



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 06:51 am BST

PDB ID : 6BOK
Title : E. coli release factor 1 (containing deletion 302-304) bound to the 70S ribosome
Authors : Svidritskiy, E.; Korostelev, A.A.
Deposited on : 2017-11-20
Resolution : 3.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

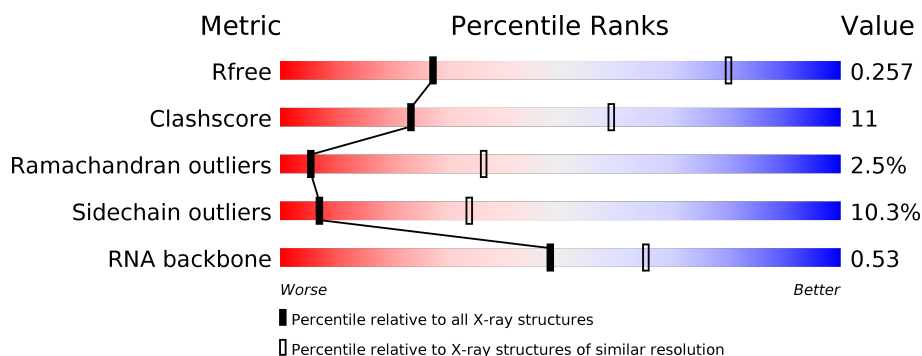
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 Å.

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




























| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1020 (3.62-3.50) |
| Clashscore | 141614 | 1100 (3.62-3.50) |
| Ramachandran outliers | 138981 | 1065 (3.62-3.50) |
| Sidechain outliers | 138945 | 1066 (3.62-3.50) |
| RNA backbone | 3102 | 1008 (4.10-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1507 | 50% 41% 8% . |
| 1 | DB | 1507 | 50% 41% 9% . |
| 2 | B | 2880 | 44% 41% 14% . |
| 2 | EB | 2880 | 48% 39% 12% . |
| 3 | C | 120 | 53% 37% 9% . |
| 3 | FB | 120 | 53% 39% 7% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | D | 77 |  |
| 4 | GB | 77 |  |
| 4 | IA | 77 |  |
| 4 | LC | 77 |  |
| 5 | E | 275 |  |
| 5 | HB | 275 |  |
| 6 | F | 206 |  |
| 6 | IB | 206 |  |
| 7 | G | 205 |  |
| 7 | JB | 205 |  |
| 8 | H | 182 |  |
| 8 | KB | 182 |  |
| 9 | I | 180 |  |
| 9 | LB | 180 |  |
| 10 | J | 148 |  |
| 10 | MB | 148 |  |
| 11 | K | 140 |  |
| 11 | NB | 140 |  |
| 12 | L | 122 |  |
| 12 | OB | 122 |  |
| 13 | M | 150 |  |
| 13 | PB | 150 |  |
| 14 | N | 141 |  |
| 14 | QB | 141 |  |
| 15 | O | 118 |  |















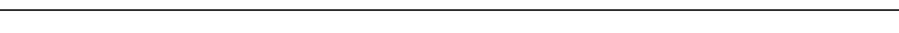




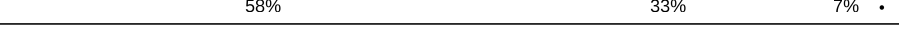





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | RB | 118 | |
| 16 | P | 112 | |
| 16 | SB | 112 | |
| 17 | Q | 146 | |
| 17 | TB | 146 | |
| 18 | R | 118 | |
| 18 | UB | 118 | |
| 19 | S | 101 | |
| 19 | VB | 101 | |
| 20 | T | 113 | |
| 20 | WB | 113 | |
| 21 | U | 96 | |
| 21 | XB | 96 | |
| 22 | V | 110 | |
| 22 | YB | 110 | |
| 23 | W | 206 | |
| 23 | ZB | 206 | |
| 24 | AC | 85 | |
| 24 | X | 85 | |
| 25 | BC | 98 | |
| 25 | Y | 98 | |
| 26 | CC | 72 | |
| 26 | Z | 72 | |
| 27 | AA | 60 | |
| 27 | DC | 60 | |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | BA | 71 |  |
| 28 | EC | 71 |  |
| 29 | CA | 60 |  |
| 29 | FC | 60 |  |
| 30 | DA | 54 |  |
| 30 | GC | 54 |  |
| 31 | EA | 49 |  |
| 31 | HC | 49 |  |
| 32 | FA | 65 |  |
| 32 | IC | 65 |  |
| 33 | GA | 37 |  |
| 33 | JC | 37 |  |
| 34 | HA | 27 |  |
| 34 | KC | 27 |  |
| 35 | JA | 256 |  |
| 35 | MC | 256 |  |
| 36 | KA | 239 |  |
| 36 | NC | 239 |  |
| 37 | LA | 209 |  |
| 37 | OC | 209 |  |
| 38 | MA | 162 |  |
| 38 | PC | 162 |  |
| 39 | NA | 101 |  |
| 39 | QC | 101 |  |
| 40 | OA | 156 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 40 | RC | 156 |  |
| 41 | PA | 138 |  |
| 41 | SC | 138 |  |
| 42 | QA | 128 |  |
| 42 | TC | 128 |  |
| 43 | RA | 105 |  |
| 43 | UC | 105 |  |
| 44 | SA | 129 |  |
| 44 | VC | 129 |  |
| 45 | TA | 132 |  |
| 45 | WC | 132 |  |
| 46 | UA | 126 |  |
| 46 | XC | 126 |  |
| 47 | VA | 61 |  |
| 47 | YC | 61 |  |
| 48 | WA | 89 |  |
| 48 | ZC | 89 |  |
| 49 | AD | 88 |  |
| 49 | XA | 88 |  |
| 50 | BD | 105 |  |
| 50 | YA | 105 |  |
| 51 | CD | 88 |  |
| 51 | ZA | 88 |  |
| 52 | AB | 93 |  |
| 52 | DD | 93 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | BB | 106 | |
| 53 | ED | 106 | |
| 54 | CB | 27 | |
| 54 | FD | 27 | |
| 55 | GD | 365 | |
| 55 | HD | 365 | |

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 299566 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | A | 1507 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32394 | 14424 | 5998 | 10465 | 1507 | | | |
| 1 | DB | 1507 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32394 | 14424 | 5998 | 10465 | 1507 | | | |

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 2 | B | 2880 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62031 | 27612 | 11589 | 19950 | 2880 | | | |
| 2 | EB | 2880 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62031 | 27612 | 11589 | 19950 | 2880 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|-------------|
| B | 154A | C | UNK | conflict | GB 46197919 |
| EB | 154A | C | UNK | conflict | GB 46197919 |

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 3 | C | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2576 | 1146 | 476 | 834 | 120 | | | |
| 3 | FB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2576 | 1146 | 476 | 834 | 120 | | | |

- Molecule 4 is a RNA chain called 16S ribosomal RNA.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 4 | D | 77 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1642 | 734 | 297 | 534 | 76 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---|---------|---------|-------|
| 4 | IA | 77 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1642 | 734 | 297 | 534 | 76 | 1 | | | |
| 4 | GB | 77 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1642 | 734 | 297 | 534 | 76 | 1 | | | |
| 4 | LC | 77 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 1642 | 734 | 297 | 534 | 76 | 1 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | E | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2145 | 1353 | 428 | 361 | 3 | | | |
| 5 | HB | 275 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2145 | 1353 | 428 | 361 | 3 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | F | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1563 | 988 | 299 | 270 | 6 | | | |
| 6 | IB | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1563 | 988 | 299 | 270 | 6 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7 | G | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1586 | 1011 | 297 | 275 | 3 | | | |
| 7 | JB | 202 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1586 | 1011 | 297 | 275 | 3 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | H | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1471 | 940 | 267 | 260 | 4 | | | |
| 8 | KB | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1471 | 940 | 267 | 260 | 4 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | I | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |
| 9 | LB | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | J | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1137 | 727 | 201 | 208 | 1 | | | |
| 10 | MB | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1137 | 727 | 201 | 208 | 1 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | K | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 722 | 208 | 187 | 4 | | | |
| 11 | NB | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 722 | 208 | 187 | 4 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | L | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 587 | 171 | 170 | 4 | | | |
| 12 | OB | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 932 | 587 | 171 | 170 | 4 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | M | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |
| 13 | PB | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1145 | 712 | 232 | 198 | 3 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | N | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 715 | 212 | 187 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | QB | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1121 | 715 | 212 | 187 | 7 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | O | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |
| 15 | RB | 118 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 968 | 604 | 203 | 160 | 1 | | | |

- Molecule 16 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | P | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 553 | 175 | 149 | | | | |
| 16 | SB | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 553 | 175 | 149 | | | | |

- Molecule 17 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | Q | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1143 | 713 | 234 | 195 | 1 | | | |
| 17 | TB | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1143 | 713 | 234 | 195 | 1 | | | |

- Molecule 18 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | R | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |
| 18 | UB | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 964 | 610 | 202 | 151 | 1 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | S | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |
| 19 | VB | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 779 | 501 | 142 | 135 | 1 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | T | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 175 | 153 | 2 | | | |
| 20 | WB | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 890 | 560 | 175 | 153 | 2 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | U | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |
| 21 | XB | 95 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 750 | 488 | 135 | 126 | 1 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | V | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 814 | 523 | 154 | 131 | 6 | | | |
| 22 | YB | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 814 | 523 | 154 | 131 | 6 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | W | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1495 | 953 | 266 | 273 | 3 | | | |
| 23 | ZB | 189 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1495 | 953 | 266 | 273 | 3 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | X | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 410 | 140 | 111 | 1 | | | |
| 24 | AC | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 662 | 410 | 140 | 111 | 1 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| X | 11 | ARG | LYS | conflict | UNP Q72HR3 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| AC | 11 | ARG | LYS | conflict | UNP Q72HR3 |

- Molecule 25 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | Y | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 761 | 478 | 151 | 131 | 1 | | | |
| 25 | BC | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 761 | 478 | 151 | 131 | 1 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | Z | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 592 | 368 | 119 | 103 | 2 | | | |
| 26 | CC | 70 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 592 | 368 | 119 | 103 | 2 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | AA | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 477 | 303 | 91 | 82 | 1 | | | |
| 27 | DC | 60 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 477 | 303 | 91 | 82 | 1 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28 | BA | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 552 | 349 | 99 | 99 | 5 | | | |
| 28 | EC | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 552 | 349 | 99 | 99 | 5 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | CA | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 460 | 290 | 90 | 75 | 5 | | | |
| 29 | FC | 59 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 460 | 290 | 90 | 75 | 5 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | DA | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |
| 30 | GC | 53 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 453 | 281 | 91 | 77 | 4 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 31 | EA | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |
| 31 | HC | 48 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 418 | 257 | 104 | 55 | 2 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 32 | FA | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |
| 32 | IC | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 517 | 331 | 102 | 82 | 2 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 33 | GA | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |
| 33 | JC | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 307 | 188 | 68 | 47 | 4 | | | |

- Molecule 34 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|---------|-------|
| 34 | HA | 11 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 220 | 98 | 44 | 67 | 11 | | | |
| 34 | KC | 11 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 220 | 98 | 44 | 67 | 11 | | | |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | MA | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |
| 38 | PC | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1155 | 729 | 218 | 204 | 4 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | TA | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 604 | 193 | 159 | 2 | | | |
| 45 | WC | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 604 | 193 | 159 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | UA | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 577 | 192 | 162 | 2 | | | |
| 46 | XC | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 577 | 192 | 162 | 2 | | | |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | YA | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 152 | 141 | 2 | | | |
| 50 | BD | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 528 | 152 | 141 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 51 | ZA | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |
| 51 | CD | 70 | Total | C | N | O | 0 | 0 | 0 |
| | | | 574 | 367 | 112 | 95 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | AB | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 424 | 124 | 115 | 2 | | | |
| 52 | DD | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 424 | 124 | 115 | 2 | | | |

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

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

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

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

- Molecule 55 is a protein called Peptide chain release factor 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 55 | GD | 255 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1980 | 1214 | 374 | 384 | 8 | | | |
| 55 | HD | 255 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1980 | 1214 | 374 | 384 | 8 | | | |

There are 22 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| GD | ? | - | ASP | deletion | UNP B7MKB3 |
| GD | ? | - | ARG | deletion | UNP B7MKB3 |
| GD | ? | - | SER | deletion | UNP B7MKB3 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| GD | 361 | LEU | - | expression tag | UNP B7MKB3 |
| GD | 362 | GLU | - | expression tag | UNP B7MKB3 |
| GD | 363 | HIS | - | expression tag | UNP B7MKB3 |
| GD | 364 | HIS | - | expression tag | UNP B7MKB3 |
| GD | 365 | HIS | - | expression tag | UNP B7MKB3 |
| GD | 366 | HIS | - | expression tag | UNP B7MKB3 |
| GD | 367 | HIS | - | expression tag | UNP B7MKB3 |
| GD | 368 | HIS | - | expression tag | UNP B7MKB3 |
| HD | ? | - | ASP | deletion | UNP B7MKB3 |
| HD | ? | - | ARG | deletion | UNP B7MKB3 |
| HD | ? | - | SER | deletion | UNP B7MKB3 |
| HD | 361 | LEU | - | expression tag | UNP B7MKB3 |
| HD | 362 | GLU | - | expression tag | UNP B7MKB3 |
| HD | 363 | HIS | - | expression tag | UNP B7MKB3 |
| HD | 364 | HIS | - | expression tag | UNP B7MKB3 |
| HD | 365 | HIS | - | expression tag | UNP B7MKB3 |
| HD | 366 | HIS | - | expression tag | UNP B7MKB3 |
| HD | 367 | HIS | - | expression tag | UNP B7MKB3 |
| HD | 368 | HIS | - | expression tag | UNP B7MKB3 |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 56 | CA | 1 | Total Mg 1 1 | 0 | 0 |
| 56 | AB | 1 | Total Mg 1 1 | 0 | 0 |
| 56 | RC | 2 | Total Mg 2 2 | 0 | 0 |
| 56 | PA | 2 | Total Mg 2 2 | 0 | 0 |
| 56 | LC | 8 | Total Mg 8 8 | 0 | 0 |
| 56 | V | 5 | Total Mg 5 5 | 0 | 0 |
| 56 | A | 160 | Total Mg 160 160 | 0 | 0 |
| 56 | BC | 1 | Total Mg 1 1 | 0 | 0 |
| 56 | PB | 2 | Total Mg 2 2 | 0 | 0 |
| 56 | NA | 2 | Total Mg 2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | JA | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | HC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | FB | 17 | Total 17 | Mg 17 | 0 | 0 |
| 56 | YB | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | Q | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | WC | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | H | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | C | 23 | Total 23 | Mg 23 | 0 | 0 |
| 56 | OB | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | MC | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | CD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | YA | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | KA | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AC | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | EB | 395 | Total 395 | Mg 395 | 0 | 0 |
| 56 | SC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | S | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | J | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | TA | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | E | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | IC | 2 | Total 2 | Mg 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | GD | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | EA | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XB | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | TB | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | VA | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | Z | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | RA | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | U | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | L | 7 | Total 7 | Mg 7 | 0 | 0 |
| 56 | PC | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | G | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | Y | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | NB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | ED | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | JB | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | FC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DB | 177 | Total 177 | Mg 177 | 0 | 0 |
| 56 | WB | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | W | 12 | Total 12 | Mg 12 | 0 | 0 |
| 56 | N | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | OA | 3 | Total 3 | Mg 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 56 | MB | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | ZC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | SB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QC | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | AD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | MA | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | I | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | IB | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | KC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | ZA | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | LA | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | XC | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | HD | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | TC | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | VB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | RB | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | IA | 8 | Total 8 | Mg 8 | 0 | 0 |
| 56 | P | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | K | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | JC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | LB | 5 | Total 5 | Mg 5 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | B | 514 | Total 514 | Mg 514 | 0 | 0 |
| 56 | HA | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | WA | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | T | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | R | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | HB | 8 | Total 8 | Mg 8 | 0 | 0 |
| 56 | M | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | FA | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | D | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | YC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | UC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | SA | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | O | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | QB | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | KB | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BD | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | GB | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | ZB | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | F | 1 | Total 1 | Mg 1 | 0 | 0 |

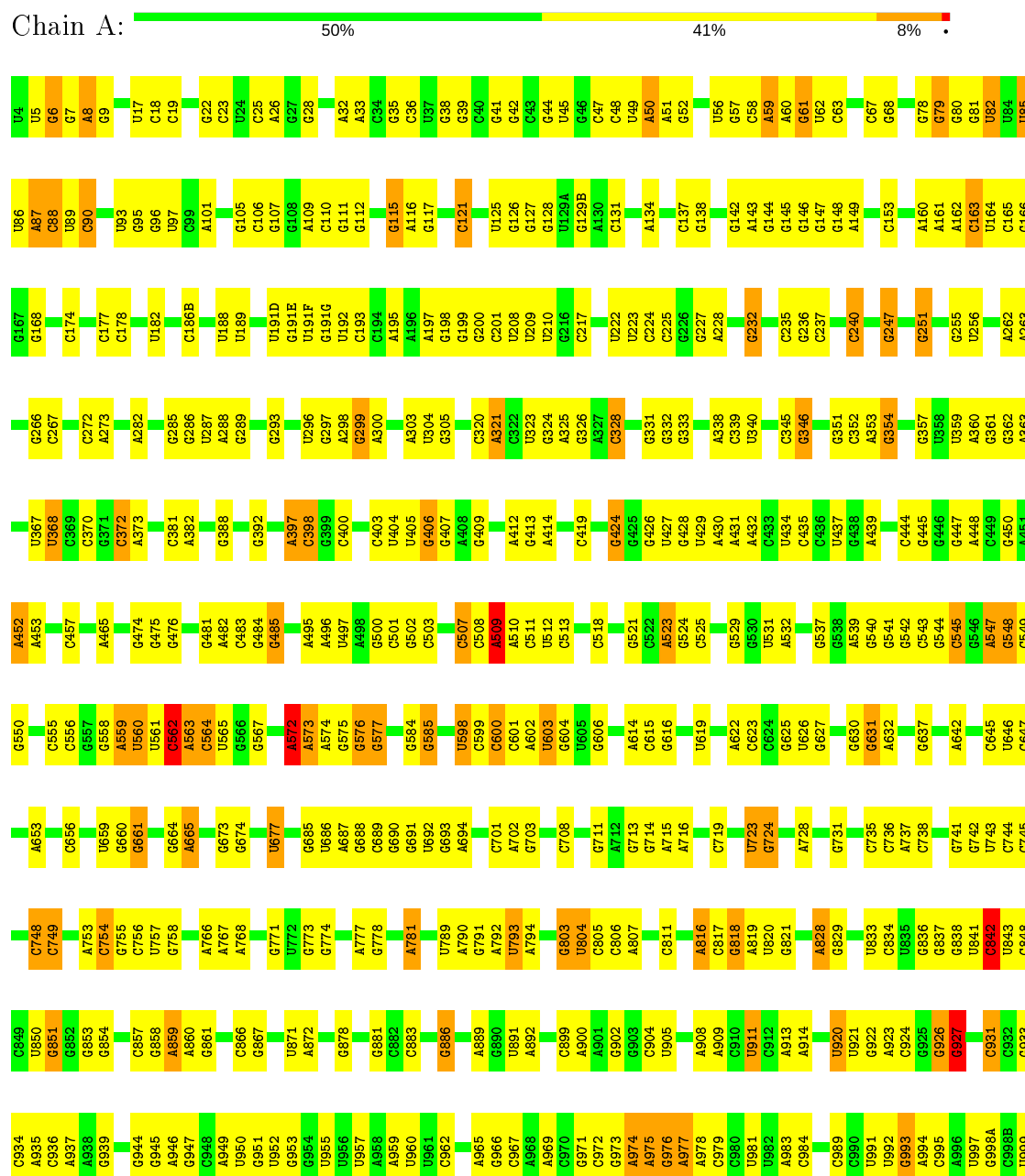
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

