# wwPDB EM Validation Summary Report (i)

Apr 16, 2024 – 03:19 am BST

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|---|---|---|
| PDB ID | : | 5LZA |
| EMDB ID | : | EMD-4121 |
| Title | : | Structure of the 70S ribosome with SECIS-mRNA and P-site tRNA (Initial complex, IC) |
| Authors | : | Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H. |
| Deposited on | : | 2016-09-29 |
| Resolution | : | 3.60 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.

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

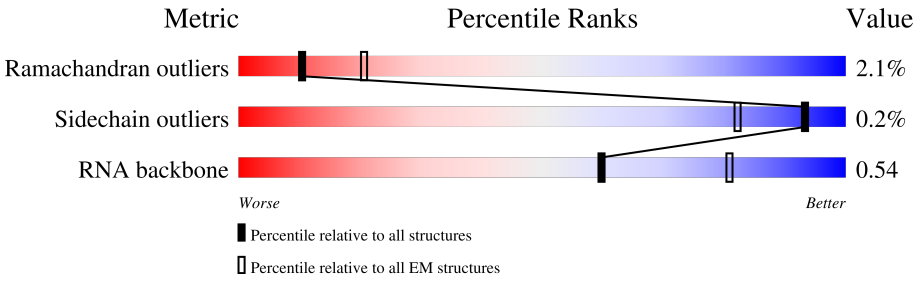
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 3.60 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%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | a | 1539 | 73% 24% . |
| 2 | b | 218 | 96% .. |
| 3 | c | 206 | 100% |
| 4 | d | 205 | 99% . |
| 5 | e | 157 | 94% .. |
| 6 | f | 100 | 93% 5% . |
| 7 | g | 151 | 97% .. |
| 8 | h | 129 | 98% . |
| 9 | i | 127 | 94% 6% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | j | 98 | 93% 5% |
| 11 | k | 116 | 97% |
| 12 | l | 123 | 91% 8% |
| 13 | m | 114 | 96% |
| 14 | n | 100 | 97% |
| 15 | o | 88 | 98% |
| 16 | p | 82 | 95% |
| 17 | q | 80 | 95% |
| 18 | r | 65 | 91% 8% |
| 19 | s | 79 | 97% |
| 20 | t | 85 | 100% |
| 21 | u | 65 | 94% |
| 22 | v | 77 | 64% 34% |
| 23 | x | 48 | 52% 48% |
| 24 | A | 2903 | 72% 24% |
| 25 | B | 120 | 72% 24% |
| 26 | C | 271 | 98% |
| 27 | D | 209 | 100% |
| 28 | E | 201 | 98% |
| 29 | F | 177 | 97% |
| 30 | G | 176 | 95% |
| 31 | I | 141 | 98% |
| 32 | H | 149 | 96% |
| 33 | J | 142 | 100% |
| 34 | K | 122 | 93% 6% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 35 | L | 143 | 95% |
| 36 | M | 136 | 97% |
| 37 | N | 120 | 100% |
| 38 | O | 116 | 98% |
| 39 | P | 114 | 99% |
| 40 | Q | 117 | 99% |
| 41 | R | 103 | 98% |
| 42 | S | 110 | 99% |
| 43 | T | 93 | 97% |
| 44 | U | 102 | 93% 5% |
| 45 | V | 94 | 100% |
| 46 | W | 75 | 99% |
| 47 | X | 77 | 99% |
| 48 | Y | 63 | 98% |
| 49 | Z | 58 | 100% |
| 50 | 0 | 56 | 96% |
| 51 | 1 | 50 | 94% 6% |
| 52 | 2 | 46 | 98% |
| 53 | 3 | 64 | 97% |
| 54 | 4 | 38 | 95% 5% |
| 55 | 6 | 66 | 98% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 1 | G7M | a | 527 | X | - | - | - |
| 24 | G7M | A | 2069 | X | - | - | - |

# 2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 146037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | a | 1539 | 33119 | 14778 | 6072 | 10726 | 1543 | 4 | 0 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | b | 218 | 1705 | 1081 | 305 | 312 | 7 | 0 | 0 |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | c | 206 | 1625 | 1028 | 305 | 289 | 3 | 0 | 0 |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | d | 205 | 1643 | 1026 | 315 | 298 | 4 | 0 | 0 |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | e | 157 | 1157 | 719 | 218 | 214 | 6 | 0 | 0 |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | f | 100 | 818 | 515 | 148 | 149 | 6 | 0 | 0 |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | g | 151 | Total | C | N | O | S | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | h | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | i | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | j | 98 | Total | C | N | O | S | 0 | 0 |
| | | | 787 | 493 | 150 | 143 | 1 | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | k | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 870 | 535 | 173 | 159 | 3 | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | l | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | m | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | n | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 794 | 495 | 164 | 132 | 3 | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | o | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | p | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | q | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 18 | r | 65 | Total | C | N | O | 0 | 0 |
| | | | 505 | 317 | 96 | 92 | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | s | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | t | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 21 | u | 65 | Total | C | N | O | S | 0 | 0 |
| | | | 496 | 307 | 100 | 88 | 1 | | |

- Molecule 22 is a RNA chain called fMet-tRNAfMet.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | v | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1644 | 733 | 297 | 536 | 77 | 1 | | |

- Molecule 23 is a RNA chain called SECIS mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | x | 48 | Total | C | N | O | P | 0 | 0 |
| | | | 1025 | 457 | 183 | 337 | 48 | | |

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | A | 2900 | Total | C | N | O | P | 1 | 0 |
| | | | 62296 | 27797 | 11464 | 20134 | 2901 | | |

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | B | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2570 | 1144 | 468 | 838 | 120 | | |

- Molecule 26 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | C | 271 | Total | C | N | O | S | 0 | 0 |
| | | | 2083 | 1288 | 423 | 365 | 7 | | |

- Molecule 27 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | D | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 28 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | E | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 29 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | F | 177 | Total | C | N | O | S | 0 | 0 |
| | | | 1411 | 899 | 249 | 257 | 6 | | |

- Molecule 30 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | G | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 31 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | I | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | |

- Molecule 32 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | H | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | |

- Molecule 33 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | J | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 34 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | K | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 939 | 587 | 180 | 166 | 6 | | |

- Molecule 35 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | L | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | |

- Molecule 36 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | M | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 37 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | N | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 961 | 593 | 196 | 167 | 5 | | |

- Molecule 38 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 38 | O | 116 | Total | C | N | O | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | |

- Molecule 39 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | P | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 40 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 40 | Q | 117 | Total | C | N | O | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | |

- Molecule 41 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | R | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 42 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | S | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 43 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | T | 93 | Total | C | N | O | S | 0 | 0 |
| | | | 739 | 466 | 139 | 132 | 2 | | |

- Molecule 44 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 44 | U | 102 | Total | C | N | O | 0 | 0 |
| | | | 780 | 492 | 146 | 142 | | |

- Molecule 45 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | V | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 46 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | W | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 575 | 356 | 116 | 102 | 1 | | |

- Molecule 47 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | X | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

- Molecule 48 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | Y | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | |

- Molecule 49 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | Z | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | 0 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 51 | 1 | 50 | Total | C | N | O | 0 | 0 |
| | | | 410 | 263 | 75 | 72 | | |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | 2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 53 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | 3 | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 54 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | 4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | 6 | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 523 | 323 | 99 | 95 | 6 | | |

