# wwPDB X-ray Structure Validation Summary Report (i)

Mar 24, 2024 – 12:07 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 4V4I |
| Title | : | Crystal Structure of a 70S Ribosome-tRNA Complex Reveals Functional Interactions and Rearrangements. |
| Authors | : | Korostelev, A.; Trakhanov, S.; Laurberg, M.; Noller, H.F. |
| Deposited on | : | 2007-02-15 |
| Resolution | : | 3.71 Å(reported) |

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

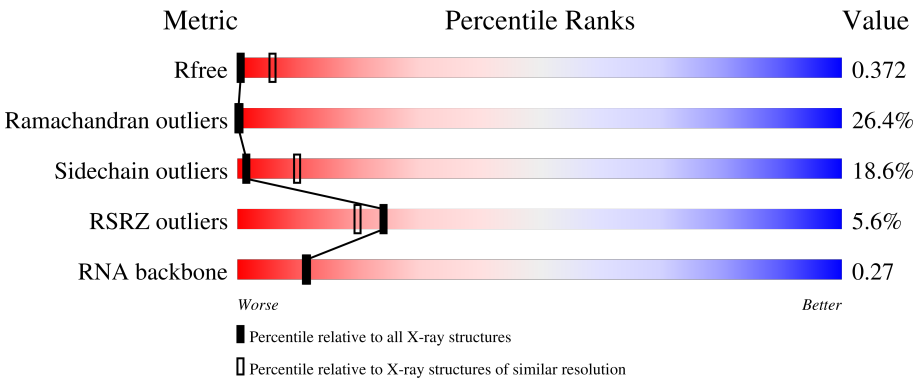
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.71 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1089 (3.90-3.54) |
| Ramachandran outliers | 138981 | 1114 (3.90-3.54) |
| Sidechain outliers | 138945 | 1110 (3.90-3.54) |
| RSRZ outliers | 127900 | 1020 (3.90-3.54) |
| RNA backbone | 3102 | 1027 (4.40-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | w | 2889 | 3% 57% 39% • |
| 2 | x | 121 | 61% 36% • • |
| 3 | A | 229 | 3% 39% 14% • 45% |
| 4 | B | 276 | 5% 57% 38% • • |
| 5 | C | 206 | 5% 56% 34% 7% • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 6 | D | 205 | 4% 55% 35% 5% 5% |
| 7 | E | 182 | 5% 64% 32% |
| 8 | F | 180 | 6% 65% 28% |
| 9 | G | 148 | 2% 59% 38% |
| 10 | H | 163 | 7% 47% 30% 8% 15% |
| 11 | I | 122 | 8% 59% 38% |
| 12 | J | 150 | 6% 55% 38% |
| 13 | K | 141 | 26% 54% 36% 7% |
| 14 | L | 118 | 3% 61% 36% |
| 15 | M | 112 | 18% 56% 31% 7% 5% |
| 16 | N | 146 | % 55% 34% 5% 6% |
| 17 | O | 118 | 17% 70% 25% |
| 18 | P | 101 | 16% 52% 47% |
| 19 | Q | 113 | 12% 61% 31% |
| 20 | R | 96 | 17% 54% 36% 5% |
| 21 | S | 110 | 23% 61% 27% 5% 6% |
| 22 | T | 206 | % 63% 25% 10% |
| 23 | U | 85 | 13% 59% 26% 5% 11% |
| 24 | V | 98 | 21% 58% 24% 7% 10% |
| 25 | W | 72 | 46% 31% 10% 14% |
| 26 | X | 60 | 70% 23% 7% |
| 27 | Y | 60 | 18% 55% 35% 7% |
| 28 | Z | 49 | 2% 61% 31% 6% |
| 29 | a | 65 | 12% 57% 29% 11% |
| 30 | b | 37 | 49% 70% 24% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 31 | y | 1522 | 2%, 62%, 32% |
| 32 | z | 76 | %, 59%, 28%, 13% |
| 33 | 0 | 76 | %, 58%, 37%, 5% |
| 34 | 1 | 10 | 40%, 20%, 40% |
| 35 | c | 256 | %, 55%, 32%, 5%, 9% |
| 36 | d | 239 | 5%, 53%, 30%, 14% |
| 37 | e | 209 | 2%, 56%, 40% |
| 38 | f | 162 | 6%, 66%, 24%, 7% |
| 39 | g | 101 | 3%, 74%, 23% |
| 40 | h | 156 | 8%, 72%, 25% |
| 41 | i | 138 | 4%, 67%, 28%, 5% |
| 42 | j | 128 | 12%, 73%, 24% |
| 43 | k | 105 | %, 64%, 27%, 7% |
| 44 | l | 129 | 6%, 58%, 30%, 10% |
| 45 | m | 132 | 5%, 54%, 36%, 6% |
| 46 | n | 126 | 8%, 63%, 32% |
| 47 | o | 61 | 38%, 61%, 31%, 7% |
| 48 | p | 89 | 3%, 69%, 26% |
| 49 | q | 88 | 14%, 65%, 27%, 6% |
| 50 | r | 105 | 7%, 65%, 26%, 9% |
| 51 | s | 88 | 55%, 24%, 5%, 17% |
| 52 | t | 93 | %, 55%, 26%, 5%, 14% |
| 53 | u | 106 | 20%, 71%, 23%, 7% |
| 54 | v | 27 | 7%, 63%, 26%, 11% |

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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 32 | H2U | z | 16 | - | - | - | X |

# 2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 146532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S LARGE SUBUNIT RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | w | 2889 | 62213 | 27690 | 11624 | 20011 | 2888 | 0 | 0 | 0 |

- Molecule 2 is a RNA chain called 5S LARGE SUBUNIT RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 2 | x | 120 | 2573 | 1146 | 476 | 832 | 119 | 0 | 0 | 0 |

- Molecule 3 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | A | 127 | 996 | 627 | 184 | 184 | 1 | 0 | 0 | 0 |

- Molecule 4 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | B | 272 | 2115 | 1335 | 420 | 357 | 3 | 0 | 0 | 0 |

- Molecule 5 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 5 | C | 201 | 1541 | 974 | 295 | 267 | 5 | 0 | 0 | 0 |

- Molecule 6 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 6 | D | 194 | 1517 | 969 | 283 | 263 | 2 | 0 | 0 | 0 |

- Molecule 7 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 7 | E | 180 | 1468 | 938 | 267 | 259 | 4 | 0 | 0 | 0 |

- Molecule 8 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 8 | F | 173 | 1319 | 839 | 245 | 234 | 1 | 0 | 0 | 0 |

- Molecule 9 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 9 | G | 148 | 1156 | 737 | 204 | 214 | 1 | 0 | 0 | 0 |

- Molecule 10 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 10 | H | 138 | 1103 | 712 | 206 | 182 | 3 | 0 | 0 | 0 |

- Molecule 11 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 11 | I | 122 | 932 | 587 | 171 | 170 | 4 | 0 | 0 | 0 |

- Molecule 12 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 12 | J | 146 | 1114 | 692 | 227 | 193 | 2 | 0 | 0 | 0 |

- Molecule 13 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 13 | K | 137 | 1089 | 698 | 207 | 177 | 7 | 0 | 0 | 0 |

- Molecule 14 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 14 | L | 118 | 968 | 604 | 203 | 160 | 1 | 0 | 0 | 0 |

- Molecule 15 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 15 | M | 106 | 846 | 534 | 168 | 144 | 0 | 0 | 0 |

- Molecule 16 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 16 | N | 137 | 1143 | 713 | 234 | 195 | 1 | 0 | 0 | 0 |

- Molecule 17 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 17 | O | 117 | 964 | 610 | 202 | 151 | 1 | 0 | 0 | 0 |

- Molecule 18 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 18 | P | 101 | 779 | 501 | 142 | 135 | 1 | 0 | 0 | 0 |

- Molecule 19 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 19 | Q | 109 | 868 | 547 | 170 | 150 | 1 | 0 | 0 | 0 |

- Molecule 20 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 20 | R | 92 | 725 | 471 | 131 | 123 | 0 | 0 | 0 |

- Molecule 21 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 21 | S | 103 | 793 | 510 | 151 | 126 | 6 | 0 | 0 | 0 |

- Molecule 22 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 22 | T | 185 | 1475 | 941 | 262 | 269 | 3 | 0 | 0 | 0 |

- Molecule 23 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 23 | U | 76 | 605 | 376 | 126 | 102 | 1 | 0 | 0 | 0 |

- Molecule 24 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 24 | V | 88 | 694 | 435 | 141 | 118 | 0 | 0 | 0 |

- Molecule 25 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 25 | W | 62 | 520 | 325 | 102 | 91 | 2 | 0 | 0 | 0 |

- Molecule 26 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 26 | X | 60 | 477 | 303 | 91 | 82 | 1 | 0 | 0 | 0 |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 27 | Y | 56 | 436 | 275 | 84 | 72 | 5 | 0 | 0 | 0 |

- Molecule 28 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 28 | Z | 48 | 418 | 257 | 104 | 55 | 2 | 0 | 0 | 0 |

- Molecule 29 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 29 | a | 63 | 507 | 326 | 101 | 78 | 2 | 0 | 0 | 0 |

- Molecule 30 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 30 | b | 35 | 294 | 181 | 66 | 44 | 3 | 0 | 0 | 0 |

- Molecule 31 is a RNA chain called 16S SMALL SUBUNIT RIBOSOMAL RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 31 | y | 1502 | 32302 | 14386 | 5984 | 10431 | 1501 | 0 | 0 | 0 |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| y | 450 | G | C | conflict | GB 155076 |
| y | 516 | PSU | U | modified residue | GB 155076 |
| y | 527 | 7MG | G | modified residue | GB 155076 |
| y | 966 | M2G | G | modified residue | GB 155076 |
| y | 967 | 5MC | C | modified residue | GB 155076 |
| y | 1207 | 2MG | G | modified residue | GB 155076 |
| y | 1400 | 5MC | C | modified residue | GB 155076 |
| y | 1402 | 4OC | C | modified residue | GB 155076 |
| y | 1404 | 5MC | C | modified residue | GB 155076 |
| y | 1407 | 5MC | C | modified residue | GB 155076 |
| y | 1498 | UR3 | U | modified residue | GB 155076 |
| y | 1518 | MA6 | A | modified residue | GB 155076 |
| y | 1519 | MA6 | A | modified residue | GB 155076 |

- Molecule 32 is a RNA chain called P-site PHE-tRNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | | | |
| 32 | z | 76 | 1628 | 731 | 290 | 530 | 75 | 2 | 0 | 0 | 0 |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| z | 8 | 4SU | U | modified residue | GB 174422 |
| z | 16 | H2U | U | modified residue | GB 174422 |
| z | 20 | H2U | U | modified residue | GB 174422 |
| z | 32 | PSU | U | modified residue | GB 174422 |
| z | 37 | MIA | A | modified residue | GB 174422 |
| z | 39 | PSU | U | modified residue | GB 174422 |
| z | 46 | 7MG | G | modified residue | GB 174422 |
| z | 54 | 5MU | U | modified residue | GB 174422 |
| z | 55 | PSU | U | modified residue | GB 174422 |

- Molecule 33 is a RNA chain called E-TRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 33 | 0 | 76 | 1621 | 725 | 293 | 528 | 75 | 0 | 0 | 0 |

- Molecule 34 is a RNA chain called MRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 34 | 1 | 6 | 122 | 56 | 19 | 42 | 5 | 0 | 0 | 0 |

- Molecule 35 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 35 | c | 234 | 1900 | 1213 | 341 | 341 | 5 | 0 | 0 | 0 |

- Molecule 36 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 36 | d | 206 | 1612 | 1016 | 314 | 281 | 1 | 0 | 0 | 0 |

- Molecule 37 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 37 | e | 208 | 1703 | 1066 | 339 | 291 | 7 | 0 | 0 | 0 |

- Molecule 38 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 38 | f | 150 | 1146 | 724 | 217 | 201 | 4 | 0 | 0 | 0 |

- Molecule 39 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 39 | g | 101 | 843 | 531 | 155 | 154 | 3 | 0 | 0 | 0 |

- Molecule 40 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 40 | h | 155 | 1257 | 781 | 252 | 218 | 6 | 0 | 0 | 0 |

- Molecule 41 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 41 | i | 138 | 1116 | 705 | 215 | 193 | 3 | 0 | 0 | 0 |

- Molecule 42 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 42 | j | 127 | 1011 | 639 | 198 | 174 | 0 | 0 | 0 |

- Molecule 43 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 43 | k | 98 | 794 | 499 | 156 | 138 | 1 | 0 | 0 | 0 |

- Molecule 44 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 44 | l | 116 | 864 | 537 | 164 | 160 | 3 | 0 | 0 | 0 |

- Molecule 45 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 45 | m | 124 | 970 | 611 | 195 | 163 | 1 | 0 | 0 | 0 |

- Molecule 46 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 46 | n | 125 | 997 | 617 | 207 | 171 | 2 | 0 | 0 | 0 |

- Molecule 47 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 47 | o | 60 | 492 | 312 | 104 | 72 | 4 | 0 | 0 | 0 |

- Molecule 48 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 48 | p | 88 | 734 | 459 | 147 | 126 | 2 | 0 | 0 | 0 |

- Molecule 49 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 49 | q | 83 | 700 | 443 | 139 | 117 | 1 | 0 | 0 | 0 |

- Molecule 50 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 50 | r | 104 | 857 | 547 | 161 | 147 | 2 | 0 | 0 | 0 |

- Molecule 51 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 51 | s | 73 | 598 | 381 | 118 | 99 | 0 | 0 | 0 |

- Molecule 52 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 52 | t | 80 | 647 | 414 | 119 | 112 | 2 | 0 | 0 | 0 |

- Molecule 53 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 53 | u | 99 | 762 | 469 | 162 | 129 | 2 | 0 | 0 | 0 |

- Molecule 54 is a protein called 30S ribosomal protein Thx.

