



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:01 PM BST

PDB ID : 4V71
EMDB ID: : EMD-1717
Title : E. coli 70S-fMetVal-tRNAVal-tRNAfMet complex in intermediate pre-translocation state (pre2)
Authors : Blau, C.; Bock, L.V.; Schroder, G.F.; Davydov, I.; Fischer, N.; Stark, H.; Rodnina, M.V.; Vaiana, A.C.; Grubmuller, H.
Deposited on : 2013-10-14
Resolution : 20.00 Å(reported)
Based on PDB ID : 3I1O, 2HGP, 2WRI, 2K4C

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

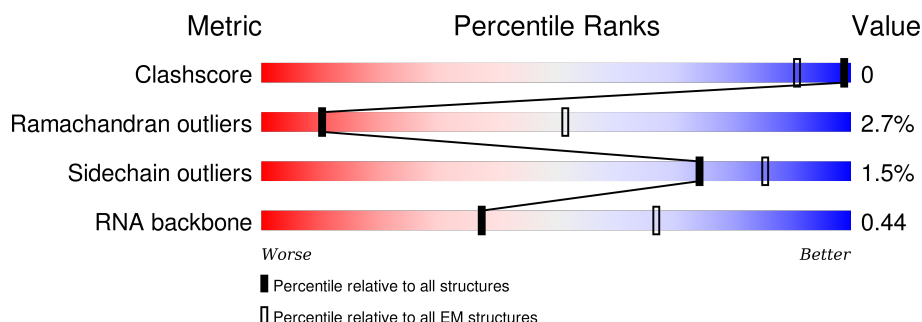
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

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















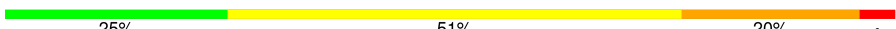
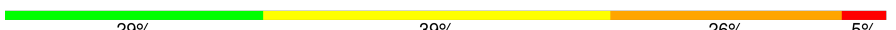
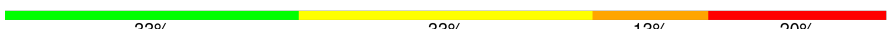
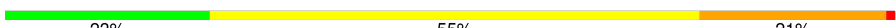






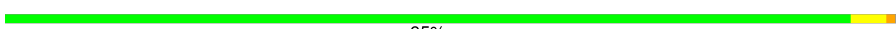


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |
| RNA backbone | 3027 | 244 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AB | 220 | 92% 7% |
| 2 | AC | 208 | 89% 11% |
| 3 | AD | 206 | 90% 9% |
| 4 | AE | 152 | 90% 10% |
| 5 | AF | 101 | 90% 10% |
| 6 | AG | 152 | 89% 11% |
| 7 | AH | 130 | 90% 9% . |
| 8 | AI | 128 | 86% 13% . |












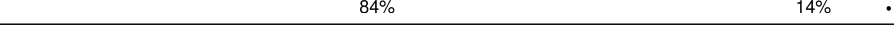

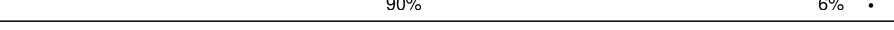







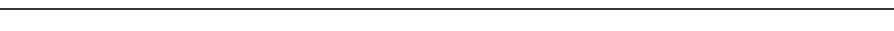

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | AJ | 100 |  85% 12% . |
| 10 | AK | 118 |  86% 13% . |
| 11 | AL | 124 |  87% 12% . |
| 12 | AM | 115 |  85% 14% . |
| 13 | AN | 101 |  88% 11% . |
| 14 | AO | 89 |  87% 12% . |
| 15 | AP | 81 |  85% 15% |
| 16 | AQ | 82 |  88% 12% |
| 17 | AR | 57 |  88% 12% |
| 18 | AS | 81 |  89% 9% . |
| 19 | AT | 86 |  91% 9% |
| 20 | AU | 53 |  77% 23% |
| 21 | AA | 1533 |  25% 51% 20% . |
| 22 | A1 | 76 |  29% 39% 26% 5% |
| 23 | A2 | 15 |  33% 33% 13% 20% |
| 24 | A3 | 77 |  23% 55% 21% . |
| 25 | BC | 273 |  88% 11% |
| 26 | BD | 209 |  89% 11% |
| 27 | BE | 201 |  92% 8% |
| 28 | BF | 179 |  88% 11% . |
| 29 | BG | 177 |  92% 7% .. |
| 30 | BH | 149 |  95% 5% |
| 31 | BI | 142 |  95% . .. |
| 32 | BJ | 142 |  89% 11% |
| 33 | BK | 123 |  90% 9% . |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 34 | BL | 144 |  90% 9% . |
| 35 | BM | 136 |  85% 15% |
| 36 | BN | 121 |  83% 17% . |
| 37 | BO | 117 |  89% 9% .. |
| 38 | BP | 115 |  82% 17% .. |
| 39 | BQ | 118 |  85% 13% .. |
| 40 | BR | 103 |  90% 10% |
| 41 | BS | 110 |  90% 9% . |
| 42 | BT | 94 |  86% 14% |
| 43 | BU | 104 |  90% 7% .. |
| 44 | BV | 94 |  89% 11% |
| 45 | BW | 80 |  84% 14% . |
| 46 | BX | 79 |  84% 13% .. |
| 47 | BY | 63 |  90% 6% . |
| 48 | BZ | 59 |  88% 10% . |
| 49 | B0 | 57 |  84% 14% . |
| 50 | B1 | 52 |  92% 8% |
| 51 | B2 | 46 |  76% 22% . |
| 52 | B3 | 65 |  91% 8% . |
| 53 | B4 | 38 |  82% 18% |
| 54 | BA | 2903 |  23% 50% 23% . |
| 55 | BB | 118 |  25% 49% 22% .. |
| 56 | B5 | 234 |  89% 6% 5% |

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | AB | 220 | Total | C | N | O | S | 0 | 1 |
| | | | 1708 | 1083 | 306 | 312 | 7 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AB | 7 | ACE | - | ACETYLATION | UNP P0A7V0 |
| AB | 226 | NH2 | - | AMIDATION | UNP P0A7V0 |

- Molecule 2 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2 | AC | 207 | Total | C | N | O | S | 0 | 1 |
| | | | 1625 | 1028 | 306 | 288 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| AC | 207 | NH2 | - | AMIDATION | UNP P0A7V3 |

- Molecule 3 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3 | AD | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | |

- Molecule 4 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4 | AE | 152 | Total | C | N | O | S | 0 | 1 |
| | | | 1109 | 689 | 212 | 202 | 6 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AE | 8 | ACE | - | ACETYLATION | UNP P0A7W1 |
| AE | 159 | NH2 | - | AMIDATION | UNP P0A7W1 |

- Molecule 5 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5 | AF | 101 | Total | C | N | O | S | 0 | 1 |
| | | | 818 | 515 | 149 | 148 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| AF | 101 | NH2 | - | AMIDATION | UNP P02358 |

- Molecule 6 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6 | AG | 152 | Total | C | N | O | S | 0 | 1 |
| | | | 1178 | 732 | 227 | 215 | 4 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AG | 1 | ACE | - | ACETYLATION | UNP P02359 |
| AG | 152 | NH2 | - | AMIDATION | UNP P02359 |

- Molecule 7 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7 | AH | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | |

- Molecule 8 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | AI | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1025 | 636 | 206 | 180 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AI | 2 | ACE | - | ACETYLATION | UNP P0A7X3 |

- Molecule 9 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | AJ | 100 | Total | C | N | O | S | 0 | 1 |
| | | | 790 | 495 | 151 | 143 | 1 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AJ | 4 | ACE | - | ACETYLATION | UNP P0A7R5 |
| AJ | 103 | NH2 | - | AMIDATION | UNP P0A7R5 |

- Molecule 10 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | AK | 118 | Total | C | N | O | S | 0 | 0 |
| | | | 880 | 542 | 174 | 161 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AK | 11 | ACE | - | ACETYLATION | UNP P0A7R9 |

- Molecule 11 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | AL | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | |

- Molecule 12 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | AM | 114 | Total | C | N | O | S | 0 | 1 |
| | | | 877 | 541 | 178 | 155 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| AM | 114 | NH2 | - | AMIDATION | UNP P0A7S9 |

- Molecule 13 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | AN | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 499 | 164 | 139 | 3 | | |

- Molecule 14 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | AO | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | |

- Molecule 15 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | AP | 81 | Total | C | N | O | S | 0 | 1 |
| | | | 639 | 400 | 127 | 111 | 1 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| AP | 81 | NH2 | - | AMIDATION | UNP P0A7T3 |

- Molecule 16 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | AQ | 82 | Total | C | N | O | S | 0 | 1 |
| | | | 652 | 413 | 122 | 114 | 3 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AQ | 2 | ACE | - | ACETYLATION | UNP P0AG63 |
| AQ | 83 | NH2 | - | AMIDATION | UNP P0AG63 |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 17 | AR | 57 | Total | C | N | O | 0 | 1 |
| | | | 459 | 290 | 87 | 82 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AR | 18 | ACE | - | ACETYLATION | UNP P0A7T7 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| AR | 74 | NH2 | - | AMIDATION | UNP P0A7T7 |

- Molecule 18 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | AS | 81 | Total | C | N | O | S | 0 | 1 |
| | | | 641 | 410 | 121 | 108 | 2 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AS | 1 | ACE | - | ACETYLATION | UNP P0A7U3 |
| AS | 81 | NH2 | - | AMIDATION | UNP P0A7U3 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | AT | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 668 | 413 | 137 | 115 | 3 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AT | 1 | ACE | - | ACETYLATION | UNP P0A7U7 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20 | AU | 53 | Total | C | N | O | S | 0 | 1 |
| | | | 429 | 267 | 87 | 74 | 1 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| AU | 2 | ACE | - | ACETYLATION | UNP P68679 |
| AU | 54 | NH2 | - | AMIDATION | UNP P68679 |

- Molecule 21 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 21 | AA | 1530 | Total | C | N | O | P | 0 | 0 |
| | | | 32828 | 14642 | 6024 | 10633 | 1529 | | |

- Molecule 22 is a RNA chain called fMet-Val-tRNA-Val.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 22 | A1 | 76 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1627 | 728 | 292 | 531 | 75 | 1 | | |

- Molecule 23 is a RNA chain called 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 23 | A2 | 15 | Total | C | N | O | P | 0 | 0 |
| | | | 309 | 140 | 46 | 109 | 14 | | |

- Molecule 24 is a RNA chain called tRNA-fMet.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 24 | A3 | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1642 | 734 | 297 | 534 | 76 | 1 | | |

- Molecule 25 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25 | BC | 272 | Total | C | N | O | S | 0 | 1 |
| | | | 2083 | 1288 | 424 | 364 | 7 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| BC | 272 | NH2 | - | AMIDATION | UNP P60422 |

- Molecule 26 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26 | BD | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 27 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27 | BE | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 28 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28 | BF | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | |

- Molecule 29 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | BG | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 30 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | BH | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | |

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

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

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | BJ | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | BK | 123 | Total | C | N | O | S | 0 | 1 |
| | | | 939 | 587 | 181 | 165 | 6 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| BK | 123 | NH2 | - | AMIDATION | UNP P0ADY3 |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | BL | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | |

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | BM | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | BN | 121 | Total | C | N | O | S | 0 | 1 |
| | | | 961 | 593 | 197 | 166 | 5 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| BN | 121 | NH2 | - | AMIDATION | UNP P0AG44 |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 37 | BO | 116 | Total | C | N | O | | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | BP | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 39 | BQ | 117 | Total | C | N | O | | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | BR | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | BS | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | BT | 94 | Total | C | N | O | S | 0 | 1 |
| | | | 739 | 466 | 140 | 131 | 2 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| BT | 94 | NH2 | - | AMIDATION | UNP P0ADZ0 |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 43 | BU | 103 | Total | C | N | O | 0 | 1 |
| | | | 780 | 492 | 147 | 141 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| BU | 103 | NH2 | - | AMIDATION | UNP P60624 |

