



wwPDB X-ray Structure Validation Summary Report

Sep 15, 2014 – 11:19 AM EDT

PDB ID : 1VVM
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-07
Resolution : 3.22 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

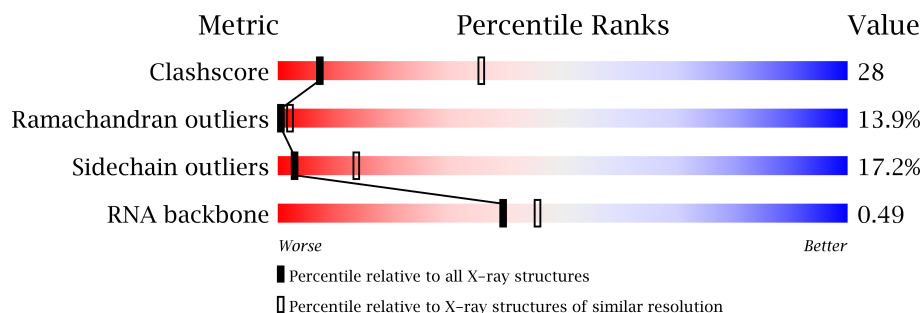
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.22 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 79885 | 1072 (3.28-3.16) |
| Ramachandran outliers | 78287 | 1052 (3.28-3.16) |
| Sidechain outliers | 78261 | 1051 (3.28-3.16) |
| RNA backbone | 1838 | 1004 (3.74-2.70) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 2916 | |
| 2 | B | 122 | |
| 3 | D | 276 | |
| 4 | E | 206 | |
| 5 | F | 210 | |
| 6 | G | 182 | |
| 7 | H | 180 | |
| 8 | I | 148 | |
| 9 | N | 140 | |
| 10 | O | 122 | |
| 11 | P | 150 | |
| 12 | Q | 141 | |
| 13 | R | 118 | |
| 14 | S | 112 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | T | 146 | |
| 16 | U | 118 | |
| 17 | V | 101 | |
| 18 | W | 113 | |
| 19 | X | 96 | |
| 20 | Y | 110 | |
| 21 | Z | 206 | |
| 22 | 0 | 85 | |
| 23 | 1 | 98 | |
| 24 | 2 | 72 | |
| 25 | 3 | 60 | |
| 26 | 4 | 71 | |
| 27 | 5 | 60 | |
| 28 | 6 | 54 | |
| 29 | 7 | 49 | |
| 30 | 8 | 65 | |
| 31 | 9 | 37 | |
| 32 | a | 3 | |

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92246 atoms, of which 0 are hydrogen and 0 are deuterium.

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 rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | A | 2882 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62071 | 27627 | 11611 | 19952 | 2881 | | | |

- Molecule 2 is a RNA chain called 5S rRNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | E | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1568 | 991 | 300 | 271 | 6 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | F | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1011 | 297 | 275 | 2 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | G | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1474 | 942 | 268 | 260 | 4 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | H | 170 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1307 | 829 | 245 | 232 | 1 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | I | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1136 | 726 | 201 | 208 | 1 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | N | 138 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1104 | 712 | 206 | 182 | 4 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | O | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | P | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | Q | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1122 | 715 | 212 | 188 | 7 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | R | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14 | S | 111 | Total | C | N | O | 0 | 0 | 0 |
| | | | 882 | 556 | 176 | 150 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | T | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1141 | 710 | 234 | 196 | 1 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | U | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | V | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | W | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 566 | 177 | 155 | 2 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19 | X | 92 | Total | C | N | O | 0 | 0 | 0 |
| | | | 725 | 471 | 131 | 123 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | Y | 102 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 785 | 505 | 150 | 125 | 5 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | Z | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1461 | 933 | 260 | 265 | 3 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | 0 | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 401 | 138 | 108 | 1 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | 1 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 481 | 150 | 131 | 1 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | 2 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 358 | 118 | 104 | 1 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 25 | 3 | 59 | Total | C | N | O | 0 | 0 | 0 |
| | | | 469 | 298 | 90 | 81 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | 4 | 71 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 581 | 364 | 108 | 104 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | 5 | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 459 | 288 | 90 | 76 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | 6 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 424 | 264 | 87 | 69 | 4 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29 | 7 | 49 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 430 | 263 | 108 | 57 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30 | 8 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | 9 | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 32 is a RNA chain called tRNA acceptor end mimic.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 32 | a | 3 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 74 | 40 | 13 | 19 | 2 | | | |

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 33 | P | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 33 | 0 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 33 | E | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 33 | B | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 33 | 5 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 33 | A | 241 | Total 241 | Mg 241 | 0 | 0 |
| 33 | U | 1 | Total 1 | Mg 1 | 0 | 0 |
| 33 | 8 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 33 | R | 1 | Total 1 | Mg 1 | 0 | 0 |
| 33 | F | 1 | Total 1 | Mg 1 | 0 | 0 |

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 34 | 9 | 1 | Total 1 | Zn 1 | 0 | 0 |

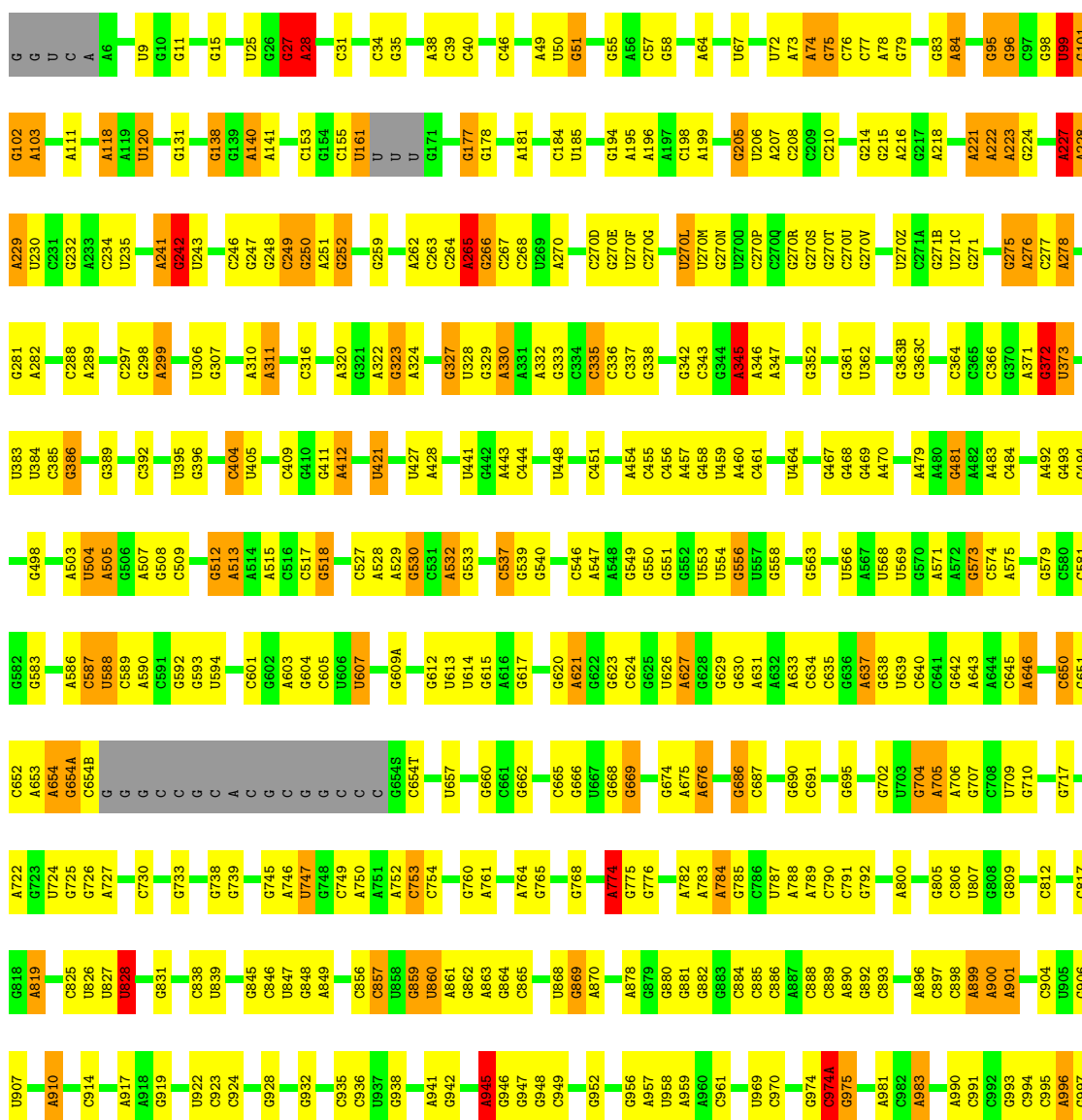
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