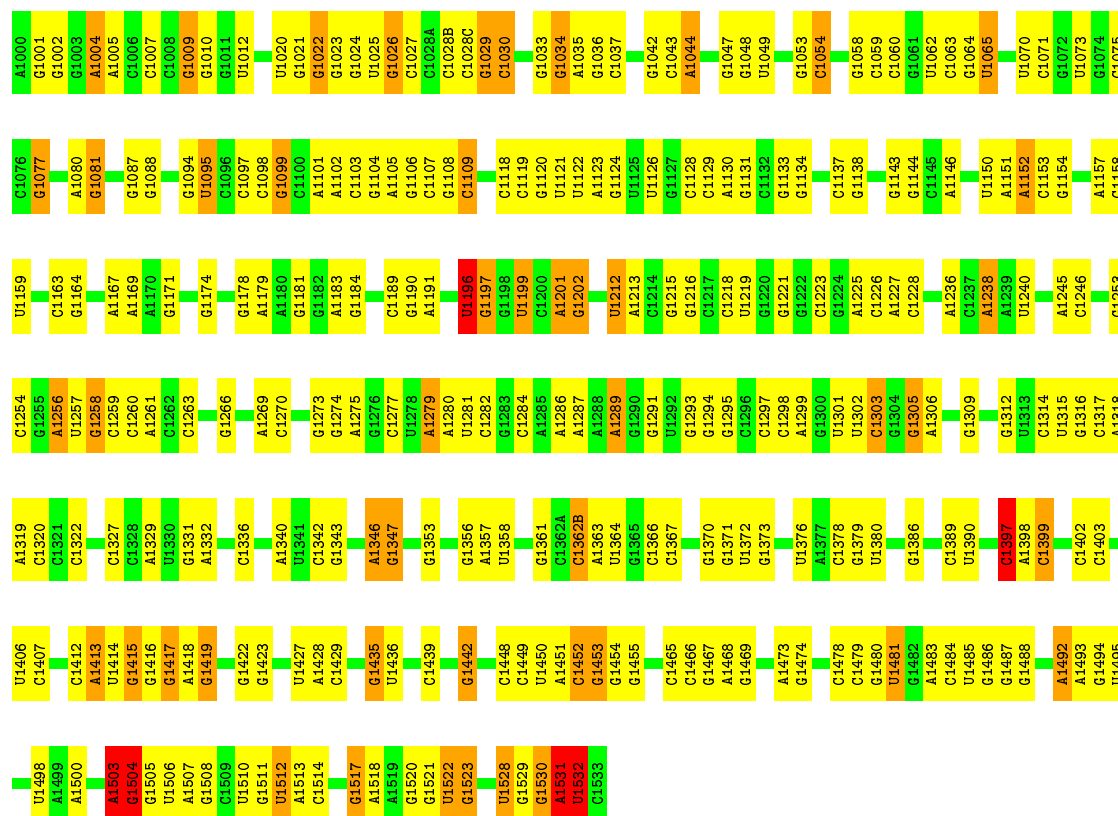
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57 | YB | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | BA | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | CA | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | JC | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | V | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | GA | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | DA | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | GC | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | EC | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | FC | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

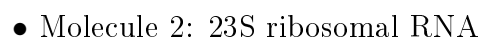
3 Residue-property plots

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







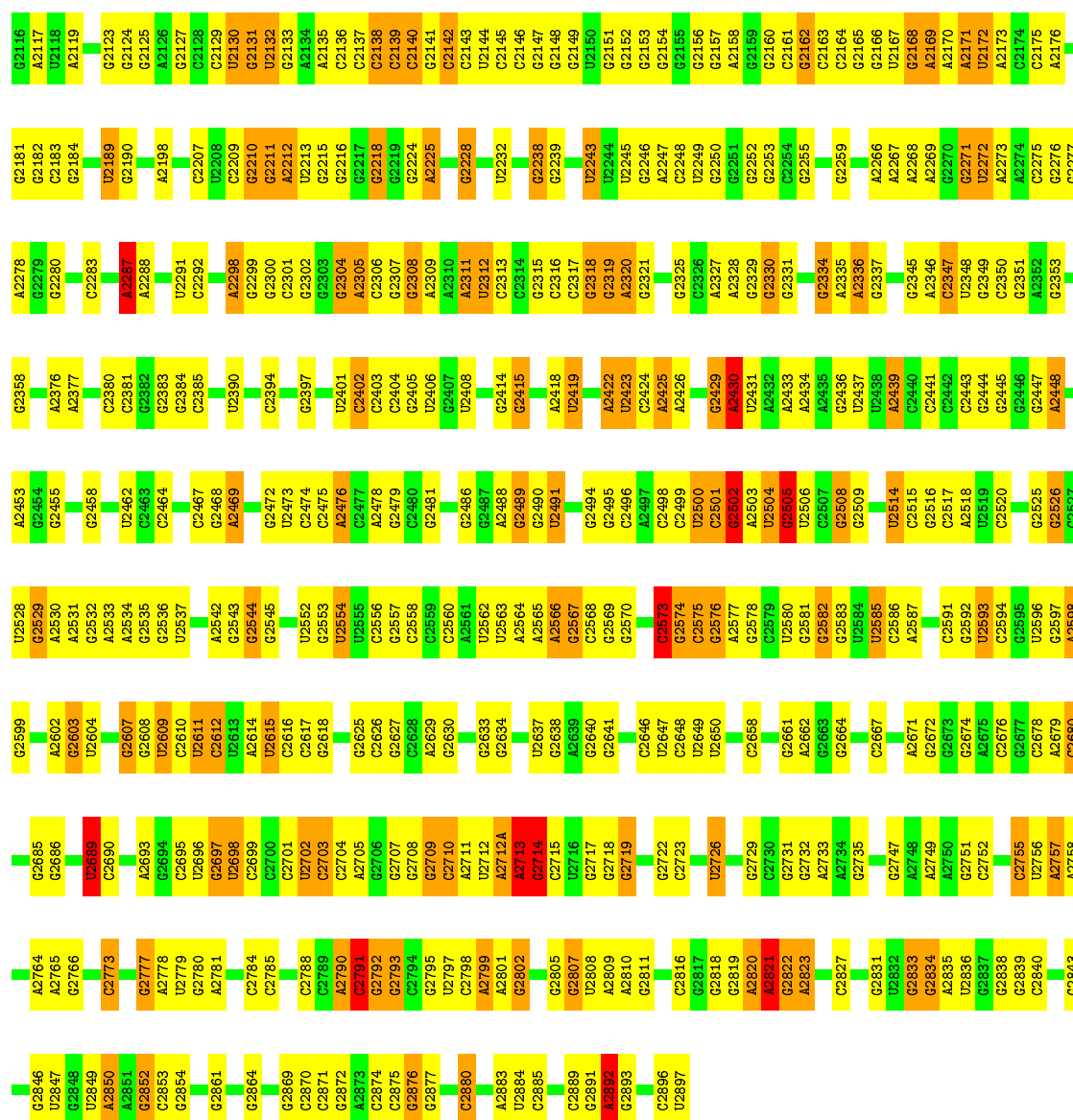
| | | |
|------|-------|-----|
| A152 | G89 | A6 |
| G139 | U90 | G7 |
| A190 | A91 | G10 |
| A191 | G92 | G14 |
| C192 | G93 | A14 |
| G193 | G94 | G15 |
| G194 | G95 | G16 |
| A195 | G96 | G17 |
| A196 | G101 | C18 |
| A197 | G102 | C19 |
| C198 | A103 | C22 |
| A199 | U104 | G23 |
| U200 | U108 | G26 |
| C203 | G109 | G27 |
| A204 | G115 | G30 |
| G205 | A118 | C31 |
| A207 | A119 | G34 |
| C208 | U120 | G35 |
| G212 | G121 | A38 |
| A213 | G122 | C39 |
| G214 | G123 | C40 |
| G215 | G124 | C41 |
| A216 | G125 | G43 |
| G220 | A126 | C46 |
| A222 | A127 | G51 |
| G223 | C128 | G55 |
| A225 | G129 | G58 |
| G226 | G133 | U59 |
| A227 | G136 | G60 |
| A228 | C137A | G61 |
| A229 | A225 | G68 |
| C238 | G226 | C69 |
| U239 | A227 | G70 |
| G240 | A228 | A71 |
| A241 | C150 | A74 |
| G242 | C151 | G75 |
| U243 | C154A | G76 |
| A244 | C155 | C77 |
| G245 | U165 | A78 |
| C246 | G171 | G79 |
| G247 | G176 | G80 |
| G248 | G177 | G81 |
| C249 | G178 | G82 |
| G250 | G179 | G83 |
| A251 | G180 | A84 |
| G252 | A181 | G85 |
| C253 | G182 | G86 |
| G254 | G183 | G87 |
| C255 | G184 | G88 |

WORLDWIDE
PDB
PROTEIN DATA BANK

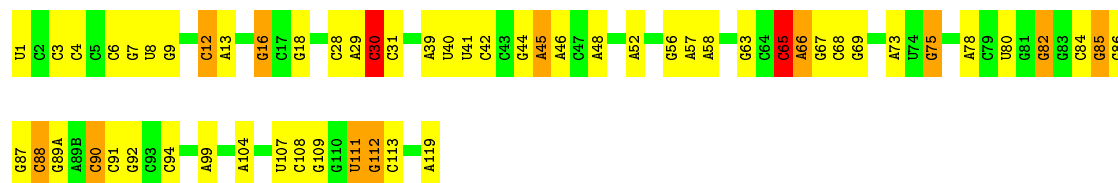
| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|
| G2526 | G2454 | C2209 | U2130 | A2054 | U1976 | G1906 | A1810 | G1728 | A1641 | G1567 | G1488 | U1397 |
| C2527 | G2455 | G2210 | G2131 | C2055 | C1979 | G1907 | A1811 | A1729 | G1642 | G1568 | U1489 | C1402 |
| U2528 | G2456 | A2211 | U2132 | G2056 | G1980 | C1908 | A1812 | U1730 | G1643 | A1569 | C1493 | |
| G2458 | G2457 | A2212 | C2133 | A2057 | A1981 | C1909 | G1813 | A1732 | G1646 | G1573 | A1494 | U1405 |
| A2530 | G2461 | G2215 | A2134 | A2058 | A1982 | A1913 | G1814 | C1742 | G1647 | U1578 | U1497 | C1407 |
| C2532 | U2462 | G2216 | C2135 | A2059 | C1983 | C1914 | A1815 | G1743 | C1648 | | | C1408 |
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| G2464 | G2384 | G2218 | C2137 | A2061 | G1989 | | A1817 | | | | | G1410 |
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| G2466 | G2386 | A2225 | C2139 | C2063 | G1993 | C1920 | A1819 | C1751 | A1652 | C1582 | A1508 | |
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| | | A2248 | G2156 | C2085 | G2010 | A1936 | G1843 | | | U1602 | A1434 | |
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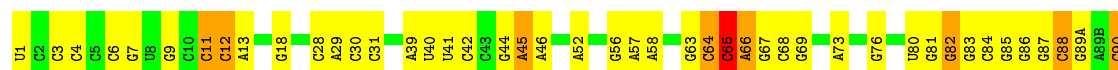
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| C2108 | U1943 | G1845 | U1768 | A1602 | C1518 | G1422 | A1253 | A1143 | U963 | |
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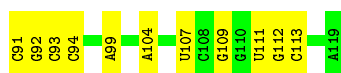


• Molecule 3: 5S ribosomal RNA

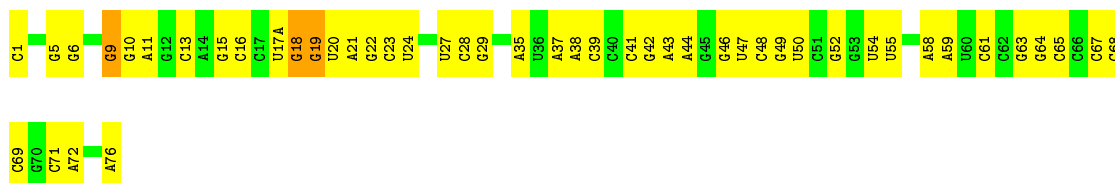


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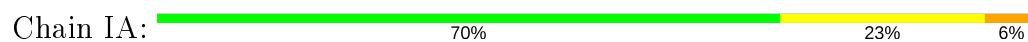




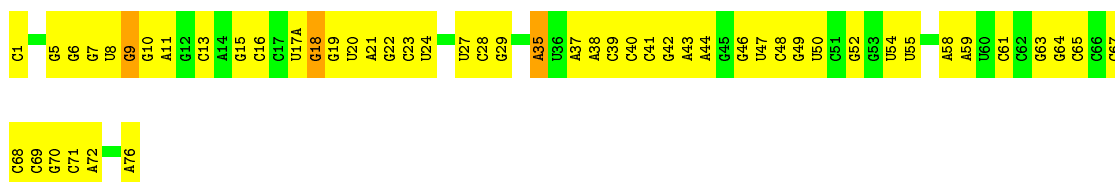
- Molecule 4: 16S ribosomal RNA



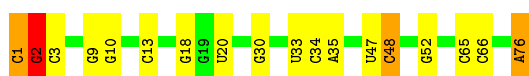
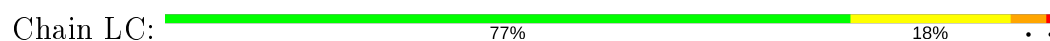
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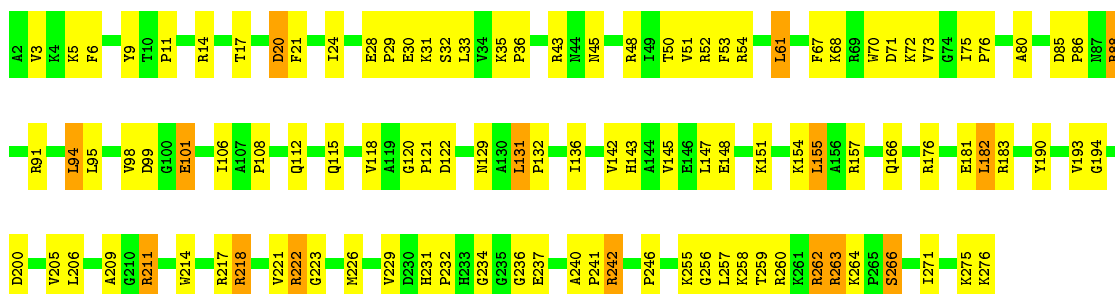
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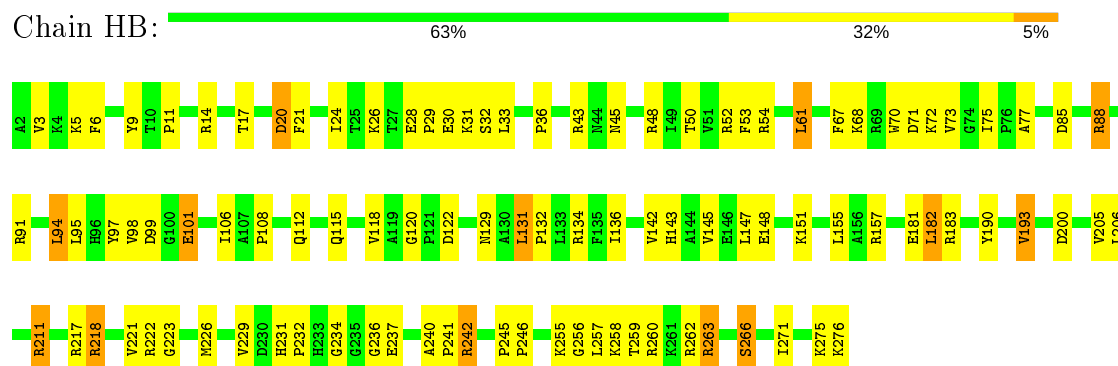
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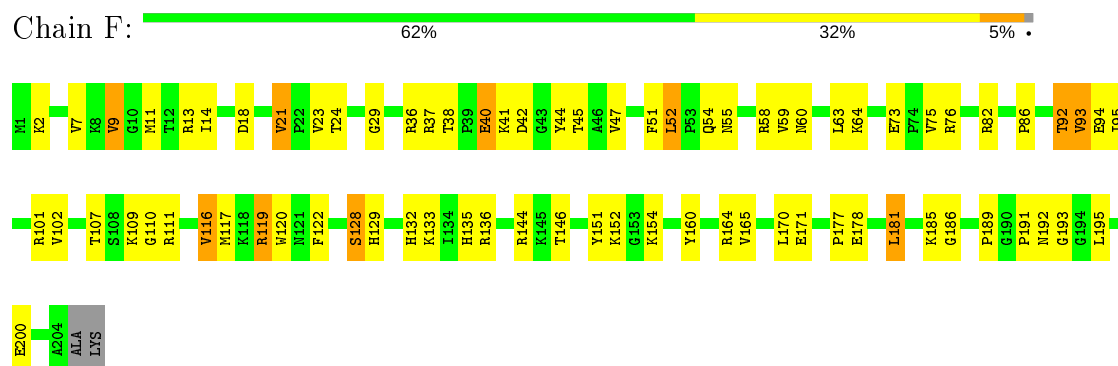
- Molecule 5: 50S ribosomal protein L2



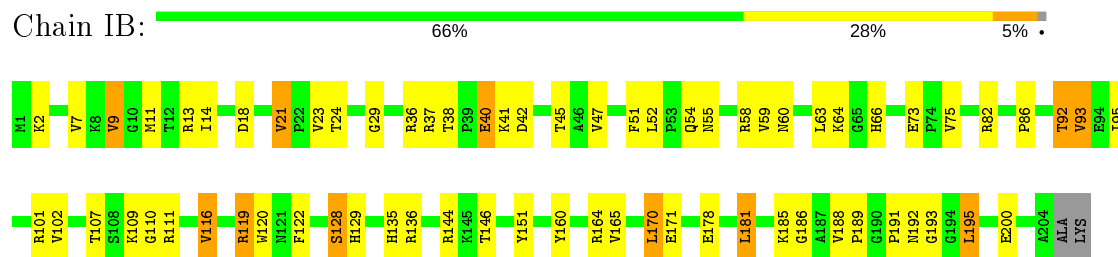
- Molecule 5: 50S ribosomal protein L2



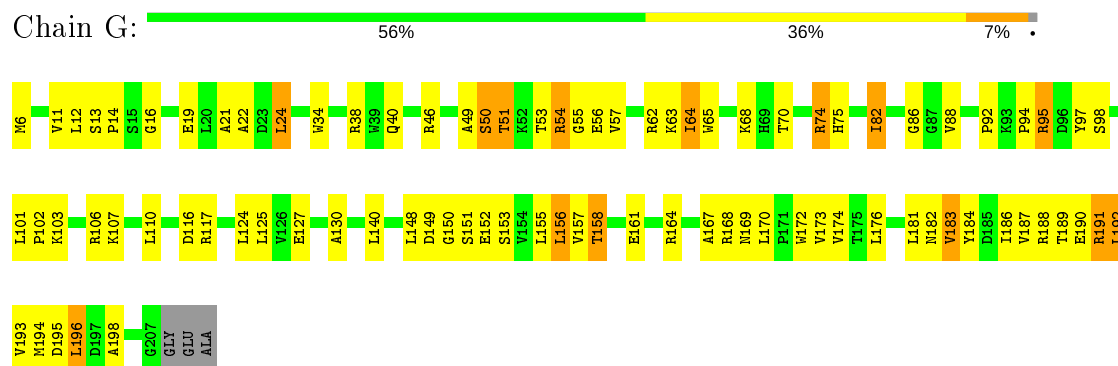
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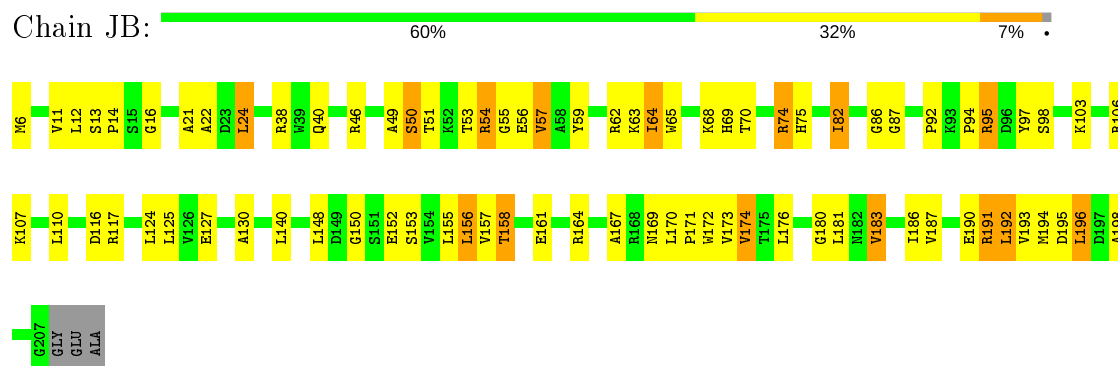
- Molecule 6: 50S ribosomal protein L3



