



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 11, 2019 – 02:49 AM EST

PDB ID : 4V6P
EMDB ID: : EMD-5364
Title : Structural characterization of mRNA-tRNA translocation intermediates (class 4b of the six classes)
Authors : Agirrezabala, X.; Liao, H.; Schreiner, E.; Fu, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on : 2011-12-08
Resolution : 13.50 Å (reported)
Based on PDB ID : 2I2U

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

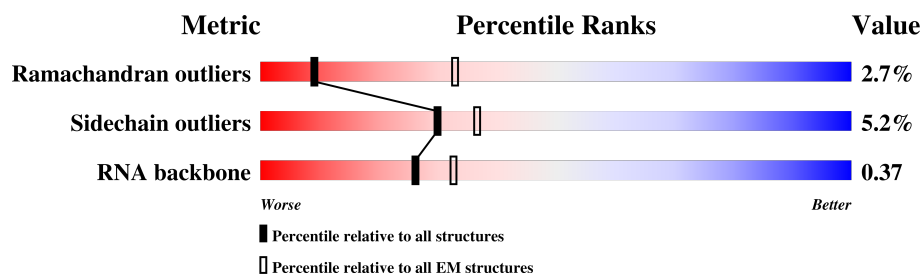
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.50 Å.

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




























| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 132723 | 1663 |
| Sidechain outliers | 132532 | 1531 |
| RNA backbone | 3747 | 458 |

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 | AA | 1542 | |
| 2 | AB | 76 | |
| 3 | AC | 47 | |
| 4 | AD | 77 | |
| 5 | AE | 240 | |
| 6 | AF | 232 | |
| 7 | AG | 205 | |
| 8 | AH | 166 | |
| 9 | AI | 135 | |

























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 10 | AJ | 178 |  80% 18% . |
| 11 | AK | 129 |  80% 20% |
| 12 | AL | 129 |  81% 17% . |
| 13 | AM | 103 |  72% 23% 5% |
| 14 | AN | 128 |  84% 15% . |
| 15 | AO | 123 |  73% 24% . |
| 16 | AP | 117 |  80% 18% . |
| 17 | AQ | 100 |  73% 24% .. |
| 18 | AR | 88 |  81% 18% . |
| 19 | AS | 82 |  80% 17% . |
| 20 | AT | 83 |  75% 20% 5% |
| 21 | AU | 74 |  64% 27% 8% . |
| 22 | AV | 91 |  76% 21% . |
| 23 | AW | 86 |  83% 15% . |
| 24 | AX | 70 |  57% 41% . |
| 25 | BA | 120 |  31% 59% 10% |
| 26 | BB | 2904 |  32% 54% 13% . |
| 27 | BC | 234 |  83% 16% . |
| 28 | BD | 272 |  77% 20% . |
| 29 | BE | 209 |  78% 19% . |
| 30 | BF | 201 |  77% 18% . |
| 31 | BG | 178 |  69% 26% 5% |
| 32 | BH | 176 |  74% 22% . |
| 33 | BI | 149 |  83% 16% . |
| 34 | BJ | 164 |  82% 15% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 35 | BK | 141 |  85% 13% . |
| 36 | BL | 142 |  79% 17% . . |
| 37 | BM | 123 |  74% 23% . |
| 38 | BN | 144 |  78% 21% . . |
| 39 | BO | 136 |  79% 16% . |
| 40 | BP | 127 |  75% 20% 5% |
| 41 | BQ | 117 |  77% 20% . |
| 42 | BR | 114 |  69% 28% . |
| 43 | BS | 117 |  73% 22% 5% |
| 44 | BT | 103 |  80% 17% . |
| 45 | BU | 110 |  79% 18% . |
| 46 | BV | 100 |  70% 25% 5% |
| 47 | BW | 103 |  81% 17% . |
| 48 | BX | 94 |  74% 21% . |
| 49 | BY | 84 |  69% 25% 6% |
| 50 | BZ | 77 |  70% 29% . |
| 51 | B0 | 63 |  83% 16% . |
| 52 | B1 | 58 |  83% 17% |
| 53 | B2 | 70 |  74% 19% 6% . |
| 54 | B3 | 56 |  73% 23% . |
| 55 | B4 | 54 |  78% 19% . |
| 56 | B5 | 46 |  74% 24% . |
| 57 | B6 | 64 |  80% 19% . |
| 58 | B7 | 38 |  79% 18% . |

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 152351 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1 | AA | 1542 | Total | C | N | O | P | 0 | 0 |
| | | | 33089 | 14767 | 6064 | 10717 | 1541 | | |

- Molecule 2 is a RNA chain called A site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 2 | AB | 76 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1627 | 731 | 287 | 532 | 75 | 2 | | |

- Molecule 3 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3 | AC | 47 | Total | C | N | O | P | 0 | 0 |
| | | | 993 | 445 | 167 | 335 | 46 | | |

- Molecule 4 is a RNA chain called P site tRNA.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|-------|
| 4 | AD | 77 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1641 | 734 | 297 | 533 | 76 | 1 | | |

- Molecule 5 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | AE | 240 | Total | C | N | O | S | 0 | 0 |
| | | | 1872 | 1180 | 332 | 352 | 8 | | |

- Molecule 6 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6 | AF | 232 | Total | C | N | O | S | 0 | 0 |
| | | | 1822 | 1149 | 346 | 323 | 4 | | |

- Molecule 7 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7 | AG | 205 | Total | C | N | O | S | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | |

- Molecule 8 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8 | AH | 166 | Total | C | N | O | S | 0 | 0 |
| | | | 1225 | 761 | 232 | 226 | 6 | | |

- Molecule 9 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9 | AI | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1101 | 677 | 198 | 219 | 7 | | |

- Molecule 10 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | AJ | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1400 | 874 | 269 | 253 | 4 | | |

- Molecule 11 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11 | AK | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | |

- Molecule 12 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12 | AL | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1036 | 642 | 208 | 183 | 3 | | |

- Molecule 13 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13 | AM | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 825 | 514 | 158 | 151 | 2 | | |

- Molecule 14 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14 | AN | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 965 | 595 | 196 | 171 | 3 | | |

- Molecule 15 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15 | AO | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | |

- Molecule 16 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16 | AP | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 910 | 564 | 183 | 160 | 3 | | |

- Molecule 17 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17 | AQ | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 499 | 164 | 139 | 3 | | |

- Molecule 18 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | AR | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 716 | 440 | 146 | 129 | 1 | | |

- Molecule 19 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19 | AS | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | |

- Molecule 20 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20 | AT | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 672 | 425 | 124 | 120 | 3 | | |

- Molecule 21 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21 | AU | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 626 | 395 | 123 | 107 | 1 | | |

- Molecule 22 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22 | AV | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 727 | 464 | 139 | 122 | 2 | | |

- Molecule 23 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23 | AW | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 670 | 414 | 138 | 115 | 3 | | |

- Molecule 24 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 24 | AX | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 590 | 366 | 125 | 98 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 25 | BA | 120 | Total | C | N | O | P | 0 | 0 |
| | | | 2566 | 1144 | 468 | 835 | 119 | | |

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 26 | BB | 2904 | Total | C | N | O | P | 0 | 0 |
| | | | 62351 | 27824 | 11469 | 20155 | 2903 | | |

- Molecule 27 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27 | BC | 234 | Total | C | N | O | S | 0 | 0 |
| | | | 1733 | 1081 | 315 | 330 | 7 | | |

- Molecule 28 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28 | BD | 272 | Total | C | N | O | S | 0 | 0 |
| | | | 2092 | 1294 | 425 | 366 | 7 | | |

- Molecule 29 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | BE | 209 | Total | C | N | O | S | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | |

- Molecule 30 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | BF | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | |

- Molecule 31 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31 | BG | 178 | Total | C | N | O | S | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | |

- Molecule 32 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32 | BH | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | |

- Molecule 33 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33 | BI | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | |

- Molecule 34 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | BJ | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1233 | 776 | 220 | 231 | 6 | | |

- Molecule 35 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | BK | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | |

- Molecule 36 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36 | BL | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | |

- Molecule 37 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37 | BM | 123 | Total | C | N | O | S | 0 | 0 |
| | | | 947 | 593 | 181 | 167 | 6 | | |

- Molecule 38 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38 | BN | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | |

- Molecule 39 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39 | BO | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | |

- Molecule 40 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40 | BP | 127 | Total | C | N | O | S | 0 | 0 |
| | | | 1008 | 621 | 204 | 178 | 5 | | |

- Molecule 41 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | BQ | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 900 | 557 | 179 | 163 | 1 | | |

- Molecule 42 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42 | BR | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | |

- Molecule 43 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 43 | BS | 117 | Total | C | N | O | | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44 | BT | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | |

- Molecule 45 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45 | BU | 110 | Total | C | N | O | S | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | |

- Molecule 46 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46 | BV | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 787 | 496 | 146 | 143 | 2 | | |

- Molecule 47 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 47 | BW | 103 | Total | C | N | O | | 0 | 0 |
| | | | 789 | 498 | 148 | 143 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | BX | 94 | Total | C | N | O | S | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | |

- Molecule 49 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49 | BY | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 634 | 391 | 129 | 113 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50 | BZ | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | |

- Molecule 51 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51 | B0 | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | |

- Molecule 52 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 52 | B1 | 58 | Total | C | N | O | S | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | |

- Molecule 53 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | B2 | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 549 | 339 | 104 | 100 | 6 | | |

- Molecule 54 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54 | B3 | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | |

- Molecule 55 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 55 | B4 | 54 | Total | C | N | O | 0 | 0 |
| | | | 441 | 284 | 81 | 76 | | |

- Molecule 56 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 56 | B5 | 46 | Total | C | N | O | S | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | |

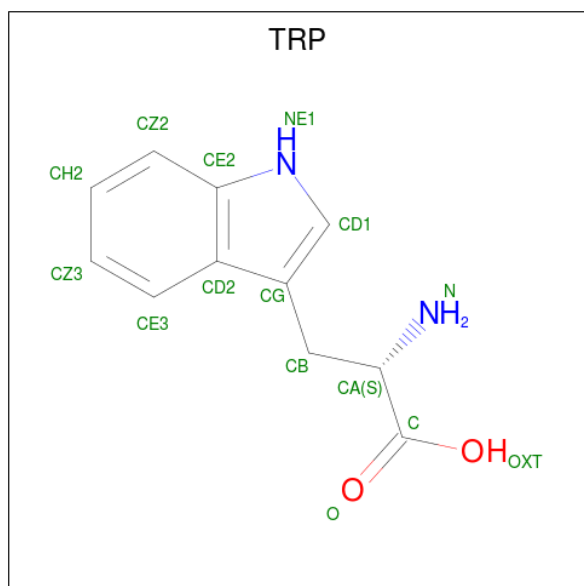
- Molecule 57 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 57 | B6 | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | |

- Molecule 58 is a protein called 50S ribosomal protein L36.

