



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:05 am GMT

PDB ID : 4V55
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin and ribosome recycling factor (RRF).
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-17
Resolution : 4.00 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

<http://wwpdb.org/validation/2016/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 | : | 1.7.2 (RC1), CSD as538be (2017) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | trunk28620 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | recalc28972 |

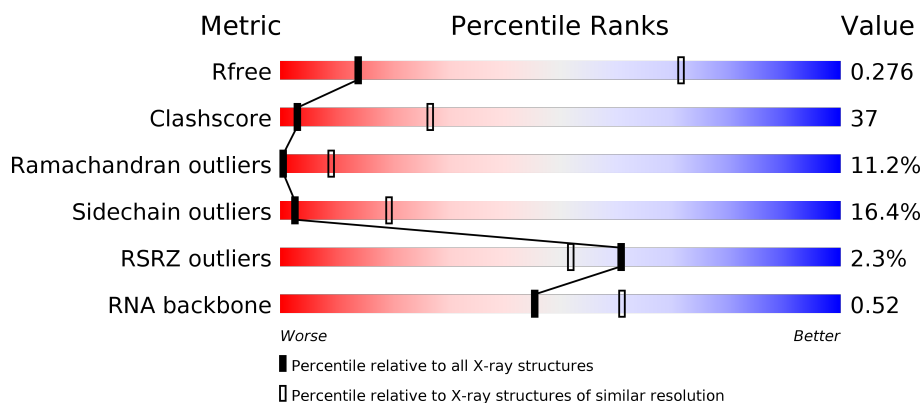
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1088 (4.40-3.60) |
| Clashscore | 112137 | 1187 (4.40-3.60) |
| Ramachandran outliers | 110173 | 1139 (4.40-3.60) |
| Sidechain outliers | 110143 | 1126 (4.40-3.60) |
| RSRZ outliers | 101464 | 1099 (4.40-3.60) |
| RNA backbone | 2435 | 1026 (5.04-2.90) |

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | AA | 1542 | <div> <div></div> <div>24% 63% 12% ..</div> </div> |
| 1 | CA | 1542 | <div> <div></div> <div>22% 65% 12% ..</div> </div> |
| 2 | AC | 232 | <div> <div></div> <div>29% 48% 11% 11%</div> </div> |
| 2 | CC | 232 | <div> <div></div> <div>28% 49% 12% 11%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AD | 205 | |
| 3 | CD | 205 | |
| 4 | AE | 166 | |
| 4 | CE | 166 | |
| 5 | AF | 135 | |
| 5 | CF | 135 | |
| 6 | AG | 178 | |
| 6 | CG | 178 | |
| 7 | AH | 129 | |
| 7 | CH | 129 | |
| 8 | AI | 129 | |
| 8 | CI | 129 | |
| 9 | AJ | 103 | |
| 9 | CJ | 103 | |
| 10 | AK | 128 | |
| 10 | CK | 128 | |
| 11 | AL | 123 | |
| 11 | CL | 123 | |
| 12 | AM | 117 | |
| 12 | CM | 117 | |
| 13 | AN | 100 | |
| 13 | CN | 100 | |
| 14 | AO | 89 | |
| 14 | CO | 89 | |
| 15 | AP | 82 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | CP | 82 | |
| 16 | AQ | 83 | |
| 16 | CQ | 83 | |
| 17 | AR | 74 | |
| 17 | CR | 74 | |
| 18 | AS | 91 | |
| 18 | CS | 91 | |
| 19 | AT | 86 | |
| 19 | CT | 86 | |
| 20 | AB | 240 | |
| 20 | CB | 240 | |
| 21 | AU | 70 | |
| 21 | CU | 70 | |
| 22 | BA | 120 | |
| 22 | DA | 120 | |
| 23 | BB | 2904 | |
| 23 | DB | 2904 | |
| 24 | BI | 141 | |
| 24 | DI | 141 | |
| 25 | BC | 272 | |
| 25 | DC | 272 | |
| 26 | BD | 209 | |
| 26 | DD | 209 | |
| 27 | BK | 123 | |
| 27 | DK | 123 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | BP | 114 | |
| 28 | DP | 114 | |
| 29 | BE | 201 | |
| 29 | DE | 201 | |
| 30 | BY | 58 | |
| 30 | DY | 58 | |
| 31 | B0 | 56 | |
| 31 | D0 | 56 | |
| 32 | B4 | 38 | |
| 32 | D4 | 38 | |
| 33 | B1 | 54 | |
| 33 | D1 | 54 | |
| 34 | B3 | 64 | |
| 34 | D3 | 64 | |
| 35 | BV | 94 | |
| 35 | DV | 94 | |
| 36 | B2 | 46 | |
| 36 | D2 | 46 | |
| 37 | BL | 144 | |
| 37 | DL | 144 | |
| 38 | BM | 136 | |
| 38 | DM | 136 | |
| 39 | BX | 63 | |
| 39 | DX | 63 | |
| 40 | BH | 149 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | DH | 149 | |
| 41 | BJ | 142 | |
| 41 | DJ | 142 | |
| 42 | BN | 127 | |
| 42 | DN | 127 | |
| 43 | BO | 117 | |
| 43 | DO | 117 | |
| 44 | BQ | 117 | |
| 44 | DQ | 117 | |
| 45 | BS | 110 | |
| 45 | DS | 110 | |
| 46 | BU | 103 | |
| 46 | DU | 103 | |
| 47 | BF | 178 | |
| 47 | DF | 178 | |
| 48 | BG | 176 | |
| 48 | DG | 176 | |
| 49 | BR | 103 | |
| 49 | DR | 103 | |
| 50 | BT | 100 | |
| 50 | DT | 100 | |
| 51 | BZ | 78 | |
| 51 | DZ | 78 | |
| 52 | BW | 84 | |
| 52 | DW | 84 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | B6 | 185 | |
| 53 | D6 | 185 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | DB | 3059 | - | - | - | X |
| 55 | LLL | BB | 3111 | - | - | - | X |
| 55 | LLL | DB | 3112 | - | - | - | X |

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287083 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 rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1530 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32831 | 14642 | 6024 | 10635 | 1530 | | | |
| 1 | CA | 1530 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32831 | 14642 | 6024 | 10635 | 1530 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | | |
| 2 | CC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | AE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |
| 4 | CE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |
| 5 | CF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AG | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1174 | 730 | 226 | 214 | 4 | | | |
| 6 | CG | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1196 | 745 | 230 | 217 | 4 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 8 | CI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1021 | 634 | 206 | 178 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | AJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |
| 9 | CJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | CK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | | |
| 12 | CM | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 876 | 541 | 177 | 155 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |
| 13 | CN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 15 | CP | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 400 | 126 | 111 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | | |
| 16 | CQ | 81 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 657 | 417 | 122 | 115 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17 | AR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |
| 17 | CR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | AS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 637 | 408 | 120 | 107 | 2 | | | |
| 18 | CS | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 644 | 413 | 121 | 108 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |
| 19 | CT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 20 | AB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |
| 20 | CB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21 | AU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |
| 21 | CU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |

- Molecule 22 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 22 | BA | 117 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2507 | 1116 | 459 | 815 | 117 | | | |
| 22 | DA | 117 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2507 | 1116 | 459 | 815 | 117 | | | |

- Molecule 23 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 23 | BB | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60995 | 27210 | 11229 | 19715 | 2841 | | | |
| 23 | DB | 2841 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60995 | 27210 | 11229 | 19715 | 2841 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | BI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 24 | DI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 25 | BC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |
| 25 | DC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |

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

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

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | BK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |
| 27 | DK | 121 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 930 | 582 | 179 | 164 | 5 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | BP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |
| 28 | DP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | BE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 29 | DE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 30 | BY | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |
| 30 | DY | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | B0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 31 | D0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 32 | B4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 32 | D4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 33 | B1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |
| 33 | D1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 34 | B3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 34 | D3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | BV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 35 | DV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 36 | B2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 36 | D2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |
| 37 | DL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |
| 38 | DM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |

- Molecule 39 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 39 | BX | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |
| 39 | DX | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |
| 40 | DH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1111 | 699 | 197 | 214 | 1 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |
| 41 | DJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | DN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 43 | BO | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |
| 43 | DO | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |

- Molecule 44 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 44 | BQ | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |
| 44 | DQ | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |

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

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 46 | BU | 102 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | | |
| 46 | DU | 102 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | | |

- Molecule 47 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | BF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |
| 47 | DF | 178 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1420 | 905 | 251 | 258 | 6 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | BG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 48 | DG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | BR | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |
| 49 | DR | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50 | BT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |
| 50 | DT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51 | BZ | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 51 | DZ | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | BW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |
| 52 | DW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |

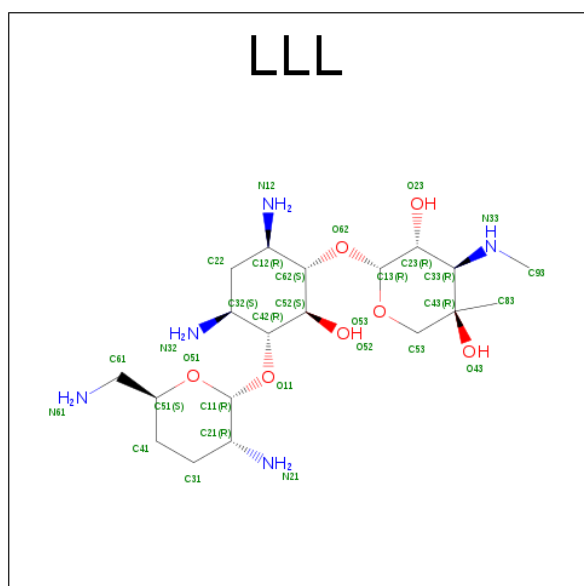
- Molecule 53 is a protein called 50S ribosomal protein RRF.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53 | B6 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1478 | 924 | 270 | 282 | 2 | | | |
| 53 | D6 | 185 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1478 | 924 | 270 | 282 | 2 | | | |

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54 | DB | 111 | Total | Mg | 0 | 0 |
| | | | 111 | 111 | | |
| 54 | BB | 110 | Total | Mg | 0 | 0 |
| | | | 110 | 110 | | |
| 54 | AA | 60 | Total | Mg | 0 | 0 |
| | | | 60 | 60 | | |
| 54 | CA | 61 | Total | Mg | 0 | 0 |
| | | | 61 | 61 | | |
| 54 | CE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 55 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 55 | AA | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 55 | BB | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 55 | CA | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |
| 55 | DB | 1 | Total | C | N | O | 0 | 0 |
| | | | 31 | 19 | 5 | 7 | | |

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

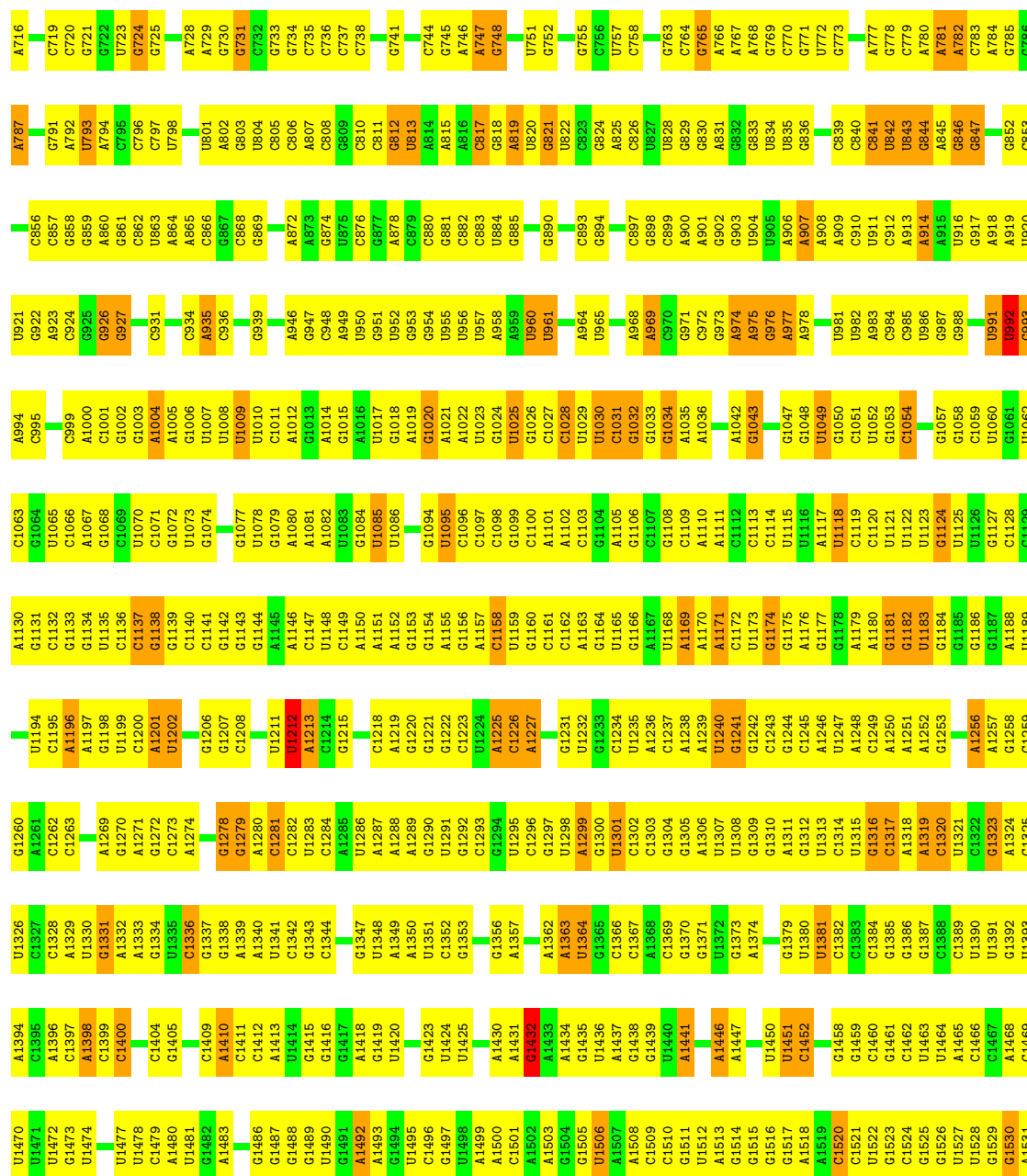
- Molecule 57 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57 | AA | 287 | Total | O | 0 | 0 |
| | | | 287 | 287 | | |
| 57 | AE | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | AK | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | AL | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | AN | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 57 | AT | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 57 | BB | 492 | Total | O | 0 | 0 |
| | | | 492 | 492 | | |
| 57 | BC | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 57 | BD | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 57 | BE | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | BL | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 57 | BT | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

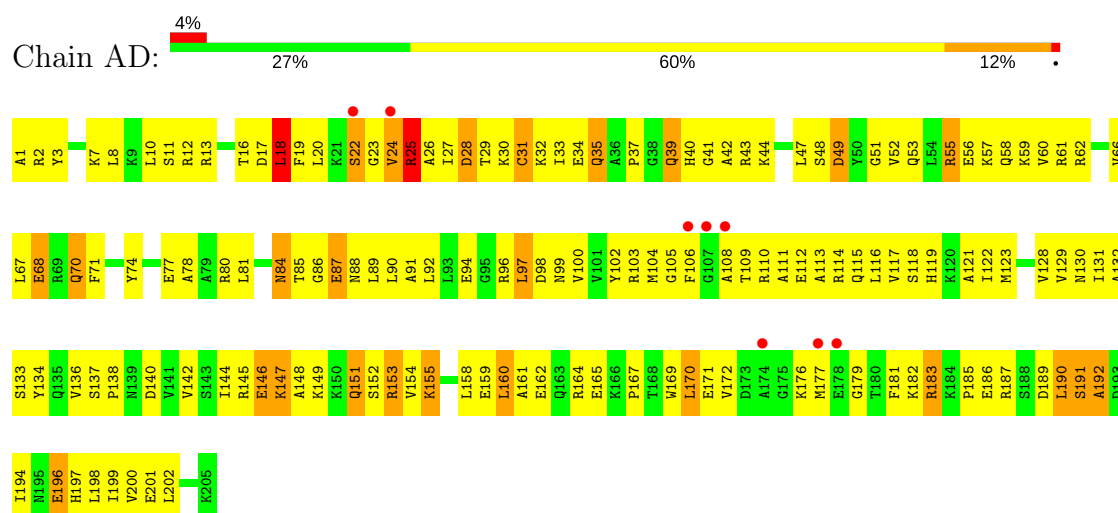
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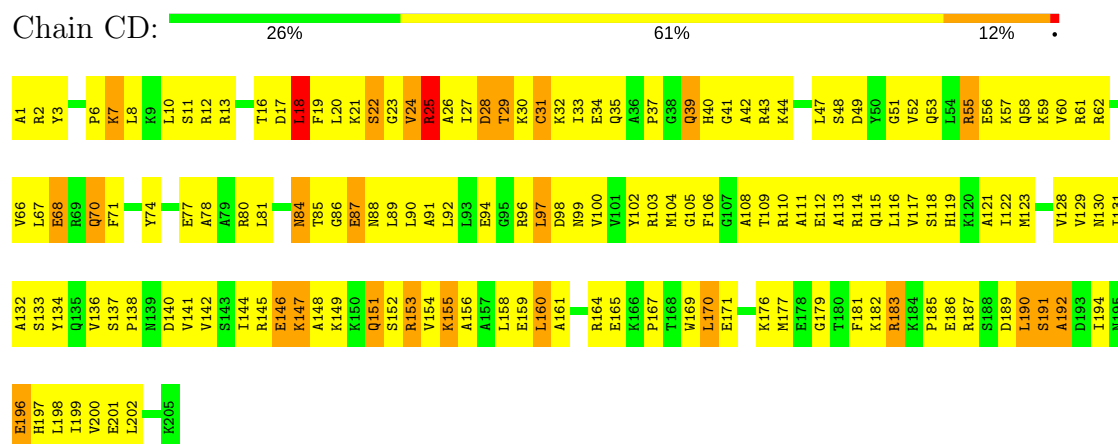
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 57 | CA | 296 | Total 296 | O 296 | 0 | 0 |
| 57 | CE | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | CK | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | CL | 3 | Total 3 | O 3 | 0 | 0 |
| 57 | CN | 4 | Total 4 | O 4 | 0 | 0 |
| 57 | CT | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | DB | 500 | Total 500 | O 500 | 0 | 0 |
| 57 | DC | 6 | Total 6 | O 6 | 0 | 0 |
| 57 | DE | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | DL | 2 | Total 2 | O 2 | 0 | 0 |
| 57 | DR | 1 | Total 1 | O 1 | 0 | 0 |
| 57 | DT | 1 | Total 1 | O 1 | 0 | 0 |