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

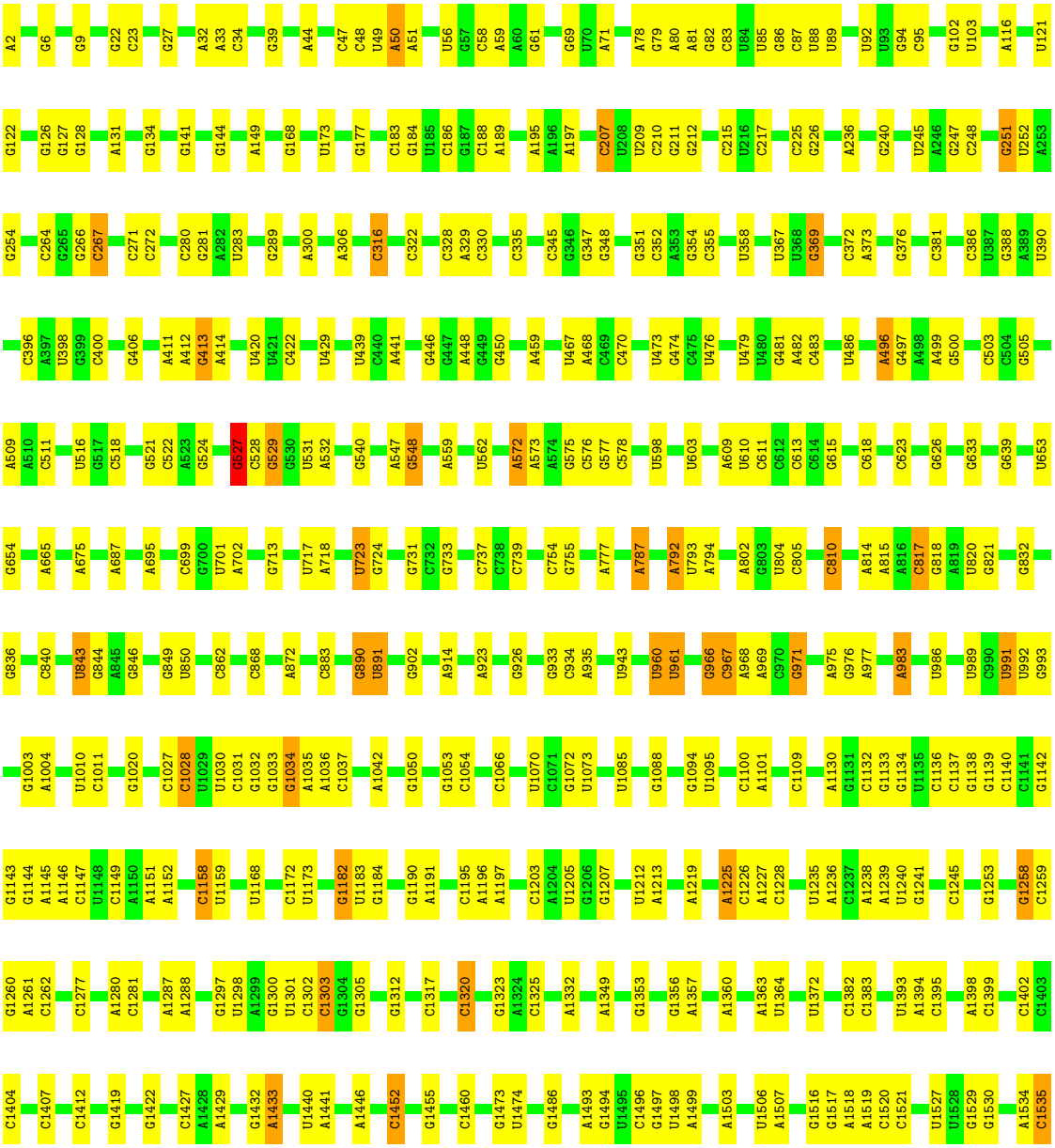
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 56 | 4 | 1 | Total Zn<br>1 1 | 0 |
| 56 | 6 | 1 | Total Zn<br>1 1 | 0 |

# 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

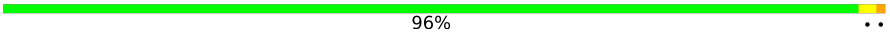
- Molecule 1: 16S ribosomal RNA

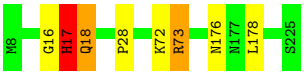
Chain a:


• Molecule 2: 30S ribosomal protein S2

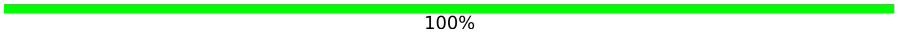
Chain b:




• Molecule 3: 30S ribosomal protein S3

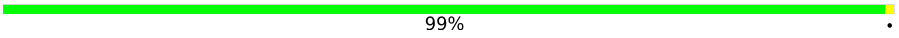
Chain c:

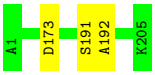




• Molecule 4: 30S ribosomal protein S4

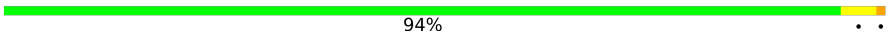
Chain d:




• Molecule 5: 30S ribosomal protein S5

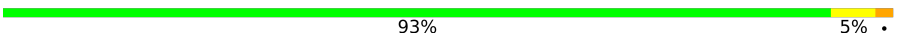
Chain e:





• Molecule 6: 30S ribosomal protein S6

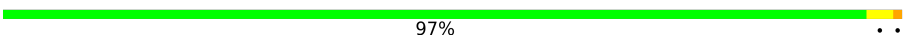
Chain f:

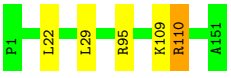




• Molecule 7: 30S ribosomal protein S7

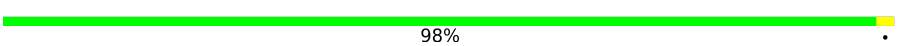
Chain g:

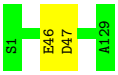



• Molecule 8: 30S ribosomal protein S8

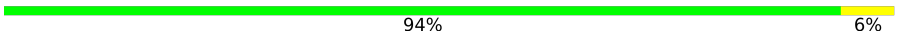
Chain h:

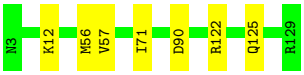





• Molecule 9: 30S ribosomal protein S9

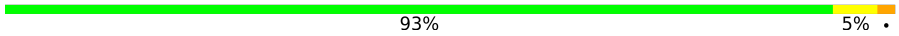
Chain i:

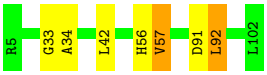



• Molecule 10: 30S ribosomal protein S10

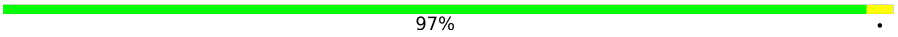
Chain j:

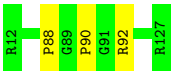



• Molecule 11: 30S ribosomal protein S11

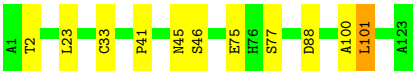
Chain k:



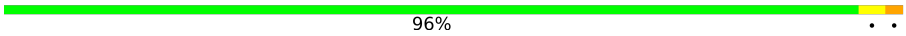

• Molecule 12: 30S ribosomal protein S12

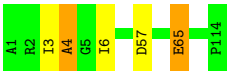
Chain l:


• Molecule 13: 30S ribosomal protein S13

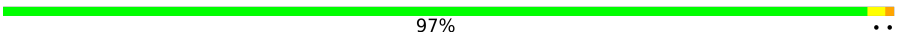
Chain m:




• Molecule 14: 30S ribosomal protein S14

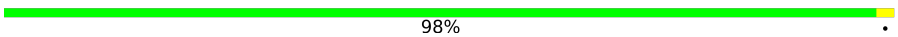
Chain n:

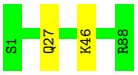




• Molecule 15: 30S ribosomal protein S15

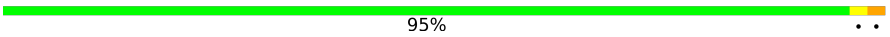
Chain o:

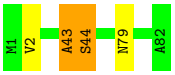





• Molecule 16: 30S ribosomal protein S16

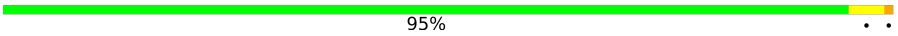
Chain p:

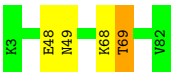



• Molecule 17: 30S ribosomal protein S17

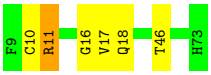
Chain q:



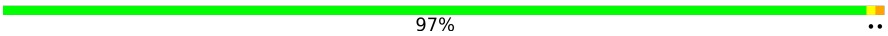

• Molecule 18: 30S ribosomal protein S18

Chain r:


• Molecule 19: 30S ribosomal protein S19

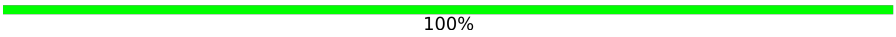
Chain s:





• Molecule 20: 30S ribosomal protein S20

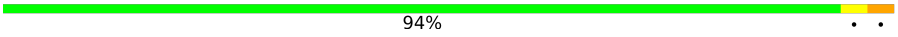
Chain t:

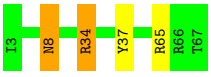



There are no outlier residues recorded for this chain.