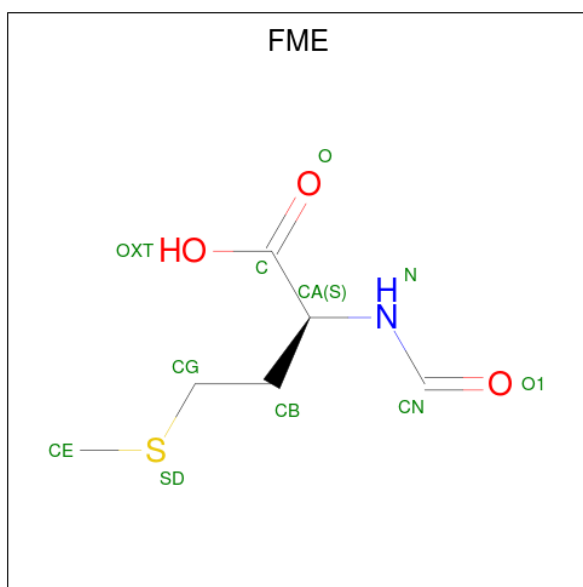
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 58 | B7 | 38 | Total | C | N | O | S | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | |

- Molecule 59 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 59 | AB | 1 | Total | C | N | O | 0 |
| | | | 14 | 11 | 2 | 1 | |

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

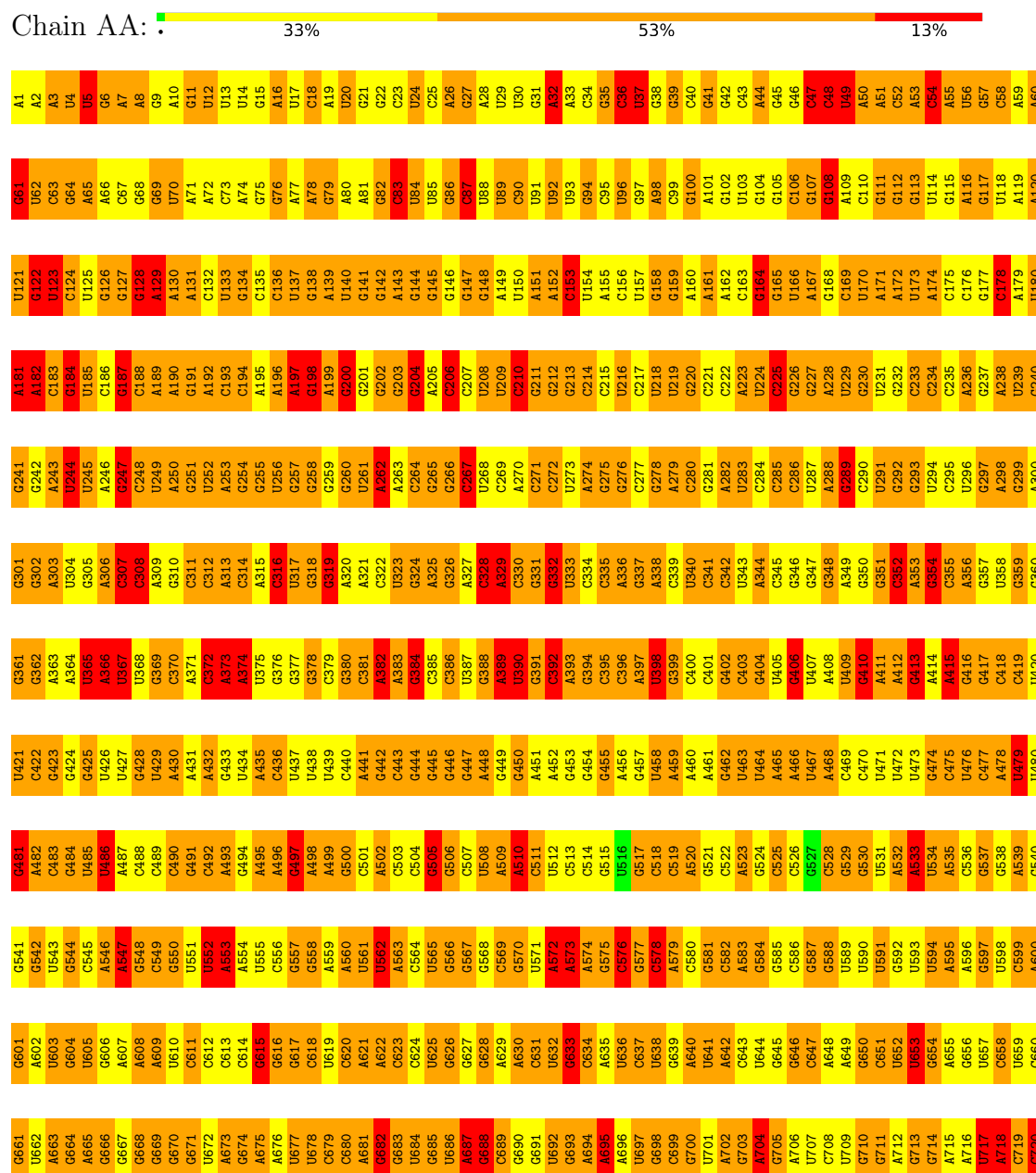


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| | | | Total | C | N | O | S | |
| 60 | BB | 1 | 10 | 6 | 1 | 2 | 1 | 0 |

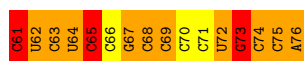
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

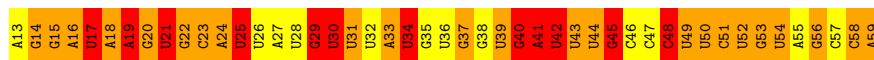
• Molecule 1: 16S ribosomal RNA



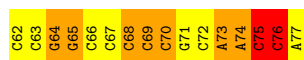


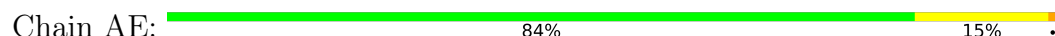
- Molecule 3: mRNA



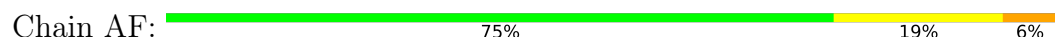
- Molecule 4: P site tRNA



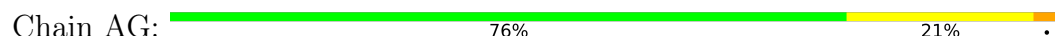
- Molecule 5: 30S ribosomal protein S2



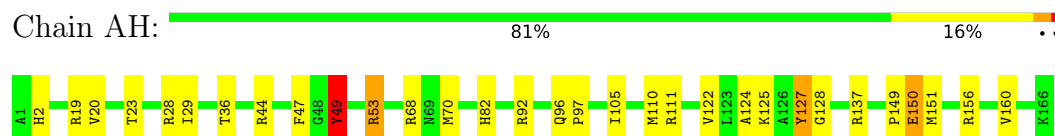
- Molecule 6: 30S ribosomal protein S3



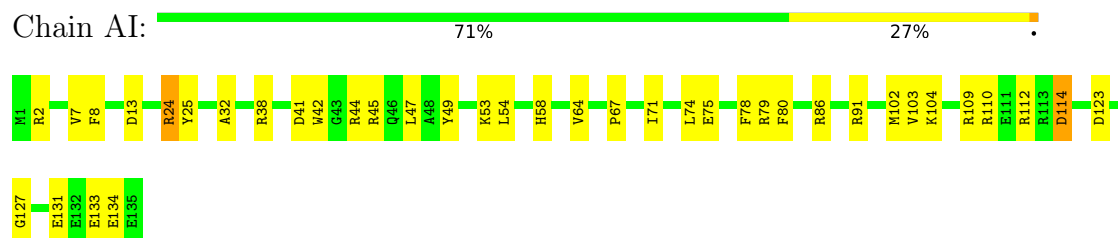
- Molecule 7: 30S ribosomal protein S4



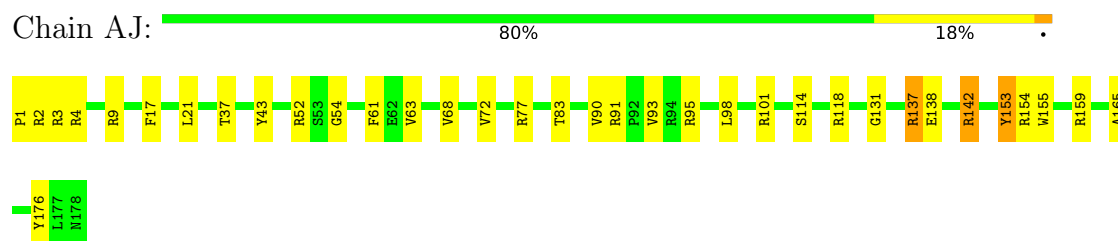
- Molecule 8: 30S ribosomal protein S5



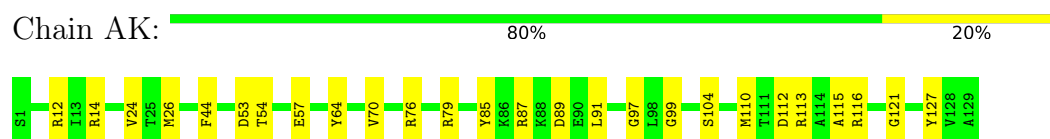
- Molecule 9: 30S ribosomal protein S6



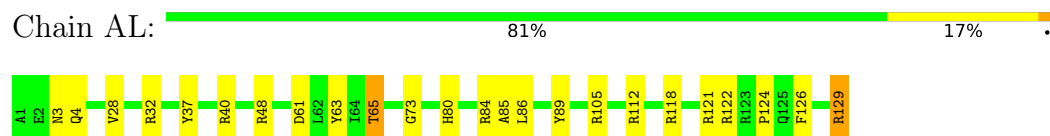
- Molecule 10: 30S ribosomal protein S7



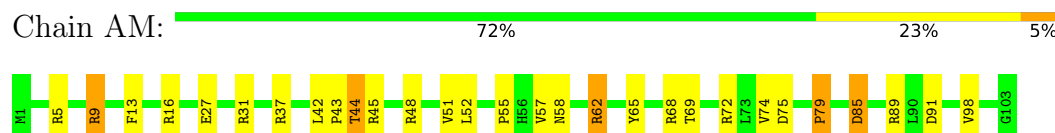
- Molecule 11: 30S ribosomal protein S8



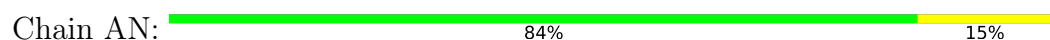
- Molecule 12: 30S ribosomal protein S9



- Molecule 13: 30S ribosomal protein S10



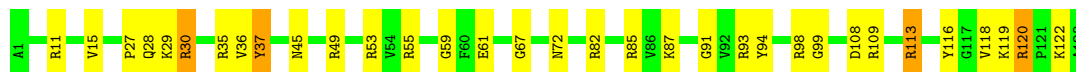
- Molecule 14: 30S ribosomal protein S11





- Molecule 15: 30S ribosomal protein S12

Chain AO: 73% 24% .



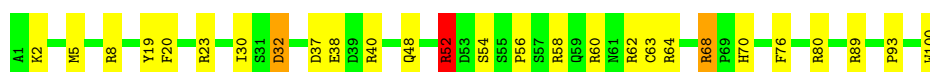
- Molecule 16: 30S ribosomal protein S13

Chain AP: 80% 18% .



- Molecule 17: 30S ribosomal protein S14

Chain AQ: 73% 24% ..



- Molecule 18: 30S ribosomal protein S15

Chain AR: 81% 18% .



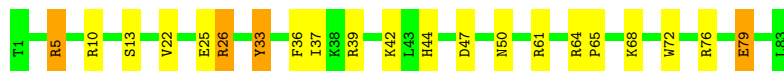
- Molecule 19: 30S ribosomal protein S16

Chain AS: 80% 17% .