- Molecule 44 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | BV | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 45 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | BW | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 599 | 369 | 120 | 109 | 1 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| BW | 5 | ACE | - | ACETYLATION | UNP P0A7L8 |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | BX | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| BX | -1 | ACE | - | ACETYLATION | UNP P0A7M2 |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 47 | BY | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 48 | BZ | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49 | B0 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 50 | B1 | 52 | Total | C | N | O | 0 | 1 |
| | | | 413 | 265 | 76 | 72 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-------------|------------|
| B1 | 2 | ACE | - | ACETYLATION | UNP P0A7N9 |
| B1 | 53 | NH2 | - | AMIDATION | UNP P0A7N9 |

- Molecule 51 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51 | B2 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

- Molecule 52 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 52 | B3 | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 53 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 53 | B4 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 54 | BA | 2903 | Total | C | N | O | P | 0 | 0 |
| | | | 62317 | 27801 | 11467 | 20147 | 2902 | | |

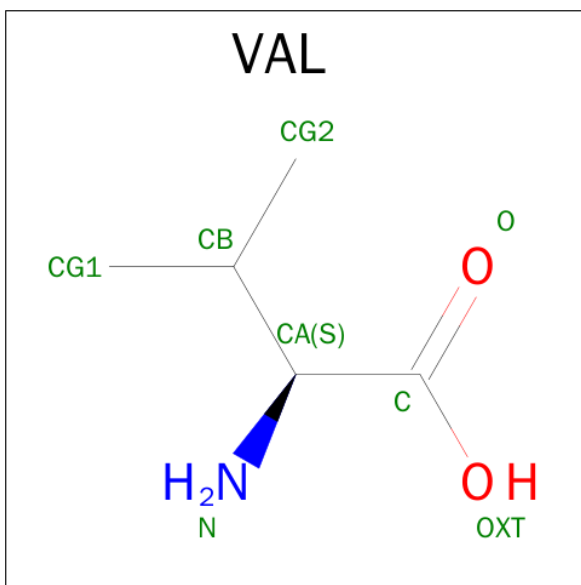
- Molecule 55 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 55 | BB | 117 | Total | C | N | O | P | 0 | 0 |
| | | | 2504 | 1116 | 459 | 813 | 116 | | |

- Molecule 56 is a protein called 50S ribosomal protein L1.

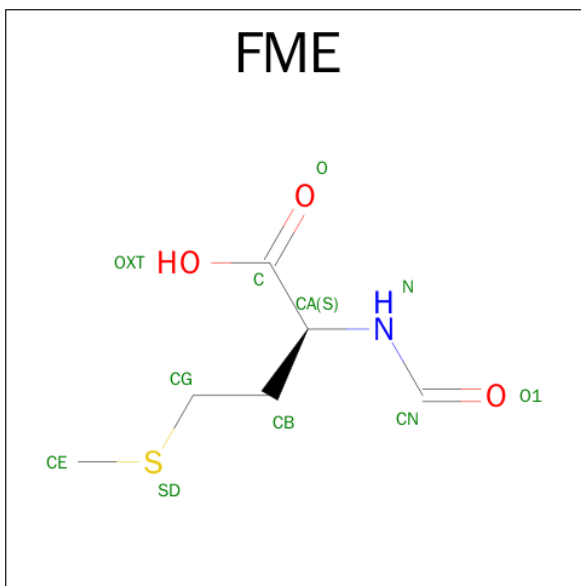
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56 | B5 | 223 | Total | C | N | O | S | 0 | 0 |
| | | | 1658 | 1038 | 302 | 312 | 6 | | |

- Molecule 57 is VALINE (three-letter code: VAL) (formula: C₅H₁₁NO₂).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 57 | A1 | 1 | Total | C | N | O | 0 |
| | | | 7 | 5 | 1 | 1 | |

- Molecule 58 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

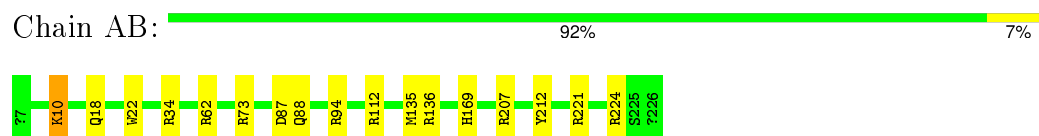


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 58 | A1 | 1 | Total | C | N | O | S | 0 |
| | | | 10 | 6 | 1 | 2 | 1 | |

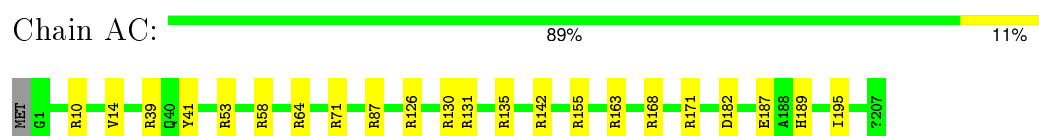
3 Residue-property plots [i](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

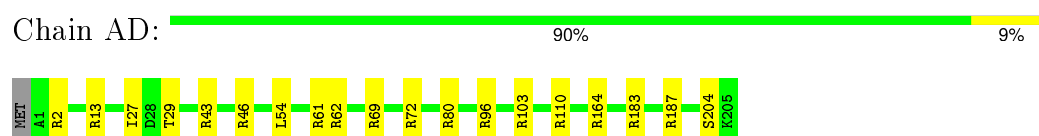
- Molecule 1: 30S ribosomal protein S2



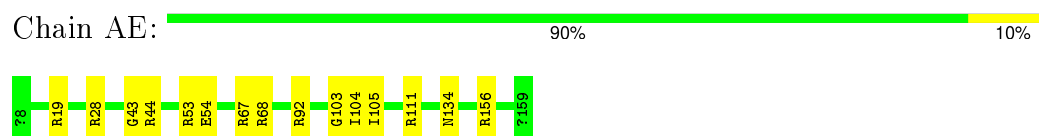
- Molecule 2: 30S ribosomal protein S3



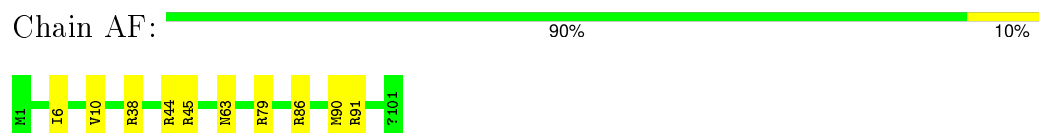
- Molecule 3: 30S ribosomal protein S4



- Molecule 4: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S6



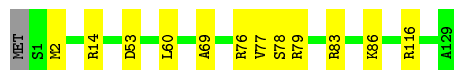
- Molecule 6: 30S ribosomal protein S7





- Molecule 7: 30S ribosomal protein S8

Chain AH: 90% 9%



- Molecule 8: 30S ribosomal protein S9

Chain AI: 86% 13%



- Molecule 9: 30S ribosomal protein S10

Chain AJ: 85% 12%



- Molecule 10: 30S ribosomal protein S11

Chain AK: 86% 13%



- Molecule 11: 30S ribosomal protein S12

Chain AL: 87% 12%



- Molecule 12: 30S ribosomal protein S13

Chain AM: 85% 14%



- Molecule 13: 30S ribosomal protein S14

Chain AN: 88% 11%




- Molecule 14: 30S ribosomal protein S15

Chain AO:  87% 12%



- Molecule 15: 30S ribosomal protein S16

Chain AP:  85% 15%



- Molecule 16: 30S ribosomal protein S17

Chain AQ:  88% 12%




- Molecule 17: 30S ribosomal protein S18

Chain AR:  88% 12%



- Molecule 18: 30S ribosomal protein S19

Chain AS:  89% 9%




- Molecule 19: 30S ribosomal protein S20

Chain AT:  91% 9%



- Molecule 20: 30S ribosomal protein S21

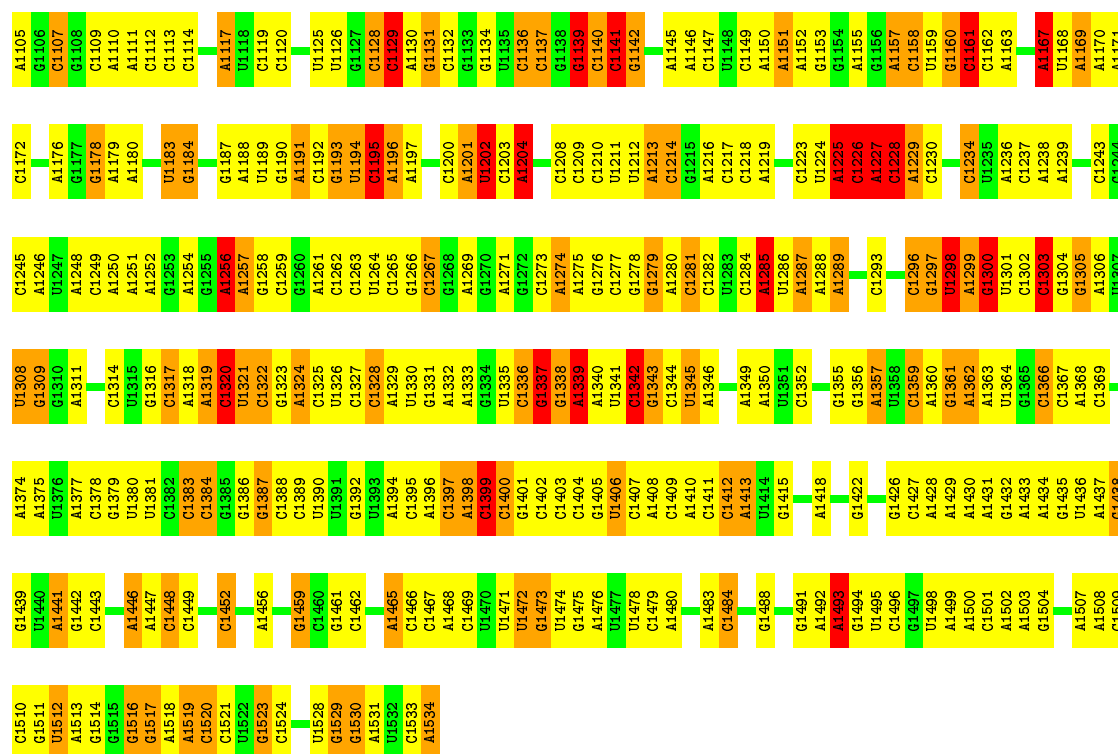
Chain AU:  77% 23%



- Molecule 21: 16S ribosomal RNA

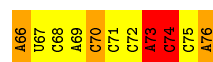
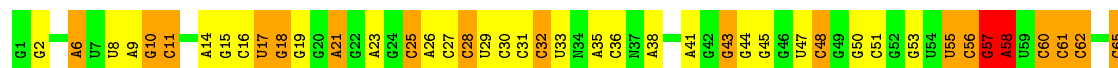
Chain AA:  25% 51% 20%