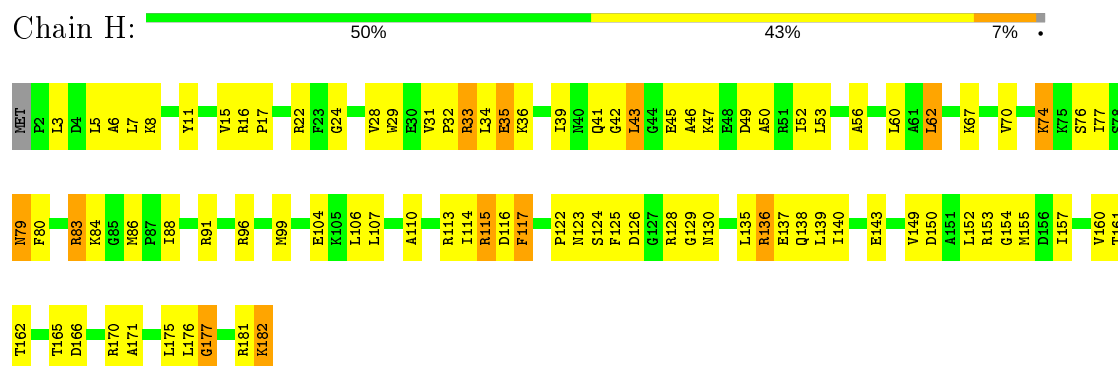
- Molecule 7: 50S ribosomal protein L4



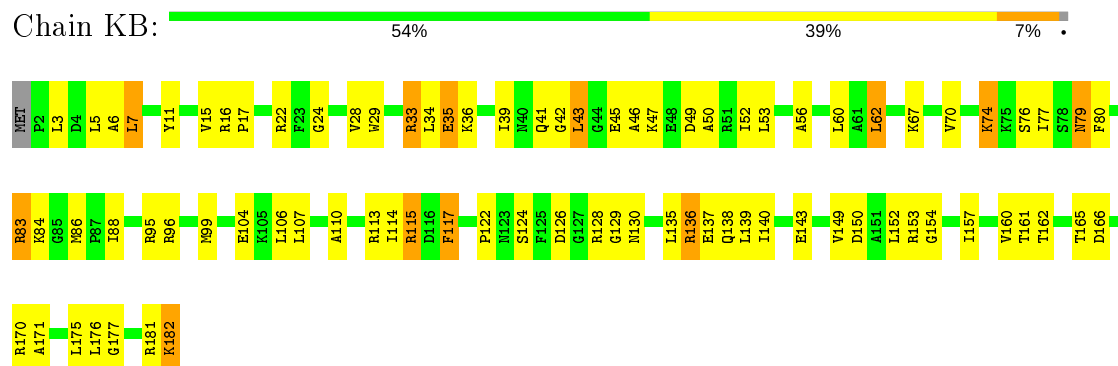
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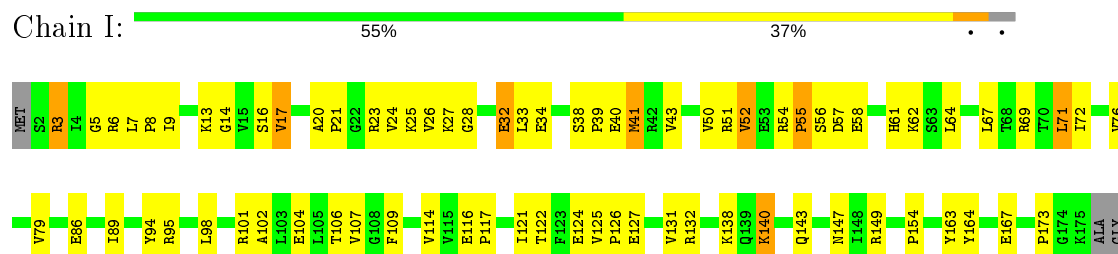
- Molecule 8: 50S ribosomal protein L5



- Molecule 8: 50S ribosomal protein L5



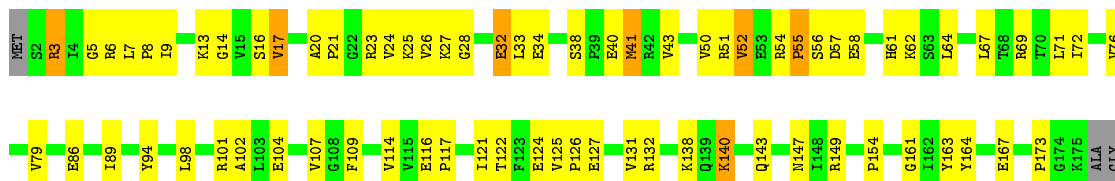
- Molecule 9: 50S ribosomal protein L6



ALA
LYS
LYS

- Molecule 9: 50S ribosomal protein L6

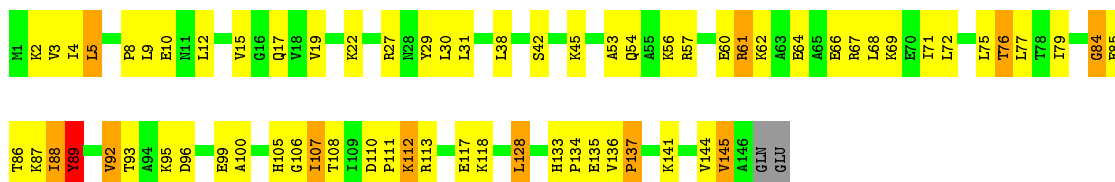
Chain LB:  56% 37%



ALA
LYS
LYS

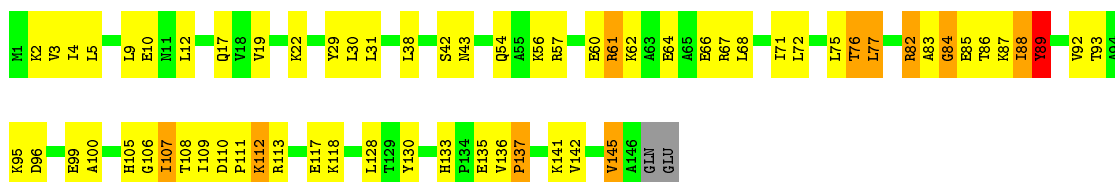
- Molecule 10: 50S ribosomal protein L9

Chain J:  53% 38% 7%



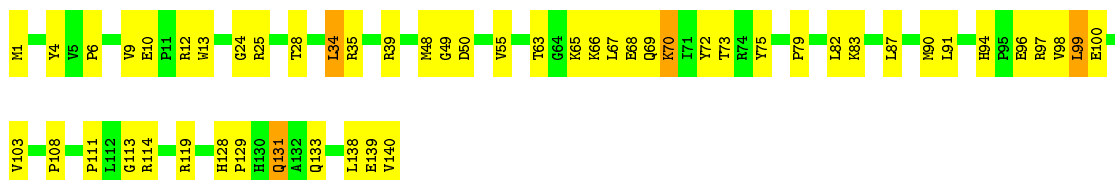
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Chain MB:  55% 36% 7%



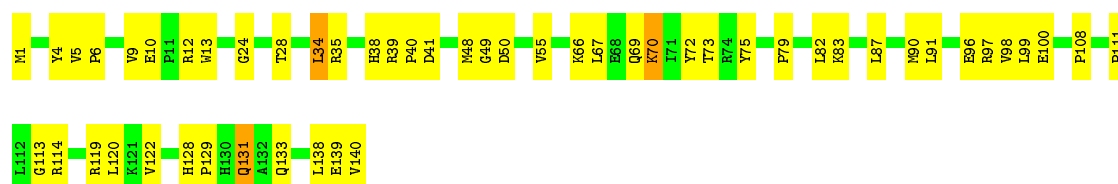
- Molecule 11: 50S ribosomal protein L13

Chain K:  63% 34%

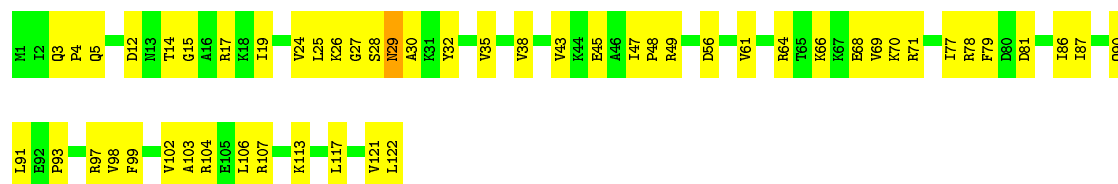


- Molecule 11: 50S ribosomal protein L13

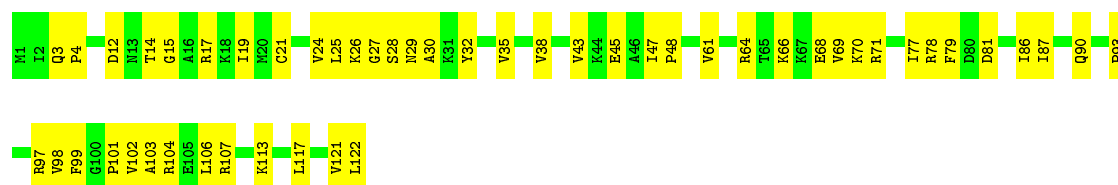
Chain NB:  63% 35%



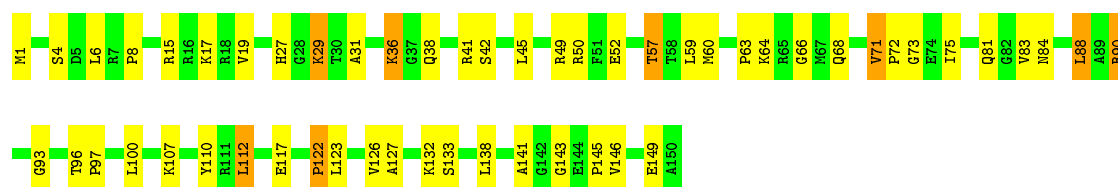
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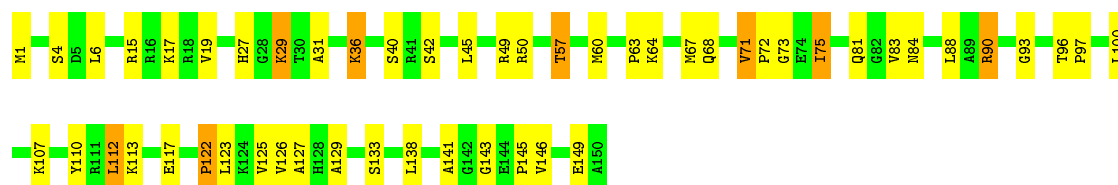
- Molecule 12: 50S ribosomal protein L14



- Molecule 13: 50S ribosomal protein L15

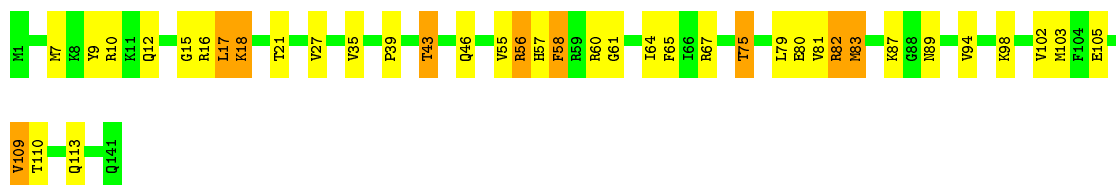


- Molecule 13: 50S ribosomal protein L15



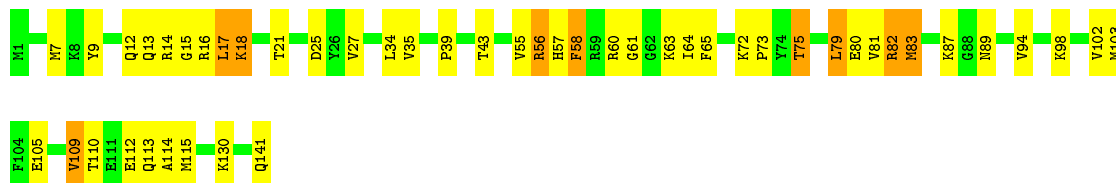
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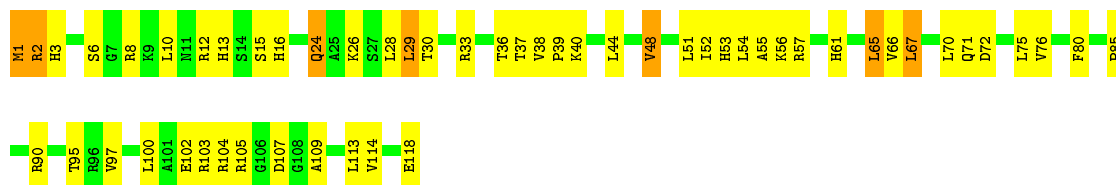
- Molecule 14: 50S ribosomal protein L16

Chain QB: 66% 28% 6%



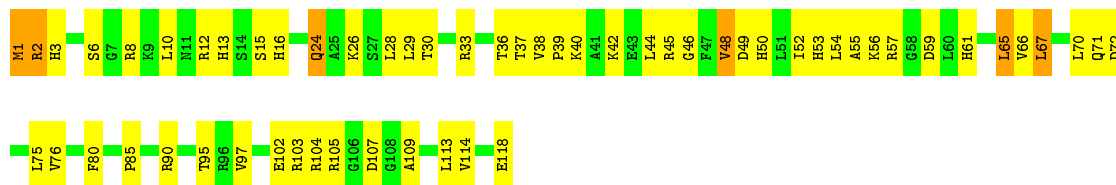
- Molecule 15: 50S ribosomal protein L17

Chain O: 54% 40% 6%



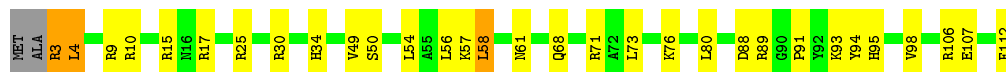
- Molecule 15: 50S ribosomal protein L17

Chain RB: 51% 44% 5%



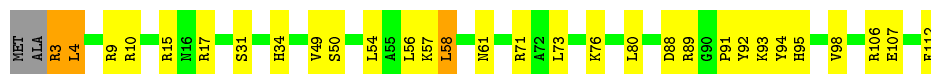
- Molecule 16: 50S ribosomal protein L18

Chain P: 71% 25% 4%

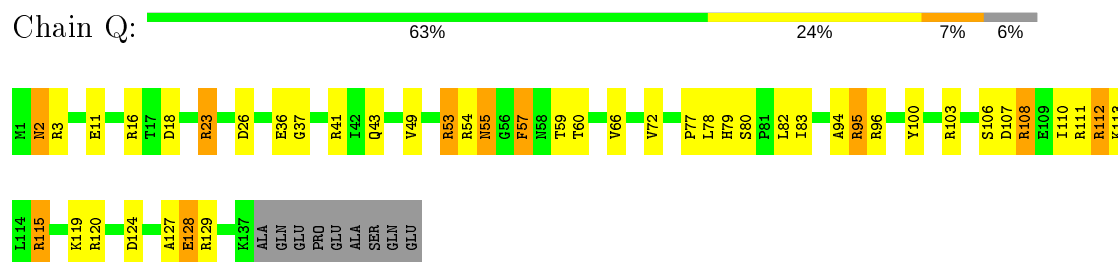


- Molecule 16: 50S ribosomal protein L18

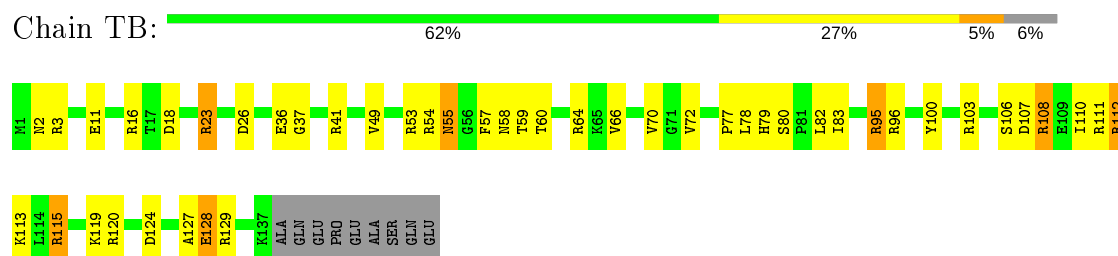
Chain SB: 71% 24% 5%



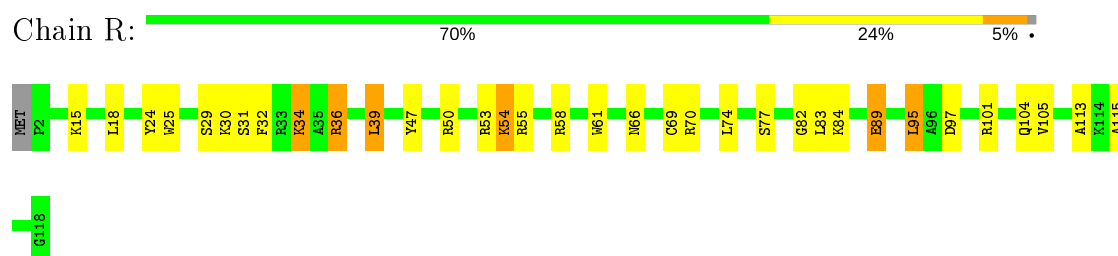
- Molecule 17: 50S ribosomal protein L19



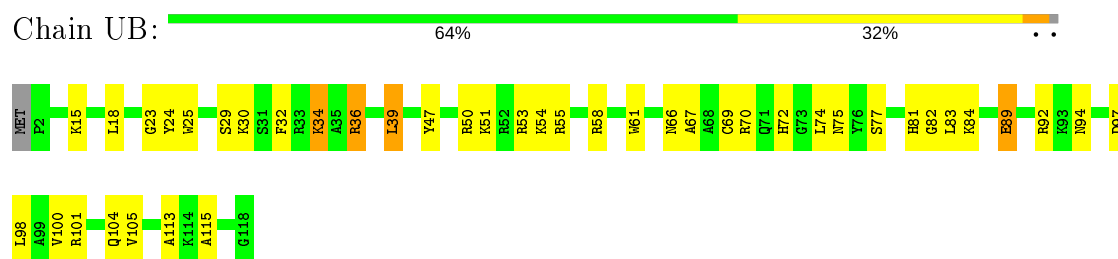
- Molecule 17: 50S ribosomal protein L19



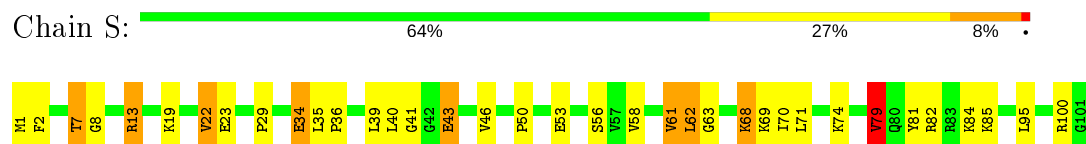
- Molecule 18: 50S ribosomal protein L20



- Molecule 18: 50S ribosomal protein L20



- Molecule 19: 50S ribosomal protein L21



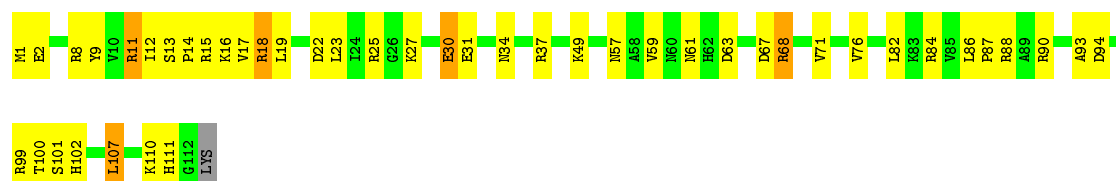
- Molecule 19: 50S ribosomal protein L21

Chain VB: 



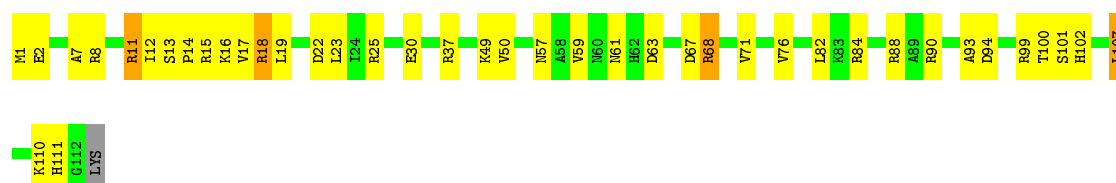
- Molecule 20: 50S ribosomal protein L22

Chain T: 




- Molecule 20: 50S ribosomal protein L22

Chain WB: 




- Molecule 21: 50S ribosomal protein L23

Chain U: 



- Molecule 21: 50S ribosomal protein L23

Chain XB: 



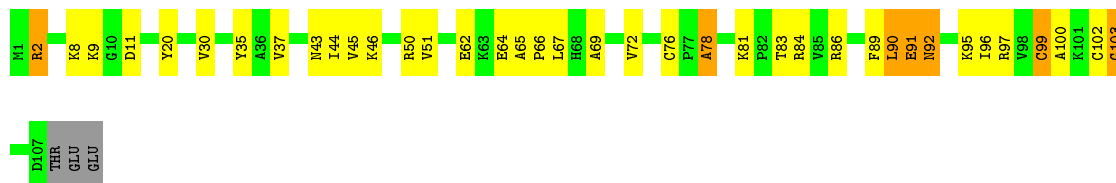
- Molecule 22: 50S ribosomal protein L24

Chain V: 



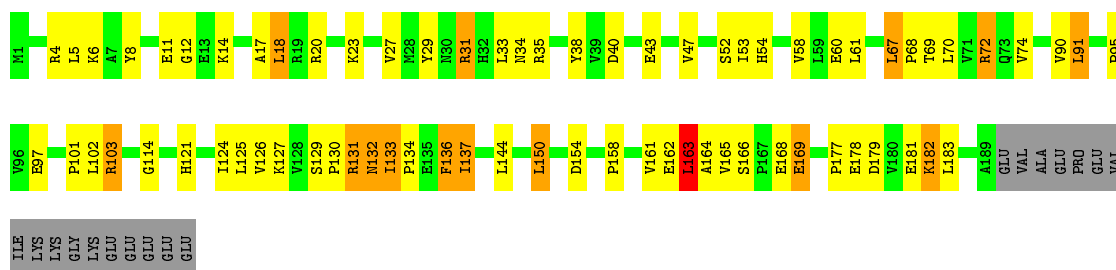
- Molecule 22: 50S ribosomal protein L24