- Molecule 20: 30S ribosomal protein S17

Chain AT: 75% 20% 5%

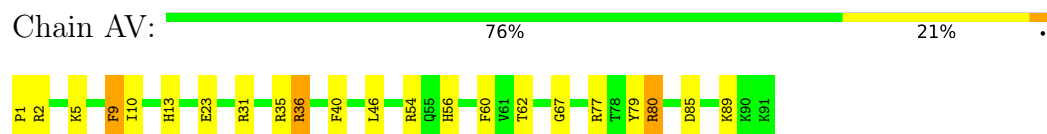


- Molecule 21: 30S ribosomal protein S18

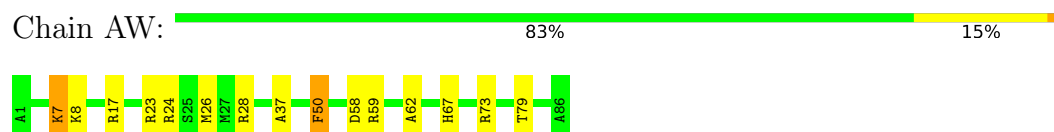
Chain AU: 64% 27% 8%



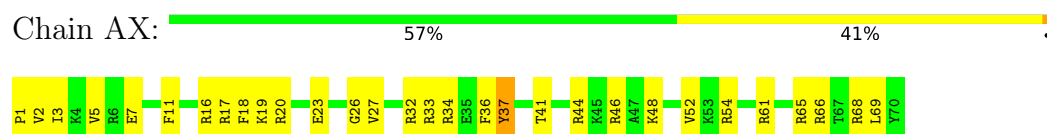
- Molecule 22: 30S ribosomal protein S19



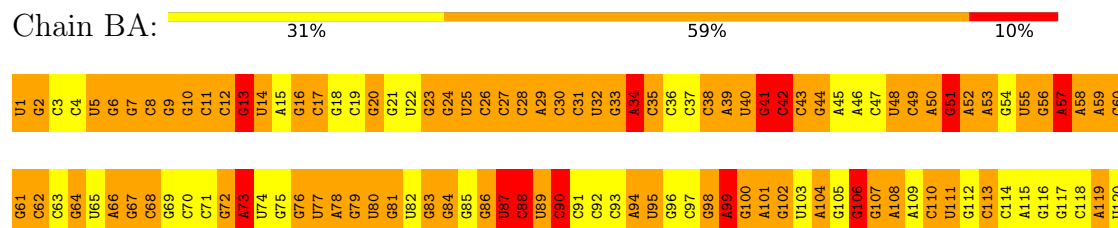
- Molecule 23: 30S ribosomal protein S20



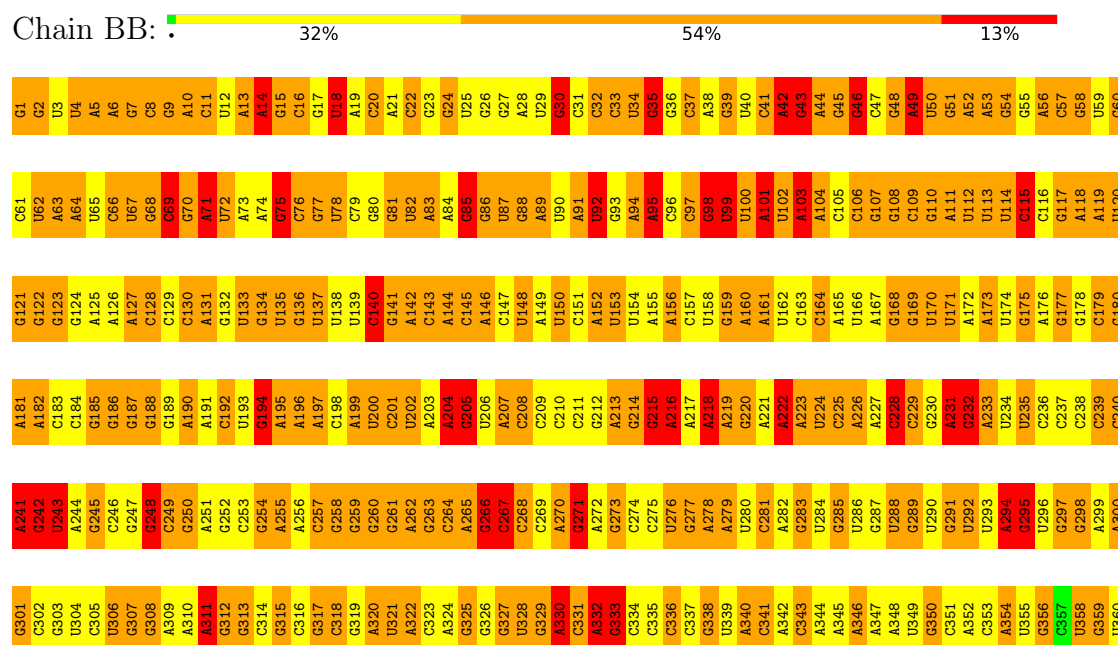
- Molecule 24: 30S ribosomal protein S21



- Molecule 25: 5S ribosomal RNA



- Molecule 26: 23S ribosomal RNA

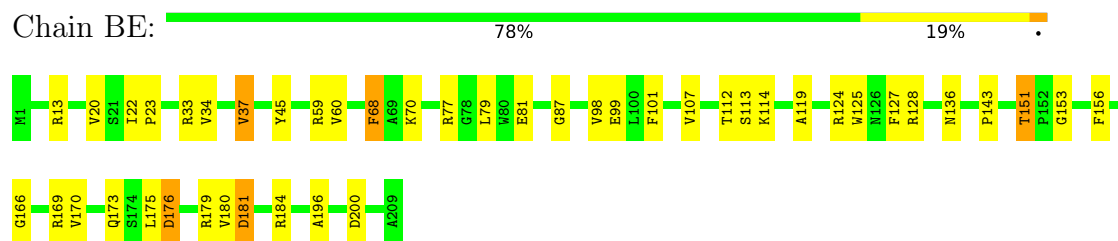


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| A1322 | A1262 | G1202 | A1142 | U1082 | G1022 | G962 | C902 | U842 | A782 | A722 | G662 | A602 | C542 | A482 | A422 | A362 |
| C1323 | U1263 | U1203 | A1143 | U1083 | U1023 | U963 | C903 | G843 | A783 | C723 | G663 | A603 | G543 | A483 | A423 | G363 |
| A1324 | A1264 | U1204 | A1144 | A1084 | G1024 | G964 | C904 | A844 | G784 | U724 | U664 | G604 | U544 | C484 | G424 | C364 |
| U1325 | A1265 | A1205 | C1145 | A1085 | G1025 | C965 | A905 | A845 | G785 | G725 | U665 | G605 | U545 | C485 | C425 | U365 |
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| U1329 | A1269 | U1209 | A1149 | A1089 | A1029 | G969 | A909 | A849 | A789 | G729 | G669 | A609 | G549 | G489 | A429 | U369 |
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| C1333 | U1273 | A1213 | C1153 | G1093 | U1033 | A973 | C913 | C853 | A793 | G733 | G673 | A613 | G553 | G493 | C433 | U373 |
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| G1346 | A1286 | A1226 | G1166 | G1106 | A1046 | C986 | C926 | A866 | C806 | U746 | U686 | A626 | U566 | G506 | C446 | G386 |
| A1347 | A1287 | G1227 | C1167 | G1107 | G1047 | C987 | A927 | U867 | U807 | U747 | G687 | A627 | C567 | A507 | A447 | U387 |
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| C1376 | U1316 | G1256 | C1196 | G1136 | C1076 | G1016 | U956 | A896 | G836 | G776 | A716 | G656 | U596 | G536 | G476 | U416 |
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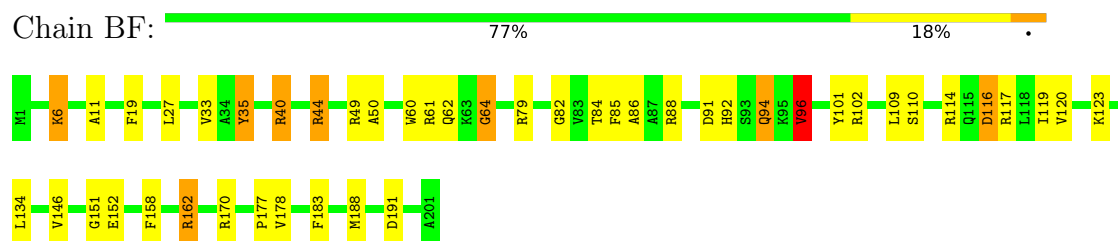
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| U2299 | G2239 | C2179 | A2119 | A2059 | C1999 | U1939 | C1879 | A1819 | A1759 | G1699 | C1639 | G1519 | G1459 | C1399 |
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| C2301 | A2241 | U2181 | G2121 | G2061 | C2001 | G1941 | C1881 | A1821 | C1761 | A1641 | G1641 | G1521 | C1461 | G1401 |
| U2302 | G2242 | U2182 | U2122 | A2062 | G2002 | C1942 | U1882 | C1822 | G1762 | G1702 | G1642 | U1522 | C1462 | U1402 |
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| G2307 | A2247 | U2187 | G2127 | G2067 | U2007 | G1947 | C1887 | G1827 | G1767 | U1707 | U1647 | G1527 | U1467 | G1407 |
| G2308 | G2248 | U2188 | G2128 | U2068 | C2008 | C1948 | G1888 | G1828 | C1768 | C1708 | U1648 | A1528 | U1468 | G1408 |
| A2309 | U2249 | U2189 | C2129 | G2069 | A2009 | G1949 | A1889 | A1829 | U1769 | U1709 | G1649 | G1529 | U1469 | U1409 |
| C2310 | G2250 | U2190 | U2130 | A2070 | G2010 | G1950 | A1890 | C1830 | G1770 | C1710 | A1650 | G1530 | A1470 | G1410 |
| A2311 | G2251 | A2191 | U2131 | A2071 | U2011 | U1951 | G1891 | G1831 | C1771 | U1711 | G1651 | C1531 | G1471 | U1411 |
| U2312 | G2252 | U2192 | U2132 | C2072 | G2012 | A1952 | C1892 | G1832 | A1772 | U1712 | A1652 | A1532 | C1472 | U1412 |
| G2313 | G2253 | G2193 | G2133 | C2073 | A2013 | A1953 | C1893 | G1833 | A1773 | C1713 | G1653 | A1533 | G1473 | A1413 |
| A2314 | C2254 | U2194 | A2134 | U2074 | A2014 | G1954 | C1894 | A1834 | C1774 | U1714 | A1654 | U1534 | U1474 | C1414 |
| G2315 | G2255 | U2195 | A2135 | U2075 | A2015 | U1955 | C1895 | G1835 | U1775 | G1715 | A1655 | U1535 | G1475 | U1415 |
| G2316 | G2256 | C2196 | G2136 | U2076 | U2016 | U1956 | G1896 | C1836 | G1776 | U1716 | C1656 | C1536 | U1476 | G1416 |
| U2317 | U2257 | U2197 | U2137 | A2077 | U2017 | C1957 | G1897 | G1837 | U1777 | U1717 | U1657 | G1537 | U1477 | C1417 |
| G2318 | C2258 | A2198 | G2138 | C2078 | G2018 | C1958 | U1898 | C1838 | U1778 | G1718 | C1658 | G1538 | G1478 | G1418 |
| U2319 | U2259 | A2199 | U2139 | U2079 | A2019 | G1959 | A1899 | G1839 | U1779 | G1719 | G1659 | U1539 | G1479 | A1419 |
| U2320 | C2260 | C2200 | G2140 | A2080 | A2020 | A1960 | A1900 | G1840 | A1780 | U1720 | G1660 | G1540 | C1480 | A1420 |
| A2321 | G2261 | G2201 | G2141 | U2081 | C2021 | C1961 | A1901 | U1841 | U1781 | G1721 | G1661 | G1541 | G1481 | G1421 |
| U2322 | U2262 | U2202 | A2142 | A2082 | U2022 | C1962 | C1902 | G1842 | U1782 | A1722 | U1662 | U1542 | G1482 | G1422 |
| G2323 | G2263 | U2203 | C2143 | G2083 | C2023 | U1963 | G1903 | C1843 | A1783 | G1723 | G1663 | A1603 | G1483 | G1423 |
| U2324 | C2264 | G2204 | G2144 | C2084 | G2024 | G1964 | G1904 | C1844 | A1784 | G1724 | A1664 | A1544 | U1484 | G1424 |
| U2265 | U2265 | A2205 | C2145 | U2085 | C2025 | C1965 | C1905 | G1845 | A1785 | U1725 | A1665 | A1545 | U1485 | G1425 |
| A2266 | C2266 | C2206 | C2146 | U2086 | U2026 | A1966 | G1906 | G1846 | A1786 | C1726 | G1666 | G1546 | U1486 | G1426 |
| U2267 | G2267 | G2207 | A2147 | G2087 | G2027 | C1967 | G1907 | A1847 | A1787 | G1727 | G1667 | C1547 | U1487 | A1427 |
| A2268 | G2268 | C2208 | G2148 | A2088 | U2028 | G1968 | C1908 | A1848 | C1788 | G1728 | A1668 | A1548 | C1488 | C1428 |
| U2329 | G2269 | G2209 | U2149 | C2089 | G2029 | A1969 | C1909 | G1849 | A1789 | U1729 | A1669 | A1549 | C1489 | G1429 |
| G2330 | A2270 | U2210 | C2150 | A2090 | A2030 | A1970 | G1910 | G1850 | C1790 | G1730 | C1670 | A1550 | A1490 | G1430 |
| C2331 | G2271 | A2211 | U2151 | C2091 | A2031 | U1971 | U1911 | U1851 | A1791 | G1731 | U1671 | A1551 | G1491 | A1431 |
| U2272 | U2272 | A2212 | G2152 | U2092 | G2032 | C1972 | A1912 | G1852 | G1792 | C1732 | A1672 | A1552 | G1492 | G1432 |
| A2333 | G2273 | U2213 | C2153 | A2093 | A2033 | G1973 | A1913 | A1853 | C1793 | G1733 | G1673 | A1553 | C1493 | A1433 |
| U2334 | A2274 | C2214 | A2154 | A2094 | U2034 | C1974 | A1914 | A1854 | A1794 | G1674 | G1674 | U1554 | A1494 | A1434 |
| G2275 | G2275 | U2155 | U2155 | A2095 | G2035 | G1975 | G1915 | A1855 | A1735 | C1675 | G1675 | G1555 | G1495 | G1435 |
| A2335 | G2276 | G2216 | G2156 | C2096 | C2036 | U1976 | A1916 | U1856 | U1796 | U1736 | A1676 | A1556 | A1496 | G1436 |
| G2277 | G2277 | G2217 | G2157 | A2097 | A2037 | A1977 | U1917 | G1857 | G1797 | G1737 | A1677 | C1557 | U1497 | C1437 |
| A2278 | U2278 | A2218 | A2158 | U2098 | G2038 | A1978 | A1918 | A1858 | U1798 | G1738 | A1678 | C1558 | C1498 | U1438 |
| G2279 | G2279 | U2219 | C2159 | U2099 | U2039 | A1979 | A1919 | U1859 | G1799 | G1739 | A1679 | C1559 | C1499 | A1439 |
| A2340 | G2280 | U2220 | C2160 | G2100 | G2040 | G1980 | C1920 | G1860 | C1800 | G1740 | U1680 | G1560 | G1500 | U1440 |