| | | | | | | | | | | | | | | | | |
|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| G1034 | A969 | U905 | U843 | G778 | G711 | U644 | A579 | C513 | A451 | U587 | A327 | G265 | G200 | C136 | G67 | A |
| A1035 | C970 | A906 | G844 | C779 | A712 | G845 | C580 | C514 | A452 | G388 | C328 | G266 | G201 | U137 | G68 | A |
| A1036 | G971 | A907 | A845 | A780 | G713 | G846 | G581 | | A453 | A389 | A329 | C267 | G202 | U138 | G69 | U |
| C1037 | C972 | A908 | G846 | A781 | G714 | G847 | C582 | G517 | A454 | U390 | C330 | U268 | G203 | A139 | U70 | U5 |
| C1038 | G973 | A909 | G847 | A782 | A715 | A648 | A583 | C518 | A455 | G391 | G331 | C269 | G204 | U140 | A71 | G6 |
| | G974 | C910 | C848 | A783 | A716 | A649 | A584 | C519 | A456 | C392 | G332 | A270 | G205 | | A72 | A7 |
| A1042 | A975 | U911 | | A784 | U717 | G850 | G585 | A520 | A457 | A393 | U333 | C271 | C206 | A143 | C73 | A8 |
| G1043 | G976 | C912 | G851 | G785 | A718 | C851 | C586 | G521 | U458 | G394 | C334 | C272 | C207 | | A74 | G9 |
| A1044 | A977 | A913 | G852 | A786 | C719 | U852 | G587 | C522 | A459 | C395 | C335 | U273 | U208 | G148 | G75 | A10 |
| C1045 | A978 | A914 | C853 | A787 | C720 | U853 | G588 | A523 | A460 | C396 | A336 | U274 | U209 | A149 | A76 | G11 |
| A1046 | C979 | A915 | | U788 | | G854 | U589 | G524 | A461 | C397 | G337 | | C210 | U150 | A77 | U12 |
| G1047 | G980 | U916 | C856 | U789 | U723 | A655 | | C525 | A462 | U398 | A338 | C277 | G211 | A151 | A78 | |
| G1048 | U981 | C917 | C857 | A790 | G724 | | G592 | C526 | U463 | G399 | C339 | G278 | G212 | A152 | G79 | A16 |
| U1049 | U982 | A918 | G858 | G791 | G725 | C858 | | G527 | U464 | C400 | U340 | A279 | G213 | C153 | A80 | U17 |
| G1050 | A983 | A919 | G859 | A792 | G726 | U859 | A595 | C528 | A465 | C401 | C341 | C280 | C214 | C154 | A81 | C18 |
| C1051 | C984 | | A860 | U793 | G727 | G660 | A596 | G529 | A466 | G402 | C342 | G281 | C215 | U154 | G82 | A19 |
| U1052 | C985 | A923 | G861 | A794 | A728 | U661 | G597 | C530 | U467 | C403 | C343 | A282 | C216 | C156 | U83 | U20 |
| G1053 | U986 | C924 | C862 | C795 | A729 | U662 | U598 | U531 | G404 | G404 | A344 | U283 | C217 | U157 | U84 | G21 |
| C1054 | G987 | G925 | U863 | C796 | | A663 | C599 | A532 | C469 | U405 | C345 | C284 | | G158 | U85 | G22 |
| A1055 | G988 | G926 | A864 | C797 | C732 | G664 | A600 | A533 | | U406 | G346 | C285 | G220 | G159 | G86 | C23 |
| U1056 | U989 | G927 | A865 | U798 | G733 | A665 | G601 | A534 | | G407 | G347 | C286 | C221 | A160 | C87 | C24 |
| G1057 | C990 | G928 | C866 | | G734 | G666 | A602 | A535 | U473 | A408 | A348 | C287 | C222 | A161 | C88 | C25 |
| U1058 | U991 | G929 | U867 | C735 | G735 | | U603 | C536 | C474 | U409 | A349 | A288 | C223 | A162 | A26 | A26 |
| C1059 | U992 | C930 | G868 | C736 | C736 | U672 | G604 | G537 | C475 | G410 | G350 | G289 | U224 | G163 | G94 | G27 |
| U1060 | G993 | C931 | C869 | C737 | C737 | A673 | | G538 | U476 | A411 | G351 | C290 | | G164 | C95 | U29 |
| G1061 | A994 | C932 | U870 | C738 | C738 | G674 | A607 | A539 | C477 | A412 | C352 | U291 | G226 | G165 | U96 | U30 |
| U1062 | C995 | G933 | U871 | C739 | | A675 | A608 | G540 | U478 | G413 | G353 | G292 | G227 | U166 | G97 | G31 |
| C1063 | A996 | C934 | A872 | U740 | U740 | A676 | A609 | A545 | U479 | A414 | G354 | G293 | A228 | A167 | G98 | A32 |
| G1064 | U997 | A935 | A873 | C908 | G741 | U677 | U610 | C546 | U480 | G415 | C355 | U294 | | G168 | C99 | A33 |
| | C998 | G936 | G874 | G809 | G742 | U678 | G611 | A546 | G481 | G416 | A356 | C295 | | C169 | G100 | |
| A1067 | U999 | A937 | U875 | C810 | A743 | C679 | G612 | A547 | A482 | G417 | G357 | U296 | G232 | U170 | A101 | C34 |
| G1068 | A1000 | A938 | C876 | C744 | C744 | C680 | G613 | G548 | G483 | C418 | U358 | G297 | C233 | A171 | | G35 |
| C1069 | C1001 | C940 | G877 | G745 | G745 | A681 | | C549 | G484 | G420 | G359 | A298 | C234 | A172 | C36 | C36 |
| U1070 | G1002 | C941 | A878 | U746 | A747 | G682 | G614 | | | U421 | G360 | G299 | C235 | U173 | U37 | U37 |
| C1071 | G1003 | C942 | G883 | G683 | G683 | G683 | | U552 | A487 | A422 | G361 | A300 | A236 | C174 | G38 | G38 |
| G1072 | A1004 | U943 | U886 | U686 | U748 | U686 | G618 | A553 | C488 | G423 | G362 | G301 | G237 | C175 | G107 | G39 |
| U1073 | A1005 | G944 | G881 | A815 | A749 | A887 | U619 | A554 | C489 | G424 | A363 | G302 | A238 | C176 | G108 | |
| | G1006 | G945 | C882 | C817 | C750 | A887 | G620 | U555 | C490 | G425 | A364 | A303 | U239 | G177 | A109 | |
| | | A946 | C883 | G818 | | G688 | A621 | C556 | G491 | U426 | U365 | U304 | G240 | C178 | C110 | C43 |
| | | G947 | U884 | A819 | G752 | C889 | A622 | G557 | C492 | G426 | A366 | G305 | G241 | A179 | G111 | C44 |
| A1080 | C1011 | U947 | G885 | C823 | A753 | G690 | C624 | G558 | A493 | G428 | U368 | A306 | A242 | U180 | G112 | |
| A1081 | A1012 | A949 | G886 | G824 | C754 | G691 | G625 | A559 | G494 | G429 | G369 | C307 | G243 | A181 | G113 | C47 |
| A1082 | G1013 | G950 | G887 | A825 | C755 | | U625 | A560 | A495 | U430 | C370 | C308 | U244 | A182 | U114 | C48 |
| U1083 | A1014 | G951 | G888 | G826 | C756 | A894 | G626 | U561 | A496 | A430 | C371 | A309 | U245 | C183 | U69 | |
| G1084 | G1015 | | A889 | C827 | U757 | A895 | G627 | U562 | G497 | A431 | A371 | G310 | A246 | G184 | A50 | A50 |
| U1085 | A1016 | G954 | G890 | U827 | C758 | A896 | G628 | A563 | A498 | A432 | C372 | G311 | G247 | U185 | A51 | |
| | | U955 | U891 | U828 | A759 | A897 | A629 | C564 | A499 | | A373 | C312 | C248 | C186 | A119 | C52 |
| A1092 | A1019 | U956 | A892 | G829 | G760 | G698 | A630 | U565 | C500 | C435 | A374 | A313 | U249 | G187 | A120 | A53 |
| A1093 | G1020 | U957 | C893 | G830 | | C699 | C631 | G566 | G501 | C436 | U375 | C314 | A250 | C188 | U121 | C54 |
| G1094 | A1021 | A958 | C894 | A831 | G763 | G700 | U632 | G567 | A502 | | G376 | A315 | G251 | A189 | G122 | A55 |
| U1095 | A1022 | A959 | G895 | G832 | C764 | U701 | G633 | G568 | C503 | C440 | G377 | C316 | U252 | A190 | U123 | |
| C1096 | | U960 | C896 | G833 | C765 | A702 | G634 | C569 | G504 | A441 | G378 | U317 | A253 | G191 | C124 | C58 |
| C1097 | U1025 | U961 | C897 | A766 | A766 | G703 | A635 | G505 | G505 | A442 | C379 | | G254 | A192 | U125 | A59 |
| C1098 | G1026 | C962 | G898 | A767 | A767 | A704 | U636 | G506 | C443 | C443 | G390 | | G255 | C193 | U126 | A60 |
| G1099 | C1027 | G963 | C899 | U837 | G768 | G705 | C637 | A572 | C507 | G446 | C381 | A321 | U256 | C194 | A129 | G61 |
| C1100 | C1028 | A964 | A900 | G838 | G769 | A706 | | A574 | U508 | G447 | A382 | C322 | G257 | A195 | U62 | U62 |
| A1101 | | U965 | A901 | C839 | C770 | U707 | A640 | G575 | A509 | G447 | A383 | U323 | | A196 | A130 | C63 |
| A1102 | C1031 | G966 | G902 | C840 | G771 | U708 | U641 | G576 | A510 | G448 | G384 | G324 | A262 | A197 | A131 | C64 |
| C1103 | G1032 | C967 | G903 | C841 | | U709 | A642 | G577 | C511 | G449 | C385 | A325 | G264 | G198 | A65 | |
| G1104 | G1033 | A968 | U904 | U842 | A777 | G710 | C643 | C578 | U512 | G450 | C386 | G326 | | A199 | C135 | A66 |



• Molecule 22: fMet-Val-tRNA-Val

Chain A1: 29% 39% 26% 5%



• Molecule 23: 5'-R(*AP*CP*UP*AP*UP*GP*GP*UP*UP*UP*UP*UP*AP*UP*U)-3'

