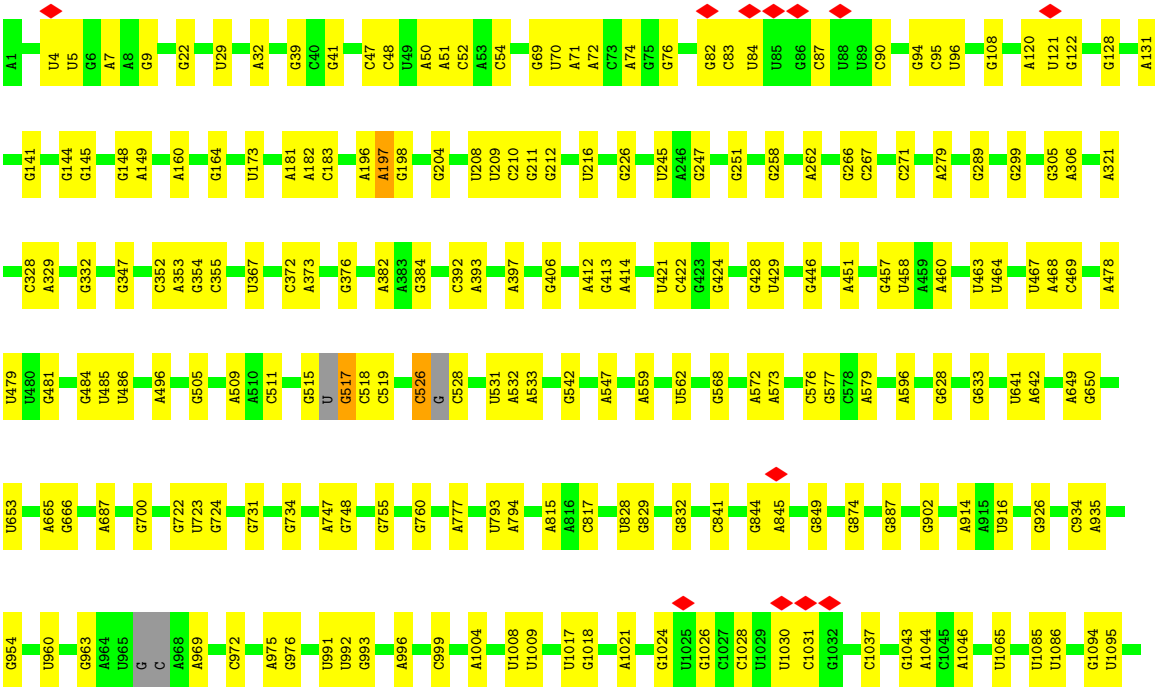

- Molecule 17: 30S ribosomal protein S18

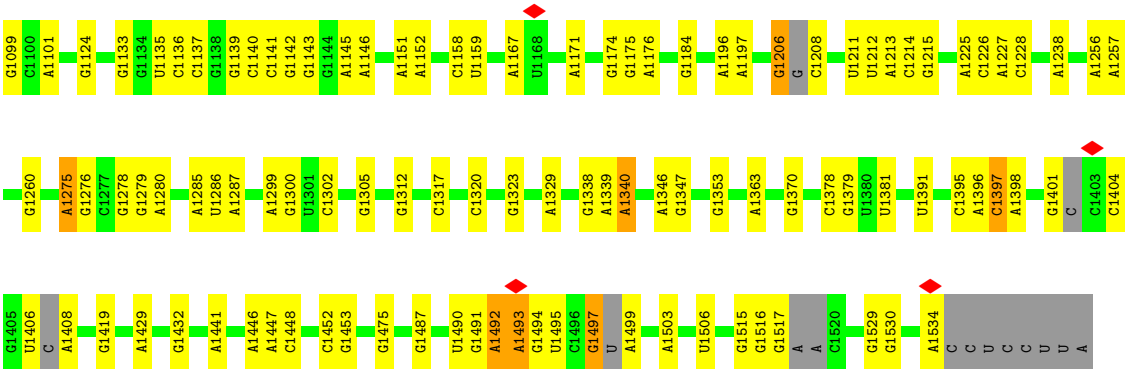
Chain C:




- Molecule 18: 16S rRNA

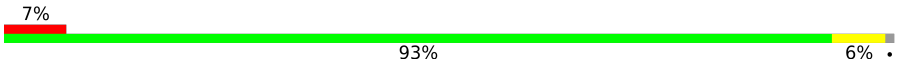
Chain D:

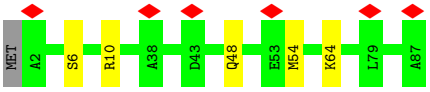





- Molecule 19: 30S ribosomal protein S20

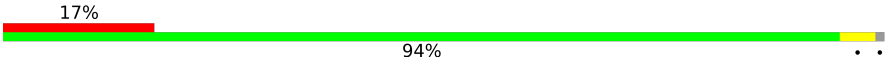
Chain E:

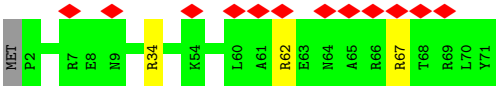



- Molecule 20: 30S ribosomal protein S21

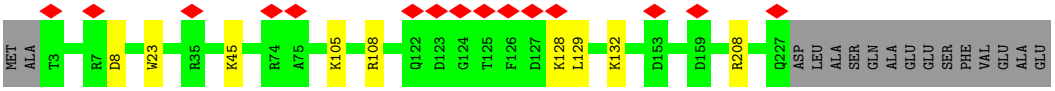
Chain F:



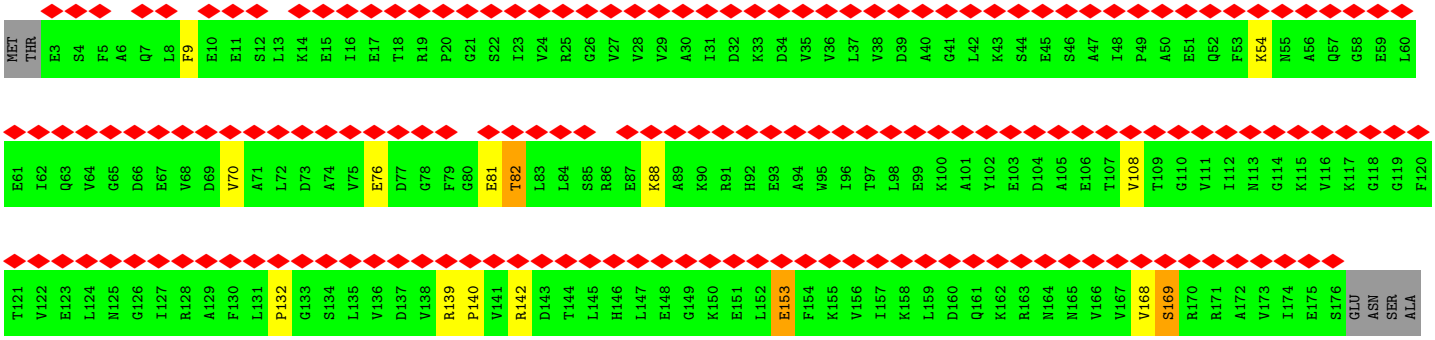

- Molecule 21: 30S ribosomal protein S2

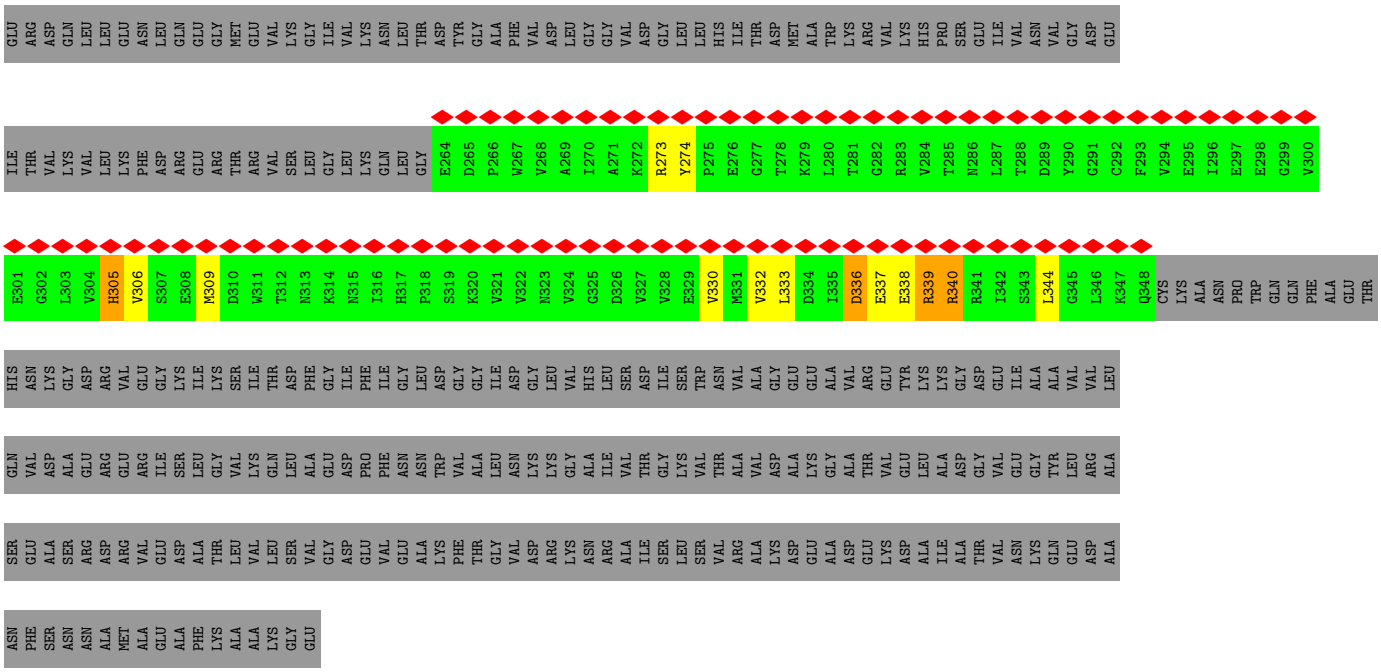
Chain G:




- Molecule 22: 30S ribosomal protein S1

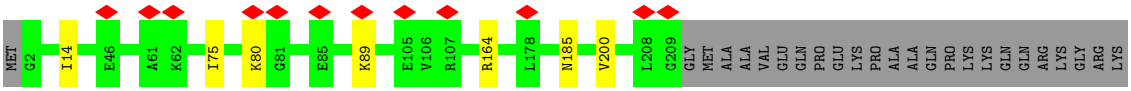
Chain H:





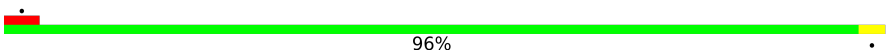

- Molecule 23: 30S ribosomal protein S3

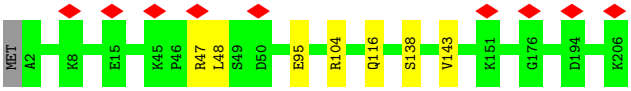
Chain I:




- Molecule 24: 30S ribosomal protein S4

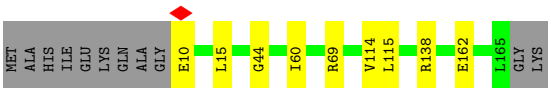
Chain J:



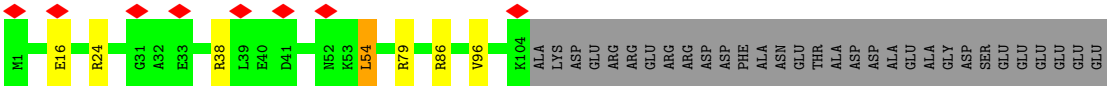

- Molecule 25: 30S ribosomal protein S5

Chain K:



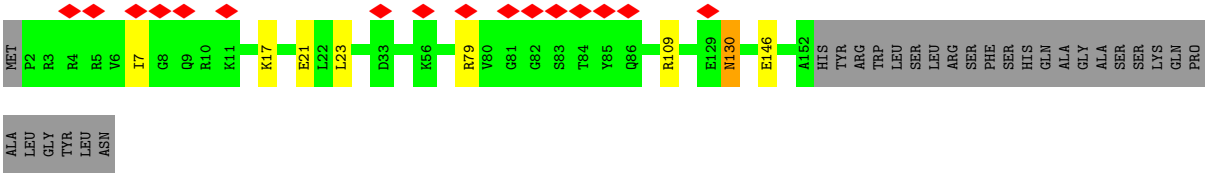

- Molecule 26: 30S ribosomal protein S6

Chain L:



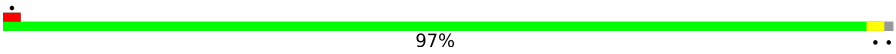
• Molecule 27: 30S ribosomal protein S7

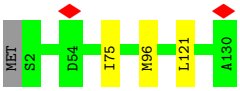
Chain M:




• Molecule 28: 30S ribosomal protein S8

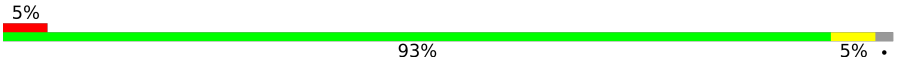
Chain N:

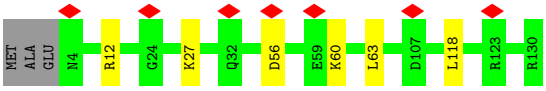



• Molecule 29: 30S ribosomal protein S9

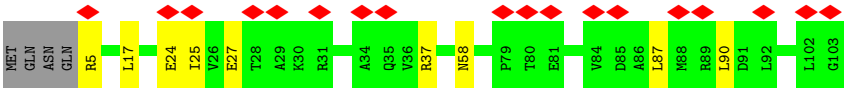
Chain O:



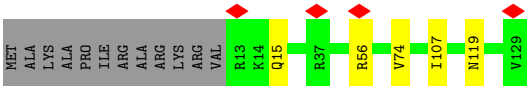

• Molecule 30: 30S ribosomal protein S10

Chain P:



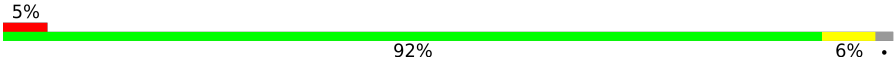

• Molecule 31: 30S ribosomal protein S11

Chain Q:



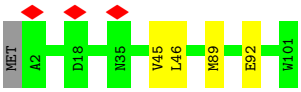

• Molecule 32: 30S ribosomal protein S12

Chain R:



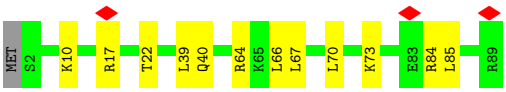
• Molecule 33: 30S ribosomal protein S14

Chain S: 95%



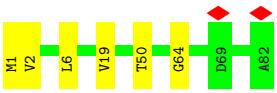

• Molecule 34: 30S ribosomal protein S15

Chain T: 85% 13%



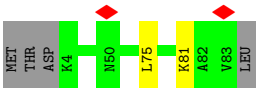

• Molecule 35: 30S ribosomal protein S16

Chain U: 93% 7%



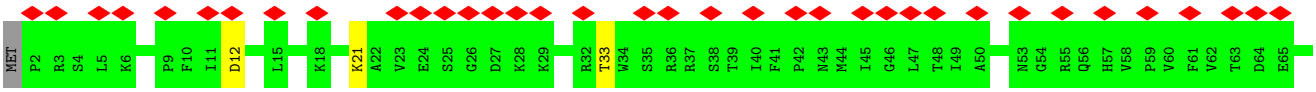

• Molecule 36: 30S ribosomal protein S17

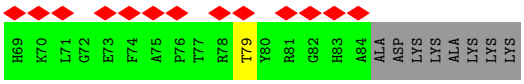
Chain V: 93% 5%




• Molecule 37: 30S ribosomal protein S19

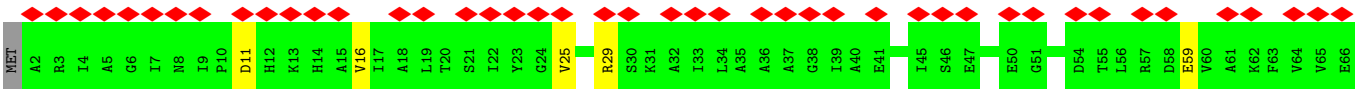
Chain W: 53% 86% 10%

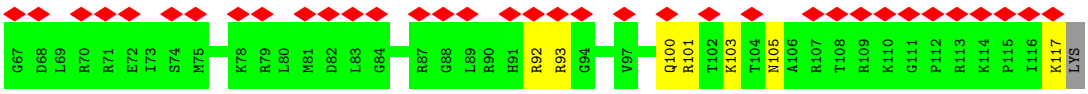



• Molecule 38: 30S ribosomal protein S13

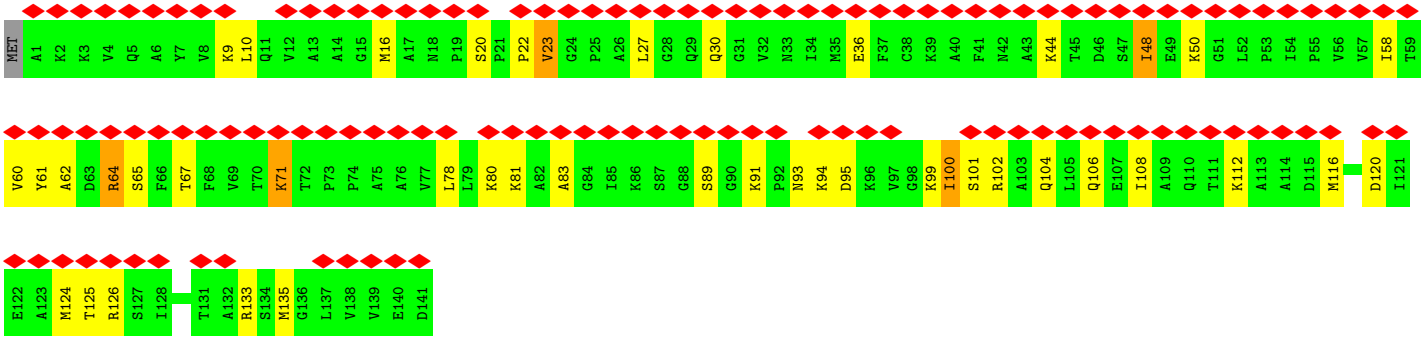
Chain X: 67% 88% 10%



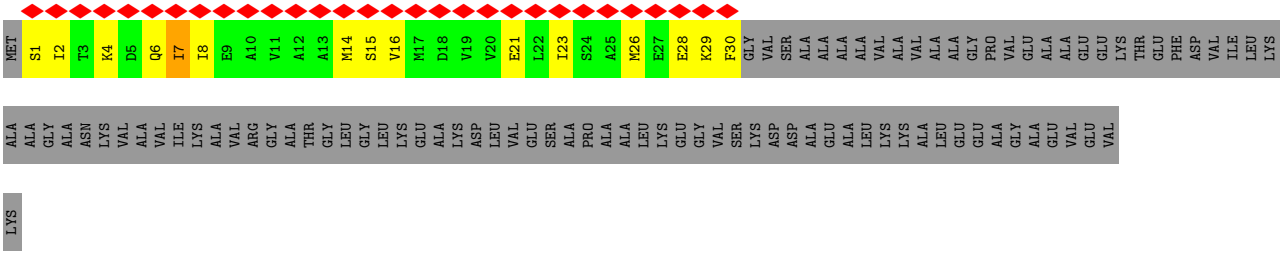
- Molecule 39: 50S ribosomal protein L11

Chain Y:



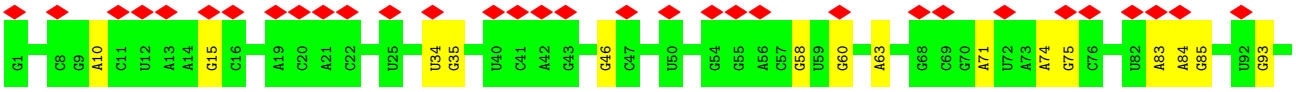

- Molecule 40: 50S ribosomal protein L7/L12

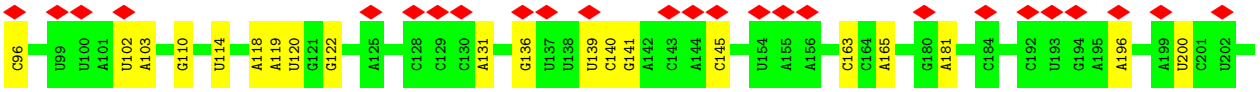
Chain Z:

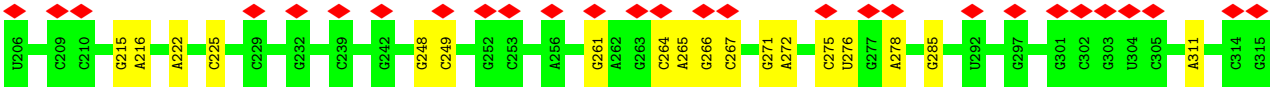


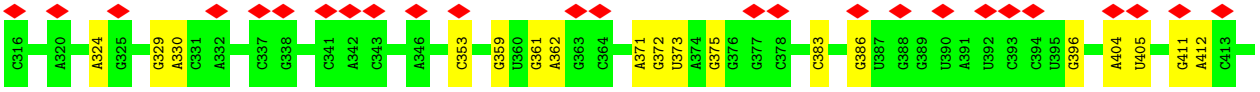

- Molecule 41: 23S rRNA

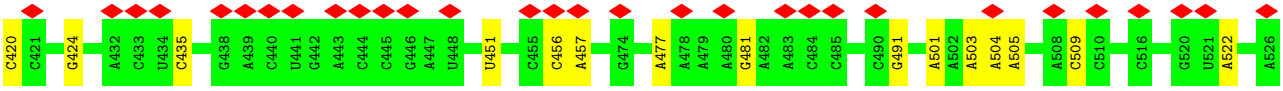
Chain a:

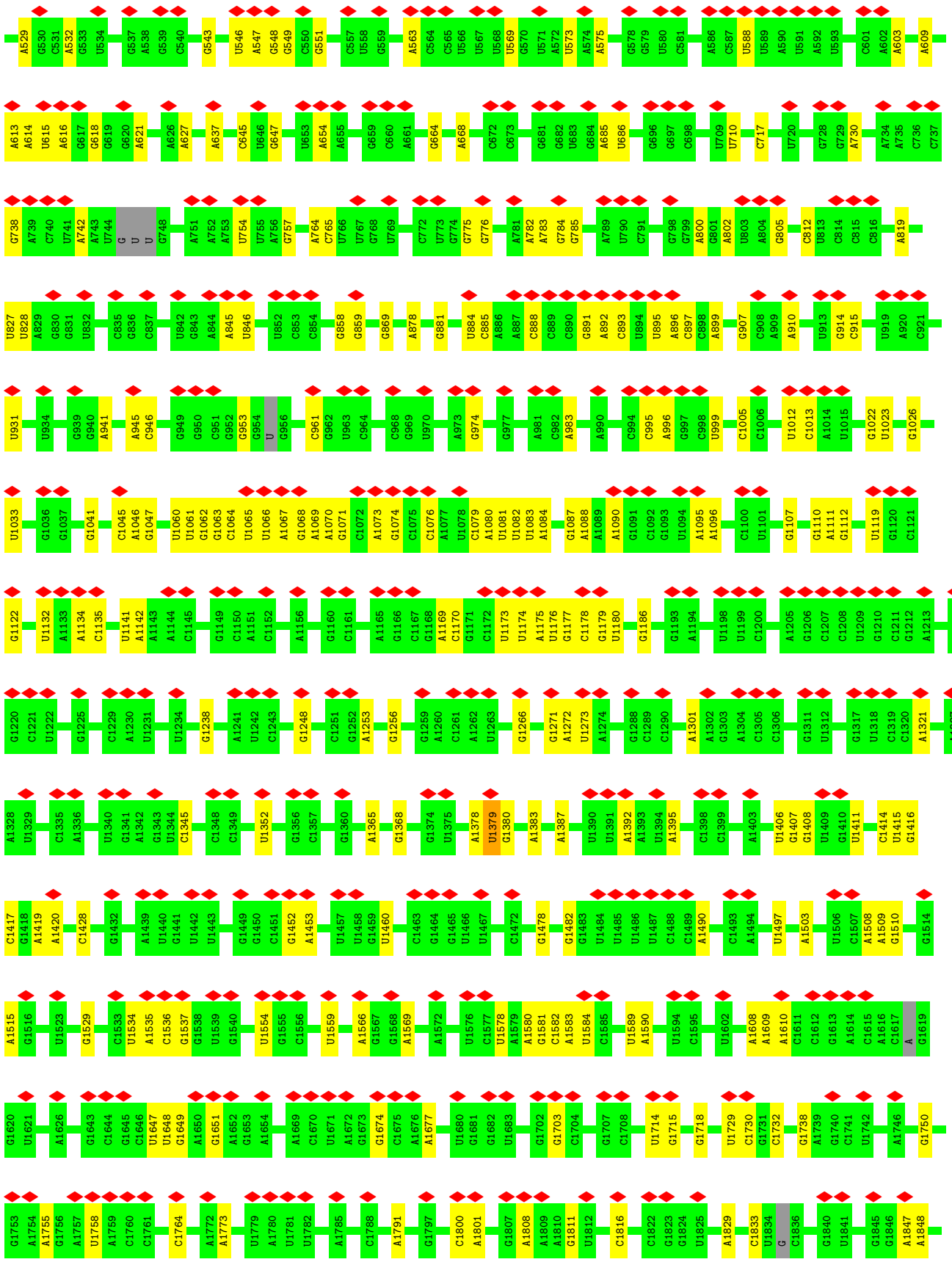


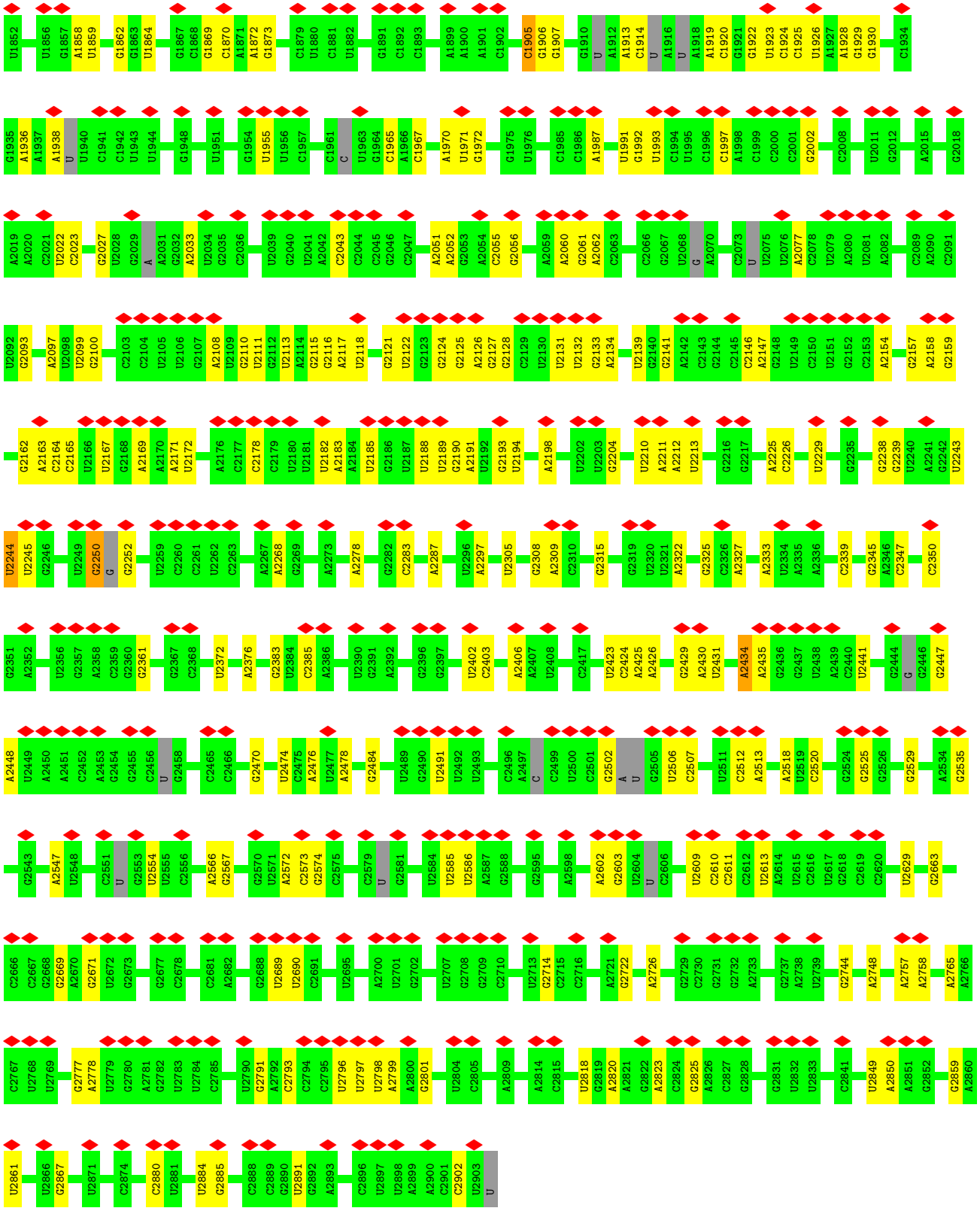




A529 G530 C531 A532 G533 U534 G537 A538 G539 C540 G543 U546 A547 G548 G549 C550 G551 C557 U558 G559 A563 C564 C565 U566 U567 U568 U569 G570 U571 A572 U573 A574 A575 G578 G579 U580 C581 A586 C587 U588 U589 A590 U591 A592 U593 C601 A602 A603 A609
A613 A614 U615 A616 G617 G618 G619 G620 A621 A626 A627 A637 C645 U646 G647 U653 A654 A655 G659 C660 A661 G664 A668 C672 C673 G681 G682 U683 G684 A685 U686 G696 G697 C698 U709 U710 C717 U720 G728 G729 A730 A734 A735 C736 C737
G738 A739 C740 U741 A742 A743 U744 G U U G748 A751 A752 A753 U754 U755 A756 G757 A764 C765 U766 U767 G768 U769 C772 U773 G774 G775 G776 A781 A782 A783 G784 G785 A789 U790 C791 G798 G799 A800 G801 A802 U803 A804 G805 C812 U813 C814 C815 C816 A819
U827 U828 A829 G830 G831 U832 C835 G836 C837 U842 G843 A844 A845 U846 U852 C853 C854 G858 G859 G869 A878 G881 U884 C885 A886 A887 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 G907 C908 A909 A910 U913 G914 C915 U919 A920 C921
U931 U934 G939 G940 A941 A945 C946 G949 G950 C951 G952 G953 G954 U U G956 C961 G962 U963 C964 G968 G969 U970 A973 G974 G977 A981 C982 A983 A990 C994 C995 A996 G997 C998 U999 C1005 C1006 U1012 C1013 A1014 U1015 G1022 U1023 G1026
U1033 G1036 G1037 G1041 C1045 A1046 G1047 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 C1100 U1101 G1107 G1110 A1111 G1112 U1119 G1120 C1121
G1122 U1132 A1133 A1134 C1135 U1141 A1142 A1143 A1144 C1145 G1149 C1150 A1151 C1152 A1156 G1160 C1161 A1165 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 G1186 G1193 A1194 U1198 U1199 C1200 A1205 G1206 C1207 C1208 U1209 G1210 C1211 G1212 A1213 U1219
G1220 C1221 U1222 G1225 C1229 A1230 U1231 U1234 G1238 A1241 U1242 C1243 G1248 C1251 G1252 A1253 G1256 G1259 A1260 C1261 A1262 U1263 G1266 G1271 A1272 U1273 A1274 G1288 C1289 C1290 A1301 A1302 G1303 A1304 C1305 C1306 G1311 U1312 G1317 U1318 C1319 C1320 A1321 A1327
A1328 U1329 C1335 A1336 U1340 G1341 A1342 G1343 U1344 C1345 C1348 C1349 U1352 G1356 C1357 G1360 A1365 G1368 G1374 U1375 A1378 U1379 G1380 A1383 A1387 U1390 U1391 A1392 A1393 U1394 A1395 C1398 C1399 A1403 U1406 G1407 G1408 U1409 G1410 U1411 C1414 U1415 G1416
C1417 G1418 A1419 A1420 C1428 G1432 A1439 U1440 G1441 U1442 U1443 G1449 G1450 C1451 G1452 A1453 U1457 U1458 G1459 U1460 C1463 G1464 G1465 U1466 U1467 C1472 G1478 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489 A1490 C1493 A1494 U1497 A1503 U1506 C1507 A1508 A1509 G1510 G1514
A1515 G1516 U1523 G1529 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 U1554 G1555 C1556 U1559 A1566 G1567 G1568 A1569 A1572 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 U1589 A1590 U1594 C1595 U1602 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A G1619
G1620 U1621 A1626 G1643 C1644 G1645 C1646 U1647 U1648 G1649 A1650 G1651 A1652 G1653 A1654 A1669 C1670 U1671 A1672 G1673 G1674 C1675 A1676 A1677 U1680 G1681 G1682 U1683 G1702 G1703 C1704 G1707 C1708 U1714 G1715 G1718 U1729 C1730 G1731 C1732 G1738 A1739 G1740 C1741 U1742 A1746 G1750
G1753 A1754 A1755 G1756 A1757 U1758 A1759 C1760 C1761 C1764 A1772 A1773 U1779 A1780 U1781 U1782 A1785 C1788 A1791 G1797 C1800 A1801 G1807 A1808 A1809 A1810 G1811 U1812 C1816 C1822 G1823 G1824 U1825 A1829 C1833 U1834 G C1836 G1840 U1841 G1845 G1846 A1847 A1848

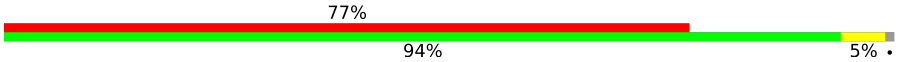


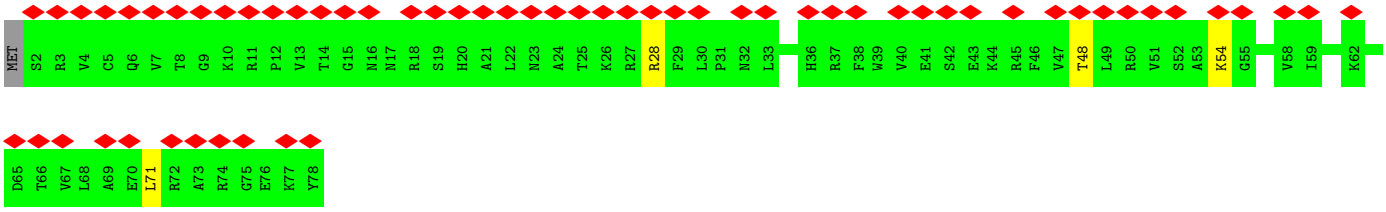
- Molecule 42: 50S ribosomal protein L27

Chain b:

• Molecule 43: 50S ribosomal protein L28

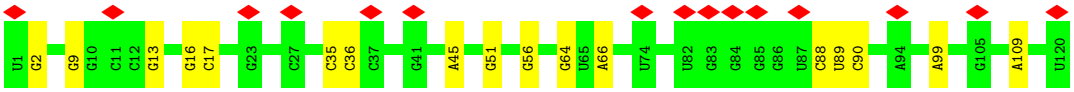
Chain c:



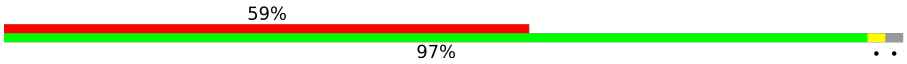

• Molecule 44: 5S rRNA

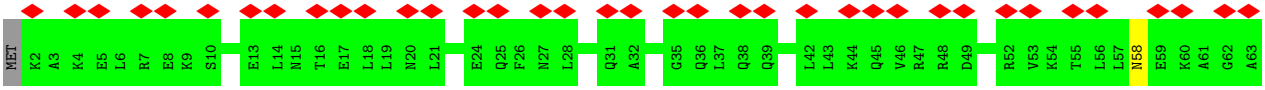
Chain d:




• Molecule 45: 50S ribosomal protein L29

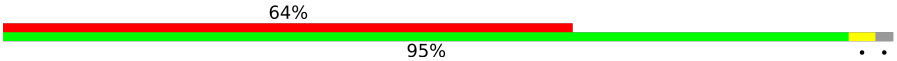
Chain e:

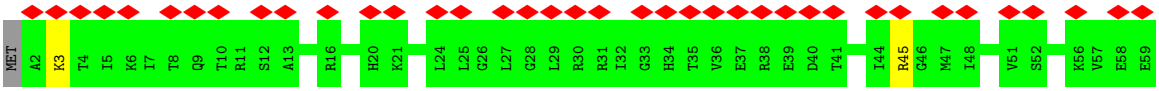



• Molecule 46: 50S ribosomal protein L30

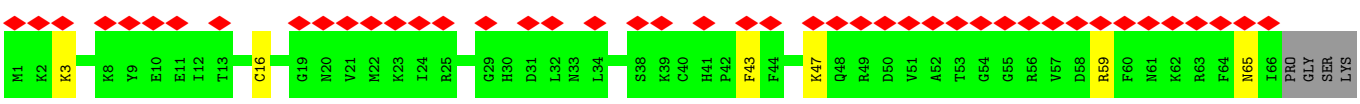
Chain f:



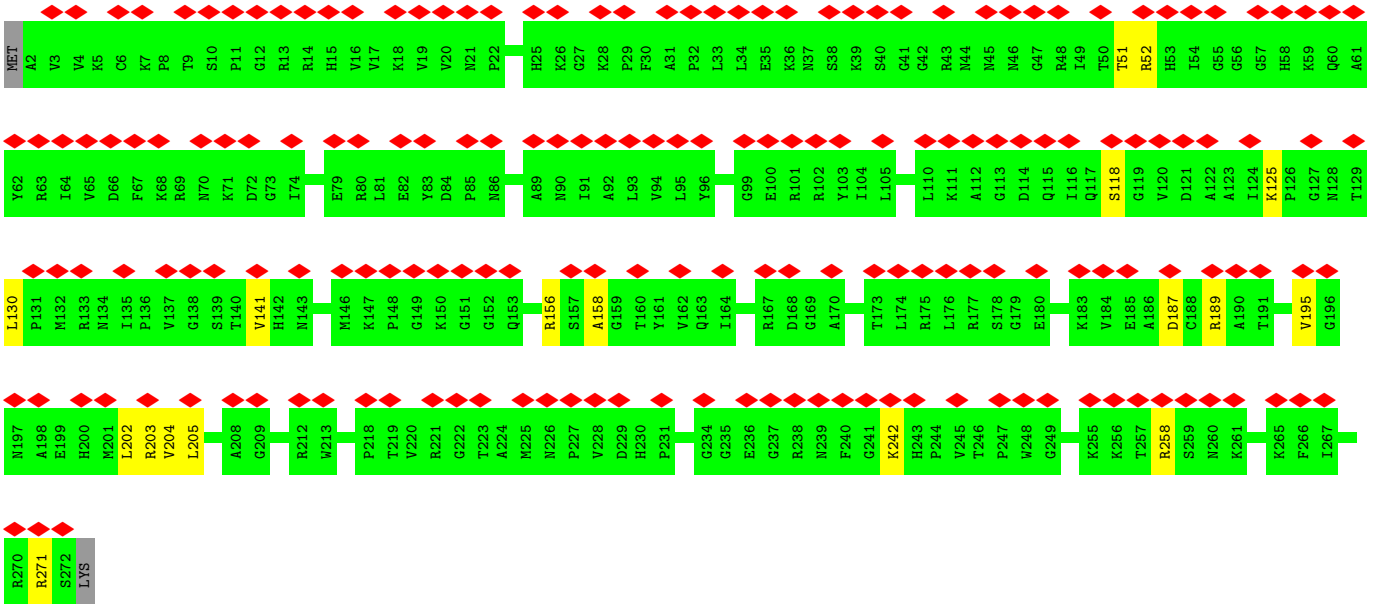

• Molecule 47: 50S ribosomal protein L31

Chain g:




• Molecule 48: 50S ribosomal protein L2

Chain h: 66% 93% 7%

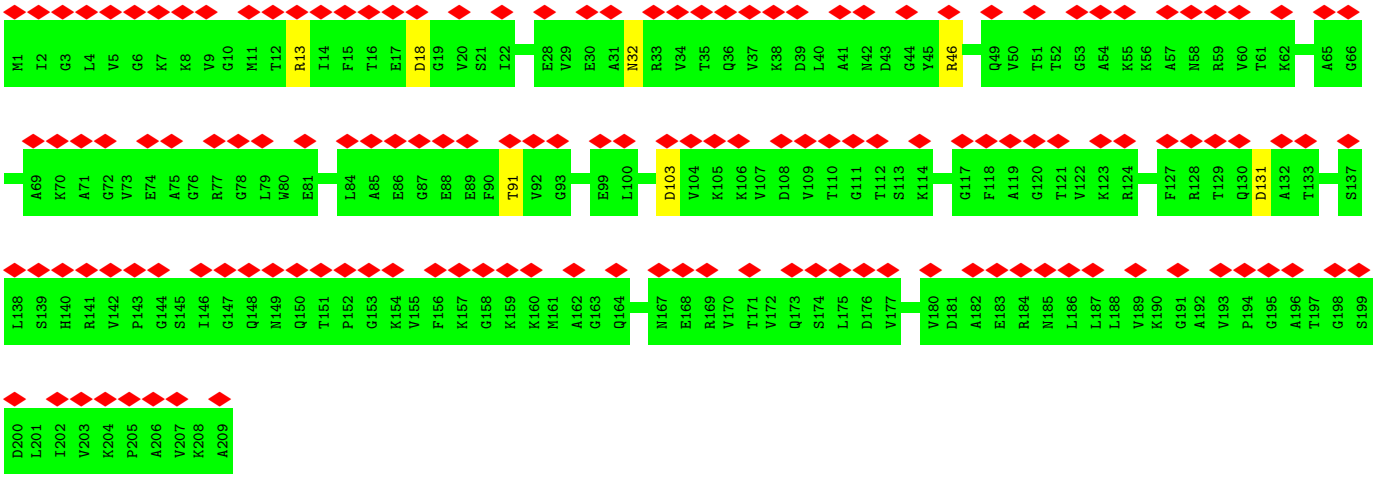



- Molecule 49: 50S ribosomal protein L32

Chain i: 61% 88% 11%

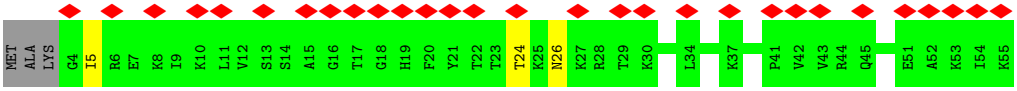
- Molecule 50: 50S ribosomal protein L3

Chain j: 69% 97%



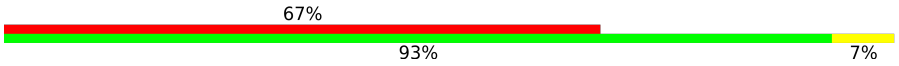

- Molecule 51: 50S ribosomal protein L33

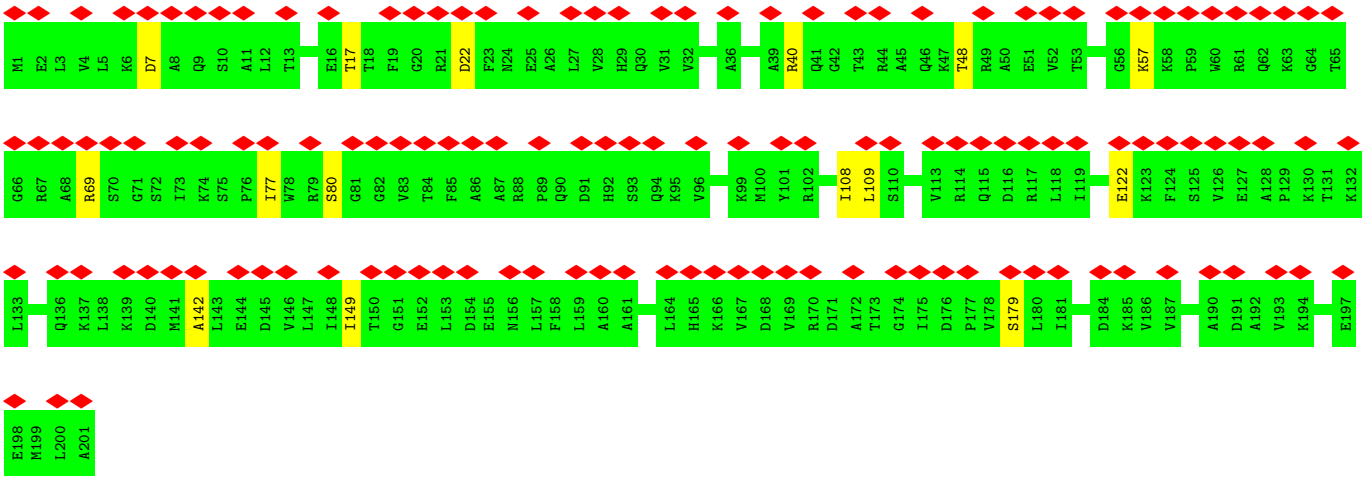
Chain k: 53% 89% 5% 5%




- Molecule 52: 50S ribosomal protein L4

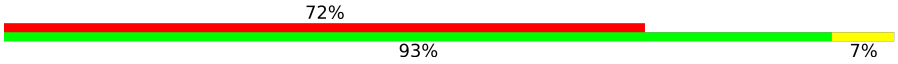
Chain l:

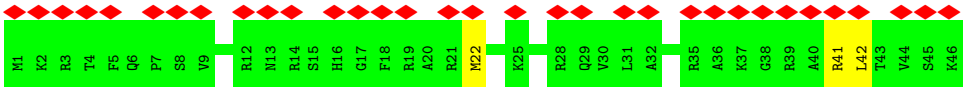



- Molecule 53: 50S ribosomal protein L34

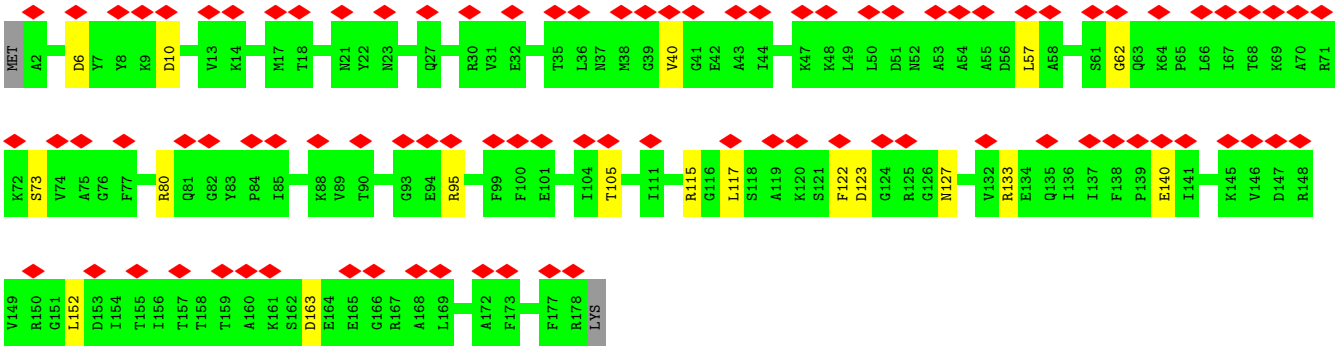
Chain m:



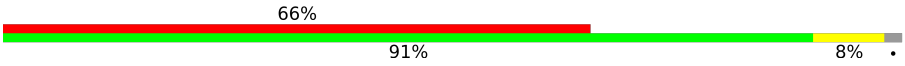

- Molecule 54: 50S ribosomal protein L5

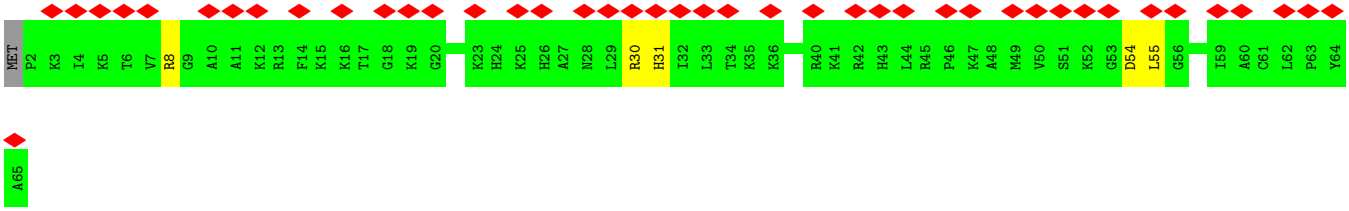
Chain n:




- Molecule 55: 50S ribosomal protein L35

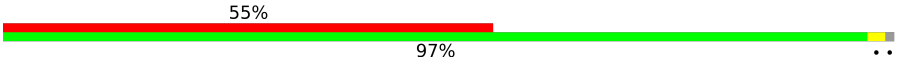
Chain o:

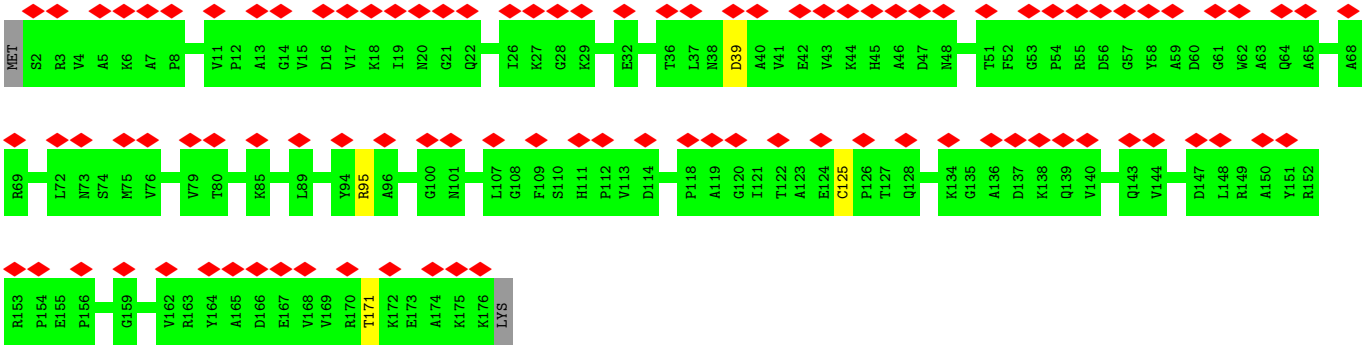





• Molecule 56: 50S ribosomal protein L6

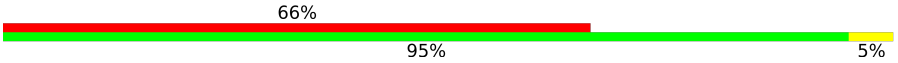
Chain p:

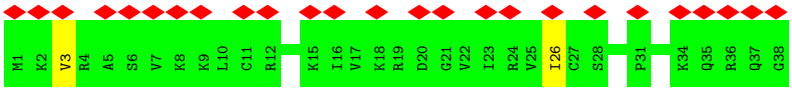



• Molecule 57: 50S ribosomal protein L36

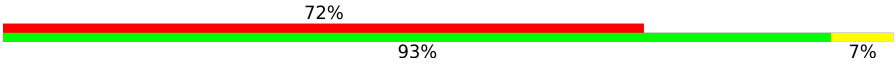
Chain q:

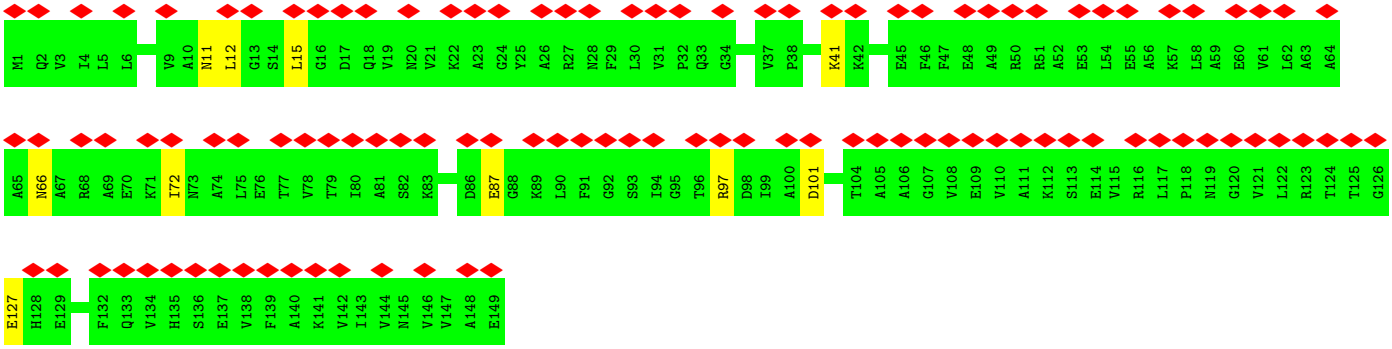



• Molecule 58: 50S ribosomal protein L9

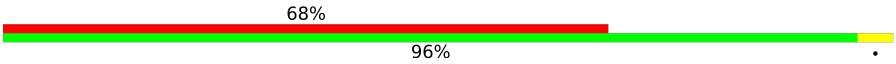
Chain r:



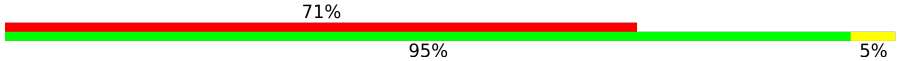

• Molecule 59: 50S ribosomal protein L13

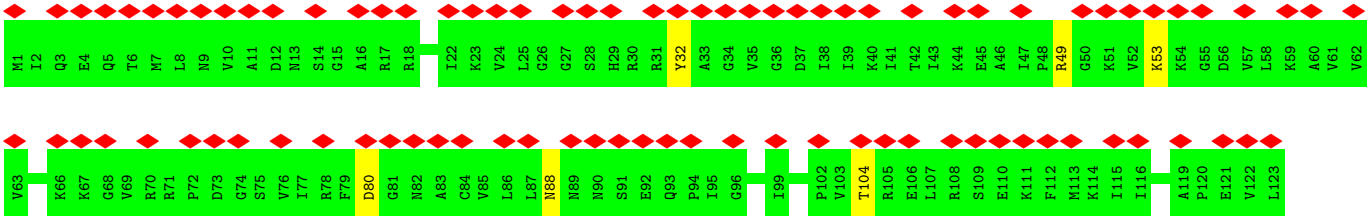
Chain s:



- Molecule 60: 50S ribosomal protein L14

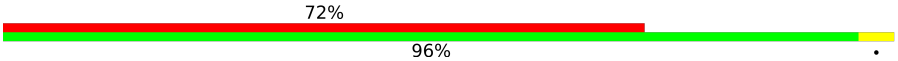
Chain t:

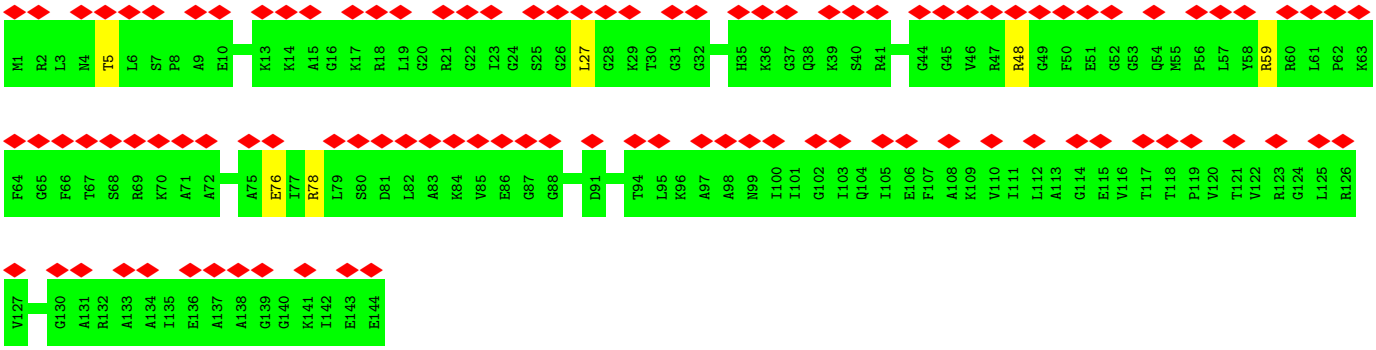



- Molecule 61: 50S ribosomal protein L15

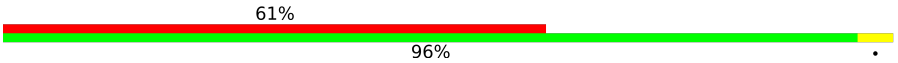
Chain u:

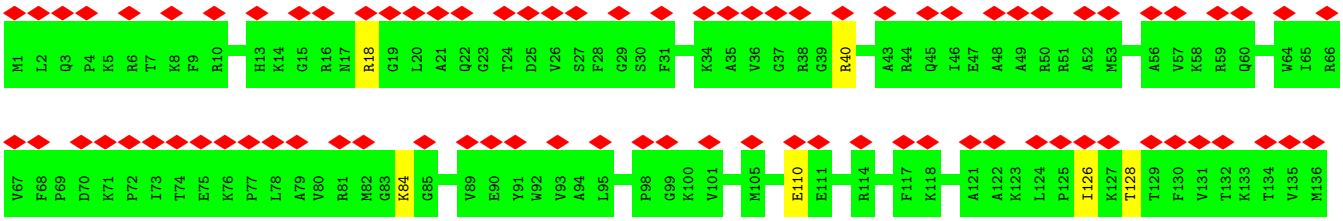



- Molecule 62: 50S ribosomal protein L16

Chain v:



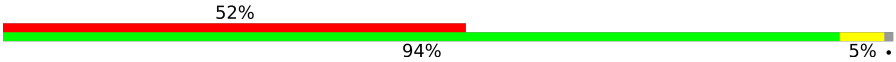



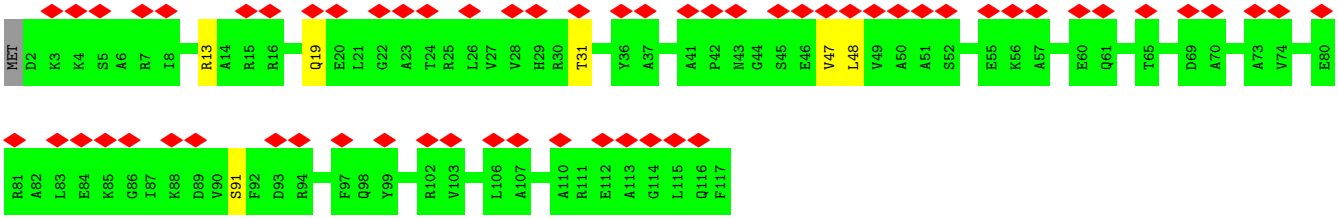

- Molecule 63: 50S ribosomal protein L17

Chain w:

- Molecule 64: 50S ribosomal protein L18

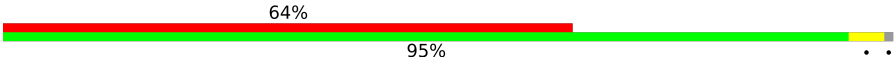
Chain x:

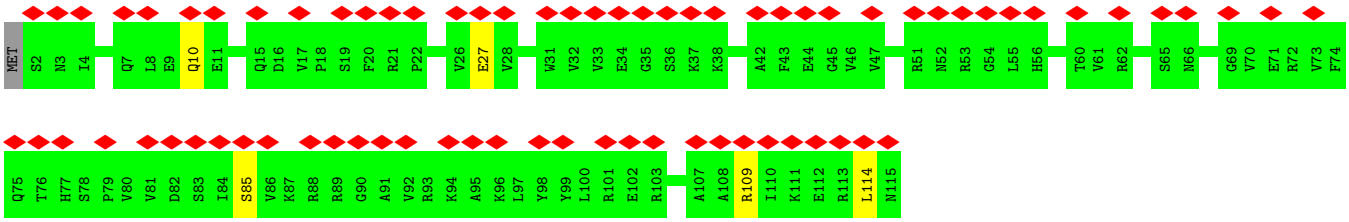



- Molecule 65: 50S ribosomal protein L19

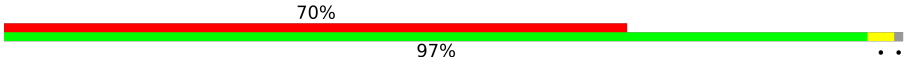
Chain y:

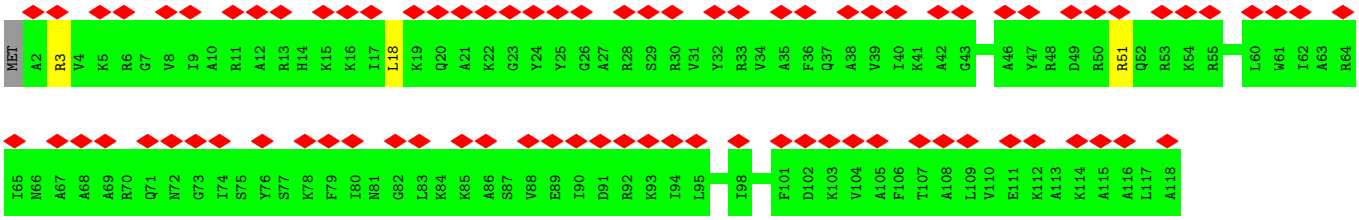



- Molecule 66: 50S ribosomal protein L20

Chain z:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 38957 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 45 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.065 | Depositor |
| Minimum map value | -0.026 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.014 | Depositor |
| Map size (Å) | 532.48, 532.48, 532.48 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.04, 1.04, 1.04 | 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: MG, ZN

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | 0 | 0.38 | 0/829 | 0.67 | 0/1107 |
| 2 | 1 | 0.49 | 0/864 | 0.82 | 0/1156 |
| 3 | 2 | 0.41 | 0/752 | 0.71 | 0/1005 |
| 4 | 3 | 0.35 | 0/796 | 0.66 | 2/1062 (0.2%) |
| 5 | 4 | 0.40 | 0/766 | 0.68 | 0/1025 |
| 6 | 5 | 1.13 | 6/528 (1.1%) | 0.97 | 1/810 (0.1%) |
| 7 | 6 | 1.11 | 4/603 (0.7%) | 0.96 | 0/926 |
| 8 | 7 | 0.74 | 7/761 (0.9%) | 0.99 | 3/1178 (0.3%) |
| 9 | 9 | 0.79 | 2/1131 (0.2%) | 0.64 | 1/1524 (0.1%) |
| 10 | A | 0.38 | 0/1810 | 0.75 | 1/2821 (0.0%) |
| 10 | B | 0.46 | 2/1810 (0.1%) | 0.85 | 7/2821 (0.2%) |
| 11 | AA | 0.44 | 1/10736 (0.0%) | 0.61 | 2/14487 (0.0%) |
| 12 | AB | 0.68 | 2/1310 (0.2%) | 0.67 | 2/1766 (0.1%) |
| 13 | AC | 0.38 | 0/2113 | 0.58 | 0/2877 |
| 13 | AD | 0.34 | 0/2096 | 0.59 | 0/2854 |
| 14 | AE | 0.52 | 4/10545 (0.0%) | 0.66 | 6/14236 (0.0%) |
| 15 | AF | 0.33 | 0/652 | 0.57 | 0/879 |
| 16 | AG | 0.65 | 2/3897 (0.1%) | 0.89 | 31/5273 (0.6%) |
| 17 | C | 0.48 | 0/553 | 0.83 | 0/743 |
| 18 | D | 0.33 | 10/36610 (0.0%) | 0.73 | 30/57091 (0.1%) |
| 19 | E | 0.57 | 0/675 | 0.85 | 0/895 |
| 20 | F | 0.56 | 0/597 | 0.87 | 0/792 |
| 21 | G | 0.48 | 0/1791 | 0.71 | 0/2413 |
| 22 | H | 0.54 | 1/1746 (0.1%) | 1.03 | 13/2382 (0.5%) |
| 23 | I | 0.43 | 0/1663 | 0.71 | 0/2241 |
| 24 | J | 0.47 | 0/1665 | 0.73 | 0/2227 |
| 25 | K | 0.45 | 0/1165 | 0.75 | 0/1568 |
| 26 | L | 0.43 | 0/867 | 0.76 | 1/1171 (0.1%) |
| 27 | M | 0.50 | 0/1195 | 0.81 | 0/1602 |
| 28 | N | 0.41 | 0/989 | 0.69 | 0/1326 |
| 29 | O | 0.43 | 0/1034 | 0.75 | 0/1375 |
| 30 | P | 0.43 | 0/800 | 0.75 | 0/1082 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 31 | Q | 0.40 | 0/893 | 0.70 | 0/1205 |
| 32 | R | 0.35 | 0/952 | 0.74 | 0/1274 |
| 33 | S | 0.49 | 0/817 | 0.79 | 0/1088 |
| 34 | T | 0.53 | 0/722 | 0.86 | 0/964 |
| 35 | U | 0.44 | 0/659 | 0.78 | 0/884 |
| 36 | V | 0.34 | 0/657 | 0.61 | 0/881 |
| 37 | W | 0.38 | 0/680 | 0.62 | 0/915 |
| 38 | X | 0.49 | 0/909 | 0.86 | 0/1215 |
| 39 | Y | 0.66 | 0/1046 | 0.58 | 0/1410 |
| 40 | Z | 0.69 | 0/227 | 0.57 | 0/304 |
| 41 | a | 0.38 | 3/69247 (0.0%) | 0.72 | 18/107985 (0.0%) |
| 42 | b | 0.39 | 0/589 | 0.71 | 0/779 |
| 43 | c | 0.48 | 0/635 | 0.81 | 2/848 (0.2%) |
| 44 | d | 0.29 | 0/2872 | 0.69 | 0/4478 |
| 45 | e | 0.54 | 0/502 | 0.82 | 0/667 |
| 46 | f | 0.45 | 0/452 | 0.78 | 0/605 |
| 47 | g | 0.43 | 0/531 | 0.68 | 0/709 |
| 48 | h | 0.39 | 0/2121 | 0.78 | 0/2852 |
| 49 | i | 0.40 | 0/450 | 0.79 | 0/599 |
| 50 | j | 0.43 | 0/1586 | 0.69 | 0/2134 |
| 51 | k | 0.35 | 0/433 | 0.65 | 0/576 |
| 52 | l | 0.46 | 0/1571 | 0.77 | 0/2113 |
| 53 | m | 0.53 | 0/380 | 0.99 | 0/498 |
| 54 | n | 0.49 | 0/1434 | 0.88 | 3/1926 (0.2%) |
| 55 | o | 0.45 | 0/513 | 0.83 | 0/676 |
| 56 | p | 0.39 | 0/1333 | 0.67 | 0/1805 |
| 57 | q | 0.37 | 0/303 | 0.77 | 0/397 |
| 58 | r | 0.43 | 0/1122 | 0.69 | 0/1515 |
| 59 | s | 0.50 | 0/1152 | 0.75 | 0/1551 |
| 60 | t | 0.41 | 0/955 | 0.78 | 0/1279 |
| 61 | u | 0.40 | 0/1062 | 0.76 | 0/1413 |
| 62 | v | 0.46 | 0/1093 | 0.81 | 0/1460 |
| 63 | w | 0.52 | 0/964 | 0.87 | 0/1289 |
| 64 | x | 0.46 | 0/902 | 0.81 | 0/1209 |
| 65 | y | 0.41 | 0/929 | 0.72 | 1/1242 (0.1%) |
| 66 | z | 0.60 | 0/960 | 0.91 | 0/1278 |
| All | All | 0.43 | 44/195002 (0.0%) | 0.73 | 124/286738 (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 |
|---|---|---|---|
| 10 | A | 0 | 2 |
| 10 | B | 0 | 2 |
| 13 | AC | 0 | 3 |
| 13 | AD | 0 | 1 |
| 14 | AE | 0 | 5 |
| 16 | AG | 0 | 6 |
| 22 | H | 0 | 3 |
| 38 | X | 0 | 1 |
| All | All | 0 | 23 |

The worst 5 of 44 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | 9 | 130 | PRO | N-CA | 13.75 | 1.70 | 1.47 |
| 18 | D | 1516 | G | O3'-P | -13.40 | 1.45 | 1.61 |
| 12 | AB | 124 | PRO | N-CA | 13.13 | 1.69 | 1.47 |
| 18 | D | 1339 | A | O3'-P | 10.58 | 1.73 | 1.61 |
| 14 | AE | 88 | CYS | CB-SG | -10.21 | 1.64 | 1.82 |

The worst 5 of 124 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | D | 1516 | G | P-O3'-C3' | -19.01 | 96.89 | 119.70 |
| 18 | D | 1516 | G | O3'-P-O5' | 13.81 | 130.24 | 104.00 |
| 16 | AG | 104 | ARG | C-N-CA | 13.00 | 154.21 | 121.70 |
| 41 | a | 2252 | G | N9-C1'-C2' | -10.96 | 99.75 | 114.00 |
| 12 | AB | 124 | PRO | CA-N-CD | -10.70 | 96.53 | 111.50 |