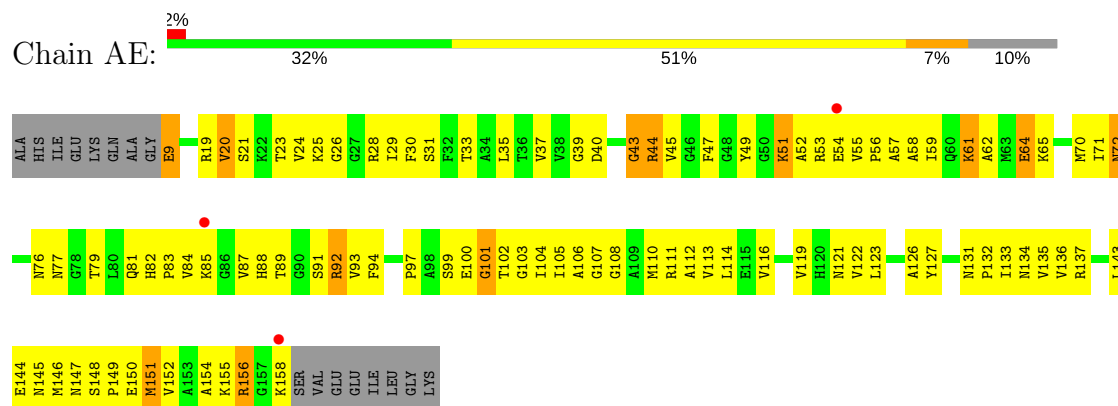


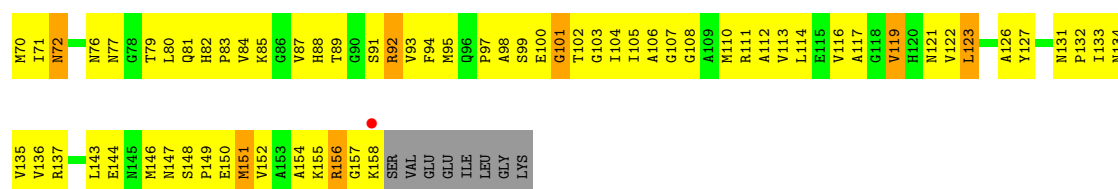


• Molecule 3: 30S ribosomal protein S4

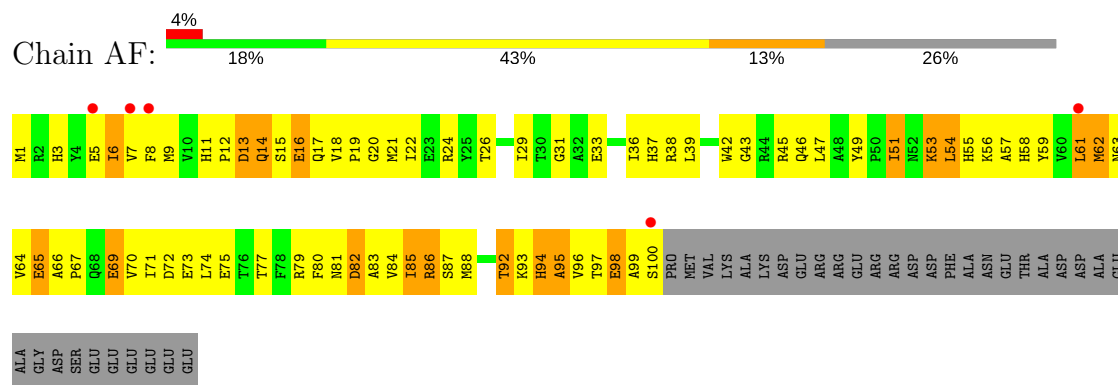


• Molecule 4: 30S ribosomal protein S5

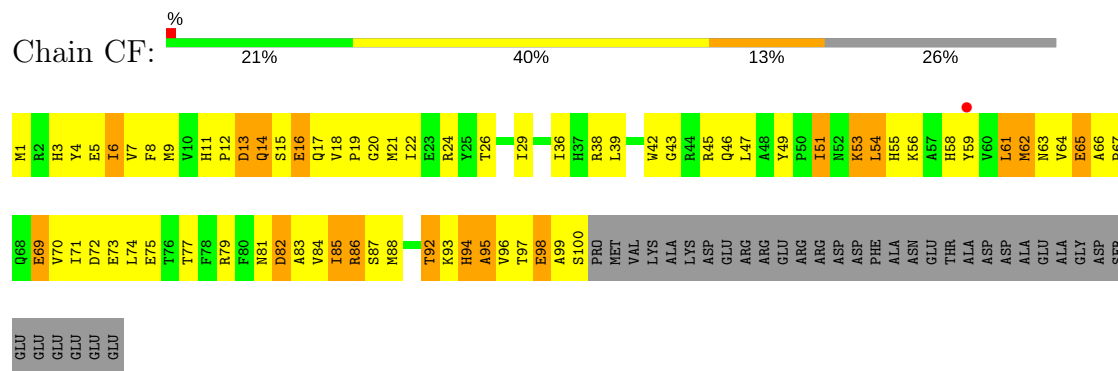




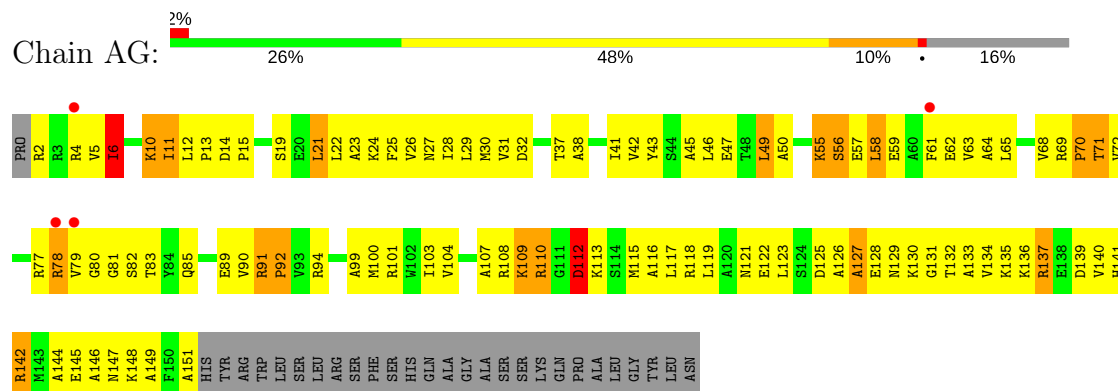
• Molecule 5: 30S ribosomal protein S6

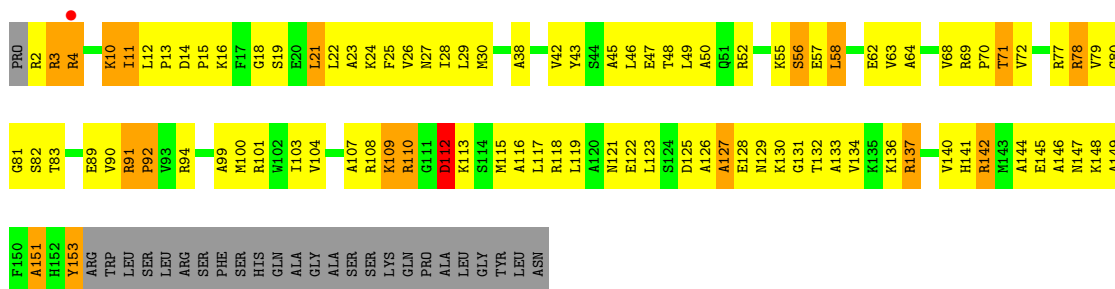


• Molecule 5: 30S ribosomal protein S6

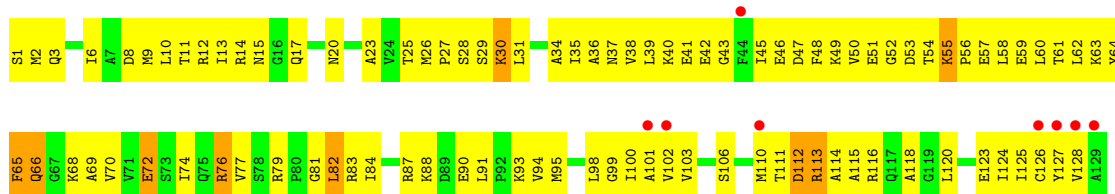


• Molecule 6: 30S ribosomal protein S7

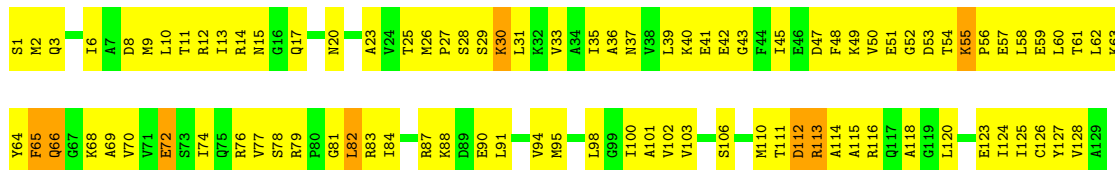




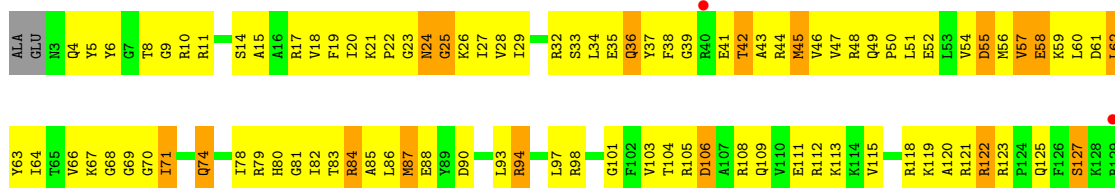
• Molecule 7: 30S ribosomal protein S8



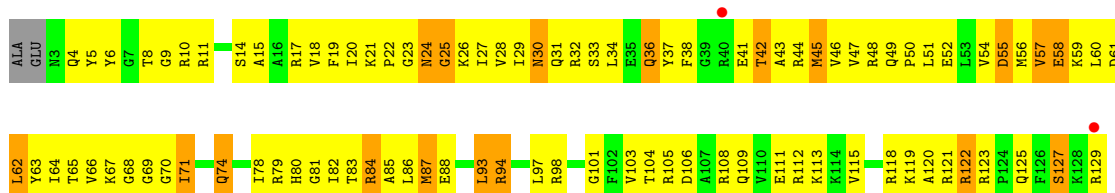
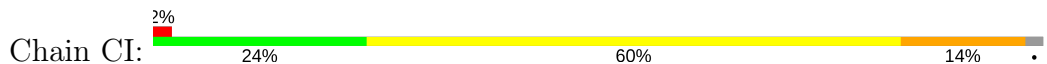
• Molecule 7: 30S ribosomal protein S8



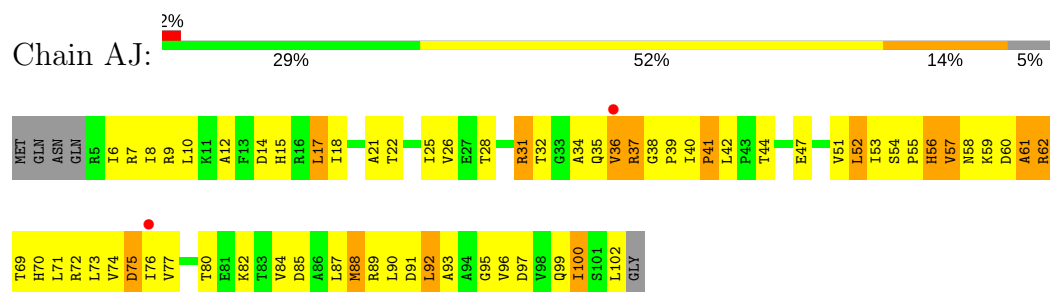
• Molecule 8: 30S ribosomal protein S9



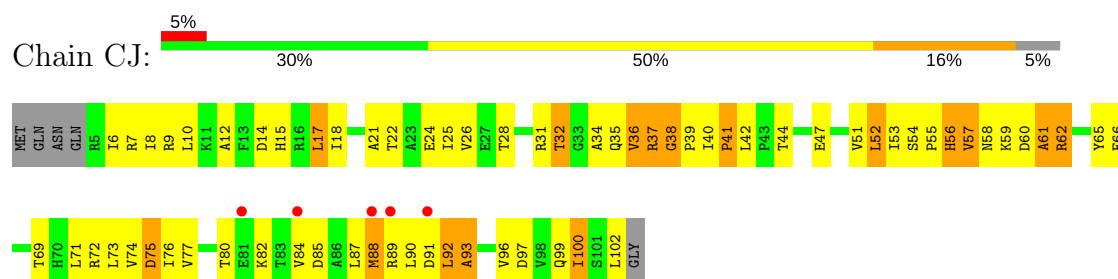
• Molecule 8: 30S ribosomal protein S9



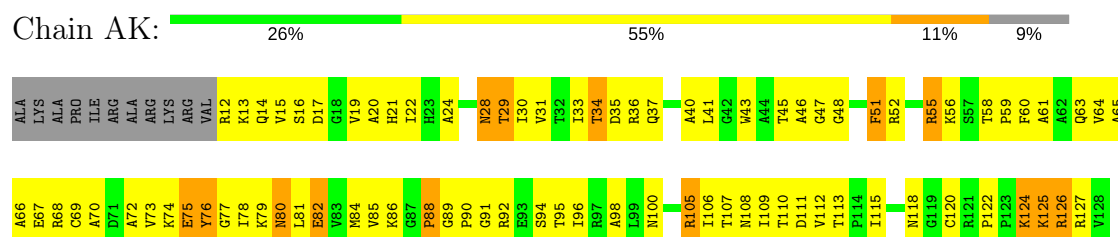
- Molecule 9: 30S ribosomal protein S10



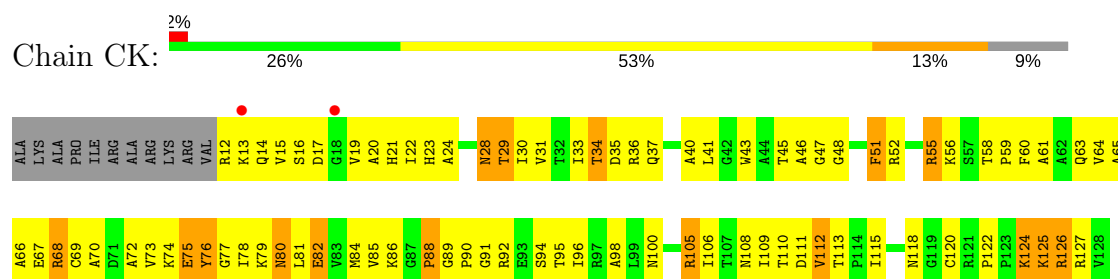
- Molecule 9: 30S ribosomal protein S10



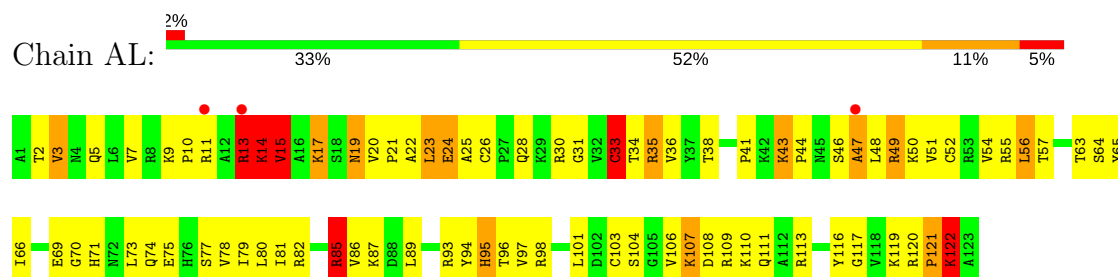
- Molecule 10: 30S ribosomal protein S11



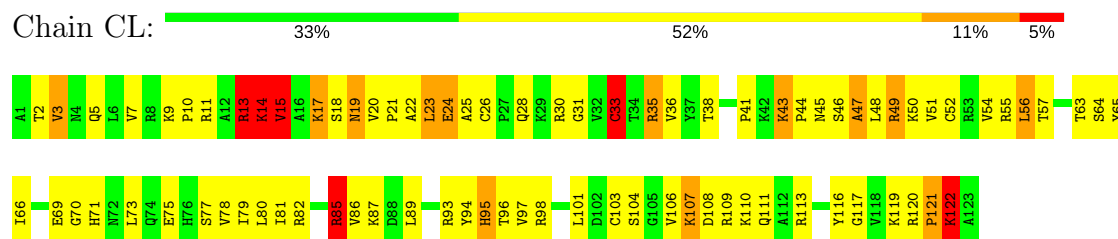
- Molecule 10: 30S ribosomal protein S11



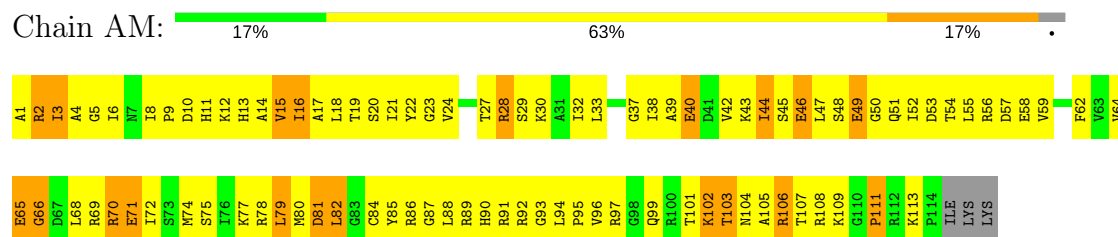
- Molecule 11: 30S ribosomal protein S12



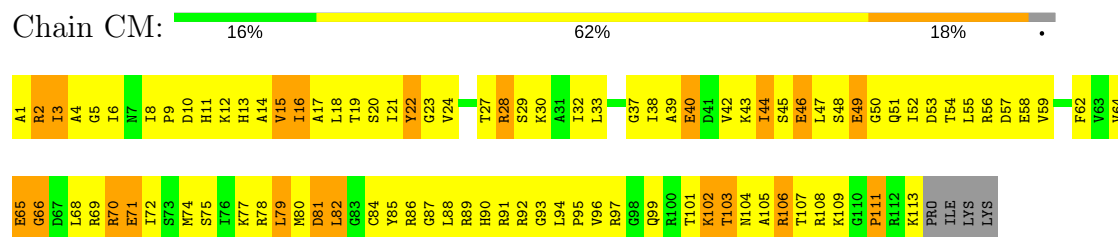
- Molecule 11: 30S ribosomal protein S12



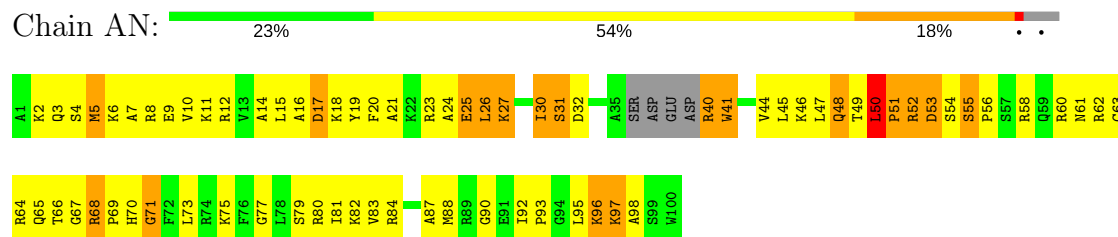
- Molecule 12: 30S ribosomal protein S13



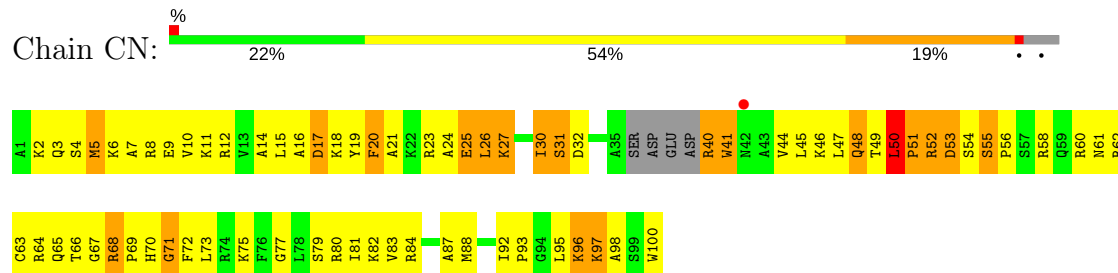
- Molecule 12: 30S ribosomal protein S13



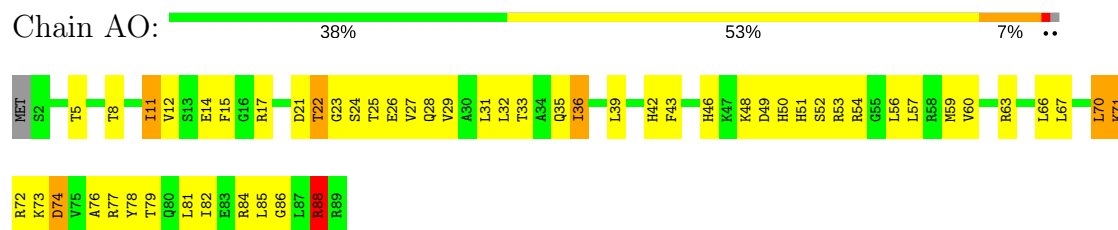
- Molecule 13: 30S ribosomal protein S14