Chain A2: 33% 33% 13% 20%

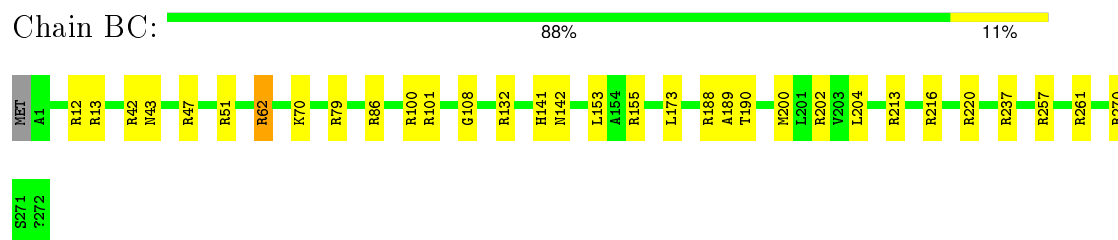


• Molecule 24: tRNA-fMet

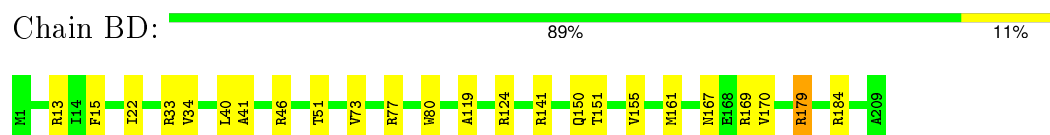
Chain A3: 23% 55% 21%



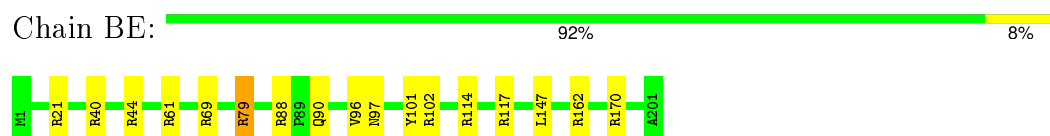
• Molecule 25: 50S ribosomal protein L2



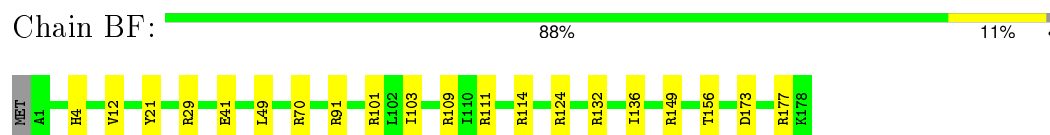
- Molecule 26: 50S ribosomal protein L3



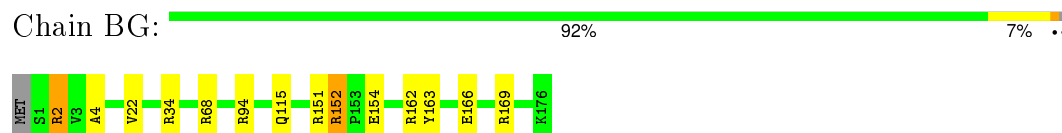
- Molecule 27: 50S ribosomal protein L4



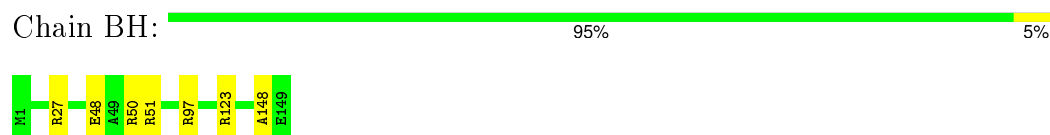
- Molecule 28: 50S ribosomal protein L5



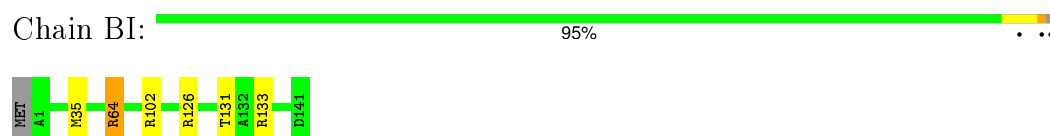
- Molecule 29: 50S ribosomal protein L6




- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L11



- Molecule 32: 50S ribosomal protein L13

Chain BJ:  89% 11%



- Molecule 33: 50S ribosomal protein L14

Chain BK:  90% 9%



- Molecule 34: 50S ribosomal protein L15

Chain BL:  90% 9%




- Molecule 35: 50S ribosomal protein L16

Chain BM:  85% 15%



- Molecule 36: 50S ribosomal protein L17

Chain BN:  83% 17%




- Molecule 37: 50S ribosomal protein L18

Chain BO:  89% 9%




- Molecule 38: 50S ribosomal protein L19

Chain BP:  82% 17%



- Molecule 39: 50S ribosomal protein L20

Chain BQ:  85% 13%



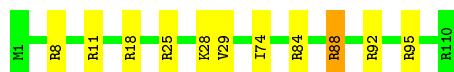
- Molecule 40: 50S ribosomal protein L21

Chain BR: 90% 10%



- Molecule 41: 50S ribosomal protein L22

Chain BS: 90% 9% .



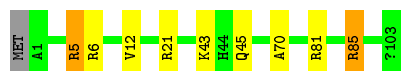
- Molecule 42: 50S ribosomal protein L23

Chain BT: 86% 14%



- Molecule 43: 50S ribosomal protein L24

Chain BU: 90% 7% ..



- Molecule 44: 50S ribosomal protein L25

Chain BV: 89% 11%



- Molecule 45: 50S ribosomal protein L27

Chain BW: 84% 14% .



- Molecule 46: 50S ribosomal protein L28

Chain BX: 84% 13% ..



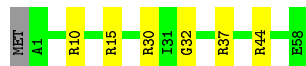
- Molecule 47: 50S ribosomal protein L29

Chain BY:  90% 6%




- Molecule 48: 50S ribosomal protein L30

Chain BZ:  88% 10%



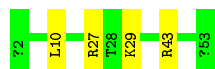
- Molecule 49: 50S ribosomal protein L32