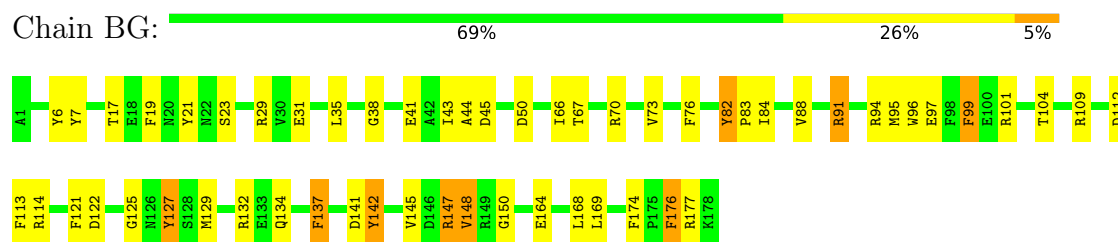
- Molecule 29: 50S ribosomal protein L3



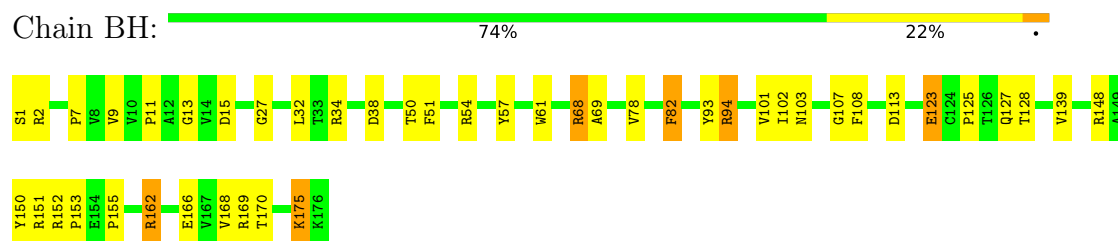
- Molecule 30: 50S ribosomal protein L4



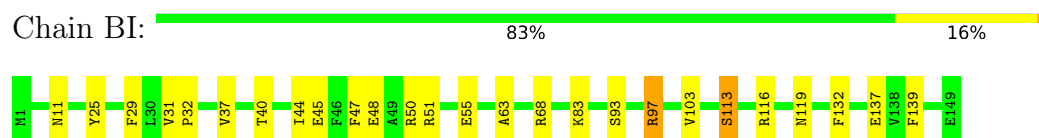
- Molecule 31: 50S ribosomal protein L5



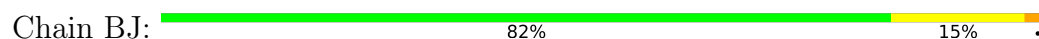
- Molecule 32: 50S ribosomal protein L6

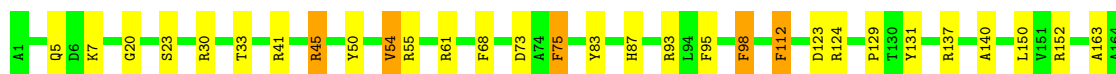


- Molecule 33: 50S ribosomal protein L9



- Molecule 34: 50S ribosomal protein L10





- Molecule 35: 50S ribosomal protein L11

Chain BK: 85% 13%



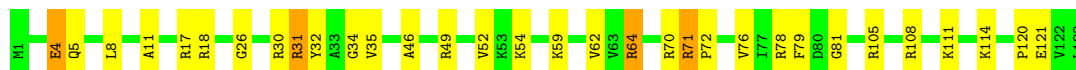
- Molecule 36: 50S ribosomal protein L13

Chain BL: 79% 17%



- Molecule 37: 50S ribosomal protein L14

Chain BM: 74% 23%



- Molecule 38: 50S ribosomal protein L15

Chain BN: 78% 21%



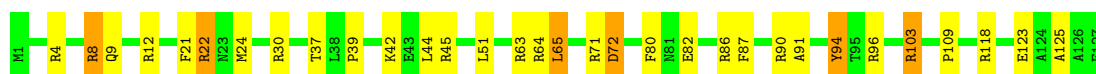
- Molecule 39: 50S ribosomal protein L16

Chain BO: 79% 16%



- Molecule 40: 50S ribosomal protein L17

Chain BP: 75% 20% 5%



- Molecule 41: 50S ribosomal protein L18

Chain BQ: 77% 20%



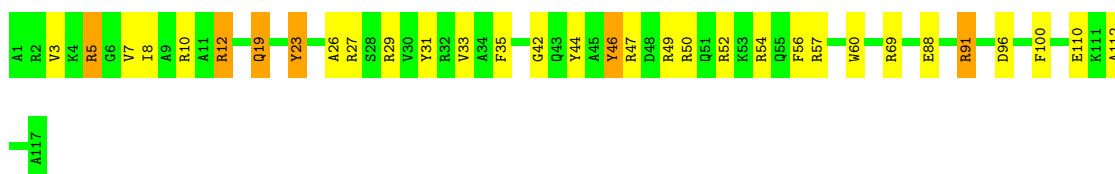
- Molecule 42: 50S ribosomal protein L19

Chain BR: 69% 28%



- Molecule 43: 50S ribosomal protein L20

Chain BS: 73% 22% 5%



- Molecule 44: 50S ribosomal protein L21

Chain BT: 80% 17%



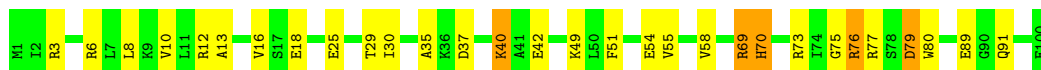
- Molecule 45: 50S ribosomal protein L22

Chain BU: 79% 18%



- Molecule 46: 50S ribosomal protein L23

Chain BV: 70% 25% 5%

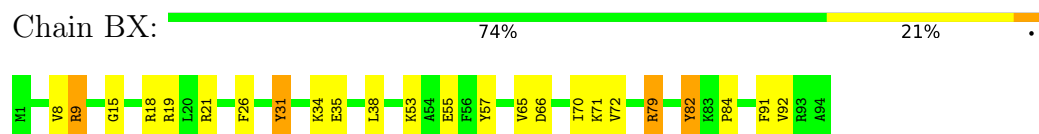


- Molecule 47: 50S ribosomal protein L24

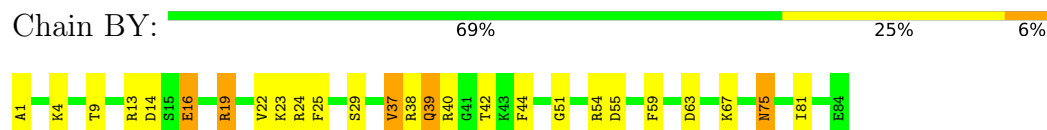
Chain BW: 81% 17%



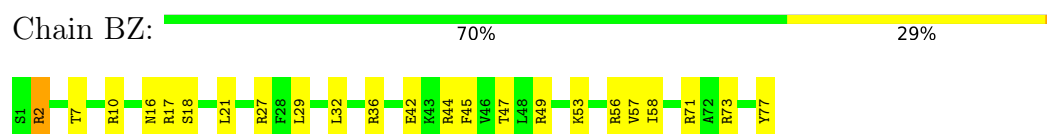
• Molecule 48: 50S ribosomal protein L25



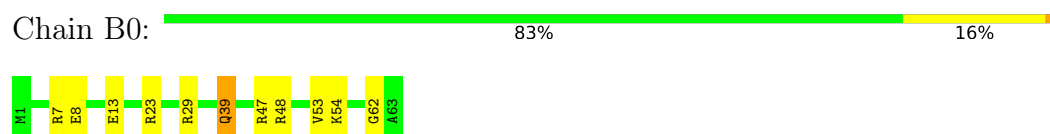
• Molecule 49: 50S ribosomal protein L27