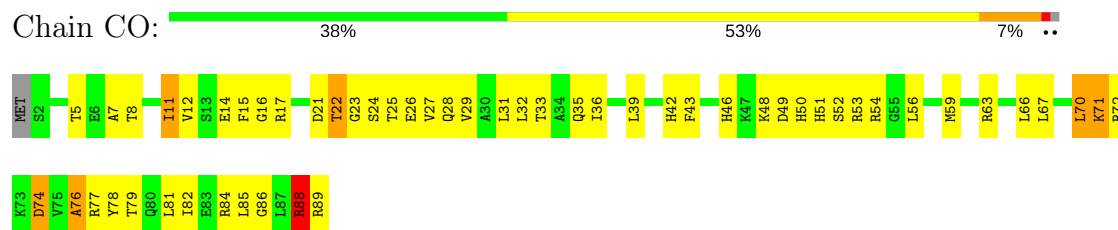
- Molecule 13: 30S ribosomal protein S14



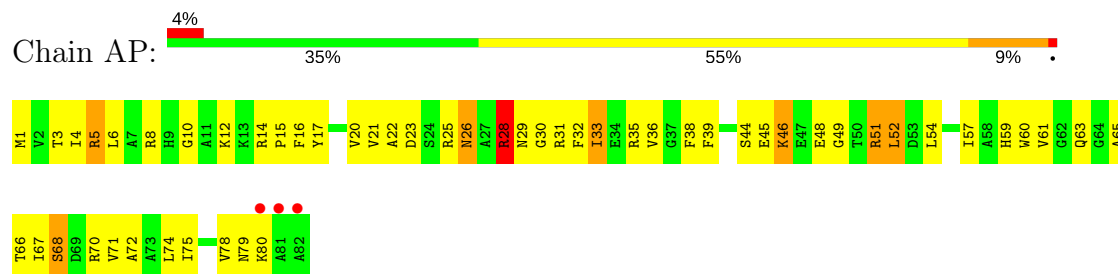
- Molecule 14: 30S ribosomal protein S15



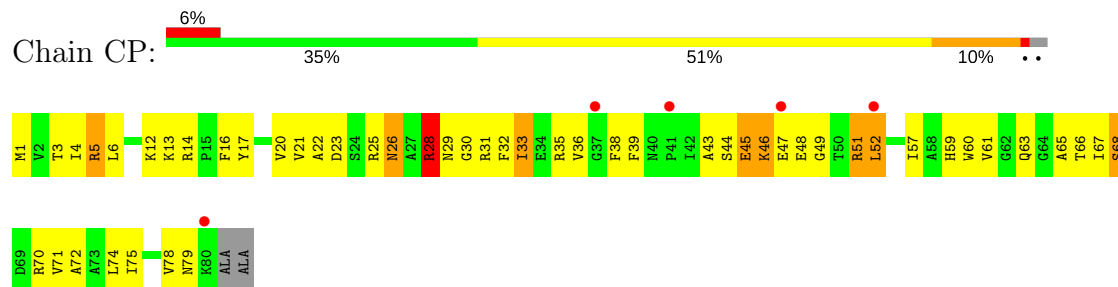
• Molecule 14: 30S ribosomal protein S15



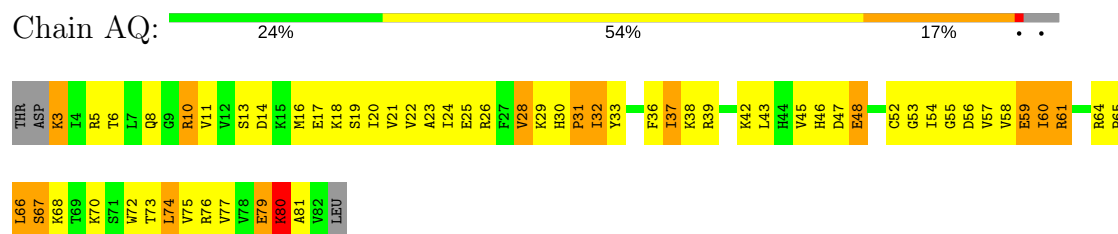
• Molecule 15: 30S ribosomal protein S16



• Molecule 15: 30S ribosomal protein S16

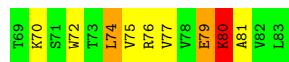


• Molecule 16: 30S ribosomal protein S17

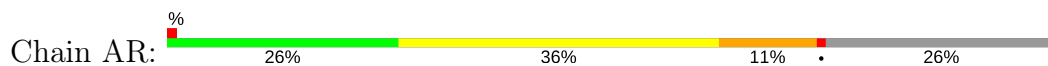


• Molecule 16: 30S ribosomal protein S17

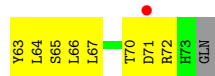
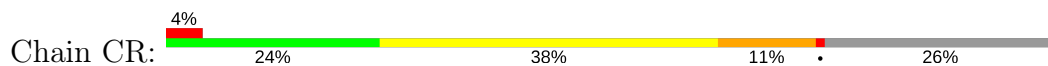




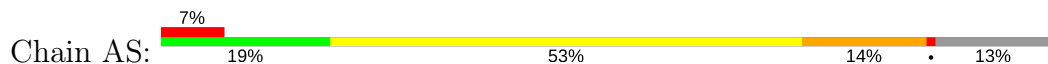
- Molecule 17: 30S ribosomal protein S18



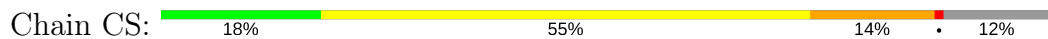
- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19

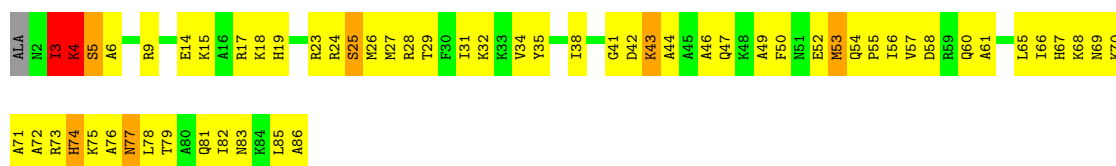


- Molecule 18: 30S ribosomal protein S19



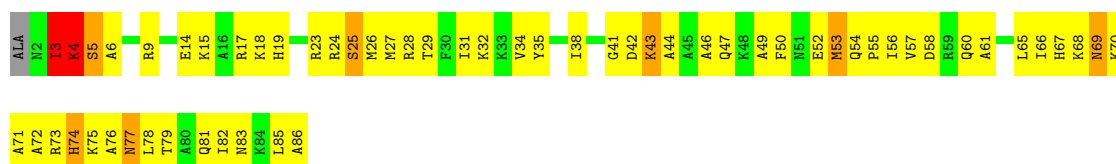
- Molecule 19: 30S ribosomal protein S20





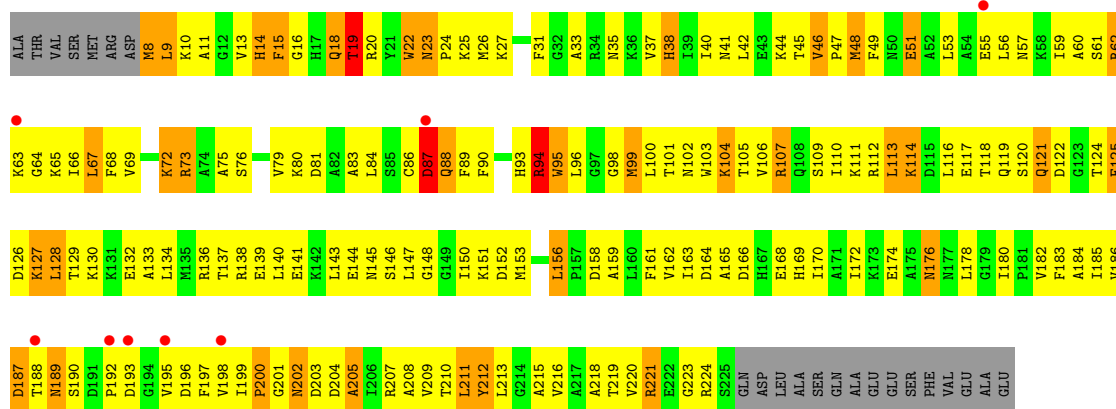
• Molecule 19: 30S ribosomal protein S20

Chain CT: 30% 58% 8%



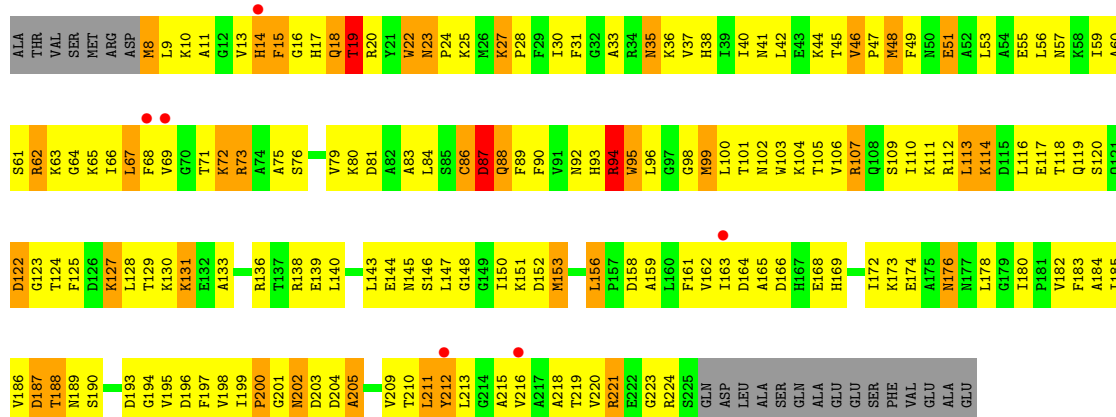
• Molecule 20: 30S ribosomal protein S2

Chain AB: 3% 21% 54% 15% 9%

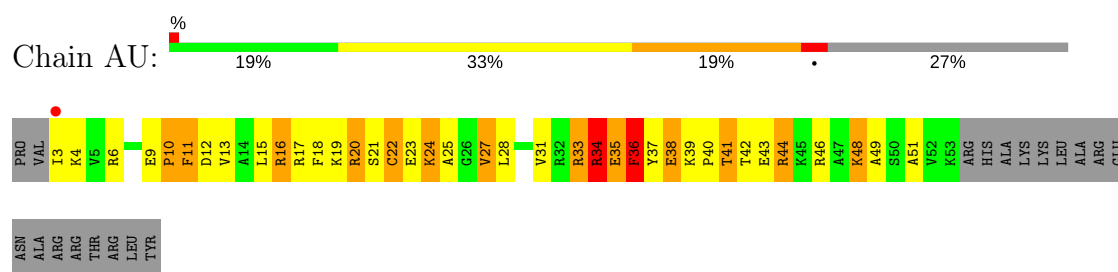


• Molecule 20: 30S ribosomal protein S2

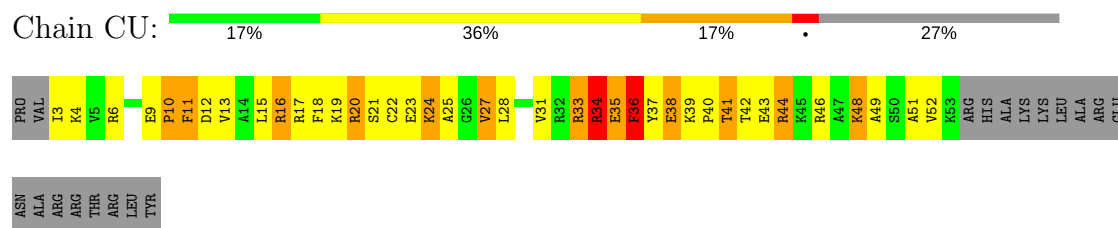
Chain CB: 3% 21% 53% 15% 9%



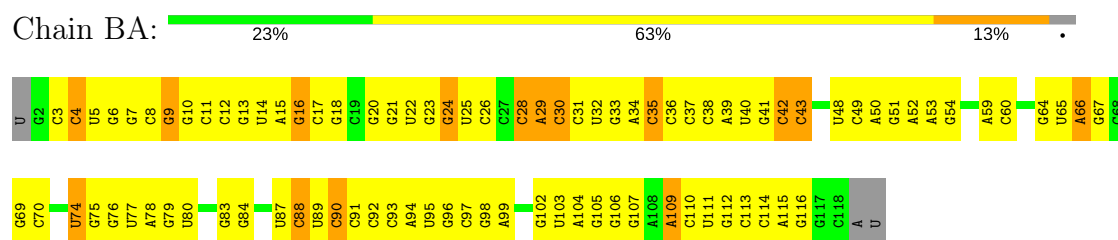
• Molecule 21: 30S ribosomal protein S21



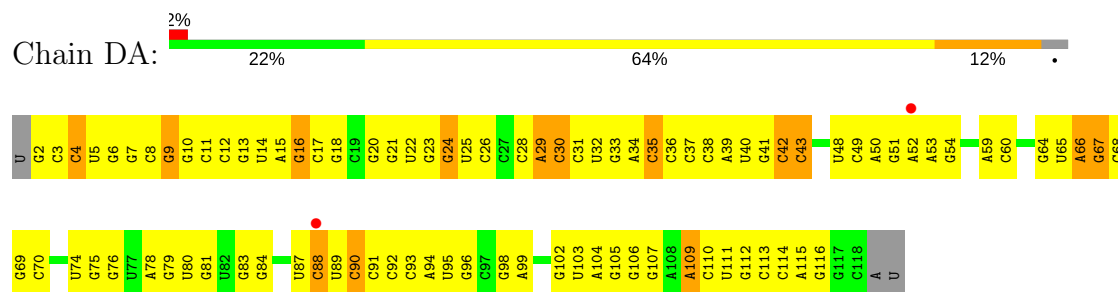
- Molecule 21: 30S ribosomal protein S21



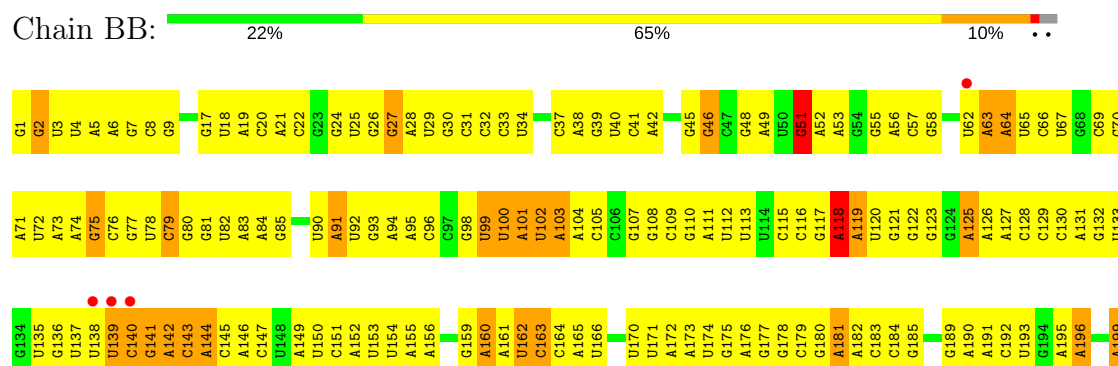
- Molecule 22: 5S rRNA



- Molecule 22: 5S rRNA



- Molecule 23: 23S rRNA

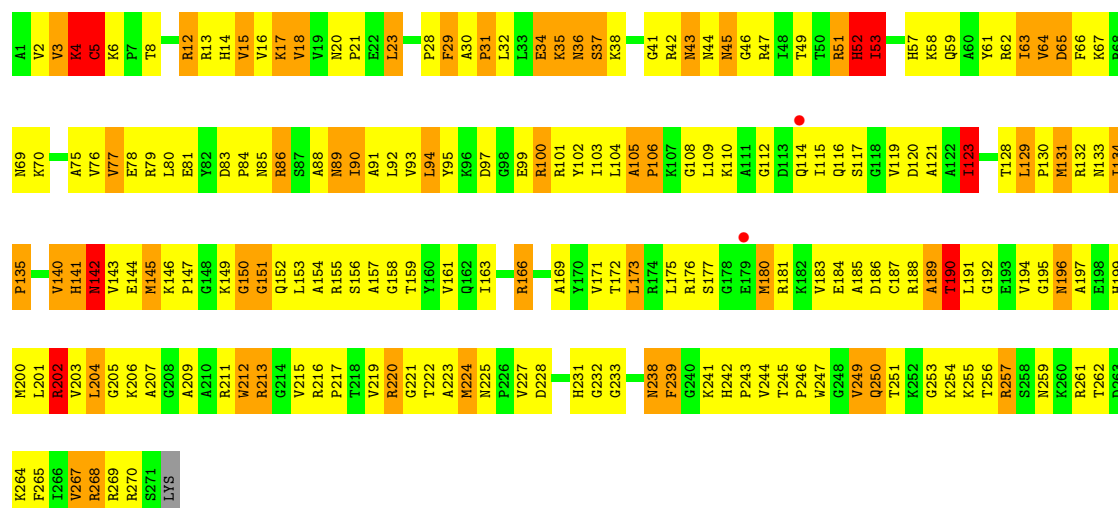


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| U1201 | C1135 | A1069 | C995 | A933 | A863 | G799 | C732 | A668 | C545 | A472 | U405 | C334 | C267 | C201 |
| G1202 | G1136 | A1070 | A996 | U934 | G864 | U803 | G733 | G669 | U546 | A473 | G408 | C335 | C268 | U202 |
| A1203 | G1137 | A1071 | C996 | C935 | C865 | A804 | A734 | A609 | U547 | C476 | G409 | C336 | C269 | A203 |
| A1204 | G1138 | A1072 | A1001 | A936 | A866 | G805 | A735 | C611 | G548 | A478 | G410 | C337 | A270 | G204 |
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| U1209 | A1143 | U1078 | A941 | A941 | U873 | U810 | C740 | A616 | U554 | A483 | C415 | A345 | C275 | C209 |
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| C2295 | U2039 | C1967 | C1894 | U1826 | G1766 | | | C1564 | A1439 | G1377 | G1309 | G1310 |
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| C2308 | G2052 | U1982 | A1913 | C1843 | U1777 | A1711 | U1647 | U1575 | C1512 | C1451 | G1388 | A1322 |
| A2309 | G2053 | G1983 | C1914 | C1844 | U1778 | U1712 | U1648 | U1576 | G1513 | G1452 | G1389 | C1323 |
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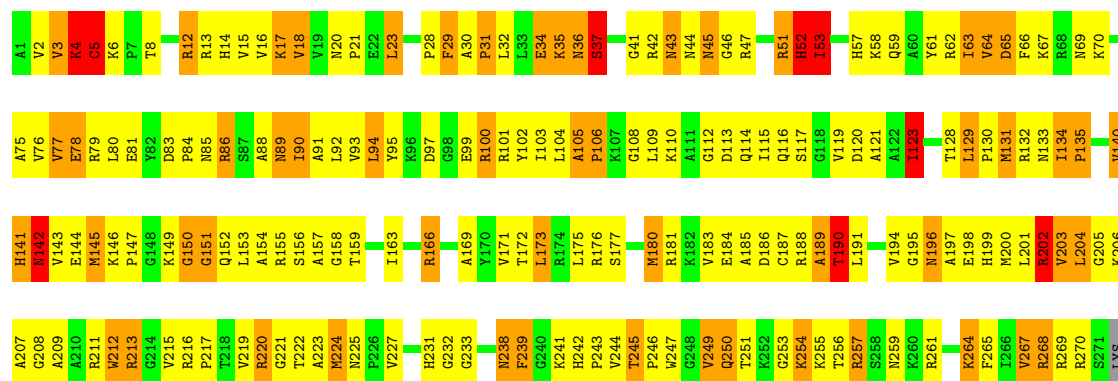