• Molecule 21: 30S ribosomal protein S21

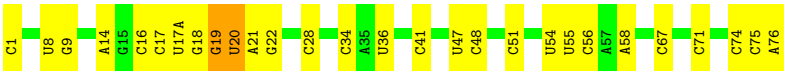
Chain u:



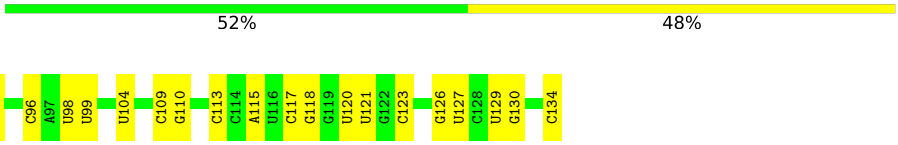

• Molecule 22: fMet-tRNAfMet

Chain v:

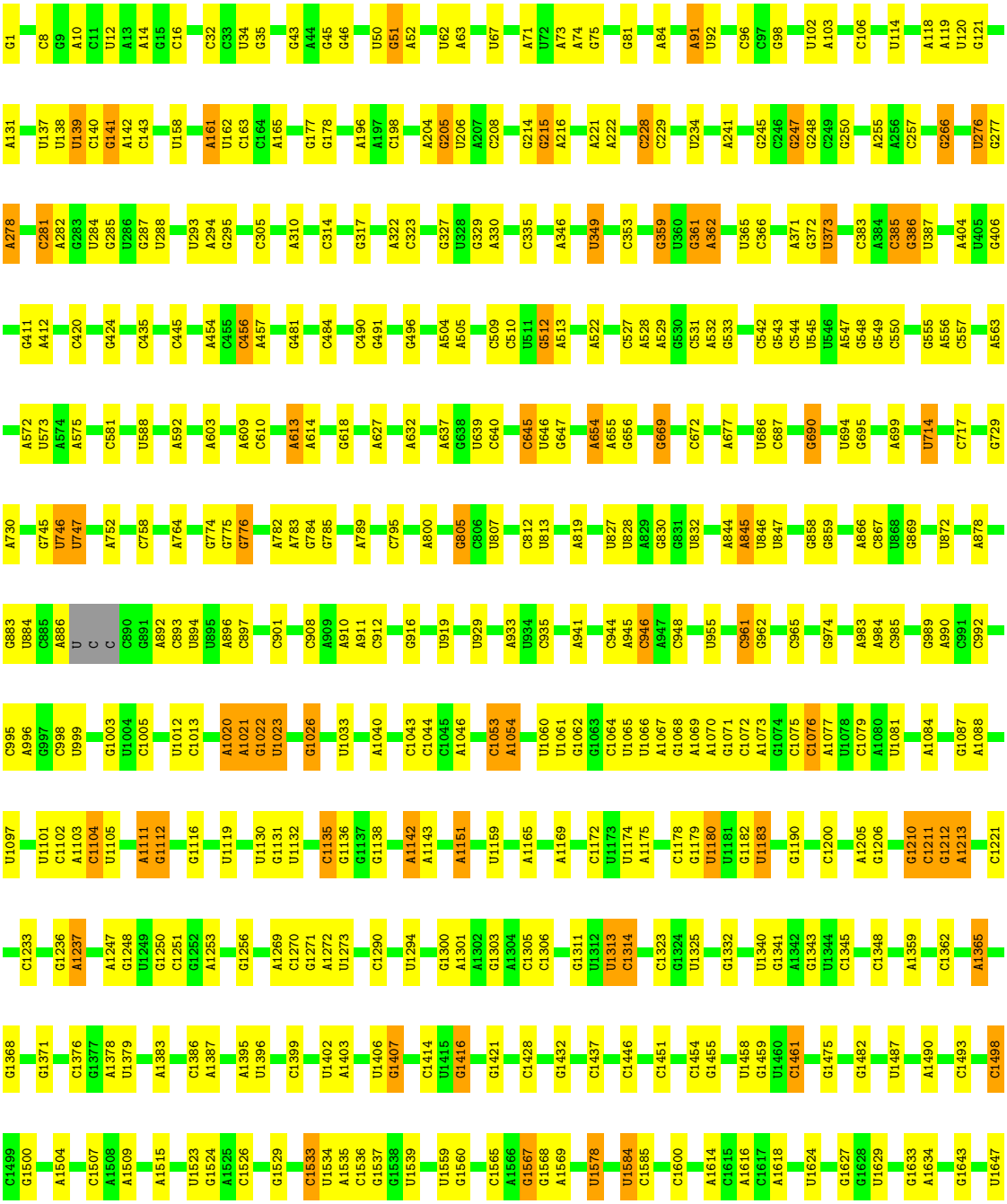
• Molecule 23: SECIS mRNA

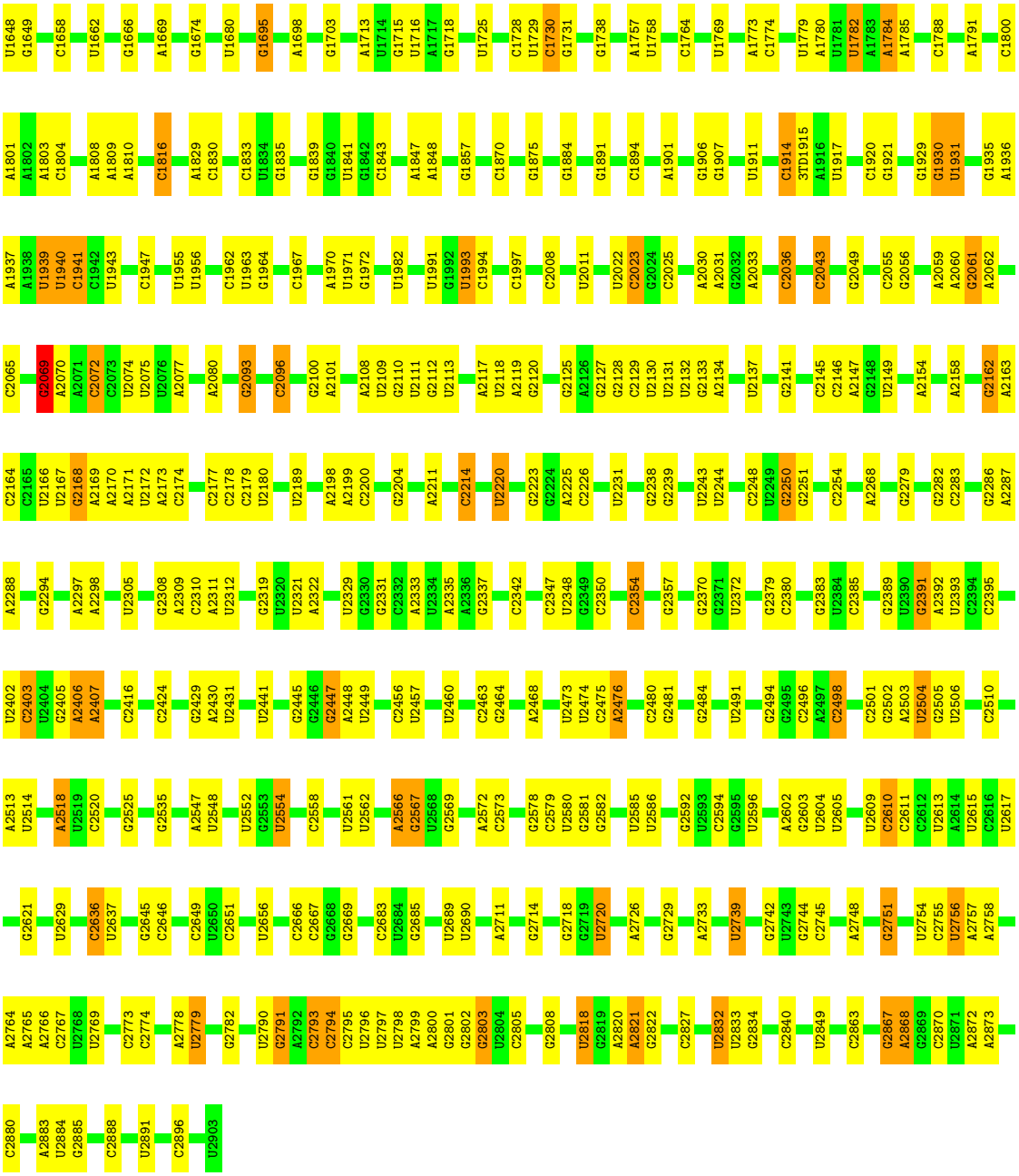
Chain x:




• Molecule 24: 23S ribosomal RNA

Chain A:

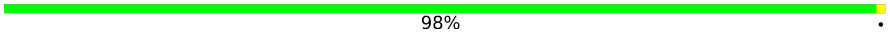


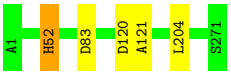
• Molecule 25: 5S ribosomal RNA

Chain B:


• Molecule 26: 50S ribosomal protein L2

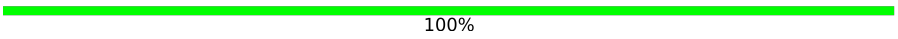
Chain C:






• Molecule 27: 50S ribosomal protein L3

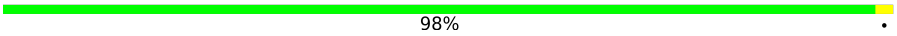
Chain D:





• Molecule 28: 50S ribosomal protein L4

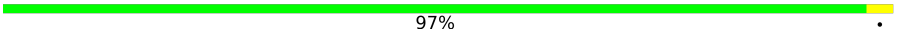
Chain E:





• Molecule 29: 50S ribosomal protein L5

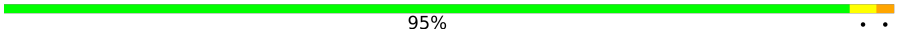
Chain F:





• Molecule 30: 50S ribosomal protein L6

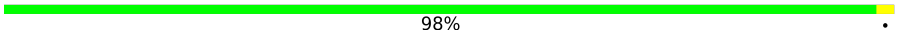
Chain G:

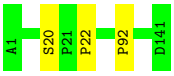




• Molecule 31: 50S ribosomal protein L11

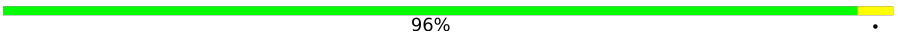
Chain I:

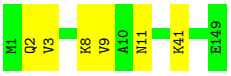



• Molecule 32: 50S ribosomal protein L9

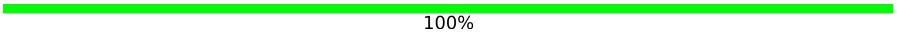
Chain H:




• Molecule 33: 50S ribosomal protein L13

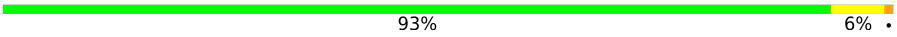
Chain J:




There are no outlier residues recorded for this chain.

• Molecule 34: 50S ribosomal protein L14

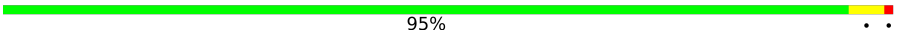
Chain K:





• Molecule 35: 50S ribosomal protein L15

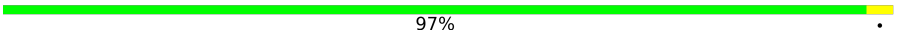
Chain L:

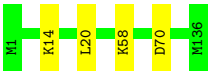




• Molecule 36: 50S ribosomal protein L16

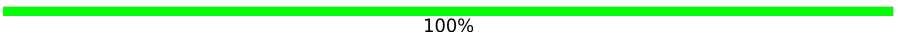
Chain M:




• Molecule 37: 50S ribosomal protein L17

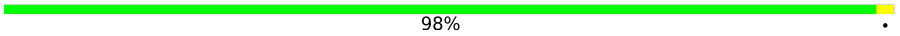
Chain N:

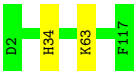



There are no outlier residues recorded for this chain.

• Molecule 38: 50S ribosomal protein L18

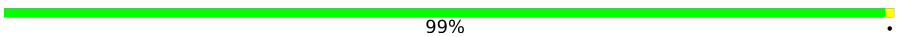
Chain O:




• Molecule 39: 50S ribosomal protein L19

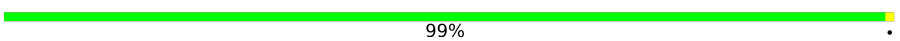
Chain P:





• Molecule 40: 50S ribosomal protein L20

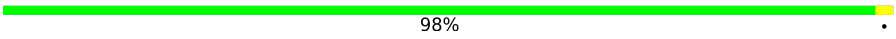
Chain Q:

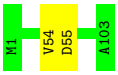




• Molecule 41: 50S ribosomal protein L21

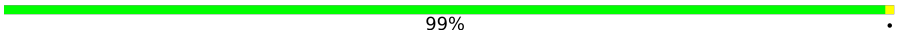
Chain R:




• Molecule 42: 50S ribosomal protein L22

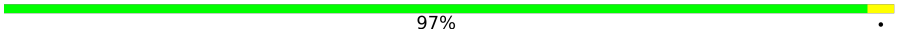
Chain S:

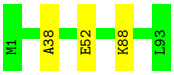




• Molecule 43: 50S ribosomal protein L23

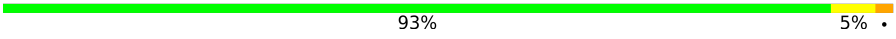
Chain T:




• Molecule 44: 50S ribosomal protein L24

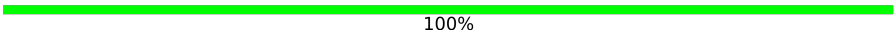
Chain U:





• Molecule 45: 50S ribosomal protein L25

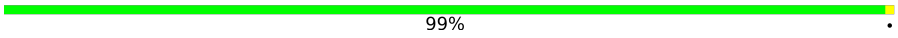
Chain V:




There are no outlier residues recorded for this chain.

• Molecule 46: 50S ribosomal protein L27

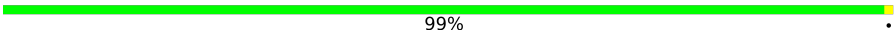
Chain W:





• Molecule 47: 50S ribosomal protein L28

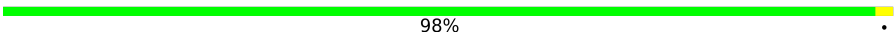
Chain X:



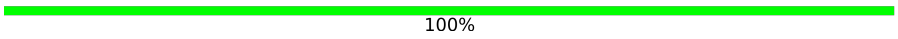


• Molecule 48: 50S ribosomal protein L29

Chain Y:

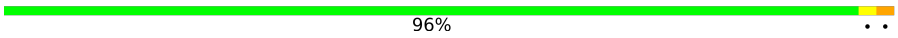



• Molecule 49: 50S ribosomal protein L30

Chain Z: 

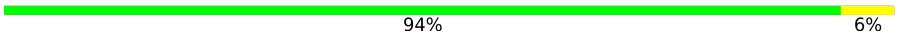

There are no outlier residues recorded for this chain.