Chain YB: 



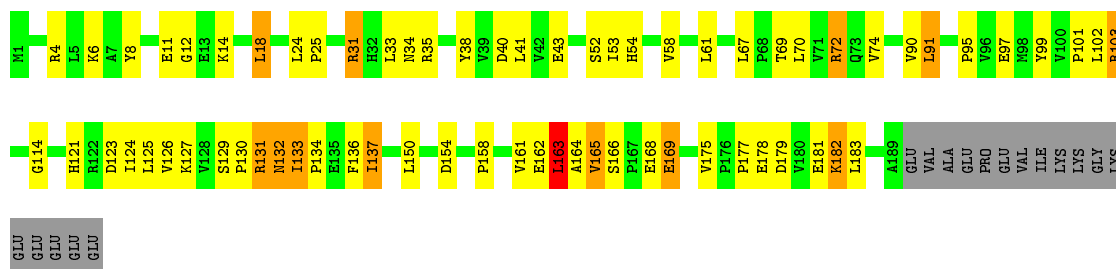
- Molecule 23: 50S ribosomal protein L25

Chain W: 



- Molecule 23: 50S ribosomal protein L25

Chain ZB: 



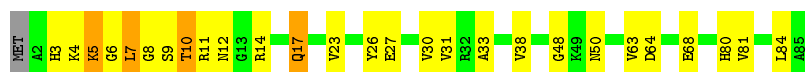
- Molecule 24: 50S ribosomal protein L27

Chain X: 

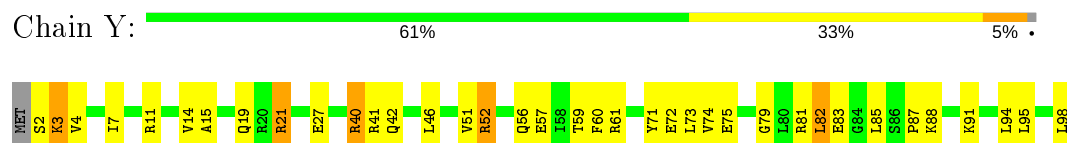


- Molecule 24: 50S ribosomal protein L27

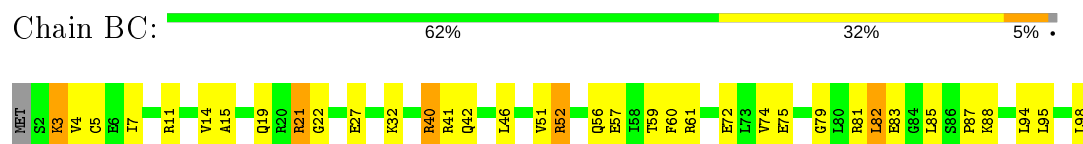
Chain AC: 



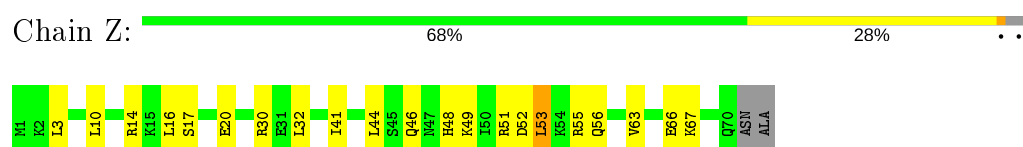
- Molecule 25: 50S ribosomal protein L28



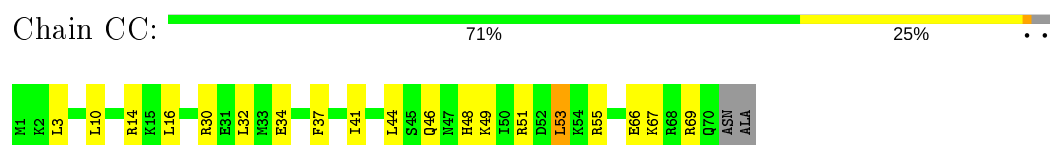
- Molecule 25: 50S ribosomal protein L28



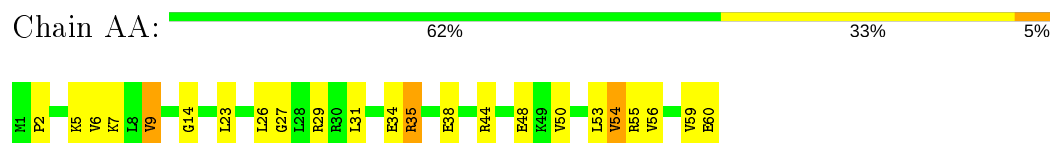
- Molecule 26: 50S ribosomal protein L29



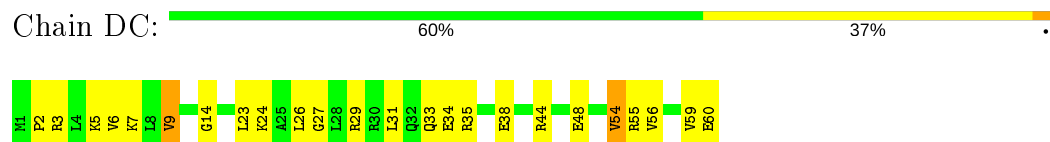
- Molecule 26: 50S ribosomal protein L29



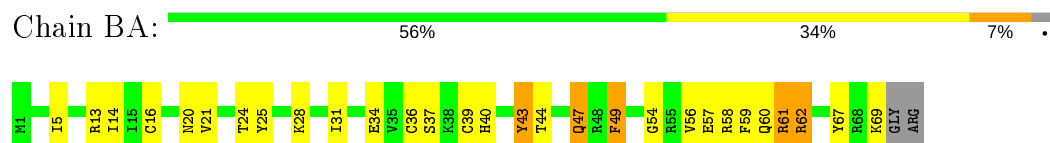
- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L31

Chain EC:  58% 32% 7% .



- Molecule 29: 50S ribosomal protein L32

Chain CA:  62% 32% 5% .



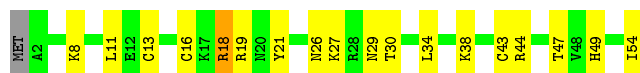
- Molecule 29: 50S ribosomal protein L32

Chain FC:  60% 33% 5% .



- Molecule 30: 50S ribosomal protein L33

Chain DA:  65% 31% ..



- Molecule 30: 50S ribosomal protein L33

Chain GC:  65% 31% ..



- Molecule 31: 50S ribosomal protein L34

Chain EA:  53% 37% 8% .



- Molecule 31: 50S ribosomal protein L34

Chain HC:  49% 43% 6% .



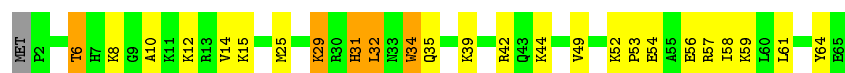
- Molecule 32: 50S ribosomal protein L35

Chain FA:  66% 23% 9%



- Molecule 32: 50S ribosomal protein L35

Chain IC:  60% 31% 8%



- Molecule 33: 50S ribosomal protein L36

Chain GA:  51% 46%



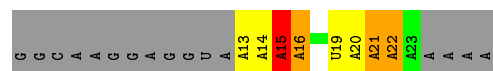
- Molecule 33: 50S ribosomal protein L36