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| A2476 | A2147 | G2023 | G2087 | G2023 | G1945 | C1883 | C1816 | A1744 | A1678 | C1541 | C1541 | U1476 |
| G2484 | G2148 | G2024 | A2088 | G2024 | U1946 | G1884 | G1817 | A1745 | A1679 | U1542 | U1542 | A1477 |
| G2485 | U2149 | C2025 | C2089 | C2025 | C1947 | A1885 | U1818 | A1746 | C1606 | G1543 | G1543 | G1478 |
| G2486 | C2150 | U2026 | A2090 | U2026 | G1948 | U1886 | A1819 | A1754 | C1607 | A1544 | A1544 | G1479 |
| G2487 | U2151 | G2027 | C2091 | G2027 | G1949 | C1887 | U1820 | | A1608 | A1545 | C1480 | U1480 |
| G2488 | G2152 | U2092 | G2093 | U2092 | U1955 | A1888 | A1821 | | U1683 | G1546 | G1546 | U1481 |
| G2489 | C2153 | G2028 | G2093 | G2028 | U1956 | A1889 | A1822 | U1758 | A1609 | C1547 | C1547 | G1482 |
| U2491 | A2154 | A2030 | A2094 | A2030 | C1957 | A1890 | G1823 | A1759 | C1611 | A1548 | A1548 | G1483 |
| U2492 | U2155 | A2031 | A2095 | A2031 | C1958 | G1891 | U1824 | C1760 | C1612 | A1549 | A1549 | U1484 |
| G2493 | U2156 | G2032 | C2096 | G2032 | G1958 | C1892 | U1825 | C1761 | G1613 | U1550 | C1550 | U1485 |
| G2494 | G2157 | U2033 | A2097 | U2033 | G1959 | C1893 | G1826 | A1762 | C1557 | A1551 | C1557 | U1486 |
| G2495 | A | U2034 | U2098 | U2034 | U1963 | C1894 | U1827 | G1763 | A1616 | A1553 | A1553 | U1487 |
| G2496 | C | G2035 | U2099 | G2035 | G1964 | C1895 | G1828 | C1764 | G1620 | U1554 | U1554 | C1488 |
| G2497 | C | C2036 | C2100 | C2036 | C1965 | G1896 | A1829 | U1765 | G1620 | U1554 | U1554 | C1488 |
| G2498 | C | A2037 | A2101 | A2037 | C1966 | G1897 | C1830 | U1766 | G1620 | U1554 | U1554 | C1488 |
| G2499 | G | G2038 | C2102 | G2038 | A1966 | U1898 | G1831 | C1767 | C1556 | U1555 | C1556 | A1490 |
| G2500 | A | U2039 | C2103 | U2039 | C1967 | A1899 | C1832 | C1768 | C1557 | C1557 | C1557 | G1491 |
| G2501 | C | G2040 | C2104 | G2040 | G1968 | A1900 | C1833 | U1769 | C1558 | C1493 | C1493 | G1492 |
| G2502 | U | U2041 | U2105 | U2041 | A1969 | A1901 | U1834 | G1770 | U1559 | A1494 | A1494 | C1493 |
| G2503 | U | A2042 | U2106 | A2042 | A1970 | C1902 | U1834 | C1771 | C1560 | A1495 | A1495 | A1496 |
| G2504 | U | C2043 | G2107 | C2043 | U1971 | G1903 | U1841 | A1772 | C1561 | A1496 | A1496 | U1497 |
| G2505 | A | G2044 | A2108 | G2044 | G1972 | G1904 | G1842 | A1773 | U1562 | U1562 | U1562 | G1501 |
| G2506 | A | C2045 | U2109 | C2045 | G1973 | C1905 | C1843 | C1774 | C1563 | U1563 | U1563 | G1501 |
| G2507 | A | G2046 | G2110 | G2046 | C1974 | G1906 | C1844 | U1775 | C1564 | C1564 | C1564 | A1502 |
| G2508 | U | A2047 | U | A2047 | A1977 | G1907 | G1845 | G1776 | C1565 | A1503 | A1503 | A1503 |
| G2509 | A | A2051 | G | A2051 | G1983 | C1908 | G1846 | U1777 | C1566 | A1504 | A1504 | A1504 |
| G2510 | A | G2052 | A | G2052 | G1984 | C1909 | A1847 | U1778 | C1567 | A1505 | A1505 | A1505 |
| G2511 | C | A2053 | G | A2053 | C1985 | U1911 | A1848 | U1779 | C1568 | U1506 | U1506 | U1506 |
| G2512 | C | G2054 | G | G2054 | C1986 | A1912 | G1849 | | A1570 | A1570 | A1570 | C1507 |
| G2513 | C | C2055 | A | C2055 | A1987 | A1913 | U1853 | A1783 | C1569 | A1507 | A1507 | A1507 |
| G2514 | C | G2056 | A | G2056 | G1988 | C1914 | A1854 | A1784 | C1570 | A1508 | A1508 | A1508 |
| G2515 | A | A2060 | G | A2060 | G1988 | U1915 | U1855 | A1785 | U1571 | A1509 | A1509 | A1509 |
| G2516 | G | G2061 | U | G2061 | U1991 | A1916 | U1856 | U1786 | U1572 | A1510 | A1510 | G1510 |
| G2517 | U | A2062 | G | A2062 | G1992 | U1917 | U1857 | A1787 | C1573 | G1511 | G1511 | G1511 |
| G2518 | G | G2063 | U | G2063 | G1993 | A1918 | G1858 | C1788 | C1574 | C1574 | C1574 | C1512 |
| G2519 | G | C2064 | G | C2064 | U1994 | A1919 | A1859 | A1789 | G1575 | U1512 | U1512 | U1512 |
| G2520 | G | G2065 | G | G2065 | C1994 | A1919 | G1860 | C1791 | C1576 | U1513 | U1513 | U1513 |
| G2521 | A | U2066 | A | U2066 | U1995 | U1923 | G1861 | G1792 | C1577 | A1514 | A1514 | A1514 |
| G2522 | G | C2067 | G | C2067 | C1996 | C1924 | G1862 | C1793 | C1578 | A1515 | A1515 | A1515 |
| G2523 | G | U2068 | G | U2068 | U1998 | U1926 | G1863 | C1794 | C1579 | A1516 | A1516 | A1516 |
| G2524 | G | U2068 | G | U2068 | U1998 | U1926 | G1863 | C1794 | C1579 | A1516 | A1516 | A1516 |
| G2525 | G | U2068 | G | U2068 | U1998 | U1926 | G1863 | C1794 | C1579 | A1516 | A1516 | A1516 |



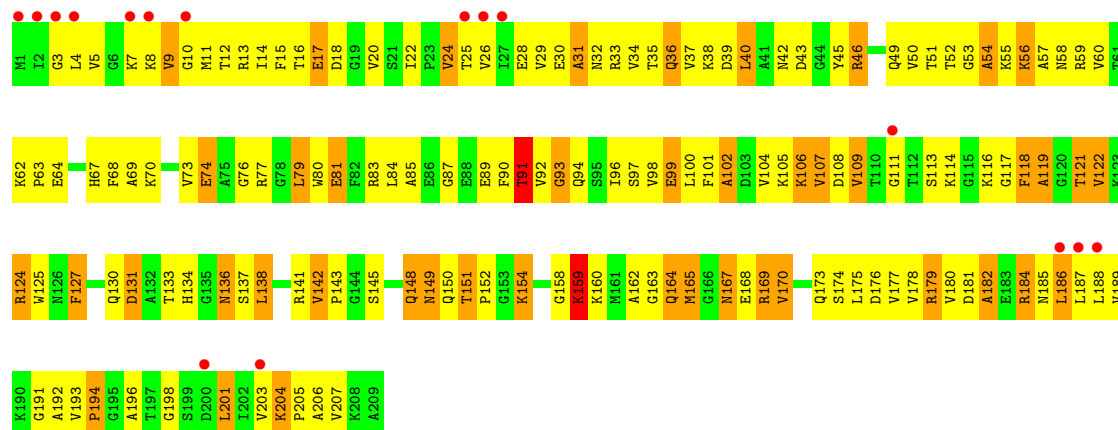
- Molecule 25: 50S ribosomal protein L2

Chain DC: 29% 47% 20%

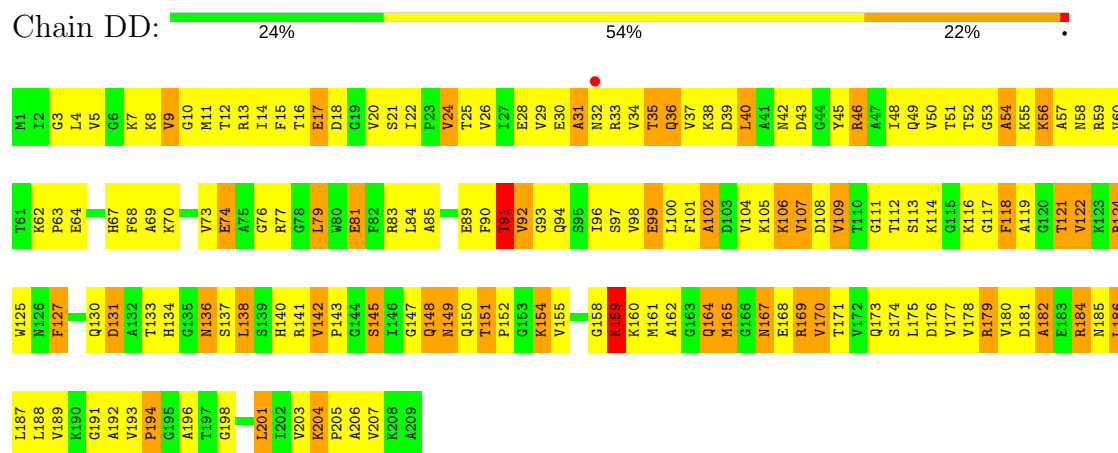


- Molecule 26: 50S ribosomal protein L3

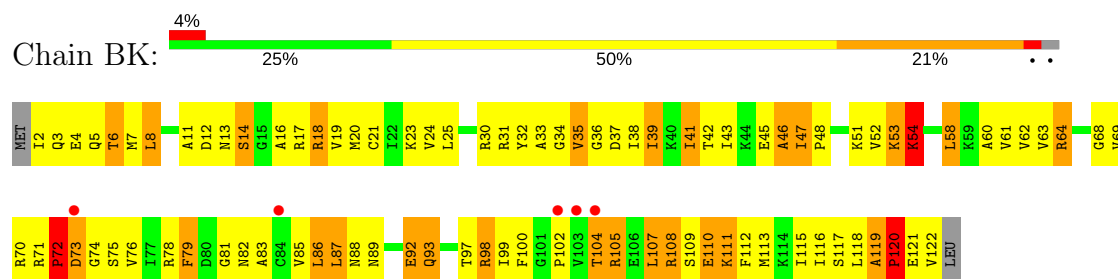
Chain BD: 8% 26% 52% 21%



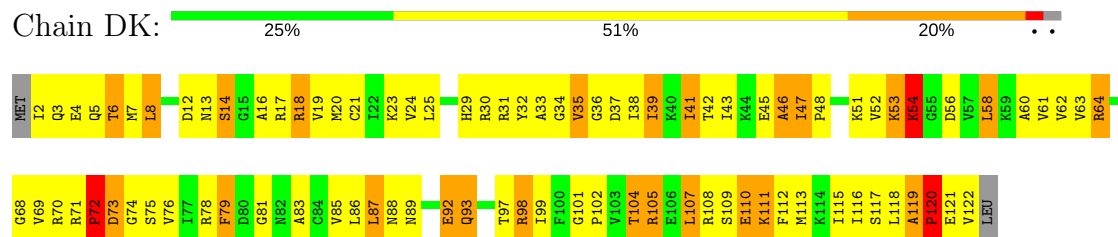
- Molecule 26: 50S ribosomal protein L3



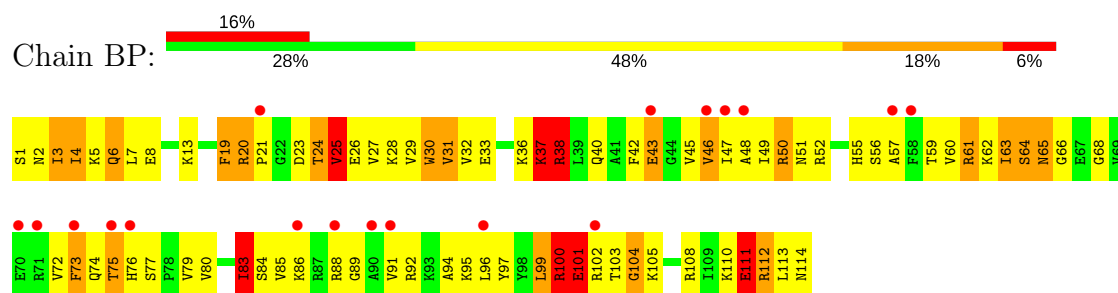
- Molecule 27: 50S ribosomal protein L14



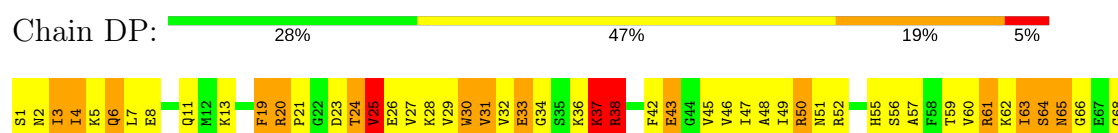
- Molecule 27: 50S ribosomal protein L14



- Molecule 28: 50S ribosomal protein L19

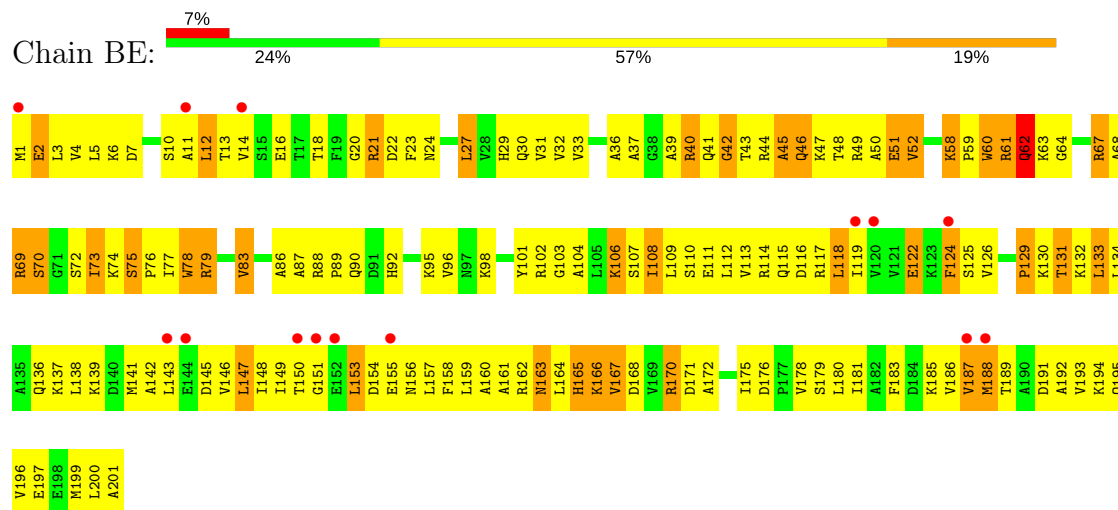


- Molecule 28: 50S ribosomal protein L19

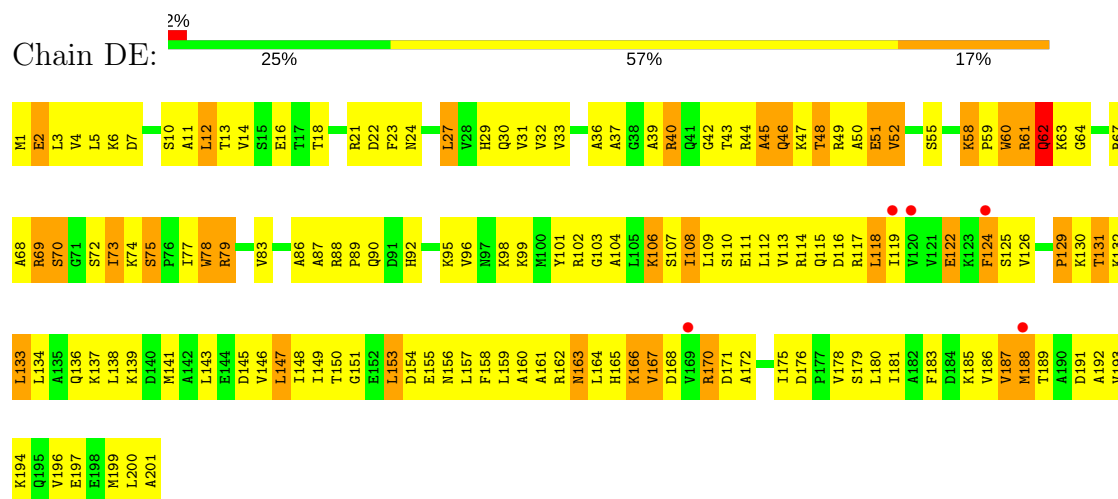




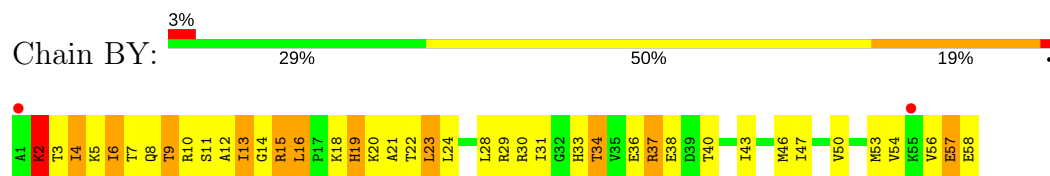
• Molecule 29: 50S ribosomal protein L4



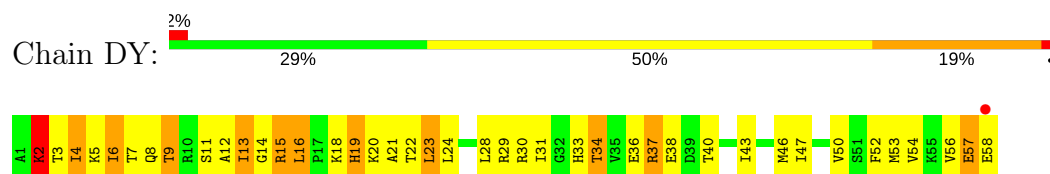
• Molecule 29: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L30




• Molecule 30: 50S ribosomal protein L30






- Molecule 34: 50S ribosomal protein L35



- Chain BV: 

- Chain DV:

- Chain B2: 
- | Category | Percentage |
|----------|------------|
| Green | 33% |
| Orange | 43% |
| Red | 22% |
- 

- Chain D2: 
- | Chain | Category | Percentage |
|----------|----------|------------|
| Chain D2 | M1 | Yellow |
| | K2 | Yellow |
| | R3 | Yellow |
| | T4 | Yellow |
| | F5 | Yellow |
| | Q6 | Yellow |
| | P7 | Yellow |
| | S8 | Green |
| | V9 | Yellow |
| | L10 | Yellow |
| | K11 | Yellow |
| | R12 | Yellow |
| | M13 | Yellow |
| | N14 | Yellow |
| | S15 | Green |
| | H16 | Yellow |
| | G17 | Yellow |
| | F18 | Green |
| | R19 | Yellow |
| | A20 | Green |
| R21 | Yellow | |
| K22 | Red | |
| A23 | Green | |
| T24 | Yellow | |
| K25 | Green | |
| N26 | Yellow | |
| G27 | Yellow | |
| R28 | Yellow | |
| Q29 | Yellow | |
| V30 | Yellow | |
| L31 | Yellow | |
| A32 | Yellow | |
| R33 | Yellow | |
| R34 | Yellow | |
| R35 | Yellow | |
| A40 | Green | |
| R41 | Yellow | |
| L42 | Yellow | |
| T43 | Yellow | |
| V44 | Yellow | |
| S45 | Yellow | |
| K46 | Green | |

- Chain BL:
-
- 27% 53% 18%
- ..

A137
A138
G139
G140
K141
I142
E143
E144

• Molecule 37: 50S ribosomal protein L15

Chain DL: 26% 54% 18% ..

MET R2 L3 N4 T5 L6 S7 P8 S12 S17 K17 R18 L19 L20 G20 R21 G22 I23 G28 G29 T30 G31 G32 R33 R36 R40 S40 R41 S42 S43 G43 G44 R47 R48 V110 V111 G49 F50 E51 E52 G53 Q54 V116 T117 M55 P56 L57 P119 V120 Y58 R59 T121 T122 V122 R60 L61 P62 K63 P64 G65 F66 T67 S68 R69 A71 A72

I73 T74 A75 E76 I77 R78 L79 S80 D81 L82 A83 K84 V85 V89 V90 L91 L92 L93 N93 T94 L95 L96 A97 A98 G99 I100 I101 G102 I103 G104 I105 S106 E106 F107 K109 A108 V110 V111 L112 A113 G114 E115 V116 T117 M118 P119 V120 Y121 T122 V123 R123 G124 L125 L126 P127 G65 F66 T128 A131 A134 I135 A136

A137
A138
G139
G140
K141
I142
E143
E144

• Molecule 38: 50S ribosomal protein L16

Chain BM: 3% 26% 53% 18% .