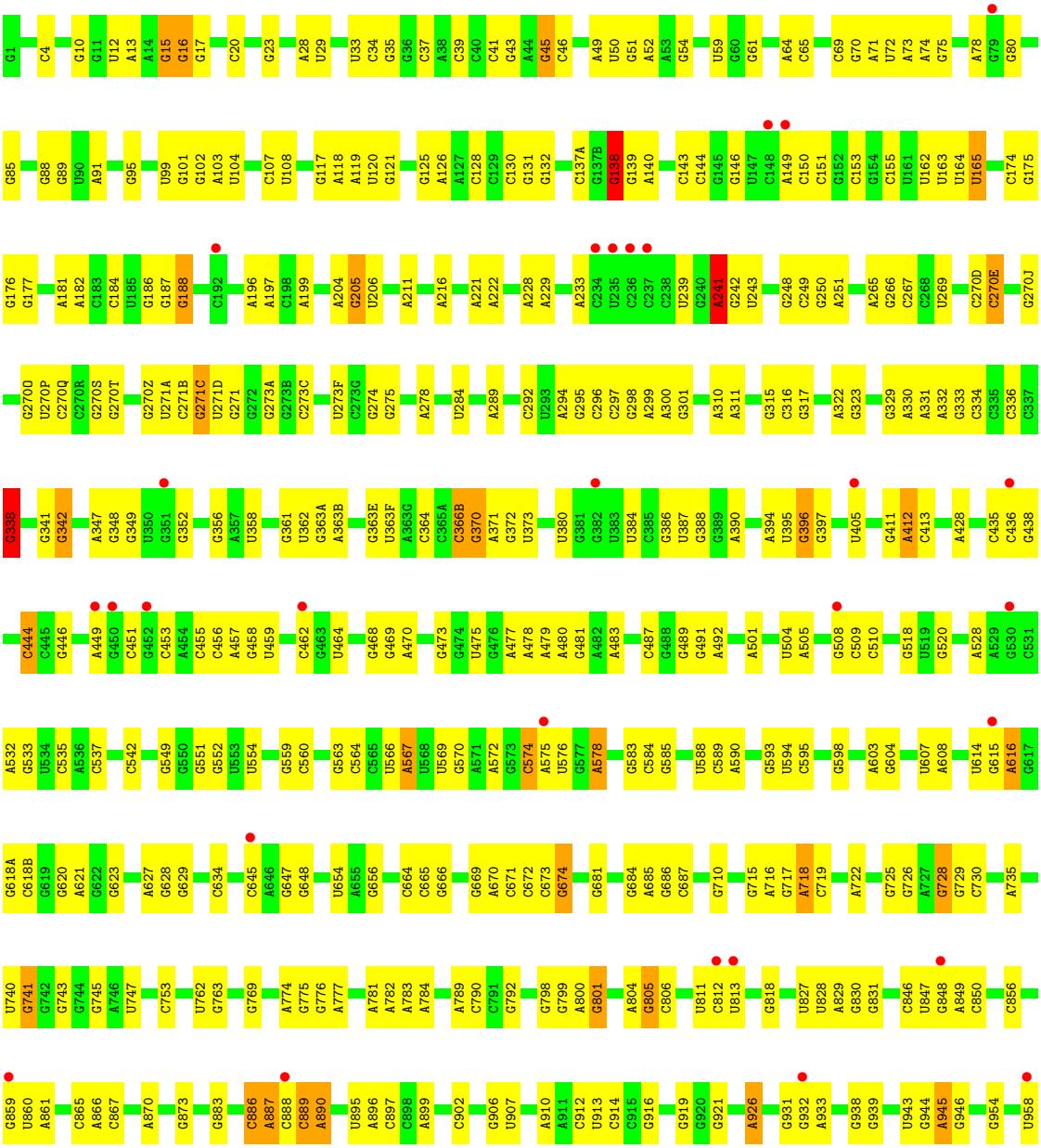
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 54 | v | 24 | 208 | 128 | 50 | 30 | 0 | 0 | 0 |

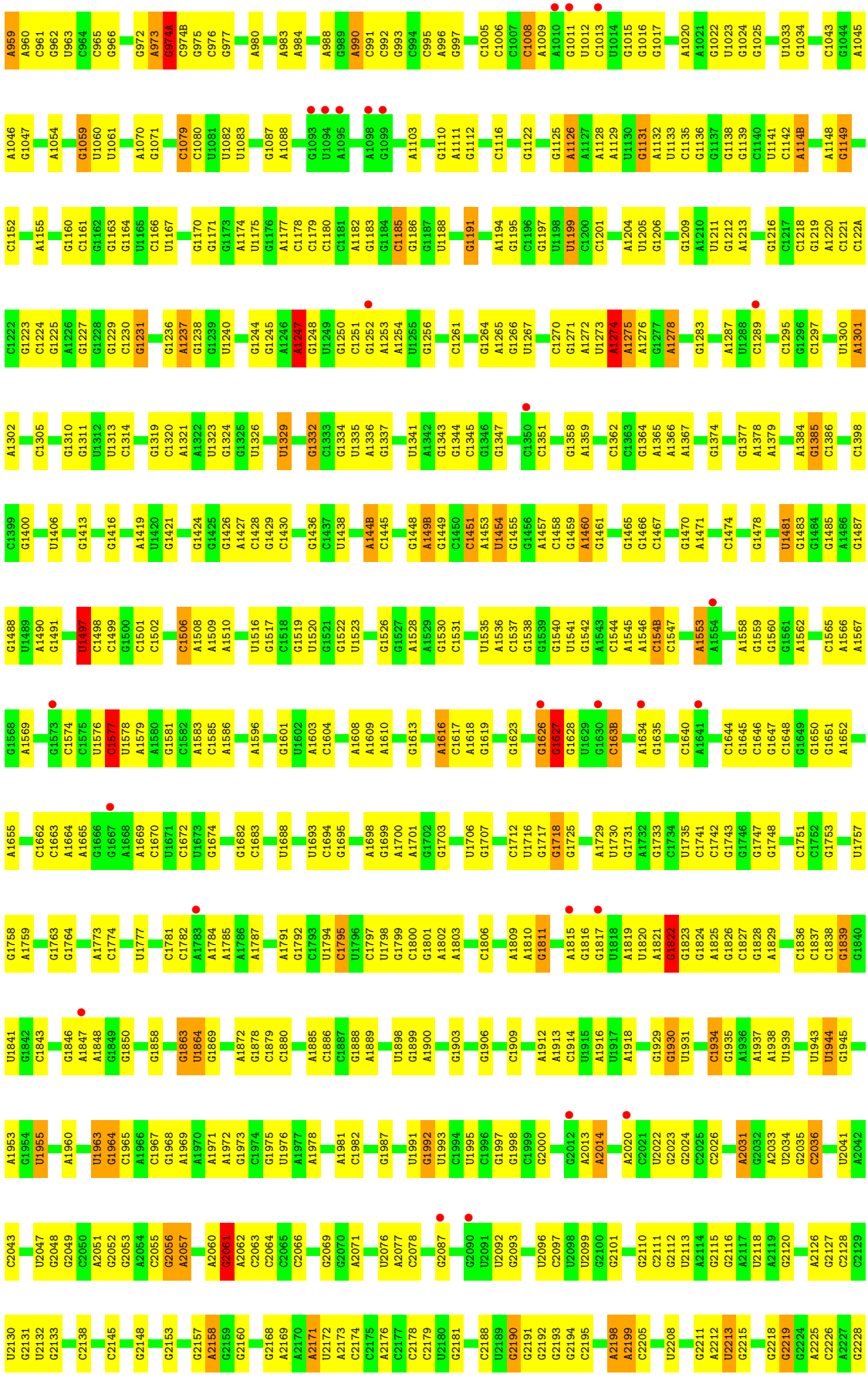
# 3 Residue-property plots (i)

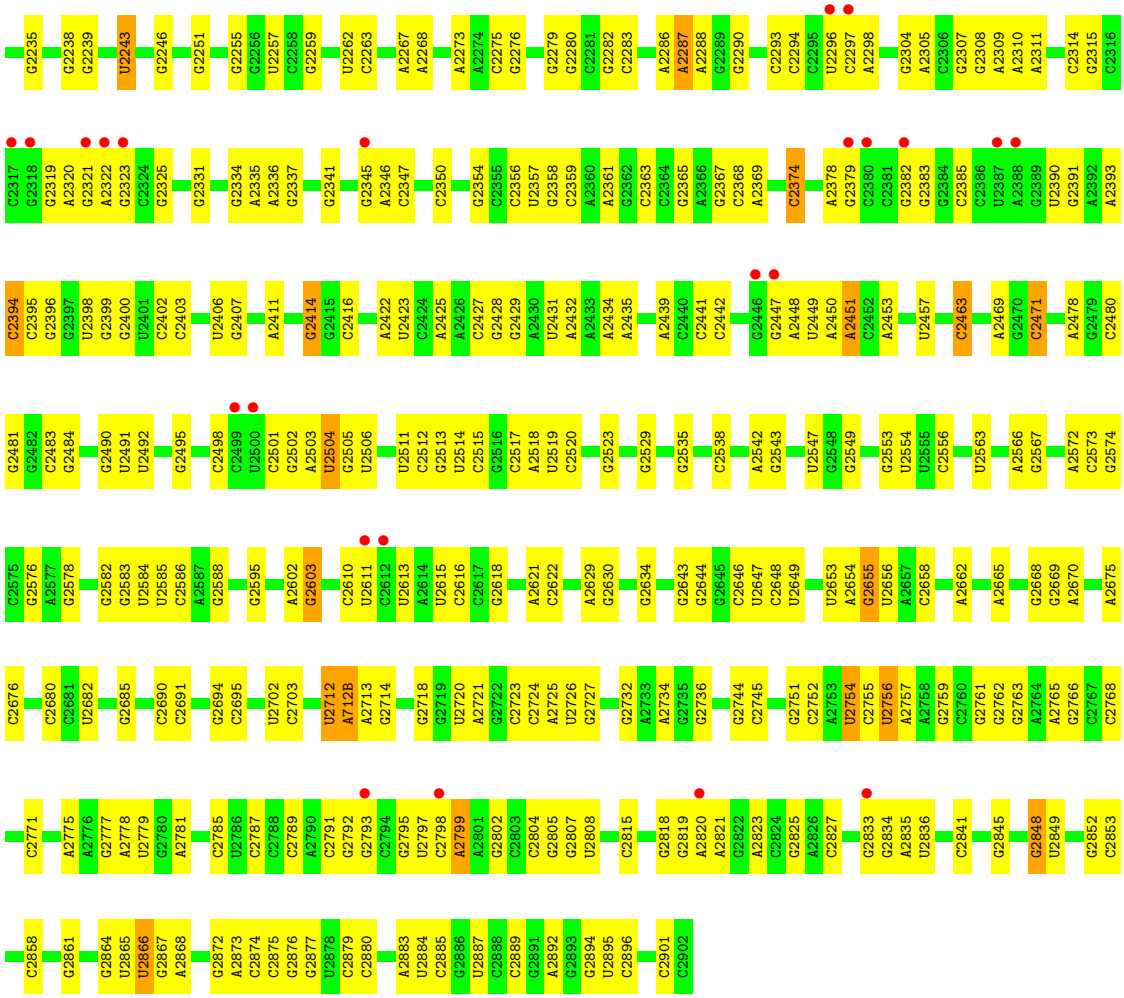
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: 23S LARGE SUBUNIT RIBOSOMAL RNA

Chain w: 3% 57% 39%




A959 A960 C961 G962 U963 C964 C965 G966 G972 A973 G974A C974B G975 C976 G977 A980 A983 A984 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 G1016 G1017 A1020 A1021 G1022 U1023 G1024 G1025 U1033 G1034 C1043 G1044 A1045
A1046 G1047 A1054 G1059 U1060 U1061 A1070 G1071 C1079 C1080 U1081 U1082 U1083 G1087 A1088 G1093 U1094 A1095 A1098 G1099 A1103 G1110 A1111 G1112 C1116 G1122 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 C1142 A114B A1148 G1149
C1152 A1155 G1160 C1161 G1162 G1163 G1164 U1165 C1166 U1167 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 G1186 G1187 U1188 G1191 A1194 G1195 C1196 G1197 U1198 U1199 C1200 C1201 A1204 U1205 G1206 G1209 A1210 U1211 G1212 A1213 G1216 C1217 C1218 G1219 A1220 C1221 C122A
C1222 G1223 C1224 G1225 A1226 G1227 G1228 G1229 C1230 G1231 G1236 A1237 G1238 G1239 U1240 G1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1261 G1264 A1265 G1266 U1267 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278 G1283 A1287 U1288 C1289 C1295 G1296 C1297 U1300 A1301
A1302 C1305 G1310 G1311 U1312 U1313 C1314 G1319 C1320 A1321 A1322 U1323 G1324 G1325 U1326 U1329 G1332 C1333 G1334 U1335 A1336 G1337 U1341 A1342 G1343 G1344 C1345 G1346 G1347 C1350 C1351 G1358 A1359 C1362 C1363 G1364 A1365 A1366 A1367 G1374 G1377 A1378 A1379 A1384 G1385 C1386 C1398
C1399 G1400 U1406 G1413 G1416 A1419 U1420 G1421 G1424 G1425 G1426 A1427 C1428 G1429 C1430 G1436 C1437 U1438 A144B C1445 G1448 A149B G1449 C1450 C1451 A1453 U1454 G1455 G1456 A1457 C1458 G1459 A1460 G1461 G1465 G1466 C1467 G1470 A1471 C1474 G1478 U1481 G1483 G1484 G1485 A1486 G1487
G1488 U1489 A1490 G1491 U1497 C1498 C1499 G1500 C1501 C1502 C1506 A1508 A1509 A1510 U1516 G1517 C1518 G1519 U1520 G1521 G1522 U1523 G1526 G1527 A1528 A1529 G1530 C1531 U1535 A1536 C1537 G1538 G1539 G1540 U1541 G1542 A1543 C1544 A1545 A1546 C154B C1547 A1553 A1554 A1558 G1559 G1560 G1561 A1562 C1565 A1566 A1567
G1568 A1569 G1573 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1585 A1586 A1596 G1601 U1602 A1603 C1604 A1608 A1609 A1610 G1613 A1616 C1617 A1618 G1619 G1623 G1626 G1627 G1628 U1629 G1630 C163B A1634 G1635 C1640 A1641 C1644 G1645 C1646 G1647 C1648 G1649 G1650 G1651 A1652
A1655 C1662 C1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 C1672 U1673 G1674 G1682 C1683 U1688 U1693 C1694 G1695 A1698 G1699 A1700 A1701 G1702 G1703 U1706 G1707 C1712 U1716 G1717 G1718 G1725 A1729 U1730 G1731 A1732 G1733 C1734 U1735 C1741 C1742 G1743 G1746 G1747 G1748 C1751 C1752 G1753 U1757
G1758 A1759 G1763 G1764 A1773 C1774 U1777 C1781 C1782 A1783 A1784 A1785 A1786 A1787 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1806 A1809 A1810 G1811 A1815 G1816 G1817 U1818 A1819 U1820 A1821 G1822 G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1836 C1837 C1838 G1839 G1840
U1841 G1842 C1843 G1846 A1847 A1848 G1849 G1850 G1858 G1863 U1864 G1869 A1872 G1878 C1879 C1880 A1885 C1886 C1887 G1888 A1889 U1898 G1899 A1900 G1903 G1906 C1909 A1912 A1913 C1914 U1915 A1916 U1917 A1918 G1929 G1930 U1931 C1934 G1935 A1936 A1937 A1938 U1939 U1943 U1944 G1945
A1953 G1954 U1955 A1960 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1975 U1976 A1977 A1978 A1981 C1982 G1987 U1991 G1992 U1993 C1994 U1995 C1996 G1997 G1998 C1999 G2000 G2012 A2013 A2014 A2020 C2021 U2022 G2023 G2024 C2025 C2026 A2031 G2032 A2033 U2034 G2035 C2036 U2041 A2042
C2043 U2047 G2048 G2049 C2050 A2051 G2052 C2053 A2054 C2055 G2056 A2057 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 G2070 A2071 U2076 A2077 C2078 G2087 G2090 U2091 U2092 G2093 U2096 C2097 U2098 U2099 G2100 G2101 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 A2126 G2127 C2128 C2129
U2130 G2131 U2132 G2133 C2138 C2145 G2148 G2153 G2157 A2158 G2159 G2160 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 C2188 U2189 G2190 G2191 G2192 G2193 G2194 C2195 A2198 A2199 C2205 U2208 G2211 A2212 U2213 G2215 G2218 G2219 G2224 A2225 C2226 A2227 G2228