Chain B0:  84% 14%




- Molecule 50: 50S ribosomal protein L33

Chain B1:  92% 8%



- Molecule 51: 50S ribosomal protein L34

Chain B2:  76% 22%




- Molecule 52: 50S ribosomal protein L35

Chain B3:  91% 8%



- Molecule 53: 50S ribosomal protein L36

Chain B4:  82% 18%

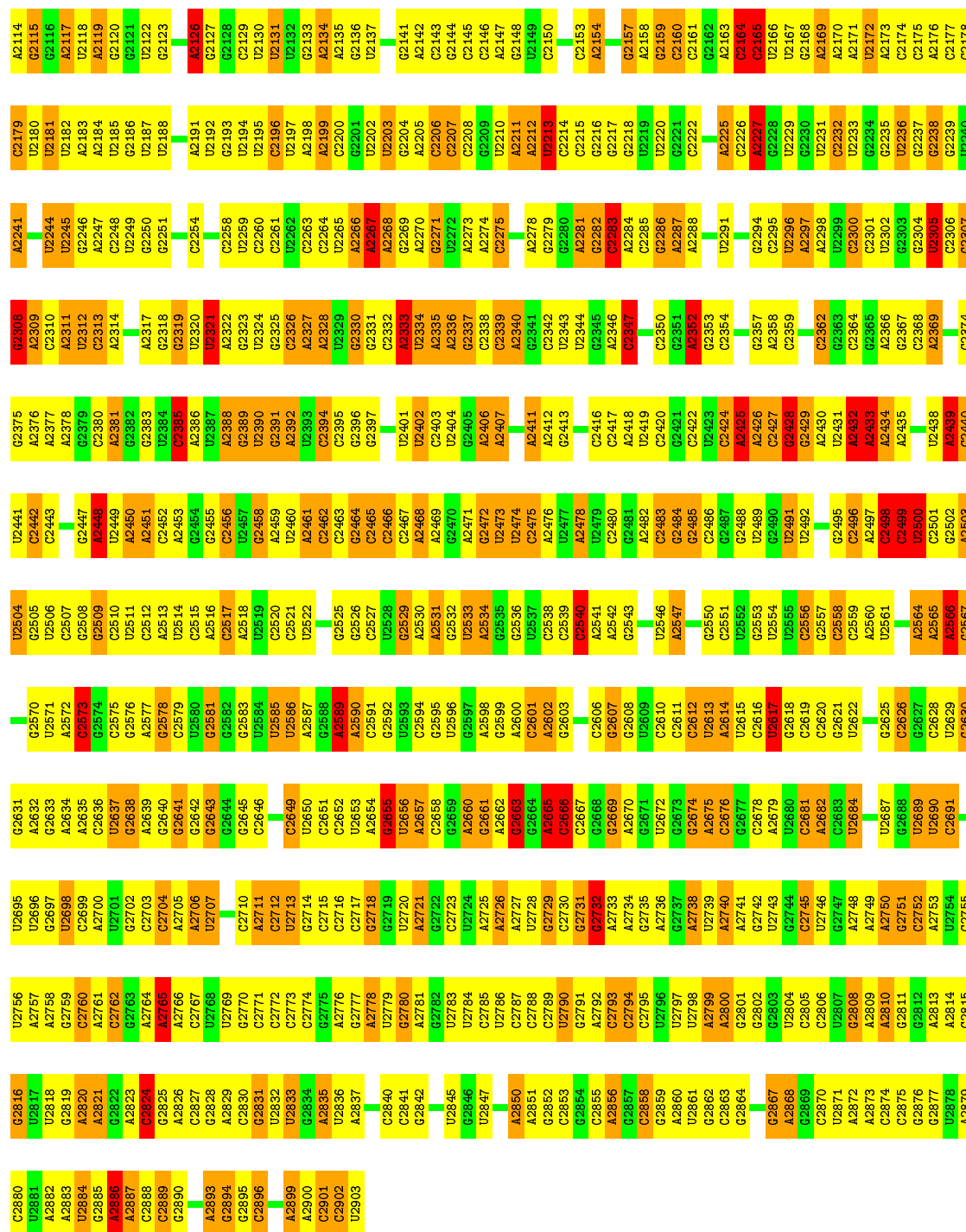


- Molecule 54: 23S ribosomal RNA

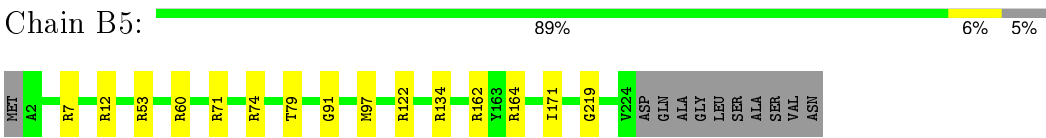
Chain BA:  23% 50% 23%

| | | | | | | | | | | | | | | | | |
|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| U1035 | A973 | A911 | U846 | A783 | C717 | G648 | A586 | G518 | G452 | G388 | C323 | A256 | G194 | A131 | G68 | G1 |
| G1036 | G974 | C912 | U847 | G784 | A718 | G649 | C587 | A522 | A453 | G389 | A324 | C257 | A195 | G132 | C69 | G2 |
| A1039 | A975 | U913 | C848 | G785 | C719 | G851 | U589 | A523 | A454 | U390 | G325 | G258 | A196 | U133 | C70 | A5 |
| A1040 | G976 | C915 | A849 | G786 | U720 | U652 | C523 | C523 | C455 | U391 | G134 | A71 | A197 | G134 | A71 | A6 |
| G1041 | A979 | G916 | C850 | C787 | A721 | U653 | U591 | U524 | A456 | U392 | A262 | G263 | C198 | U135 | A72 | A7 |
| G1042 | A880 | A917 | U852 | A788 | A722 | A854 | A592 | A526 | G458 | C393 | G329 | G264 | A199 | U138 | A73 | A8 |
| C1043 | C981 | A918 | C853 | A789 | C723 | A855 | A593 | C527 | U459 | C394 | A330 | C265 | U200 | U139 | A74 | A9 |
| C1044 | C982 | U919 | C854 | C790 | U724 | | C595 | A328 | A460 | U395 | C331 | A266 | C201 | U140 | C75 | A10 |
| C1045 | A983 | A920 | | A792 | G726 | | U596 | A529 | A461 | C398 | A332 | G267 | U202 | U141 | C76 | A11 |
| A1046 | A984 | C921 | | A793 | G727 | | G597 | G330 | C462 | U399 | G333 | C268 | A203 | G141 | C77 | A12 |
| G1047 | C985 | C922 | | A794 | G728 | | U598 | C531 | C463 | G400 | C334 | C269 | A204 | A142 | U78 | A13 |
| A1048 | C986 | | | C795 | G729 | | A599 | A532 | U464 | A401 | C335 | A270 | U205 | C143 | C79 | A14 |
| C1049 | C987 | A925 | | C796 | A730 | | G600 | G533 | G465 | A402 | C336 | G271 | C206 | A144 | | A15 |
| A1050 | A988 | G926 | | | C731 | | C601 | | A466 | U403 | C337 | A272 | A207 | C145 | U82 | A16 |
| G1051 | G989 | A927 | | G799 | C732 | | A602 | G537 | A470 | A404 | A340 | A273 | C208 | A146 | A83 | A17 |
| C1052 | A990 | A928 | | A800 | C733 | | G603 | A538 | A471 | U405 | C341 | G274 | C209 | C147 | A84 | A18 |
| C1053 | C991 | G929 | | G801 | A734 | | G604 | G539 | A472 | G406 | A342 | C275 | C211 | U148 | U87 | A19 |
| A1054 | C992 | A802 | | A802 | G735 | | G605 | C540 | A473 | G407 | C343 | U276 | G212 | U150 | G88 | A20 |
| G1055 | G993 | U803 | | U803 | C736 | | U606 | C541 | A474 | G410 | A344 | A277 | A213 | C151 | A89 | A21 |
| C994 | C994 | A804 | | A804 | G737 | | C671 | C542 | G474 | A411 | A345 | A278 | A216 | A152 | U90 | A22 |
| C995 | C995 | G805 | | G805 | C738 | | A608 | G543 | C475 | G412 | A346 | A279 | A217 | U153 | A91 | A23 |
| A996 | A996 | U934 | | C673 | A739 | | A609 | C544 | A476 | A413 | A347 | U280 | A218 | U154 | U92 | A24 |
| | | C935 | | G674 | C740 | | C610 | U545 | A477 | C413 | A348 | C281 | A219 | A155 | G93 | A25 |
| C997 | C997 | A836 | | A675 | U741 | | C611 | U546 | A478 | C414 | U349 | A282 | A220 | A156 | A94 | A26 |
| U1061 | C998 | C937 | | A676 | A742 | | G612 | A547 | A479 | A415 | G350 | G283 | G221 | C157 | A95 | A27 |
| G1062 | U871 | U872 | | A677 | A743 | | A613 | G548 | A480 | U416 | A351 | U284 | A221 | U158 | C96 | A28 |
| G1063 | C873 | C874 | | A678 | U744 | | A614 | G549 | C481 | G417 | A352 | | A222 | U159 | C97 | A29 |
| C1064 | G875 | G876 | | C679 | A745 | | U615 | C550 | A482 | C418 | C353 | U288 | A223 | A160 | G98 | A30 |
| U1065 | A941 | C942 | | A680 | U746 | | U616 | G551 | A483 | U419 | A354 | U290 | G225 | A161 | U99 | A31 |
| A1066 | C942 | G943 | | G674 | U747 | | C624 | G559 | C490 | C420 | A355 | G291 | A226 | U162 | U100 | A32 |
| A1067 | C943 | A943 | | A685 | G748 | | G625 | U554 | C491 | C421 | C357 | | A227 | C163 | C37 | A33 |
| G1068 | C944 | C944 | | U886 | A749 | | A626 | G555 | A492 | A422 | U358 | U294 | A228 | C164 | U102 | A34 |
| A1069 | C945 | A945 | | C887 | A750 | | A627 | A556 | A493 | A423 | C359 | A294 | C229 | U166 | A103 | A35 |
| U1070 | C946 | A946 | | U888 | A751 | | G622 | C557 | C488 | G424 | U360 | G295 | C230 | A167 | A104 | A36 |
| C1071 | A947 | C948 | | A689 | A752 | | C623 | U558 | G489 | C426 | C361 | | G231 | A168 | A105 | A37 |
| A1072 | C948 | A948 | | C821 | A753 | | G624 | G559 | C490 | U427 | A362 | A299 | A231 | U170 | G106 | A38 |
| G1073 | A1009 | G950 | | G822 | U754 | | G625 | C560 | C491 | A428 | C363 | A300 | G232 | U171 | G107 | A39 |
| C1075 | C951 | C951 | | C823 | U755 | | A626 | A563 | A492 | A429 | C364 | G301 | A233 | U172 | G108 | A40 |
| A1076 | G952 | G952 | | U824 | A756 | | A627 | A563 | A493 | A430 | U365 | C302 | U234 | A172 | G109 | A41 |
| C1077 | C953 | G953 | | A825 | G757 | | G628 | C564 | A497 | U431 | C366 | G303 | U235 | A173 | G110 | A42 |
| U1078 | G954 | C954 | | G696 | C758 | | G629 | C565 | | A432 | G367 | U304 | C236 | | G47 | A43 |
| C1079 | U955 | U955 | | G697 | C759 | | G630 | U566 | G500 | C433 | A368 | C305 | C237 | A176 | G48 | A44 |
| A1080 | C956 | C956 | | C698 | G760 | | A631 | U567 | A501 | U434 | U369 | U306 | C238 | A177 | A49 | A45 |
| U1081 | C957 | C957 | | A699 | A761 | | A632 | U568 | A502 | C435 | G370 | U307 | C239 | G177 | U113 | A46 |
| | U958 | U958 | | G830 | U762 | | A633 | A503 | A503 | C436 | A371 | G308 | C240 | G178 | U114 | A47 |
| A1084 | A1020 | A1021 | | U702 | A763 | | C634 | A572 | A504 | A439 | G372 | A309 | A241 | C179 | C115 | A52 |
| A1085 | G1022 | A1086 | | U703 | A764 | | C635 | U573 | U505 | U440 | U373 | A310 | G180 | G181 | C116 | A53 |
| G1087 | U1023 | A833 | | G704 | C765 | | A636 | A574 | G506 | U441 | A374 | A311 | A181 | G117 | G117 | A54 |
| A1088 | G1024 | G962 | | A705 | U766 | | A637 | A575 | A507 | G442 | G312 | G313 | A244 | A182 | G55 | A55 |
| A1089 | G1025 | U963 | | A706 | | | G638 | U576 | A508 | G443 | C378 | G314 | G246 | C183 | A119 | A56 |
| A1090 | G1026 | C964 | | G707 | | | U639 | G577 | C509 | A444 | G379 | C314 | G247 | G185 | U120 | C57 |
| C1092 | A1027 | C965 | | C772 | | | C640 | G578 | C510 | C445 | G380 | G315 | G248 | G186 | G121 | |
| | A1028 | G966 | | U773 | | | U641 | G579 | U511 | C446 | G381 | G316 | C249 | G187 | G124 | C61 |
| | A1029 | U967 | | U774 | | | U642 | U580 | G512 | G446 | A382 | G317 | G250 | G188 | A62 | A63 |
| | C1030 | C968 | | G712 | | | A643 | U581 | G513 | A447 | C383 | C318 | A251 | G189 | A126 | A64 |
| A1095 | G1031 | G969 | | G713 | | | A644 | C581 | A514 | U448 | C384 | G319 | G252 | A190 | A127 | A65 |
| A1096 | U1032 | U970 | | G714 | | | A645 | G583 | A515 | G449 | A385 | A320 | C253 | G189 | C128 | A66 |
| A1098 | U1033 | G971 | | A715 | | | U646 | C584 | A516 | G450 | G386 | U321 | G254 | A191 | C129 | A67 |
| G1099 | G1034 | A972 | | A716 | | | G647 | G585 | C517 | U451 | U387 | A322 | A255 | U193 | C130 | |

| | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A2054 | C1994 | A1932 | G1869 | A1802 | G1738 | U1671 | A1610 | A1549 | U1487 | A1419 | G1355 | C1293 | A1226 | G1162 | C1100 |
| C2055 | U1995 | G1933 | C1870 | A1803 | A1739 | A1672 | C1611 | C1550 | U1488 | A1420 | G1356 | U1294 | A1227 | G1163 | U1101 |
| G2056 | C1996 | A1934 | A1871 | C1804 | G1740 | G1673 | C1612 | A1551 | C1488 | G1423 | G1357 | C1295 | G1228 | C1164 | C1102 |
| G2057 | C1997 | G1935 | A1872 | A1805 | C1741 | G1674 | G1613 | A1552 | C1489 | G1424 | G1358 | G1296 | A1230 | A1165 | A1103 |
| A2058 | A1998 | G1873 | C1806 | G1807 | U1742 | C1675 | A1614 | A1553 | A1490 | G1425 | G1359 | C1297 | G1233 | G1166 | C1104 |
| A2059 | C1999 | G1874 | G1807 | G1807 | G1743 | A1676 | C1615 | U1554 | G1491 | G1426 | G1360 | C1298 | G1234 | G1167 | U1105 |
| A2060 | C2000 | G1875 | A1808 | A1808 | A1744 | A1677 | A1616 | G1555 | G1492 | A1427 | G1361 | G1299 | G1235 | G1168 | G1106 |
| G2061 | C2001 | A1876 | A1809 | A1809 | A1745 | A1678 | C1617 | C1556 | C1493 | A1428 | C1362 | G1300 | U1234 | A1169 | U1107 |
| A2062 | G2002 | A1877 | A1810 | A1810 | A1746 | A1679 | A1618 | C1557 | A1494 | G1429 | G1363 | A1301 | G1236 | C1170 | G1108 |
| C2063 | A2003 | G1878 | G1811 | G1811 | U1747 | U1680 | G1619 | U1558 | A1496 | G1430 | G1364 | A1302 | A1237 | G1171 | C1109 |
| C2064 | G2004 | U1812 | U1812 | U1812 | C1748 | G1681 | G1620 | U1559 | A1497 | G1432 | A1365 | G1303 | A1238 | C1172 | G1110 |
| C2065 | A2005 | G1813 | U1880 | G1813 | A1749 | G1682 | U1621 | G1560 | U1498 | G1433 | A1366 | A1304 | G1239 | U1173 | A1111 |
| C2066 | C2006 | G1814 | G1881 | G1814 | A1749 | G1683 | G1622 | C1499 | C1498 | A1434 | A1367 | C1305 | U1240 | U1174 | G1112 |
| G2067 | U2007 | A1815 | U1882 | A1815 | C1752 | G1684 | G1623 | U1562 | C1499 | A1434 | G1368 | C1306 | A1241 | A1175 | U1113 |
| U2068 | C2008 | C1816 | U1883 | C1816 | G1753 | C1685 | U1624 | U1563 | G1500 | G1437 | G1369 | A1307 | U1242 | U1176 | C1114 |
| G2069 | A2009 | G1817 | A1884 | G1817 | A1754 | C1686 | C1625 | C1564 | G1501 | C1370 | C1370 | A1308 | U1243 | G1177 | G1115 |
| A2070 | G2010 | U1818 | A1885 | U1818 | A1755 | G1687 | A1626 | C1565 | A1502 | U1438 | G1371 | C1309 | C1243 | C1178 | G1116 |
| A2071 | U2011 | A1819 | U1886 | A1819 | G1756 | A1688 | G1627 | A1566 | A1503 | U1439 | U1372 | G1310 | A1244 | G1179 | C1117 |
| C2072 | G2012 | U1820 | C1887 | U1820 | A1757 | A1689 | U1628 | G1567 | A1504 | U1440 | A1373 | G1311 | G1245 | U1180 | C1118 |
| C2073 | A2013 | A1821 | G1888 | A1821 | U1758 | A1690 | U1629 | G1568 | A1505 | G1441 | G1374 | U1312 | A1246 | U1119 | U1119 |
| U2074 | C2014 | C1822 | G1889 | C1822 | A1759 | C1691 | A1630 | U1569 | U1506 | U1442 | U1375 | C1313 | A1247 | U1183 | G1120 |
| U2075 | A2015 | G1823 | A1890 | G1823 | C1760 | G1692 | A1631 | A1570 | C1507 | U1443 | C1376 | C1314 | U1248 | U1184 | C1121 |
| U2076 | U2016 | G1824 | C1891 | G1824 | C1761 | G1693 | G1633 | A1571 | A1508 | U1444 | G1377 | C1315 | G1252 | G1185 | G1122 |
| A2077 | U2017 | U1825 | C1892 | U1825 | A1762 | G1695 | A1634 | A1572 | A1509 | G1445 | A1378 | U1316 | A1253 | G1186 | C1123 |
| C2078 | G2018 | G1826 | C1893 | G1826 | G1763 | G1696 | U1635 | G1573 | C1512 | C1446 | U1379 | U1317 | A1254 | G1124 | G1125 |
| U2079 | A2019 | U1827 | C1894 | U1827 | C1764 | A1698 | U1636 | C1574 | C1513 | C1447 | G1380 | U1318 | A1255 | A1189 | C1124 |
| A2080 | A2020 | G1828 | C1895 | G1828 | U1765 | G1699 | A1637 | C1575 | U1513 | G1448 | G1381 | C1319 | U1256 | G1190 | A1126 |
| U2081 | C2021 | G1829 | G1896 | A1829 | G1766 | A1700 | C1638 | A1576 | G1514 | G1449 | G1382 | G1320 | G1257 | A1127 | U1127 |
| A2082 | U2022 | G1830 | C1897 | G1830 | G1767 | A1701 | C1639 | C1577 | A1515 | G1450 | A1383 | A1321 | C1257 | G1128 | G1128 |
| G2083 | C2023 | U1831 | U1898 | G1831 | C1768 | G1702 | A1640 | C1578 | A1515 | G1451 | A1384 | A1322 | A1257 | A1194 | A1129 |
| C2084 | G2024 | G1832 | C1899 | G1832 | U1769 | C1704 | A1641 | A1579 | U1518 | G1452 | A1385 | C1323 | A1260 | G1195 | G1137 |
| U2085 | C2025 | A1833 | A1900 | G1833 | G1770 | A1705 | G1642 | A1580 | U1519 | A1483 | C1386 | G1324 | C1261 | C1196 | U1132 |
| U2086 | U2026 | U1834 | A1901 | U1834 | C1771 | C1706 | G1643 | G1581 | U1520 | C1484 | A1387 | U1325 | A1262 | A1197 | A1133 |
| G2087 | G2027 | G1835 | C1902 | G1835 | A1772 | G1707 | C1644 | C1582 | G1521 | G1455 | G1388 | U1326 | U1263 | U1198 | A1134 |
| C2088 | U2028 | U1836 | G1903 | G1836 | A1773 | C1708 | G1645 | A1583 | A1522 | G1456 | G1389 | A1327 | A1264 | U1199 | C1135 |
| C2089 | G2029 | C1837 | U1905 | C1837 | C1774 | U1709 | C1646 | U1584 | U1523 | G1459 | U1391 | A1328 | A1265 | C1200 | G1136 |
| C2091 | A2030 | C1838 | G1906 | C1838 | U1775 | G1710 | U1647 | C1585 | G1524 | U1460 | A1392 | G1331 | G1266 | U1201 | G1137 |
| U2092 | C2031 | G1842 | C1907 | G1842 | U1776 | A1711 | U1648 | A1586 | U1525 | U1461 | A1393 | G1332 | U1267 | G1202 | G1138 |
| G2093 | A2032 | C1843 | U1908 | C1843 | U1777 | G1712 | G1649 | G1587 | C1526 | C1462 | U1394 | G1332 | A1268 | U1203 | G1139 |
| A2094 | G2033 | G1844 | C1909 | G1844 | U1713 | U1714 | A1650 | C1527 | G1527 | C1463 | A1395 | A1204 | A1269 | A1204 | C1140 |
| A2095 | U2034 | C1845 | A1912 | G1845 | A1717 | A1717 | A1651 | A1590 | G1528 | C1463 | A1396 | A1205 | C1270 | A1205 | U1141 |
| A2096 | G2035 | G1846 | A1913 | G1846 | U1718 | A1718 | A1652 | A1591 | G1529 | G1464 | U1396 | A1336 | G1271 | G1206 | A1142 |
| A2097 | C2036 | A1847 | C1914 | A1847 | A1785 | A1785 | A1653 | C1592 | G1530 | G1465 | U1397 | G1337 | A1272 | C1207 | A1143 |
| A2098 | U2037 | U1848 | U1915 | A1848 | A1786 | U1720 | A1654 | A1593 | C1531 | U1466 | C1398 | G1338 | U1273 | C1208 | A1144 |
| U2099 | G2038 | A1849 | U1916 | A1849 | A1787 | G1721 | A1655 | U1594 | A1532 | U1467 | C1399 | G1339 | A1274 | U1209 | C1145 |
| G2100 | U2039 | A1853 | A1917 | A1853 | C1788 | G1722 | C1656 | C1595 | G1533 | U1468 | U1468 | U1340 | A1275 | G1210 | C1146 |
| A2101 | C2040 | G1854 | U1917 | G1854 | A1789 | A1722 | U1657 | A1596 | U1534 | A1469 | A1403 | G1341 | A1276 | C1211 | A1147 |
| G2102 | U2041 | A1854 | A1918 | A1854 | G1723 | C1723 | C1658 | A1597 | A1535 | A1470 | C1404 | A1342 | A1277 | G1212 | U1148 |
| C2103 | A2042 | G1857 | C1920 | G1857 | G1790 | G1724 | G1659 | A1598 | C1536 | G1471 | G1343 | A1343 | C1278 | A1213 | G1149 |
| C2104 | C2043 | U1857 | U1920 | U1857 | A1791 | A1725 | G1660 | U1599 | G1537 | C1472 | U1344 | U1344 | A1214 | C1150 | C1150 |
| U2105 | G2044 | A1858 | G1792 | A1858 | G1792 | C1727 | G1661 | C1600 | U1538 | G1473 | U1409 | C1345 | G1283 | G1215 | A1151 |
| G2106 | C2045 | C1861 | C1793 | G1861 | C1728 | C1728 | U1662 | G1601 | G1539 | U1474 | U1410 | C1346 | A1284 | G1216 | C1152 |
| G2107 | U2046 | G1862 | A1794 | G1862 | U1729 | U1729 | G1663 | U1602 | G1540 | U1475 | U1411 | A1347 | U1217 | C1153 | C1153 |
| G2108 | C2047 | C1863 | C1795 | G1863 | C1730 | A1603 | A1664 | A1603 | C1541 | U1476 | U1412 | C1348 | A1286 | G1154 | G1154 |
| U2109 | G2048 | G1864 | U1796 | G1864 | G1731 | A1604 | A1665 | A1604 | C1541 | A1477 | A1413 | C1349 | A1287 | A1155 | A1155 |
| G2110 | G2049 | U1865 | G1797 | U1865 | C1732 | C1732 | G1666 | C1605 | A1544 | G1478 | C1414 | G1350 | G1288 | C1221 | A1156 |
| U2111 | C2050 | A1866 | U1798 | A1866 | G1667 | G1667 | G1667 | C1606 | A1545 | U1479 | U1415 | C1351 | C1289 | U1222 | G1157 |
| G2112 | A2051 | G1867 | G1799 | A1867 | U1735 | U1735 | A1668 | C1607 | G1546 | C1480 | G1416 | U1352 | C1290 | G1223 | C1158 |
| U2113 | G2052 | C1868 | U1931 | C1868 | U1736 | U1736 | A1669 | U1608 | C1547 | U1481 | C1417 | U1353 | C1291 | U1224 | G1159 |
| | G2053 | A1868 | G1737 | A1868 | G1737 | G1737 | C1670 | A1609 | A1548 | G1492 | G1418 | A1354 | G1292 | G1225 | C1161 |