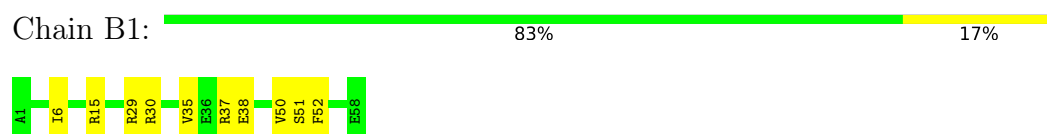
• Molecule 50: 50S ribosomal protein L28



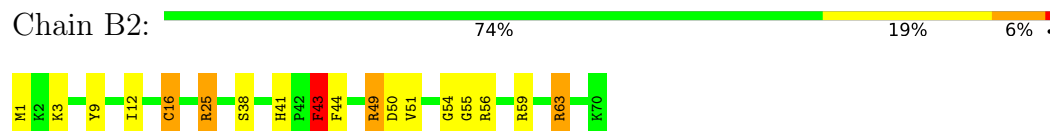
• Molecule 51: 50S ribosomal protein L29



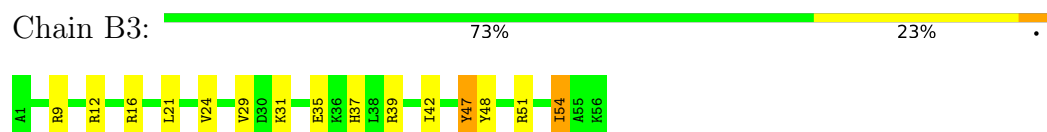
• Molecule 52: 50S ribosomal protein L30



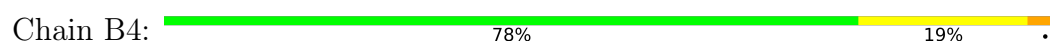
• Molecule 53: 50S ribosomal protein L31



• Molecule 54: 50S ribosomal protein L32

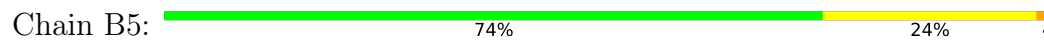


• Molecule 55: 50S ribosomal protein L33

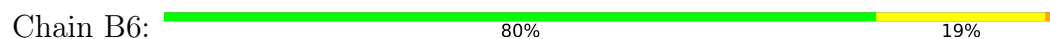




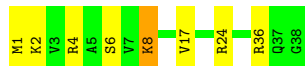
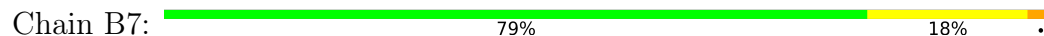
- Molecule 56: 50S ribosomal protein L34



- Molecule 57: 50S ribosomal protein L35



- Molecule 58: 50S ribosomal protein L36



4 Experimental information

| Property | Value | Source |
|--------------------------------------|--|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 21000 | Depositor |
| Resolution determination method | FSC 0.5 CUT-OFF | Depositor |
| CTF correction method | Volumes were CTF-corrected in defocus groups | Depositor |
| Microscope | FEI TECNAI F30 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 25 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 58269 | Depositor |
| Image detector | TVIPS TEMCAM-F415 (4k x 4k) | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 3TD, CH, OMG, 5MC, MA6, MIA, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, FME, 4SU, 7MG, 5MU, 1MG, 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 | AA | 3.07 | 3842/36769 (10.4%) | 3.54 | 8339/57354 (14.5%) |
| 10 | AJ | 1.51 | 5/1422 (0.4%) | 1.96 | 30/1908 (1.6%) |
| 11 | AK | 1.47 | 6/989 (0.6%) | 1.83 | 20/1326 (1.5%) |
| 12 | AL | 1.57 | 2/1048 (0.2%) | 1.98 | 28/1394 (2.0%) |
| 13 | AM | 1.46 | 3/835 (0.4%) | 2.17 | 31/1127 (2.8%) |
| 14 | AN | 1.51 | 2/982 (0.2%) | 1.85 | 20/1323 (1.5%) |
| 15 | AO | 1.51 | 3/969 (0.3%) | 2.08 | 29/1300 (2.2%) |
| 16 | AP | 1.55 | 1/919 (0.1%) | 1.88 | 20/1226 (1.6%) |
| 17 | AQ | 1.45 | 4/817 (0.5%) | 2.05 | 21/1088 (1.9%) |
| 18 | AR | 1.50 | 2/724 (0.3%) | 2.03 | 16/966 (1.7%) |
| 19 | AS | 1.50 | 4/659 (0.6%) | 2.09 | 14/884 (1.6%) |
| 2 | AB | 3.16 | 182/1600 (11.4%) | 3.61 | 372/2492 (14.9%) |
| 20 | AT | 1.46 | 2/681 (0.3%) | 2.02 | 24/913 (2.6%) |
| 21 | AU | 1.68 | 6/637 (0.9%) | 2.13 | 28/851 (3.3%) |
| 22 | AV | 1.44 | 3/744 (0.4%) | 1.80 | 16/995 (1.6%) |
| 23 | AW | 1.44 | 0/676 | 1.87 | 16/895 (1.8%) |
| 24 | AX | 1.54 | 3/598 (0.5%) | 2.37 | 30/792 (3.8%) |
| 25 | BA | 2.99 | 281/2869 (9.8%) | 3.51 | 651/4474 (14.6%) |
| 26 | BB | 3.08 | 7353/69257 (10.6%) | 3.54 | 15900/108040 (14.7%) |
| 27 | BC | 1.44 | 5/1748 (0.3%) | 1.89 | 32/2355 (1.4%) |
| 28 | BD | 1.55 | 11/2131 (0.5%) | 1.90 | 52/2863 (1.8%) |
| 29 | BE | 1.44 | 3/1586 (0.2%) | 1.91 | 40/2134 (1.9%) |
| 3 | AC | 3.10 | 124/1108 (11.2%) | 3.72 | 275/1724 (16.0%) |
| 30 | BF | 1.46 | 7/1571 (0.4%) | 1.94 | 37/2113 (1.8%) |
| 31 | BG | 1.58 | 11/1444 (0.8%) | 2.03 | 47/1937 (2.4%) |
| 32 | BH | 1.57 | 11/1343 (0.8%) | 1.89 | 39/1816 (2.1%) |
| 33 | BI | 1.56 | 7/1122 (0.6%) | 1.83 | 20/1515 (1.3%) |
| 34 | BJ | 1.49 | 3/1247 (0.2%) | 1.95 | 37/1679 (2.2%) |
| 35 | BK | 1.46 | 3/1046 (0.3%) | 1.85 | 17/1410 (1.2%) |
| 36 | BL | 1.48 | 6/1152 (0.5%) | 1.94 | 27/1551 (1.7%) |
| 37 | BM | 1.49 | 3/956 (0.3%) | 2.06 | 24/1279 (1.9%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------------|-------------|----------------------|
| | | RMSZ | # Z >2 | RMSZ | # Z >2 |
| 38 | BN | 1.52 | 5/1062 (0.5%) | 1.88 | 26/1413 (1.8%) |
| 39 | BO | 1.49 | 4/1093 (0.4%) | 1.95 | 25/1460 (1.7%) |
| 4 | AD | 3.15 | 181/1721 (10.5%) | 3.52 | 392/2683 (14.6%) |
| 40 | BP | 1.52 | 4/1021 (0.4%) | 2.12 | 32/1364 (2.3%) |
| 41 | BQ | 1.54 | 4/910 (0.4%) | 1.99 | 23/1219 (1.9%) |
| 42 | BR | 1.55 | 5/929 (0.5%) | 1.93 | 26/1242 (2.1%) |
| 43 | BS | 1.57 | 10/960 (1.0%) | 2.05 | 33/1278 (2.6%) |
| 44 | BT | 1.50 | 3/829 (0.4%) | 1.84 | 16/1107 (1.4%) |
| 45 | BU | 1.49 | 1/864 (0.1%) | 1.95 | 26/1156 (2.2%) |
| 46 | BV | 1.54 | 3/794 (0.4%) | 1.91 | 18/1060 (1.7%) |
| 47 | BW | 1.53 | 1/797 (0.1%) | 1.83 | 15/1062 (1.4%) |
| 48 | BX | 1.46 | 3/766 (0.4%) | 1.89 | 22/1025 (2.1%) |
| 49 | BY | 1.57 | 4/642 (0.6%) | 2.03 | 20/848 (2.4%) |
| 5 | AE | 1.46 | 6/1904 (0.3%) | 1.85 | 30/2565 (1.2%) |
| 50 | BZ | 1.58 | 2/635 (0.3%) | 1.97 | 14/848 (1.7%) |
| 51 | B0 | 1.43 | 1/510 (0.2%) | 2.10 | 9/677 (1.3%) |
| 52 | B1 | 1.40 | 0/453 | 2.08 | 9/605 (1.5%) |
| 53 | B2 | 1.45 | 1/559 (0.2%) | 2.02 | 17/745 (2.3%) |
| 54 | B3 | 1.52 | 4/450 (0.9%) | 1.89 | 10/599 (1.7%) |
| 55 | B4 | 1.48 | 0/448 | 1.91 | 6/594 (1.0%) |
| 56 | B5 | 1.65 | 1/380 (0.3%) | 2.10 | 13/498 (2.6%) |
| 57 | B6 | 1.47 | 0/513 | 1.90 | 7/676 (1.0%) |
| 58 | B7 | 1.51 | 2/303 (0.7%) | 2.07 | 8/397 (2.0%) |
| 6 | AF | 1.47 | 6/1852 (0.3%) | 2.14 | 61/2490 (2.4%) |
| 7 | AG | 1.54 | 7/1665 (0.4%) | 1.95 | 47/2227 (2.1%) |
| 8 | AH | 1.48 | 3/1239 (0.2%) | 1.96 | 33/1664 (2.0%) |
| 9 | AI | 1.50 | 5/1121 (0.4%) | 1.99 | 30/1509 (2.0%) |
| All | All | 2.69 | 12164/164069 (7.4%) | 3.18 | 27220/244735 (11.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AA | 0 | 881 |
| 10 | AJ | 0 | 4 |
| 11 | AK | 0 | 2 |
| 12 | AL | 0 | 2 |
| 14 | AN | 0 | 3 |
| 15 | AO | 0 | 4 |
| 16 | AP | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 17 | AQ | 0 | 4 |
| 18 | AR | 0 | 1 |
| 19 | AS | 0 | 2 |
| 2 | AB | 0 | 40 |
| 20 | AT | 0 | 1 |
| 21 | AU | 0 | 3 |
| 22 | AV | 0 | 2 |
| 23 | AW | 0 | 1 |
| 24 | AX | 0 | 2 |
| 25 | BA | 0 | 75 |
| 26 | BB | 0 | 1720 |
| 27 | BC | 0 | 2 |
| 28 | BD | 0 | 9 |
| 29 | BE | 0 | 4 |
| 3 | AC | 0 | 28 |
| 30 | BF | 0 | 3 |
| 31 | BG | 0 | 6 |
| 32 | BH | 0 | 3 |
| 33 | BI | 0 | 1 |
| 34 | BJ | 0 | 5 |
| 35 | BK | 0 | 3 |
| 36 | BL | 0 | 2 |
| 37 | BM | 0 | 5 |
| 38 | BN | 0 | 2 |
| 39 | BO | 0 | 3 |
| 4 | AD | 0 | 42 |
| 40 | BP | 0 | 4 |
| 41 | BQ | 0 | 6 |
| 42 | BR | 0 | 4 |
| 43 | BS | 0 | 6 |
| 44 | BT | 0 | 4 |
| 45 | BU | 0 | 5 |
| 46 | BV | 0 | 2 |
| 48 | BX | 0 | 4 |
| 49 | BY | 0 | 5 |
| 5 | AE | 0 | 3 |
| 50 | BZ | 0 | 2 |
| 51 | B0 | 0 | 1 |
| 52 | B1 | 0 | 1 |
| 53 | B2 | 0 | 4 |
| 54 | B3 | 0 | 1 |
| 55 | B4 | 0 | 4 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 56 | B5 | 0 | 2 |
| 57 | B6 | 0 | 2 |
| 6 | AF | 0 | 11 |
| 7 | AG | 0 | 6 |
| 8 | AH | 0 | 2 |
| 9 | AI | 0 | 4 |
| All | All | 0 | 2949 |