Chain JC:  49% 49%



- Molecule 34: mRNA

Chain HA:  11% 15% 11% 59%



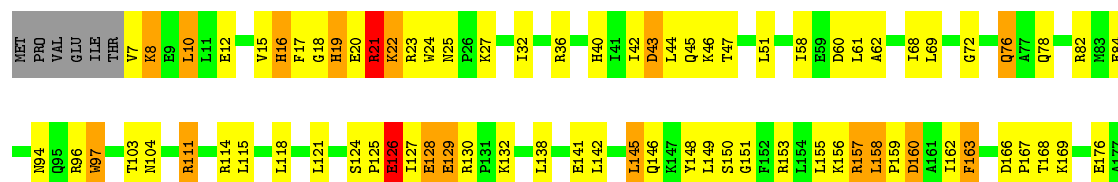
- Molecule 34: mRNA

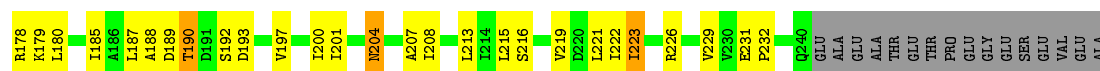
Chain KC:  7% 22% 11% 59%



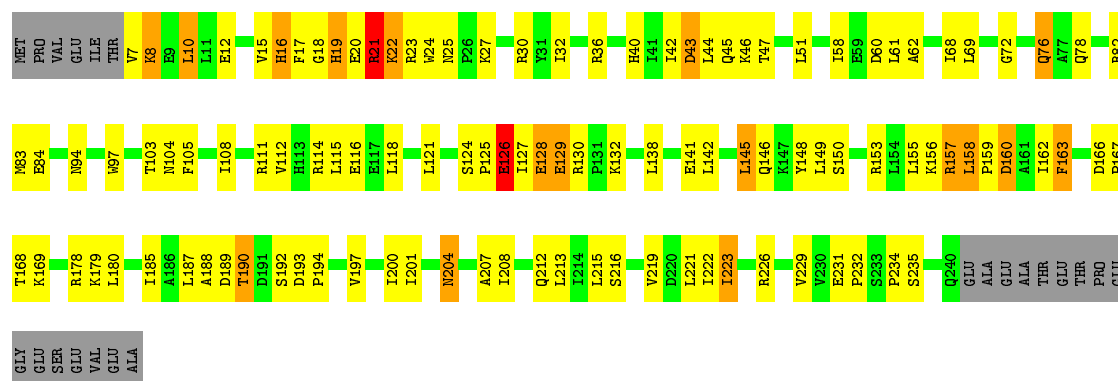
- Molecule 35: 30S ribosomal protein S2

Chain JA:  50% 33% 7% 9%

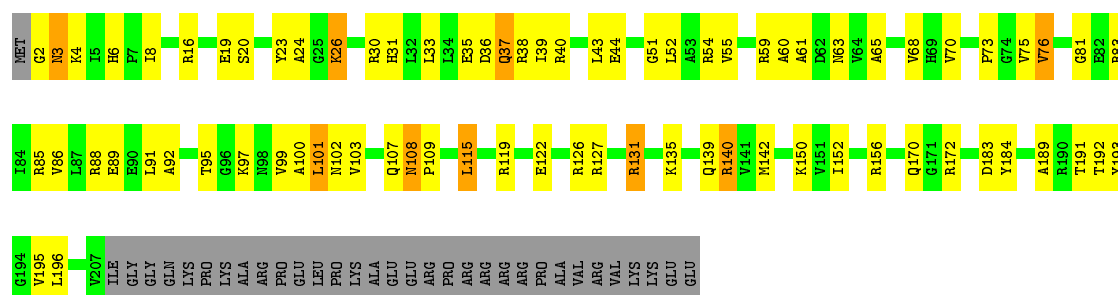




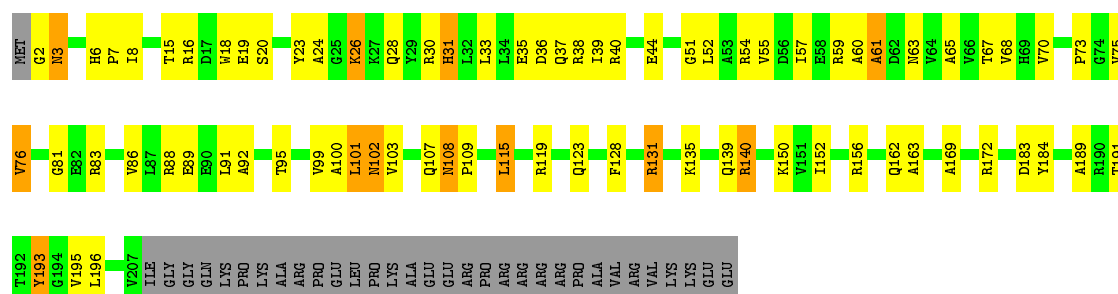
• Molecule 35: 30S ribosomal protein S2



• Molecule 36: 30S ribosomal protein S3

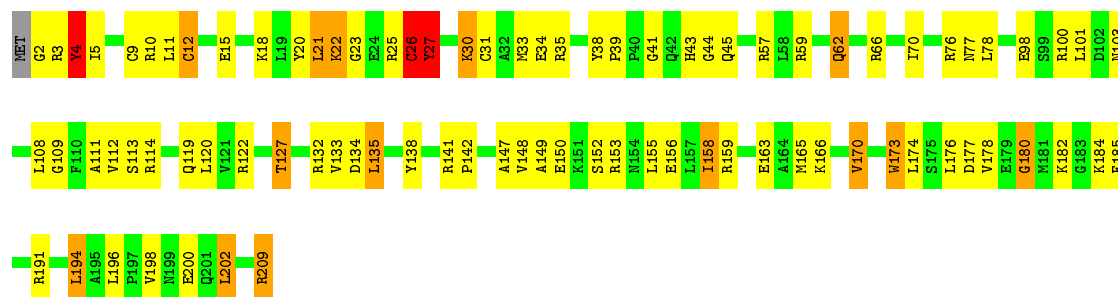


• Molecule 36: 30S ribosomal protein S3



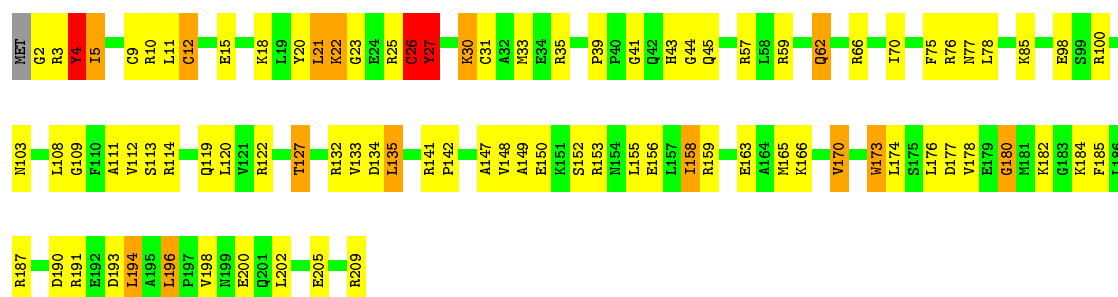
• Molecule 37: 30S ribosomal protein S4





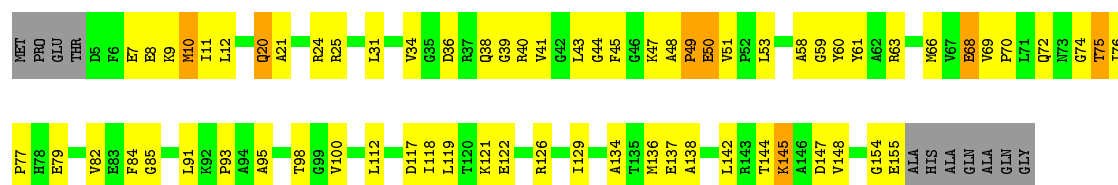
- Molecule 37: 30S ribosomal protein S4

Chain OC: 57% 34% 7%



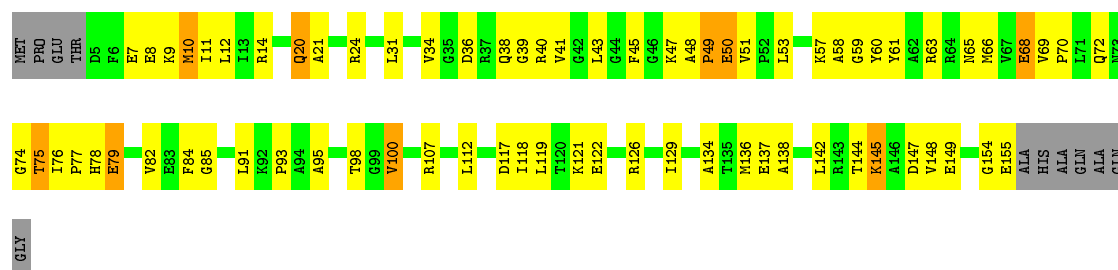
- Molecule 38: 30S ribosomal protein S5

Chain MA: 51% 38% 7%



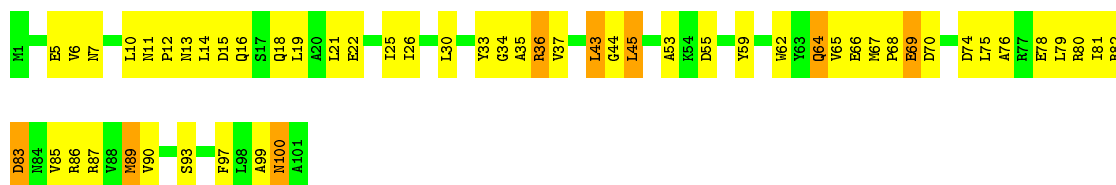
- Molecule 38: 30S ribosomal protein S5

Chain PC: 49% 39% 6% 7%

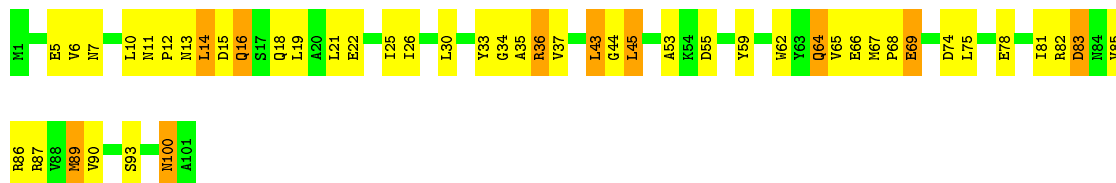


- Molecule 39: 30S ribosomal protein S6

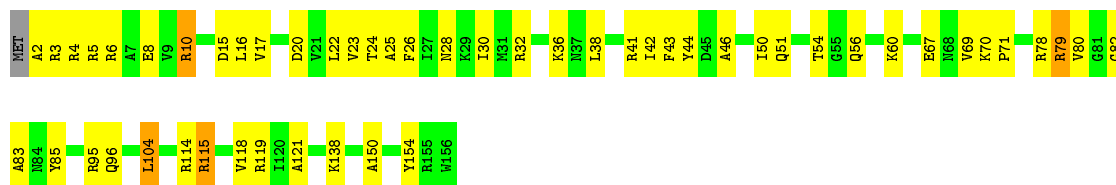
Chain NA: 47% 46% 8%



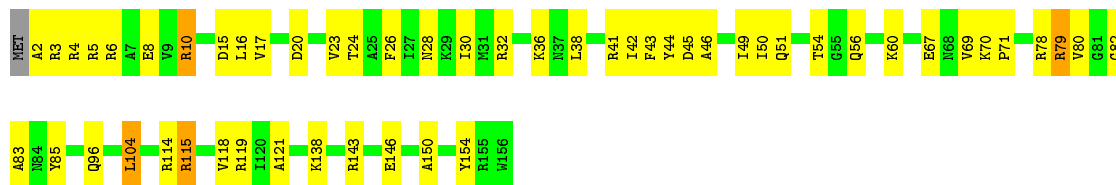
- Molecule 39: 30S ribosomal protein S6



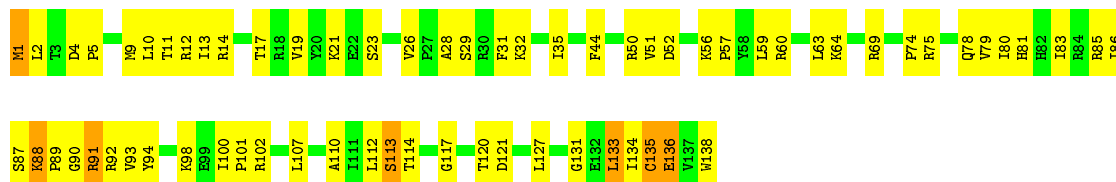
- Molecule 40: 30S ribosomal protein S7



- Molecule 40: 30S ribosomal protein S7

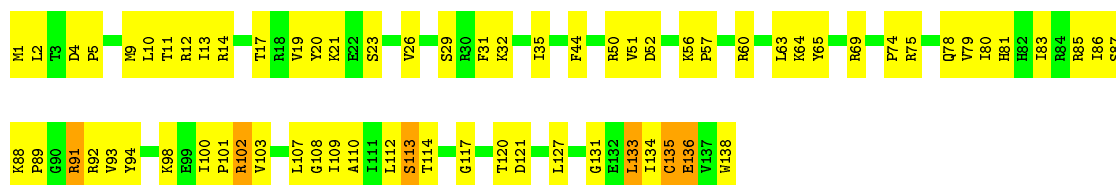


- Molecule 41: 30S ribosomal protein S8

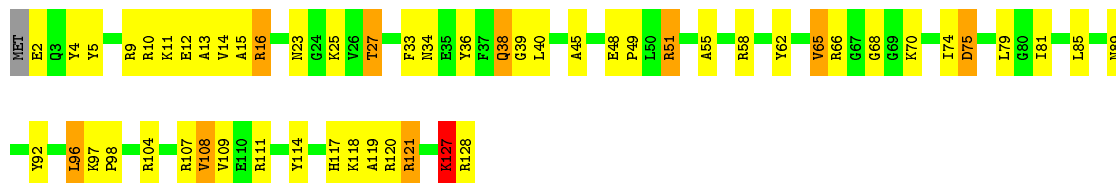


- Molecule 41: 30S ribosomal protein S8

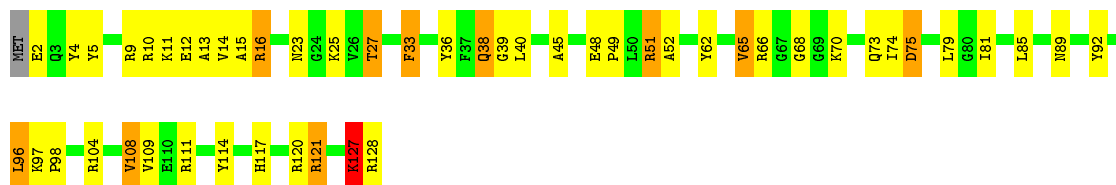




• Molecule 42: 30S ribosomal protein S9



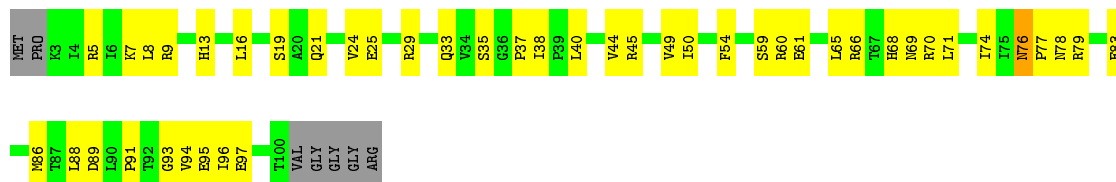
• Molecule 42: 30S ribosomal protein S9



• Molecule 43: 30S ribosomal protein S10

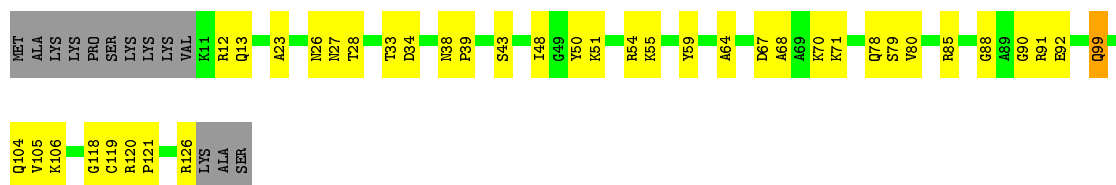


• Molecule 43: 30S ribosomal protein S10



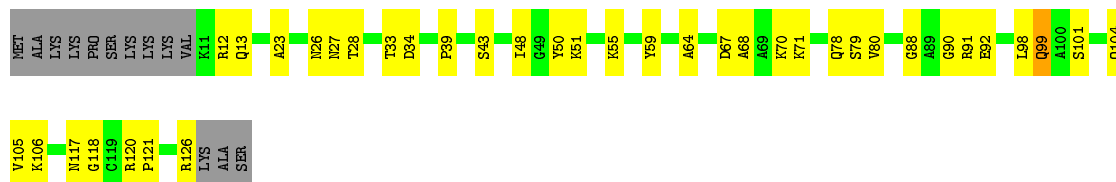
• Molecule 44: 30S ribosomal protein S11





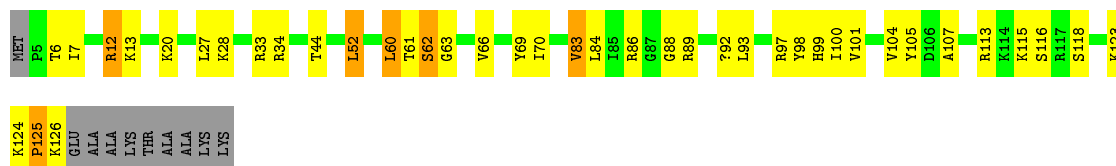
- Molecule 44: 30S ribosomal protein S11

Chain VC: 60% 29% 10%



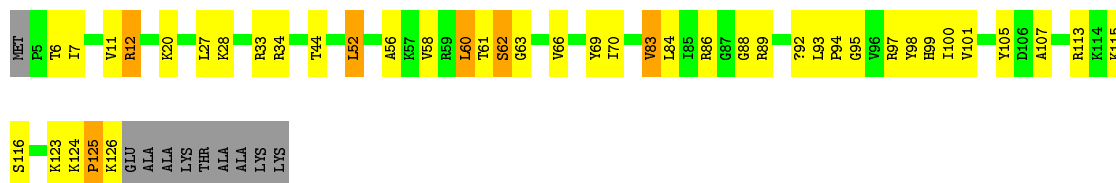
- Molecule 45: 30S ribosomal protein S12

Chain TA: 61% 27% 5% 8%



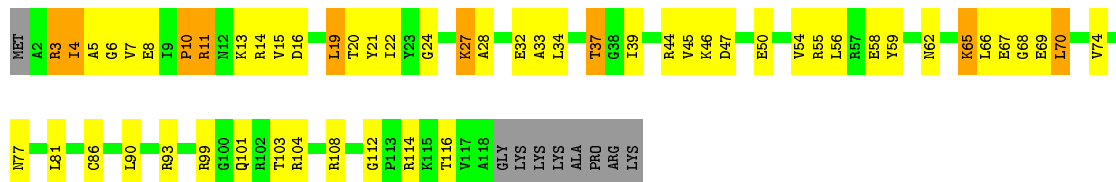
- Molecule 45: 30S ribosomal protein S12

Chain WC: 60% 28% 5% 8%



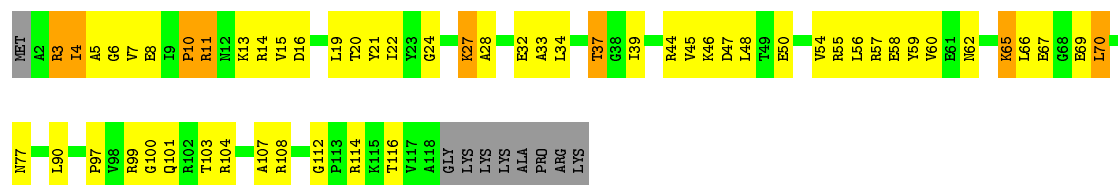
- Molecule 46: 30S ribosomal protein S13

Chain UA: 49% 37% 7% 7%



- Molecule 46: 30S ribosomal protein S13

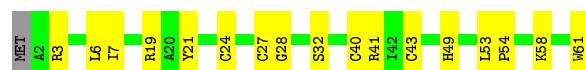
Chain XC: 48% 38% 6% 7%



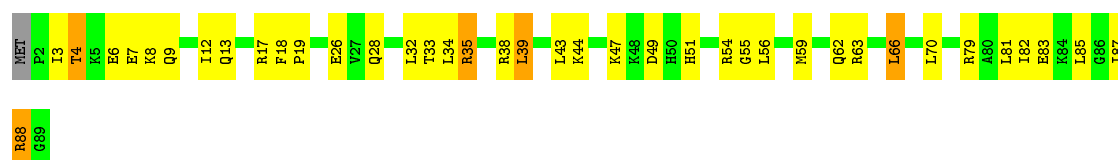
- Molecule 47: 30S ribosomal protein S14 type Z



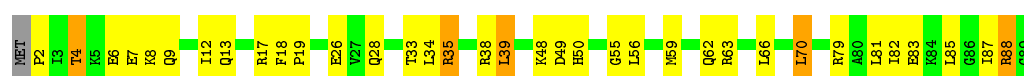
- Molecule 47: 30S ribosomal protein S14 type Z



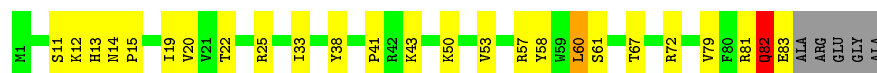
- Molecule 48: 30S ribosomal protein S15



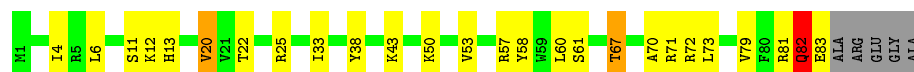
- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16



- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17

Chain YA: 



- Molecule 50: 30S ribosomal protein S17

Chain BD: 



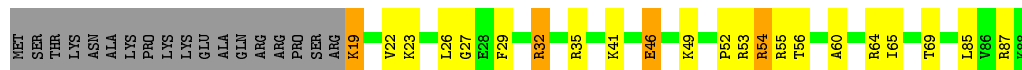
- Molecule 51: 30S ribosomal protein S18

Chain ZA: 



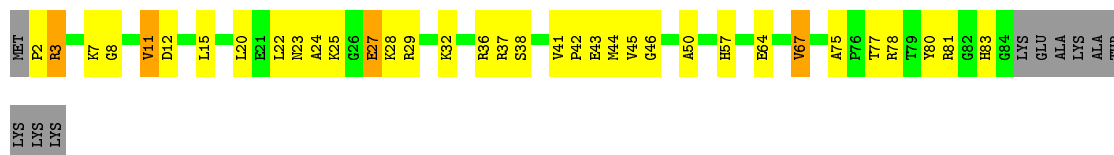
- Molecule 51: 30S ribosomal protein S18

Chain CD: 



- Molecule 52: 30S ribosomal protein S19

Chain AB: 



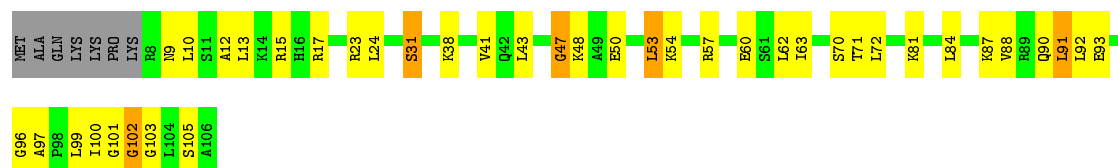
- Molecule 52: 30S ribosomal protein S19

Chain DD: 

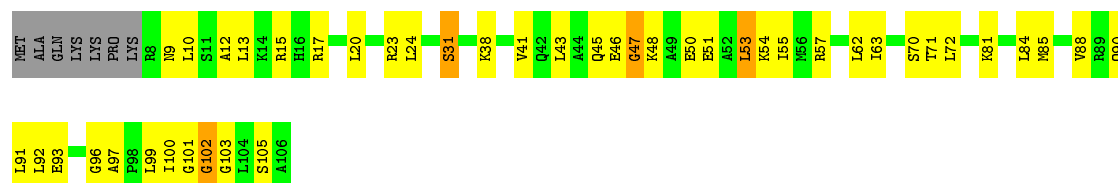


- Molecule 53: 30S ribosomal protein S20

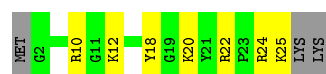
Chain BB: 



- Molecule 53: 30S ribosomal protein S20



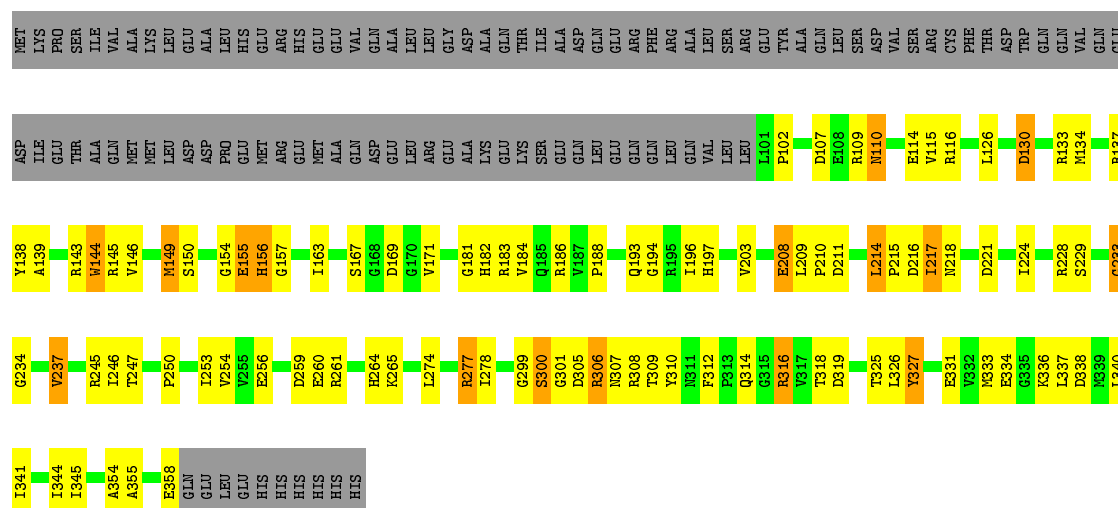
- Molecule 54: 30S ribosomal protein Thx



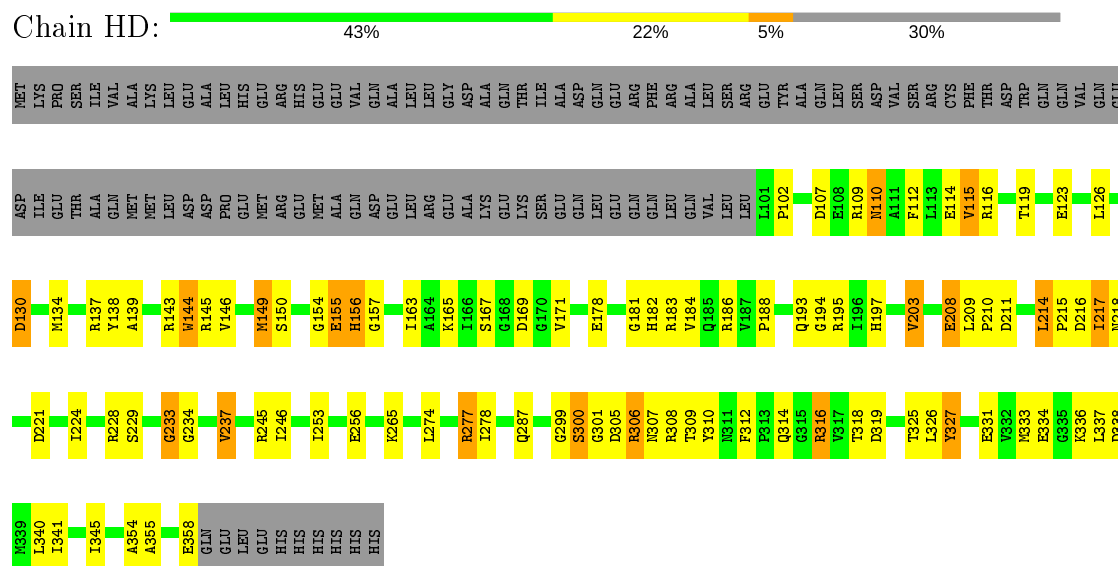
- Molecule 54: 30S ribosomal protein Thx



- Molecule 55: Peptide chain release factor 1



- Molecule 55: Peptide chain release factor 1



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 210.82Å 450.45Å 615.17Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.55 68.93 – 3.55 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (50.00-3.55) 99.9 (68.93-3.55) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.28 (at 3.58Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | (Not available) , (Not available) 0.221 , 0.257 | Depositor DCC |
| R_{free} test set | 13965 reflections (2.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 124.9 | Xtriage |
| Anisotropy | 0.055 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 81.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 299566 | wwPDB-VP |
| Average B, all atoms (Å ²) | 128.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, M2G, OMG, 2MU, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 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 > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.66 | 8/35961 (0.0%) | 1.15 | 147/56125 (0.3%) |
| 1 | DB | 0.69 | 5/35961 (0.0%) | 1.18 | 176/56125 (0.3%) |
| 2 | B | 1.01 | 76/69214 (0.1%) | 1.49 | 1088/108048 (1.0%) |
| 2 | EB | 0.88 | 60/69214 (0.1%) | 1.38 | 770/108048 (0.7%) |
| 3 | C | 0.69 | 0/2881 | 1.20 | 18/4494 (0.4%) |
| 3 | FB | 0.61 | 0/2881 | 1.09 | 11/4494 (0.2%) |
| 4 | D | 0.47 | 0/1744 | 0.88 | 0/2719 |
| 4 | GB | 0.48 | 0/1744 | 0.88 | 0/2719 |
| 4 | IA | 0.74 | 0/1744 | 1.17 | 7/2719 (0.3%) |
| 4 | LC | 0.70 | 1/1744 (0.1%) | 1.12 | 5/2719 (0.2%) |
| 5 | E | 0.78 | 4/2195 (0.2%) | 0.74 | 0/2955 |
| 5 | HB | 0.70 | 3/2195 (0.1%) | 0.72 | 0/2955 |
| 6 | F | 0.63 | 0/1596 | 0.67 | 0/2153 |
| 6 | IB | 0.57 | 0/1596 | 0.65 | 0/2153 |
| 7 | G | 0.70 | 0/1621 | 0.69 | 0/2194 |
| 7 | JB | 0.61 | 0/1621 | 0.65 | 0/2194 |
| 8 | H | 0.44 | 0/1496 | 0.57 | 0/2013 |
| 8 | KB | 0.40 | 0/1496 | 0.56 | 0/2013 |
| 9 | I | 0.52 | 0/1356 | 0.56 | 0/1834 |
| 9 | LB | 0.38 | 0/1356 | 0.52 | 0/1834 |
| 10 | J | 0.51 | 0/1152 | 0.58 | 0/1559 |
| 10 | MB | 0.47 | 0/1152 | 0.58 | 0/1559 |
| 11 | K | 0.62 | 0/1148 | 0.66 | 0/1547 |
| 11 | NB | 0.51 | 0/1148 | 0.63 | 0/1547 |
| 12 | L | 0.67 | 0/942 | 0.68 | 0/1268 |
| 12 | OB | 0.67 | 0/942 | 0.67 | 0/1268 |
| 13 | M | 0.64 | 0/1162 | 0.69 | 0/1544 |
| 13 | PB | 0.56 | 0/1162 | 0.67 | 0/1544 |
| 14 | N | 0.67 | 0/1142 | 0.63 | 0/1525 |
| 14 | QB | 0.60 | 0/1142 | 0.63 | 0/1525 |
| 15 | O | 0.60 | 0/982 | 0.72 | 0/1312 |
| 15 | RB | 0.57 | 0/982 | 0.68 | 0/1312 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | P | 0.45 | 0/887 | 0.58 | 0/1180 |
| 16 | SB | 0.40 | 0/887 | 0.53 | 0/1180 |
| 17 | Q | 0.61 | 0/1157 | 0.65 | 0/1544 |
| 17 | TB | 0.58 | 0/1157 | 0.65 | 0/1544 |
| 18 | R | 0.67 | 0/982 | 0.68 | 0/1306 |
| 18 | UB | 0.57 | 0/982 | 0.65 | 0/1306 |
| 19 | S | 0.65 | 0/790 | 0.67 | 0/1057 |
| 19 | VB | 0.56 | 0/790 | 0.65 | 0/1057 |
| 20 | T | 0.74 | 0/901 | 0.73 | 0/1209 |
| 20 | WB | 0.65 | 0/901 | 0.69 | 0/1209 |
| 21 | U | 0.76 | 0/764 | 0.69 | 0/1025 |
| 21 | XB | 0.63 | 0/764 | 0.65 | 0/1025 |
| 22 | V | 0.64 | 0/827 | 0.66 | 0/1103 |
| 22 | YB | 0.60 | 0/827 | 0.65 | 0/1103 |
| 23 | W | 0.49 | 0/1527 | 0.58 | 0/2073 |
| 23 | ZB | 0.43 | 0/1527 | 0.55 | 0/2073 |
| 24 | AC | 0.61 | 0/671 | 0.71 | 0/892 |
| 24 | X | 0.71 | 0/671 | 0.73 | 0/892 |
| 25 | BC | 0.65 | 0/768 | 0.71 | 0/1021 |
| 25 | Y | 0.70 | 0/768 | 0.72 | 0/1021 |
| 26 | CC | 0.57 | 0/594 | 0.60 | 0/785 |
| 26 | Z | 0.68 | 0/594 | 0.64 | 0/785 |
| 27 | AA | 0.60 | 0/482 | 0.62 | 0/646 |
| 27 | DC | 0.57 | 0/482 | 0.63 | 0/646 |
| 28 | BA | 0.42 | 0/565 | 0.46 | 0/761 |
| 28 | EC | 0.39 | 0/565 | 0.46 | 0/761 |
| 29 | CA | 0.60 | 0/474 | 0.63 | 0/640 |
| 29 | FC | 0.55 | 0/474 | 0.64 | 0/640 |
| 30 | DA | 0.41 | 0/460 | 0.50 | 0/613 |
| 30 | GC | 0.40 | 0/460 | 0.48 | 0/613 |
| 31 | EA | 0.79 | 0/426 | 0.89 | 3/561 (0.5%) |
| 31 | HC | 0.69 | 0/426 | 0.78 | 1/561 (0.2%) |
| 32 | FA | 0.74 | 1/525 (0.2%) | 0.68 | 0/691 |
| 32 | IC | 0.61 | 0/525 | 0.66 | 0/691 |
| 33 | GA | 0.45 | 0/310 | 0.53 | 0/407 |
| 33 | JC | 0.46 | 0/310 | 0.53 | 0/407 |
| 34 | HA | 1.01 | 0/247 | 1.24 | 3/382 (0.8%) |
| 34 | KC | 1.01 | 0/247 | 1.14 | 0/382 |
| 35 | JA | 0.41 | 0/1935 | 0.55 | 0/2609 |
| 35 | MC | 0.41 | 0/1935 | 0.54 | 0/2609 |
| 36 | KA | 0.41 | 0/1636 | 0.53 | 0/2205 |
| 36 | NC | 0.40 | 0/1636 | 0.53 | 0/2205 |
| 37 | LA | 0.51 | 1/1733 (0.1%) | 0.60 | 1/2318 (0.0%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 37 | OC | 0.58 | 1/1733 (0.1%) | 0.62 | 1/2318 (0.0%) |
| 38 | MA | 0.48 | 0/1171 | 0.61 | 0/1576 |
| 38 | PC | 0.51 | 0/1171 | 0.63 | 0/1576 |
| 39 | NA | 0.53 | 0/856 | 0.59 | 0/1154 |
| 39 | QC | 0.50 | 0/856 | 0.59 | 0/1154 |
| 40 | OA | 0.42 | 0/1276 | 0.51 | 0/1709 |
| 40 | RC | 0.44 | 0/1276 | 0.52 | 0/1709 |
| 41 | PA | 0.45 | 0/1136 | 0.59 | 0/1527 |
| 41 | SC | 0.46 | 0/1136 | 0.60 | 0/1527 |
| 42 | QA | 0.36 | 0/1029 | 0.49 | 0/1378 |
| 42 | TC | 0.36 | 0/1029 | 0.49 | 0/1378 |
| 43 | RA | 0.38 | 0/807 | 0.49 | 0/1085 |
| 43 | UC | 0.38 | 0/807 | 0.49 | 0/1085 |
| 44 | SA | 0.52 | 0/879 | 0.61 | 0/1187 |
| 44 | VC | 0.50 | 0/879 | 0.61 | 0/1187 |
| 45 | TA | 0.55 | 0/963 | 0.63 | 0/1287 |
| 45 | WC | 0.56 | 0/963 | 0.63 | 0/1287 |
| 46 | UA | 0.38 | 0/943 | 0.53 | 0/1265 |
| 46 | XC | 0.38 | 0/943 | 0.52 | 0/1265 |
| 47 | VA | 0.42 | 0/501 | 0.54 | 0/664 |
| 47 | YC | 0.39 | 0/501 | 0.53 | 0/664 |
| 48 | WA | 0.50 | 0/745 | 0.56 | 0/992 |
| 48 | ZC | 0.51 | 0/745 | 0.56 | 0/992 |
| 49 | AD | 0.49 | 0/716 | 0.58 | 0/963 |
| 49 | XA | 0.40 | 0/716 | 0.55 | 0/963 |
| 50 | BD | 0.53 | 0/836 | 0.58 | 0/1117 |
| 50 | YA | 0.52 | 0/836 | 0.59 | 0/1117 |
| 51 | CD | 0.50 | 0/579 | 0.55 | 0/768 |
| 51 | ZA | 0.52 | 0/579 | 0.57 | 0/768 |
| 52 | AB | 0.36 | 0/680 | 0.51 | 0/915 |
| 52 | DD | 0.35 | 0/680 | 0.51 | 0/915 |
| 53 | BB | 0.40 | 0/764 | 0.52 | 0/1006 |
| 53 | ED | 0.44 | 0/764 | 0.55 | 0/1006 |
| 54 | CB | 0.35 | 0/212 | 0.46 | 0/277 |
| 54 | FD | 0.36 | 0/212 | 0.46 | 0/277 |
| 55 | GD | 0.54 | 0/2012 | 0.62 | 0/2713 |
| 55 | HD | 0.48 | 0/2012 | 0.60 | 0/2713 |
| All | All | 0.77 | 160/322204 (0.0%) | 1.18 | 2231/481240 (0.5%) |