- Molecule 56: 50S ribosomal protein L1



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-----------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | 1904 | Depositor |
| Resolution determination method | FSC at 0.5 cut-off | Depositor |
| CTF correction method | local | Depositor |
| Microscope | FEI/PHILIPS CM200FEG | Depositor |
| Voltage (kV) | 160 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 20 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | 161000 | Depositor |
| Image detector | 4k CCD camera (TVIPS) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, FME, ACE, H2U, CM0, 6MZ, NH2, 4SU, 7MG, PSU

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 | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | AB | 0.71 | 0/1736 | 1.09 | 15/2340 (0.6%) |
| 10 | AK | 0.75 | 0/894 | 1.23 | 11/1207 (0.9%) |
| 11 | AL | 0.75 | 0/969 | 1.25 | 14/1300 (1.1%) |
| 12 | AM | 0.73 | 0/884 | 1.22 | 11/1181 (0.9%) |
| 13 | AN | 0.78 | 0/817 | 1.22 | 9/1088 (0.8%) |
| 14 | AO | 0.71 | 0/722 | 1.15 | 8/964 (0.8%) |
| 15 | AP | 0.74 | 0/648 | 1.35 | 12/870 (1.4%) |
| 16 | AQ | 0.70 | 0/658 | 1.19 | 8/883 (0.9%) |
| 17 | AR | 0.80 | 0/463 | 1.21 | 6/623 (1.0%) |
| 18 | AS | 0.76 | 0/653 | 1.15 | 9/879 (1.0%) |
| 19 | AT | 0.68 | 0/672 | 1.11 | 4/890 (0.4%) |
| 2 | AC | 0.72 | 0/1651 | 1.15 | 16/2225 (0.7%) |
| 20 | AU | 0.83 | 0/431 | 1.66 | 13/572 (2.3%) |
| 21 | AA | 1.53 | 1/36759 (0.0%) | 2.22 | 1937/57346 (3.4%) |
| 22 | A1 | 1.54 | 0/1668 | 2.21 | 86/2595 (3.3%) |
| 23 | A2 | 1.54 | 0/343 | 2.22 | 16/531 (3.0%) |
| 24 | A3 | 1.54 | 0/1722 | 2.22 | 99/2685 (3.7%) |
| 25 | BC | 0.73 | 0/2121 | 1.23 | 23/2852 (0.8%) |
| 26 | BD | 0.68 | 0/1586 | 1.12 | 8/2134 (0.4%) |
| 27 | BE | 0.67 | 0/1571 | 1.16 | 12/2113 (0.6%) |
| 28 | BF | 0.74 | 0/1444 | 1.17 | 11/1937 (0.6%) |
| 29 | BG | 0.69 | 0/1343 | 1.14 | 9/1816 (0.5%) |
| 3 | AD | 0.76 | 0/1665 | 1.19 | 16/2227 (0.7%) |
| 30 | BH | 0.66 | 0/1122 | 1.11 | 5/1515 (0.3%) |
| 31 | BI | 0.65 | 0/1046 | 1.07 | 4/1410 (0.3%) |
| 32 | BJ | 0.73 | 0/1152 | 1.25 | 12/1551 (0.8%) |
| 33 | BK | 0.70 | 0/947 | 1.21 | 9/1268 (0.7%) |
| 34 | BL | 0.72 | 0/1054 | 1.22 | 10/1403 (0.7%) |
| 35 | BM | 0.75 | 0/1093 | 1.27 | 11/1460 (0.8%) |
| 36 | BN | 0.75 | 0/973 | 1.38 | 18/1301 (1.4%) |
| 37 | BO | 0.72 | 0/902 | 1.26 | 13/1209 (1.1%) |
| 38 | BP | 0.74 | 0/929 | 1.34 | 15/1242 (1.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|--------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 39 | BQ | 0.78 | 0/960 | 1.30 | 14/1278 (1.1%) |
| 4 | AE | 0.71 | 0/1119 | 1.11 | 10/1506 (0.7%) |
| 40 | BR | 0.70 | 0/829 | 1.19 | 6/1107 (0.5%) |
| 41 | BS | 0.66 | 0/864 | 1.22 | 10/1156 (0.9%) |
| 42 | BT | 0.64 | 0/744 | 1.18 | 6/994 (0.6%) |
| 43 | BU | 0.68 | 0/787 | 1.07 | 5/1051 (0.5%) |
| 44 | BV | 0.70 | 0/766 | 1.13 | 5/1025 (0.5%) |
| 45 | BW | 0.75 | 0/604 | 1.32 | 8/799 (1.0%) |
| 46 | BX | 0.73 | 0/635 | 1.34 | 10/848 (1.2%) |
| 47 | BY | 0.69 | 0/510 | 1.23 | 4/677 (0.6%) |
| 48 | BZ | 0.68 | 0/453 | 1.23 | 7/605 (1.2%) |
| 49 | B0 | 0.74 | 0/450 | 1.28 | 5/599 (0.8%) |
| 5 | AF | 0.73 | 0/835 | 1.12 | 7/1128 (0.6%) |
| 50 | B1 | 0.73 | 0/417 | 1.05 | 2/556 (0.4%) |
| 51 | B2 | 0.81 | 0/380 | 1.62 | 11/498 (2.2%) |
| 52 | B3 | 0.72 | 0/513 | 1.15 | 5/676 (0.7%) |
| 53 | B4 | 0.67 | 0/303 | 1.36 | 6/397 (1.5%) |
| 54 | BA | 1.40 | 1/69796 (0.0%) | 2.21 | 4031/108888 (3.7%) |
| 55 | BB | 1.42 | 0/2800 | 2.15 | 146/4367 (3.3%) |
| 56 | B5 | 0.64 | 0/1673 | 1.09 | 11/2255 (0.5%) |
| 6 | AG | 0.74 | 0/1188 | 1.23 | 14/1593 (0.9%) |
| 7 | AH | 0.69 | 0/989 | 1.02 | 5/1326 (0.4%) |
| 8 | AI | 0.81 | 0/1035 | 1.33 | 17/1377 (1.2%) |
| 9 | AJ | 0.71 | 0/797 | 1.28 | 10/1079 (0.9%) |
| All | All | 1.28 | 2/160085 (0.0%) | 2.00 | 6805/239402 (2.8%) |

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 |
|-----|-------|---------------------|---------------------|
| 14 | AO | 0 | 1 |
| 21 | AA | 0 | 372 |
| 22 | A1 | 0 | 21 |
| 23 | A2 | 0 | 5 |
| 24 | A3 | 0 | 7 |
| 27 | BE | 0 | 1 |
| 3 | AD | 0 | 1 |
| 37 | BO | 0 | 1 |
| 39 | BQ | 0 | 1 |
| 45 | BW | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 54 | BA | 0 | 726 |
| 55 | BB | 0 | 20 |
| 8 | AI | 0 | 1 |
| All | All | 0 | 1158 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 21 | AA | 1060 | U | C5'-C4' | 5.13 | 1.57 | 1.51 |
| 54 | BA | 2428 | G | C2-N2 | -5.06 | 1.29 | 1.34 |

The worst 5 of 6805 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 54 | BA | 982 | C | N3-C2-O2 | -13.80 | 112.24 | 121.90 |
| 54 | BA | 574 | A | N1-C6-N6 | -13.05 | 110.77 | 118.60 |
| 21 | AA | 676 | A | N1-C6-N6 | -12.48 | 111.11 | 118.60 |
| 21 | AA | 964 | A | N1-C6-N6 | -12.38 | 111.17 | 118.60 |
| 54 | BA | 1932 | A | N1-C6-N6 | -12.22 | 111.27 | 118.60 |

There are no chirality outliers.