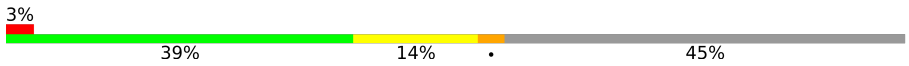


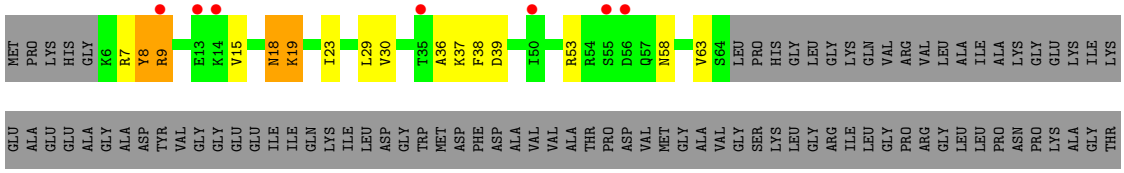

- Molecule 2: 5S LARGE SUBUNIT RIBOSOMAL RNA

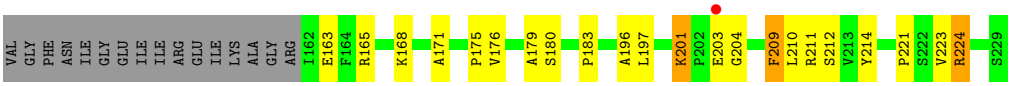
Chain x:

- Molecule 3: 50S ribosomal protein L1

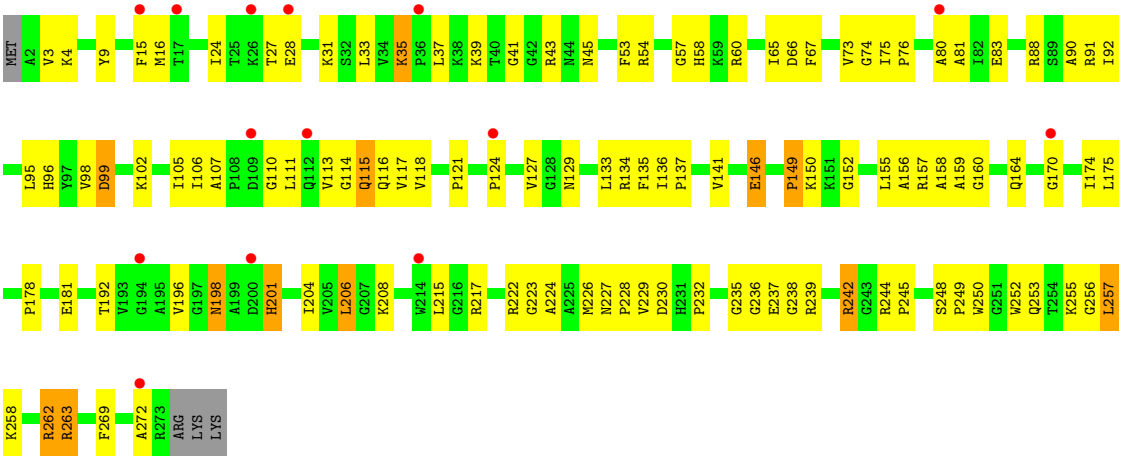
Chain A:



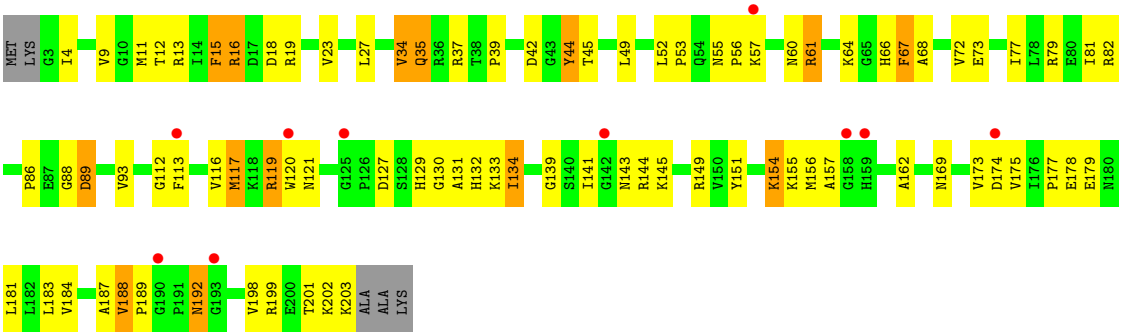





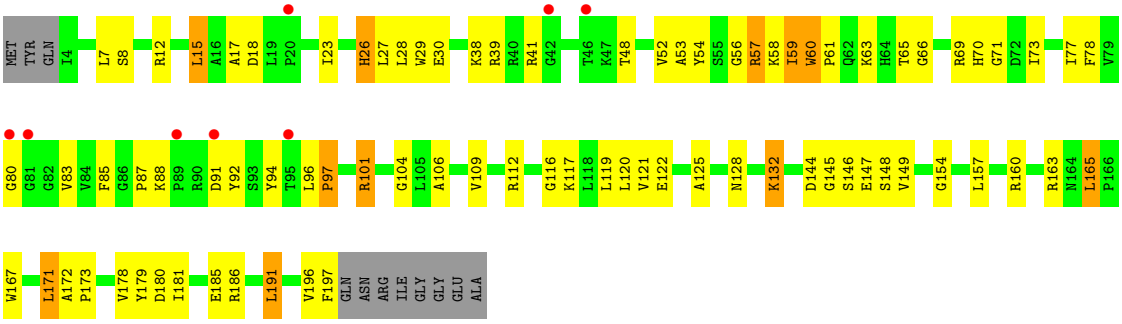

• Molecule 4: 50S ribosomal protein L2




• Molecule 5: 50S ribosomal protein L3

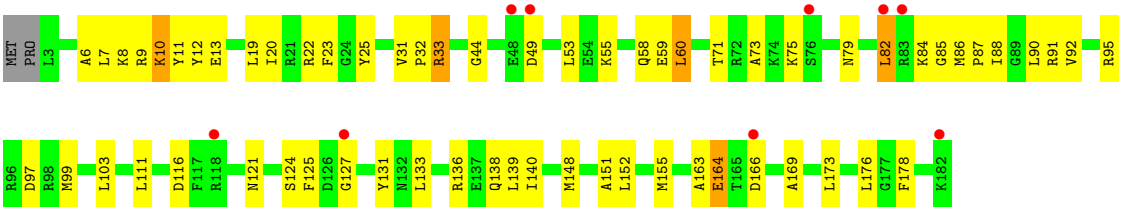



• Molecule 6: 50S ribosomal protein L4



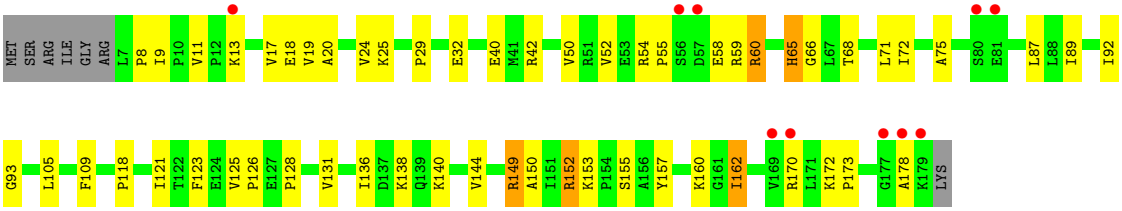
• Molecule 7: 50S ribosomal protein L5

Chain E:



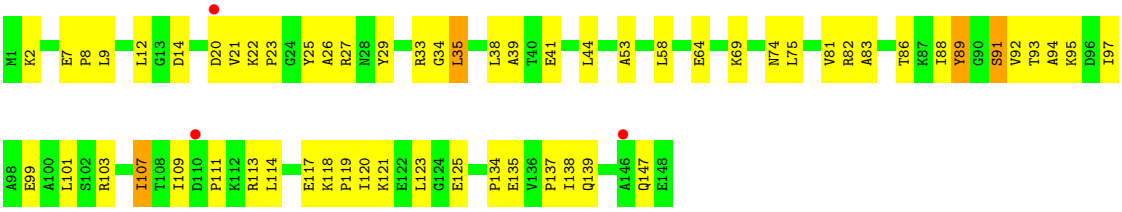

• Molecule 8: 50S ribosomal protein L6

Chain F:



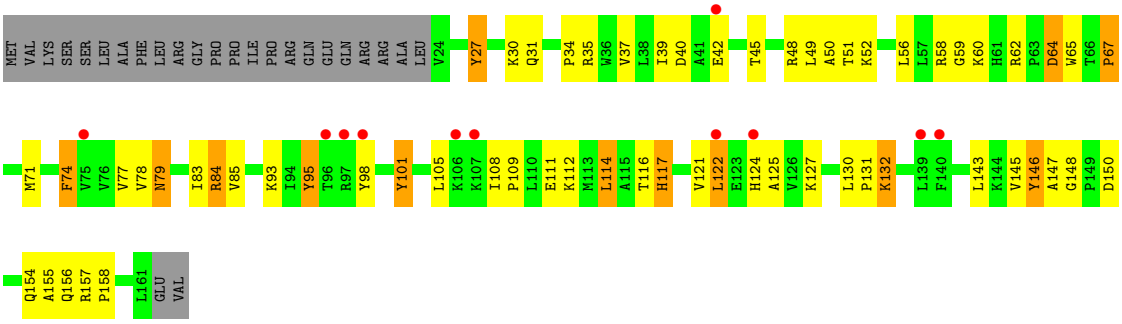

• Molecule 9: 50S ribosomal protein L9

Chain G:



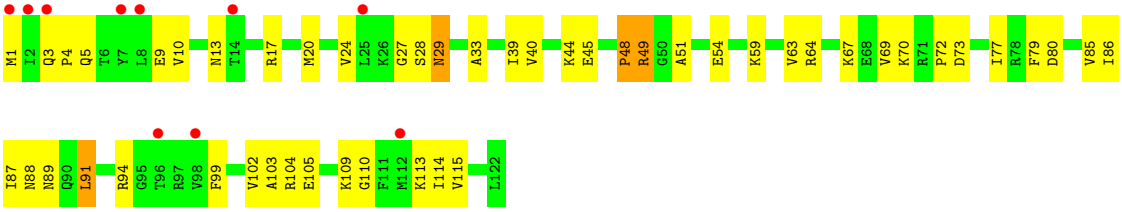

• Molecule 10: 50S ribosomal protein L13

Chain H:



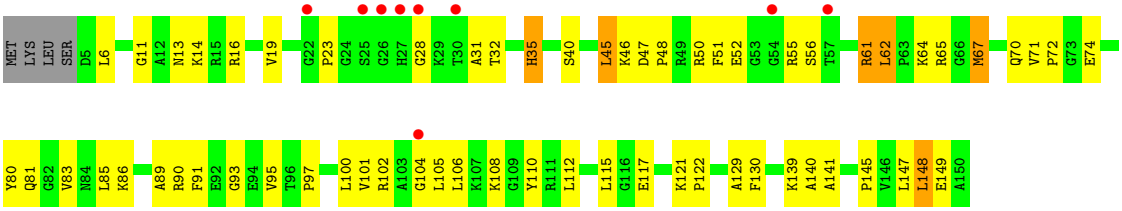

• Molecule 11: 50S ribosomal protein L14

Chain I:



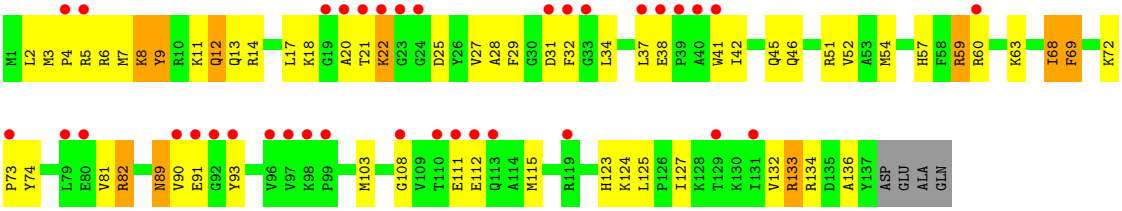

• Molecule 12: 50S ribosomal protein L15

Chain J:



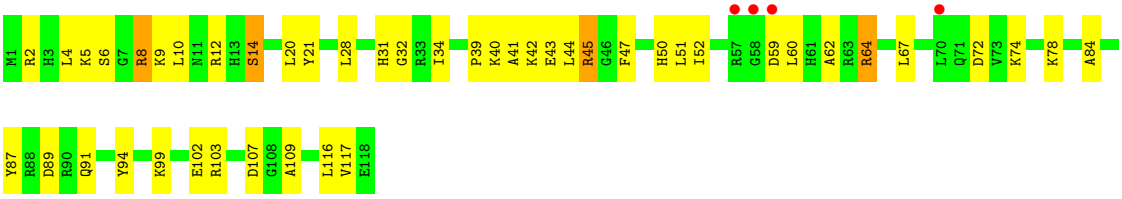

• Molecule 13: 50S ribosomal protein L16

Chain K:



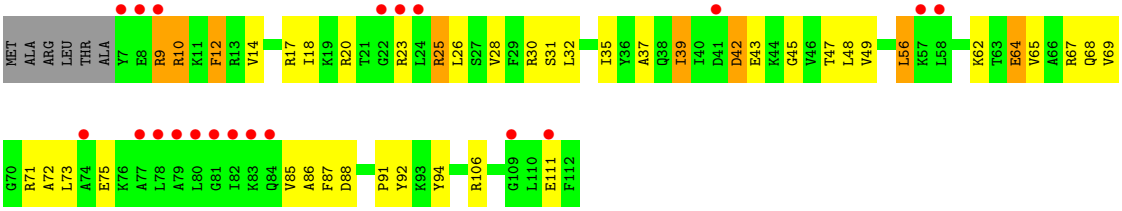

• Molecule 14: 50S ribosomal protein L17

Chain L:



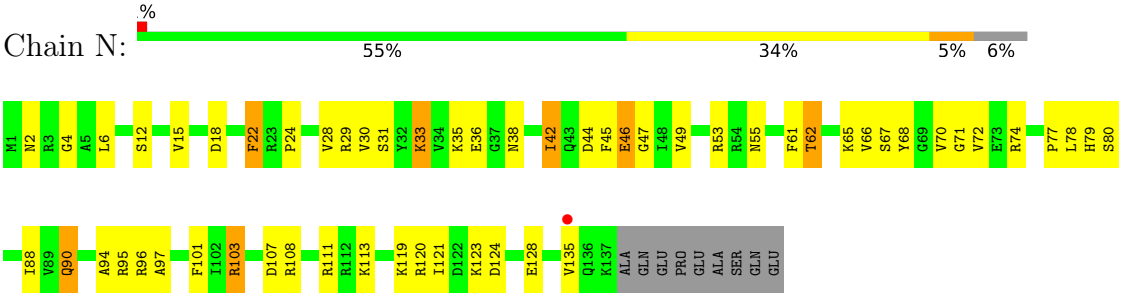

• Molecule 15: 50S ribosomal protein L18

Chain M:



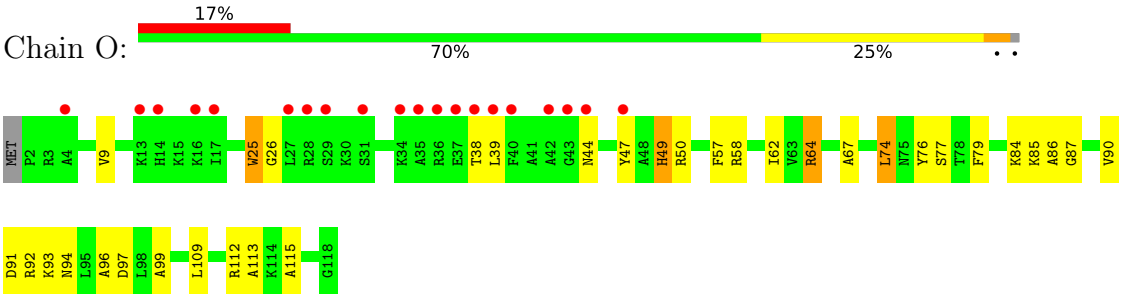
• Molecule 16: 50S ribosomal protein L19

Chain N:



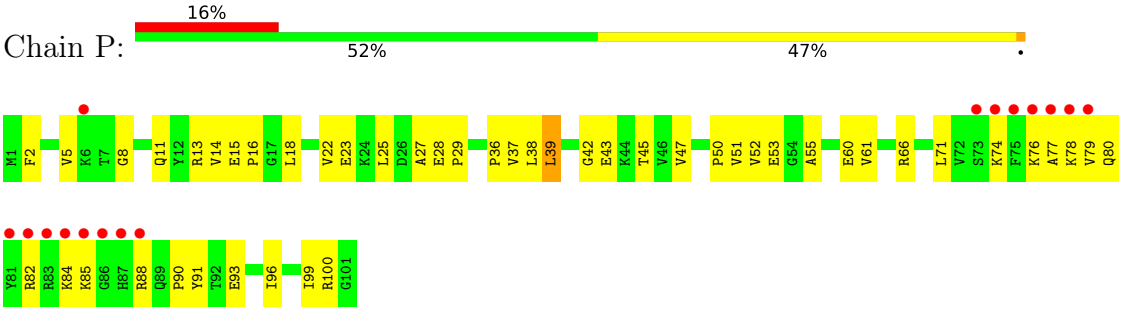

• Molecule 17: 50S ribosomal protein L20

Chain O:



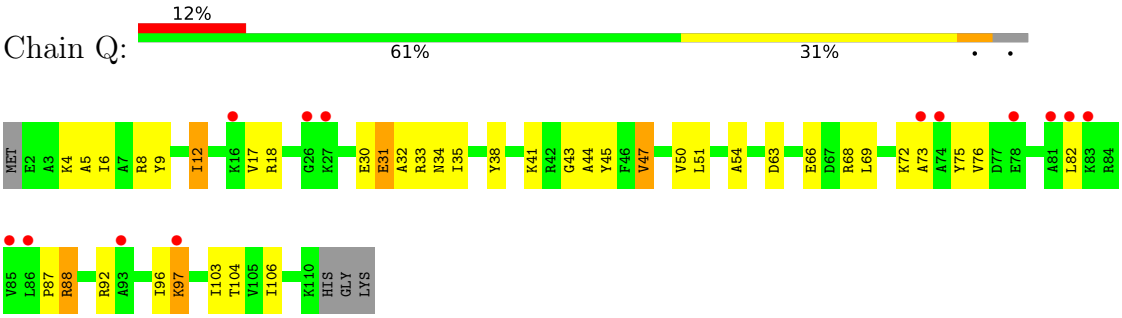

• Molecule 18: 50S ribosomal protein L21

Chain P:



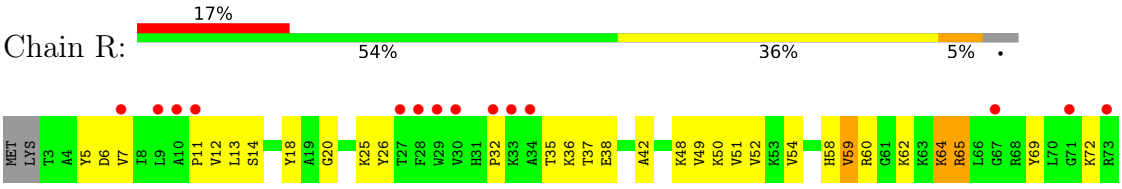

• Molecule 19: 50S ribosomal protein L22

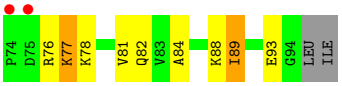
Chain Q:




• Molecule 20: 50S ribosomal protein L23

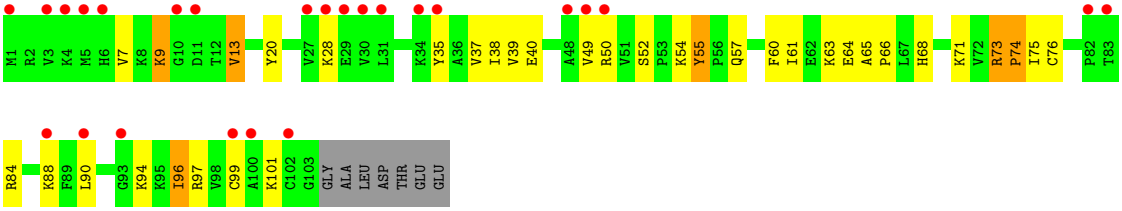
Chain R:





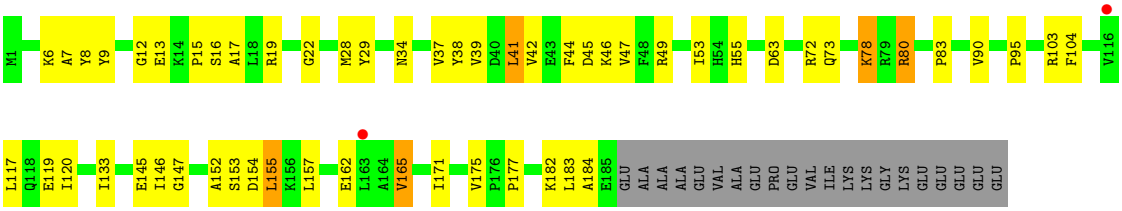

• Molecule 21: 50S ribosomal protein L24

Chain S:



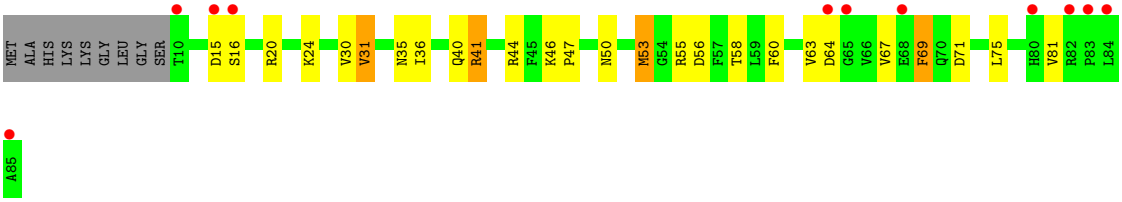

• Molecule 22: 50S ribosomal protein L25

Chain T:



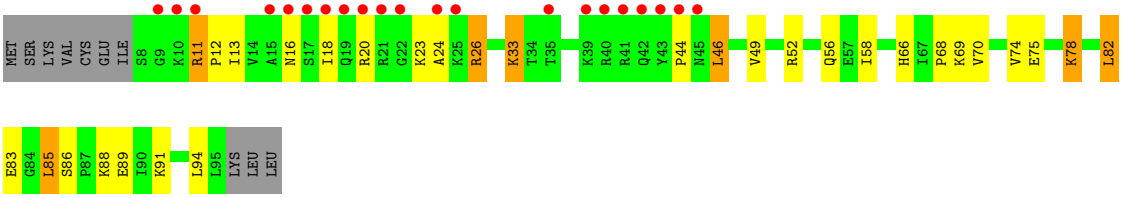

• Molecule 23: 50S ribosomal protein L27

Chain U:



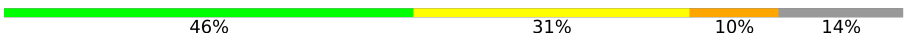

• Molecule 24: 50S ribosomal protein L28

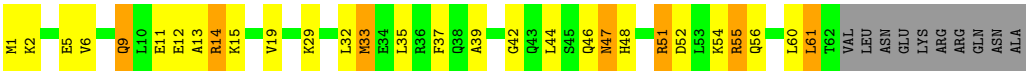
Chain V:




• Molecule 25: 50S ribosomal protein L29

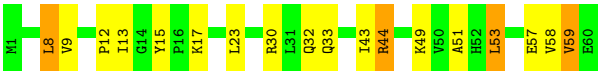
Chain W:





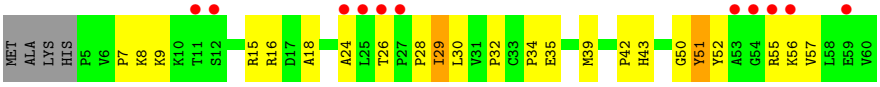

- Molecule 26: 50S ribosomal protein L30

Chain X:



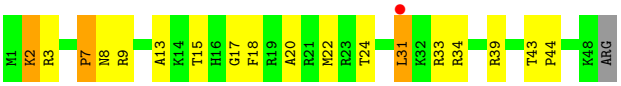

- Molecule 27: 50S ribosomal protein L32

Chain Y:



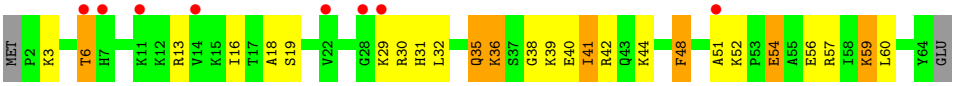

- Molecule 28: 50S ribosomal protein L34

Chain Z:



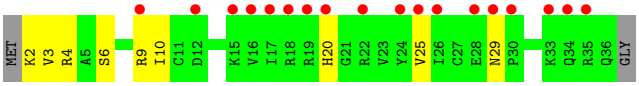

- Molecule 29: 50S ribosomal protein L35

Chain a:



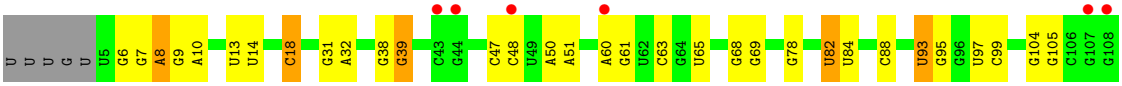

- Molecule 30: 50S ribosomal protein L36

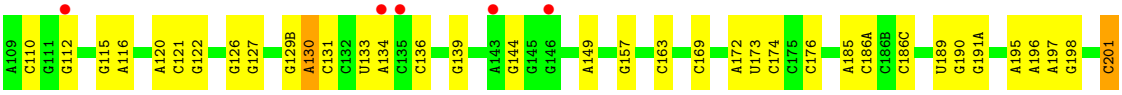
Chain b:

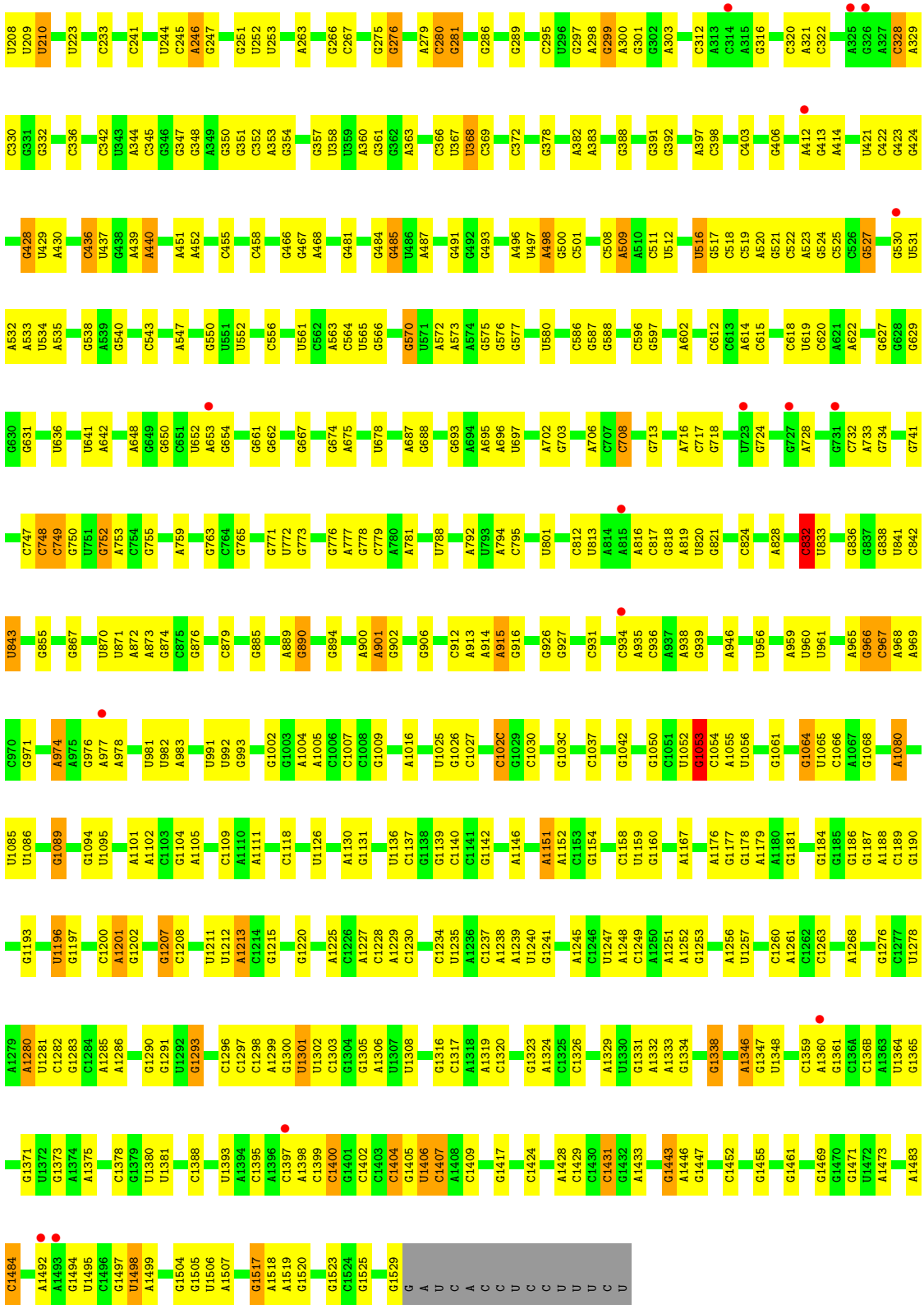



- Molecule 31: 16S SMALL SUBUNIT RIBOSOMAL RNA

Chain y:

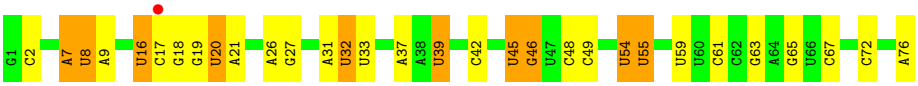




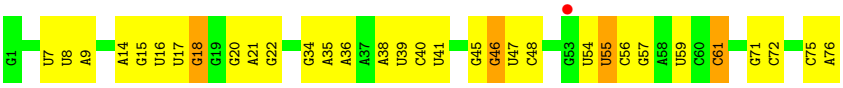

- Molecule 32: P-site PHE-tRNA

Chain z:



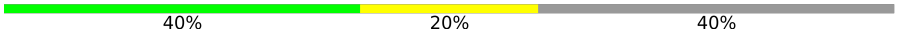

- Molecule 33: E-TRNA

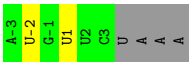
Chain 0:




- Molecule 34: MRNA

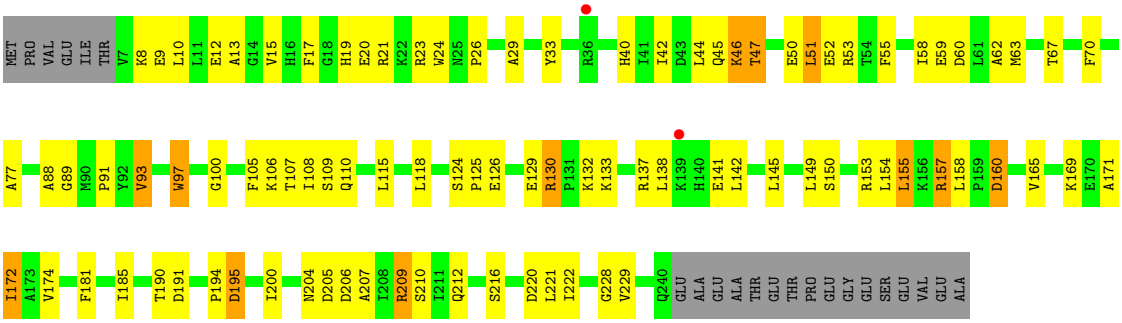
Chain 1:



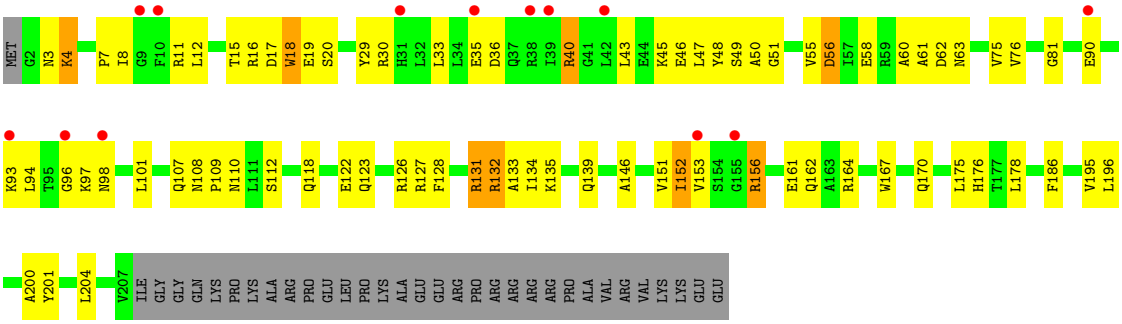

- Molecule 35: 30S ribosomal protein S2

Chain c:



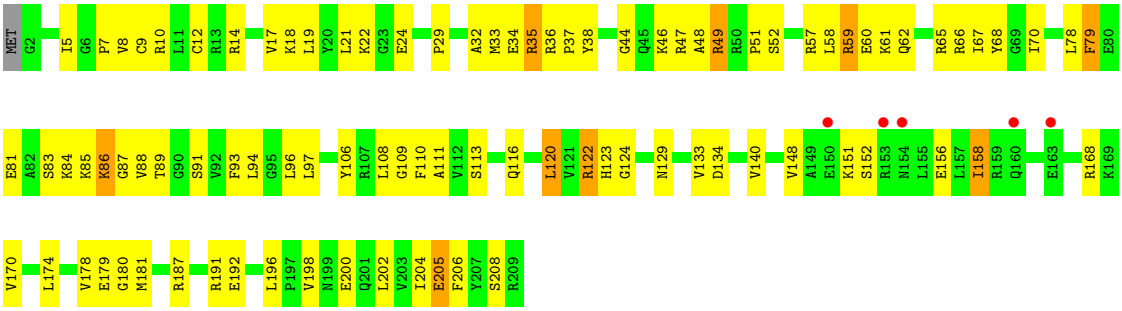

- Molecule 36: 30S ribosomal protein S3

Chain d:



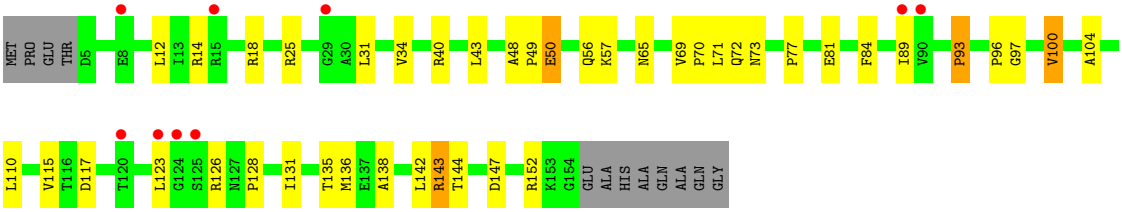

- Molecule 37: 30S ribosomal protein S4

Chain e:



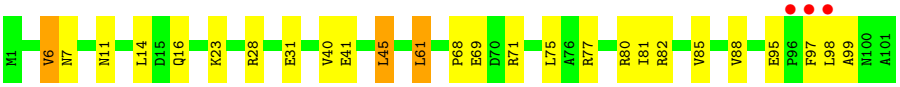

- Molecule 38: 30S ribosomal protein S5

Chain f:



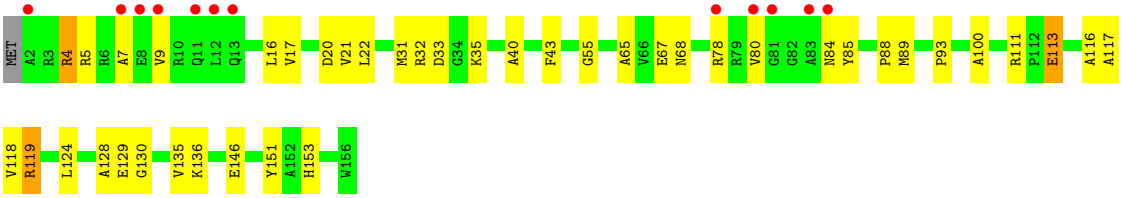

- Molecule 39: 30S ribosomal protein S6

Chain g:



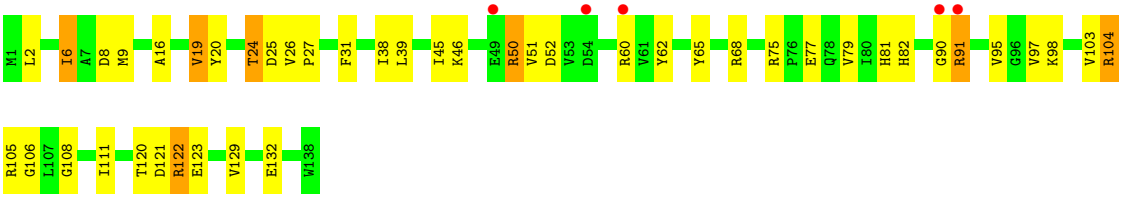

- Molecule 40: 30S ribosomal protein S7

Chain h:



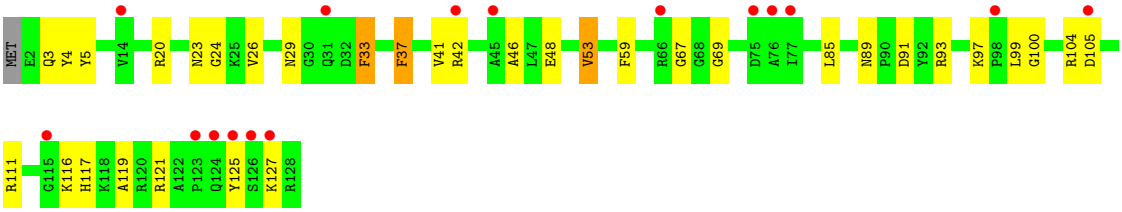

- Molecule 41: 30S ribosomal protein S8

Chain i:



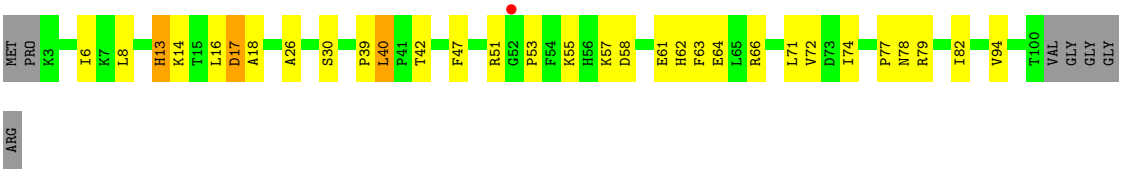

- Molecule 42: 30S ribosomal protein S9

Chain j:




- Molecule 43: 30S ribosomal protein S10

Chain k:

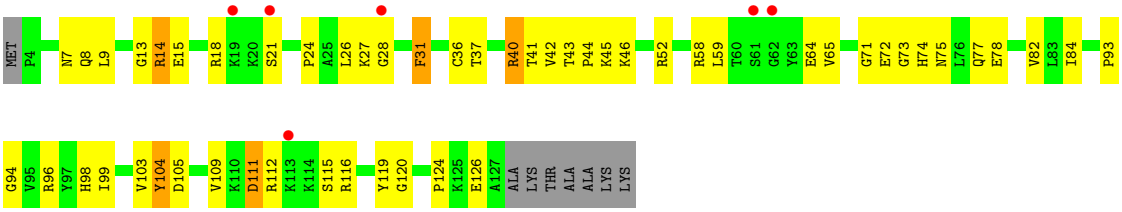



- Molecule 44: 30S ribosomal protein S11

Chain l:

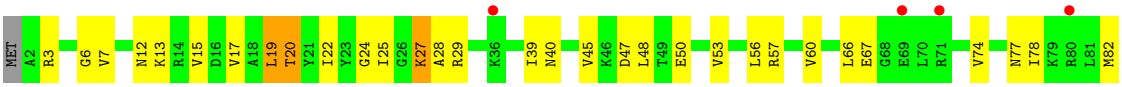
- Molecule 45: 30S ribosomal protein S12

Chain m:



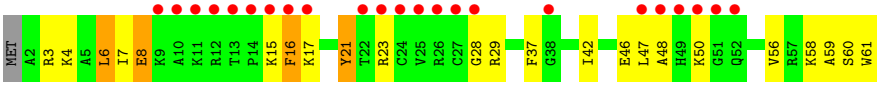

- Molecule 46: 30S ribosomal protein S13

Chain n:



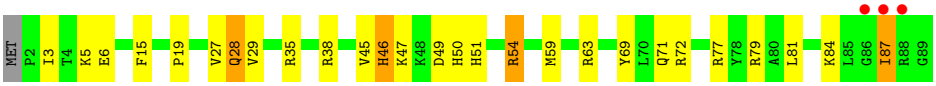
• Molecule 47: 30S ribosomal protein S14

Chain o:



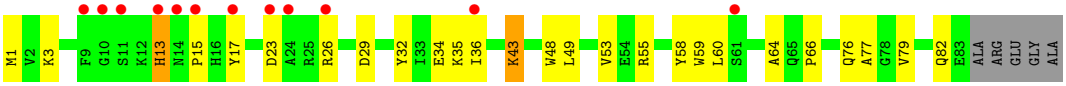

• Molecule 48: 30S ribosomal protein S15

Chain p:



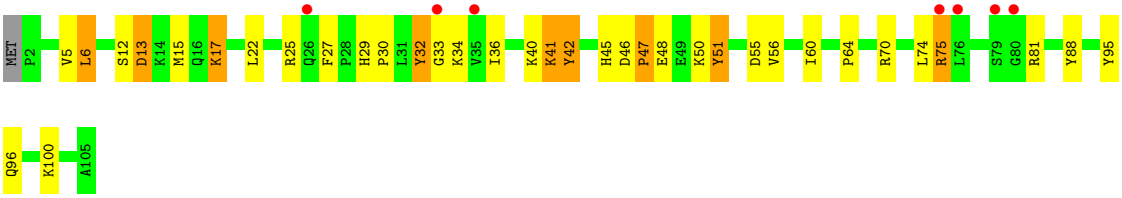

• Molecule 49: 30S ribosomal protein S16

Chain q:



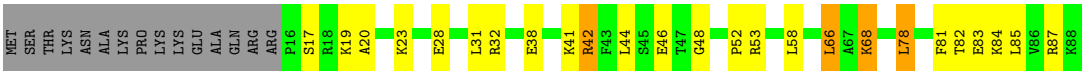

• Molecule 50: 30S ribosomal protein S17

Chain r:



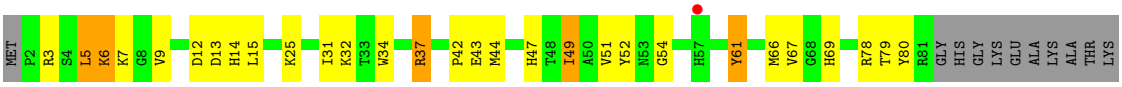

• Molecule 51: 30S ribosomal protein S18

Chain s:

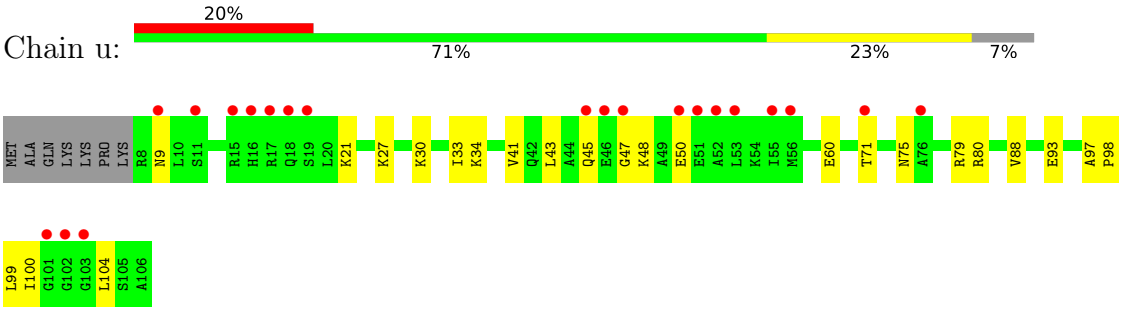



• Molecule 52: 30S ribosomal protein S19

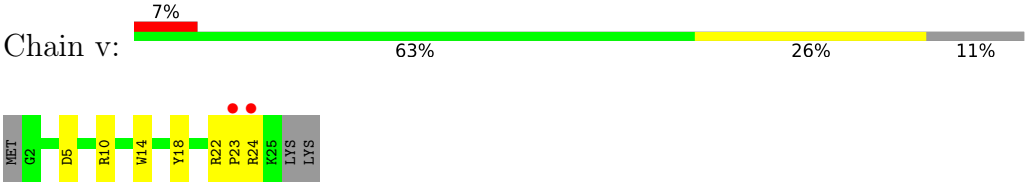
Chain t:



• Molecule 53: 30S ribosomal protein S20




• Molecule 54: 30S ribosomal protein Thx



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | I 4 2 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 507.81Å 507.81Å 689.52Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 3.71<br>72.78 – 3.70 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 100.0 (30.00-3.71)<br>97.9 (72.78-3.70) | Depositor<br>EDS |
| $R_{merge}$ | 0.15 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.68 (at 3.67Å) | Xtriage |
| Refinement program | REFMAC 5.2.0019, CNS | Depositor |
| R, $R_{free}$ | 0.348 , 0.353<br>0.367 , 0.372 | Depositor<br>DCC |
| $R_{free}$ test set | 11428 reflections (2.48%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 40.4 | Xtriage |
| Anisotropy | 0.192 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | (Not available) , (Not available) | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.26$, $< L^2 > = 0.11$ | Xtriage |
| Estimated twinning fraction | 0.228 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k<br>0.219 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k | Xtriage |
| $F_o$,$F_c$ correlation | 0.76 | EDS |
| Total number of atoms | 146532 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 40.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 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: MIA, 4OC, PSU, 7MG, 5MC, M2G, 4SU, H2U, MA6, 5MU, 2MG, UR3

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 | w | 1.06 | 48/69679 (0.1%) | 1.11 | 232/108779 (0.2%) |
| 2 | x | 0.89 | 0/2878 | 1.03 | 11/4490 (0.2%) |
| 3 | A | 0.50 | 0/1015 | 0.57 | 0/1369 |
| 4 | B | 0.49 | 0/2165 | 0.63 | 0/2919 |
| 5 | C | 0.57 | 0/1574 | 0.68 | 0/2125 |
| 6 | D | 0.57 | 0/1551 | 0.66 | 0/2101 |
| 7 | E | 0.55 | 0/1492 | 0.65 | 0/2006 |
| 8 | F | 0.55 | 0/1345 | 0.66 | 1/1819 (0.1%) |
| 9 | G | 0.53 | 0/1171 | 0.65 | 0/1583 |
| 10 | H | 0.47 | 0/1130 | 0.59 | 0/1525 |
| 11 | I | 0.54 | 0/942 | 0.66 | 0/1268 |
| 12 | J | 0.50 | 0/1131 | 0.64 | 0/1504 |
| 13 | K | 0.62 | 0/1110 | 0.71 | 1/1483 (0.1%) |
| 14 | L | 0.51 | 0/982 | 0.65 | 0/1312 |
| 15 | M | 0.54 | 0/856 | 0.63 | 0/1138 |
| 16 | N | 0.49 | 0/1157 | 0.62 | 0/1544 |
| 17 | O | 0.54 | 0/982 | 0.67 | 0/1306 |
| 18 | P | 0.51 | 0/790 | 0.62 | 0/1057 |
| 19 | Q | 0.56 | 0/878 | 0.66 | 0/1179 |
| 20 | R | 0.59 | 0/739 | 0.69 | 0/993 |
| 21 | S | 0.58 | 0/806 | 0.64 | 0/1074 |
| 22 | T | 0.54 | 0/1507 | 0.64 | 0/2045 |
| 23 | U | 0.57 | 0/613 | 0.65 | 0/816 |
| 24 | V | 0.49 | 0/701 | 0.60 | 0/932 |
| 25 | W | 0.52 | 0/522 | 0.65 | 0/690 |
| 26 | X | 0.56 | 0/482 | 0.73 | 0/646 |
| 27 | Y | 0.45 | 0/449 | 0.55 | 0/606 |
| 28 | Z | 0.80 | 0/426 | 0.73 | 0/561 |
| 29 | a | 0.58 | 0/515 | 0.69 | 0/679 |
| 30 | b | 0.55 | 0/297 | 0.61 | 0/392 |
| 31 | y | 0.97 | 13/35859 (0.0%) | 1.07 | 96/55966 (0.2%) |
| 32 | z | 0.98 | 1/1603 (0.1%) | 1.05 | 3/2497 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 33 | 0 | 0.89 | 1/1791 (0.1%) | 0.97 | 2/2791 (0.1%) |
| 34 | 1 | 0.94 | 0/135 | 1.02 | 0/208 |
| 35 | c | 0.55 | 0/1935 | 0.60 | 0/2609 |
| 36 | d | 0.51 | 0/1636 | 0.62 | 0/2205 |
| 37 | e | 0.53 | 0/1733 | 0.62 | 1/2318 (0.0%) |
| 38 | f | 0.51 | 0/1162 | 0.60 | 0/1564 |
| 39 | g | 0.56 | 0/856 | 0.63 | 0/1154 |
| 40 | h | 0.53 | 0/1276 | 0.57 | 0/1709 |
| 41 | i | 0.51 | 0/1136 | 0.62 | 0/1527 |
| 42 | j | 0.47 | 0/1029 | 0.53 | 0/1378 |
| 43 | k | 0.52 | 0/807 | 0.59 | 0/1085 |
| 44 | l | 0.49 | 0/879 | 0.59 | 0/1187 |
| 45 | m | 0.57 | 0/986 | 0.72 | 0/1320 |
| 46 | n | 0.52 | 0/1008 | 0.61 | 0/1347 |
| 47 | o | 0.53 | 0/501 | 0.57 | 0/664 |
| 48 | p | 0.49 | 0/745 | 0.58 | 0/992 |
| 49 | q | 0.49 | 0/716 | 0.63 | 0/963 |
| 50 | r | 0.55 | 0/870 | 0.63 | 0/1159 |
| 51 | s | 0.51 | 0/604 | 0.63 | 0/801 |
| 52 | t | 0.54 | 0/661 | 0.64 | 0/890 |
| 53 | u | 0.21 | 0/764 | 0.44 | 0/1006 |
| 54 | v | 0.57 | 0/212 | 0.52 | 0/277 |
| All | All | 0.91 | 63/158789 (0.0%) | 0.99 | 347/237558 (0.1%) |

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 | w | 0 | 24 |
| 2 | x | 2 | 0 |
| 31 | y | 0 | 8 |
| All | All | 2 | 32 |

The worst 5 of 63 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | w | 926 | A | O3'-P | 30.08 | 1.97 | 1.61 |
| 1 | w | 1506 | C | O3'-P | 29.80 | 1.97 | 1.61 |
| 1 | w | 1171 | G | O3'-P | 28.10 | 1.94 | 1.61 |
| 1 | w | 890 | A | O3'-P | 28.02 | 1.94 | 1.61 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | w | 1481 | U | O3'-P | 24.13 | 1.90 | 1.61 |

The worst 5 of 347 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | w | 1822 | G | N9-C1'-C2' | -18.71 | 89.67 | 114.00 |
| 1 | w | 1577 | C | N1-C1'-C2' | -15.42 | 93.96 | 114.00 |
| 1 | w | 712(B) | A | P-O3'-C3' | -14.26 | 102.58 | 119.70 |
| 31 | y | 93 | U | N1-C1'-C2' | -14.11 | 95.66 | 114.00 |
| 31 | y | 832 | C | N1-C1'-C2' | -13.21 | 96.82 | 114.00 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 2 | x | 14 | U | C3' |
| 2 | x | 24 | G | C3' |