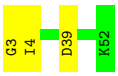
• Molecule 50: 50S ribosomal protein L32

Chain 0: 

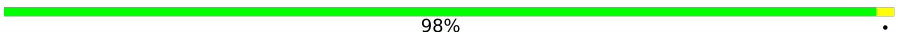


• Molecule 51: 50S ribosomal protein L33

Chain 1: 

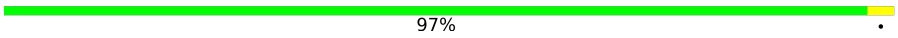




• Molecule 52: 50S ribosomal protein L34

Chain 2: 

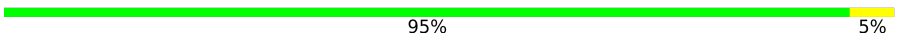


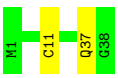
• Molecule 53: 50S ribosomal protein L35

Chain 3: 

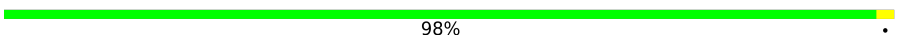


• Molecule 54: 50S ribosomal protein L36

Chain 4: 


• Molecule 55: 50S ribosomal protein L31

Chain 6: 


# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 75176 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 30 | Depositor |
| Minimum defocus (nm) | 700 | Depositor |
| Maximum defocus (nm) | 2600 | Depositor |
| Magnification | 59000 | Depositor |
| Image detector | FEI FALCON II (4k x 4k) | 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: G7M, 4OC, OMC, OMG, 5MU, PSU, UR3, 6MZ, MA6, 1MG, 2MA, 4SU, OMU, H2U, ZN, 3TD, 5MC, 2MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | a | 0.61 | 4/36803 (0.0%) | 1.26 | 322/57406 (0.6%) |
| 2 | b | 0.43 | 0/1736 | 0.66 | 3/2338 (0.1%) |
| 3 | c | 0.40 | 0/1652 | 0.60 | 0/2225 |
| 4 | d | 0.43 | 0/1665 | 0.62 | 0/2227 |
| 5 | e | 0.44 | 0/1170 | 0.80 | 2/1573 (0.1%) |
| 6 | f | 0.49 | 0/836 | 0.83 | 2/1128 (0.2%) |
| 7 | g | 0.43 | 0/1196 | 0.70 | 3/1602 (0.2%) |
| 8 | h | 0.42 | 0/989 | 0.66 | 0/1326 |
| 9 | i | 0.41 | 0/1034 | 0.69 | 0/1375 |
| 10 | j | 0.37 | 0/797 | 0.74 | 0/1077 |
| 11 | k | 0.40 | 0/886 | 0.71 | 0/1195 |
| 12 | l | 0.43 | 0/969 | 0.82 | 2/1300 (0.2%) |
| 13 | m | 0.46 | 0/893 | 0.78 | 3/1193 (0.3%) |
| 14 | n | 0.45 | 0/806 | 0.66 | 1/1074 (0.1%) |
| 15 | o | 0.40 | 0/722 | 0.61 | 0/964 |
| 16 | p | 0.45 | 0/659 | 0.70 | 1/884 (0.1%) |
| 17 | q | 0.45 | 0/658 | 0.78 | 1/881 (0.1%) |
| 18 | r | 0.42 | 0/512 | 0.70 | 0/689 |
| 19 | s | 0.41 | 0/653 | 0.75 | 1/877 (0.1%) |
| 20 | t | 0.42 | 0/671 | 0.60 | 0/888 |
| 21 | u | 0.53 | 0/501 | 0.84 | 1/668 (0.1%) |
| 22 | v | 0.55 | 1/1747 (0.1%) | 1.29 | 19/2721 (0.7%) |
| 23 | x | 0.58 | 1/1145 (0.1%) | 1.09 | 1/1781 (0.1%) |
| 24 | A | 0.66 | 9/69196 (0.0%) | 1.26 | 616/107943 (0.6%) |
| 25 | B | 0.59 | 1/2873 (0.0%) | 1.25 | 29/4478 (0.6%) |
| 26 | C | 0.48 | 0/2122 | 0.73 | 1/2852 (0.0%) |
| 27 | D | 0.44 | 0/1586 | 0.67 | 0/2134 |
| 28 | E | 0.43 | 0/1571 | 0.63 | 0/2113 |
| 29 | F | 0.43 | 0/1435 | 0.71 | 2/1926 (0.1%) |
| 30 | G | 0.42 | 0/1343 | 0.67 | 4/1816 (0.2%) |
| 31 | I | 0.38 | 0/1046 | 0.61 | 0/1410 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 32 | H | 0.38 | 0/1122 | 0.63 | 0/1515 |
| 33 | J | 0.46 | 0/1152 | 0.61 | 0/1551 |
| 34 | K | 0.46 | 0/948 | 0.69 | 0/1268 |
| 35 | L | 0.44 | 0/1054 | 0.74 | 1/1403 (0.1%) |
| 36 | M | 0.46 | 0/1093 | 0.72 | 1/1460 (0.1%) |
| 37 | N | 0.44 | 0/974 | 0.65 | 0/1301 |
| 38 | O | 0.42 | 0/902 | 0.59 | 0/1209 |
| 39 | P | 0.45 | 0/929 | 0.67 | 0/1242 |
| 40 | Q | 0.47 | 0/960 | 0.60 | 1/1278 (0.1%) |
| 41 | R | 0.45 | 0/829 | 0.72 | 0/1107 |
| 42 | S | 0.40 | 0/864 | 0.62 | 0/1156 |
| 43 | T | 0.40 | 0/745 | 0.63 | 0/994 |
| 44 | U | 0.44 | 0/788 | 0.78 | 2/1051 (0.2%) |
| 45 | V | 0.40 | 0/766 | 0.60 | 0/1025 |
| 46 | W | 0.41 | 0/582 | 0.62 | 0/769 |
| 47 | X | 0.38 | 0/635 | 0.59 | 0/848 |
| 48 | Y | 0.42 | 0/510 | 0.64 | 0/677 |
| 49 | Z | 0.40 | 0/453 | 0.60 | 0/605 |
| 50 | 0 | 0.41 | 0/450 | 0.72 | 0/599 |
| 51 | 1 | 0.42 | 0/417 | 0.84 | 1/554 (0.2%) |
| 52 | 2 | 0.41 | 0/380 | 0.67 | 0/498 |
| 53 | 3 | 0.47 | 0/513 | 0.65 | 0/676 |
| 54 | 4 | 0.67 | 1/303 (0.3%) | 0.78 | 0/397 |
| 55 | 6 | 0.42 | 0/532 | 0.62 | 0/709 |
| All | All | 0.59 | 17/157773 (0.0%) | 1.14 | 1020/235956 (0.4%) |

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 |
|---|---|---|---|
| 1 | a | 2 | 0 |
| 2 | b | 0 | 4 |
| 5 | e | 0 | 4 |
| 6 | f | 0 | 1 |
| 7 | g | 0 | 2 |
| 8 | h | 0 | 1 |
| 9 | i | 0 | 1 |
| 10 | j | 0 | 5 |
| 12 | l | 0 | 1 |
| 13 | m | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 16 | p | 0 | 1 |
| 17 | q | 0 | 2 |
| 18 | r | 0 | 3 |
| 19 | s | 0 | 1 |
| 21 | u | 0 | 1 |
| 24 | A | 2 | 0 |
| 26 | C | 0 | 1 |
| 28 | E | 0 | 1 |
| 30 | G | 0 | 3 |
| 32 | H | 0 | 2 |
| 34 | K | 0 | 3 |
| 35 | L | 0 | 4 |
| 42 | S | 0 | 1 |
| 44 | U | 0 | 3 |
| 48 | Y | 0 | 1 |
| 50 | 0 | 0 | 2 |
| 51 | 1 | 0 | 1 |
| 53 | 3 | 0 | 1 |
| All | All | 4 | 51 |

The worst 5 of 17 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 23 | x | 87 | A | OP3-P | -10.73 | 1.48 | 1.61 |
| 24 | A | 1 | G | OP3-P | -10.59 | 1.48 | 1.61 |
| 25 | B | 1 | U | OP3-P | -10.53 | 1.48 | 1.61 |
| 22 | v | 1 | C | OP3-P | -10.52 | 1.48 | 1.61 |
| 1 | a | 2 | A | OP3-P | -10.51 | 1.48 | 1.61 |