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 10 | A | 19 | G | Sidechain |
| 10 | A | 7 | G | Sidechain |
| 13 | AC | 192 | VAL | Peptide |
| 13 | AC | 319 | GLU | Peptide |
| 13 | AC | 321 | TRP | 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 | 101/103 (98%) | 97 (96%) | 3 (3%) | 1 (1%) | 15 54 |
| 2 | 1 | 108/110 (98%) | 104 (96%) | 4 (4%) | 0 | 100 100 |
| 3 | 2 | 92/100 (92%) | 90 (98%) | 2 (2%) | 0 | 100 100 |
| 4 | 3 | 101/104 (97%) | 96 (95%) | 4 (4%) | 1 (1%) | 15 54 |
| 5 | 4 | 92/94 (98%) | 91 (99%) | 1 (1%) | 0 | 100 100 |
| 9 | 9 | 146/165 (88%) | 95 (65%) | 37 (25%) | 14 (10%) | 0 3 |
| 11 | AA | 1338/1342 (100%) | 1206 (90%) | 126 (9%) | 6 (0%) | 34 69 |
| 12 | AB | 158/181 (87%) | 119 (75%) | 26 (16%) | 13 (8%) | 1 5 |
| 13 | AC | 295/329 (90%) | 274 (93%) | 19 (6%) | 2 (1%) | 22 61 |
| 13 | AD | 293/329 (89%) | 269 (92%) | 24 (8%) | 0 | 100 100 |
| 14 | AE | 1329/1407 (94%) | 1199 (90%) | 121 (9%) | 9 (1%) | 22 61 |
| 15 | AF | 80/91 (88%) | 77 (96%) | 3 (4%) | 0 | 100 100 |
| 16 | AG | 493/495 (100%) | 376 (76%) | 86 (17%) | 31 (6%) | 1 10 |
| 17 | C | 64/75 (85%) | 63 (98%) | 1 (2%) | 0 | 100 100 |
| 19 | E | 84/87 (97%) | 83 (99%) | 1 (1%) | 0 | 100 100 |
| 20 | F | 68/71 (96%) | 68 (100%) | 0 | 0 | 100 100 |
| 21 | G | 223/241 (92%) | 210 (94%) | 13 (6%) | 0 | 100 100 |
| 22 | H | 255/557 (46%) | 188 (74%) | 55 (22%) | 12 (5%) | 2 17 |
| 23 | I | 206/233 (88%) | 196 (95%) | 9 (4%) | 1 (0%) | 29 67 |
| 24 | J | 203/206 (98%) | 198 (98%) | 5 (2%) | 0 | 100 100 |
| 25 | K | 154/167 (92%) | 146 (95%) | 7 (4%) | 1 (1%) | 25 64 |
| 26 | L | 102/135 (76%) | 97 (95%) | 4 (4%) | 1 (1%) | 15 54 |
| 27 | M | 149/179 (83%) | 144 (97%) | 4 (3%) | 1 (1%) | 22 61 |
| 28 | N | 127/130 (98%) | 121 (95%) | 5 (4%) | 1 (1%) | 19 58 |
| 29 | O | 125/130 (96%) | 115 (92%) | 9 (7%) | 1 (1%) | 19 58 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 30 | P | 97/103 (94%) | 88 (91%) | 8 (8%) | 1 (1%) | 15 | 54 |
| 31 | Q | 115/129 (89%) | 104 (90%) | 9 (8%) | 2 (2%) | 9 | 42 |
| 32 | R | 117/124 (94%) | 116 (99%) | 1 (1%) | 0 | 100 | 100 |
| 33 | S | 98/101 (97%) | 96 (98%) | 2 (2%) | 0 | 100 | 100 |
| 34 | T | 86/89 (97%) | 82 (95%) | 4 (5%) | 0 | 100 | 100 |
| 35 | U | 80/82 (98%) | 75 (94%) | 4 (5%) | 1 (1%) | 12 | 47 |
| 36 | V | 78/84 (93%) | 74 (95%) | 4 (5%) | 0 | 100 | 100 |
| 37 | W | 81/92 (88%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 38 | X | 114/118 (97%) | 107 (94%) | 5 (4%) | 2 (2%) | 8 | 41 |
| 39 | Y | 139/142 (98%) | 102 (73%) | 25 (18%) | 12 (9%) | 1 | 4 |
| 40 | Z | 28/121 (23%) | 19 (68%) | 7 (25%) | 2 (7%) | 1 | 8 |
| 42 | b | 74/85 (87%) | 69 (93%) | 5 (7%) | 0 | 100 | 100 |
| 43 | c | 75/78 (96%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |
| 45 | e | 60/63 (95%) | 57 (95%) | 3 (5%) | 0 | 100 | 100 |
| 46 | f | 56/59 (95%) | 53 (95%) | 3 (5%) | 0 | 100 | 100 |
| 47 | g | 64/70 (91%) | 63 (98%) | 1 (2%) | 0 | 100 | 100 |
| 48 | h | 269/273 (98%) | 259 (96%) | 9 (3%) | 1 (0%) | 34 | 69 |
| 49 | i | 54/57 (95%) | 51 (94%) | 3 (6%) | 0 | 100 | 100 |
| 50 | j | 207/209 (99%) | 198 (96%) | 9 (4%) | 0 | 100 | 100 |
| 51 | k | 50/55 (91%) | 50 (100%) | 0 | 0 | 100 | 100 |
| 52 | l | 199/201 (99%) | 190 (96%) | 8 (4%) | 1 (0%) | 29 | 67 |
| 53 | m | 44/46 (96%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 54 | n | 175/179 (98%) | 162 (93%) | 11 (6%) | 2 (1%) | 14 | 51 |
| 55 | o | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 56 | p | 173/177 (98%) | 161 (93%) | 12 (7%) | 0 | 100 | 100 |
| 57 | q | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 58 | r | 147/149 (99%) | 136 (92%) | 11 (8%) | 0 | 100 | 100 |
| 59 | s | 140/142 (99%) | 135 (96%) | 5 (4%) | 0 | 100 | 100 |
| 60 | t | 121/123 (98%) | 111 (92%) | 10 (8%) | 0 | 100 | 100 |
| 61 | u | 142/144 (99%) | 135 (95%) | 7 (5%) | 0 | 100 | 100 |
| 62 | v | 134/136 (98%) | 129 (96%) | 5 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 63 | w | 117/127 (92%) | 107 (92%) | 10 (8%) | 0 | 100 | 100 |
| 64 | x | 114/117 (97%) | 108 (95%) | 6 (5%) | 0 | 100 | 100 |
| 65 | y | 112/115 (97%) | 105 (94%) | 7 (6%) | 0 | 100 | 100 |
| 66 | z | 115/118 (98%) | 110 (96%) | 4 (4%) | 1 (1%) | 17 | 56 |
| All | All | 10159/11072 (92%) | 9261 (91%) | 778 (8%) | 120 (1%) | 17 | 49 |

5 of 120 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | 9 | 88 | HIS |
| 11 | AA | 888 | THR |
| 12 | AB | 121 | LYS |
| 12 | AB | 122 | PRO |
| 12 | AB | 123 | ARG |

### 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 | 84/84 (100%) | 78 (93%) | 6 (7%) | 14 | 47 |
| 2 | 1 | 93/93 (100%) | 84 (90%) | 9 (10%) | 8 | 31 |
| 3 | 2 | 81/84 (96%) | 76 (94%) | 5 (6%) | 18 | 53 |
| 4 | 3 | 84/85 (99%) | 78 (93%) | 6 (7%) | 14 | 47 |
| 5 | 4 | 78/78 (100%) | 74 (95%) | 4 (5%) | 24 | 60 |
| 9 | 9 | 112/123 (91%) | 65 (58%) | 47 (42%) | 0 | 0 |
| 11 | AA | 1155/1157 (100%) | 1142 (99%) | 13 (1%) | 73 | 88 |
| 12 | AB | 138/158 (87%) | 104 (75%) | 34 (25%) | 0 | 2 |
| 13 | AC | 186/286 (65%) | 186 (100%) | 0 | 100 | 100 |
| 13 | AD | 185/286 (65%) | 185 (100%) | 0 | 100 | 100 |
| 14 | AE | 1120/1168 (96%) | 1051 (94%) | 69 (6%) | 18 | 53 |
| 15 | AF | 70/75 (93%) | 70 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 16 | AG | 409/409 (100%) | 297 (73%) | 112 (27%) | 0 | 1 |
| 17 | C | 57/65 (88%) | 55 (96%) | 2 (4%) | 36 | 69 |
| 19 | E | 65/66 (98%) | 60 (92%) | 5 (8%) | 13 | 44 |
| 20 | F | 60/61 (98%) | 57 (95%) | 3 (5%) | 24 | 60 |
| 21 | G | 187/199 (94%) | 178 (95%) | 9 (5%) | 25 | 61 |
| 22 | H | 137/461 (30%) | 128 (93%) | 9 (7%) | 16 | 51 |
| 23 | I | 171/190 (90%) | 165 (96%) | 6 (4%) | 36 | 69 |
| 24 | J | 172/173 (99%) | 165 (96%) | 7 (4%) | 30 | 66 |
| 25 | K | 119/126 (94%) | 111 (93%) | 8 (7%) | 16 | 50 |
| 26 | L | 91/116 (78%) | 85 (93%) | 6 (7%) | 16 | 51 |
| 27 | M | 124/147 (84%) | 116 (94%) | 8 (6%) | 17 | 51 |
| 28 | N | 104/105 (99%) | 102 (98%) | 2 (2%) | 57 | 81 |
| 29 | O | 105/107 (98%) | 100 (95%) | 5 (5%) | 25 | 61 |
| 30 | P | 86/90 (96%) | 78 (91%) | 8 (9%) | 9 | 33 |
| 31 | Q | 90/99 (91%) | 87 (97%) | 3 (3%) | 38 | 71 |
| 32 | R | 101/104 (97%) | 94 (93%) | 7 (7%) | 15 | 49 |
| 33 | S | 83/84 (99%) | 79 (95%) | 4 (5%) | 25 | 61 |
| 34 | T | 76/77 (99%) | 64 (84%) | 12 (16%) | 2 | 12 |
| 35 | U | 65/65 (100%) | 60 (92%) | 5 (8%) | 13 | 44 |
| 36 | V | 74/78 (95%) | 72 (97%) | 2 (3%) | 44 | 75 |
| 37 | W | 72/79 (91%) | 68 (94%) | 4 (6%) | 21 | 57 |
| 38 | X | 94/96 (98%) | 85 (90%) | 9 (10%) | 8 | 32 |
| 39 | Y | 109/110 (99%) | 72 (66%) | 37 (34%) | 0 | 0 |
| 40 | Z | 26/85 (31%) | 12 (46%) | 14 (54%) | 0 | 0 |
| 42 | b | 58/63 (92%) | 57 (98%) | 1 (2%) | 60 | 83 |
| 43 | c | 67/68 (98%) | 64 (96%) | 3 (4%) | 27 | 63 |
| 45 | e | 54/55 (98%) | 53 (98%) | 1 (2%) | 57 | 81 |
| 46 | f | 48/49 (98%) | 46 (96%) | 2 (4%) | 30 | 65 |
| 47 | g | 59/62 (95%) | 53 (90%) | 6 (10%) | 7 | 29 |
| 48 | h | 216/218 (99%) | 199 (92%) | 17 (8%) | 12 | 43 |
| 49 | i | 47/48 (98%) | 41 (87%) | 6 (13%) | 4 | 20 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 50 | j | 164/164 (100%) | 157 (96%) | 7 (4%) | 29 | 64 |
| 51 | k | 47/49 (96%) | 44 (94%) | 3 (6%) | 17 | 52 |
| 52 | l | 165/165 (100%) | 151 (92%) | 14 (8%) | 10 | 38 |
| 53 | m | 38/38 (100%) | 35 (92%) | 3 (8%) | 12 | 43 |
| 54 | n | 148/150 (99%) | 134 (90%) | 14 (10%) | 8 | 32 |
| 55 | o | 51/52 (98%) | 46 (90%) | 5 (10%) | 8 | 31 |
| 56 | p | 136/138 (99%) | 132 (97%) | 4 (3%) | 42 | 74 |
| 57 | q | 34/34 (100%) | 32 (94%) | 2 (6%) | 19 | 54 |
| 58 | r | 114/114 (100%) | 104 (91%) | 10 (9%) | 10 | 36 |
| 59 | s | 116/116 (100%) | 110 (95%) | 6 (5%) | 23 | 59 |
| 60 | t | 104/104 (100%) | 98 (94%) | 6 (6%) | 20 | 55 |
| 61 | u | 103/103 (100%) | 97 (94%) | 6 (6%) | 20 | 55 |
| 62 | v | 109/109 (100%) | 103 (94%) | 6 (6%) | 21 | 57 |
| 63 | w | 99/103 (96%) | 91 (92%) | 8 (8%) | 11 | 42 |
| 64 | x | 86/87 (99%) | 80 (93%) | 6 (7%) | 15 | 48 |
| 65 | y | 99/100 (99%) | 95 (96%) | 4 (4%) | 31 | 66 |
| 66 | z | 89/90 (99%) | 87 (98%) | 2 (2%) | 52 | 79 |
| All | All | 8314/9148 (91%) | 7692 (92%) | 622 (8%) | 17 | 45 |

5 of 622 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 39 | Y | 126 | ARG |
| 58 | r | 72 | ILE |
| 40 | Z | 26 | MET |
| 39 | Y | 125 | THR |
| 50 | j | 91 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | AD | 227 | GLN |
| 38 | X | 105 | ASN |
| 16 | AG | 194 | GLN |
| 16 | AG | 428 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | AF | 31 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 10 | A | 75/76 (98%) | 29 (38%) | 6 (8%) |
| 10 | B | 75/76 (98%) | 35 (46%) | 6 (8%) |
| 18 | D | 1514/1542 (98%) | 288 (19%) | 34 (2%) |
| 41 | a | 2859/2904 (98%) | 533 (18%) | 0 |
| 44 | d | 119/120 (99%) | 17 (14%) | 0 |
| 8 | 7 | 32/41 (78%) | 19 (59%) | 4 (12%) |
| All | All | 4674/4759 (98%) | 921 (19%) | 50 (1%) |

5 of 921 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 7 | -18 | G |
| 8 | 7 | -17 | U |
| 8 | 7 | -16 | U |
| 8 | 7 | -14 | U |
| 8 | 7 | -13 | U |

5 of 50 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | D | 531 | U |
| 18 | D | 992 | U |
| 18 | D | 1493 | A |
| 18 | D | 532 | A |
| 18 | D | 722 | G |

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

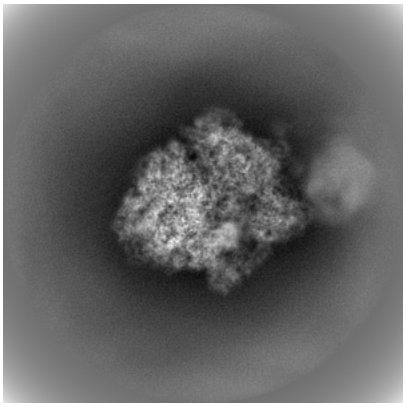
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22082. These allow visual inspection of the internal detail of the map and identification of artifacts.