M1 L2 R6 F9 R10 H13 R16 N17 R18 G19 L20 A21 G22 G23 T24 D25 V26 S27 F31 G32 L33 K34 A35 V36 G37 R38 G39 R40 L41 T42 A43 R44 Q45 T46 E47 A48 A49 R50 M53 T54 R55 A56 V57 K58 R59 Q60 G61 K62 I63 T64 T65 R66 V67 P68

P69 D70 K71 P72 I73 L78 M82 G83 K84 G85 K86 G87 E90 Y91 W92 V93 A94 L95 L96 P96 Q97 P98 G99 K100 V101 L102 Y103 I104 M105 G106 G107 V108 P109 T109 E110 E111 L112 E115 A116 F117 K118 L119 A120 K123 L124 P125 L126 K127 T128 T129 F130 V131 I63 T132 K133 T134 V135 M136

• Molecule 38: 50S ribosomal protein L16

Chain DM: 3% 28% 53% 17% .

M1 L2 R6 R10 H13 R16 N17 R18 G19 L20 A21 G22 G23 T24 D25 V26 S27 F28 G29 S30 F31 G32 L33 K34 A35 V36 G37 R38 G39 R40 L41 T42 A43 R44 Q45 T46 E47 A48 A49 R50 M53 T54 R55 A56 V57 K58 R59 Q60 G61 K62 I63 T64 T65 R66 V67

P68 P69 D70 K71 P72 I73 L78 M82 G83 K84 G85 K86 G87 E90 Y91 W92 V93 A94 L95 L96 P96 Q97 P98 G99 K100 V101 L102 Y103 I104 M105 G106 G107 V108 P109 T109 E110 E111 L112 E115 A116 F117 K118 L119 A120 K123 L124 P125 L126 K127 T128 T129 F130 V131 I63 T132 K133 T134 V135 M136

M136

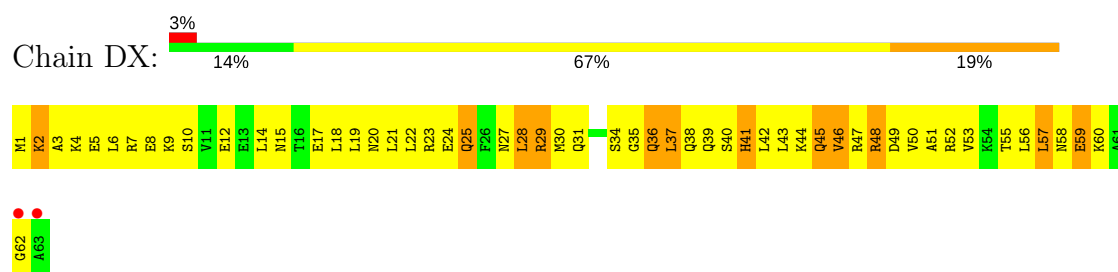
• Molecule 39: 50S ribosomal protein L29

Chain BX: 3% 17% 67% 16%

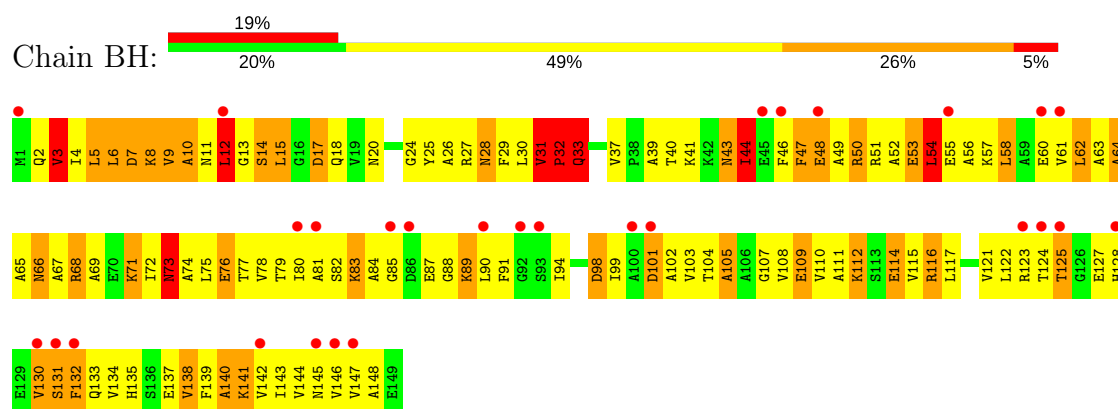
M1 K2 A3 K4 E5 L6 R7 E8 K9 V11 E12 E13 L14 M15 T16 E17 L18 L19 N20 N21 L21 L22 R23 R24 E25 F26 S27 N27 L28 R29 R30 M30 Q31 S34 G35 Q36 L37 Q38 Q39 S40 H41 L42 L43 K44 Q45 V46 R47 R48 D49 V50 A51 R52 R53 K54 T55 L56 L57 M58 E59 K60 A61

G62
A63

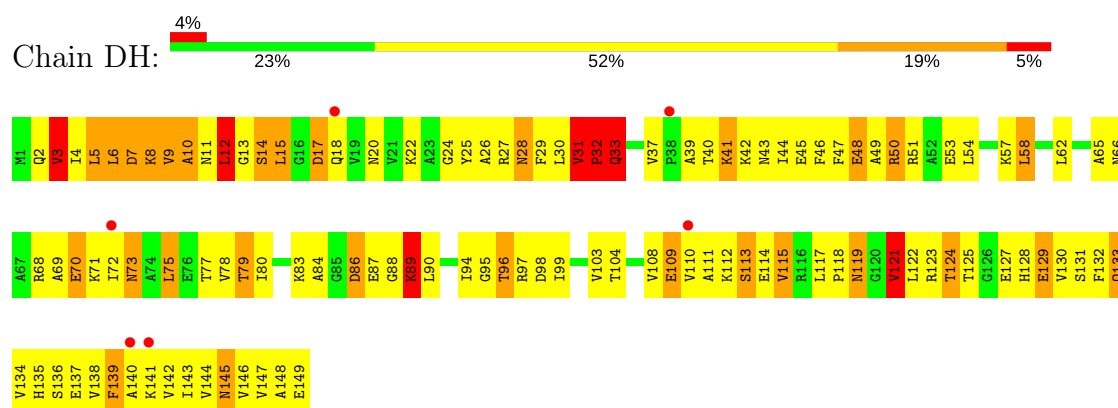
• Molecule 39: 50S ribosomal protein L29



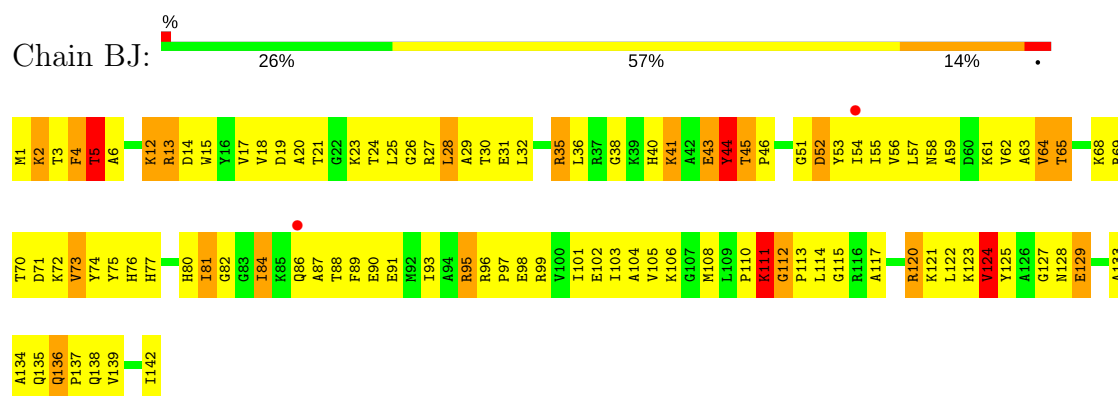
• Molecule 40: 50S ribosomal protein L9



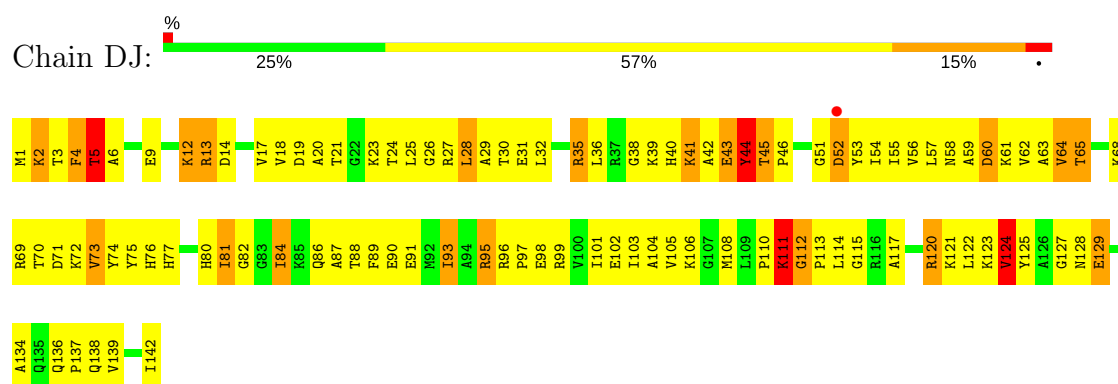
• Molecule 40: 50S ribosomal protein L9



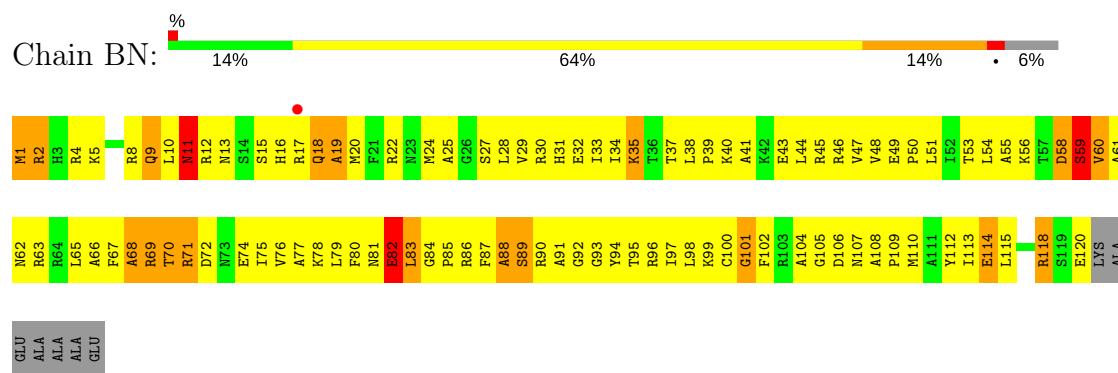
• Molecule 41: 50S ribosomal protein L13



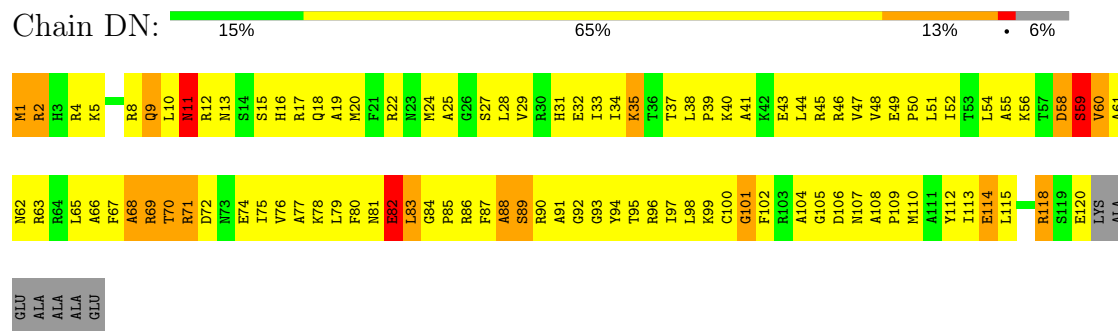
• Molecule 41: 50S ribosomal protein L13



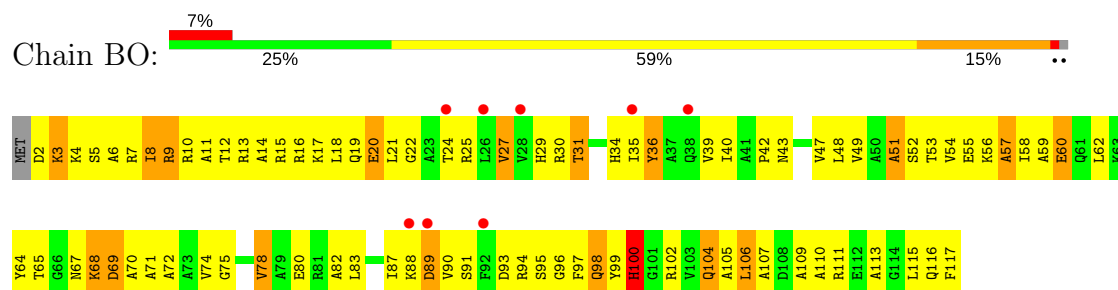
• Molecule 42: 50S ribosomal protein L17



• Molecule 42: 50S ribosomal protein L17

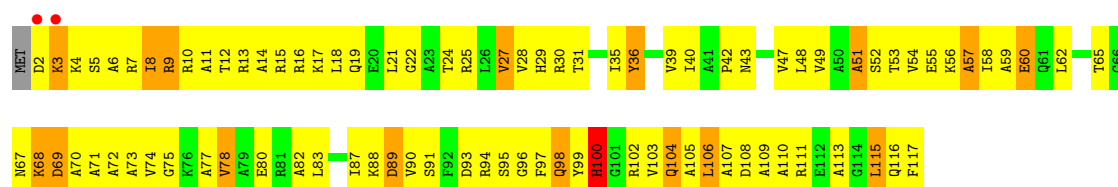


• Molecule 43: 50S ribosomal protein L18



• Molecule 43: 50S ribosomal protein L18

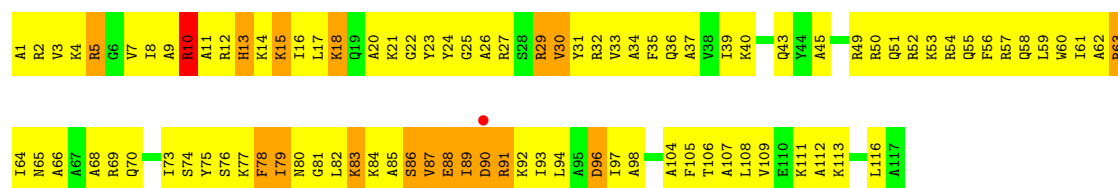




• Molecule 44: 50S ribosomal protein L20



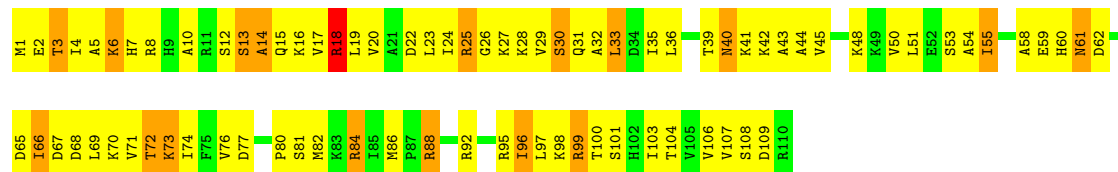
• Molecule 44: 50S ribosomal protein L20



• Molecule 45: 50S ribosomal protein L22

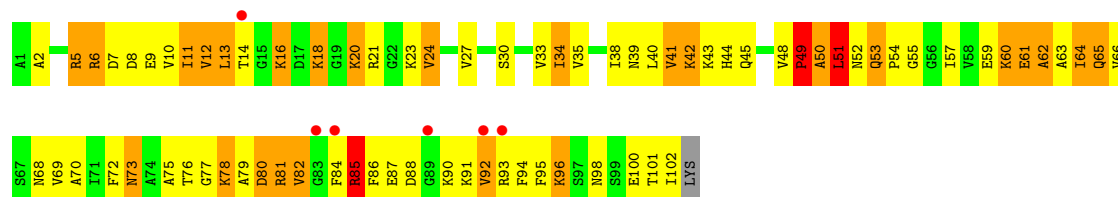


• Molecule 45: 50S ribosomal protein L22

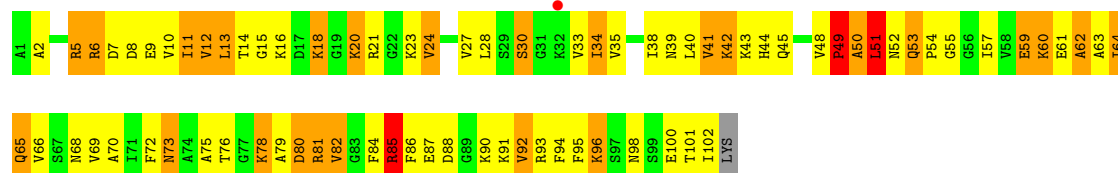


• Molecule 46: 50S ribosomal protein L24

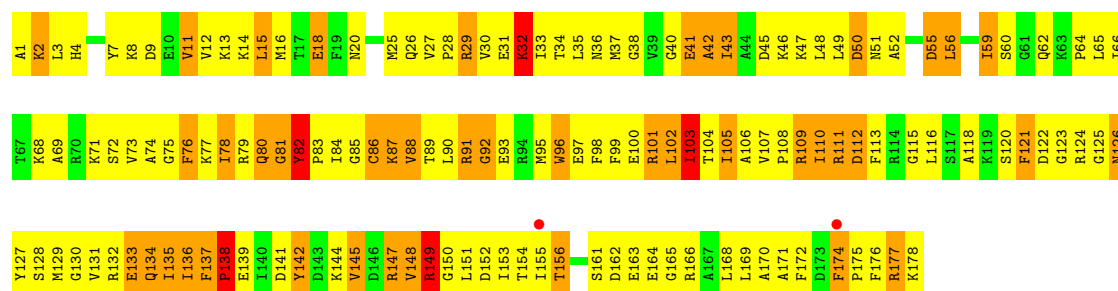
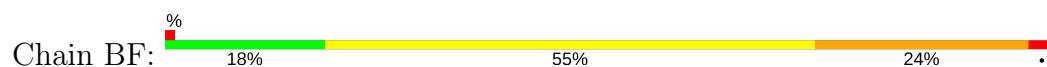




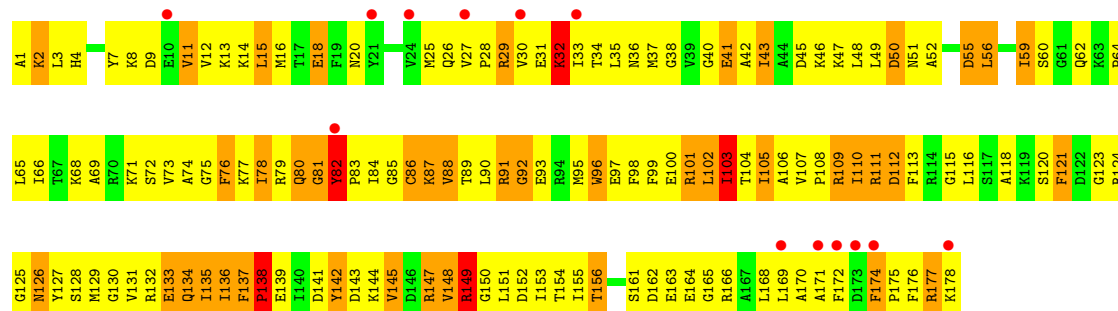
• Molecule 46: 50S ribosomal protein L24