The worst 5 of 12164 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 26 | BB | 659 | G | N7-C5 | 18.05 | 1.50 | 1.39 |
| 26 | BB | 2104 | C | P-O5' | 17.37 | 1.77 | 1.59 |
| 26 | BB | 2168 | G | N7-C5 | 16.73 | 1.49 | 1.39 |
| 26 | BB | 268 | C | N1-C6 | 16.25 | 1.47 | 1.37 |
| 1 | AA | 1072 | G | P-O5' | 16.08 | 1.75 | 1.59 |

The worst 5 of 27220 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 51 | B0 | 48 | ARG | NE-CZ-NH1 | 24.22 | 132.41 | 120.30 |
| 26 | BB | 2494 | G | N3-C4-C5 | -22.56 | 117.32 | 128.60 |
| 51 | B0 | 48 | ARG | NE-CZ-NH2 | -21.50 | 109.55 | 120.30 |
| 26 | BB | 93 | G | C2-N3-C4 | 20.63 | 122.22 | 111.90 |
| 26 | BB | 1478 | G | N1-C6-O6 | -20.46 | 107.62 | 119.90 |

There are no chirality outliers.

5 of 2949 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 11 | G | Sidechain |
| 1 | AA | 3 | A | Sidechain |
| 1 | AA | 4 | U | Sidechain |
| 1 | AA | 5 | U | Sidechain |
| 1 | AA | 6 | G | 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 | AA | 33089 | 0 | 16619 | 0 | 0 |
| 2 | AB | 1627 | 0 | 844 | 0 | 0 |
| 3 | AC | 993 | 0 | 501 | 0 | 0 |
| 4 | AD | 1641 | 0 | 840 | 0 | 0 |
| 5 | AE | 1872 | 0 | 1885 | 0 | 0 |
| 6 | AF | 1822 | 0 | 1913 | 0 | 0 |
| 7 | AG | 1643 | 0 | 1710 | 0 | 0 |
| 8 | AH | 1225 | 0 | 1273 | 0 | 0 |
| 9 | AI | 1101 | 0 | 1050 | 0 | 0 |
| 10 | AJ | 1400 | 0 | 1449 | 0 | 0 |
| 11 | AK | 979 | 0 | 1034 | 0 | 0 |
| 12 | AL | 1036 | 0 | 1084 | 0 | 0 |
| 13 | AM | 825 | 0 | 865 | 0 | 0 |
| 14 | AN | 965 | 0 | 997 | 0 | 0 |
| 15 | AO | 955 | 0 | 1019 | 0 | 0 |
| 16 | AP | 910 | 0 | 981 | 0 | 0 |
| 17 | AQ | 805 | 0 | 847 | 0 | 0 |
| 18 | AR | 716 | 0 | 742 | 0 | 0 |
| 19 | AS | 649 | 0 | 666 | 0 | 0 |
| 20 | AT | 672 | 0 | 716 | 0 | 0 |
| 21 | AU | 626 | 0 | 651 | 0 | 0 |
| 22 | AV | 727 | 0 | 769 | 0 | 0 |
| 23 | AW | 670 | 0 | 722 | 0 | 0 |
| 24 | AX | 590 | 0 | 631 | 0 | 0 |
| 25 | BA | 2566 | 0 | 1296 | 0 | 0 |
| 26 | BB | 62351 | 0 | 31238 | 0 | 0 |
| 27 | BC | 1733 | 0 | 1824 | 0 | 0 |
| 28 | BD | 2092 | 0 | 2170 | 0 | 0 |
| 29 | BE | 1565 | 0 | 1616 | 0 | 0 |
| 30 | BF | 1552 | 0 | 1619 | 0 | 0 |
| 31 | BG | 1420 | 0 | 1460 | 0 | 0 |
| 32 | BH | 1323 | 0 | 1374 | 0 | 0 |
| 33 | BI | 1111 | 0 | 1148 | 0 | 0 |
| 34 | BJ | 1233 | 0 | 1283 | 0 | 0 |
| 35 | BK | 1032 | 0 | 1088 | 0 | 0 |
| 36 | BL | 1129 | 0 | 1162 | 0 | 0 |
| 37 | BM | 947 | 0 | 1023 | 0 | 0 |
| 38 | BN | 1053 | 0 | 1129 | 0 | 0 |
| 39 | BO | 1074 | 0 | 1157 | 0 | 0 |
| 40 | BP | 1008 | 0 | 1045 | 0 | 0 |
| 41 | BQ | 900 | 0 | 935 | 0 | 0 |
| 42 | BR | 917 | 0 | 965 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 43 | BS | 947 | 0 | 1022 | 0 | 0 |
| 44 | BT | 816 | 0 | 839 | 0 | 0 |
| 45 | BU | 857 | 0 | 922 | 0 | 0 |
| 46 | BV | 787 | 0 | 846 | 0 | 0 |
| 47 | BW | 789 | 0 | 847 | 0 | 0 |
| 48 | BX | 753 | 0 | 780 | 0 | 0 |
| 49 | BY | 634 | 0 | 656 | 0 | 0 |
| 50 | BZ | 625 | 0 | 655 | 0 | 0 |
| 51 | B0 | 509 | 0 | 543 | 0 | 0 |
| 52 | B1 | 449 | 0 | 491 | 0 | 0 |
| 53 | B2 | 549 | 0 | 552 | 0 | 0 |
| 54 | B3 | 444 | 0 | 461 | 0 | 0 |
| 55 | B4 | 441 | 0 | 485 | 0 | 0 |
| 56 | B5 | 377 | 0 | 418 | 0 | 0 |
| 57 | B6 | 504 | 0 | 574 | 0 | 0 |
| 58 | B7 | 302 | 0 | 343 | 0 | 0 |
| 59 | AB | 14 | 0 | 9 | 0 | 0 |
| 60 | BB | 10 | 0 | 10 | 0 | 0 |
| All | All | 152351 | 0 | 103793 | 0 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 5 | AE | 238/240 (99%) | 211 (89%) | 24 (10%) | 3 (1%) | 13 | 54 |
| 6 | AF | 230/232 (99%) | 204 (89%) | 20 (9%) | 6 (3%) | 6 | 38 |
| 7 | AG | 203/205 (99%) | 182 (90%) | 17 (8%) | 4 (2%) | 8 | 45 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 8 | AH | 164/166 (99%) | 146 (89%) | 15 (9%) | 3 (2%) | 9 | 47 |
| 9 | AI | 133/135 (98%) | 118 (89%) | 12 (9%) | 3 (2%) | 7 | 41 |
| 10 | AJ | 176/178 (99%) | 163 (93%) | 11 (6%) | 2 (1%) | 16 | 58 |
| 11 | AK | 127/129 (98%) | 116 (91%) | 9 (7%) | 2 (2%) | 11 | 50 |
| 12 | AL | 127/129 (98%) | 118 (93%) | 7 (6%) | 2 (2%) | 11 | 50 |
| 13 | AM | 101/103 (98%) | 92 (91%) | 5 (5%) | 4 (4%) | 3 | 29 |
| 14 | AN | 126/128 (98%) | 111 (88%) | 15 (12%) | 0 | 100 | 100 |
| 15 | AO | 121/123 (98%) | 103 (85%) | 14 (12%) | 4 (3%) | 4 | 33 |
| 16 | AP | 115/117 (98%) | 101 (88%) | 11 (10%) | 3 (3%) | 6 | 38 |
| 17 | AQ | 98/100 (98%) | 79 (81%) | 13 (13%) | 6 (6%) | 1 | 22 |
| 18 | AR | 86/88 (98%) | 82 (95%) | 3 (4%) | 1 (1%) | 14 | 56 |
| 19 | AS | 80/82 (98%) | 75 (94%) | 4 (5%) | 1 (1%) | 13 | 54 |
| 20 | AT | 81/83 (98%) | 66 (82%) | 14 (17%) | 1 (1%) | 14 | 56 |
| 21 | AU | 72/74 (97%) | 63 (88%) | 6 (8%) | 3 (4%) | 3 | 28 |
| 22 | AV | 89/91 (98%) | 79 (89%) | 6 (7%) | 4 (4%) | 3 | 28 |
| 23 | AW | 84/86 (98%) | 78 (93%) | 4 (5%) | 2 (2%) | 6 | 40 |
| 24 | AX | 68/70 (97%) | 53 (78%) | 13 (19%) | 2 (3%) | 5 | 36 |
| 27 | BC | 232/234 (99%) | 207 (89%) | 20 (9%) | 5 (2%) | 7 | 42 |
| 28 | BD | 270/272 (99%) | 232 (86%) | 30 (11%) | 8 (3%) | 5 | 35 |
| 29 | BE | 207/209 (99%) | 171 (83%) | 31 (15%) | 5 (2%) | 6 | 40 |
| 30 | BF | 199/201 (99%) | 171 (86%) | 16 (8%) | 12 (6%) | 2 | 22 |
| 31 | BG | 176/178 (99%) | 142 (81%) | 24 (14%) | 10 (6%) | 2 | 23 |
| 32 | BH | 174/176 (99%) | 149 (86%) | 22 (13%) | 3 (2%) | 10 | 49 |
| 33 | BI | 147/149 (99%) | 124 (84%) | 21 (14%) | 2 (1%) | 12 | 52 |
| 34 | BJ | 162/164 (99%) | 147 (91%) | 13 (8%) | 2 (1%) | 14 | 56 |
| 35 | BK | 139/141 (99%) | 126 (91%) | 12 (9%) | 1 (1%) | 24 | 67 |
| 36 | BL | 140/142 (99%) | 112 (80%) | 21 (15%) | 7 (5%) | 2 | 26 |
| 37 | BM | 121/123 (98%) | 104 (86%) | 13 (11%) | 4 (3%) | 4 | 33 |
| 38 | BN | 142/144 (99%) | 121 (85%) | 17 (12%) | 4 (3%) | 5 | 37 |
| 39 | BO | 134/136 (98%) | 116 (87%) | 14 (10%) | 4 (3%) | 5 | 35 |
| 40 | BP | 125/127 (98%) | 116 (93%) | 8 (6%) | 1 (1%) | 21 | 65 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 41 | BQ | 115/117 (98%) | 109 (95%) | 4 (4%) | 2 (2%) | 10 | 49 |
| 42 | BR | 112/114 (98%) | 88 (79%) | 22 (20%) | 2 (2%) | 9 | 47 |
| 43 | BS | 115/117 (98%) | 106 (92%) | 7 (6%) | 2 (2%) | 10 | 49 |
| 44 | BT | 101/103 (98%) | 90 (89%) | 8 (8%) | 3 (3%) | 5 | 35 |
| 45 | BU | 108/110 (98%) | 101 (94%) | 4 (4%) | 3 (3%) | 5 | 37 |
| 46 | BV | 98/100 (98%) | 78 (80%) | 14 (14%) | 6 (6%) | 1 | 22 |
| 47 | BW | 101/103 (98%) | 85 (84%) | 13 (13%) | 3 (3%) | 5 | 35 |
| 48 | BX | 92/94 (98%) | 82 (89%) | 9 (10%) | 1 (1%) | 16 | 58 |
| 49 | BY | 82/84 (98%) | 60 (73%) | 18 (22%) | 4 (5%) | 2 | 26 |
| 50 | BZ | 75/77 (97%) | 65 (87%) | 6 (8%) | 4 (5%) | 2 | 25 |
| 51 | B0 | 61/63 (97%) | 55 (90%) | 5 (8%) | 1 (2%) | 11 | 50 |
| 52 | B1 | 56/58 (97%) | 50 (89%) | 5 (9%) | 1 (2%) | 9 | 47 |
| 53 | B2 | 68/70 (97%) | 45 (66%) | 18 (26%) | 5 (7%) | 1 | 18 |
| 54 | B3 | 54/56 (96%) | 44 (82%) | 9 (17%) | 1 (2%) | 9 | 45 |
| 55 | B4 | 52/54 (96%) | 45 (86%) | 4 (8%) | 3 (6%) | 2 | 23 |
| 56 | B5 | 44/46 (96%) | 40 (91%) | 2 (4%) | 2 (4%) | 3 | 28 |
| 57 | B6 | 62/64 (97%) | 54 (87%) | 6 (10%) | 2 (3%) | 4 | 34 |
| 58 | B7 | 36/38 (95%) | 31 (86%) | 4 (11%) | 1 (3%) | 5 | 37 |
| All | All | 6319/6423 (98%) | 5506 (87%) | 643 (10%) | 170 (3%) | 9 | 38 |