5 of 32 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | w | 138 | G | Sidechain |
| 1 | w | 241 | A | Sidechain |
| 1 | w | 338 | G | Sidechain |
| 1 | w | 566 | U | Sidechain |
| 1 | w | 74 | A | Sidechain |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | A | 123/229 (54%) | 54 (44%) | 39 (32%) | 30 (24%) | 0 | 0 |
| 4 | B | 270/276 (98%) | 103 (38%) | 84 (31%) | 83 (31%) | 0 | 0 |
| 5 | C | 199/206 (97%) | 89 (45%) | 48 (24%) | 62 (31%) | 0 | 0 |
| 6 | D | 192/205 (94%) | 76 (40%) | 54 (28%) | 62 (32%) | 0 | 0 |
| 7 | E | 178/182 (98%) | 84 (47%) | 53 (30%) | 41 (23%) | 0 | 0 |
| 8 | F | 171/180 (95%) | 76 (44%) | 53 (31%) | 42 (25%) | 0 | 0 |
| 9 | G | 146/148 (99%) | 75 (51%) | 30 (20%) | 41 (28%) | 0 | 0 |
| 10 | H | 136/163 (83%) | 48 (35%) | 40 (29%) | 48 (35%) | 0 | 0 |
| 11 | I | 120/122 (98%) | 50 (42%) | 37 (31%) | 33 (28%) | 0 | 0 |
| 12 | J | 144/150 (96%) | 59 (41%) | 39 (27%) | 46 (32%) | 0 | 0 |
| 13 | K | 135/141 (96%) | 52 (38%) | 44 (33%) | 39 (29%) | 0 | 0 |
| 14 | L | 116/118 (98%) | 60 (52%) | 28 (24%) | 28 (24%) | 0 | 0 |
| 15 | M | 104/112 (93%) | 40 (38%) | 31 (30%) | 33 (32%) | 0 | 0 |
| 16 | N | 135/146 (92%) | 59 (44%) | 36 (27%) | 40 (30%) | 0 | 0 |
| 17 | O | 115/118 (98%) | 64 (56%) | 27 (24%) | 24 (21%) | 0 | 1 |
| 18 | P | 99/101 (98%) | 30 (30%) | 32 (32%) | 37 (37%) | 0 | 0 |
| 19 | Q | 107/113 (95%) | 49 (46%) | 30 (28%) | 28 (26%) | 0 | 0 |
| 20 | R | 90/96 (94%) | 28 (31%) | 29 (32%) | 33 (37%) | 0 | 0 |
| 21 | S | 101/110 (92%) | 36 (36%) | 34 (34%) | 31 (31%) | 0 | 0 |
| 22 | T | 183/206 (89%) | 104 (57%) | 41 (22%) | 38 (21%) | 0 | 1 |
| 23 | U | 74/85 (87%) | 35 (47%) | 23 (31%) | 16 (22%) | 0 | 1 |
| 24 | V | 86/98 (88%) | 30 (35%) | 31 (36%) | 25 (29%) | 0 | 0 |
| 25 | W | 60/72 (83%) | 28 (47%) | 12 (20%) | 20 (33%) | 0 | 0 |
| 26 | X | 58/60 (97%) | 32 (55%) | 15 (26%) | 11 (19%) | 0 | 1 |
| 27 | Y | 54/60 (90%) | 22 (41%) | 12 (22%) | 20 (37%) | 0 | 0 |
| 28 | Z | 46/49 (94%) | 25 (54%) | 9 (20%) | 12 (26%) | 0 | 0 |
| 29 | a | 61/65 (94%) | 20 (33%) | 22 (36%) | 19 (31%) | 0 | 0 |
| 30 | b | 33/37 (89%) | 22 (67%) | 5 (15%) | 6 (18%) | 0 | 2 |
| 35 | c | 232/256 (91%) | 109 (47%) | 66 (28%) | 57 (25%) | 0 | 0 |
| 36 | d | 204/239 (85%) | 98 (48%) | 49 (24%) | 57 (28%) | 0 | 0 |
| 37 | e | 206/209 (99%) | 99 (48%) | 44 (21%) | 63 (31%) | 0 | 0 |
| 38 | f | 148/162 (91%) | 89 (60%) | 33 (22%) | 26 (18%) | 0 | 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 39 | g | 99/101 (98%) | 61 (62%) | 24 (24%) | 14 (14%) | 0 | 4 |
| 40 | h | 153/156 (98%) | 84 (55%) | 40 (26%) | 29 (19%) | 0 | 1 |
| 41 | i | 136/138 (99%) | 71 (52%) | 35 (26%) | 30 (22%) | 0 | 1 |
| 42 | j | 125/128 (98%) | 73 (58%) | 31 (25%) | 21 (17%) | 0 | 3 |
| 43 | k | 96/105 (91%) | 50 (52%) | 24 (25%) | 22 (23%) | 0 | 0 |
| 44 | l | 114/129 (88%) | 59 (52%) | 28 (25%) | 27 (24%) | 0 | 0 |
| 45 | m | 122/132 (92%) | 51 (42%) | 32 (26%) | 39 (32%) | 0 | 0 |
| 46 | n | 123/126 (98%) | 53 (43%) | 35 (28%) | 35 (28%) | 0 | 0 |
| 47 | o | 58/61 (95%) | 22 (38%) | 19 (33%) | 17 (29%) | 0 | 0 |
| 48 | p | 86/89 (97%) | 46 (54%) | 23 (27%) | 17 (20%) | 0 | 1 |
| 49 | q | 81/88 (92%) | 37 (46%) | 28 (35%) | 16 (20%) | 0 | 1 |
| 50 | r | 102/105 (97%) | 46 (45%) | 31 (30%) | 25 (24%) | 0 | 0 |
| 51 | s | 71/88 (81%) | 42 (59%) | 12 (17%) | 17 (24%) | 0 | 0 |
| 52 | t | 78/93 (84%) | 26 (33%) | 31 (40%) | 21 (27%) | 0 | 0 |
| 53 | u | 97/106 (92%) | 42 (43%) | 37 (38%) | 18 (19%) | 0 | 1 |
| 54 | v | 22/27 (82%) | 11 (50%) | 7 (32%) | 4 (18%) | 0 | 2 |
| All | All | 5689/6186 (92%) | 2619 (46%) | 1567 (28%) | 1503 (26%) | 0 | 0 |

5 of 1503 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 63 | VAL |
| 3 | A | 179 | ALA |
| 3 | A | 180 | SER |
| 3 | A | 201 | LYS |
| 3 | A | 203 | GLU |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 3 | A | 106/181 (59%) | 91 (86%) | 15 (14%) | 3 | 20 |
| 4 | B | 214/218 (98%) | 169 (79%) | 45 (21%) | 1 | 7 |
| 5 | C | 163/166 (98%) | 126 (77%) | 37 (23%) | 1 | 6 |
| 6 | D | 154/162 (95%) | 123 (80%) | 31 (20%) | 1 | 8 |
| 7 | E | 154/156 (99%) | 127 (82%) | 27 (18%) | 2 | 12 |
| 8 | F | 142/148 (96%) | 124 (87%) | 18 (13%) | 4 | 23 |
| 9 | G | 124/124 (100%) | 103 (83%) | 21 (17%) | 2 | 13 |
| 10 | H | 117/139 (84%) | 90 (77%) | 27 (23%) | 1 | 6 |
| 11 | I | 100/100 (100%) | 79 (79%) | 21 (21%) | 1 | 7 |
| 12 | J | 112/116 (97%) | 89 (80%) | 23 (20%) | 1 | 7 |
| 13 | K | 108/111 (97%) | 77 (71%) | 31 (29%) | 0 | 2 |
| 14 | L | 101/101 (100%) | 79 (78%) | 22 (22%) | 1 | 6 |
| 15 | M | 84/88 (96%) | 66 (79%) | 18 (21%) | 1 | 7 |
| 16 | N | 121/128 (94%) | 97 (80%) | 24 (20%) | 1 | 8 |
| 17 | O | 93/94 (99%) | 79 (85%) | 14 (15%) | 3 | 18 |
| 18 | P | 82/82 (100%) | 70 (85%) | 12 (15%) | 3 | 18 |
| 19 | Q | 89/92 (97%) | 72 (81%) | 17 (19%) | 1 | 9 |
| 20 | R | 74/78 (95%) | 62 (84%) | 12 (16%) | 2 | 15 |
| 21 | S | 86/91 (94%) | 75 (87%) | 11 (13%) | 4 | 23 |
| 22 | T | 163/179 (91%) | 140 (86%) | 23 (14%) | 3 | 20 |
| 23 | U | 61/67 (91%) | 47 (77%) | 14 (23%) | 1 | 6 |
| 24 | V | 73/83 (88%) | 60 (82%) | 13 (18%) | 2 | 11 |
| 25 | W | 58/67 (87%) | 42 (72%) | 16 (28%) | 0 | 3 |
| 26 | X | 52/52 (100%) | 41 (79%) | 11 (21%) | 1 | 7 |
| 27 | Y | 49/52 (94%) | 44 (90%) | 5 (10%) | 7 | 31 |
| 28 | Z | 41/42 (98%) | 32 (78%) | 9 (22%) | 1 | 6 |
| 29 | a | 53/55 (96%) | 39 (74%) | 14 (26%) | 0 | 3 |
| 30 | b | 33/34 (97%) | 30 (91%) | 3 (9%) | 9 | 36 |
| 35 | c | 202/220 (92%) | 154 (76%) | 48 (24%) | 0 | 5 |
| 36 | d | 160/188 (85%) | 130 (81%) | 30 (19%) | 1 | 10 |
| 37 | e | 180/181 (99%) | 143 (79%) | 37 (21%) | 1 | 7 |
| 38 | f | 115/123 (94%) | 94 (82%) | 21 (18%) | 1 | 10 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 39 | g | 90/90 (100%) | 75 (83%) | 15 (17%) | 2 | 14 |
| 40 | h | 126/127 (99%) | 110 (87%) | 16 (13%) | 4 | 23 |
| 41 | i | 119/119 (100%) | 97 (82%) | 22 (18%) | 1 | 10 |
| 42 | j | 98/99 (99%) | 82 (84%) | 16 (16%) | 2 | 15 |
| 43 | k | 88/92 (96%) | 76 (86%) | 12 (14%) | 3 | 21 |
| 44 | l | 88/99 (89%) | 72 (82%) | 16 (18%) | 1 | 10 |
| 45 | m | 104/109 (95%) | 85 (82%) | 19 (18%) | 1 | 10 |
| 46 | n | 100/101 (99%) | 85 (85%) | 15 (15%) | 3 | 18 |
| 47 | o | 49/50 (98%) | 39 (80%) | 10 (20%) | 1 | 7 |
| 48 | p | 79/80 (99%) | 65 (82%) | 14 (18%) | 2 | 12 |
| 49 | q | 72/74 (97%) | 60 (83%) | 12 (17%) | 2 | 14 |
| 50 | r | 96/97 (99%) | 76 (79%) | 20 (21%) | 1 | 7 |
| 51 | s | 64/77 (83%) | 52 (81%) | 12 (19%) | 1 | 10 |
| 52 | t | 71/80 (89%) | 58 (82%) | 13 (18%) | 1 | 10 |
| 53 | u | 76/82 (93%) | 70 (92%) | 6 (8%) | 12 | 42 |
| 54 | v | 19/22 (86%) | 16 (84%) | 3 (16%) | 2 | 16 |
| All | All | 4803/5116 (94%) | 3912 (81%) | 891 (19%) | 1 | 10 |

5 of 891 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 24 | V | 11 | ARG |
| 53 | u | 79 | ARG |
| 35 | c | 195 | ASP |
| 52 | t | 32 | LYS |
| 46 | n | 110 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 38 | f | 73 | ASN |
| 44 | l | 116 | HIS |
| 39 | g | 27 | GLN |
| 42 | j | 73 | GLN |
| 48 | p | 13 | GLN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | w | 2888/2889 (99%) | 1138 (39%) | 0 |
| 2 | x | 119/121 (98%) | 42 (35%) | 0 |
| 31 | y | 1498/1522 (98%) | 502 (33%) | 0 |
| 32 | z | 74/76 (97%) | 28 (37%) | 0 |
| 33 | 0 | 75/76 (98%) | 30 (40%) | 5 (6%) |
| 34 | 1 | 5/10 (50%) | 2 (40%) | 0 |
| All | All | 4659/4694 (99%) | 1742 (37%) | 5 (0%) |

5 of 1742 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | w | 10 | G |
| 1 | w | 12 | U |
| 1 | w | 13 | A |
| 1 | w | 15 | G |
| 1 | w | 16 | G |

All (5) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | 0 | 7 | U |
| 33 | 0 | 9 | A |
| 33 | 0 | 46 | G |
| 33 | 0 | 48 | C |
| 33 | 0 | 56 | C |

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

22 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 | $\#\|Z\| > 2$ |
| 31 | 5MC | y | 1407 | 31 | 18,22,23 | 0.92 | 1 (5%) | 26,32,35 | 1.47 | 5 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 32 | MIA | z | 37 | 32 | 24,31,32 | 2.36 | 6 (25%) | 26,44,47 | 2.58 | 6 (23%) |
| 31 | MA6 | y | 1519 | 31 | 19,26,27 | 2.16 | 2 (10%) | 18,38,41 | 1.90 | 4 (22%) |
| 32 | PSU | z | 39 | 32 | 18,21,22 | 2.29 | 4 (22%) | 22,30,33 | 1.83 | 7 (31%) |
| 31 | 5MC | y | 1404 | 31 | 18,22,23 | 1.04 | 1 (5%) | 26,32,35 | 1.52 | 5 (19%) |
| 31 | 5MC | y | 1400 | 31 | 18,22,23 | 1.07 | 2 (11%) | 26,32,35 | 1.46 | 2 (7%) |
| 32 | 4SU | z | 8 | 32 | 18,21,22 | 1.82 | 3 (16%) | 26,30,33 | 2.31 | 9 (34%) |
| 31 | 2MG | y | 1207 | 31 | 18,26,27 | 1.73 | 3 (16%) | 16,38,41 | 1.70 | 5 (31%) |
| 32 | PSU | z | 32 | 32 | 18,21,22 | 2.03 | 4 (22%) | 22,30,33 | 2.11 | 6 (27%) |
| 31 | MA6 | y | 1518 | 31 | 19,26,27 | 1.80 | 3 (15%) | 18,38,41 | 2.29 | 6 (33%) |
| 32 | 5MU | z | 54 | 32 | 19,22,23 | 1.79 | 2 (10%) | 28,32,35 | 1.52 | 7 (25%) |
| 31 | 4OC | y | 1402 | 31 | 20,23,24 | 1.39 | 3 (15%) | 26,32,35 | 1.55 | 5 (19%) |
| 31 | 5MC | y | 967 | 31 | 18,22,23 | 0.77 | 1 (5%) | 26,32,35 | 1.16 | 3 (11%) |
| 32 | PSU | z | 55 | 32 | 18,21,22 | 1.96 | 4 (22%) | 22,30,33 | 1.94 | 6 (27%) |
| 31 | PSU | y | 516 | 31 | 18,21,22 | 1.89 | 4 (22%) | 22,30,33 | 1.87 | 7 (31%) |
| 31 | 7MG | y | 527 | 31 | 22,26,27 | 3.72 | 3 (13%) | 29,39,42 | 1.67 | 6 (20%) |
| 31 | UR3 | y | 1498 | 31 | 19,22,23 | 1.62 | 1 (5%) | 26,32,35 | 1.52 | 6 (23%) |
| 31 | M2G | y | 966 | 31 | 20,27,28 | 2.24 | 6 (30%) | 22,40,43 | 1.56 | 4 (18%) |
| 32 | H2U | z | 20 | 32 | 18,21,22 | 0.76 | 0 | 21,30,33 | 0.89 | 1 (4%) |
| 32 | H2U | z | 16 | 32 | 18,21,22 | 0.97 | 1 (5%) | 21,30,33 | 0.93 | 1 (4%) |
| 32 | 7MG | z | 46 | 32 | 22,26,27 | 3.56 | 4 (18%) | 29,39,42 | 1.81 | 6 (20%) |
| 33 | PSU | 0 | 55 | 33 | 18,21,22 | 3.41 | 5 (27%) | 22,30,33 | 2.05 | 6 (27%) |