The worst 5 of 160 bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|--------|-------------|----------|
| 2 | B | 1762 | A | N9-C4 | 14.42 | 1.46 | 1.37 |
| 2 | EB | 1762 | A | N9-C4 | 13.35 | 1.45 | 1.37 |
| 2 | B | 1142(B) | A | N9-C4 | -10.33 | 1.31 | 1.37 |
| 1 | A | 1503 | A | N9-C4 | 9.28 | 1.43 | 1.37 |
| 1 | A | 1531 | A | N9-C4 | 9.11 | 1.43 | 1.37 |

The worst 5 of 2231 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 2 | EB | 2053 | G | N1-C6-O6 | 19.40 | 131.54 | 119.90 |
| 2 | EB | 2053 | G | C5-C6-O6 | -15.62 | 119.23 | 128.60 |
| 2 | B | 2053 | G | N1-C6-O6 | 15.42 | 129.15 | 119.90 |
| 2 | B | 2593 | U | N3-C4-C5 | -14.85 | 105.69 | 114.60 |
| 2 | B | 1602 | U | N3-C4-C5 | -14.74 | 105.75 | 114.60 |

There are no chirality outliers.

There are no planarity outliers.

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 | A | 32394 | 0 | 16367 | 505 | 0 |
| 1 | DB | 32394 | 0 | 16367 | 492 | 0 |
| 2 | B | 62031 | 0 | 31275 | 829 | 0 |
| 2 | EB | 62031 | 0 | 31275 | 802 | 0 |
| 3 | C | 2576 | 0 | 1305 | 35 | 0 |
| 3 | FB | 2576 | 0 | 1305 | 35 | 0 |
| 4 | D | 1642 | 0 | 841 | 26 | 0 |
| 4 | GB | 1642 | 0 | 841 | 29 | 0 |
| 4 | IA | 1642 | 0 | 841 | 12 | 0 |
| 4 | LC | 1642 | 0 | 841 | 10 | 0 |
| 5 | E | 2145 | 0 | 2234 | 91 | 0 |
| 5 | HB | 2145 | 0 | 2234 | 78 | 0 |
| 6 | F | 1563 | 0 | 1629 | 61 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | IB | 1563 | 0 | 1629 | 55 | 0 |
| 7 | G | 1586 | 0 | 1632 | 65 | 0 |
| 7 | JB | 1586 | 0 | 1632 | 61 | 0 |
| 8 | H | 1471 | 0 | 1526 | 67 | 0 |
| 8 | KB | 1471 | 0 | 1526 | 62 | 0 |
| 9 | I | 1330 | 0 | 1407 | 57 | 0 |
| 9 | LB | 1330 | 0 | 1407 | 51 | 0 |
| 10 | J | 1137 | 0 | 1225 | 50 | 0 |
| 10 | MB | 1137 | 0 | 1225 | 40 | 0 |
| 11 | K | 1121 | 0 | 1195 | 34 | 0 |
| 11 | NB | 1121 | 0 | 1195 | 31 | 0 |
| 12 | L | 932 | 0 | 994 | 32 | 0 |
| 12 | OB | 932 | 0 | 994 | 27 | 0 |
| 13 | M | 1145 | 0 | 1228 | 40 | 0 |
| 13 | PB | 1145 | 0 | 1228 | 35 | 0 |
| 14 | N | 1121 | 0 | 1179 | 36 | 0 |
| 14 | QB | 1121 | 0 | 1179 | 42 | 0 |
| 15 | O | 968 | 0 | 1033 | 39 | 0 |
| 15 | RB | 968 | 0 | 1033 | 43 | 0 |
| 16 | P | 877 | 0 | 938 | 28 | 0 |
| 16 | SB | 877 | 0 | 938 | 29 | 0 |
| 17 | Q | 1143 | 0 | 1211 | 37 | 0 |
| 17 | TB | 1143 | 0 | 1211 | 33 | 0 |
| 18 | R | 964 | 0 | 1022 | 25 | 0 |
| 18 | UB | 964 | 0 | 1022 | 30 | 0 |
| 19 | S | 779 | 0 | 852 | 28 | 0 |
| 19 | VB | 779 | 0 | 852 | 29 | 0 |
| 20 | T | 890 | 0 | 951 | 34 | 0 |
| 20 | WB | 890 | 0 | 951 | 26 | 0 |
| 21 | U | 750 | 0 | 814 | 14 | 0 |
| 21 | XB | 750 | 0 | 814 | 14 | 0 |
| 22 | V | 814 | 0 | 907 | 28 | 0 |
| 22 | YB | 814 | 0 | 907 | 25 | 0 |
| 23 | W | 1495 | 0 | 1521 | 51 | 0 |
| 23 | ZB | 1495 | 0 | 1521 | 50 | 0 |
| 24 | AC | 662 | 0 | 688 | 23 | 0 |
| 24 | X | 662 | 0 | 688 | 23 | 0 |
| 25 | BC | 761 | 0 | 837 | 28 | 0 |
| 25 | Y | 761 | 0 | 837 | 30 | 0 |
| 26 | CC | 592 | 0 | 654 | 16 | 0 |
| 26 | Z | 592 | 0 | 654 | 16 | 0 |
| 27 | AA | 477 | 0 | 529 | 16 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27 | DC | 477 | 0 | 529 | 16 | 0 |
| 28 | BA | 552 | 0 | 537 | 23 | 0 |
| 28 | EC | 552 | 0 | 537 | 22 | 0 |
| 29 | CA | 460 | 0 | 484 | 17 | 0 |
| 29 | FC | 460 | 0 | 484 | 19 | 0 |
| 30 | DA | 453 | 0 | 477 | 11 | 0 |
| 30 | GC | 453 | 0 | 477 | 11 | 0 |
| 31 | EA | 418 | 0 | 467 | 17 | 0 |
| 31 | HC | 418 | 0 | 467 | 17 | 0 |
| 32 | FA | 517 | 0 | 582 | 17 | 0 |
| 32 | IC | 517 | 0 | 582 | 19 | 0 |
| 33 | GA | 307 | 0 | 338 | 15 | 0 |
| 33 | JC | 307 | 0 | 337 | 16 | 0 |
| 34 | HA | 220 | 0 | 108 | 7 | 0 |
| 34 | KC | 220 | 0 | 108 | 9 | 0 |
| 35 | JA | 1900 | 0 | 1951 | 69 | 0 |
| 35 | MC | 1900 | 0 | 1951 | 69 | 0 |
| 36 | KA | 1612 | 0 | 1677 | 49 | 0 |
| 36 | NC | 1612 | 0 | 1677 | 48 | 0 |
| 37 | LA | 1703 | 0 | 1765 | 74 | 0 |
| 37 | OC | 1703 | 0 | 1765 | 68 | 0 |
| 38 | MA | 1155 | 0 | 1213 | 45 | 0 |
| 38 | PC | 1155 | 0 | 1213 | 51 | 0 |
| 39 | NA | 843 | 0 | 857 | 44 | 0 |
| 39 | QC | 843 | 0 | 857 | 40 | 0 |
| 40 | OA | 1257 | 0 | 1296 | 38 | 0 |
| 40 | RC | 1257 | 0 | 1296 | 42 | 0 |
| 41 | PA | 1116 | 0 | 1177 | 49 | 0 |
| 41 | SC | 1116 | 0 | 1177 | 48 | 0 |
| 42 | QA | 1011 | 0 | 1043 | 43 | 0 |
| 42 | TC | 1011 | 0 | 1043 | 43 | 0 |
| 43 | RA | 794 | 0 | 840 | 25 | 0 |
| 43 | UC | 794 | 0 | 840 | 27 | 0 |
| 44 | SA | 864 | 0 | 881 | 25 | 0 |
| 44 | VC | 864 | 0 | 881 | 21 | 0 |
| 45 | TA | 958 | 0 | 1047 | 31 | 0 |
| 45 | WC | 958 | 0 | 1047 | 31 | 0 |
| 46 | UA | 933 | 0 | 992 | 50 | 0 |
| 46 | XC | 933 | 0 | 992 | 47 | 0 |
| 47 | VA | 492 | 0 | 533 | 20 | 0 |
| 47 | YC | 492 | 0 | 533 | 17 | 0 |
| 48 | WA | 734 | 0 | 771 | 31 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48 | ZC | 734 | 0 | 771 | 27 | 0 |
| 49 | AD | 700 | 0 | 720 | 20 | 0 |
| 49 | XA | 700 | 0 | 720 | 20 | 0 |
| 50 | BD | 823 | 0 | 893 | 24 | 0 |
| 50 | YA | 823 | 0 | 893 | 21 | 0 |
| 51 | CD | 574 | 0 | 644 | 17 | 0 |
| 51 | ZA | 574 | 0 | 644 | 19 | 0 |
| 52 | AB | 665 | 0 | 686 | 28 | 0 |
| 52 | DD | 665 | 0 | 686 | 29 | 0 |
| 53 | BB | 762 | 0 | 859 | 27 | 0 |
| 53 | ED | 762 | 0 | 859 | 27 | 0 |
| 54 | CB | 208 | 0 | 221 | 4 | 0 |
| 54 | FD | 208 | 0 | 221 | 12 | 0 |
| 55 | GD | 1980 | 0 | 1942 | 69 | 0 |
| 55 | HD | 1980 | 0 | 1942 | 63 | 0 |
| 56 | A | 160 | 0 | 0 | 0 | 0 |
| 56 | AB | 1 | 0 | 0 | 0 | 0 |
| 56 | AC | 2 | 0 | 0 | 0 | 0 |
| 56 | AD | 1 | 0 | 0 | 0 | 0 |
| 56 | B | 514 | 0 | 0 | 0 | 0 |
| 56 | BB | 1 | 0 | 0 | 0 | 0 |
| 56 | BC | 1 | 0 | 0 | 0 | 0 |
| 56 | BD | 2 | 0 | 0 | 0 | 0 |
| 56 | C | 23 | 0 | 0 | 0 | 0 |
| 56 | CA | 1 | 0 | 0 | 0 | 0 |
| 56 | CD | 2 | 0 | 0 | 0 | 0 |
| 56 | D | 6 | 0 | 0 | 0 | 0 |
| 56 | DB | 177 | 0 | 0 | 0 | 0 |
| 56 | DC | 1 | 0 | 0 | 0 | 0 |
| 56 | E | 4 | 0 | 0 | 0 | 0 |
| 56 | EA | 1 | 0 | 0 | 0 | 0 |
| 56 | EB | 395 | 0 | 0 | 0 | 0 |
| 56 | ED | 1 | 0 | 0 | 0 | 0 |
| 56 | F | 1 | 0 | 0 | 0 | 0 |
| 56 | FA | 1 | 0 | 0 | 0 | 0 |
| 56 | FB | 17 | 0 | 0 | 0 | 0 |
| 56 | FC | 1 | 0 | 0 | 0 | 0 |
| 56 | G | 4 | 0 | 0 | 0 | 0 |
| 56 | GB | 5 | 0 | 0 | 0 | 0 |
| 56 | GD | 5 | 0 | 0 | 0 | 0 |
| 56 | H | 1 | 0 | 0 | 0 | 0 |
| 56 | HA | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56 | HB | 8 | 0 | 0 | 0 | 0 |
| 56 | HC | 1 | 0 | 0 | 0 | 0 |
| 56 | HD | 3 | 0 | 0 | 0 | 0 |
| 56 | I | 3 | 0 | 0 | 0 | 0 |
| 56 | IA | 8 | 0 | 0 | 0 | 0 |
| 56 | IB | 3 | 0 | 0 | 0 | 0 |
| 56 | IC | 2 | 0 | 0 | 0 | 0 |
| 56 | J | 5 | 0 | 0 | 0 | 0 |
| 56 | JA | 3 | 0 | 0 | 0 | 0 |
| 56 | JB | 2 | 0 | 0 | 0 | 0 |
| 56 | JC | 1 | 0 | 0 | 0 | 0 |
| 56 | K | 2 | 0 | 0 | 0 | 0 |
| 56 | KA | 1 | 0 | 0 | 0 | 0 |
| 56 | KB | 1 | 0 | 0 | 0 | 0 |
| 56 | KC | 1 | 0 | 0 | 0 | 0 |
| 56 | L | 7 | 0 | 0 | 0 | 0 |
| 56 | LA | 1 | 0 | 0 | 0 | 0 |
| 56 | LB | 5 | 0 | 0 | 0 | 0 |
| 56 | LC | 8 | 0 | 0 | 0 | 0 |
| 56 | M | 4 | 0 | 0 | 0 | 0 |
| 56 | MA | 3 | 0 | 0 | 0 | 0 |
| 56 | MB | 2 | 0 | 0 | 0 | 0 |
| 56 | MC | 3 | 0 | 0 | 0 | 0 |
| 56 | N | 3 | 0 | 0 | 0 | 0 |
| 56 | NA | 2 | 0 | 0 | 0 | 0 |
| 56 | NB | 1 | 0 | 0 | 0 | 0 |
| 56 | O | 1 | 0 | 0 | 0 | 0 |
| 56 | OA | 3 | 0 | 0 | 0 | 0 |
| 56 | OB | 3 | 0 | 0 | 0 | 0 |
| 56 | P | 2 | 0 | 0 | 0 | 0 |
| 56 | PA | 2 | 0 | 0 | 0 | 0 |
| 56 | PB | 2 | 0 | 0 | 0 | 0 |
| 56 | PC | 2 | 0 | 0 | 0 | 0 |
| 56 | Q | 3 | 0 | 0 | 0 | 0 |
| 56 | QB | 3 | 0 | 0 | 0 | 0 |
| 56 | QC | 2 | 0 | 0 | 0 | 0 |
| 56 | R | 4 | 0 | 0 | 0 | 0 |
| 56 | RA | 2 | 0 | 0 | 0 | 0 |
| 56 | RB | 5 | 0 | 0 | 0 | 0 |
| 56 | RC | 2 | 0 | 0 | 0 | 0 |
| 56 | S | 3 | 0 | 0 | 0 | 0 |
| 56 | SA | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56 | SB | 1 | 0 | 0 | 0 | 0 |
| 56 | SC | 1 | 0 | 0 | 0 | 0 |
| 56 | T | 2 | 0 | 0 | 0 | 0 |
| 56 | TA | 3 | 0 | 0 | 0 | 0 |
| 56 | TB | 5 | 0 | 0 | 0 | 0 |
| 56 | TC | 2 | 0 | 0 | 0 | 0 |
| 56 | U | 2 | 0 | 0 | 0 | 0 |
| 56 | UC | 1 | 0 | 0 | 0 | 0 |
| 56 | V | 5 | 0 | 0 | 0 | 0 |
| 56 | VA | 2 | 0 | 0 | 0 | 0 |
| 56 | VB | 1 | 0 | 0 | 0 | 0 |
| 56 | W | 12 | 0 | 0 | 0 | 0 |
| 56 | WA | 3 | 0 | 0 | 0 | 0 |
| 56 | WB | 3 | 0 | 0 | 0 | 0 |
| 56 | WC | 2 | 0 | 0 | 0 | 0 |
| 56 | XB | 2 | 0 | 0 | 0 | 0 |
| 56 | XC | 2 | 0 | 0 | 0 | 0 |
| 56 | Y | 4 | 0 | 0 | 0 | 0 |
| 56 | YA | 2 | 0 | 0 | 0 | 0 |
| 56 | YB | 3 | 0 | 0 | 0 | 0 |
| 56 | YC | 1 | 0 | 0 | 0 | 0 |
| 56 | Z | 3 | 0 | 0 | 0 | 0 |
| 56 | ZA | 1 | 0 | 0 | 0 | 0 |
| 56 | ZB | 2 | 0 | 0 | 0 | 0 |
| 56 | ZC | 1 | 0 | 0 | 0 | 0 |
| 57 | BA | 1 | 0 | 0 | 0 | 0 |
| 57 | CA | 1 | 0 | 0 | 0 | 0 |
| 57 | DA | 1 | 0 | 0 | 0 | 0 |
| 57 | EC | 1 | 0 | 0 | 0 | 0 |
| 57 | FC | 1 | 0 | 0 | 0 | 0 |
| 57 | GA | 1 | 0 | 0 | 0 | 0 |
| 57 | GC | 1 | 0 | 0 | 0 | 0 |
| 57 | JC | 1 | 0 | 0 | 0 | 0 |
| 57 | V | 1 | 0 | 0 | 0 | 0 |
| 57 | YB | 1 | 0 | 0 | 0 | 0 |
| All | All | 299566 | 0 | 203671 | 5481 | 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 11.