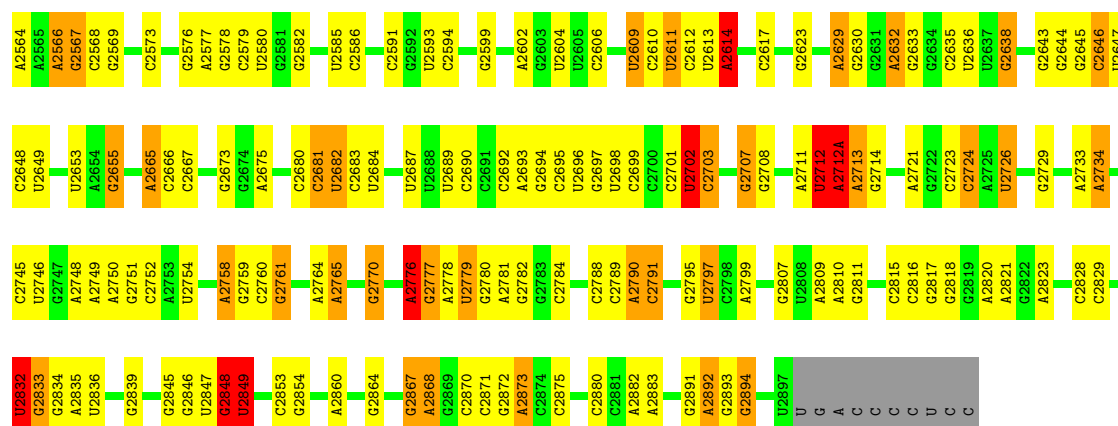
Note EDS was not executed.

• Molecule 1: 23S rRNA

Chain A:

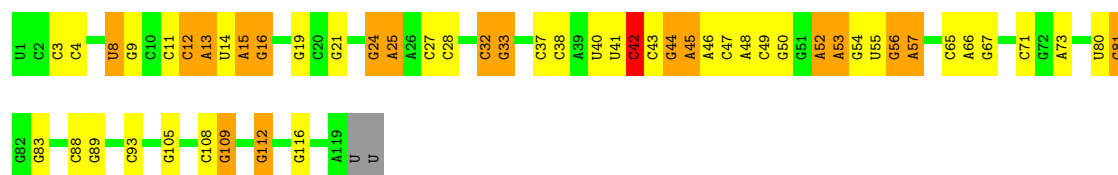


| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|--------|-------|-------|
| U2462 | G2382 | A2398 | C2183 | G2087 | G1863 | C1771 | C1648 | A1536 | A1444A | U1341 | G1256 | G1154 | C1076 | G1003 |
| C2463 | G2383 | G2299 | G2184 | U2099 | U1864 | G1772 | G1653 | C1537 | C1445 | A1342 | C1257 | A1155 | A1077 | C1004 |
| C2466 | G2384 | G2304 | G2190 | C1989 | G1869 | A1773 | A1654 | G1538 | C1445 | G1348 | C1258 | C1161 | C1078 | C1005 |
| C2467 | C2385 | A2305 | G2191 | C1990 | C1870 | C1773 | G1655 | A1542 | G1449 | A1349 | U1263 | G1162 | C1079 | C1006 |
| G2468 | G2388 | C2306 | G2192 | G1991 | A1871 | A1780 | C1656 | G1543 | G1449A | A1349 | U1263 | U1081 | U1080 | C1007 |
| A2469 | A2388 | G2307 | C2193 | G1992 | A1872 | C1782 | C1657 | C1544 | U1454 | A1354 | G1264 | U1165 | U1082 | C1008 |
| G2470 | G2392 | G2308 | U2197 | C1998 | C1882 | A1786 | C1659 | A1545 | G1455 | A1359 | U1266 | C1166 | U1083 | A1009 |
| C2474 | A2393 | A2311 | A2198 | C1999 | A1883 | A1787 | C1660 | C1547 | G1458 | G1364 | G1271 | G1169 | A1084 | A1010 |
| G2475 | C2394 | U2312 | A2199 | G2009 | A1884 | C1790 | G1661 | U1554 | C1458 | A1365 | U1272 | G1170 | A1085 | G1011 |
| A2476 | C2395 | C2313 | U2208 | G2010 | A1885 | A1791 | G1667 | A1558 | C1459 | A1365 | U1273 | G1171 | A1086 | U1012 |
| C2477 | G2396 | C2314 | C2209 | U2011 | A1889 | G1792 | A1668 | A1569 | A1460 | G1368 | U1278 | G1172 | A1087 | C1013 |
| G2481 | G2397 | G2318 | G2210 | G2012 | A1896 | C1795 | A1669 | G1569 | C1461 | G1369 | A1279 | U1175 | A1088 | U1014 |
| C2482 | U2398 | A2320 | A2211 | A2013 | G1896 | C1796 | G1674 | U1577 | C1462 | G1370 | G1278 | A1177 | U1090 | G1015 |
| G2483 | G2401 | G2326 | G2212 | A2014 | G1899 | C1797 | G1678 | C1577 | C1464 | U1371 | G1279 | U1176 | G1093 | U1019 |
| G2484 | C2403 | G2326 | G2213 | A2015 | A1900 | U1798 | G1682 | U1578 | A1471 | G1380 | U1287 | G1184 | U1094 | A1020 |
| G2485 | G2404 | A2326 | G2214 | G2018 | A1901 | C1799 | U1688 | A1580 | A1477 | A1384 | C1291 | G1187 | U1095 | A1021 |
| G2490 | G2405 | C2326 | G2215 | A2019 | G1902 | C1800 | U1689 | G1581 | U1482 | G1385 | U1292 | A1188 | A1096 | G1022 |
| G2494 | G2406 | G2326 | G2216 | G2020 | G1903 | A1801 | A1689 | C1588 | U1483 | G1386 | C1293 | A1189 | U1101 | U1023 |
| G2499 | G2407 | G2326 | G2217 | G2021 | G1904 | G1802 | U1693 | C1589 | G1487 | C1398 | U1309 | G1190 | U1102 | G1024 |
| G2502 | G2408 | G2326 | G2218 | G2022 | G1905 | A1803 | U1694 | U1590 | U1490 | G1401 | A1302 | G1191 | U1103 | G1025 |
| A2503 | G2409 | G2326 | G2219 | G2023 | G1906 | A1804 | U1695 | U1591 | C1493 | C1402 | A1303 | G1192 | U1104 | U1026 |
| U2504 | G2410 | G2326 | G2220 | G2024 | G1907 | A1805 | U1696 | U1592 | C1494 | C1403 | A1304 | G1193 | U1105 | A1045 |
| G2505 | A2411 | G2326 | G2221 | G2025 | G1908 | A1806 | U1697 | U1593 | A1496 | U1406 | C1306 | G1194 | U1106 | A1046 |
| U2506 | G2412 | G2326 | G2222 | G2026 | G1909 | A1807 | U1698 | U1594 | U1497 | C1407 | G1309 | G1122 | G1047 | G1047 |
| C2507 | G2413 | G2326 | G2223 | G2027 | G1910 | A1808 | U1699 | U1595 | C1498 | A1408 | G1310 | G1123 | A1048 | A1048 |
| G2508 | U2422 | G2326 | G2224 | G2028 | G1911 | A1809 | U1700 | U1596 | C1505 | C1411 | U1311 | G1124 | C1049 | A1050 |
| C2517 | U2423 | G2326 | G2225 | G2029 | G1912 | A1810 | U1701 | U1597 | C1506 | C1412 | U1312 | G1125 | A1064 | A1064 |
| U2518 | G2424 | G2326 | G2226 | G2030 | G1913 | A1811 | U1702 | U1598 | C1507 | A1413 | U1313 | G1126 | G1055 | G1055 |
| U2519 | A2425 | G2326 | G2227 | G2031 | G1914 | A1812 | U1703 | U1599 | C1508 | G1414 | U1314 | A1129 | U1060 | G1056 |
| G2527 | G2426 | G2326 | G2228 | G2032 | G1915 | A1813 | U1704 | U1600 | C1509 | U1415 | U1315 | G1130 | U1061 | G1057 |
| U2528 | U2430 | G2326 | G2229 | G2033 | G1916 | A1814 | U1705 | U1601 | C1510 | U1416 | U1316 | G1131 | G1058 | G1058 |
| G2529 | G2431 | G2326 | G2230 | G2034 | G1917 | A1815 | U1706 | U1602 | C1511 | G1417 | U1317 | C1135 | G1059 | G1059 |
| A2530 | U2432 | G2326 | G2231 | G2035 | G1918 | A1816 | U1707 | U1603 | C1512 | G1418 | U1318 | G1136 | U1060 | U1060 |
| U2537 | G2433 | G2326 | G2232 | G2036 | G1919 | A1817 | U1708 | U1604 | C1513 | G1419 | U1319 | G1137 | U1061 | U1061 |
| C2538 | U2434 | G2326 | G2233 | G2037 | G1920 | A1818 | U1709 | U1605 | C1514 | U1420 | U1320 | G1138 | G1062 | G1062 |
| A2542 | G2435 | G2326 | G2234 | G2038 | G1921 | A1819 | U1710 | U1606 | C1515 | U1421 | U1321 | G1139 | G1063 | G1063 |
| G2543 | U2436 | G2326 | G2235 | G2039 | G1922 | A1820 | U1711 | U1607 | C1516 | U1422 | U1322 | C1140 | U1064 | G1064 |
| G2544 | G2437 | G2326 | G2236 | G2040 | G1923 | A1821 | U1712 | U1608 | C1517 | U1423 | U1323 | U1141 | U1065 | U1065 |
| U2554 | U2438 | G2326 | G2237 | G2041 | G1924 | A1822 | U1713 | U1609 | C1518 | U1424 | U1324 | U1142 | U1066 | U1066 |
| G2555 | G2439 | G2326 | G2238 | G2042 | G1925 | A1823 | U1714 | U1610 | C1519 | U1425 | U1325 | A1142A | A1067 | A1067 |
| G2556 | U2440 | G2326 | G2239 | G2043 | G1926 | A1824 | U1715 | U1611 | C1520 | U1426 | U1326 | G1149 | G1068 | G1068 |
| G2557 | C2441 | G2326 | G2240 | G2044 | G1927 | A1825 | U1716 | U1612 | C1521 | U1427 | U1327 | C1150 | A1069 | A1069 |
| U2558 | G2442 | G2326 | G2241 | G2045 | G1928 | A1826 | U1717 | U1613 | C1522 | C1428 | U1328 | C1151 | A1070 | A1070 |
| G2559 | U2443 | G2326 | G2242 | G2046 | G1929 | A1827 | U1718 | U1614 | C1523 | C1429 | U1329 | C1152 | G1071 | G1071 |
| U2562 | G2444 | G2326 | G2243 | G2047 | G1930 | A1828 | U1719 | U1615 | C1524 | C1430 | U1330 | G1153 | C1152 | C1152 |
| U2563 | U2445 | G2326 | G2244 | G2048 | G1931 | A1829 | U1720 | U1616 | C1525 | U1431 | U1331 | C1154 | C1153 | C1153 |
| | G2446 | G2326 | G2245 | G2049 | G1932 | A1830 | U1721 | U1617 | C1526 | U1432 | U1332 | G1155 | | |
| | U2447 | G2326 | G2246 | G2050 | G1933 | A1831 | U1722 | U1618 | C1527 | U1433 | U1333 | G1156 | | |
| | G2448 | G2326 | G2247 | G2051 | G1934 | A1832 | U1723 | U1619 | C1528 | U1434 | U1334 | G1157 | | |
| | U2449 | G2326 | G2248 | G2052 | G1935 | A1833 | U1724 | U1620 | C1529 | U1435 | U1335 | G1158 | | |
| | G2450 | G2326 | G2249 | G2053 | G1936 | A1834 | U1725 | U1621 | C1530 | U1436 | U1336 | G1159 | | |
| | U2451 | G2326 | G2250 | G2054 | G1937 | A1835 | U1726 | U1622 | C1531 | U1437 | U1337 | G1160 | | |
| | A2452 | G2326 | G2251 | G2055 | A1937 | A1836 | U1727 | U1623 | C1532 | U1438 | U1338 | G1161 | | |
| | G2453 | G2326 | G2252 | G2056 | A1938 | A1837 | U1728 | U1624 | C1533 | U1439 | U1339 | G1162 | | |
| | U2454 | G2326 | G2253 | G2057 | A1939 | A1838 | U1729 | U1625 | C1534 | U1440 | U1340 | G1163 | | |
| | G2455 | G2326 | G2254 | G2058 | U1940 | A1839 | U1730 | U1626 | C1535 | U1441 | U1341 | G1164 | | |
| | U2456 | G2326 | G2255 | G2059 | U1941 | A1840 | U1731 | U1627 | C1536 | U1442 | U1342 | G1165 | | |
| | G2457 | G2326 | G2256 | G2060 | U1942 | A1841 | U1732 | U1628 | C1537 | U1443 | U1343 | G1166 | | |
| | U2458 | G2326 | G2257 | G2061 | U1943 | A1842 | U1733 | U1629 | C1538 | U1444 | U1344 | G1167 | | |
| | G2459 | G2326 | G2258 | G2062 | U1944 | A1843 | U1734 | U1630 | C1539 | U1445 | U1345 | G1168 | | |
| | U2460 | G2326 | G2259 | G2063 | U1945 | A1844 | U1735 | U1631 | C1540 | U1446 | U1346 | G1169 | | |
| | G2461 | G2326 | G2260 | G2064 | U1946 | A1845 | U1736 | U1632 | C1541 | U1447 | U1347 | G1170 | | |
| | U2462 | G2326 | G2261 | G2065 | U1947 | A1846 | U1737 | U1633 | C1542 | U1448 | U1348 | G1171 | | |
| | G2463 | G2326 | G2262 | G2066 | U1948 | A1847 | U1738 | U1634 | C1543 | U1449 | U1349 | G1172 | | |
| | U2464 | G2326 | G2263 | G2067 | U1949 | A1848 | U1739 | U1635 | C1544 | U1450 | U1350 | G1173 | | |
| | G2465 | G2326 | G2264 | G2068 | U1950 | A1849 | U1740 | U1636 | C1545 | U1451 | U1351 | G1174 | | |
| | U2466 | G2326 | G2265 | G2069 | U1951 | A1850 | U1741 | U1637 | C1546 | U1452 | U1352 | G1175 | | |
| | G2467 | G2326 | G2266 | G2070 | U1952 | A1851 | U1742 | U1638 | C1547 | U1453 | U1353 | G1176 | | |
| | U2468 | G2326 | G2267 | G2071 | U1953 | A1852 | U1743 | U1639 | C1548 | U1454 | U1354 | G1177 | | |
| | G2469 | G2326 | G2268 | G2072 | U1954 | A1853 | U1744 | U1640 | C1549 | U1455 | U1355 | G1178 | | |
| | U2470 | G2326 | G2269 | G2073 | U1955 | A1854 | U1745 | U1641 | C1550 | U1456 | U1356 | G1179 | | |
| | G2471 | G2326 | G2270 | G2074 | U1956 | A1855 | U1746 | U1642 | C1551 | U1457 | U1357 | G1180 | | |
| | U2472 | G2326 | G2271 | G2075 | U1957 | A1856 | U1747 | U1643 | C1552 | U1458 | U1358 | G1181 | | |
| | G2473 | G2326 | G2272 | G2076 | U1958 | A1857 | U1748 | U1644 | C1553 | U1459 | U1359 | G1182 | | |
| | U2474 | G2326 | G2273 | G2077 | U1959 | A1858 | U1749 | U1645 | C1554 | U1460 | U1360 | G1183 | | |
| | G2475 | G2326 | G2274 | G2078 | U1960 | A1859 | U1750 | U1646 | C1555 | U1461 | U1361 | G1184 | | |
| | U2476 | G2326 | G2275 | G2079 | U1961 | A1860 | U1751 | U1647 | C1556 | U1462 | U1362 | G1185 | | |
| | G2477 | G2326 | G2276 | G2080 | U1962 | A1861 | U1752 | U1648 | C1557 | U1463 | U1363 | G1186 | | |
| | U2478 | G2326 | G2277 | G2081 | U1963 | A1862 | U1753 | U1649 | C1558 | U1464 | U1364 | G1187 | | |
| | G2479 | G2326 | G2278 | G2082 | U1964 | A1863 | U1754 | U1650 | C1559 | U1465 | U1365 | G1188 | | |
| | U2480 | G2326 | G2279 | G2083 | U1965 | A1864 | U1755 | U1651 | C1560 | U1466 | U1366 | G1189 | | |
| | G2481 | G2326 | G2280 | G2084 | U1966 | A1865 | U1756 | U1652 | C1561 | U1467 | U1367 | G1190 | | |
| | U2482 | G2326 | G2281 | G2085 | U1967 | A1866 | U1757 | U1653 | C1562 | U1468 | U1368 | G1191 | | |
| | G2483 | G2326 | G2282 | G2086 | U1968 | A1867 | U1758 | U1654 | C1563 | U1469 | U1369 | G1192 | | |
| | U2484 | G2326 | G2283 | G2087 | U1969 | A1868 | U1759 | U1655 | C1564 | U1470 | U1370 | G1193 | | |
| | G2485 | G2326 | G2284 | G2088 | U1970 | A1869 | U1760 | U1656 | C1565 | U1471 | U1371 | G1194 | | |
| | U2486 | G2326 | G2285 | G2089 | U1971 | A1870 | U1761 | U1657 | C1566 | U1472 | U1372 | G1195 | | |
| | G2487 | G2326 | G2286 | G2090 | U1972 | A1871 | U1762 | U1658 | C1567 | U1473 | U1373 | G1196 | | |
| | U2488 | G2326 | G2287 | G2091 | U1973 | A1872 | U1763 | U1659 | C1568 | U1474 | U1374 | G1197 | | |
| | G2489 | G2326 | G2288 | G2092 | U1974 | A1873 | U1764 | U1660 | C1569 | U1475 | U1375 | G1198 | | |