• Molecule 47: 50S ribosomal protein L5

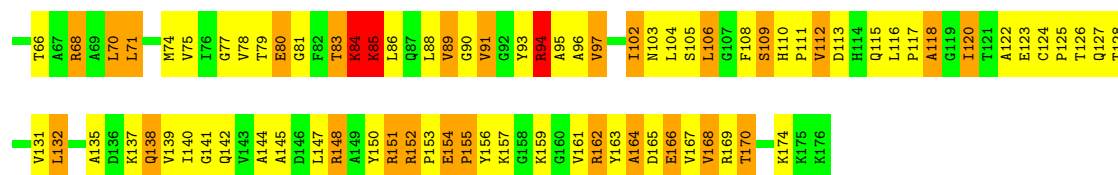


• Molecule 47: 50S ribosomal protein L5

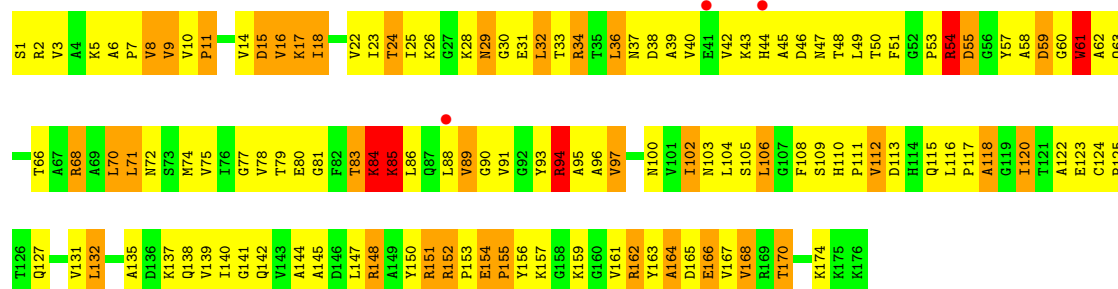


• Molecule 48: 50S ribosomal protein L6

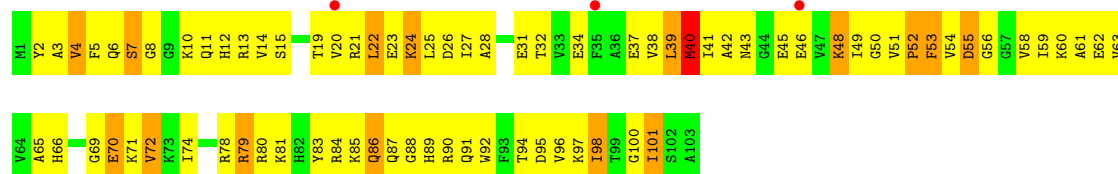




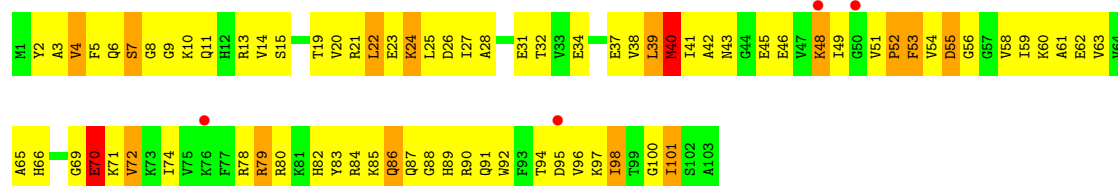
• Molecule 48: 50S ribosomal protein L6



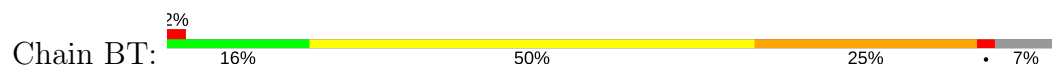
• Molecule 49: 50S ribosomal protein L21



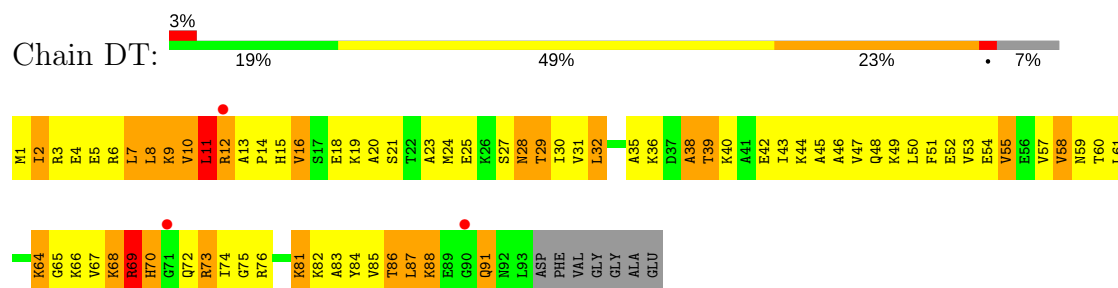
• Molecule 49: 50S ribosomal protein L21



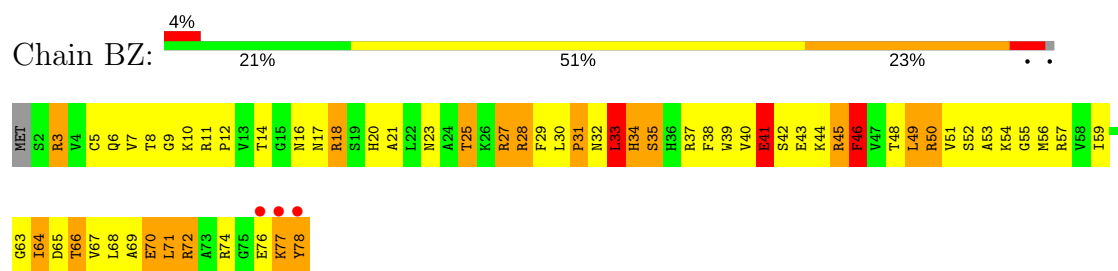
• Molecule 50: 50S ribosomal protein L23



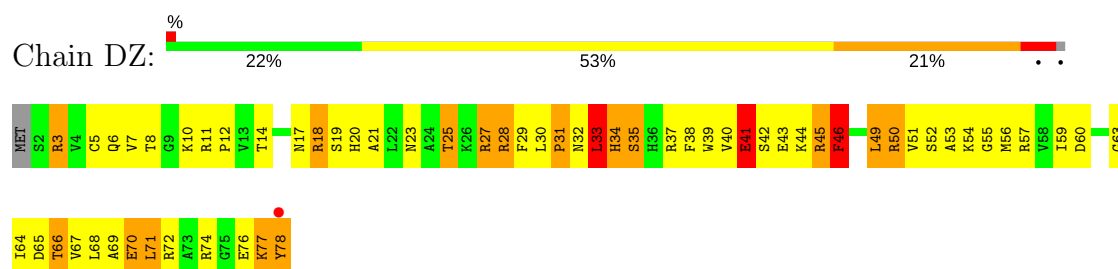
• Molecule 50: 50S ribosomal protein L23



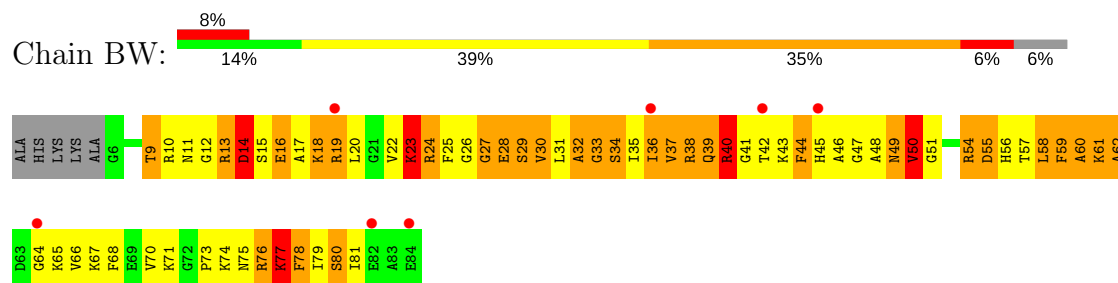
• Molecule 51: 50S ribosomal protein L28



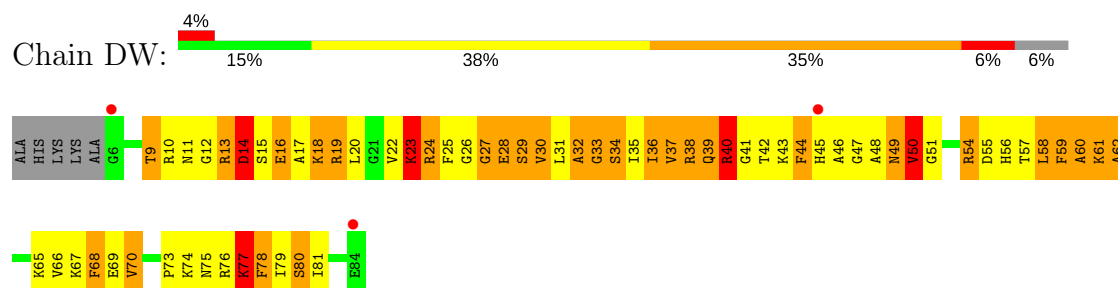
• Molecule 51: 50S ribosomal protein L28



• Molecule 52: 50S ribosomal protein L27

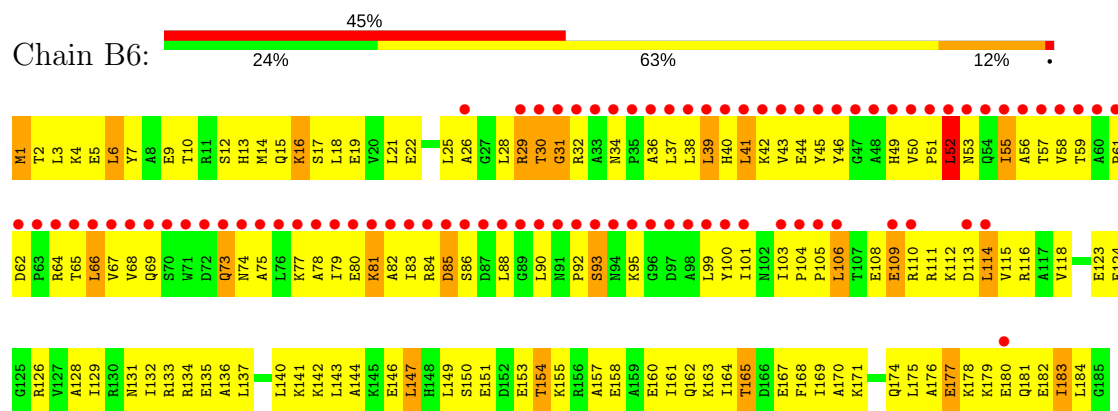


• Molecule 52: 50S ribosomal protein L27



• Molecule 53: 50S ribosomal protein RRF

Chain B6:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.54Å 378.89Å 736.90Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 4.00 138.07 – 4.15 | Depositor EDS |
| % Data completeness (in resolution range) | 87.4 (40.00-4.00) 87.4 (138.07-4.15) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.14 (at 4.15Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.261 , 0.305 0.238 , 0.276 | Depositor DCC |
| R_{free} test set | 18876 reflections (5.19%) | DCC |
| Wilson B-factor (Å ²) | 133.1 | Xtriage |
| Anisotropy | 0.323 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.22 , 74.2 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 287083 | wwPDB-VP |
| Average B, all atoms (Å ²) | 72.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: ZN, MG, LLL

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 | AA | 0.29 | 3/36762 (0.0%) | 0.78 | 21/57350 (0.0%) |
| 1 | CA | 0.29 | 4/36762 (0.0%) | 0.78 | 22/57350 (0.0%) |
| 2 | AC | 0.23 | 0/1651 | 0.44 | 0/2225 |
| 2 | CC | 0.23 | 0/1651 | 0.44 | 0/2225 |
| 3 | AD | 0.23 | 0/1665 | 0.44 | 0/2227 |
| 3 | CD | 0.23 | 0/1665 | 0.44 | 0/2227 |
| 4 | AE | 0.23 | 0/1118 | 0.46 | 0/1504 |
| 4 | CE | 0.23 | 0/1118 | 0.46 | 0/1504 |
| 5 | AF | 0.24 | 0/835 | 0.45 | 0/1128 |
| 5 | CF | 0.24 | 0/835 | 0.45 | 0/1128 |
| 6 | AG | 0.23 | 0/1187 | 0.46 | 0/1591 |
| 6 | CG | 0.23 | 0/1211 | 0.46 | 0/1624 |
| 7 | AH | 0.23 | 0/989 | 0.44 | 0/1326 |
| 7 | CH | 0.23 | 0/989 | 0.44 | 0/1326 |
| 8 | AI | 0.24 | 0/1034 | 0.46 | 0/1375 |
| 8 | CI | 0.24 | 0/1033 | 0.46 | 0/1375 |
| 9 | AJ | 0.22 | 0/796 | 0.48 | 0/1077 |
| 9 | CJ | 0.22 | 0/796 | 0.48 | 0/1077 |
| 10 | AK | 0.24 | 0/893 | 0.46 | 0/1205 |
| 10 | CK | 0.24 | 0/893 | 0.46 | 0/1205 |
| 11 | AL | 0.22 | 0/969 | 0.50 | 0/1300 |
| 11 | CL | 0.22 | 0/969 | 0.50 | 0/1300 |
| 12 | AM | 0.21 | 0/892 | 0.46 | 0/1193 |
| 12 | CM | 0.21 | 0/884 | 0.46 | 0/1181 |
| 13 | AN | 0.24 | 0/785 | 0.45 | 0/1043 |
| 13 | CN | 0.24 | 0/785 | 0.45 | 0/1043 |
| 14 | AO | 0.23 | 0/722 | 0.47 | 0/964 |
| 14 | CO | 0.23 | 0/722 | 0.47 | 0/964 |
| 15 | AP | 0.25 | 0/659 | 0.46 | 0/884 |
| 15 | CP | 0.25 | 0/648 | 0.47 | 0/870 |
| 16 | AQ | 0.24 | 0/657 | 0.47 | 0/881 |
| 16 | CQ | 0.24 | 0/666 | 0.47 | 0/892 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AR | 0.23 | 0/462 | 0.46 | 0/621 |
| 17 | CR | 0.23 | 0/462 | 0.46 | 0/621 |
| 18 | AS | 0.25 | 0/652 | 0.47 | 0/877 |
| 18 | CS | 0.25 | 0/660 | 0.48 | 0/888 |
| 19 | AT | 0.23 | 0/671 | 0.39 | 0/888 |
| 19 | CT | 0.23 | 0/671 | 0.39 | 0/888 |
| 20 | AB | 0.25 | 0/1735 | 0.45 | 0/2338 |
| 20 | CB | 0.25 | 0/1735 | 0.45 | 0/2338 |
| 21 | AU | 0.26 | 0/430 | 0.48 | 0/570 |
| 21 | CU | 0.26 | 0/430 | 0.48 | 0/570 |
| 22 | BA | 0.28 | 0/2803 | 0.76 | 1/4371 (0.0%) |
| 22 | DA | 0.28 | 0/2803 | 0.76 | 0/4371 |
| 23 | BB | 0.28 | 6/68314 (0.0%) | 0.78 | 48/106569 (0.0%) |
| 23 | DB | 0.30 | 6/68314 (0.0%) | 0.79 | 48/106569 (0.0%) |
| 24 | BI | 0.24 | 0/1046 | 0.47 | 0/1410 |
| 24 | DI | 0.25 | 0/1046 | 0.48 | 0/1410 |
| 25 | BC | 0.22 | 0/2121 | 0.48 | 0/2852 |
| 25 | DC | 0.22 | 0/2121 | 0.48 | 0/2852 |
| 26 | BD | 0.24 | 0/1586 | 0.49 | 0/2134 |
| 26 | DD | 0.24 | 0/1586 | 0.49 | 0/2134 |
| 27 | BK | 0.24 | 0/939 | 0.55 | 0/1258 |
| 27 | DK | 0.24 | 0/939 | 0.55 | 0/1258 |
| 28 | BP | 0.24 | 0/929 | 0.51 | 0/1242 |
| 28 | DP | 0.24 | 0/929 | 0.51 | 0/1242 |
| 29 | BE | 0.24 | 0/1571 | 0.51 | 0/2113 |
| 29 | DE | 0.24 | 0/1571 | 0.51 | 0/2113 |
| 30 | BY | 0.23 | 0/453 | 0.49 | 0/605 |
| 30 | DY | 0.23 | 0/453 | 0.49 | 0/605 |
| 31 | B0 | 0.22 | 0/450 | 0.55 | 0/599 |
| 31 | D0 | 0.23 | 0/450 | 0.55 | 0/599 |
| 32 | B4 | 0.23 | 0/303 | 0.47 | 0/397 |
| 32 | D4 | 0.23 | 0/303 | 0.47 | 0/397 |
| 33 | B1 | 0.27 | 0/416 | 0.49 | 0/554 |
| 33 | D1 | 0.27 | 0/416 | 0.49 | 0/554 |
| 34 | B3 | 0.24 | 0/513 | 0.48 | 0/676 |
| 34 | D3 | 0.24 | 0/513 | 0.48 | 0/676 |
| 35 | BV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 35 | DV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 36 | B2 | 0.25 | 0/380 | 0.48 | 0/498 |
| 36 | D2 | 0.25 | 0/380 | 0.48 | 0/498 |
| 37 | BL | 0.23 | 0/1054 | 0.48 | 0/1403 |
| 37 | DL | 0.23 | 0/1054 | 0.48 | 0/1403 |
| 38 | BM | 0.25 | 0/1093 | 0.48 | 0/1460 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DM | 0.25 | 0/1093 | 0.48 | 0/1460 |
| 39 | BX | 0.24 | 0/510 | 0.53 | 0/677 |
| 39 | DX | 0.24 | 0/510 | 0.53 | 0/677 |
| 40 | BH | 0.25 | 0/1122 | 0.48 | 0/1515 |
| 40 | DH | 0.25 | 0/1122 | 0.48 | 0/1515 |
| 41 | BJ | 0.24 | 0/1152 | 0.48 | 0/1551 |
| 41 | DJ | 0.23 | 0/1152 | 0.48 | 0/1551 |
| 42 | BN | 0.24 | 0/973 | 0.51 | 0/1301 |
| 42 | DN | 0.24 | 0/973 | 0.51 | 0/1301 |
| 43 | BO | 0.23 | 0/902 | 0.49 | 0/1209 |
| 43 | DO | 0.23 | 0/902 | 0.49 | 0/1209 |
| 44 | BQ | 0.25 | 0/960 | 0.49 | 0/1278 |
| 44 | DQ | 0.26 | 0/960 | 0.49 | 0/1278 |
| 45 | BS | 0.22 | 0/864 | 0.52 | 0/1156 |
| 45 | DS | 0.22 | 0/864 | 0.52 | 0/1156 |
| 46 | BU | 0.25 | 0/787 | 0.47 | 0/1051 |
| 46 | DU | 0.25 | 0/787 | 0.47 | 0/1051 |
| 47 | BF | 0.26 | 0/1444 | 0.52 | 0/1937 |
| 47 | DF | 0.26 | 0/1444 | 0.52 | 0/1937 |
| 48 | BG | 0.23 | 0/1343 | 0.47 | 0/1816 |
| 48 | DG | 0.23 | 0/1343 | 0.47 | 0/1816 |
| 49 | BR | 0.25 | 0/829 | 0.50 | 0/1107 |
| 49 | DR | 0.25 | 0/829 | 0.50 | 0/1107 |
| 50 | BT | 0.23 | 0/744 | 0.55 | 0/994 |
| 50 | DT | 0.22 | 0/744 | 0.55 | 0/994 |
| 51 | BZ | 0.25 | 0/635 | 0.51 | 0/848 |
| 51 | DZ | 0.25 | 0/635 | 0.52 | 0/848 |
| 52 | BW | 0.28 | 0/603 | 0.51 | 0/797 |
| 52 | DW | 0.28 | 0/603 | 0.51 | 0/797 |
| 53 | B6 | 0.23 | 0/1497 | 0.52 | 1/2017 (0.0%) |
| 53 | D6 | 0.30 | 0/1497 | 0.58 | 1/2017 (0.0%) |
| All | All | 0.28 | 19/309353 (0.0%) | 0.71 | 142/462003 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AA | 0 | 16 |
| 1 | CA | 0 | 17 |
| 23 | BB | 0 | 35 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 23 | DB | 0 | 47 |
| All | All | 0 | 115 |

The worst 5 of 19 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23 | BB | 1086 | A | C5-C6 | -16.56 | 1.26 | 1.41 |
| 23 | DB | 1086 | A | C5-C6 | -16.53 | 1.26 | 1.41 |
| 23 | DB | 1088 | A | C6-N1 | -10.57 | 1.28 | 1.35 |
| 23 | BB | 1088 | A | C6-N1 | -10.52 | 1.28 | 1.35 |
| 1 | CA | 1213 | A | P-OP1 | -9.61 | 1.32 | 1.49 |

The worst 5 of 142 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | CA | 1213 | A | O5'-P-OP1 | -31.90 | 72.42 | 110.70 |
| 1 | AA | 1213 | A | O5'-P-OP2 | -30.12 | 74.56 | 110.70 |
| 23 | DB | 2204 | G | O5'-P-OP1 | -29.74 | 75.02 | 110.70 |
| 23 | BB | 2204 | G | O5'-P-OP2 | -28.90 | 76.02 | 110.70 |
| 23 | BB | 2791 | G | O5'-P-OP1 | -28.07 | 77.02 | 110.70 |

There are no chirality outliers.