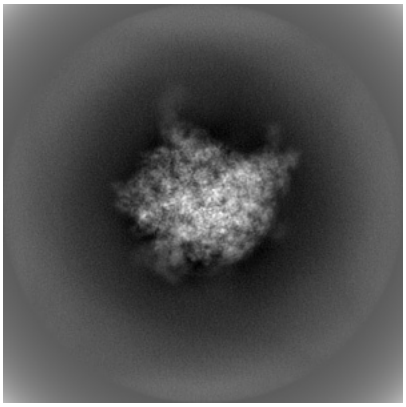
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

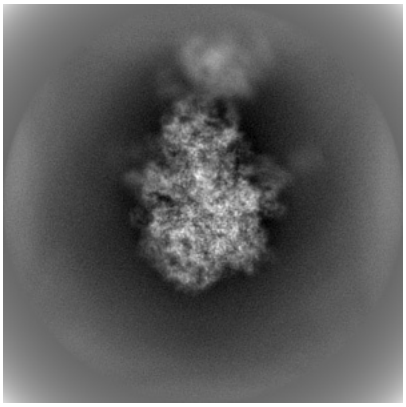
### 6.1.1 Primary map



X



Y

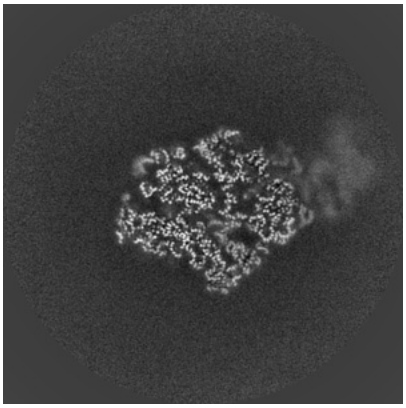


Z

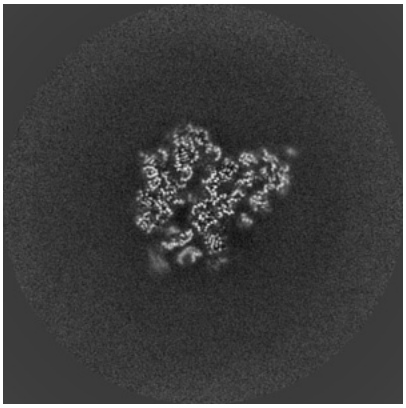
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

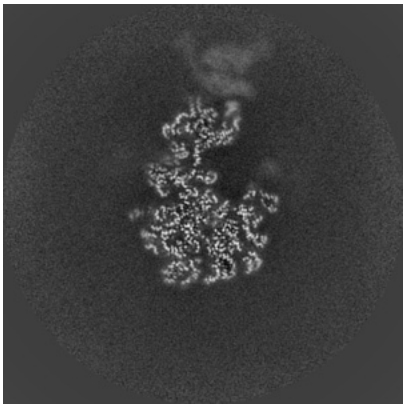
### 6.2.1 Primary map



X Index: 256



Y Index: 256

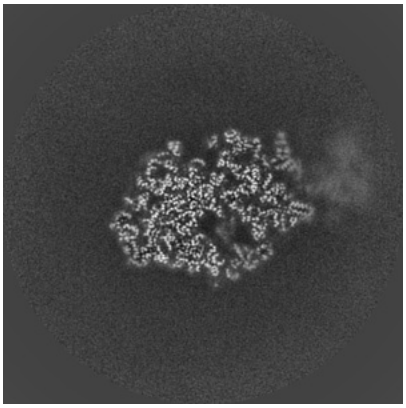


Z Index: 256

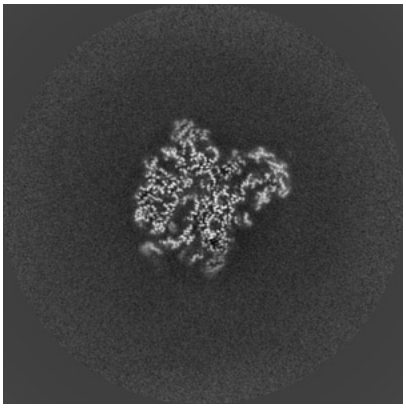
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

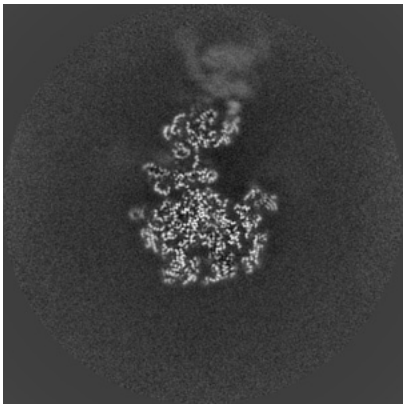
### 6.3.1 Primary map



X Index: 242



Y Index: 250



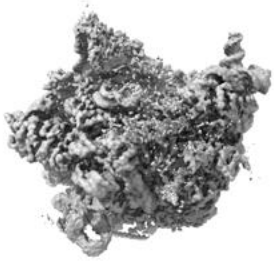
Z Index: 259

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

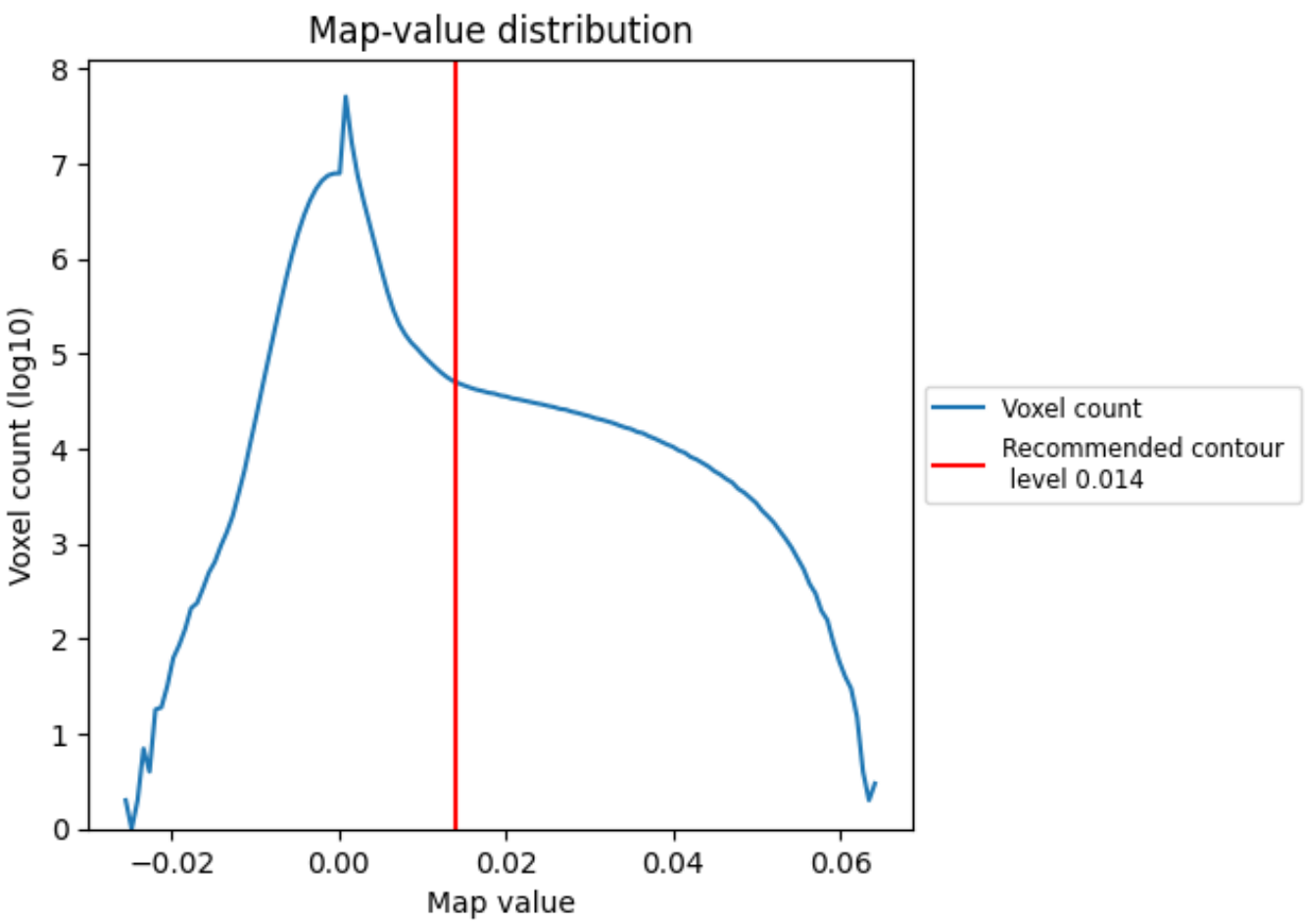
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

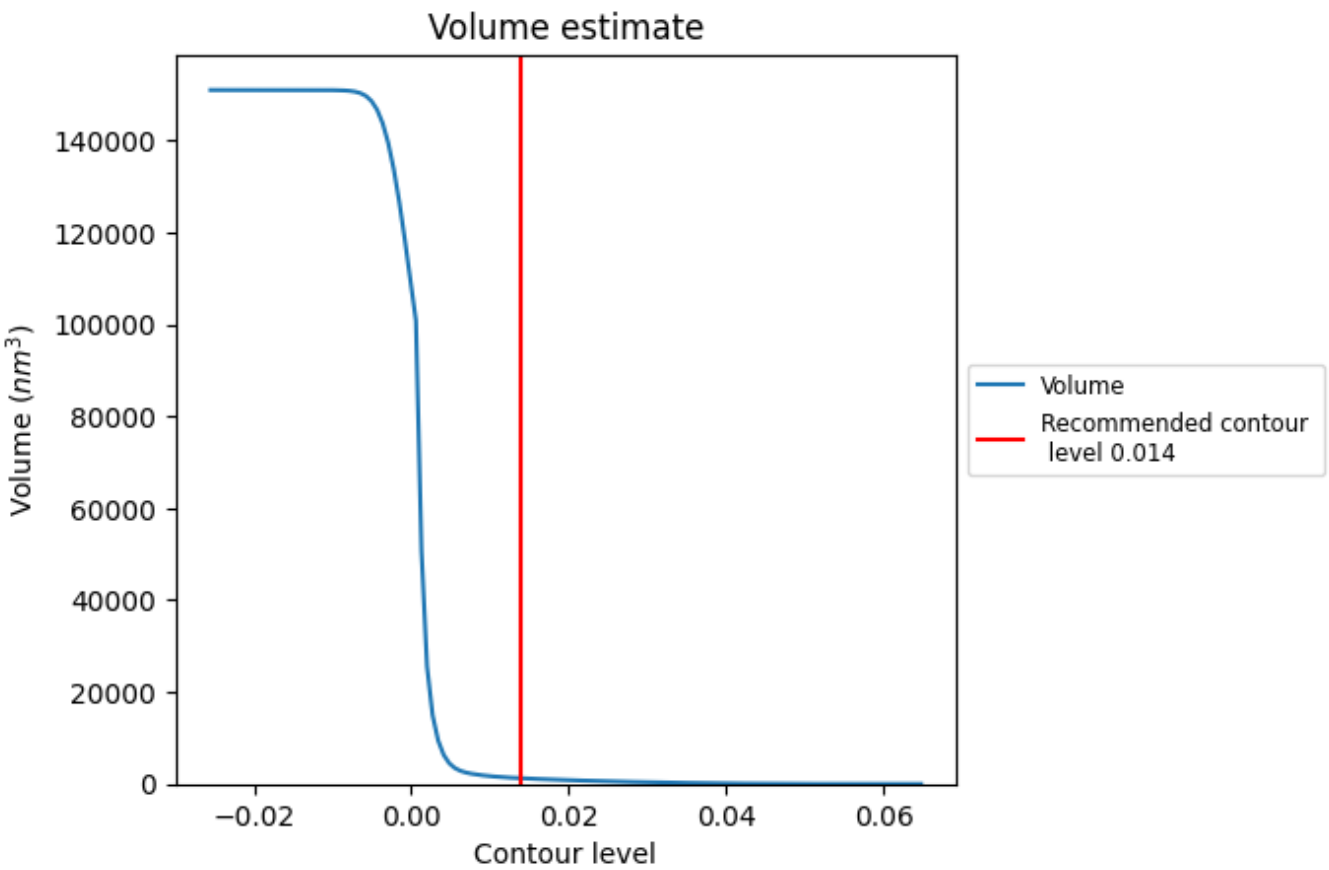
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