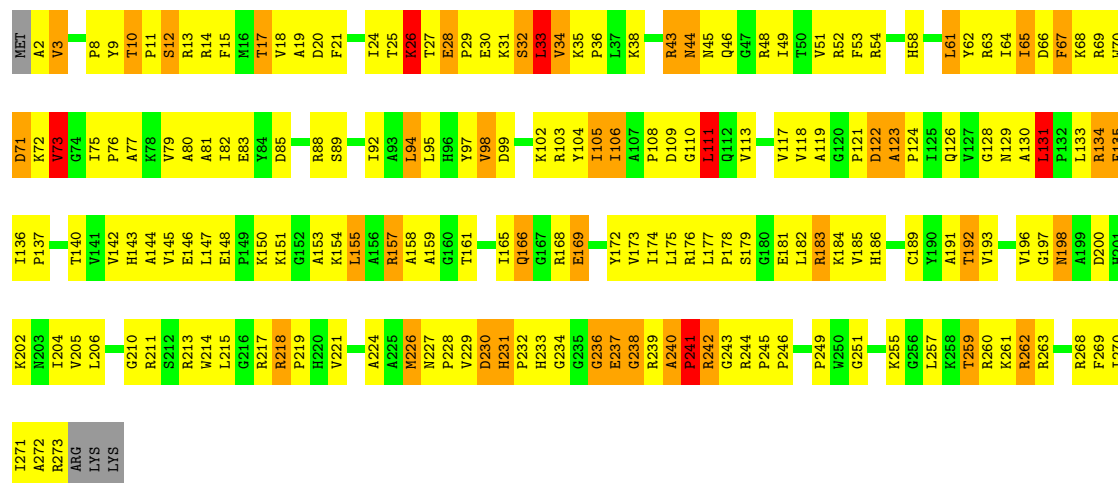
• Molecule 2: 5S rRNA

Chain B:



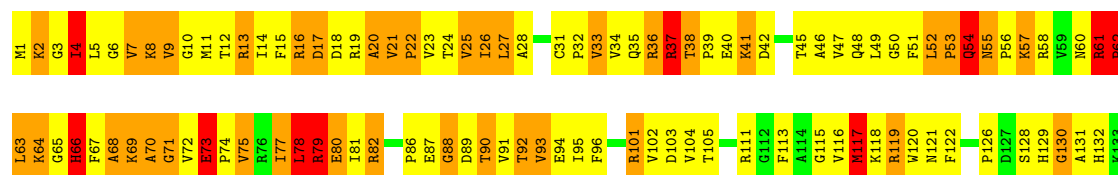
• Molecule 3: 50S ribosomal protein L2

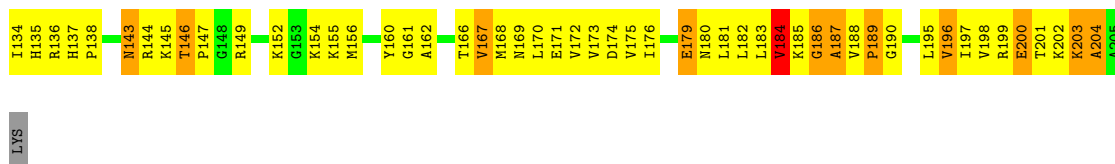
Chain D:



• Molecule 4: 50S ribosomal protein L3

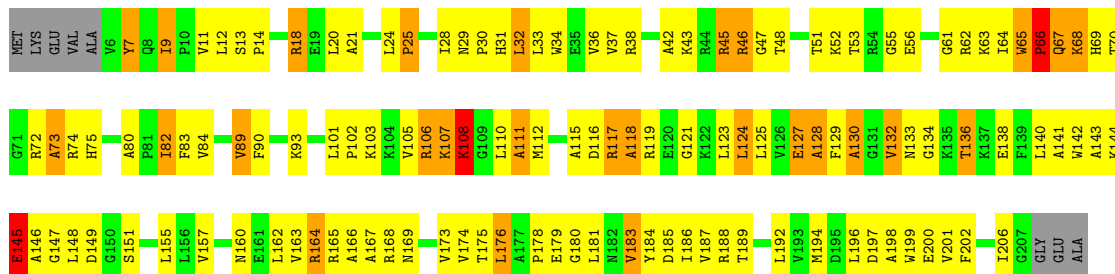
Chain E:





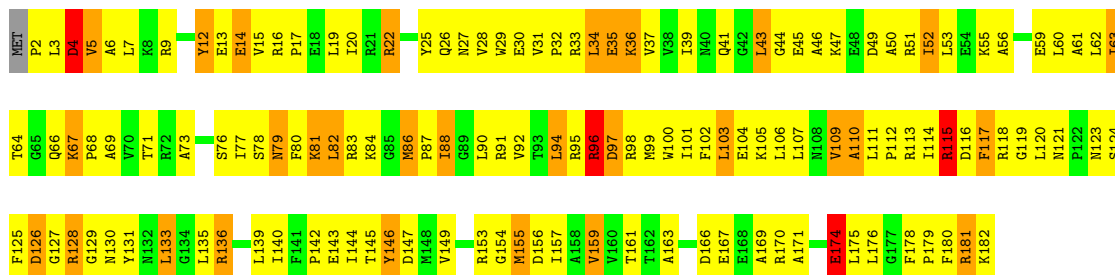
• Molecule 5: 50S ribosomal protein L4

Chain F:



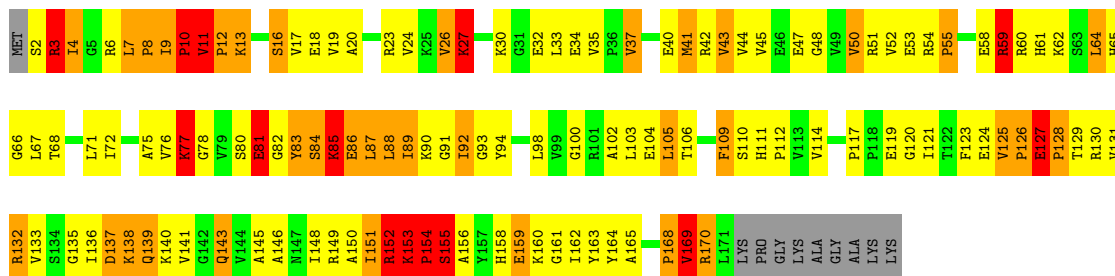
• Molecule 6: 50S ribosomal protein L5

Chain G:



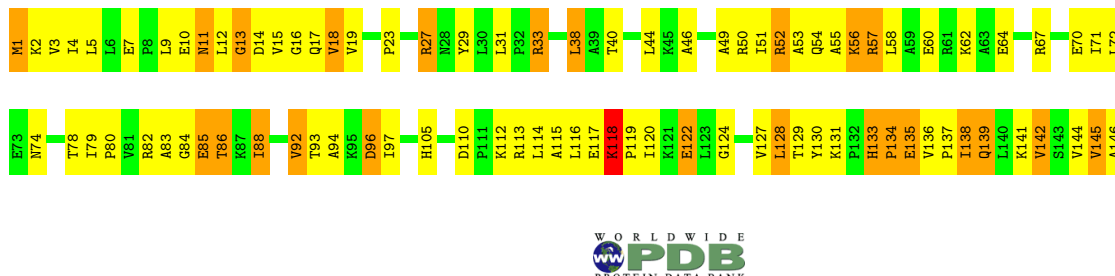
• Molecule 7: 50S ribosomal protein L6

Chain H:



• Molecule 8: 50S ribosomal protein L9

Chain I:



GLN
GLU

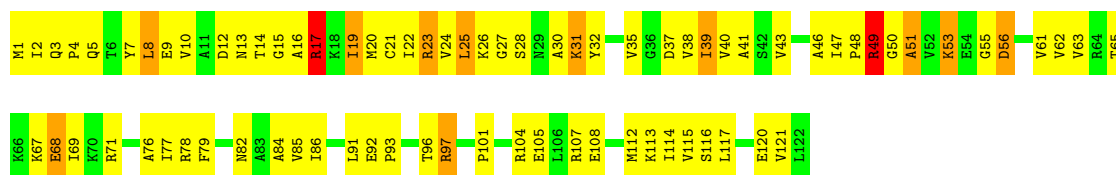
- Molecule 9: 50S ribosomal protein L13

Chain N:



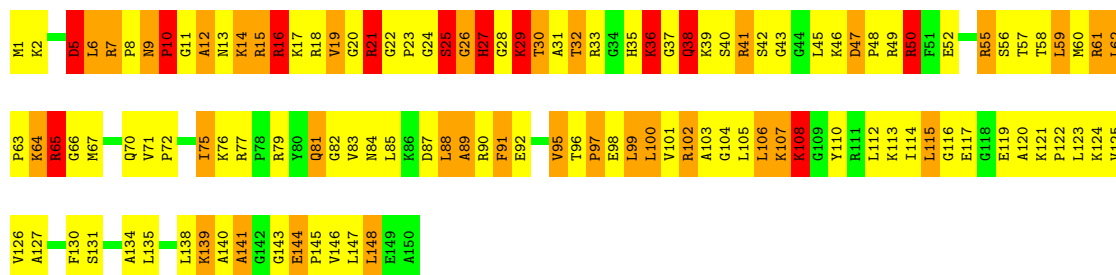
- Molecule 10: 50S ribosomal protein L14

Chain O:



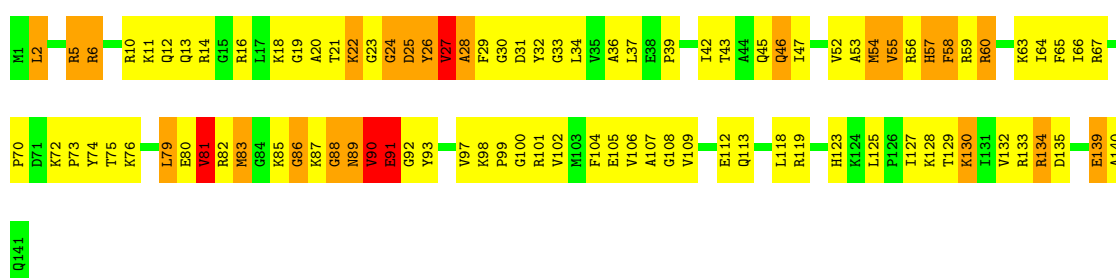
- Molecule 11: 50S ribosomal protein L15

Chain P:



- Molecule 12: 50S ribosomal protein L16

Chain Q:



- Molecule 13: 50S ribosomal protein L17

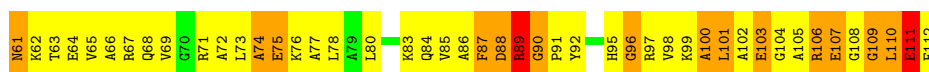
Chain R:





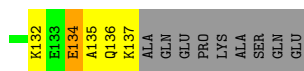
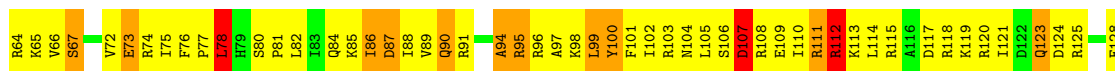
• Molecule 14: 50S ribosomal protein L18

Chain S:



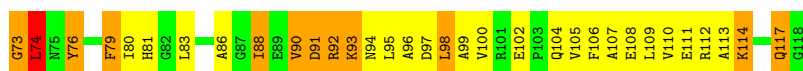
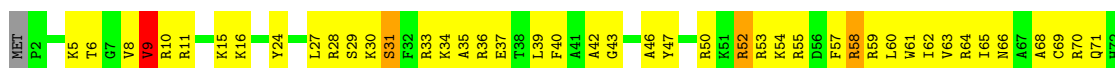
• Molecule 15: 50S ribosomal protein L19

Chain T:



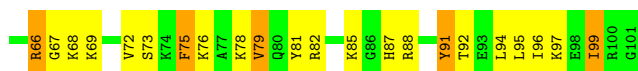
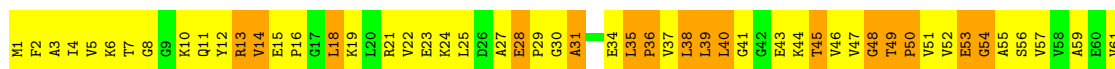
• Molecule 16: 50S ribosomal protein L20

Chain U:



• Molecule 17: 50S ribosomal protein L21

Chain V:



• Molecule 18: 50S ribosomal protein L22

Chain W:





• Molecule 19: 50S ribosomal protein L23

Chain X:



• Molecule 20: 50S ribosomal protein L24

Chain Y:



• Molecule 21: 50S ribosomal protein L25

Chain Z:



• Molecule 22: 50S ribosomal protein L27

Chain 0:



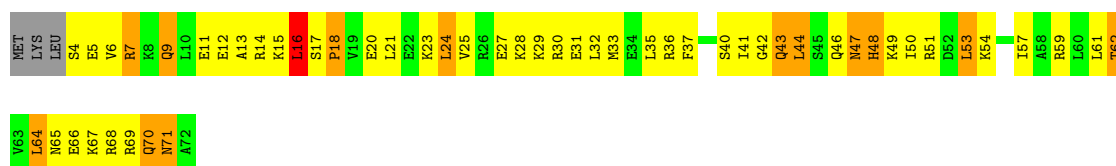
• Molecule 23: 50S ribosomal protein L28

Chain 1:



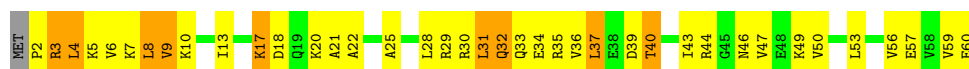
• Molecule 24: 50S ribosomal protein L29

Chain 2:



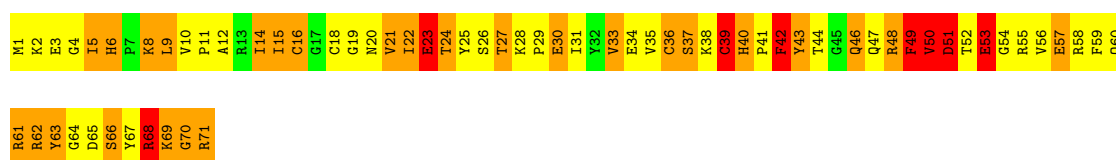
- Molecule 25: 50S ribosomal protein L30

Chain 3:



- Molecule 26: 50S ribosomal protein L31

Chain 4:



- Molecule 27: 50S ribosomal protein L32

Chain 5:



- Molecule 28: 50S ribosomal protein L33

Chain 6:



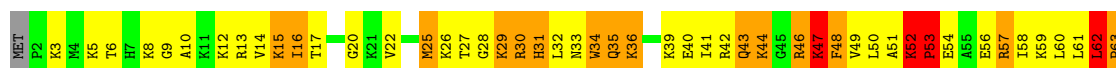
- Molecule 29: 50S ribosomal protein L34

Chain 7:



- Molecule 30: 50S ribosomal protein L35

Chain 8:



- Molecule 31: 50S ribosomal protein L36

Chain 9:





- Molecule 32: tRNA acceptor end mimic

Chain a: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.20Å 450.23Å 621.74Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 34.97 – 3.22 | Depositor |
| % Data completeness (in resolution range) | 98.5 (34.97-3.22) | Depositor |
| R_{merge} | 0.25 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.229 , 0.260 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 92246 | wwPDB-VP |
| Average B, all atoms (Å ²) | 90.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 0.39 | 1/69521 (0.0%) | 0.91 | 95/108529 (0.1%) |
| 2 | B | 0.34 | 0/2878 | 0.89 | 3/4490 (0.1%) |
| 3 | D | 0.59 | 2/2165 (0.1%) | 0.90 | 4/2919 (0.1%) |
| 4 | E | 0.52 | 0/1601 | 0.91 | 2/2160 (0.1%) |
| 5 | F | 0.50 | 0/1620 | 0.76 | 0/2194 |
| 6 | G | 0.40 | 0/1499 | 0.66 | 0/2016 |
| 7 | H | 0.45 | 0/1332 | 0.85 | 3/1802 (0.2%) |
| 8 | I | 0.29 | 0/1151 | 0.63 | 0/1558 |
| 9 | N | 0.46 | 0/1131 | 0.78 | 1/1525 (0.1%) |
| 10 | O | 0.53 | 0/943 | 0.71 | 0/1269 |
| 11 | P | 0.50 | 0/1162 | 0.94 | 3/1544 (0.2%) |
| 12 | Q | 0.54 | 0/1143 | 0.90 | 3/1527 (0.2%) |
| 13 | R | 0.45 | 0/982 | 0.80 | 1/1312 (0.1%) |
| 14 | S | 0.46 | 0/892 | 0.82 | 1/1187 (0.1%) |
| 15 | T | 0.47 | 0/1155 | 0.73 | 2/1542 (0.1%) |
| 16 | U | 0.48 | 0/982 | 0.78 | 0/1306 |
| 17 | V | 0.47 | 0/790 | 0.82 | 0/1057 |
| 18 | W | 0.45 | 0/911 | 0.75 | 0/1220 |
| 19 | X | 0.56 | 0/739 | 0.77 | 0/993 |
| 20 | Y | 0.52 | 0/798 | 0.80 | 0/1064 |
| 21 | Z | 0.32 | 0/1493 | 0.60 | 0/2026 |
| 22 | 0 | 0.30 | 0/657 | 0.56 | 0/874 |
| 23 | 1 | 0.49 | 0/770 | 0.85 | 1/1022 (0.1%) |
| 24 | 2 | 0.51 | 0/583 | 0.83 | 1/771 (0.1%) |
| 25 | 3 | 0.47 | 0/474 | 0.72 | 0/635 |
| 26 | 4 | 0.38 | 0/594 | 0.78 | 1/795 (0.1%) |
| 27 | 5 | 0.51 | 0/473 | 0.74 | 0/639 |
| 28 | 6 | 0.42 | 0/431 | 0.76 | 0/575 |
| 29 | 7 | 0.56 | 0/438 | 0.76 | 0/575 |
| 30 | 8 | 0.62 | 0/525 | 0.93 | 1/691 (0.1%) |
| 31 | 9 | 0.35 | 0/310 | 0.59 | 0/407 |
| 32 | a | 0.79 | 0/40 | 1.79 | 1/60 (1.7%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.41 | 3/100183 (0.0%) | 0.88 | 123/150284 (0.1%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 3 | D | 236 | GLY | C-N | 8.55 | 1.53 | 1.34 |
| 1 | A | 654(T) | C | C1'-N1 | 5.71 | 1.57 | 1.48 |
| 3 | D | 241 | PRO | N-CD | 5.15 | 1.55 | 1.47 |