The worst 5 of 1020 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A | 1313 | U | N3-C2-O2 | -14.71 | 111.90 | 122.20 |
| 24 | A | 2072 | C | C6-N1-C2 | -14.04 | 114.69 | 120.30 |
| 1 | a | 89 | U | C5-C4-O4 | -13.94 | 117.53 | 125.90 |
| 1 | a | 529 | G | C5-C6-O6 | -13.71 | 120.38 | 128.60 |
| 24 | A | 62 | U | N1-C2-O2 | 13.14 | 132.00 | 122.80 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | a | 527 | G7M | C4',C3' |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 24 | A | 2069 | G7M | C4',C3' |

5 of 51 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | b | 16 | GLY | Peptide |
| 2 | b | 17 | HIS | Mainchain,Peptide |
| 2 | b | 72 | LYS | Peptide |
| 5 | e | 76 | ASN | Peptide |
| 5 | e | 88 | HIS | 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 |
|---|---|---|---|---|---|---|
| 2 | b | 216/218 (99%) | 189 (88%) | 23 (11%) | 4 (2%) | 8 42 |
| 3 | c | 204/206 (99%) | 190 (93%) | 13 (6%) | 1 (0%) | 29 68 |
| 4 | d | 203/205 (99%) | 187 (92%) | 14 (7%) | 2 (1%) | 15 55 |
| 5 | e | 155/157 (99%) | 134 (86%) | 16 (10%) | 5 (3%) | 4 31 |
| 6 | f | 98/100 (98%) | 82 (84%) | 10 (10%) | 6 (6%) | 1 17 |
| 7 | g | 149/151 (99%) | 135 (91%) | 11 (7%) | 3 (2%) | 7 41 |
| 8 | h | 127/129 (98%) | 115 (91%) | 11 (9%) | 1 (1%) | 19 59 |
| 9 | i | 125/127 (98%) | 104 (83%) | 15 (12%) | 6 (5%) | 2 22 |
| 10 | j | 96/98 (98%) | 82 (85%) | 10 (10%) | 4 (4%) | 3 25 |
| 11 | k | 114/116 (98%) | 100 (88%) | 11 (10%) | 3 (3%) | 5 35 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 12 | l | 121/123 (98%) | 98 (81%) | 14 (12%) | 9 (7%) | 1 | 13 |
| 13 | m | 112/114 (98%) | 97 (87%) | 12 (11%) | 3 (3%) | 5 | 35 |
| 14 | n | 98/100 (98%) | 83 (85%) | 13 (13%) | 2 (2%) | 7 | 41 |
| 15 | o | 86/88 (98%) | 73 (85%) | 11 (13%) | 2 (2%) | 6 | 38 |
| 16 | p | 80/82 (98%) | 71 (89%) | 6 (8%) | 3 (4%) | 3 | 27 |
| 17 | q | 78/80 (98%) | 66 (85%) | 10 (13%) | 2 (3%) | 5 | 35 |
| 18 | r | 63/65 (97%) | 57 (90%) | 2 (3%) | 4 (6%) | 1 | 17 |
| 19 | s | 77/79 (98%) | 70 (91%) | 6 (8%) | 1 (1%) | 12 | 50 |
| 20 | t | 83/85 (98%) | 77 (93%) | 6 (7%) | 0 | 100 | 100 |
| 21 | u | 63/65 (97%) | 50 (79%) | 9 (14%) | 4 (6%) | 1 | 17 |
| 26 | C | 269/271 (99%) | 246 (91%) | 20 (7%) | 3 (1%) | 14 | 53 |
| 27 | D | 207/209 (99%) | 193 (93%) | 13 (6%) | 1 (0%) | 29 | 68 |
| 28 | E | 199/201 (99%) | 184 (92%) | 12 (6%) | 3 (2%) | 10 | 47 |
| 29 | F | 175/177 (99%) | 158 (90%) | 13 (7%) | 4 (2%) | 6 | 38 |
| 30 | G | 174/176 (99%) | 157 (90%) | 11 (6%) | 6 (3%) | 3 | 31 |
| 31 | I | 139/141 (99%) | 121 (87%) | 15 (11%) | 3 (2%) | 6 | 39 |
| 32 | H | 147/149 (99%) | 129 (88%) | 14 (10%) | 4 (3%) | 5 | 35 |
| 33 | J | 140/142 (99%) | 136 (97%) | 4 (3%) | 0 | 100 | 100 |
| 34 | K | 120/122 (98%) | 105 (88%) | 10 (8%) | 5 (4%) | 3 | 25 |
| 35 | L | 141/143 (99%) | 129 (92%) | 9 (6%) | 3 (2%) | 7 | 40 |
| 36 | M | 134/136 (98%) | 124 (92%) | 7 (5%) | 3 (2%) | 6 | 39 |
| 37 | N | 118/120 (98%) | 106 (90%) | 12 (10%) | 0 | 100 | 100 |
| 38 | O | 114/116 (98%) | 104 (91%) | 8 (7%) | 2 (2%) | 8 | 43 |
| 39 | P | 112/114 (98%) | 104 (93%) | 7 (6%) | 1 (1%) | 17 | 57 |
| 40 | Q | 115/117 (98%) | 108 (94%) | 7 (6%) | 0 | 100 | 100 |
| 41 | R | 101/103 (98%) | 91 (90%) | 8 (8%) | 2 (2%) | 7 | 41 |
| 42 | S | 108/110 (98%) | 102 (94%) | 6 (6%) | 0 | 100 | 100 |
| 43 | T | 91/93 (98%) | 81 (89%) | 7 (8%) | 3 (3%) | 4 | 31 |
| 44 | U | 100/102 (98%) | 89 (89%) | 6 (6%) | 5 (5%) | 2 | 21 |
| 45 | V | 92/94 (98%) | 90 (98%) | 2 (2%) | 0 | 100 | 100 |
| 46 | W | 73/75 (97%) | 68 (93%) | 4 (6%) | 1 (1%) | 11 | 48 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 47 | X | 75/77 (97%) | 71 (95%) | 4 (5%) | 0 | 100 100 |
| 48 | Y | 61/63 (97%) | 57 (93%) | 4 (7%) | 0 | 100 100 |
| 49 | Z | 56/58 (97%) | 53 (95%) | 3 (5%) | 0 | 100 100 |
| 50 | 0 | 54/56 (96%) | 49 (91%) | 4 (7%) | 1 (2%) | 8 42 |
| 51 | 1 | 48/50 (96%) | 45 (94%) | 2 (4%) | 1 (2%) | 7 40 |
| 52 | 2 | 44/46 (96%) | 41 (93%) | 2 (4%) | 1 (2%) | 6 38 |
| 53 | 3 | 62/64 (97%) | 57 (92%) | 4 (6%) | 1 (2%) | 9 46 |
| 54 | 4 | 36/38 (95%) | 33 (92%) | 2 (6%) | 1 (3%) | 5 34 |
| 55 | 6 | 64/66 (97%) | 59 (92%) | 4 (6%) | 1 (2%) | 9 46 |
| All | All | 5717/5817 (98%) | 5150 (90%) | 447 (8%) | 120 (2%) | 10 40 |