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 |
|---|---|---|---|---|---|---|---|
| 31 | 5MC | y | 1407 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MIA | z | 37 | 32 | - | 5/11/33/34 | 0/3/3/3 |
| 31 | MA6 | y | 1519 | 31 | - | 1/7/29/30 | 0/3/3/3 |
| 32 | PSU | z | 39 | 32 | - | 4/7/25/26 | 0/2/2/2 |
| 31 | 5MC | y | 1404 | 31 | - | 2/7/25/26 | 0/2/2/2 |
| 31 | 5MC | y | 1400 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 4SU | z | 8 | 32 | - | 2/7/25/26 | 0/2/2/2 |
| 31 | 2MG | y | 1207 | 31 | - | 0/5/27/28 | 0/3/3/3 |
| 32 | PSU | z | 32 | 32 | - | 3/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 31 | MA6 | y | 1518 | 31 | - | 2/7/29/30 | 0/3/3/3 |
| 32 | 5MU | z | 54 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 31 | 4OC | y | 1402 | 31 | - | 3/9/29/30 | 0/2/2/2 |
| 31 | 5MC | y | 967 | 31 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | PSU | z | 55 | 32 | - | 1/7/25/26 | 0/2/2/2 |
| 31 | PSU | y | 516 | 31 | - | 4/7/25/26 | 0/2/2/2 |
| 31 | 7MG | y | 527 | 31 | - | 0/7/37/38 | 0/3/3/3 |
| 31 | UR3 | y | 1498 | 31 | - | 6/7/25/26 | 0/2/2/2 |
| 31 | M2G | y | 966 | 31 | - | 0/7/29/30 | 0/3/3/3 |
| 32 | H2U | z | 20 | 32 | - | 2/7/38/39 | 0/2/2/2 |
| 32 | H2U | z | 16 | 32 | - | 2/7/38/39 | 0/2/2/2 |
| 32 | 7MG | z | 46 | 32 | - | 0/7/37/38 | 0/3/3/3 |
| 33 | PSU | 0 | 55 | 33 | - | 2/7/25/26 | 0/2/2/2 |

The worst 5 of 63 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 31 | y | 527 | 7MG | C8-N9 | -16.62 | 1.36 | 1.46 |
| 32 | z | 46 | 7MG | C8-N9 | -15.58 | 1.37 | 1.46 |
| 33 | 0 | 55 | PSU | O2-C2 | 12.05 | 1.48 | 1.23 |
| 32 | z | 39 | PSU | O2-C2 | 6.95 | 1.38 | 1.23 |
| 32 | z | 54 | 5MU | O4-C4 | 6.87 | 1.36 | 1.23 |

The worst 5 of 113 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 32 | z | 37 | MIA | C12-C13-C14 | -8.50 | 110.60 | 127.14 |
| 31 | y | 1518 | MA6 | N1-C6-N6 | 6.39 | 123.78 | 117.06 |
| 31 | y | 527 | 7MG | N9-C8-N7 | 5.61 | 111.41 | 103.38 |
| 32 | z | 37 | MIA | C12-N6-C6 | -5.50 | 114.41 | 122.55 |
| 32 | z | 46 | 7MG | N9-C8-N7 | 5.45 | 111.17 | 103.38 |

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 31 | y | 516 | PSU | C2'-C1'-C5-C4 |
| 31 | y | 516 | PSU | C2'-C1'-C5-C6 |
| 31 | y | 1402 | 4OC | C1'-C2'-O2'-CM2 |
| 31 | y | 1518 | MA6 | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 31 | y | 1518 | MA6 | C3'-C4'-C5'-O5' |

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)

There are no ligands in this entry.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | w | 31 |
| 31 | y | 5 |

The worst 5 of 36 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | w | 926:A | O3' | 928:G | P | 1.97 |
| 1 | w | 1506:C | O3' | 1508:A | P | 1.96 |
| 1 | w | 890:A | O3' | 892:G | P | 1.94 |
| 1 | w | 1171:G | O3' | 1173:G | P | 1.94 |
| 1 | w | 1481:U | O3' | 1483:G | P | 1.90 |

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | w | 2889/2889 (100%) | 0.35 | 77 (2%) 54 46 | 5, 5, 117, 159 | 0 |
| 2 | x | 120/121 (99%) | 0.24 | 0 100 100 | 5, 13, 95, 127 | 0 |
| 3 | A | 127/229 (55%) | -0.05 | 8 (6%) 20 15 | 5, 50, 148, 151 | 0 |
| 4 | B | 272/276 (98%) | 0.14 | 14 (5%) 28 24 | 5, 60, 148, 155 | 0 |
| 5 | C | 201/206 (97%) | 0.09 | 10 (4%) 28 25 | 5, 49, 148, 159 | 0 |
| 6 | D | 194/205 (94%) | -0.19 | 8 (4%) 37 31 | 5, 55, 148, 165 | 0 |
| 7 | E | 180/182 (98%) | -0.39 | 9 (5%) 28 25 | 5, 58, 148, 156 | 0 |
| 8 | F | 173/180 (96%) | -0.29 | 10 (5%) 23 18 | 5, 67, 148, 160 | 0 |
| 9 | G | 148/148 (100%) | -0.33 | 3 (2%) 65 58 | 5, 43, 148, 151 | 0 |
| 10 | H | 138/163 (84%) | 0.37 | 11 (7%) 12 10 | 5, 52, 147, 152 | 0 |
| 11 | I | 122/122 (100%) | 0.37 | 10 (8%) 11 10 | 5, 35, 142, 148 | 0 |
| 12 | J | 146/150 (97%) | -0.12 | 9 (6%) 20 16 | 5, 90, 150, 160 | 0 |
| 13 | K | 137/141 (97%) | 1.03 | 36 (26%) 0 0 | 5, 24, 148, 152 | 0 |
| 14 | L | 118/118 (100%) | -0.11 | 4 (3%) 45 37 | 5, 44, 148, 148 | 0 |
| 15 | M | 106/112 (94%) | 0.54 | 20 (18%) 1 1 | 5, 48, 148, 160 | 0 |
| 16 | N | 137/146 (93%) | -0.20 | 1 (0%) 87 85 | 5, 74, 150, 167 | 0 |
| 17 | O | 117/118 (99%) | 0.28 | 20 (17%) 1 1 | 5, 35, 114, 148 | 0 |
| 18 | P | 101/101 (100%) | 0.23 | 16 (15%) 2 1 | 5, 79, 148, 159 | 0 |
| 19 | Q | 109/113 (96%) | 0.34 | 13 (11%) 4 4 | 5, 33, 137, 149 | 0 |
| 20 | R | 92/96 (95%) | 0.46 | 16 (17%) 1 1 | 5, 73, 148, 161 | 0 |
| 21 | S | 103/110 (93%) | 0.81 | 25 (24%) 0 0 | 5, 86, 160, 163 | 0 |
| 22 | T | 185/206 (89%) | -0.48 | 2 (1%) 80 76 | 5, 50, 148, 161 | 0 |
| 23 | U | 76/85 (89%) | 0.35 | 11 (14%) 2 2 | 5, 57, 151, 166 | 0 |
| 24 | V | 88/98 (89%) | 0.98 | 21 (23%) 0 0 | 5, 91, 148, 154 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 25 | W | 62/72 (86%) | -0.38 | 0 | 100 | 100 | 5, 88, 149, 155 | 0 |
| 26 | X | 60/60 (100%) | -0.78 | 0 | 100 | 100 | 5, 36, 148, 150 | 0 |
| 27 | Y | 56/60 (93%) | 0.42 | 11 (19%) | 1 | 1 | 7, 77, 164, 168 | 0 |
| 28 | Z | 48/49 (97%) | 0.21 | 1 (2%) | 63 | 56 | 5, 5, 42, 126 | 0 |
| 29 | a | 63/65 (96%) | 0.67 | 8 (12%) | 3 | 4 | 5, 50, 151, 157 | 0 |
| 30 | b | 35/37 (94%) | 2.44 | 18 (51%) | 0 | 0 | 5, 102, 149, 153 | 0 |
| 31 | y | 1490/1522 (97%) | 0.32 | 27 (1%) | 68 | 62 | 5, 9, 113, 163 | 0 |
| 32 | z | 67/76 (88%) | 0.24 | 1 (1%) | 73 | 68 | 5, 6, 82, 117 | 0 |
| 33 | 0 | 75/76 (98%) | 0.26 | 1 (1%) | 77 | 72 | 5, 37, 128, 148 | 0 |
| 34 | 1 | 6/10 (60%) | 0.27 | 0 | 100 | 100 | 5, 5, 54, 67 | 0 |
| 35 | c | 234/256 (91%) | -0.60 | 2 (0%) | 84 | 80 | 5, 50, 151, 164 | 0 |
| 36 | d | 206/239 (86%) | -0.11 | 13 (6%) | 20 | 15 | 5, 57, 148, 151 | 0 |
| 37 | e | 208/209 (99%) | -0.27 | 5 (2%) | 59 | 51 | 5, 50, 148, 157 | 0 |
| 38 | f | 150/162 (92%) | -0.06 | 9 (6%) | 21 | 16 | 5, 62, 148, 154 | 0 |
| 39 | g | 101/101 (100%) | -0.42 | 3 (2%) | 50 | 40 | 5, 72, 148, 156 | 0 |
| 40 | h | 155/156 (99%) | -0.16 | 12 (7%) | 13 | 11 | 5, 73, 155, 163 | 0 |
| 41 | i | 138/138 (100%) | -0.13 | 5 (3%) | 42 | 35 | 5, 43, 148, 149 | 0 |
| 42 | j | 127/128 (99%) | 0.36 | 16 (12%) | 3 | 4 | 5, 85, 150, 154 | 0 |
| 43 | k | 98/105 (93%) | -0.25 | 1 (1%) | 82 | 78 | 5, 83, 151, 164 | 0 |
| 44 | l | 116/129 (89%) | -0.33 | 8 (6%) | 16 | 12 | 5, 71, 150, 162 | 0 |
| 45 | m | 124/132 (93%) | 0.02 | 6 (4%) | 30 | 26 | 5, 30, 148, 152 | 0 |
| 46 | n | 125/126 (99%) | -0.22 | 10 (8%) | 12 | 10 | 5, 74, 148, 162 | 0 |
| 47 | o | 60/61 (98%) | 1.78 | 23 (38%) | 0 | 0 | 5, 66, 151, 161 | 0 |
| 48 | p | 88/89 (98%) | -0.43 | 3 (3%) | 45 | 37 | 5, 57, 148, 163 | 0 |
| 49 | q | 83/88 (94%) | 0.52 | 12 (14%) | 2 | 2 | 5, 50, 148, 148 | 0 |
| 50 | r | 104/105 (99%) | 0.11 | 7 (6%) | 17 | 13 | 5, 52, 148, 158 | 0 |
| 51 | s | 73/88 (82%) | -0.75 | 0 | 100 | 100 | 5, 69, 149, 157 | 0 |
| 52 | t | 80/93 (86%) | -0.39 | 1 (1%) | 77 | 72 | 5, 52, 148, 159 | 0 |
| 53 | u | 99/106 (93%) | 0.90 | 21 (21%) | 0 | 1 | 10, 66, 199, 199 | 0 |
| 54 | v | 24/27 (88%) | 0.17 | 2 (8%) | 11 | 9 | 5, 47, 139, 142 | 0 |
| All | All | 10434/10880 (95%) | 0.17 | 580 (5%) | 24 | 20 | 5, 32, 148, 199 | 0 |

The worst 5 of 580 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 15 | M | 81 | GLY | 10.0 |
| 15 | M | 82 | ILE | 8.0 |
| 8 | F | 179 | LYS | 8.0 |
| 44 | l | 125 | PHE | 7.7 |
| 47 | o | 13 | THR | 7.7 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 32 | PSU | z | 55 | 20/21 | 0.64 | 0.30 | 40,50,52,53 | 0 |
| 33 | PSU | 0 | 55 | 20/21 | 0.75 | 0.22 | 36,36,36,36 | 0 |
| 31 | 4OC | y | 1402 | 22/23 | 0.80 | 0.28 | 10,13,16,16 | 0 |
| 32 | H2U | z | 16 | 20/21 | 0.80 | 0.55 | 80,92,93,95 | 0 |
| 32 | MIA | z | 37 | 29/30 | 0.81 | 0.28 | 20,26,32,32 | 0 |
| 31 | 5MC | y | 967 | 21/22 | 0.81 | 0.39 | 124,124,133,133 | 0 |
| 32 | H2U | z | 20 | 20/21 | 0.81 | 0.38 | 124,124,133,133 | 0 |
| 31 | PSU | y | 516 | 20/21 | 0.82 | 0.20 | 137,138,148,148 | 0 |
| 32 | 7MG | z | 46 | 24/25 | 0.82 | 0.20 | 5,5,12,12 | 0 |
| 31 | MA6 | y | 1519 | 24/25 | 0.84 | 0.25 | 5,5,6,8 | 0 |
| 31 | MA6 | y | 1518 | 24/25 | 0.85 | 0.20 | 31,39,52,53 | 0 |
| 31 | M2G | y | 966 | 25/26 | 0.85 | 0.28 | 15,16,20,31 | 0 |
| 32 | 4SU | z | 8 | 20/21 | 0.85 | 0.24 | 5,5,5,5 | 0 |
| 31 | 5MC | y | 1404 | 21/22 | 0.89 | 0.33 | 5,6,8,9 | 0 |
| 32 | PSU | z | 32 | 20/21 | 0.89 | 0.30 | 42,52,58,59 | 0 |
| 31 | 2MG | y | 1207 | 24/25 | 0.90 | 0.23 | 21,22,26,26 | 0 |
| 32 | 5MU | z | 54 | 21/22 | 0.90 | 0.23 | 5,5,5,5 | 0 |
| 31 | 7MG | y | 527 | 24/25 | 0.90 | 0.23 | 7,10,24,26 | 0 |
| 32 | PSU | z | 39 | 20/21 | 0.90 | 0.22 | 5,5,5,5 | 0 |
| 31 | 5MC | y | 1400 | 21/22 | 0.93 | 0.21 | 5,5,5,5 | 0 |
| 31 | UR3 | y | 1498 | 21/22 | 0.94 | 0.20 | 5,5,5,5 | 0 |
| 31 | 5MC | y | 1407 | 21/22 | 0.95 | 0.16 | 25,28,30,30 | 0 |

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.