The worst 5 of 123 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 4 | E | 21 | VAL | C-N-CD | -10.07 | 98.45 | 120.60 |
| 1 | A | 945 | A | P-O3'-C3' | 9.62 | 131.25 | 119.70 |
| 12 | Q | 81 | VAL | CB-CA-C | -8.65 | 94.97 | 111.40 |
| 1 | A | 2506 | U | N3-C2-O2 | -7.87 | 116.69 | 122.20 |
| 23 | 1 | 79 | GLY | N-CA-C | -7.84 | 93.51 | 113.10 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 62071 | 0 | 31285 | 849 | 0 |
| 2 | B | 2573 | 0 | 1306 | 58 | 0 |
| 3 | D | 2115 | 0 | 2195 | 317 | 0 |
| 4 | E | 1568 | 0 | 1634 | 271 | 0 |
| 5 | F | 1585 | 0 | 1632 | 177 | 0 |
| 6 | G | 1474 | 0 | 1535 | 204 | 0 |
| 7 | H | 1307 | 0 | 1382 | 226 | 0 |
| 8 | I | 1136 | 0 | 1223 | 69 | 0 |
| 9 | N | 1104 | 0 | 1180 | 194 | 0 |
| 10 | O | 933 | 0 | 996 | 121 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11 | P | 1145 | 0 | 1227 | 245 | 0 |
| 12 | Q | 1122 | 0 | 1179 | 158 | 0 |
| 13 | R | 968 | 0 | 1033 | 112 | 0 |
| 14 | S | 882 | 0 | 943 | 160 | 0 |
| 15 | T | 1141 | 0 | 1202 | 149 | 0 |
| 16 | U | 964 | 0 | 1022 | 129 | 0 |
| 17 | V | 779 | 0 | 852 | 129 | 0 |
| 18 | W | 900 | 0 | 964 | 98 | 0 |
| 19 | X | 725 | 0 | 778 | 67 | 0 |
| 20 | Y | 785 | 0 | 878 | 169 | 0 |
| 21 | Z | 1461 | 0 | 1493 | 77 | 0 |
| 22 | 0 | 648 | 0 | 672 | 27 | 0 |
| 23 | 1 | 763 | 0 | 848 | 138 | 0 |
| 24 | 2 | 581 | 0 | 629 | 81 | 0 |
| 25 | 3 | 469 | 0 | 518 | 39 | 0 |
| 26 | 4 | 581 | 0 | 574 | 133 | 0 |
| 27 | 5 | 459 | 0 | 480 | 74 | 0 |
| 28 | 6 | 424 | 0 | 450 | 92 | 0 |
| 29 | 7 | 430 | 0 | 480 | 43 | 0 |
| 30 | 8 | 517 | 0 | 582 | 103 | 0 |
| 31 | 9 | 307 | 0 | 335 | 18 | 0 |
| 32 | a | 74 | 0 | 51 | 0 | 0 |
| 33 | 0 | 1 | 0 | 0 | 0 | 0 |
| 33 | 5 | 1 | 0 | 0 | 0 | 0 |
| 33 | 8 | 1 | 0 | 0 | 0 | 0 |
| 33 | A | 241 | 0 | 0 | 0 | 0 |
| 33 | B | 2 | 0 | 0 | 0 | 0 |
| 33 | D | 1 | 0 | 0 | 0 | 0 |
| 33 | E | 2 | 0 | 0 | 0 | 0 |
| 33 | F | 1 | 0 | 0 | 0 | 0 |
| 33 | P | 2 | 0 | 0 | 0 | 0 |
| 33 | R | 1 | 0 | 0 | 0 | 0 |
| 33 | U | 1 | 0 | 0 | 0 | 0 |
| 34 | 9 | 1 | 0 | 0 | 0 | 0 |
| All | All | 92246 | 0 | 61558 | 4274 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 4274 close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|----------------|-----------------|-------------|----------|
| 7:H:127:GLU:CG | 7:H:128:PRO:HD3 | 1.36 | 1.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|----------------|-------------|----------|
| 23:1:81:LYS:NZ | 23:1:81:LYS:HA | 1.43 | 1.34 |
| 21:Z:115:GLY:CA | 21:Z:175:VAL:O | 1.83 | 1.26 |
| 23:1:81:LYS:HE2 | 23:1:81:LYS:N | 1.50 | 1.26 |
| 21:Z:115:GLY:HA2 | 21:Z:175:VAL:O | 1.14 | 1.26 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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 | D | 270/276 (98%) | 203 (75%) | 48 (18%) | 19 (7%) | 2 | 14 |
| 4 | E | 203/206 (98%) | 120 (59%) | 41 (20%) | 42 (21%) | 0 | 0 |
| 5 | F | 200/210 (95%) | 144 (72%) | 36 (18%) | 20 (10%) | 1 | 7 |
| 6 | G | 179/182 (98%) | 119 (66%) | 39 (22%) | 21 (12%) | 1 | 4 |
| 7 | H | 168/180 (93%) | 94 (56%) | 36 (21%) | 38 (23%) | 0 | 0 |
| 8 | I | 144/148 (97%) | 101 (70%) | 26 (18%) | 17 (12%) | 1 | 4 |
| 9 | N | 136/140 (97%) | 84 (62%) | 30 (22%) | 22 (16%) | 0 | 1 |
| 10 | O | 120/122 (98%) | 90 (75%) | 21 (18%) | 9 (8%) | 2 | 12 |
| 11 | P | 148/150 (99%) | 97 (66%) | 19 (13%) | 32 (22%) | 0 | 0 |
| 12 | Q | 139/141 (99%) | 95 (68%) | 30 (22%) | 14 (10%) | 1 | 7 |
| 13 | R | 116/118 (98%) | 82 (71%) | 20 (17%) | 14 (12%) | 1 | 4 |
| 14 | S | 109/112 (97%) | 62 (57%) | 28 (26%) | 19 (17%) | 0 | 1 |
| 15 | T | 135/146 (92%) | 83 (62%) | 32 (24%) | 20 (15%) | 0 | 1 |
| 16 | U | 115/118 (98%) | 86 (75%) | 20 (17%) | 9 (8%) | 1 | 11 |
| 17 | V | 99/101 (98%) | 73 (74%) | 16 (16%) | 10 (10%) | 1 | 7 |
| 18 | W | 111/113 (98%) | 75 (68%) | 22 (20%) | 14 (13%) | 0 | 3 |
| 19 | X | 90/96 (94%) | 77 (86%) | 8 (9%) | 5 (6%) | 3 | 23 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|-----|
| 20 | Y | 100/110 (91%) | 58 (58%) | 16 (16%) | 26 (26%) | 0 | 0 |
| 21 | Z | 181/206 (88%) | 118 (65%) | 39 (22%) | 24 (13%) | 0 | 2 |
| 22 | 0 | 80/85 (94%) | 69 (86%) | 8 (10%) | 3 (4%) | 5 | 34 |
| 23 | 1 | 95/98 (97%) | 64 (67%) | 20 (21%) | 11 (12%) | 1 | 4 |
| 24 | 2 | 67/72 (93%) | 47 (70%) | 11 (16%) | 9 (13%) | 0 | 2 |
| 25 | 3 | 57/60 (95%) | 45 (79%) | 9 (16%) | 3 (5%) | 3 | 24 |
| 26 | 4 | 69/71 (97%) | 23 (33%) | 20 (29%) | 26 (38%) | 0 | 0 |
| 27 | 5 | 57/60 (95%) | 33 (58%) | 9 (16%) | 15 (26%) | 0 | 0 |
| 28 | 6 | 47/54 (87%) | 15 (32%) | 18 (38%) | 14 (30%) | 0 | 0 |
| 29 | 7 | 47/49 (96%) | 37 (79%) | 7 (15%) | 3 (6%) | 2 | 17 |
| 30 | 8 | 62/65 (95%) | 36 (58%) | 15 (24%) | 11 (18%) | 0 | 1 |
| 31 | 9 | 35/37 (95%) | 31 (89%) | 4 (11%) | 0 | 100 | 100 |
| All | All | 3379/3526 (96%) | 2261 (67%) | 648 (19%) | 470 (14%) | 0 | 2 |