5 of 120 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | b | 17 | HIS |
| 2 | b | 18 | GLN |
| 2 | b | 73 | ARG |
| 4 | d | 192 | ALA |
| 5 | e | 77 | ASN |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | b | 180/180 (100%) | 178 (99%) | 2 (1%) | 73 88 |
| 3 | c | 170/170 (100%) | 170 (100%) | 0 | 100 100 |
| 4 | d | 172/172 (100%) | 171 (99%) | 1 (1%) | 86 94 |
| 5 | e | 119/119 (100%) | 119 (100%) | 0 | 100 100 |
| 6 | f | 87/87 (100%) | 87 (100%) | 0 | 100 100 |
| 7 | g | 124/124 (100%) | 124 (100%) | 0 | 100 100 |
| 8 | h | 104/104 (100%) | 104 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 9 | i | 105/105 (100%) | 105 (100%) | 0 | 100 | 100 |
| 10 | j | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 11 | k | 89/89 (100%) | 89 (100%) | 0 | 100 | 100 |
| 12 | l | 103/103 (100%) | 102 (99%) | 1 (1%) | 76 | 88 |
| 13 | m | 92/92 (100%) | 92 (100%) | 0 | 100 | 100 |
| 14 | n | 79/83 (95%) | 78 (99%) | 1 (1%) | 69 | 86 |
| 15 | o | 76/76 (100%) | 76 (100%) | 0 | 100 | 100 |
| 16 | p | 65/65 (100%) | 64 (98%) | 1 (2%) | 65 | 84 |
| 17 | q | 74/74 (100%) | 74 (100%) | 0 | 100 | 100 |
| 18 | r | 48/56 (86%) | 48 (100%) | 0 | 100 | 100 |
| 19 | s | 70/70 (100%) | 70 (100%) | 0 | 100 | 100 |
| 20 | t | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 21 | u | 44/55 (80%) | 44 (100%) | 0 | 100 | 100 |
| 26 | C | 216/216 (100%) | 215 (100%) | 1 (0%) | 88 | 95 |
| 27 | D | 164/164 (100%) | 164 (100%) | 0 | 100 | 100 |
| 28 | E | 165/165 (100%) | 165 (100%) | 0 | 100 | 100 |
| 29 | F | 148/148 (100%) | 148 (100%) | 0 | 100 | 100 |
| 30 | G | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 31 | I | 109/109 (100%) | 109 (100%) | 0 | 100 | 100 |
| 32 | H | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 33 | J | 116/116 (100%) | 116 (100%) | 0 | 100 | 100 |
| 34 | K | 103/103 (100%) | 102 (99%) | 1 (1%) | 76 | 88 |
| 35 | L | 102/102 (100%) | 101 (99%) | 1 (1%) | 76 | 88 |
| 36 | M | 109/109 (100%) | 109 (100%) | 0 | 100 | 100 |
| 37 | N | 100/100 (100%) | 100 (100%) | 0 | 100 | 100 |
| 38 | O | 86/86 (100%) | 86 (100%) | 0 | 100 | 100 |
| 39 | P | 99/99 (100%) | 99 (100%) | 0 | 100 | 100 |
| 40 | Q | 89/89 (100%) | 89 (100%) | 0 | 100 | 100 |
| 41 | R | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 42 | S | 93/93 (100%) | 93 (100%) | 0 | 100 | 100 |
| 43 | T | 80/80 (100%) | 80 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 44 | U | 83/83 (100%) | 83 (100%) | 0 | 100 100 |
| 45 | V | 78/78 (100%) | 78 (100%) | 0 | 100 100 |
| 46 | W | 57/57 (100%) | 57 (100%) | 0 | 100 100 |
| 47 | X | 67/67 (100%) | 66 (98%) | 1 (2%) | 65 84 |
| 48 | Y | 55/55 (100%) | 55 (100%) | 0 | 100 100 |
| 49 | Z | 48/48 (100%) | 48 (100%) | 0 | 100 100 |
| 50 | 0 | 47/47 (100%) | 46 (98%) | 1 (2%) | 53 78 |
| 51 | 1 | 45/45 (100%) | 45 (100%) | 0 | 100 100 |
| 52 | 2 | 38/38 (100%) | 38 (100%) | 0 | 100 100 |
| 53 | 3 | 51/51 (100%) | 51 (100%) | 0 | 100 100 |
| 54 | 4 | 34/34 (100%) | 34 (100%) | 0 | 100 100 |
| 55 | 6 | 59/59 (100%) | 59 (100%) | 0 | 100 100 |
| All | All | 4728/4751 (100%) | 4717 (100%) | 11 (0%) | 93 98 |

5 of 11 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 34 | K | 21 | CYS |
| 35 | L | 27 | LEU |
| 50 | 0 | 2 | VAL |
| 47 | X | 4 | CYS |
| 14 | n | 34 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 44 | U | 39 | ASN |
| 37 | N | 81 | ASN |
| 27 | D | 49 | GLN |
| 37 | N | 62 | ASN |
| 26 | C | 44 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | a | 1531/1539 (99%) | 260 (16%) | 0 |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 22 | v | 76/77 (98%) | 15 (19%) | 0 |
| 23 | x | 47/48 (97%) | 21 (44%) | 0 |
| 24 | A | 2893/2903 (99%) | 540 (18%) | 34 (1%) |
| 25 | B | 119/120 (99%) | 17 (14%) | 3 (2%) |
| All | All | 4666/4687 (99%) | 853 (18%) | 37 (0%) |

5 of 853 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | a | 6 | G |
| 1 | a | 9 | G |
| 1 | a | 22 | G |
| 1 | a | 32 | A |
| 1 | a | 39 | G |