5 of 115 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 187 | G | Sidechain |
| 1 | AA | 281 | G | Sidechain |
| 1 | AA | 324 | G | Sidechain |
| 1 | AA | 437 | U | Sidechain |
| 1 | AA | 86 | G | Sidechain |

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32831 | 0 | 16521 | 1290 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | CA | 32831 | 0 | 16521 | 1350 | 0 |
| 2 | AC | 1624 | 0 | 1699 | 140 | 0 |
| 2 | CC | 1624 | 0 | 1699 | 146 | 0 |
| 3 | AD | 1643 | 0 | 1710 | 174 | 0 |
| 3 | CD | 1643 | 0 | 1710 | 170 | 0 |
| 4 | AE | 1105 | 0 | 1148 | 95 | 0 |
| 4 | CE | 1105 | 0 | 1148 | 96 | 0 |
| 5 | AF | 817 | 0 | 808 | 96 | 0 |
| 5 | CF | 817 | 0 | 808 | 94 | 0 |
| 6 | AG | 1174 | 0 | 1230 | 112 | 0 |
| 6 | CG | 1196 | 0 | 1246 | 106 | 0 |
| 7 | AH | 979 | 0 | 1034 | 95 | 0 |
| 7 | CH | 979 | 0 | 1034 | 96 | 0 |
| 8 | AI | 1022 | 0 | 1070 | 149 | 0 |
| 8 | CI | 1021 | 0 | 1070 | 149 | 0 |
| 9 | AJ | 786 | 0 | 828 | 77 | 0 |
| 9 | CJ | 786 | 0 | 828 | 80 | 0 |
| 10 | AK | 877 | 0 | 887 | 111 | 0 |
| 10 | CK | 877 | 0 | 887 | 114 | 0 |
| 11 | AL | 955 | 0 | 1019 | 92 | 0 |
| 11 | CL | 955 | 0 | 1019 | 91 | 0 |
| 12 | AM | 883 | 0 | 944 | 119 | 0 |
| 12 | CM | 876 | 0 | 937 | 120 | 0 |
| 13 | AN | 774 | 0 | 827 | 121 | 0 |
| 13 | CN | 774 | 0 | 827 | 131 | 0 |
| 14 | AO | 714 | 0 | 734 | 60 | 0 |
| 14 | CO | 714 | 0 | 734 | 54 | 0 |
| 15 | AP | 649 | 0 | 666 | 56 | 0 |
| 15 | CP | 638 | 0 | 656 | 57 | 0 |
| 16 | AQ | 648 | 0 | 691 | 71 | 0 |
| 16 | CQ | 657 | 0 | 702 | 67 | 0 |
| 17 | AR | 455 | 0 | 478 | 51 | 0 |
| 17 | CR | 455 | 0 | 478 | 56 | 0 |
| 18 | AS | 637 | 0 | 665 | 85 | 0 |
| 18 | CS | 644 | 0 | 675 | 87 | 0 |
| 19 | AT | 665 | 0 | 714 | 68 | 0 |
| 19 | CT | 665 | 0 | 714 | 70 | 0 |
| 20 | AB | 1704 | 0 | 1732 | 220 | 0 |
| 20 | CB | 1704 | 0 | 1732 | 211 | 0 |
| 21 | AU | 425 | 0 | 449 | 79 | 0 |
| 21 | CU | 425 | 0 | 449 | 89 | 0 |
| 22 | BA | 2507 | 0 | 1270 | 106 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22 | DA | 2507 | 0 | 1270 | 108 | 0 |
| 23 | BB | 60995 | 0 | 30678 | 2536 | 0 |
| 23 | DB | 60995 | 0 | 30678 | 2543 | 0 |
| 24 | BI | 1032 | 0 | 1088 | 119 | 0 |
| 24 | DI | 1032 | 0 | 1088 | 181 | 0 |
| 25 | BC | 2082 | 0 | 2157 | 239 | 0 |
| 25 | DC | 2082 | 0 | 2157 | 241 | 0 |
| 26 | BD | 1565 | 0 | 1616 | 206 | 0 |
| 26 | DD | 1565 | 0 | 1616 | 216 | 0 |
| 27 | BK | 930 | 0 | 1000 | 122 | 0 |
| 27 | DK | 930 | 0 | 1000 | 122 | 0 |
| 28 | BP | 917 | 0 | 965 | 102 | 0 |
| 28 | DP | 917 | 0 | 965 | 108 | 0 |
| 29 | BE | 1552 | 0 | 1619 | 194 | 0 |
| 29 | DE | 1552 | 0 | 1619 | 181 | 0 |
| 30 | BY | 449 | 0 | 491 | 49 | 0 |
| 30 | DY | 449 | 0 | 491 | 55 | 0 |
| 31 | B0 | 444 | 0 | 461 | 49 | 0 |
| 31 | D0 | 444 | 0 | 461 | 47 | 0 |
| 32 | B4 | 302 | 0 | 340 | 38 | 0 |
| 32 | D4 | 302 | 0 | 340 | 44 | 0 |
| 33 | B1 | 409 | 0 | 440 | 58 | 0 |
| 33 | D1 | 409 | 0 | 440 | 54 | 0 |
| 34 | B3 | 504 | 0 | 574 | 51 | 0 |
| 34 | D3 | 504 | 0 | 574 | 48 | 0 |
| 35 | BV | 753 | 0 | 780 | 97 | 0 |
| 35 | DV | 753 | 0 | 780 | 102 | 0 |
| 36 | B2 | 377 | 0 | 418 | 38 | 0 |
| 36 | D2 | 377 | 0 | 418 | 38 | 0 |
| 37 | BL | 1045 | 0 | 1117 | 148 | 0 |
| 37 | DL | 1045 | 0 | 1117 | 153 | 0 |
| 38 | BM | 1074 | 0 | 1157 | 129 | 0 |
| 38 | DM | 1074 | 0 | 1157 | 121 | 0 |
| 39 | BX | 509 | 0 | 543 | 55 | 0 |
| 39 | DX | 509 | 0 | 543 | 60 | 0 |
| 40 | BH | 1111 | 0 | 1148 | 186 | 0 |
| 40 | DH | 1111 | 0 | 1148 | 158 | 0 |
| 41 | BJ | 1129 | 0 | 1162 | 136 | 0 |
| 41 | DJ | 1129 | 0 | 1162 | 137 | 0 |
| 42 | BN | 960 | 0 | 1000 | 130 | 0 |
| 42 | DN | 960 | 0 | 1000 | 129 | 0 |
| 43 | BO | 892 | 0 | 923 | 94 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43 | DO | 892 | 0 | 923 | 96 | 0 |
| 44 | BQ | 947 | 0 | 1022 | 171 | 0 |
| 44 | DQ | 947 | 0 | 1022 | 178 | 0 |
| 45 | BS | 857 | 0 | 922 | 101 | 0 |
| 45 | DS | 857 | 0 | 922 | 101 | 0 |
| 46 | BU | 779 | 0 | 834 | 114 | 0 |
| 46 | DU | 779 | 0 | 834 | 109 | 0 |
| 47 | BF | 1420 | 0 | 1460 | 223 | 0 |
| 47 | DF | 1420 | 0 | 1460 | 216 | 0 |
| 48 | BG | 1323 | 0 | 1374 | 218 | 0 |
| 48 | DG | 1323 | 0 | 1374 | 195 | 0 |
| 49 | BR | 816 | 0 | 839 | 113 | 0 |
| 49 | DR | 816 | 0 | 839 | 128 | 0 |
| 50 | BT | 738 | 0 | 807 | 125 | 0 |
| 50 | DT | 738 | 0 | 807 | 121 | 0 |
| 51 | BZ | 625 | 0 | 652 | 82 | 0 |
| 51 | DZ | 625 | 0 | 652 | 82 | 0 |
| 52 | BW | 596 | 0 | 610 | 120 | 0 |
| 52 | DW | 596 | 0 | 610 | 126 | 0 |
| 53 | B6 | 1478 | 0 | 1526 | 192 | 0 |
| 53 | D6 | 1478 | 0 | 1526 | 150 | 0 |
| 54 | AA | 60 | 0 | 0 | 0 | 0 |
| 54 | BB | 110 | 0 | 0 | 0 | 0 |
| 54 | CA | 61 | 0 | 0 | 0 | 0 |
| 54 | CE | 1 | 0 | 0 | 0 | 0 |
| 54 | DB | 111 | 0 | 0 | 0 | 0 |
| 55 | AA | 31 | 0 | 39 | 0 | 0 |
| 55 | BB | 31 | 0 | 39 | 2 | 0 |
| 55 | CA | 31 | 0 | 39 | 3 | 0 |
| 55 | DB | 31 | 0 | 39 | 0 | 0 |
| 56 | B4 | 1 | 0 | 0 | 0 | 0 |
| 56 | D4 | 1 | 0 | 0 | 0 | 0 |
| 57 | AA | 287 | 0 | 0 | 1 | 0 |
| 57 | AE | 3 | 0 | 0 | 0 | 0 |
| 57 | AK | 1 | 0 | 0 | 0 | 0 |
| 57 | AL | 3 | 0 | 0 | 0 | 0 |
| 57 | AN | 4 | 0 | 0 | 0 | 0 |
| 57 | AT | 2 | 0 | 0 | 0 | 0 |
| 57 | BB | 492 | 0 | 0 | 8 | 0 |
| 57 | BC | 6 | 0 | 0 | 0 | 0 |
| 57 | BD | 1 | 0 | 0 | 0 | 0 |
| 57 | BE | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57 | BL | 3 | 0 | 0 | 0 | 0 |
| 57 | BT | 1 | 0 | 0 | 0 | 0 |
| 57 | CA | 296 | 0 | 0 | 2 | 0 |
| 57 | CE | 3 | 0 | 0 | 0 | 0 |
| 57 | CK | 1 | 0 | 0 | 0 | 0 |
| 57 | CL | 3 | 0 | 0 | 0 | 0 |
| 57 | CN | 4 | 0 | 0 | 0 | 0 |
| 57 | CT | 2 | 0 | 0 | 0 | 0 |
| 57 | DB | 500 | 0 | 0 | 7 | 0 |
| 57 | DC | 6 | 0 | 0 | 0 | 0 |
| 57 | DE | 2 | 0 | 0 | 0 | 0 |
| 57 | DL | 2 | 0 | 0 | 0 | 0 |
| 57 | DR | 1 | 0 | 0 | 0 | 0 |
| 57 | DT | 1 | 0 | 0 | 0 | 0 |
| All | All | 287083 | 0 | 193870 | 17818 | 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 37.

The worst 5 of 17818 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) |
|------------------|-------------------|--------------------------|-------------------|
| 23:DB:1099:G:H8 | 24:DI:3:LYS:N | 1.36 | 1.20 |
| 40:BH:31:VAL:HB | 40:BH:32:PRO:HD2 | 1.23 | 1.17 |
| 21:CU:36:PHE:HB3 | 21:CU:40:PRO:HD3 | 1.28 | 1.14 |
| 21:AU:36:PHE:HB3 | 21:AU:40:PRO:HD3 | 1.29 | 1.11 |
| 25:DC:144:GLU:HA | 25:DC:151:GLY:HA2 | 1.33 | 1.11 |

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 2 | AC | 204/232 (88%) | 151 (74%) | 38 (19%) | 15 (7%) | 1 | 19 |
| 2 | CC | 204/232 (88%) | 152 (74%) | 37 (18%) | 15 (7%) | 1 | 19 |
| 3 | AD | 203/205 (99%) | 151 (74%) | 39 (19%) | 13 (6%) | 1 | 24 |
| 3 | CD | 203/205 (99%) | 148 (73%) | 42 (21%) | 13 (6%) | 1 | 24 |
| 4 | AE | 148/166 (89%) | 117 (79%) | 25 (17%) | 6 (4%) | 3 | 33 |
| 4 | CE | 148/166 (89%) | 117 (79%) | 25 (17%) | 6 (4%) | 3 | 33 |
| 5 | AF | 98/135 (73%) | 64 (65%) | 25 (26%) | 9 (9%) | 1 | 14 |
| 5 | CF | 98/135 (73%) | 65 (66%) | 24 (24%) | 9 (9%) | 1 | 14 |
| 6 | AG | 148/178 (83%) | 106 (72%) | 33 (22%) | 9 (6%) | 2 | 24 |
| 6 | CG | 150/178 (84%) | 112 (75%) | 29 (19%) | 9 (6%) | 2 | 25 |
| 7 | AH | 127/129 (98%) | 98 (77%) | 23 (18%) | 6 (5%) | 3 | 30 |
| 7 | CH | 127/129 (98%) | 96 (76%) | 25 (20%) | 6 (5%) | 3 | 30 |
| 8 | AI | 125/129 (97%) | 99 (79%) | 17 (14%) | 9 (7%) | 1 | 20 |
| 8 | CI | 125/129 (97%) | 98 (78%) | 18 (14%) | 9 (7%) | 1 | 20 |
| 9 | AJ | 96/103 (93%) | 70 (73%) | 13 (14%) | 13 (14%) | 0 | 5 |
| 9 | CJ | 96/103 (93%) | 71 (74%) | 12 (12%) | 13 (14%) | 0 | 5 |
| 10 | AK | 115/128 (90%) | 87 (76%) | 22 (19%) | 6 (5%) | 2 | 28 |
| 10 | CK | 115/128 (90%) | 87 (76%) | 22 (19%) | 6 (5%) | 2 | 28 |
| 11 | AL | 121/123 (98%) | 73 (60%) | 33 (27%) | 15 (12%) | 0 | 7 |
| 11 | CL | 121/123 (98%) | 75 (62%) | 31 (26%) | 15 (12%) | 0 | 7 |
| 12 | AM | 112/117 (96%) | 79 (70%) | 24 (21%) | 9 (8%) | 1 | 17 |
| 12 | CM | 111/117 (95%) | 76 (68%) | 25 (22%) | 10 (9%) | 1 | 15 |
| 13 | AN | 92/100 (92%) | 59 (64%) | 26 (28%) | 7 (8%) | 1 | 18 |
| 13 | CN | 92/100 (92%) | 60 (65%) | 24 (26%) | 8 (9%) | 1 | 15 |
| 14 | AO | 86/89 (97%) | 59 (69%) | 22 (26%) | 5 (6%) | 2 | 25 |
| 14 | CO | 86/89 (97%) | 60 (70%) | 22 (26%) | 4 (5%) | 3 | 30 |
| 15 | AP | 80/82 (98%) | 59 (74%) | 16 (20%) | 5 (6%) | 1 | 24 |
| 15 | CP | 78/82 (95%) | 56 (72%) | 16 (20%) | 6 (8%) | 1 | 18 |
| 16 | AQ | 78/83 (94%) | 58 (74%) | 15 (19%) | 5 (6%) | 1 | 24 |
| 16 | CQ | 79/83 (95%) | 59 (75%) | 15 (19%) | 5 (6%) | 1 | 24 |
| 17 | AR | 53/74 (72%) | 41 (77%) | 9 (17%) | 3 (6%) | 2 | 26 |
| 17 | CR | 53/74 (72%) | 41 (77%) | 9 (17%) | 3 (6%) | 2 | 26 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 18 | AS | 77/91 (85%) | 60 (78%) | 12 (16%) | 5 (6%) | 1 | 23 |
| 18 | CS | 78/91 (86%) | 61 (78%) | 11 (14%) | 6 (8%) | 1 | 18 |
| 19 | AT | 83/86 (96%) | 63 (76%) | 15 (18%) | 5 (6%) | 2 | 25 |
| 19 | CT | 83/86 (96%) | 62 (75%) | 16 (19%) | 5 (6%) | 2 | 25 |
| 20 | AB | 216/240 (90%) | 142 (66%) | 57 (26%) | 17 (8%) | 1 | 17 |
| 20 | CB | 216/240 (90%) | 134 (62%) | 65 (30%) | 17 (8%) | 1 | 17 |
| 21 | AU | 49/70 (70%) | 28 (57%) | 11 (22%) | 10 (20%) | 0 | 2 |
| 21 | CU | 49/70 (70%) | 28 (57%) | 12 (24%) | 9 (18%) | 0 | 2 |
| 24 | BI | 139/141 (99%) | 120 (86%) | 14 (10%) | 5 (4%) | 4 | 37 |
| 24 | DI | 139/141 (99%) | 114 (82%) | 20 (14%) | 5 (4%) | 4 | 37 |
| 25 | BC | 269/272 (99%) | 155 (58%) | 66 (24%) | 48 (18%) | 0 | 3 |
| 25 | DC | 269/272 (99%) | 155 (58%) | 65 (24%) | 49 (18%) | 0 | 3 |
| 26 | BD | 207/209 (99%) | 122 (59%) | 54 (26%) | 31 (15%) | 0 | 4 |
| 26 | DD | 207/209 (99%) | 124 (60%) | 51 (25%) | 32 (16%) | 0 | 4 |
| 27 | BK | 119/123 (97%) | 78 (66%) | 24 (20%) | 17 (14%) | 0 | 5 |
| 27 | DK | 119/123 (97%) | 78 (66%) | 24 (20%) | 17 (14%) | 0 | 5 |
| 28 | BP | 112/114 (98%) | 61 (54%) | 32 (29%) | 19 (17%) | 0 | 4 |
| 28 | DP | 112/114 (98%) | 61 (54%) | 34 (30%) | 17 (15%) | 0 | 4 |
| 29 | BE | 199/201 (99%) | 125 (63%) | 50 (25%) | 24 (12%) | 0 | 7 |
| 29 | DE | 199/201 (99%) | 125 (63%) | 51 (26%) | 23 (12%) | 0 | 8 |
| 30 | BY | 56/58 (97%) | 39 (70%) | 12 (21%) | 5 (9%) | 1 | 15 |
| 30 | DY | 56/58 (97%) | 39 (70%) | 12 (21%) | 5 (9%) | 1 | 15 |
| 31 | B0 | 54/56 (96%) | 39 (72%) | 8 (15%) | 7 (13%) | 0 | 6 |
| 31 | D0 | 54/56 (96%) | 39 (72%) | 8 (15%) | 7 (13%) | 0 | 6 |
| 32 | B4 | 36/38 (95%) | 16 (44%) | 10 (28%) | 10 (28%) | 0 | 0 |
| 32 | D4 | 36/38 (95%) | 16 (44%) | 10 (28%) | 10 (28%) | 0 | 0 |
| 33 | B1 | 48/54 (89%) | 37 (77%) | 7 (15%) | 4 (8%) | 1 | 16 |
| 33 | D1 | 48/54 (89%) | 36 (75%) | 8 (17%) | 4 (8%) | 1 | 16 |
| 34 | B3 | 62/64 (97%) | 35 (56%) | 21 (34%) | 6 (10%) | 1 | 13 |
| 34 | D3 | 62/64 (97%) | 34 (55%) | 22 (36%) | 6 (10%) | 1 | 13 |
| 35 | BV | 92/94 (98%) | 64 (70%) | 22 (24%) | 6 (6%) | 1 | 23 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 35 | DV | 92/94 (98%) | 62 (67%) | 24 (26%) | 6 (6%) | 1 | 23 |
| 36 | B2 | 44/46 (96%) | 30 (68%) | 10 (23%) | 4 (9%) | 1 | 14 |
| 36 | D2 | 44/46 (96%) | 30 (68%) | 10 (23%) | 4 (9%) | 1 | 14 |
| 37 | BL | 141/144 (98%) | 89 (63%) | 31 (22%) | 21 (15%) | 0 | 4 |
| 37 | DL | 141/144 (98%) | 89 (63%) | 32 (23%) | 20 (14%) | 0 | 5 |
| 38 | BM | 134/136 (98%) | 84 (63%) | 29 (22%) | 21 (16%) | 0 | 4 |
| 38 | DM | 134/136 (98%) | 83 (62%) | 31 (23%) | 20 (15%) | 0 | 4 |
| 39 | BX | 61/63 (97%) | 36 (59%) | 17 (28%) | 8 (13%) | 0 | 6 |
| 39 | DX | 61/63 (97%) | 36 (59%) | 17 (28%) | 8 (13%) | 0 | 6 |
| 40 | BH | 147/149 (99%) | 76 (52%) | 46 (31%) | 25 (17%) | 0 | 4 |
| 40 | DH | 147/149 (99%) | 91 (62%) | 33 (22%) | 23 (16%) | 0 | 4 |
| 41 | BJ | 140/142 (99%) | 85 (61%) | 37 (26%) | 18 (13%) | 0 | 6 |
| 41 | DJ | 140/142 (99%) | 85 (61%) | 36 (26%) | 19 (14%) | 0 | 5 |
| 42 | BN | 118/127 (93%) | 76 (64%) | 29 (25%) | 13 (11%) | 0 | 9 |
| 42 | DN | 118/127 (93%) | 77 (65%) | 28 (24%) | 13 (11%) | 0 | 9 |
| 43 | BO | 114/117 (97%) | 74 (65%) | 29 (25%) | 11 (10%) | 1 | 13 |
| 43 | DO | 114/117 (97%) | 75 (66%) | 27 (24%) | 12 (10%) | 0 | 10 |
| 44 | BQ | 115/117 (98%) | 75 (65%) | 31 (27%) | 9 (8%) | 1 | 18 |
| 44 | DQ | 115/117 (98%) | 75 (65%) | 29 (25%) | 11 (10%) | 1 | 13 |
| 45 | BS | 108/110 (98%) | 68 (63%) | 29 (27%) | 11 (10%) | 1 | 11 |
| 45 | DS | 108/110 (98%) | 66 (61%) | 31 (29%) | 11 (10%) | 1 | 11 |
| 46 | BU | 100/103 (97%) | 58 (58%) | 23 (23%) | 19 (19%) | 0 | 2 |
| 46 | DU | 100/103 (97%) | 59 (59%) | 22 (22%) | 19 (19%) | 0 | 2 |
| 47 | BF | 176/178 (99%) | 103 (58%) | 44 (25%) | 29 (16%) | 0 | 4 |
| 47 | DF | 176/178 (99%) | 105 (60%) | 42 (24%) | 29 (16%) | 0 | 4 |
| 48 | BG | 174/176 (99%) | 99 (57%) | 42 (24%) | 33 (19%) | 0 | 2 |
| 48 | DG | 174/176 (99%) | 101 (58%) | 41 (24%) | 32 (18%) | 0 | 2 |
| 49 | BR | 101/103 (98%) | 72 (71%) | 20 (20%) | 9 (9%) | 1 | 15 |
| 49 | DR | 101/103 (98%) | 74 (73%) | 18 (18%) | 9 (9%) | 1 | 15 |
| 50 | BT | 91/100 (91%) | 48 (53%) | 23 (25%) | 20 (22%) | 0 | 1 |
| 50 | DT | 91/100 (91%) | 46 (50%) | 27 (30%) | 18 (20%) | 0 | 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 51 | BZ | 75/78 (96%) | 50 (67%) | 13 (17%) | 12 (16%) | 0 | 4 |
| 51 | DZ | 75/78 (96%) | 50 (67%) | 13 (17%) | 12 (16%) | 0 | 4 |
| 52 | BW | 77/84 (92%) | 28 (36%) | 23 (30%) | 26 (34%) | 0 | 0 |
| 52 | DW | 77/84 (92%) | 28 (36%) | 24 (31%) | 25 (32%) | 0 | 0 |
| 53 | B6 | 183/185 (99%) | 162 (88%) | 16 (9%) | 5 (3%) | 6 | 43 |
| 53 | D6 | 183/185 (99%) | 152 (83%) | 24 (13%) | 7 (4%) | 4 | 35 |
| All | All | 11607/12284 (94%) | 7731 (67%) | 2581 (22%) | 1295 (11%) | 0 | 9 |