5 of 470 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | D | 26 | LYS |
| 3 | D | 28 | GLU |
| 3 | D | 123 | ALA |
| 3 | D | 231 | HIS |
| 4 | E | 4 | ILE |

5.3.2 Protein sidechains ⓘ

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 | D | 214/218 (98%) | 177 (83%) | 37 (17%) | 3 | 13 |
| 4 | E | 165/166 (99%) | 127 (77%) | 38 (23%) | 1 | 5 |
| 5 | F | 161/166 (97%) | 140 (87%) | 21 (13%) | 6 | 28 |
| 6 | G | 155/156 (99%) | 130 (84%) | 25 (16%) | 3 | 16 |
| 7 | H | 142/148 (96%) | 114 (80%) | 28 (20%) | 2 | 9 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 8 | I | 122/124 (98%) | 94 (77%) | 28 (23%) | 1 | 5 |
| 9 | N | 117/119 (98%) | 98 (84%) | 19 (16%) | 3 | 15 |
| 10 | O | 100/100 (100%) | 90 (90%) | 10 (10%) | 11 | 41 |
| 11 | P | 116/116 (100%) | 89 (77%) | 27 (23%) | 1 | 5 |
| 12 | Q | 111/111 (100%) | 93 (84%) | 18 (16%) | 3 | 15 |
| 13 | R | 101/101 (100%) | 84 (83%) | 17 (17%) | 3 | 14 |
| 14 | S | 87/88 (99%) | 74 (85%) | 13 (15%) | 4 | 20 |
| 15 | T | 120/127 (94%) | 97 (81%) | 23 (19%) | 2 | 10 |
| 16 | U | 93/94 (99%) | 80 (86%) | 13 (14%) | 5 | 24 |
| 17 | V | 82/82 (100%) | 71 (87%) | 11 (13%) | 6 | 26 |
| 18 | W | 92/92 (100%) | 77 (84%) | 15 (16%) | 3 | 15 |
| 19 | X | 74/78 (95%) | 63 (85%) | 11 (15%) | 4 | 20 |
| 20 | Y | 85/91 (93%) | 70 (82%) | 15 (18%) | 3 | 13 |
| 21 | Z | 162/179 (90%) | 140 (86%) | 22 (14%) | 5 | 26 |
| 22 | 0 | 65/67 (97%) | 60 (92%) | 5 (8%) | 18 | 59 |
| 23 | 1 | 82/83 (99%) | 67 (82%) | 15 (18%) | 2 | 12 |
| 24 | 2 | 64/67 (96%) | 57 (89%) | 7 (11%) | 9 | 37 |
| 25 | 3 | 51/52 (98%) | 40 (78%) | 11 (22%) | 1 | 7 |
| 26 | 4 | 63/63 (100%) | 44 (70%) | 19 (30%) | 0 | 1 |
| 27 | 5 | 51/52 (98%) | 39 (76%) | 12 (24%) | 1 | 4 |
| 28 | 6 | 48/52 (92%) | 38 (79%) | 10 (21%) | 2 | 8 |
| 29 | 7 | 42/42 (100%) | 39 (93%) | 3 (7%) | 21 | 63 |
| 30 | 8 | 54/55 (98%) | 39 (72%) | 15 (28%) | 0 | 2 |
| 31 | 9 | 34/34 (100%) | 32 (94%) | 2 (6%) | 28 | 72 |
| All | All | 2853/2923 (98%) | 2363 (83%) | 490 (17%) | 3 | 14 |

5 of 490 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | P | 62 | LEU |
| 14 | S | 56 | LEU |
| 27 | 5 | 19 | ARG |
| 11 | P | 99 | LEU |
| 12 | Q | 130 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | Q | 123 | HIS |
| 15 | T | 58 | ASN |
| 24 | 2 | 47 | ASN |
| 13 | R | 3 | HIS |
| 16 | U | 94 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 2879/2916 (98%) | 623 (21%) | 73 (2%) |
| 2 | B | 119/122 (97%) | 25 (21%) | 2 (1%) |
| 32 | a | 1/3 (33%) | 0 | 0 |
| All | All | 2999/3041 (98%) | 648 (21%) | 75 (2%) |

5 of 648 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 9 | U |
| 1 | A | 11 | G |
| 1 | A | 15 | G |
| 1 | A | 28 | A |
| 1 | A | 34 | C |

5 of 75 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1026 | U |
| 1 | A | 1301 | A |
| 1 | A | 2776 | A |
| 1 | A | 1045 | A |
| 1 | A | 1178 | C |

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

1 non-standard protein/DNA/RNA residue is 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 | $\# Z > 2$ |
| 32 | PPU | a | 76 | 1,32 | 38,40,41 | 2.43 | 9 (23%) | 54,57,60 | 2.61 | 14 (25%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 32 | PPU | a | 76 | 1,32 | - | 0/26/43/44 | 0/4/4/4 |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 32 | a | 76 | PPU | O-C | 9.24 | 1.41 | 1.23 |
| 32 | a | 76 | PPU | C9-N6 | -5.45 | 1.31 | 1.45 |
| 32 | a | 76 | PPU | C-N3' | 5.40 | 1.46 | 1.34 |
| 32 | a | 76 | PPU | C10-N6 | -5.13 | 1.32 | 1.45 |
| 32 | a | 76 | PPU | C4-N9 | -3.14 | 1.33 | 1.37 |

The worst 5 of 14 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32 | a | 76 | PPU | N3-C2-N1 | -8.49 | 121.42 | 128.89 |
| 32 | a | 76 | PPU | C3'-N3'-C | -8.15 | 110.21 | 123.19 |
| 32 | a | 76 | PPU | C5-C4-N3 | -6.35 | 119.79 | 125.98 |
| 32 | a | 76 | PPU | C2'-C1'-N9 | -5.44 | 98.52 | 113.35 |
| 32 | a | 76 | PPU | C2'-C3'-N3' | 5.17 | 125.09 | 113.08 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 255 ligands modelled in this entry, 255 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.