The worst 5 of 5481 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) |
|------------------|-------------------|--------------------------|-------------------|
| 37:LA:18:LYS:NZ | 37:LA:31:CYS:SG | 2.10 | 1.23 |
| 37:OC:18:LYS:NZ | 37:OC:31:CYS:SG | 2.10 | 1.23 |
| 37:OC:12:CYS:SG | 37:OC:18:LYS:NZ | 2.24 | 1.11 |
| 10:J:60:GLU:HG3 | 10:J:61:ARG:HH12 | 1.11 | 1.09 |
| 10:MB:60:GLU:HG3 | 10:MB:61:ARG:HH12 | 1.19 | 1.05 |

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 5 | E | 273/275 (99%) | 243 (89%) | 25 (9%) | 5 (2%) | 8 | 43 |
| 5 | HB | 273/275 (99%) | 243 (89%) | 25 (9%) | 5 (2%) | 8 | 43 |
| 6 | F | 202/206 (98%) | 180 (89%) | 20 (10%) | 2 (1%) | 15 | 55 |
| 6 | IB | 202/206 (98%) | 181 (90%) | 19 (9%) | 2 (1%) | 15 | 55 |
| 7 | G | 200/205 (98%) | 187 (94%) | 9 (4%) | 4 (2%) | 7 | 42 |
| 7 | JB | 200/205 (98%) | 186 (93%) | 10 (5%) | 4 (2%) | 7 | 42 |
| 8 | H | 179/182 (98%) | 152 (85%) | 20 (11%) | 7 (4%) | 3 | 27 |
| 8 | KB | 179/182 (98%) | 151 (84%) | 22 (12%) | 6 (3%) | 3 | 31 |
| 9 | I | 172/180 (96%) | 155 (90%) | 14 (8%) | 3 (2%) | 9 | 45 |
| 9 | LB | 172/180 (96%) | 154 (90%) | 15 (9%) | 3 (2%) | 9 | 45 |
| 10 | J | 144/148 (97%) | 118 (82%) | 17 (12%) | 9 (6%) | 1 | 17 |
| 10 | MB | 144/148 (97%) | 118 (82%) | 16 (11%) | 10 (7%) | 1 | 15 |
| 11 | K | 138/140 (99%) | 125 (91%) | 12 (9%) | 1 (1%) | 22 | 62 |
| 11 | NB | 138/140 (99%) | 126 (91%) | 11 (8%) | 1 (1%) | 22 | 62 |
| 12 | L | 120/122 (98%) | 106 (88%) | 12 (10%) | 2 (2%) | 9 | 45 |
| 12 | OB | 120/122 (98%) | 106 (88%) | 12 (10%) | 2 (2%) | 9 | 45 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 13 | M | 148/150 (99%) | 132 (89%) | 11 (7%) | 5 (3%) | 3 | 31 |
| 13 | PB | 148/150 (99%) | 131 (88%) | 12 (8%) | 5 (3%) | 3 | 31 |
| 14 | N | 139/141 (99%) | 126 (91%) | 11 (8%) | 2 (1%) | 11 | 48 |
| 14 | QB | 139/141 (99%) | 125 (90%) | 12 (9%) | 2 (1%) | 11 | 48 |
| 15 | O | 116/118 (98%) | 109 (94%) | 5 (4%) | 2 (2%) | 9 | 45 |
| 15 | RB | 116/118 (98%) | 107 (92%) | 7 (6%) | 2 (2%) | 9 | 45 |
| 16 | P | 108/112 (96%) | 99 (92%) | 7 (6%) | 2 (2%) | 8 | 42 |
| 16 | SB | 108/112 (96%) | 100 (93%) | 6 (6%) | 2 (2%) | 8 | 42 |
| 17 | Q | 135/146 (92%) | 118 (87%) | 12 (9%) | 5 (4%) | 3 | 28 |
| 17 | TB | 135/146 (92%) | 118 (87%) | 13 (10%) | 4 (3%) | 4 | 33 |
| 18 | R | 115/118 (98%) | 106 (92%) | 8 (7%) | 1 (1%) | 17 | 57 |
| 18 | UB | 115/118 (98%) | 107 (93%) | 7 (6%) | 1 (1%) | 17 | 57 |
| 19 | S | 99/101 (98%) | 91 (92%) | 6 (6%) | 2 (2%) | 7 | 42 |
| 19 | VB | 99/101 (98%) | 89 (90%) | 8 (8%) | 2 (2%) | 7 | 42 |
| 20 | T | 110/113 (97%) | 104 (94%) | 4 (4%) | 2 (2%) | 8 | 43 |
| 20 | WB | 110/113 (97%) | 103 (94%) | 5 (4%) | 2 (2%) | 8 | 43 |
| 21 | U | 93/96 (97%) | 84 (90%) | 8 (9%) | 1 (1%) | 14 | 54 |
| 21 | XB | 93/96 (97%) | 84 (90%) | 8 (9%) | 1 (1%) | 14 | 54 |
| 22 | V | 105/110 (96%) | 89 (85%) | 11 (10%) | 5 (5%) | 2 | 22 |
| 22 | YB | 105/110 (96%) | 91 (87%) | 9 (9%) | 5 (5%) | 2 | 22 |
| 23 | W | 187/206 (91%) | 165 (88%) | 21 (11%) | 1 (0%) | 29 | 67 |
| 23 | ZB | 187/206 (91%) | 165 (88%) | 21 (11%) | 1 (0%) | 29 | 67 |
| 24 | AC | 82/85 (96%) | 70 (85%) | 10 (12%) | 2 (2%) | 6 | 37 |
| 24 | X | 82/85 (96%) | 69 (84%) | 11 (13%) | 2 (2%) | 6 | 37 |
| 25 | BC | 95/98 (97%) | 84 (88%) | 10 (10%) | 1 (1%) | 14 | 54 |
| 25 | Y | 95/98 (97%) | 86 (90%) | 8 (8%) | 1 (1%) | 14 | 54 |
| 26 | CC | 68/72 (94%) | 65 (96%) | 3 (4%) | 0 | 100 | 100 |
| 26 | Z | 68/72 (94%) | 65 (96%) | 3 (4%) | 0 | 100 | 100 |
| 27 | AA | 58/60 (97%) | 53 (91%) | 4 (7%) | 1 (2%) | 9 | 45 |
| 27 | DC | 58/60 (97%) | 53 (91%) | 4 (7%) | 1 (2%) | 9 | 45 |
| 28 | BA | 67/71 (94%) | 47 (70%) | 19 (28%) | 1 (2%) | 10 | 47 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 28 | EC | 67/71 (94%) | 47 (70%) | 20 (30%) | 0 | 100 | 100 |
| 29 | CA | 57/60 (95%) | 52 (91%) | 4 (7%) | 1 (2%) | 8 | 43 |
| 29 | FC | 57/60 (95%) | 51 (90%) | 5 (9%) | 1 (2%) | 8 | 43 |
| 30 | DA | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |
| 30 | GC | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |
| 31 | EA | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 31 | HC | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 32 | FA | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 32 | IC | 62/65 (95%) | 58 (94%) | 4 (6%) | 0 | 100 | 100 |
| 33 | GA | 35/37 (95%) | 27 (77%) | 8 (23%) | 0 | 100 | 100 |
| 33 | JC | 35/37 (95%) | 27 (77%) | 8 (23%) | 0 | 100 | 100 |
| 35 | JA | 232/256 (91%) | 189 (82%) | 29 (12%) | 14 (6%) | 1 | 17 |
| 35 | MC | 232/256 (91%) | 188 (81%) | 30 (13%) | 14 (6%) | 1 | 17 |
| 36 | KA | 204/239 (85%) | 172 (84%) | 24 (12%) | 8 (4%) | 3 | 27 |
| 36 | NC | 204/239 (85%) | 172 (84%) | 24 (12%) | 8 (4%) | 3 | 27 |
| 37 | LA | 206/209 (99%) | 179 (87%) | 20 (10%) | 7 (3%) | 3 | 31 |
| 37 | OC | 206/209 (99%) | 182 (88%) | 16 (8%) | 8 (4%) | 3 | 27 |
| 38 | MA | 149/162 (92%) | 132 (89%) | 11 (7%) | 6 (4%) | 3 | 26 |
| 38 | PC | 149/162 (92%) | 132 (89%) | 10 (7%) | 7 (5%) | 2 | 22 |
| 39 | NA | 99/101 (98%) | 88 (89%) | 9 (9%) | 2 (2%) | 7 | 42 |
| 39 | QC | 99/101 (98%) | 89 (90%) | 8 (8%) | 2 (2%) | 7 | 42 |
| 40 | OA | 153/156 (98%) | 133 (87%) | 13 (8%) | 7 (5%) | 2 | 23 |
| 40 | RC | 153/156 (98%) | 133 (87%) | 13 (8%) | 7 (5%) | 2 | 23 |
| 41 | PA | 136/138 (99%) | 125 (92%) | 9 (7%) | 2 (2%) | 10 | 47 |
| 41 | SC | 136/138 (99%) | 126 (93%) | 9 (7%) | 1 (1%) | 22 | 62 |
| 42 | QA | 125/128 (98%) | 105 (84%) | 17 (14%) | 3 (2%) | 6 | 37 |
| 42 | TC | 125/128 (98%) | 105 (84%) | 16 (13%) | 4 (3%) | 4 | 31 |
| 43 | RA | 96/105 (91%) | 81 (84%) | 12 (12%) | 3 (3%) | 4 | 32 |
| 43 | UC | 96/105 (91%) | 81 (84%) | 12 (12%) | 3 (3%) | 4 | 32 |
| 44 | SA | 114/129 (88%) | 101 (89%) | 10 (9%) | 3 (3%) | 5 | 35 |
| 44 | VC | 114/129 (88%) | 101 (89%) | 9 (8%) | 4 (4%) | 3 | 30 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 45 | TA | 119/132 (90%) | 104 (87%) | 11 (9%) | 4 (3%) | 3 | 31 |
| 45 | WC | 119/132 (90%) | 104 (87%) | 11 (9%) | 4 (3%) | 3 | 31 |
| 46 | UA | 115/126 (91%) | 102 (89%) | 12 (10%) | 1 (1%) | 17 | 57 |
| 46 | XC | 115/126 (91%) | 102 (89%) | 11 (10%) | 2 (2%) | 9 | 45 |
| 47 | VA | 58/61 (95%) | 52 (90%) | 6 (10%) | 0 | 100 | 100 |
| 47 | YC | 58/61 (95%) | 52 (90%) | 6 (10%) | 0 | 100 | 100 |
| 48 | WA | 86/89 (97%) | 80 (93%) | 4 (5%) | 2 (2%) | 6 | 38 |
| 48 | ZC | 86/89 (97%) | 81 (94%) | 3 (4%) | 2 (2%) | 6 | 38 |
| 49 | AD | 81/88 (92%) | 73 (90%) | 7 (9%) | 1 (1%) | 13 | 52 |
| 49 | XA | 81/88 (92%) | 73 (90%) | 7 (9%) | 1 (1%) | 13 | 52 |
| 50 | BD | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 50 | YA | 97/105 (92%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 51 | CD | 68/88 (77%) | 62 (91%) | 5 (7%) | 1 (2%) | 10 | 47 |
| 51 | ZA | 68/88 (77%) | 61 (90%) | 6 (9%) | 1 (2%) | 10 | 47 |
| 52 | AB | 81/93 (87%) | 63 (78%) | 14 (17%) | 4 (5%) | 2 | 21 |
| 52 | DD | 81/93 (87%) | 63 (78%) | 14 (17%) | 4 (5%) | 2 | 21 |
| 53 | BB | 97/106 (92%) | 90 (93%) | 3 (3%) | 4 (4%) | 3 | 26 |
| 53 | ED | 97/106 (92%) | 90 (93%) | 3 (3%) | 4 (4%) | 3 | 26 |
| 54 | CB | 22/27 (82%) | 18 (82%) | 4 (18%) | 0 | 100 | 100 |
| 54 | FD | 22/27 (82%) | 18 (82%) | 4 (18%) | 0 | 100 | 100 |
| 55 | GD | 253/365 (69%) | 207 (82%) | 35 (14%) | 11 (4%) | 2 | 24 |
| 55 | HD | 253/365 (69%) | 206 (81%) | 37 (15%) | 10 (4%) | 3 | 26 |
| All | All | 11990/12846 (93%) | 10568 (88%) | 1121 (9%) | 301 (2%) | 5 | 36 |

5 of 301 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 31 | LYS |
| 6 | F | 192 | ASN |
| 7 | G | 21 | ALA |
| 7 | G | 130 | ALA |
| 8 | H | 74 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 5 | E | 217/217 (100%) | 197 (91%) | 20 (9%) | 9 | 38 |
| 5 | HB | 217/217 (100%) | 197 (91%) | 20 (9%) | 9 | 38 |
| 6 | F | 165/166 (99%) | 145 (88%) | 20 (12%) | 5 | 26 |
| 6 | IB | 165/166 (99%) | 145 (88%) | 20 (12%) | 5 | 26 |
| 7 | G | 161/162 (99%) | 142 (88%) | 19 (12%) | 5 | 28 |
| 7 | JB | 161/162 (99%) | 142 (88%) | 19 (12%) | 5 | 28 |
| 8 | H | 154/156 (99%) | 134 (87%) | 20 (13%) | 4 | 24 |
| 8 | KB | 154/156 (99%) | 136 (88%) | 18 (12%) | 5 | 28 |
| 9 | I | 144/148 (97%) | 130 (90%) | 14 (10%) | 8 | 35 |
| 9 | LB | 144/148 (97%) | 130 (90%) | 14 (10%) | 8 | 35 |
| 10 | J | 122/124 (98%) | 105 (86%) | 17 (14%) | 3 | 21 |
| 10 | MB | 122/124 (98%) | 106 (87%) | 16 (13%) | 4 | 23 |
| 11 | K | 119/119 (100%) | 107 (90%) | 12 (10%) | 7 | 34 |
| 11 | NB | 119/119 (100%) | 108 (91%) | 11 (9%) | 9 | 38 |
| 12 | L | 100/100 (100%) | 91 (91%) | 9 (9%) | 9 | 39 |
| 12 | OB | 100/100 (100%) | 90 (90%) | 10 (10%) | 7 | 35 |
| 13 | M | 116/116 (100%) | 103 (89%) | 13 (11%) | 6 | 30 |
| 13 | PB | 116/116 (100%) | 101 (87%) | 15 (13%) | 4 | 24 |
| 14 | N | 111/111 (100%) | 99 (89%) | 12 (11%) | 6 | 32 |
| 14 | QB | 111/111 (100%) | 98 (88%) | 13 (12%) | 5 | 28 |
| 15 | O | 101/101 (100%) | 89 (88%) | 12 (12%) | 5 | 27 |
| 15 | RB | 101/101 (100%) | 89 (88%) | 12 (12%) | 5 | 27 |
| 16 | P | 87/88 (99%) | 83 (95%) | 4 (5%) | 27 | 61 |
| 16 | SB | 87/88 (99%) | 83 (95%) | 4 (5%) | 27 | 61 |
| 17 | Q | 121/128 (94%) | 112 (93%) | 9 (7%) | 13 | 45 |
| 17 | TB | 121/128 (94%) | 113 (93%) | 8 (7%) | 16 | 50 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 18 | R | 93/94 (99%) | 83 (89%) | 10 (11%) | 6 | 32 |
| 18 | UB | 93/94 (99%) | 84 (90%) | 9 (10%) | 8 | 35 |
| 19 | S | 82/82 (100%) | 70 (85%) | 12 (15%) | 3 | 20 |
| 19 | VB | 82/82 (100%) | 72 (88%) | 10 (12%) | 5 | 26 |
| 20 | T | 91/92 (99%) | 81 (89%) | 10 (11%) | 6 | 31 |
| 20 | WB | 91/92 (99%) | 81 (89%) | 10 (11%) | 6 | 31 |
| 21 | U | 77/78 (99%) | 73 (95%) | 4 (5%) | 23 | 58 |
| 21 | XB | 77/78 (99%) | 73 (95%) | 4 (5%) | 23 | 58 |
| 22 | V | 87/91 (96%) | 81 (93%) | 6 (7%) | 15 | 48 |
| 22 | YB | 87/91 (96%) | 81 (93%) | 6 (7%) | 15 | 48 |
| 23 | W | 163/179 (91%) | 142 (87%) | 21 (13%) | 4 | 24 |
| 23 | ZB | 163/179 (91%) | 143 (88%) | 20 (12%) | 4 | 26 |
| 24 | AC | 66/67 (98%) | 57 (86%) | 9 (14%) | 3 | 22 |
| 24 | X | 66/67 (98%) | 57 (86%) | 9 (14%) | 3 | 22 |
| 25 | BC | 81/83 (98%) | 70 (86%) | 11 (14%) | 3 | 22 |
| 25 | Y | 81/83 (98%) | 70 (86%) | 11 (14%) | 3 | 22 |
| 26 | CC | 66/67 (98%) | 62 (94%) | 4 (6%) | 18 | 53 |
| 26 | Z | 66/67 (98%) | 62 (94%) | 4 (6%) | 18 | 53 |
| 27 | AA | 52/52 (100%) | 48 (92%) | 4 (8%) | 13 | 44 |
| 27 | DC | 52/52 (100%) | 49 (94%) | 3 (6%) | 20 | 55 |
| 28 | BA | 59/63 (94%) | 51 (86%) | 8 (14%) | 3 | 22 |
| 28 | EC | 59/63 (94%) | 51 (86%) | 8 (14%) | 3 | 22 |
| 29 | CA | 51/52 (98%) | 46 (90%) | 5 (10%) | 8 | 35 |
| 29 | FC | 51/52 (98%) | 46 (90%) | 5 (10%) | 8 | 35 |
| 30 | DA | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 43 |
| 30 | GC | 51/52 (98%) | 46 (90%) | 5 (10%) | 8 | 35 |
| 31 | EA | 41/42 (98%) | 35 (85%) | 6 (15%) | 3 | 20 |
| 31 | HC | 41/42 (98%) | 35 (85%) | 6 (15%) | 3 | 20 |
| 32 | FA | 54/55 (98%) | 47 (87%) | 7 (13%) | 4 | 24 |
| 32 | IC | 54/55 (98%) | 48 (89%) | 6 (11%) | 6 | 31 |
| 33 | GA | 34/34 (100%) | 30 (88%) | 4 (12%) | 5 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 33 | JC | 34/34 (100%) | 30 (88%) | 4 (12%) | 5 | 28 |
| 35 | JA | 202/220 (92%) | 177 (88%) | 25 (12%) | 4 | 25 |
| 35 | MC | 202/220 (92%) | 177 (88%) | 25 (12%) | 4 | 25 |
| 36 | KA | 160/188 (85%) | 146 (91%) | 14 (9%) | 10 | 40 |
| 36 | NC | 160/188 (85%) | 145 (91%) | 15 (9%) | 8 | 37 |
| 37 | LA | 180/181 (99%) | 159 (88%) | 21 (12%) | 5 | 28 |
| 37 | OC | 180/181 (99%) | 157 (87%) | 23 (13%) | 4 | 24 |
| 38 | MA | 116/123 (94%) | 100 (86%) | 16 (14%) | 3 | 22 |
| 38 | PC | 116/123 (94%) | 99 (85%) | 17 (15%) | 3 | 19 |
| 39 | NA | 90/90 (100%) | 80 (89%) | 10 (11%) | 6 | 31 |
| 39 | QC | 90/90 (100%) | 79 (88%) | 11 (12%) | 5 | 26 |
| 40 | OA | 126/127 (99%) | 120 (95%) | 6 (5%) | 25 | 60 |
| 40 | RC | 126/127 (99%) | 120 (95%) | 6 (5%) | 25 | 60 |
| 41 | PA | 119/119 (100%) | 107 (90%) | 12 (10%) | 7 | 34 |
| 41 | SC | 119/119 (100%) | 108 (91%) | 11 (9%) | 9 | 38 |
| 42 | QA | 98/99 (99%) | 86 (88%) | 12 (12%) | 5 | 26 |
| 42 | TC | 98/99 (99%) | 86 (88%) | 12 (12%) | 5 | 26 |
| 43 | RA | 88/92 (96%) | 81 (92%) | 7 (8%) | 12 | 43 |
| 43 | UC | 88/92 (96%) | 81 (92%) | 7 (8%) | 12 | 43 |
| 44 | SA | 88/99 (89%) | 85 (97%) | 3 (3%) | 37 | 69 |
| 44 | VC | 88/99 (89%) | 85 (97%) | 3 (3%) | 37 | 69 |
| 45 | TA | 102/108 (94%) | 95 (93%) | 7 (7%) | 15 | 48 |
| 45 | WC | 102/108 (94%) | 95 (93%) | 7 (7%) | 15 | 48 |
| 46 | UA | 94/101 (93%) | 82 (87%) | 12 (13%) | 4 | 24 |
| 46 | XC | 94/101 (93%) | 83 (88%) | 11 (12%) | 5 | 28 |
| 47 | VA | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 64 |
| 47 | YC | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 64 |
| 48 | WA | 79/80 (99%) | 72 (91%) | 7 (9%) | 9 | 39 |
| 48 | ZC | 79/80 (99%) | 72 (91%) | 7 (9%) | 9 | 39 |
| 49 | AD | 72/74 (97%) | 66 (92%) | 6 (8%) | 11 | 41 |
| 49 | XA | 72/74 (97%) | 66 (92%) | 6 (8%) | 11 | 41 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|-------------|----|
| 50 | BD | 94/97 (97%) | 86 (92%) | 8 (8%) | 10 | 41 |
| 50 | YA | 94/97 (97%) | 86 (92%) | 8 (8%) | 10 | 41 |
| 51 | CD | 61/77 (79%) | 56 (92%) | 5 (8%) | 11 | 42 |
| 51 | ZA | 61/77 (79%) | 56 (92%) | 5 (8%) | 11 | 42 |
| 52 | AB | 72/80 (90%) | 65 (90%) | 7 (10%) | 8 | 35 |
| 52 | DD | 72/80 (90%) | 65 (90%) | 7 (10%) | 8 | 35 |
| 53 | BB | 76/82 (93%) | 70 (92%) | 6 (8%) | 12 | 43 |
| 53 | ED | 76/82 (93%) | 70 (92%) | 6 (8%) | 12 | 43 |
| 54 | CB | 19/22 (86%) | 18 (95%) | 1 (5%) | 22 | 58 |
| 54 | FD | 19/22 (86%) | 18 (95%) | 1 (5%) | 22 | 58 |
| 55 | GD | 206/305 (68%) | 179 (87%) | 27 (13%) | 4 | 23 |
| 55 | HD | 206/305 (68%) | 179 (87%) | 27 (13%) | 4 | 23 |
| All | All | 10114/10666 (95%) | 9077 (90%) | 1037 (10%) | 7 | 34 |