5 of 37 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | A | 2566 | A |
| 25 | B | 66 | A |
| 24 | A | 2610 | C |
| 24 | A | 2832 | U |
| 24 | A | 1070 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 24 | 5MU | A | 1939 | 24 | 19,22,23 | 1.45 | 4 (21%) | 28,32,35 | 2.18 | 5 (17%) |
| 24 | G7M | A | 2069 | 24 | 20,26,27 | 1.41 | 3 (15%) | 17,39,42 | 1.59 | 2 (11%) |
| 24 | PSU | A | 2504 | 24 | 18,21,22 | 1.44 | 3 (16%) | 22,30,33 | 1.84 | 3 (13%) |
| 22 | 4SU | v | 8 | 22 | 18,21,22 | 1.80 | 4 (22%) | 26,30,33 | 2.35 | 5 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 24 | PSU | A | 2580 | 24 | 18,21,22 | 1.51 | 3 (16%) | 22,30,33 | 1.94 | 3 (13%) |
| 24 | 2MA | A | 2503 | 24 | 17,25,26 | 1.00 | 1 (5%) | 17,37,40 | 0.96 | 2 (11%) |
| 24 | 6MZ | A | 1618 | 24 | 18,25,26 | 0.94 | 1 (5%) | 16,36,39 | 2.35 | 4 (25%) |
| 1 | PSU | a | 516 | 1 | 18,21,22 | 1.39 | 3 (16%) | 22,30,33 | 1.87 | 4 (18%) |
| 22 | PSU | v | 55 | 22 | 18,21,22 | 1.38 | 3 (16%) | 22,30,33 | 1.86 | 4 (18%) |
| 22 | H2U | v | 20 | 22 | 18,21,22 | 0.94 | 2 (11%) | 21,30,33 | 1.26 | 3 (14%) |
| 1 | UR3 | a | 1498 | 1 | 19,22,23 | 1.13 | 2 (10%) | 26,32,35 | 2.06 | 5 (19%) |
| 24 | PSU | A | 955 | 24 | 18,21,22 | 1.42 | 4 (22%) | 22,30,33 | 1.94 | 3 (13%) |
| 1 | 2MG | a | 1516 | 1 | 18,26,27 | 0.89 | 1 (5%) | 16,38,41 | 1.15 | 2 (12%) |
| 24 | PSU | A | 2457 | 24 | 18,21,22 | 1.55 | 4 (22%) | 22,30,33 | 2.11 | 5 (22%) |
| 24 | PSU | A | 746 | 24 | 18,21,22 | 1.34 | 2 (11%) | 22,30,33 | 1.74 | 4 (18%) |
| 1 | G7M | a | 527 | 1 | 20,26,27 | 1.74 | 5 (25%) | 17,39,42 | 1.94 | 6 (35%) |
| 24 | 3TD | A | 1915 | 24 | 18,22,23 | 4.06 | 7 (38%) | 22,32,35 | 1.79 | 3 (13%) |
| 1 | MA6 | a | 1519 | 1 | 18,26,27 | 0.92 | 1 (5%) | 19,38,41 | 1.84 | 4 (21%) |
| 1 | 5MC | a | 1407 | 1 | 18,22,23 | 0.89 | 2 (11%) | 26,32,35 | 1.19 | 3 (11%) |
| 1 | MA6 | a | 1518 | 1 | 18,26,27 | 0.96 | 1 (5%) | 19,38,41 | 1.69 | 4 (21%) |
| 24 | OMG | A | 2251 | 22,24 | 18,26,27 | 1.01 | 1 (5%) | 19,38,41 | 1.19 | 2 (10%) |
| 24 | 6MZ | A | 2030 | 24 | 18,25,26 | 0.95 | 1 (5%) | 16,36,39 | 2.69 | 4 (25%) |
| 24 | 5MU | A | 747 | 24 | 19,22,23 | 1.42 | 5 (26%) | 28,32,35 | 2.06 | 8 (28%) |
| 24 | 5MC | A | 1962 | 24 | 18,22,23 | 1.00 | 1 (5%) | 26,32,35 | 1.49 | 3 (11%) |
| 24 | 2MG | A | 1835 | 24 | 18,26,27 | 0.91 | 1 (5%) | 16,38,41 | 1.22 | 3 (18%) |
| 24 | PSU | A | 2605 | 24 | 18,21,22 | 1.40 | 3 (16%) | 22,30,33 | 1.90 | 4 (18%) |
| 24 | 1MG | A | 745 | 24 | 18,26,27 | 0.81 | 1 (5%) | 19,39,42 | 1.07 | 2 (10%) |
| 24 | PSU | A | 2604 | 24 | 18,21,22 | 1.48 | 3 (16%) | 22,30,33 | 1.84 | 4 (18%) |
| 1 | 4OC | a | 1402 | 1 | 20,23,24 | 0.77 | 0 | 26,32,35 | 0.98 | 2 (7%) |
| 24 | 2MG | A | 2445 | 24 | 18,26,27 | 0.98 | 1 (5%) | 16,38,41 | 1.19 | 3 (18%) |
| 24 | PSU | A | 1911 | 24 | 18,21,22 | 1.38 | 3 (16%) | 22,30,33 | 1.94 | 3 (13%) |
| 1 | 2MG | a | 1207 | 1 | 18,26,27 | 1.02 | 1 (5%) | 16,38,41 | 1.04 | 2 (12%) |
| 1 | 5MC | a | 967 | 1 | 18,22,23 | 0.92 | 2 (11%) | 26,32,35 | 1.10 | 3 (11%) |
| 1 | 2MG | a | 966 | 1 | 18,26,27 | 0.91 | 1 (5%) | 16,38,41 | 1.22 | 2 (12%) |
| 24 | OMU | A | 2552 | 24 | 19,22,23 | 1.23 | 2 (10%) | 26,31,34 | 1.94 | 7 (26%) |
| 24 | OMC | A | 2498 | 24 | 19,22,23 | 0.88 | 1 (5%) | 26,31,34 | 1.13 | 2 (7%) |
| 24 | H2U | A | 2449 | 24 | 18,21,22 | 1.05 | 2 (11%) | 21,30,33 | 1.76 | 3 (14%) |
| 22 | 5MU | v | 54 | 22 | 19,22,23 | 1.40 | 6 (31%) | 28,32,35 | 2.05 | 6 (21%) |
| 24 | PSU | A | 1917 | 24 | 18,21,22 | 1.42 | 3 (16%) | 22,30,33 | 1.93 | 3 (13%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | 5MU | A | 1939 | 24 | - | 2/7/25/26 | 0/2/2/2 |
| 24 | G7M | A | 2069 | 24 | 2/2/5/5 | 2/3/25/26 | 0/3/3/3 |
| 24 | PSU | A | 2504 | 24 | - | 2/7/25/26 | 0/2/2/2 |
| 22 | 4SU | v | 8 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | PSU | A | 2580 | 24 | - | 2/7/25/26 | 0/2/2/2 |
| 24 | 2MA | A | 2503 | 24 | - | 2/3/25/26 | 0/3/3/3 |
| 24 | 6MZ | A | 1618 | 24 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | PSU | a | 516 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | PSU | v | 55 | 22 | - | 2/7/25/26 | 0/2/2/2 |
| 22 | H2U | v | 20 | 22 | - | 0/7/38/39 | 0/2/2/2 |
| 1 | UR3 | a | 1498 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 24 | PSU | A | 955 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | a | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 24 | PSU | A | 2457 | 24 | - | 2/7/25/26 | 0/2/2/2 |
| 24 | PSU | A | 746 | 24 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | G7M | a | 527 | 1 | 2/2/5/5 | 1/3/25/26 | 0/3/3/3 |
| 24 | 3TD | A | 1915 | 24 | - | 5/7/25/26 | 0/2/2/2 |
| 1 | MA6 | a | 1519 | 1 | - | 3/7/29/30 | 0/3/3/3 |
| 1 | 5MC | a | 1407 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MA6 | a | 1518 | 1 | - | 3/7/29/30 | 0/3/3/3 |
| 24 | OMG | A | 2251 | 22,24 | - | 3/5/27/28 | 0/3/3/3 |
| 24 | 6MZ | A | 2030 | 24 | - | 3/5/27/28 | 0/3/3/3 |
| 24 | 5MU | A | 747 | 24 | - | 1/7/25/26 | 0/2/2/2 |
| 24 | 5MC | A | 1962 | 24 | - | 4/7/25/26 | 0/2/2/2 |
| 24 | 2MG | A | 1835 | 24 | - | 2/5/27/28 | 0/3/3/3 |
| 24 | PSU | A | 2605 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 1MG | A | 745 | 24 | - | 0/3/25/26 | 0/3/3/3 |
| 24 | PSU | A | 2604 | 24 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 4OC | a | 1402 | 1 | - | 0/9/29/30 | 0/2/2/2 |
| 24 | 2MG | A | 2445 | 24 | - | 3/5/27/28 | 0/3/3/3 |
| 24 | PSU | A | 1911 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | a | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | a | 967 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | 2MG | a | 966 | 1 | - | 0/5/27/28 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 24 | OMU | A | 2552 | 24 | - | 2/9/27/28 | 0/2/2/2 |
| 24 | OMC | A | 2498 | 24 | - | 2/9/27/28 | 0/2/2/2 |
| 24 | H2U | A | 2449 | 24 | - | 0/7/38/39 | 0/2/2/2 |
| 22 | 5MU | v | 54 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | PSU | A | 1917 | 24 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 94 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 24 | A | 1915 | 3TD | C6-C5 | 11.98 | 1.49 | 1.35 |
| 24 | A | 1915 | 3TD | C2-N1 | 8.97 | 1.48 | 1.37 |
| 24 | A | 1915 | 3TD | C6-N1 | 5.66 | 1.45 | 1.36 |
| 1 | a | 527 | G7M | C5-C4 | 4.81 | 1.48 | 1.39 |
| 22 | v | 8 | 4SU | C4-S4 | -4.62 | 1.59 | 1.68 |

The worst 5 of 140 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | A | 2030 | 6MZ | C9-N6-C6 | -7.16 | 116.71 | 122.87 |
| 24 | A | 2457 | PSU | N1-C2-N3 | 6.97 | 123.03 | 115.13 |
| 22 | v | 8 | 4SU | C4-N3-C2 | -6.82 | 120.71 | 127.34 |
| 24 | A | 1618 | 6MZ | C2-N1-C6 | 6.65 | 122.29 | 116.59 |
| 24 | A | 2449 | H2U | C4-N3-C2 | -6.55 | 120.36 | 125.79 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | a | 527 | G7M | C4' |
| 1 | a | 527 | G7M | C3' |
| 24 | A | 2069 | G7M | C4' |
| 24 | A | 2069 | G7M | C3' |

5 of 53 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | a | 967 | 5MC | O4'-C4'-C5'-O5' |
| 1 | a | 967 | 5MC | C3'-C4'-C5'-O5' |
| 1 | a | 1498 | UR3 | O4'-C1'-N1-C6 |
| 1 | a | 1498 | UR3 | O4'-C1'-N1-C2 |
| 1 | a | 1518 | MA6 | C5-C6-N6-C9 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4121. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

## 6.1 Orthogonal projections

This section was not generated.

## 6.2 Central slices

This section was not generated.

## 6.3 Largest variance slices

This section was not generated.

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

This section was not generated.

## 6.5 Orthogonal surface views

This section was not generated.

## 6.6 Mask visualisation

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

# 7 Map analysis

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

## 7.1 Map-value distribution

This section was not generated.

## 7.2 Volume estimate versus contour level

This section was not generated.

## 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

# 8 Fourier-Shell correlation

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

# 9 Map-model fit

This section was not generated.