5 of 1158 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 21 | AA | 10 | A | Sidechain |
| 21 | AA | 5 | U | Sidechain |
| 3 | AD | 204 | SER | Mainchain |
| 8 | AI | 105 | ARG | Sidechain |
| 14 | AO | 87 | ARG | Sidechain |

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AB | 1708 | 0 | 1736 | 0 | 0 |
| 2 | AC | 1625 | 0 | 1699 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | AD | 1643 | 0 | 1710 | 0 | 0 |
| 4 | AE | 1109 | 0 | 1152 | 0 | 0 |
| 5 | AF | 818 | 0 | 808 | 0 | 0 |
| 6 | AG | 1178 | 0 | 1234 | 0 | 0 |
| 7 | AH | 979 | 0 | 1034 | 0 | 0 |
| 8 | AI | 1025 | 0 | 1074 | 0 | 0 |
| 9 | AJ | 790 | 0 | 832 | 0 | 0 |
| 10 | AK | 880 | 0 | 891 | 1 | 0 |
| 11 | AL | 955 | 0 | 1019 | 1 | 0 |
| 12 | AM | 877 | 0 | 937 | 0 | 0 |
| 13 | AN | 805 | 0 | 844 | 0 | 0 |
| 14 | AO | 714 | 0 | 737 | 0 | 0 |
| 15 | AP | 639 | 0 | 656 | 0 | 0 |
| 16 | AQ | 652 | 0 | 695 | 0 | 0 |
| 17 | AR | 459 | 0 | 482 | 0 | 0 |
| 18 | AS | 641 | 0 | 669 | 1 | 0 |
| 19 | AT | 668 | 0 | 718 | 2 | 0 |
| 20 | AU | 429 | 0 | 453 | 0 | 0 |
| 21 | AA | 32828 | 0 | 16522 | 3 | 0 |
| 22 | A1 | 1627 | 0 | 832 | 1 | 0 |
| 23 | A2 | 309 | 0 | 158 | 0 | 0 |
| 24 | A3 | 1642 | 0 | 843 | 0 | 0 |
| 25 | BC | 2083 | 0 | 2157 | 0 | 0 |
| 26 | BD | 1565 | 0 | 1616 | 0 | 0 |
| 27 | BE | 1552 | 0 | 1619 | 0 | 0 |
| 28 | BF | 1420 | 0 | 1460 | 0 | 0 |
| 29 | BG | 1323 | 0 | 1374 | 0 | 0 |
| 30 | BH | 1111 | 0 | 1148 | 0 | 0 |
| 31 | BI | 1032 | 0 | 1088 | 0 | 0 |
| 32 | BJ | 1129 | 0 | 1162 | 0 | 0 |
| 33 | BK | 939 | 0 | 1012 | 0 | 0 |
| 34 | BL | 1045 | 0 | 1117 | 0 | 0 |
| 35 | BM | 1074 | 0 | 1157 | 1 | 0 |
| 36 | BN | 961 | 0 | 1000 | 0 | 0 |
| 37 | BO | 892 | 0 | 923 | 0 | 0 |
| 38 | BP | 917 | 0 | 965 | 0 | 0 |
| 39 | BQ | 947 | 0 | 1022 | 1 | 0 |
| 40 | BR | 816 | 0 | 839 | 0 | 0 |
| 41 | BS | 857 | 0 | 922 | 0 | 0 |
| 42 | BT | 739 | 0 | 807 | 0 | 0 |
| 43 | BU | 780 | 0 | 834 | 0 | 0 |
| 44 | BV | 753 | 0 | 780 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 45 | BW | 599 | 0 | 614 | 0 | 0 |
| 46 | BX | 625 | 0 | 655 | 0 | 0 |
| 47 | BY | 509 | 0 | 543 | 0 | 0 |
| 48 | BZ | 449 | 0 | 491 | 0 | 0 |
| 49 | B0 | 444 | 0 | 461 | 0 | 0 |
| 50 | B1 | 413 | 0 | 444 | 0 | 0 |
| 51 | B2 | 377 | 0 | 418 | 0 | 0 |
| 52 | B3 | 504 | 0 | 574 | 0 | 0 |
| 53 | B4 | 302 | 0 | 343 | 1 | 0 |
| 54 | BA | 62317 | 0 | 31343 | 6 | 0 |
| 55 | BB | 2504 | 0 | 1271 | 0 | 0 |
| 56 | B5 | 1658 | 0 | 1751 | 0 | 0 |
| 57 | A1 | 7 | 0 | 8 | 0 | 0 |
| 58 | A1 | 10 | 0 | 10 | 0 | 0 |
| All | All | 147653 | 0 | 99663 | 16 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

The worst 5 of 16 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 19:AT:40:ALA:HB1 | 19:AT:41:GLY:HA2 | 1.86 | 0.57 |
| 54:BA:1977:A:H2' | 54:BA:1978:A:C8 | 2.51 | 0.46 |
| 54:BA:1709:U:H2' | 54:BA:1710:G:C8 | 2.52 | 0.44 |
| 18:AS:78:THR:HB | 18:AS:79:TYR:HA | 1.99 | 0.44 |
| 39:BQ:40:LYS:HE2 | 39:BQ:44:TYR:CZ | 2.53 | 0.44 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | AB | 218/220 (99%) | 201 (92%) | 14 (6%) | 3 (1%) | 14 | 58 |
| 2 | AC | 205/208 (99%) | 189 (92%) | 13 (6%) | 3 (2%) | 13 | 57 |
| 3 | AD | 203/206 (98%) | 188 (93%) | 13 (6%) | 2 (1%) | 19 | 65 |
| 4 | AE | 150/152 (99%) | 135 (90%) | 10 (7%) | 5 (3%) | 5 | 40 |
| 5 | AF | 99/101 (98%) | 81 (82%) | 14 (14%) | 4 (4%) | 4 | 35 |
| 6 | AG | 150/152 (99%) | 134 (89%) | 13 (9%) | 3 (2%) | 9 | 51 |
| 7 | AH | 127/130 (98%) | 117 (92%) | 5 (4%) | 5 (4%) | 4 | 36 |
| 8 | AI | 126/128 (98%) | 106 (84%) | 16 (13%) | 4 (3%) | 5 | 41 |
| 9 | AJ | 98/100 (98%) | 91 (93%) | 2 (2%) | 5 (5%) | 2 | 30 |
| 10 | AK | 116/118 (98%) | 109 (94%) | 4 (3%) | 3 (3%) | 7 | 45 |
| 11 | AL | 121/124 (98%) | 109 (90%) | 9 (7%) | 3 (2%) | 7 | 46 |
| 12 | AM | 112/115 (97%) | 93 (83%) | 14 (12%) | 5 (4%) | 3 | 33 |
| 13 | AN | 98/101 (97%) | 88 (90%) | 9 (9%) | 1 (1%) | 19 | 65 |
| 14 | AO | 86/89 (97%) | 80 (93%) | 5 (6%) | 1 (1%) | 16 | 61 |
| 15 | AP | 79/81 (98%) | 71 (90%) | 6 (8%) | 2 (2%) | 7 | 46 |
| 16 | AQ | 80/82 (98%) | 74 (92%) | 6 (8%) | 0 | 100 | 100 |
| 17 | AR | 55/57 (96%) | 50 (91%) | 4 (7%) | 1 (2%) | 11 | 53 |
| 18 | AS | 79/81 (98%) | 69 (87%) | 9 (11%) | 1 (1%) | 15 | 60 |
| 19 | AT | 84/86 (98%) | 73 (87%) | 9 (11%) | 2 (2%) | 7 | 47 |
| 20 | AU | 51/53 (96%) | 32 (63%) | 15 (29%) | 4 (8%) | 1 | 20 |
| 25 | BC | 270/273 (99%) | 236 (87%) | 26 (10%) | 8 (3%) | 5 | 42 |
| 26 | BD | 207/209 (99%) | 178 (86%) | 15 (7%) | 14 (7%) | 1 | 23 |
| 27 | BE | 199/201 (99%) | 187 (94%) | 7 (4%) | 5 (2%) | 7 | 46 |
| 28 | BF | 176/179 (98%) | 153 (87%) | 18 (10%) | 5 (3%) | 6 | 44 |
| 29 | BG | 174/177 (98%) | 160 (92%) | 11 (6%) | 3 (2%) | 11 | 55 |
| 30 | BH | 147/149 (99%) | 136 (92%) | 9 (6%) | 2 (1%) | 14 | 58 |
| 31 | BI | 139/142 (98%) | 127 (91%) | 11 (8%) | 1 (1%) | 26 | 71 |
| 32 | BJ | 140/142 (99%) | 131 (94%) | 7 (5%) | 2 (1%) | 14 | 58 |
| 33 | BK | 121/123 (98%) | 107 (88%) | 10 (8%) | 4 (3%) | 5 | 40 |
| 34 | BL | 141/144 (98%) | 122 (86%) | 15 (11%) | 4 (3%) | 6 | 44 |
| 35 | BM | 134/136 (98%) | 121 (90%) | 8 (6%) | 5 (4%) | 4 | 38 |
| 36 | BN | 119/121 (98%) | 107 (90%) | 10 (8%) | 2 (2%) | 11 | 55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 37 | BO | 114/117 (97%) | 105 (92%) | 8 (7%) | 1 (1%) | 21 | 67 |
| 38 | BP | 112/115 (97%) | 94 (84%) | 11 (10%) | 7 (6%) | 2 | 25 |
| 39 | BQ | 115/118 (98%) | 106 (92%) | 6 (5%) | 3 (3%) | 7 | 45 |
| 40 | BR | 101/103 (98%) | 92 (91%) | 7 (7%) | 2 (2%) | 9 | 51 |
| 41 | BS | 108/110 (98%) | 100 (93%) | 5 (5%) | 3 (3%) | 6 | 44 |
| 42 | BT | 92/94 (98%) | 77 (84%) | 8 (9%) | 7 (8%) | 1 | 20 |
| 43 | BU | 101/104 (97%) | 85 (84%) | 10 (10%) | 6 (6%) | 2 | 27 |
| 44 | BV | 92/94 (98%) | 86 (94%) | 3 (3%) | 3 (3%) | 5 | 40 |
| 45 | BW | 78/80 (98%) | 56 (72%) | 16 (20%) | 6 (8%) | 1 | 20 |
| 46 | BX | 75/79 (95%) | 66 (88%) | 7 (9%) | 2 (3%) | 6 | 45 |
| 47 | BY | 61/63 (97%) | 54 (88%) | 5 (8%) | 2 (3%) | 5 | 40 |
| 48 | BZ | 56/59 (95%) | 50 (89%) | 5 (9%) | 1 (2%) | 11 | 53 |
| 49 | B0 | 54/57 (95%) | 44 (82%) | 9 (17%) | 1 (2%) | 10 | 52 |
| 50 | B1 | 50/52 (96%) | 47 (94%) | 3 (6%) | 0 | 100 | 100 |
| 51 | B2 | 44/46 (96%) | 42 (96%) | 0 | 2 (4%) | 3 | 33 |
| 52 | B3 | 62/65 (95%) | 57 (92%) | 4 (6%) | 1 (2%) | 12 | 56 |
| 53 | B4 | 36/38 (95%) | 32 (89%) | 4 (11%) | 0 | 100 | 100 |
| 56 | B5 | 221/234 (94%) | 206 (93%) | 13 (6%) | 2 (1%) | 21 | 67 |
| All | All | 5876/6008 (98%) | 5254 (89%) | 461 (8%) | 161 (3%) | 10 | 45 |