5 of 170 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | AL | 86 | LEU |
| 13 | AM | 42 | LEU |
| 13 | AM | 57 | VAL |
| 16 | AP | 22 | TYR |
| 21 | AU | 11 | ARG |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 5 | AE | 198/198 (100%) | 191 (96%) | 7 (4%) | 39 | 66 |
| 6 | AF | 189/189 (100%) | 176 (93%) | 13 (7%) | 17 | 47 |
| 7 | AG | 172/172 (100%) | 165 (96%) | 7 (4%) | 33 | 62 |
| 8 | AH | 125/125 (100%) | 119 (95%) | 6 (5%) | 28 | 58 |
| 9 | AI | 116/116 (100%) | 109 (94%) | 7 (6%) | 21 | 52 |
| 10 | AJ | 146/146 (100%) | 139 (95%) | 7 (5%) | 28 | 58 |
| 11 | AK | 104/104 (100%) | 102 (98%) | 2 (2%) | 60 | 80 |
| 12 | AL | 106/106 (100%) | 104 (98%) | 2 (2%) | 60 | 80 |
| 13 | AM | 90/90 (100%) | 82 (91%) | 8 (9%) | 11 | 36 |
| 14 | AN | 98/98 (100%) | 95 (97%) | 3 (3%) | 43 | 69 |
| 15 | AO | 103/103 (100%) | 95 (92%) | 8 (8%) | 14 | 43 |
| 16 | AP | 95/95 (100%) | 90 (95%) | 5 (5%) | 25 | 56 |
| 17 | AQ | 83/83 (100%) | 82 (99%) | 1 (1%) | 74 | 87 |
| 18 | AR | 76/76 (100%) | 74 (97%) | 2 (3%) | 49 | 73 |
| 19 | AS | 65/65 (100%) | 63 (97%) | 2 (3%) | 43 | 69 |
| 20 | AT | 77/77 (100%) | 71 (92%) | 6 (8%) | 14 | 43 |
| 21 | AU | 64/64 (100%) | 59 (92%) | 5 (8%) | 14 | 43 |
| 22 | AV | 78/78 (100%) | 72 (92%) | 6 (8%) | 14 | 44 |
| 23 | AW | 65/65 (100%) | 62 (95%) | 3 (5%) | 29 | 59 |
| 24 | AX | 60/60 (100%) | 54 (90%) | 6 (10%) | 8 | 31 |
| 27 | BC | 181/181 (100%) | 171 (94%) | 10 (6%) | 24 | 55 |
| 28 | BD | 217/217 (100%) | 208 (96%) | 9 (4%) | 33 | 62 |
| 29 | BE | 164/164 (100%) | 156 (95%) | 8 (5%) | 27 | 58 |
| 30 | BF | 165/165 (100%) | 157 (95%) | 8 (5%) | 28 | 58 |
| 31 | BG | 149/149 (100%) | 141 (95%) | 8 (5%) | 24 | 55 |
| 32 | BH | 137/137 (100%) | 128 (93%) | 9 (7%) | 18 | 48 |
| 33 | BI | 114/114 (100%) | 108 (95%) | 6 (5%) | 25 | 56 |
| 34 | BJ | 122/122 (100%) | 118 (97%) | 4 (3%) | 41 | 67 |
| 35 | BK | 109/109 (100%) | 106 (97%) | 3 (3%) | 47 | 71 |
| 36 | BL | 116/116 (100%) | 111 (96%) | 5 (4%) | 32 | 61 |
| 37 | BM | 104/104 (100%) | 97 (93%) | 7 (7%) | 18 | 48 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 38 | BN | 103/103 (100%) | 97 (94%) | 6 (6%) | 22 | 52 |
| 39 | BO | 109/109 (100%) | 101 (93%) | 8 (7%) | 15 | 46 |
| 40 | BP | 103/103 (100%) | 97 (94%) | 6 (6%) | 22 | 52 |
| 41 | BQ | 87/87 (100%) | 83 (95%) | 4 (5%) | 29 | 59 |
| 42 | BR | 99/99 (100%) | 91 (92%) | 8 (8%) | 13 | 41 |
| 43 | BS | 89/89 (100%) | 87 (98%) | 2 (2%) | 55 | 77 |
| 44 | BT | 84/84 (100%) | 79 (94%) | 5 (6%) | 21 | 52 |
| 45 | BU | 93/93 (100%) | 92 (99%) | 1 (1%) | 76 | 88 |
| 46 | BV | 84/84 (100%) | 75 (89%) | 9 (11%) | 7 | 28 |
| 47 | BW | 84/84 (100%) | 79 (94%) | 5 (6%) | 21 | 52 |
| 48 | BX | 78/78 (100%) | 75 (96%) | 3 (4%) | 36 | 64 |
| 49 | BY | 62/62 (100%) | 60 (97%) | 2 (3%) | 42 | 68 |
| 50 | BZ | 67/67 (100%) | 63 (94%) | 4 (6%) | 21 | 52 |
| 51 | B0 | 55/55 (100%) | 53 (96%) | 2 (4%) | 38 | 65 |
| 52 | B1 | 48/48 (100%) | 46 (96%) | 2 (4%) | 32 | 61 |
| 53 | B2 | 62/62 (100%) | 57 (92%) | 5 (8%) | 13 | 41 |
| 54 | B3 | 47/47 (100%) | 42 (89%) | 5 (11%) | 7 | 29 |
| 55 | B4 | 48/48 (100%) | 47 (98%) | 1 (2%) | 56 | 78 |
| 56 | B5 | 38/38 (100%) | 37 (97%) | 1 (3%) | 49 | 73 |
| 57 | B6 | 51/51 (100%) | 45 (88%) | 6 (12%) | 6 | 25 |
| 58 | B7 | 34/34 (100%) | 32 (94%) | 2 (6%) | 21 | 52 |
| All | All | 5213/5213 (100%) | 4943 (95%) | 270 (5%) | 30 | 56 |

5 of 270 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | BD | 174 | ARG |
| 32 | BH | 102 | ILE |
| 52 | B1 | 35 | VAL |
| 29 | BE | 45 | TYR |
| 30 | BF | 96 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1538/1542 (99%) | 291 (18%) | 99 (6%) |
| 2 | AB | 74/76 (97%) | 23 (31%) | 6 (8%) |
| 25 | BA | 119/120 (99%) | 16 (13%) | 10 (8%) |
| 26 | BB | 2898/2904 (99%) | 544 (18%) | 186 (6%) |
| 3 | AC | 46/47 (97%) | 18 (39%) | 6 (13%) |
| 4 | AD | 76/77 (98%) | 17 (22%) | 4 (5%) |
| All | All | 4751/4766 (99%) | 909 (19%) | 311 (6%) |

5 of 909 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 8 | A |
| 1 | AA | 32 | A |
| 1 | AA | 36 | C |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |

5 of 311 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 26 | BB | 228 | C |
| 26 | BB | 847 | U |
| 26 | BB | 2610 | C |
| 26 | BB | 265 | A |
| 26 | BB | 561 | G |