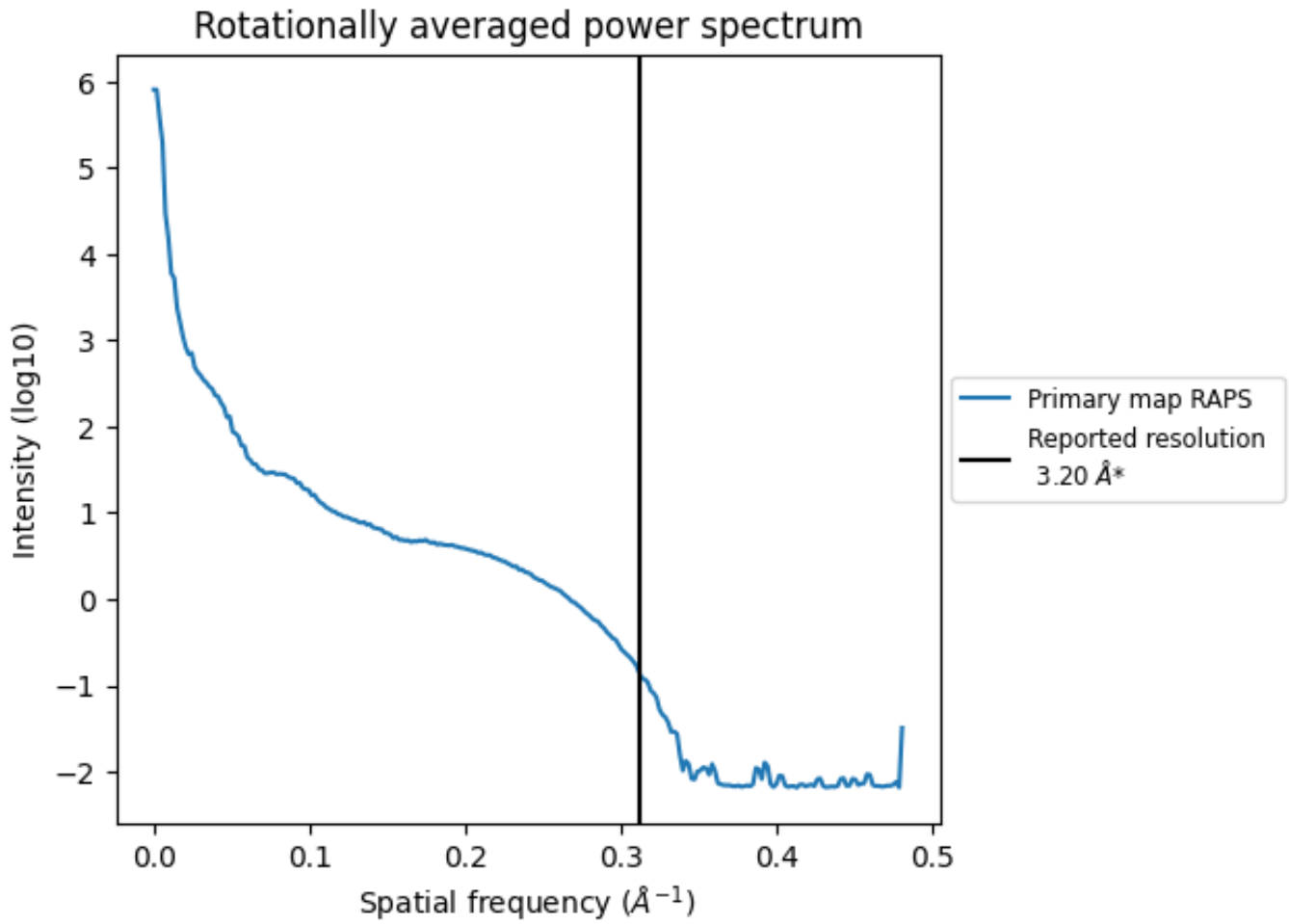
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1238 $nm^3$; this corresponds to an approximate mass of 1118 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 0.312 Å$^{-1}$

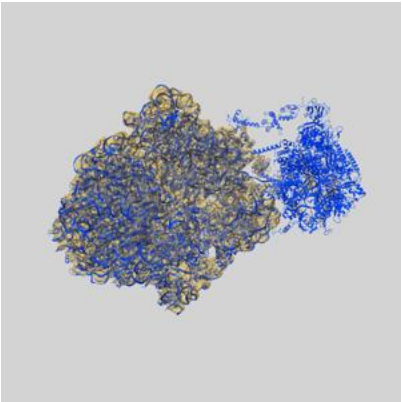
# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

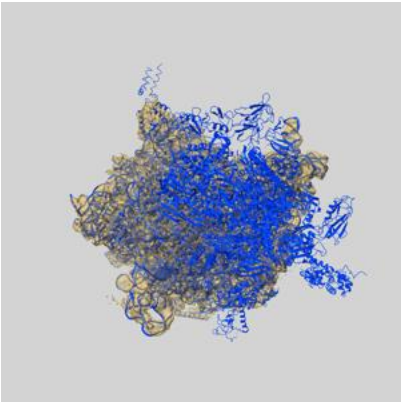
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22082 and PDB model 6X6T. Per-residue inclusion information can be found in section 3 on page 17.

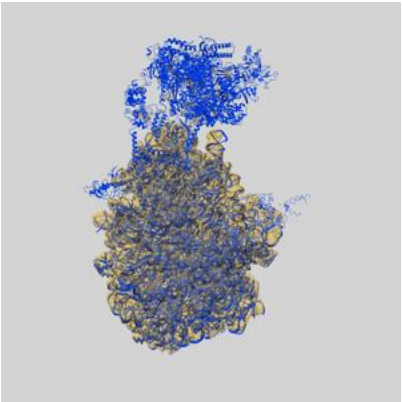
## 9.1 Map-model overlay (i)



X



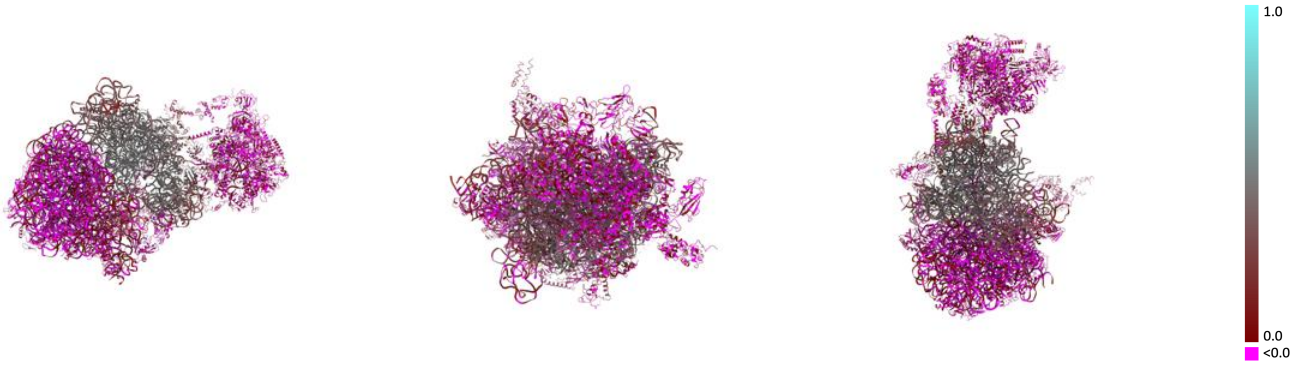
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

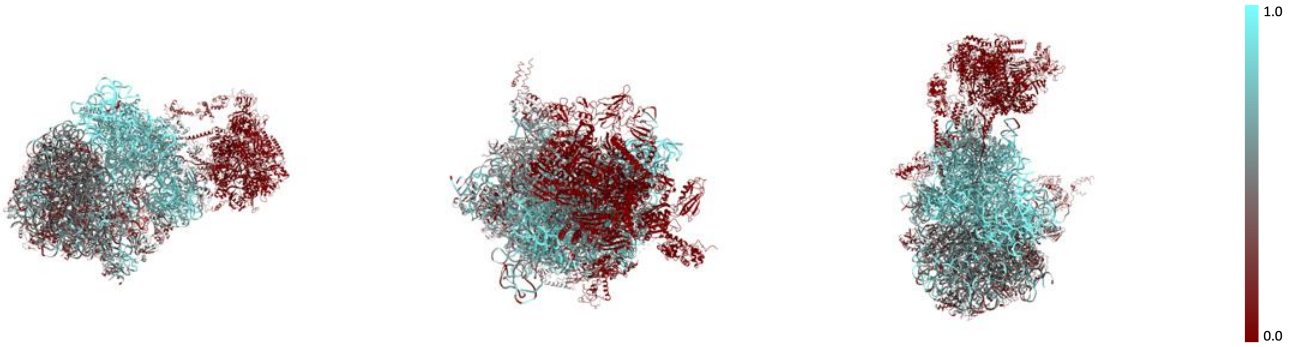
## 9.2 Q-score mapped to coordinate model (i)




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.

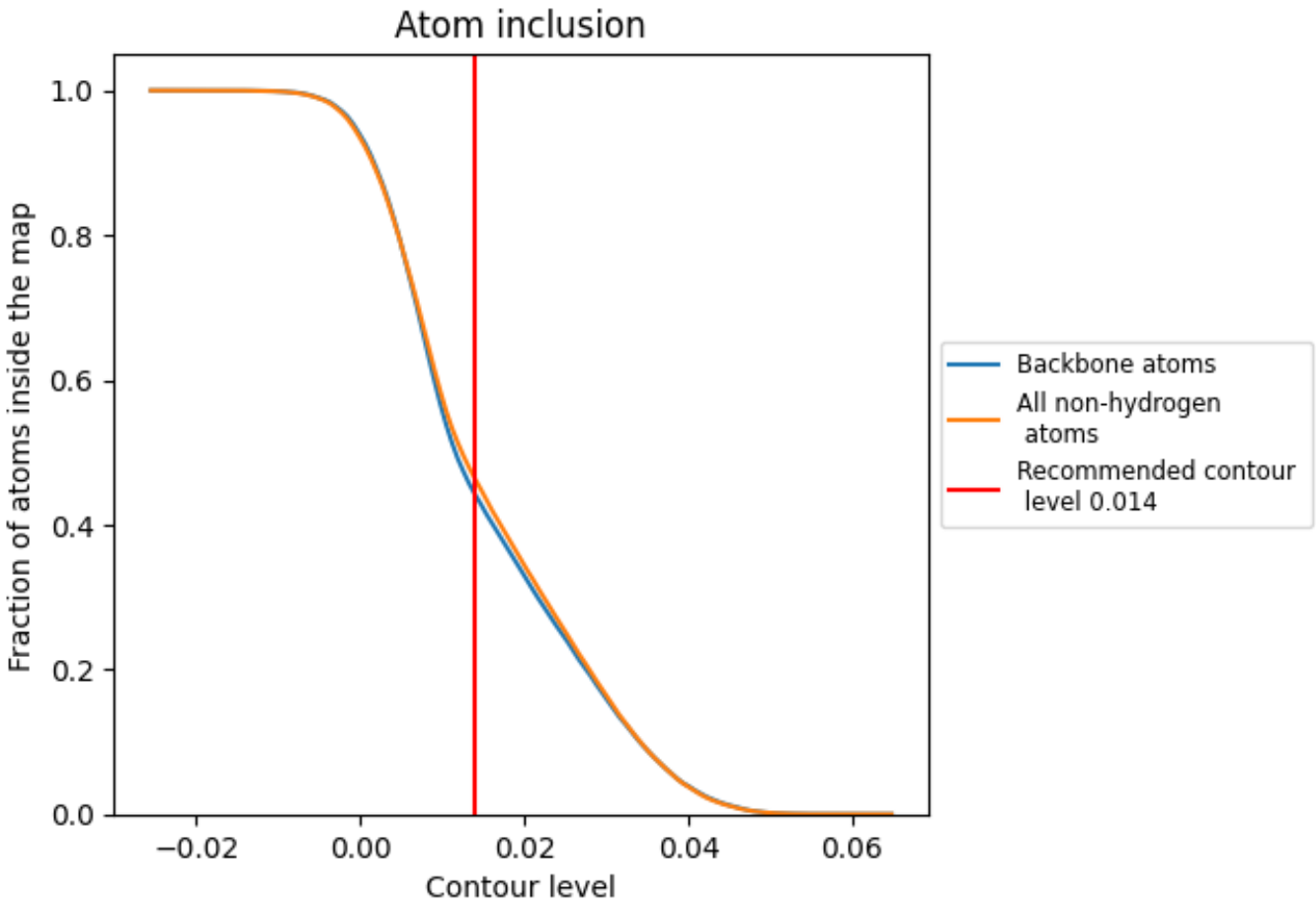
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.014).

## 9.4 Atom inclusion (i)




At the recommended contour level, 44% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4633 | 0.1180 |
| 0 | 0.3501 | -0.0380 |
| 1 | 0.3385 | -0.0430 |
| 2 | 0.3192 | -0.0530 |
| 3 | 0.3235 | -0.0190 |
| 4 | 0.3957 | 0.0260 |
| 5 | 0.0254 | 0.0380 |
| 6 | 0.0756 | 0.0390 |
| 7 | 0.1206 | 0.0400 |
| 9 | 0.2258 | 0.1050 |
| A | 0.5154 | 0.1640 |
| AA | 0.0073 | 0.0250 |
| AB | 0.1219 | 0.1120 |
| AC | 0.0005 | 0.0090 |
| AD | 0.0005 | 0.0120 |
| AE | 0.0032 | 0.0160 |
| AF | 0.0000 | 0.0220 |
| AG | 0.1944 | 0.1360 |
| B | 0.4617 | 0.0880 |
| C | 0.6750 | 0.3960 |
| D | 0.9082 | 0.4050 |
| E | 0.7049 | 0.3360 |
| F | 0.5653 | 0.3510 |
| G | 0.6721 | 0.3610 |
| H | 0.0275 | 0.0640 |
| I | 0.6629 | 0.3950 |
| J | 0.7057 | 0.4110 |
| K | 0.7257 | 0.4400 |
| L | 0.6602 | 0.3570 |
| M | 0.6337 | 0.3240 |
| N | 0.7438 | 0.4290 |
| O | 0.6813 | 0.3310 |
| P | 0.5974 | 0.3090 |
| Q | 0.7128 | 0.4160 |
| R | 0.7238 | 0.4650 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| S | 0.7028 | 0.3650 |
| T | 0.7188 | 0.3920 |
| U | 0.7241 | 0.3890 |
| V | 0.6915 | 0.4010 |
| W | 0.3617 | 0.0050 |
| X | 0.3295 | 0.0050 |
| Y | 0.0959 | 0.1150 |
| Z | 0.0000 | 0.1320 |
| a | 0.5290 | -0.0020 |
| b | 0.3728 | 0.0030 |
| c | 0.2729 | -0.0660 |
| d | 0.6353 | 0.0670 |
| e | 0.3620 | -0.0030 |
| f | 0.3211 | -0.0570 |
| g | 0.3092 | 0.0450 |
| h | 0.3105 | -0.0520 |
| i | 0.3084 | -0.0780 |
| j | 0.2978 | -0.0760 |
| k | 0.3445 | -0.0350 |
| l | 0.3079 | -0.0270 |
| m | 0.2761 | -0.0740 |
| n | 0.4151 | 0.0490 |
| o | 0.2933 | -0.0540 |
| p | 0.3831 | 0.0470 |
| q | 0.2979 | -0.0410 |
| r | 0.2555 | 0.0580 |
| s | 0.2936 | -0.0600 |
| t | 0.2834 | -0.0500 |
| u | 0.2832 | -0.0420 |
| v | 0.3570 | 0.0050 |
| w | 0.3133 | -0.0780 |
| x | 0.4148 | 0.0240 |
| y | 0.3232 | -0.0430 |
| z | 0.3249 | -0.0520 |