5 of 161 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AB | 10 | LYS |
| 5 | AF | 90 | MET |
| 6 | AG | 5 | VAL |
| 7 | AH | 77 | VAL |
| 10 | AK | 125 | LYS |

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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | AB | 180/180 (100%) | 176 (98%) | 4 (2%) | 60 | 83 |
| 2 | AC | 170/171 (99%) | 167 (98%) | 3 (2%) | 66 | 87 |
| 3 | AD | 172/173 (99%) | 171 (99%) | 1 (1%) | 90 | 95 |
| 4 | AE | 113/113 (100%) | 112 (99%) | 1 (1%) | 84 | 93 |
| 5 | AF | 87/87 (100%) | 87 (100%) | 0 | 100 | 100 |
| 6 | AG | 123/123 (100%) | 122 (99%) | 1 (1%) | 86 | 94 |
| 7 | AH | 104/105 (99%) | 102 (98%) | 2 (2%) | 65 | 86 |
| 8 | AI | 105/105 (100%) | 104 (99%) | 1 (1%) | 82 | 92 |
| 9 | AJ | 86/86 (100%) | 83 (96%) | 3 (4%) | 43 | 74 |
| 10 | AK | 90/90 (100%) | 87 (97%) | 3 (3%) | 45 | 76 |
| 11 | AL | 103/104 (99%) | 101 (98%) | 2 (2%) | 65 | 86 |
| 12 | AM | 91/92 (99%) | 91 (100%) | 0 | 100 | 100 |
| 13 | AN | 83/84 (99%) | 81 (98%) | 2 (2%) | 57 | 82 |
| 14 | AO | 76/77 (99%) | 75 (99%) | 1 (1%) | 76 | 89 |
| 15 | AP | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 16 | AQ | 74/74 (100%) | 71 (96%) | 3 (4%) | 37 | 71 |
| 17 | AR | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 18 | AS | 70/70 (100%) | 69 (99%) | 1 (1%) | 74 | 89 |
| 19 | AT | 65/65 (100%) | 65 (100%) | 0 | 100 | 100 |
| 20 | AU | 44/44 (100%) | 44 (100%) | 0 | 100 | 100 |
| 25 | BC | 216/217 (100%) | 212 (98%) | 4 (2%) | 65 | 86 |
| 26 | BD | 164/164 (100%) | 161 (98%) | 3 (2%) | 66 | 87 |
| 27 | BE | 165/165 (100%) | 165 (100%) | 0 | 100 | 100 |
| 28 | BF | 149/150 (99%) | 144 (97%) | 5 (3%) | 44 | 75 |
| 29 | BG | 137/138 (99%) | 133 (97%) | 4 (3%) | 50 | 78 |
| 30 | BH | 114/114 (100%) | 114 (100%) | 0 | 100 | 100 |
| 31 | BI | 109/110 (99%) | 107 (98%) | 2 (2%) | 66 | 87 |
| 32 | BJ | 116/116 (100%) | 114 (98%) | 2 (2%) | 68 | 87 |
| 33 | BK | 103/103 (100%) | 102 (99%) | 1 (1%) | 82 | 92 |
| 34 | BL | 102/103 (99%) | 102 (100%) | 0 | 100 | 100 |
| 35 | BM | 109/109 (100%) | 106 (97%) | 3 (3%) | 51 | 78 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 36 | BN | 100/100 (100%) | 97 (97%) | 3 (3%) | 48 | 77 |
| 37 | BO | 86/87 (99%) | 86 (100%) | 0 | 100 | 100 |
| 38 | BP | 99/100 (99%) | 98 (99%) | 1 (1%) | 82 | 92 |
| 39 | BQ | 89/90 (99%) | 88 (99%) | 1 (1%) | 80 | 91 |
| 40 | BR | 84/84 (100%) | 82 (98%) | 2 (2%) | 57 | 82 |
| 41 | BS | 93/93 (100%) | 92 (99%) | 1 (1%) | 80 | 91 |
| 42 | BT | 80/80 (100%) | 80 (100%) | 0 | 100 | 100 |
| 43 | BU | 83/84 (99%) | 83 (100%) | 0 | 100 | 100 |
| 44 | BV | 78/78 (100%) | 76 (97%) | 2 (3%) | 54 | 80 |
| 45 | BW | 59/59 (100%) | 58 (98%) | 1 (2%) | 68 | 87 |
| 46 | BX | 67/68 (98%) | 66 (98%) | 1 (2%) | 72 | 88 |
| 47 | BY | 55/55 (100%) | 53 (96%) | 2 (4%) | 42 | 74 |
| 48 | BZ | 48/49 (98%) | 48 (100%) | 0 | 100 | 100 |
| 49 | B0 | 47/48 (98%) | 45 (96%) | 2 (4%) | 35 | 70 |
| 50 | B1 | 45/45 (100%) | 43 (96%) | 2 (4%) | 35 | 69 |
| 51 | B2 | 38/38 (100%) | 38 (100%) | 0 | 100 | 100 |
| 52 | B3 | 51/52 (98%) | 51 (100%) | 0 | 100 | 100 |
| 53 | B4 | 34/34 (100%) | 33 (97%) | 1 (3%) | 50 | 78 |
| 56 | B5 | 173/181 (96%) | 170 (98%) | 3 (2%) | 68 | 87 |
| All | All | 4842/4870 (99%) | 4768 (98%) | 74 (2%) | 74 | 88 |

5 of 74 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | BD | 161 | MET |
| 29 | BG | 115 | GLN |
| 50 | B1 | 10 | LEU |
| 26 | BD | 179 | ARG |
| 28 | BF | 41 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AB | 17 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AB | 202 | ASN |
| 11 | AL | 45 | ASN |
| 36 | BN | 3 | HIS |
| 44 | BV | 44 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 21 | AA | 1530/1533 (99%) | 237 (15%) | 85 (5%) |
| 22 | A1 | 73/76 (96%) | 12 (16%) | 8 (10%) |
| 23 | A2 | 14/15 (93%) | 5 (35%) | 2 (14%) |
| 24 | A3 | 76/77 (98%) | 15 (19%) | 6 (7%) |
| 54 | BA | 2902/2903 (99%) | 487 (16%) | 135 (4%) |
| 55 | BB | 116/118 (98%) | 17 (14%) | 3 (2%) |
| All | All | 4711/4722 (99%) | 773 (16%) | 239 (5%) |

5 of 773 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21 | AA | 6 | G |
| 21 | AA | 9 | G |
| 21 | AA | 20 | U |
| 21 | AA | 21 | G |
| 21 | AA | 31 | G |

5 of 239 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 54 | BA | 99 | U |
| 54 | BA | 574 | A |
| 54 | BA | 2439 | A |
| 54 | BA | 119 | A |
| 54 | BA | 323 | C |

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

11 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 |
| 22 | CM0 | A1 | 34 | 22,23 | 15,26,27 | 1.88 | 3 (20%) | 18,37,40 | 3.02 | 3 (16%) |
| 22 | 6MZ | A1 | 37 | 22 | 17,25,26 | 0.91 | 0 | 15,36,39 | 1.12 | 1 (6%) |
| 22 | 7MG | A1 | 46 | 22 | 20,26,27 | 2.29 | 3 (15%) | 23,39,42 | 2.03 | 2 (8%) |
| 22 | 5MU | A1 | 54 | 22 | 13,22,23 | 1.07 | 1 (7%) | 16,32,35 | 4.62 | 2 (12%) |
| 22 | PSU | A1 | 55 | 22 | 15,21,22 | 2.04 | 4 (26%) | 16,30,33 | 4.15 | 6 (37%) |
| 22 | 4SU | A1 | 7 | 22 | 12,21,22 | 0.95 | 1 (8%) | 15,30,33 | 2.22 | 2 (13%) |
| 24 | H2U | A3 | 21 | 24 | 17,21,22 | 1.39 | 2 (11%) | 23,30,33 | 1.34 | 4 (17%) |
| 24 | OMC | A3 | 33 | 24 | 15,22,23 | 1.11 | 1 (6%) | 20,31,34 | 0.92 | 1 (5%) |
| 24 | 5MU | A3 | 55 | 24 | 13,22,23 | 0.92 | 1 (7%) | 16,32,35 | 4.53 | 3 (18%) |
| 24 | PSU | A3 | 56 | 24 | 15,21,22 | 1.09 | 1 (6%) | 16,30,33 | 3.30 | 4 (25%) |
| 24 | 4SU | A3 | 8 | 24 | 12,21,22 | 1.10 | 1 (8%) | 15,30,33 | 2.26 | 1 (6%) |

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 |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 22 | CM0 | A1 | 34 | 22,23 | - | 0/6/30/31 | 0/2/2/2 |
| 22 | 6MZ | A1 | 37 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | 7MG | A1 | 46 | 22 | - | 0/7/37/38 | 0/3/3/3 |
| 22 | 5MU | A1 | 54 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 22 | PSU | A1 | 55 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 4SU | A1 | 7 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 24 | H2U | A3 | 21 | 24 | - | 0/7/38/39 | 0/2/2/2 |
| 24 | OMC | A3 | 33 | 24 | - | 0/5/27/28 | 0/2/2/2 |
| 24 | 5MU | A3 | 55 | 24 | - | 0/3/25/26 | 0/2/2/2 |
| 24 | PSU | A3 | 56 | 24 | - | 0/7/25/26 | 0/2/2/2 |
| 24 | 4SU | A3 | 8 | 24 | - | 0/3/25/26 | 0/2/2/2 |

The worst 5 of 18 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 22 | A1 | 46 | 7MG | C8-N9 | -8.61 | 1.33 | 1.45 |
| 22 | A1 | 34 | CM0 | O5-C5 | -5.90 | 1.25 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 22 | A1 | 55 | PSU | C2'-C1' | -4.73 | 1.49 | 1.53 |
| 24 | A3 | 21 | H2U | C4-N3 | -3.49 | 1.32 | 1.37 |
| 24 | A3 | 21 | H2U | C2-N3 | -3.24 | 1.31 | 1.38 |

The worst 5 of 29 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 22 | A1 | 54 | 5MU | C5-C4-N3 | -13.20 | 114.27 | 125.35 |
| 24 | A3 | 55 | 5MU | C5-C4-N3 | -12.30 | 115.02 | 125.35 |
| 22 | A1 | 55 | PSU | C4-C5-C1' | -9.87 | 104.59 | 121.22 |
| 24 | A3 | 8 | 4SU | C5-C4-N3 | -8.08 | 114.99 | 123.56 |
| 22 | A1 | 7 | 4SU | C5-C4-N3 | -7.65 | 115.44 | 123.56 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | A1 | 55 | PSU | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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 | $\# Z > 2$ |
| 57 | VAL | A1 | 101 | 58,22 | 5,6,7 | 0.50 | 0 | 5,7,9 | 2.31 | 2 (40%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 58 | FME | A1 | 102 | 57 | 8,9,10 | 0.83 | 0 | 5,9,11 | 1.20 | 1 (20%) |

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 |
|-----|------|-------|-----|-------|---------|----------|---------|
| 57 | VAL | A1 | 101 | 58,22 | - | 0/4/6/8 | 0/0/0/0 |
| 58 | FME | A1 | 102 | 57 | - | 0/6/9/11 | 0/0/0/0 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 57 | A1 | 101 | VAL | O-C-CA | -4.44 | 113.56 | 125.69 |
| 58 | A1 | 102 | FME | O-C-CA | -2.52 | 118.80 | 125.69 |
| 57 | A1 | 101 | VAL | C-CA-N | 2.66 | 115.82 | 109.95 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.