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

49 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 |
| 1 | 2MG | AA | 1207 | 1 | 18,26,27 | 1.60 | 4 (22%) | 19,38,41 | 2.77 | 6 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 4OC | AA | 1402 | 1 | 16,23,24 | 1.61 | 3 (18%) | 20,32,35 | 1.58 | 1 (5%) |
| 1 | 5MC | AA | 1407 | 1 | 14,22,23 | 1.63 | 3 (21%) | 17,32,35 | 2.25 | 9 (52%) |
| 1 | UR3 | AA | 1498 | 1 | 13,22,23 | 1.69 | 5 (38%) | 15,32,35 | 1.39 | 2 (13%) |
| 1 | 2MG | AA | 1516 | 1 | 18,26,27 | 2.31 | 8 (44%) | 19,38,41 | 2.53 | 5 (26%) |
| 1 | MA6 | AA | 1518 | 1 | 16,26,27 | 1.37 | 2 (12%) | 16,38,41 | 1.57 | 5 (31%) |
| 1 | MA6 | AA | 1519 | 1 | 16,26,27 | 1.52 | 3 (18%) | 16,38,41 | 1.54 | 3 (18%) |
| 1 | PSU | AA | 516 | 1 | 16,21,22 | 2.94 | 6 (37%) | 20,30,33 | 7.15 | 10 (50%) |
| 1 | 7MG | AA | 527 | 1 | 20,26,27 | 2.00 | 6 (30%) | 24,39,42 | 1.74 | 5 (20%) |
| 1 | 2MG | AA | 966 | 1 | 18,26,27 | 1.48 | 4 (22%) | 19,38,41 | 2.51 | 6 (31%) |
| 1 | 5MC | AA | 967 | 1 | 14,22,23 | 1.99 | 4 (28%) | 17,32,35 | 1.75 | 4 (23%) |
| 2 | H2U | AB | 16 | 2 | 17,21,22 | 1.56 | 2 (11%) | 20,30,33 | 2.24 | 9 (45%) |
| 2 | H2U | AB | 17 | 2 | 17,21,22 | 1.53 | 3 (17%) | 20,30,33 | 2.31 | 6 (30%) |
| 2 | H2U | AB | 20 | 2 | 17,21,22 | 1.71 | 4 (23%) | 20,30,33 | 1.88 | 7 (35%) |
| 2 | OMC | AB | 32 | 2 | 15,22,23 | 1.78 | 3 (20%) | 20,31,34 | 1.98 | 4 (20%) |
| 2 | MIA | AB | 37 | 2 | 22,31,32 | 2.46 | 8 (36%) | 26,44,47 | 2.21 | 8 (30%) |
| 2 | 7MG | AB | 46 | 2 | 20,26,27 | 2.67 | 9 (45%) | 24,39,42 | 2.05 | 6 (25%) |
| 2 | 5MU | AB | 54 | 2 | 13,22,23 | 1.61 | 3 (23%) | 14,32,35 | 3.70 | 3 (21%) |
| 2 | PSU | AB | 55 | 2 | 16,21,22 | 1.92 | 3 (18%) | 20,30,33 | 5.42 | 7 (35%) |
| 2 | 4SU | AB | 8 | 2 | 13,21,22 | 1.47 | 2 (15%) | 14,30,33 | 2.82 | 5 (35%) |
| 4 | H2U | AD | 21 | 4 | 17,21,22 | 1.65 | 2 (11%) | 20,30,33 | 1.61 | 5 (25%) |
| 4 | OMC | AD | 33 | 4 | 15,22,23 | 1.22 | 2 (13%) | 20,31,34 | 1.71 | 4 (20%) |
| 4 | 5MU | AD | 55 | 4 | 13,22,23 | 1.93 | 5 (38%) | 14,32,35 | 3.26 | 3 (21%) |
| 4 | PSU | AD | 56 | 4 | 16,21,22 | 1.52 | 4 (25%) | 20,30,33 | 4.87 | 7 (35%) |
| 4 | 4SU | AD | 8 | 4 | 13,21,22 | 1.64 | 5 (38%) | 14,30,33 | 3.04 | 7 (50%) |
| 26 | 6MZ | BB | 1618 | 26 | 17,25,26 | 1.74 | 6 (35%) | 15,36,39 | 1.94 | 4 (26%) |
| 26 | 2MG | BB | 1835 | 26 | 18,26,27 | 1.97 | 5 (27%) | 19,38,41 | 3.20 | 6 (31%) |
| 26 | PSU | BB | 1911 | 26 | 16,21,22 | 2.27 | 2 (12%) | 20,30,33 | 5.71 | 7 (35%) |
| 26 | 3TD | BB | 1915 | 26 | 16,22,23 | 2.29 | 4 (25%) | 19,32,35 | 1.98 | 5 (26%) |
| 26 | PSU | BB | 1917 | 26 | 16,21,22 | 1.58 | 2 (12%) | 20,30,33 | 5.17 | 10 (50%) |
| 26 | 5MU | BB | 1939 | 26 | 13,22,23 | 2.06 | 3 (23%) | 14,32,35 | 2.74 | 3 (21%) |
| 26 | 5MC | BB | 1962 | 26 | 14,22,23 | 1.81 | 5 (35%) | 17,32,35 | 1.75 | 4 (23%) |
| 26 | 6MZ | BB | 2030 | 26 | 17,25,26 | 1.56 | 4 (23%) | 15,36,39 | 2.00 | 4 (26%) |
| 26 | 7MG | BB | 2069 | 26 | 20,26,27 | 2.37 | 5 (25%) | 24,39,42 | 2.33 | 6 (25%) |
| 26 | OMG | BB | 2251 | 26 | 18,26,27 | 2.03 | 6 (33%) | 22,38,41 | 2.94 | 6 (27%) |
| 26 | 2MG | BB | 2445 | 26 | 18,26,27 | 2.25 | 4 (22%) | 19,38,41 | 2.48 | 6 (31%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | H2U | BB | 2449 | 26 | 17,21,22 | 1.41 | 1 (5%) | 20,30,33 | 1.73 | 4 (20%) |
| 26 | PSU | BB | 2457 | 26 | 16,21,22 | 2.25 | 5 (31%) | 20,30,33 | 6.08 | 8 (40%) |
| 26 | OMC | BB | 2498 | 26 | 15,22,23 | 1.63 | 3 (20%) | 20,31,34 | 1.62 | 3 (15%) |
| 26 | 2MA | BB | 2503 | 26 | 16,25,26 | 1.41 | 3 (18%) | 17,37,40 | 1.76 | 5 (29%) |
| 26 | PSU | BB | 2504 | 26 | 16,21,22 | 1.53 | 3 (18%) | 20,30,33 | 5.96 | 8 (40%) |
| 26 | OMU | BB | 2552 | 26 | 14,22,23 | 2.13 | 4 (28%) | 17,31,34 | 2.06 | 9 (52%) |
| 26 | CH | BB | 2575 | 26 | 14,21,22 | 2.87 | 6 (42%) | 16,30,33 | 2.58 | 7 (43%) |
| 26 | PSU | BB | 2580 | 26 | 16,21,22 | 2.84 | 9 (56%) | 20,30,33 | 6.68 | 7 (35%) |
| 26 | PSU | BB | 2605 | 26 | 16,21,22 | 2.72 | 5 (31%) | 20,30,33 | 6.12 | 6 (30%) |
| 26 | 1MG | BB | 745 | 26 | 17,26,27 | 1.47 | 4 (23%) | 17,39,42 | 2.13 | 4 (23%) |
| 26 | PSU | BB | 746 | 26 | 16,21,22 | 2.24 | 4 (25%) | 20,30,33 | 5.55 | 8 (40%) |
| 26 | 5MU | BB | 747 | 26 | 13,22,23 | 1.41 | 2 (15%) | 14,32,35 | 3.40 | 5 (35%) |
| 26 | PSU | BB | 955 | 26 | 16,21,22 | 2.13 | 6 (37%) | 20,30,33 | 4.80 | 9 (45%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 1 | 2MG | AA | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 4OC | AA | 1402 | 1 | - | 0/7/29/30 | 0/2/2/2 |
| 1 | 5MC | AA | 1407 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | UR3 | AA | 1498 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 2MG | AA | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | MA6 | AA | 1518 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | MA6 | AA | 1519 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | PSU | AA | 516 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 7MG | AA | 527 | 1 | - | 1/7/37/38 | 0/3/3/3 |
| 1 | 2MG | AA | 966 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | AA | 967 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 2 | H2U | AB | 16 | 2 | - | 0/7/38/39 | 0/2/2/2 |
| 2 | H2U | AB | 17 | 2 | - | 1/7/38/39 | 0/2/2/2 |
| 2 | H2U | AB | 20 | 2 | - | 2/7/38/39 | 0/2/2/2 |
| 2 | OMC | AB | 32 | 2 | - | 0/5/27/28 | 0/2/2/2 |
| 2 | MIA | AB | 37 | 2 | - | 2/11/33/34 | 0/3/3/3 |
| 2 | 7MG | AB | 46 | 2 | - | 2/7/37/38 | 0/3/3/3 |
| 2 | 5MU | AB | 54 | 2 | - | 0/3/25/26 | 0/2/2/2 |
| 2 | PSU | AB | 55 | 2 | - | 1/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 2 | 4SU | AB | 8 | 2 | - | 1/3/25/26 | 0/2/2/2 |
| 4 | H2U | AD | 21 | 4 | - | 4/7/38/39 | 0/2/2/2 |
| 4 | OMC | AD | 33 | 4 | - | 0/5/27/28 | 0/2/2/2 |
| 4 | 5MU | AD | 55 | 4 | - | 0/3/25/26 | 0/2/2/2 |
| 4 | PSU | AD | 56 | 4 | - | 0/7/25/26 | 0/2/2/2 |
| 4 | 4SU | AD | 8 | 4 | - | 0/3/25/26 | 0/2/2/2 |
| 26 | 6MZ | BB | 1618 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | 2MG | BB | 1835 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | PSU | BB | 1911 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | 3TD | BB | 1915 | 26 | - | 1/7/25/26 | 0/2/2/2 |
| 26 | PSU | BB | 1917 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | 5MU | BB | 1939 | 26 | - | 0/3/25/26 | 0/2/2/2 |
| 26 | 5MC | BB | 1962 | 26 | - | 0/3/25/26 | 0/2/2/2 |
| 26 | 6MZ | BB | 2030 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | 7MG | BB | 2069 | 26 | - | 0/7/37/38 | 0/3/3/3 |
| 26 | OMG | BB | 2251 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | 2MG | BB | 2445 | 26 | - | 0/5/27/28 | 0/3/3/3 |
| 26 | H2U | BB | 2449 | 26 | - | 0/7/38/39 | 0/2/2/2 |
| 26 | PSU | BB | 2457 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | OMC | BB | 2498 | 26 | - | 0/5/27/28 | 0/2/2/2 |
| 26 | 2MA | BB | 2503 | 26 | - | 0/3/25/26 | 0/3/3/3 |
| 26 | PSU | BB | 2504 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | OMU | BB | 2552 | 26 | - | 0/5/27/28 | 0/2/2/2 |
| 26 | CH | BB | 2575 | 26 | - | 0/3/25/26 | 0/2/2/2 |
| 26 | PSU | BB | 2580 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | PSU | BB | 2605 | 26 | - | 0/7/25/26 | 0/2/2/2 |
| 26 | 1MG | BB | 745 | 26 | - | 0/3/25/26 | 0/3/3/3 |
| 26 | PSU | BB | 746 | 26 | - | 2/7/25/26 | 0/2/2/2 |
| 26 | 5MU | BB | 747 | 26 | - | 0/3/25/26 | 0/2/2/2 |
| 26 | PSU | BB | 955 | 26 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 204 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | AB | 37 | MIA | C2-S10 | -8.38 | 1.68 | 1.75 |
| 26 | BB | 2580 | PSU | C5-C1' | 7.94 | 1.59 | 1.52 |
| 26 | BB | 1915 | 3TD | C5-C1' | 7.23 | 1.58 | 1.52 |
| 26 | BB | 2445 | 2MG | C6-N1 | 7.17 | 1.45 | 1.33 |
| 1 | AA | 516 | PSU | O5'-C5' | -6.84 | 1.35 | 1.44 |

The worst 5 of 281 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 26 | BB | 2580 | PSU | N1-C2-N3 | -22.86 | 110.25 | 128.43 |
| 1 | AA | 516 | PSU | N1-C2-N3 | -21.26 | 111.53 | 128.43 |
| 26 | BB | 2605 | PSU | N1-C2-N3 | -19.70 | 112.77 | 128.43 |
| 26 | BB | 2457 | PSU | N1-C2-N3 | -18.23 | 113.93 | 128.43 |
| 1 | AA | 516 | PSU | C4-N3-C2 | 17.34 | 129.78 | 115.14 |

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 26 | BB | 746 | PSU | O4'-C1'-C5-C4 |
| 26 | BB | 746 | PSU | O4'-C1'-C5-C6 |
| 2 | AB | 46 | 7MG | C4'-C5'-O5'-P |
| 2 | AB | 20 | H2U | O4'-C4'-C5'-O5' |
| 1 | AA | 527 | 7MG | C4'-C5'-O5'-P |

There are no ring outliers.

No monomer is involved in short contacts.

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$ |
| 60 | FME | BB | 3001 | 59 | 9,9,10 | 1.18 | 2 (22%) | 6,9,11 | 1.46 | 1 (16%) |

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 |
|-----|------|-------|------|------|---------|----------|-------|
| 60 | FME | BB | 3001 | 59 | - | 2/6/9/11 | - |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 60 | BB | 3001 | FME | CB-CG | 2.19 | 1.60 | 1.51 |
| 60 | BB | 3001 | FME | CE-SD | 2.10 | 1.91 | 1.78 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 60 | BB | 3001 | FME | O-C-CA | -2.00 | 120.54 | 125.11 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|------------|
| 60 | BB | 3001 | FME | O1-CN-N-CA |
| 60 | BB | 3001 | FME | CB-CA-N-CN |

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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 26 | BB | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | BB | 2677:G | O3' | 2678:C | P | 1.76 |