5 of 1037 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | YA | 75 | ARG |
| 9 | LB | 107 | VAL |
| 50 | BD | 63 | ARG |
| 52 | AB | 15 | LEU |
| 6 | IB | 128 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | HB | 166 | GLN |
| 16 | SB | 61 | ASN |
| 55 | GD | 236 | HIS |
| 6 | IB | 132 | HIS |
| 10 | MB | 54 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | A | 1502/1507 (99%) | 228 (15%) | 10 (0%) |

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| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | DB | 1502/1507 (99%) | 223 (14%) | 10 (0%) |
| 2 | B | 2876/2880 (99%) | 498 (17%) | 15 (0%) |
| 2 | EB | 2876/2880 (99%) | 496 (17%) | 15 (0%) |
| 3 | C | 119/120 (99%) | 18 (15%) | 0 |
| 3 | FB | 119/120 (99%) | 17 (14%) | 0 |
| 34 | HA | 9/27 (33%) | 4 (44%) | 1 (11%) |
| 34 | KC | 9/27 (33%) | 4 (44%) | 1 (11%) |
| 4 | D | 76/77 (98%) | 13 (17%) | 0 |
| 4 | GB | 76/77 (98%) | 13 (17%) | 0 |
| 4 | IA | 76/77 (98%) | 7 (9%) | 0 |
| 4 | LC | 76/77 (98%) | 7 (9%) | 0 |
| All | All | 9316/9376 (99%) | 1528 (16%) | 52 (0%) |

5 of 1528 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | U |
| 1 | A | 6 | G |
| 1 | A | 8 | A |
| 1 | A | 9 | G |
| 1 | A | 32 | A |

5 of 52 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 2422 | A |
| 1 | DB | 563 | A |
| 2 | EB | 2032 | G |
| 2 | B | 2833 | G |
| 1 | DB | 115 | G |

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

64 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 | PSU | A | 516 | 1 | 17,21,22 | 1.99 | 3 (17%) | 20,30,33 | 3.91 | 6 (30%) |
| 1 | 4OC | A | 1402 | 1 | 16,23,24 | 0.99 | 1 (6%) | 17,32,35 | 2.12 | 2 (11%) |
| 1 | 7MG | A | 527 | 1 | 22,26,27 | 2.16 | 7 (31%) | 28,39,42 | 1.68 | 7 (25%) |
| 1 | 5MC | DB | 967 | 1 | 15,22,23 | 1.45 | 2 (13%) | 19,32,35 | 1.27 | 3 (15%) |
| 2 | OMG | B | 2251 | 2,4 | 18,26,27 | 1.87 | 2 (11%) | 20,38,41 | 1.89 | 4 (20%) |
| 2 | 2MU | B | 2552 | 2 | 14,22,24 | 2.68 | 5 (35%) | 14,31,36 | 1.39 | 2 (14%) |
| 1 | PSU | DB | 516 | 1 | 17,21,22 | 1.90 | 3 (17%) | 20,30,33 | 4.15 | 6 (30%) |
| 1 | 5MC | DB | 1404 | 1 | 15,22,23 | 1.45 | 2 (13%) | 19,32,35 | 1.35 | 3 (15%) |
| 2 | PSU | EB | 1917 | 2 | 17,21,22 | 1.45 | 3 (17%) | 20,30,33 | 3.34 | 6 (30%) |
| 2 | 5MC | EB | 1962 | 56,2 | 15,22,23 | 1.45 | 2 (13%) | 19,32,35 | 1.22 | 2 (10%) |
| 45 | 0TD | WC | 92 | 45 | 4,9,10 | 1.46 | 1 (25%) | 3,11,13 | 3.60 | 1 (33%) |
| 1 | MA6 | A | 1519 | 1 | 19,26,27 | 1.58 | 3 (15%) | 18,38,41 | 1.28 | 2 (11%) |
| 2 | 5MC | EB | 1942 | 2 | 15,22,23 | 1.49 | 2 (13%) | 19,32,35 | 1.60 | 4 (21%) |
| 4 | 4SU | D | 8 | 4 | 14,21,22 | 2.97 | 4 (28%) | 15,30,33 | 1.74 | 3 (20%) |
| 1 | M2G | DB | 966 | 1 | 20,27,28 | 2.09 | 3 (15%) | 22,40,43 | 1.67 | 5 (22%) |
| 2 | PSU | B | 1911 | 2 | 17,21,22 | 1.33 | 3 (17%) | 20,30,33 | 3.49 | 7 (35%) |
| 1 | 5MC | A | 967 | 1 | 15,22,23 | 1.42 | 2 (13%) | 19,32,35 | 1.24 | 2 (10%) |
| 2 | 4OC | B | 1920 | 2 | 15,22,24 | 0.93 | 1 (6%) | 17,31,35 | 1.11 | 2 (11%) |
| 1 | UR3 | A | 1498 | 1 | 14,22,23 | 1.64 | 1 (7%) | 15,32,35 | 0.68 | 0 |
| 2 | PSU | EB | 1911 | 2 | 17,21,22 | 1.38 | 3 (17%) | 20,30,33 | 3.06 | 7 (35%) |
| 4 | 5MC | IA | 32 | 4 | 15,22,23 | 1.43 | 2 (13%) | 19,32,35 | 1.64 | 5 (26%) |
| 1 | 5MC | A | 1407 | 1 | 15,22,23 | 1.45 | 2 (13%) | 19,32,35 | 1.44 | 4 (21%) |
| 1 | UR3 | DB | 1498 | 1 | 14,22,23 | 1.78 | 1 (7%) | 15,32,35 | 0.61 | 0 |
| 4 | 4SU | IA | 8 | 4 | 14,21,22 | 2.90 | 4 (28%) | 15,30,33 | 1.22 | 1 (6%) |
| 2 | 2MA | EB | 2503 | 2 | 17,25,26 | 1.39 | 2 (11%) | 19,37,40 | 1.77 | 4 (21%) |
| 2 | 5MU | B | 1939 | 2 | 15,22,23 | 1.63 | 3 (20%) | 16,32,35 | 2.08 | 4 (25%) |
| 4 | 5MC | LC | 32 | 4 | 15,22,23 | 1.38 | 1 (6%) | 19,32,35 | 1.38 | 3 (15%) |
| 1 | 5MC | DB | 1407 | 1 | 15,22,23 | 1.59 | 2 (13%) | 19,32,35 | 1.61 | 4 (21%) |
| 45 | 0TD | TA | 92 | 45 | 4,9,10 | 1.33 | 0 | 3,11,13 | 3.83 | 1 (33%) |
| 4 | 5MU | GB | 54 | 4 | 15,22,23 | 1.66 | 3 (20%) | 16,32,35 | 1.84 | 1 (6%) |
| 1 | 7MG | DB | 527 | 1 | 22,26,27 | 2.12 | 7 (31%) | 28,39,42 | 1.62 | 6 (21%) |
| 2 | 2MA | B | 2503 | 2 | 17,25,26 | 1.38 | 2 (11%) | 19,37,40 | 1.79 | 3 (15%) |
| 2 | 5MU | B | 1915 | 2 | 15,22,23 | 1.64 | 4 (26%) | 16,32,35 | 1.50 | 1 (6%) |
| 4 | 5MC | GB | 32 | 4 | 15,22,23 | 1.41 | 2 (13%) | 19,32,35 | 1.39 | 4 (21%) |
| 1 | M2G | A | 966 | 1 | 20,27,28 | 2.13 | 3 (15%) | 22,40,43 | 1.63 | 6 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | 5MU | EB | 1939 | 2 | 15,22,23 | 1.61 | 3 (20%) | 16,32,35 | 1.96 | 4 (25%) |
| 4 | 5MU | LC | 54 | 4 | 15,22,23 | 1.84 | 3 (20%) | 16,32,35 | 2.21 | 1 (6%) |
| 4 | PSU | IA | 55 | 4 | 17,21,22 | 1.64 | 4 (23%) | 20,30,33 | 3.33 | 6 (30%) |
| 1 | 2MG | A | 1207 | 1 | 19,26,27 | 2.58 | 3 (15%) | 21,38,41 | 1.89 | 7 (33%) |
| 1 | 5MC | DB | 1400 | 1 | 15,22,23 | 1.35 | 2 (13%) | 19,32,35 | 1.33 | 2 (10%) |
| 1 | MA6 | DB | 1518 | 1 | 19,26,27 | 1.43 | 3 (15%) | 18,38,41 | 1.53 | 2 (11%) |
| 2 | PSU | B | 2605 | 2 | 17,21,22 | 1.49 | 3 (17%) | 20,30,33 | 3.63 | 5 (25%) |
| 4 | 5MC | D | 32 | 4 | 15,22,23 | 1.43 | 2 (13%) | 19,32,35 | 1.39 | 4 (21%) |
| 2 | 5MC | B | 1942 | 2 | 15,22,23 | 1.44 | 2 (13%) | 19,32,35 | 1.47 | 4 (21%) |
| 1 | MA6 | DB | 1519 | 1 | 19,26,27 | 1.47 | 3 (15%) | 18,38,41 | 1.28 | 2 (11%) |
| 4 | PSU | GB | 55 | 4 | 17,21,22 | 1.68 | 3 (17%) | 20,30,33 | 3.46 | 6 (30%) |
| 4 | 4SU | LC | 8 | 4 | 14,21,22 | 2.73 | 4 (28%) | 15,30,33 | 1.94 | 3 (20%) |
| 2 | 4OC | EB | 1920 | 2 | 15,22,24 | 0.83 | 1 (6%) | 17,31,35 | 0.95 | 1 (5%) |
| 2 | OMG | EB | 2251 | 2,4 | 18,26,27 | 1.80 | 2 (11%) | 20,38,41 | 1.84 | 6 (30%) |
| 4 | 5MU | D | 54 | 4 | 15,22,23 | 1.70 | 3 (20%) | 16,32,35 | 1.96 | 1 (6%) |
| 4 | PSU | D | 55 | 4 | 17,21,22 | 1.65 | 3 (17%) | 20,30,33 | 3.58 | 5 (25%) |
| 4 | 4SU | GB | 8 | 4 | 14,21,22 | 2.90 | 5 (35%) | 15,30,33 | 2.37 | 2 (13%) |
| 2 | PSU | B | 1917 | 2 | 17,21,22 | 1.62 | 3 (17%) | 20,30,33 | 3.39 | 5 (25%) |
| 2 | 2MU | EB | 2552 | 56,2 | 14,22,24 | 2.54 | 5 (35%) | 14,31,36 | 1.21 | 1 (7%) |
| 2 | 5MU | EB | 1915 | 2 | 15,22,23 | 1.77 | 3 (20%) | 16,32,35 | 1.69 | 2 (12%) |
| 1 | 5MC | A | 1404 | 1 | 15,22,23 | 1.46 | 2 (13%) | 19,32,35 | 1.50 | 4 (21%) |
| 4 | PSU | LC | 55 | 4 | 17,21,22 | 1.65 | 3 (17%) | 20,30,33 | 3.60 | 6 (30%) |
| 1 | 4OC | DB | 1402 | 1 | 16,23,24 | 0.98 | 1 (6%) | 17,32,35 | 2.22 | 3 (17%) |
| 2 | 5MC | B | 1962 | 2 | 15,22,23 | 1.46 | 2 (13%) | 19,32,35 | 1.18 | 2 (10%) |
| 4 | 5MU | IA | 54 | 56,4 | 15,22,23 | 1.70 | 3 (20%) | 16,32,35 | 1.95 | 1 (6%) |
| 1 | 2MG | DB | 1207 | 1 | 19,26,27 | 2.48 | 2 (10%) | 21,38,41 | 1.88 | 7 (33%) |
| 2 | PSU | EB | 2605 | 2 | 17,21,22 | 1.42 | 3 (17%) | 20,30,33 | 3.42 | 5 (25%) |
| 1 | MA6 | A | 1518 | 1 | 19,26,27 | 1.53 | 3 (15%) | 18,38,41 | 1.41 | 2 (11%) |
| 1 | 5MC | A | 1400 | 1 | 15,22,23 | 1.32 | 1 (6%) | 19,32,35 | 1.15 | 2 (10%) |

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 | PSU | A | 516 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | A | 1402 | 1 | - | 4/9/29/30 | 0/2/2/2 |
| 1 | 7MG | A | 527 | 1 | - | 2/7/37/38 | 0/3/3/3 |
| 1 | 5MC | DB | 967 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 2 | OMG | B | 2251 | 2,4 | - | 1/5/27/28 | 0/3/3/3 |
| 2 | 2MU | B | 2552 | 2 | - | 0/7/27/28 | 0/2/2/2 |
| 1 | PSU | DB | 516 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | DB | 1404 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 2 | PSU | EB | 1917 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 5MC | EB | 1962 | 56,2 | - | 2/5/25/26 | 0/2/2/2 |
| 45 | 0TD | WC | 92 | 45 | - | 3/3/12/14 | - |
| 1 | MA6 | A | 1519 | 1 | - | 3/7/29/30 | 0/3/3/3 |
| 2 | 5MC | EB | 1942 | 2 | - | 0/5/25/26 | 0/2/2/2 |
| 4 | 4SU | D | 8 | 4 | - | 1/5/25/26 | 0/2/2/2 |
| 1 | M2G | DB | 966 | 1 | - | 4/7/29/30 | 0/3/3/3 |
| 2 | PSU | B | 1911 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 967 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 2 | 4OC | B | 1920 | 2 | - | 4/7/27/30 | 0/2/2/2 |
| 1 | UR3 | A | 1498 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 2 | PSU | EB | 1911 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 4 | 5MC | IA | 32 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 1407 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | UR3 | DB | 1498 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 4 | 4SU | IA | 8 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 2 | 2MA | EB | 2503 | 2 | - | 2/3/25/26 | 0/3/3/3 |
| 2 | 5MU | B | 1939 | 2 | - | 0/5/25/26 | 0/2/2/2 |
| 4 | 5MC | LC | 32 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MC | DB | 1407 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 45 | 0TD | TA | 92 | 45 | - | 2/3/12/14 | - |
| 4 | 5MU | GB | 54 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 7MG | DB | 527 | 1 | - | 2/7/37/38 | 0/3/3/3 |
| 2 | 2MA | B | 2503 | 2 | - | 2/3/25/26 | 0/3/3/3 |
| 2 | 5MU | B | 1915 | 2 | - | 0/5/25/26 | 0/2/2/2 |
| 4 | 5MC | GB | 32 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | M2G | A | 966 | 1 | - | 4/7/29/30 | 0/3/3/3 |
| 2 | 5MU | EB | 1939 | 2 | - | 0/5/25/26 | 0/2/2/2 |
| 4 | 5MU | LC | 54 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 4 | PSU | IA | 55 | 4 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MG | A | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | DB | 1400 | 1 | - | 2/5/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | MA6 | DB | 1518 | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 2 | PSU | B | 2605 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 4 | 5MC | D | 32 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 2 | 5MC | B | 1942 | 2 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | MA6 | DB | 1519 | 1 | - | 3/7/29/30 | 0/3/3/3 |
| 4 | PSU | GB | 55 | 4 | - | 0/7/25/26 | 0/2/2/2 |
| 4 | 4SU | LC | 8 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 2 | 4OC | EB | 1920 | 2 | - | 3/7/27/30 | 0/2/2/2 |
| 2 | OMG | EB | 2251 | 2,4 | - | 1/5/27/28 | 0/3/3/3 |
| 4 | 5MU | D | 54 | 4 | - | 0/5/25/26 | 0/2/2/2 |
| 4 | PSU | D | 55 | 4 | - | 0/7/25/26 | 0/2/2/2 |
| 4 | 4SU | GB | 8 | 4 | - | 1/5/25/26 | 0/2/2/2 |
| 2 | PSU | B | 1917 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 2 | 2MU | EB | 2552 | 56,2 | - | 0/7/27/28 | 0/2/2/2 |
| 2 | 5MU | EB | 1915 | 2 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MC | A | 1404 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 4 | PSU | LC | 55 | 4 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | DB | 1402 | 1 | - | 4/9/29/30 | 0/2/2/2 |
| 2 | 5MC | B | 1962 | 2 | - | 2/5/25/26 | 0/2/2/2 |
| 4 | 5MU | IA | 54 | 56,4 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 2MG | DB | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 2 | PSU | EB | 2605 | 2 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MA6 | A | 1518 | 1 | - | 2/7/29/30 | 0/3/3/3 |
| 1 | 5MC | A | 1400 | 1 | - | 2/5/25/26 | 0/2/2/2 |

The worst 5 of 171 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 1 | A | 1207 | 2MG | C2-N2 | 8.72 | 1.41 | 1.34 |
| 1 | DB | 1207 | 2MG | C2-N2 | 8.30 | 1.41 | 1.34 |
| 4 | IA | 8 | 4SU | C5-C4 | 7.11 | 1.46 | 1.38 |
| 1 | A | 527 | 7MG | O6-C6 | 7.09 | 1.42 | 1.24 |
| 4 | D | 8 | 4SU | C5-C4 | 6.77 | 1.46 | 1.38 |

The worst 5 of 222 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | DB | 516 | PSU | N1-C2-N3 | -14.88 | 116.60 | 128.43 |
| 1 | A | 516 | PSU | N1-C2-N3 | -14.00 | 117.30 | 128.43 |
| 2 | B | 2605 | PSU | N1-C2-N3 | -12.92 | 118.16 | 128.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 4 | D | 55 | PSU | N1-C2-N3 | -12.10 | 118.81 | 128.43 |
| 4 | LC | 55 | PSU | N1-C2-N3 | -12.08 | 118.83 | 128.43 |

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 1 | A | 1402 | 4OC | N3-C4-N4-CM4 |
| 1 | A | 1402 | 4OC | C5-C4-N4-CM4 |
| 2 | B | 2251 | OMG | C1'-C2'-O2'-CM2 |
| 2 | EB | 1962 | 5MC | O4'-C1'-N1-C6 |
| 2 | EB | 1962 | 5MC | C2'-C1'-N1-C6 |

There are no ring outliers.

31 monomers are involved in 42 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | A | 1402 | 4OC | 2 | 0 |
| 1 | DB | 967 | 5MC | 1 | 0 |
| 2 | B | 2552 | 2MU | 2 | 0 |
| 2 | EB | 1917 | PSU | 1 | 0 |
| 45 | WC | 92 | 0TD | 3 | 0 |
| 2 | EB | 1942 | 5MC | 1 | 0 |
| 1 | DB | 966 | M2G | 1 | 0 |
| 1 | A | 967 | 5MC | 1 | 0 |
| 2 | B | 1920 | 4OC | 1 | 0 |
| 1 | A | 1498 | UR3 | 1 | 0 |
| 1 | A | 1407 | 5MC | 1 | 0 |
| 1 | DB | 1498 | UR3 | 1 | 0 |
| 2 | EB | 2503 | 2MA | 4 | 0 |
| 2 | B | 1939 | 5MU | 2 | 0 |
| 1 | DB | 1407 | 5MC | 1 | 0 |
| 45 | TA | 92 | 0TD | 3 | 0 |
| 4 | GB | 54 | 5MU | 1 | 0 |
| 2 | B | 2503 | 2MA | 3 | 0 |
| 2 | B | 1915 | 5MU | 1 | 0 |
| 1 | A | 966 | M2G | 1 | 0 |
| 2 | EB | 1939 | 5MU | 1 | 0 |
| 1 | DB | 1518 | MA6 | 1 | 0 |
| 1 | DB | 1519 | MA6 | 1 | 0 |
| 4 | GB | 55 | PSU | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | D | 54 | 5MU | 1 | 0 |
| 4 | D | 55 | PSU | 1 | 0 |
| 4 | GB | 8 | 4SU | 1 | 0 |
| 2 | EB | 2552 | 2MU | 2 | 0 |
| 2 | EB | 1915 | 5MU | 1 | 0 |
| 1 | DB | 1402 | 4OC | 1 | 0 |
| 1 | A | 1518 | MA6 | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1528 ligands modelled in this entry, 1528 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.