5 of 1295 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AC | 14 | VAL |
| 2 | AC | 54 | ILE |
| 2 | AC | 205 | GLU |
| 3 | AD | 24 | VAL |
| 3 | AD | 25 | ARG |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | AC | 170/189 (90%) | 144 (85%) | 26 (15%) | 3 | 22 |
| 2 | CC | 170/189 (90%) | 143 (84%) | 27 (16%) | 3 | 21 |
| 3 | AD | 172/172 (100%) | 146 (85%) | 26 (15%) | 3 | 23 |
| 3 | CD | 172/172 (100%) | 147 (86%) | 25 (14%) | 4 | 24 |
| 4 | AE | 113/125 (90%) | 95 (84%) | 18 (16%) | 3 | 21 |
| 4 | CE | 113/125 (90%) | 96 (85%) | 17 (15%) | 3 | 23 |
| 5 | AF | 87/116 (75%) | 76 (87%) | 11 (13%) | 5 | 29 |
| 5 | CF | 87/116 (75%) | 76 (87%) | 11 (13%) | 5 | 29 |
| 6 | AG | 123/146 (84%) | 105 (85%) | 18 (15%) | 3 | 24 |
| 6 | CG | 125/146 (86%) | 106 (85%) | 19 (15%) | 3 | 22 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 7 | AH | 104/104 (100%) | 96 (92%) | 8 (8%) | 15 | 51 |
| 7 | CH | 104/104 (100%) | 97 (93%) | 7 (7%) | 19 | 55 |
| 8 | AI | 105/106 (99%) | 91 (87%) | 14 (13%) | 4 | 28 |
| 8 | CI | 105/106 (99%) | 89 (85%) | 16 (15%) | 3 | 22 |
| 9 | AJ | 86/90 (96%) | 76 (88%) | 10 (12%) | 6 | 33 |
| 9 | CJ | 86/90 (96%) | 76 (88%) | 10 (12%) | 6 | 33 |
| 10 | AK | 90/98 (92%) | 77 (86%) | 13 (14%) | 4 | 25 |
| 10 | CK | 90/98 (92%) | 75 (83%) | 15 (17%) | 2 | 19 |
| 11 | AL | 103/103 (100%) | 86 (84%) | 17 (16%) | 2 | 19 |
| 11 | CL | 103/103 (100%) | 85 (82%) | 18 (18%) | 2 | 16 |
| 12 | AM | 92/95 (97%) | 77 (84%) | 15 (16%) | 3 | 20 |
| 12 | CM | 91/95 (96%) | 76 (84%) | 15 (16%) | 2 | 19 |
| 13 | AN | 79/83 (95%) | 62 (78%) | 17 (22%) | 1 | 9 |
| 13 | CN | 79/83 (95%) | 62 (78%) | 17 (22%) | 1 | 9 |
| 14 | AO | 76/77 (99%) | 69 (91%) | 7 (9%) | 11 | 42 |
| 14 | CO | 76/77 (99%) | 69 (91%) | 7 (9%) | 11 | 42 |
| 15 | AP | 65/65 (100%) | 59 (91%) | 6 (9%) | 11 | 42 |
| 15 | CP | 65/65 (100%) | 59 (91%) | 6 (9%) | 11 | 42 |
| 16 | AQ | 74/77 (96%) | 61 (82%) | 13 (18%) | 2 | 16 |
| 16 | CQ | 75/77 (97%) | 63 (84%) | 12 (16%) | 3 | 20 |
| 17 | AR | 48/64 (75%) | 40 (83%) | 8 (17%) | 2 | 19 |
| 17 | CR | 48/64 (75%) | 39 (81%) | 9 (19%) | 2 | 13 |
| 18 | AS | 70/78 (90%) | 56 (80%) | 14 (20%) | 1 | 12 |
| 18 | CS | 71/78 (91%) | 57 (80%) | 14 (20%) | 1 | 12 |
| 19 | AT | 65/65 (100%) | 55 (85%) | 10 (15%) | 3 | 22 |
| 19 | CT | 65/65 (100%) | 55 (85%) | 10 (15%) | 3 | 22 |
| 20 | AB | 180/198 (91%) | 148 (82%) | 32 (18%) | 2 | 16 |
| 20 | CB | 180/198 (91%) | 150 (83%) | 30 (17%) | 2 | 19 |
| 21 | AU | 44/60 (73%) | 32 (73%) | 12 (27%) | 0 | 4 |
| 21 | CU | 44/60 (73%) | 32 (73%) | 12 (27%) | 0 | 4 |
| 24 | BI | 109/109 (100%) | 107 (98%) | 2 (2%) | 64 | 85 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 24 | DI | 109/109 (100%) | 103 (94%) | 6 (6%) | 25 | 62 |
| 25 | BC | 216/217 (100%) | 179 (83%) | 37 (17%) | 2 | 17 |
| 25 | DC | 216/217 (100%) | 176 (82%) | 40 (18%) | 2 | 14 |
| 26 | BD | 164/164 (100%) | 135 (82%) | 29 (18%) | 2 | 16 |
| 26 | DD | 164/164 (100%) | 134 (82%) | 30 (18%) | 2 | 14 |
| 27 | BK | 102/104 (98%) | 80 (78%) | 22 (22%) | 1 | 9 |
| 27 | DK | 102/104 (98%) | 81 (79%) | 21 (21%) | 1 | 10 |
| 28 | BP | 99/99 (100%) | 80 (81%) | 19 (19%) | 1 | 13 |
| 28 | DP | 99/99 (100%) | 80 (81%) | 19 (19%) | 1 | 13 |
| 29 | BE | 165/165 (100%) | 143 (87%) | 22 (13%) | 4 | 28 |
| 29 | DE | 165/165 (100%) | 142 (86%) | 23 (14%) | 4 | 27 |
| 30 | BY | 48/48 (100%) | 38 (79%) | 10 (21%) | 1 | 10 |
| 30 | DY | 48/48 (100%) | 38 (79%) | 10 (21%) | 1 | 10 |
| 31 | B0 | 47/47 (100%) | 38 (81%) | 9 (19%) | 2 | 13 |
| 31 | D0 | 47/47 (100%) | 38 (81%) | 9 (19%) | 2 | 13 |
| 32 | B4 | 34/34 (100%) | 28 (82%) | 6 (18%) | 2 | 16 |
| 32 | D4 | 34/34 (100%) | 29 (85%) | 5 (15%) | 3 | 24 |
| 33 | B1 | 45/48 (94%) | 40 (89%) | 5 (11%) | 7 | 34 |
| 33 | D1 | 45/48 (94%) | 41 (91%) | 4 (9%) | 11 | 44 |
| 34 | B3 | 51/51 (100%) | 45 (88%) | 6 (12%) | 6 | 32 |
| 34 | D3 | 51/51 (100%) | 46 (90%) | 5 (10%) | 9 | 39 |
| 35 | BV | 78/78 (100%) | 64 (82%) | 14 (18%) | 2 | 15 |
| 35 | DV | 78/78 (100%) | 64 (82%) | 14 (18%) | 2 | 15 |
| 36 | B2 | 38/38 (100%) | 28 (74%) | 10 (26%) | 0 | 5 |
| 36 | D2 | 38/38 (100%) | 28 (74%) | 10 (26%) | 0 | 5 |
| 37 | BL | 102/103 (99%) | 91 (89%) | 11 (11%) | 7 | 36 |
| 37 | DL | 102/103 (99%) | 91 (89%) | 11 (11%) | 7 | 36 |
| 38 | BM | 109/109 (100%) | 87 (80%) | 22 (20%) | 1 | 11 |
| 38 | DM | 109/109 (100%) | 87 (80%) | 22 (20%) | 1 | 11 |
| 39 | BX | 55/55 (100%) | 46 (84%) | 9 (16%) | 2 | 19 |
| 39 | DX | 55/55 (100%) | 46 (84%) | 9 (16%) | 2 | 19 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 40 | BH | 114/114 (100%) | 79 (69%) | 35 (31%) | 0 | 3 |
| 40 | DH | 114/114 (100%) | 89 (78%) | 25 (22%) | 1 | 9 |
| 41 | BJ | 116/116 (100%) | 100 (86%) | 16 (14%) | 4 | 27 |
| 41 | DJ | 116/116 (100%) | 100 (86%) | 16 (14%) | 4 | 27 |
| 42 | BN | 100/103 (97%) | 84 (84%) | 16 (16%) | 3 | 20 |
| 42 | DN | 100/103 (97%) | 84 (84%) | 16 (16%) | 3 | 20 |
| 43 | BO | 86/87 (99%) | 71 (83%) | 15 (17%) | 2 | 16 |
| 43 | DO | 86/87 (99%) | 72 (84%) | 14 (16%) | 3 | 20 |
| 44 | BQ | 89/89 (100%) | 79 (89%) | 10 (11%) | 7 | 34 |
| 44 | DQ | 89/89 (100%) | 79 (89%) | 10 (11%) | 7 | 34 |
| 45 | BS | 93/93 (100%) | 77 (83%) | 16 (17%) | 2 | 17 |
| 45 | DS | 93/93 (100%) | 77 (83%) | 16 (17%) | 2 | 17 |
| 46 | BU | 83/84 (99%) | 65 (78%) | 18 (22%) | 1 | 9 |
| 46 | DU | 83/84 (99%) | 65 (78%) | 18 (22%) | 1 | 9 |
| 47 | BF | 149/149 (100%) | 117 (78%) | 32 (22%) | 1 | 9 |
| 47 | DF | 149/149 (100%) | 117 (78%) | 32 (22%) | 1 | 9 |
| 48 | BG | 137/137 (100%) | 110 (80%) | 27 (20%) | 1 | 12 |
| 48 | DG | 137/137 (100%) | 112 (82%) | 25 (18%) | 2 | 14 |
| 49 | BR | 84/84 (100%) | 71 (84%) | 13 (16%) | 3 | 22 |
| 49 | DR | 84/84 (100%) | 70 (83%) | 14 (17%) | 2 | 19 |
| 50 | BT | 80/84 (95%) | 64 (80%) | 16 (20%) | 1 | 12 |
| 50 | DT | 80/84 (95%) | 64 (80%) | 16 (20%) | 1 | 12 |
| 51 | BZ | 67/68 (98%) | 53 (79%) | 14 (21%) | 1 | 10 |
| 51 | DZ | 67/68 (98%) | 56 (84%) | 11 (16%) | 2 | 19 |
| 52 | BW | 59/62 (95%) | 42 (71%) | 17 (29%) | 0 | 3 |
| 52 | DW | 59/62 (95%) | 42 (71%) | 17 (29%) | 0 | 3 |
| 53 | B6 | 157/157 (100%) | 137 (87%) | 20 (13%) | 5 | 29 |
| 53 | D6 | 157/157 (100%) | 134 (85%) | 23 (15%) | 3 | 24 |
| All | All | 9647/10014 (96%) | 8066 (84%) | 1581 (16%) | 2 | 19 |

5 of 1581 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | BR | 39 | LEU |
| 6 | CG | 110 | ARG |
| 47 | DF | 103 | ILE |
| 50 | BT | 68 | LYS |
| 2 | CC | 61 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 320 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48 | BG | 37 | ASN |
| 7 | CH | 3 | GLN |
| 46 | DU | 65 | GLN |
| 49 | BR | 86 | GLN |
| 2 | CC | 2 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1529/1542 (99%) | 244 (15%) | 0 |
| 1 | CA | 1529/1542 (99%) | 235 (15%) | 0 |
| 22 | BA | 116/120 (96%) | 17 (14%) | 0 |
| 22 | DA | 116/120 (96%) | 16 (13%) | 0 |
| 23 | BB | 2837/2904 (97%) | 457 (16%) | 0 |
| 23 | DB | 2837/2904 (97%) | 435 (15%) | 0 |
| All | All | 8964/9132 (98%) | 1404 (15%) | 0 |

5 of 1404 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 9 | G |
| 1 | AA | 14 | U |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 for Mogul analysis.

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$ |
| 55 | LLL | AA | 1661 | - | 30,33,33 | 2.30 | 11 (36%) | 33,49,49 | 1.31 | 4 (12%) |
| 55 | LLL | BB | 3111 | - | 30,33,33 | 2.27 | 11 (36%) | 33,49,49 | 1.22 | 3 (9%) |
| 55 | LLL | CA | 1662 | - | 30,33,33 | 2.30 | 11 (36%) | 33,49,49 | 1.30 | 4 (12%) |
| 55 | LLL | DB | 3112 | - | 30,33,33 | 2.31 | 11 (36%) | 33,49,49 | 1.26 | 4 (12%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 55 | LLL | AA | 1661 | - | - | 0/11/65/65 | 0/3/3/3 |
| 55 | LLL | BB | 3111 | - | - | 0/11/65/65 | 0/3/3/3 |
| 55 | LLL | CA | 1662 | - | - | 0/11/65/65 | 0/3/3/3 |
| 55 | LLL | DB | 3112 | - | - | 0/11/65/65 | 0/3/3/3 |

The worst 5 of 44 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 55 | BB | 3111 | LLL | C22-C32 | 2.20 | 1.58 | 1.53 |
| 55 | BB | 3111 | LLL | C31-C21 | 2.27 | 1.59 | 1.53 |
| 55 | CA | 1662 | LLL | C52-C62 | 2.29 | 1.58 | 1.52 |
| 55 | DB | 3112 | LLL | C31-C21 | 2.32 | 1.59 | 1.53 |
| 55 | CA | 1662 | LLL | C31-C21 | 2.34 | 1.59 | 1.53 |

The worst 5 of 15 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 55 | AA | 1661 | LLL | O43-C43-C83 | -2.58 | 102.47 | 108.10 |
| 55 | DB | 3112 | LLL | O43-C43-C83 | -2.55 | 102.54 | 108.10 |
| 55 | BB | 3111 | LLL | O43-C43-C83 | -2.49 | 102.66 | 108.10 |
| 55 | CA | 1662 | LLL | O43-C43-C83 | -2.46 | 102.73 | 108.10 |
| 55 | DB | 3112 | LLL | C13-O62-C62 | 2.09 | 123.08 | 118.00 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 55 | BB | 3111 | LLL | 2 | 0 |
| 55 | CA | 1662 | LLL | 3 | 0 |

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 ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1 | AA | 1530/1542 (99%) | -0.34 | 8 (0%) 90 86 | 13, 75, 157, 180 | 0 |
| 1 | CA | 1530/1542 (99%) | -0.40 | 1 (0%) 95 94 | 8, 52, 139, 180 | 0 |
| 2 | AC | 206/232 (88%) | -0.19 | 3 (1%) 74 64 | 5, 72, 147, 180 | 0 |
| 2 | CC | 206/232 (88%) | -0.10 | 1 (0%) 90 86 | 6, 72, 131, 180 | 0 |
| 3 | AD | 205/205 (100%) | 0.19 | 8 (3%) 40 31 | 20, 95, 159, 180 | 0 |
| 3 | CD | 205/205 (100%) | -0.17 | 0 100 100 | 5, 56, 145, 180 | 0 |
| 4 | AE | 150/166 (90%) | 0.16 | 3 (2%) 65 56 | 7, 69, 146, 180 | 0 |
| 4 | CE | 150/166 (90%) | 0.16 | 3 (2%) 65 56 | 5, 49, 112, 180 | 0 |
| 5 | AF | 100/135 (74%) | 0.24 | 5 (5%) 30 23 | 5, 69, 150, 177 | 0 |
| 5 | CF | 100/135 (74%) | -0.01 | 1 (1%) 82 74 | 5, 72, 143, 166 | 0 |
| 6 | AG | 150/178 (84%) | 0.01 | 4 (2%) 55 44 | 20, 97, 159, 175 | 0 |
| 6 | CG | 152/178 (85%) | -0.14 | 1 (0%) 87 82 | 29, 85, 147, 180 | 0 |
| 7 | AH | 129/129 (100%) | 0.26 | 8 (6%) 21 16 | 26, 80, 143, 177 | 0 |
| 7 | CH | 129/129 (100%) | 0.00 | 0 100 100 | 6, 49, 117, 174 | 0 |
| 8 | AI | 127/129 (98%) | 0.01 | 2 (1%) 72 63 | 18, 89, 171, 180 | 0 |
| 8 | CI | 127/129 (98%) | -0.05 | 2 (1%) 72 63 | 22, 92, 160, 180 | 0 |
| 9 | AJ | 98/103 (95%) | 0.21 | 2 (2%) 65 56 | 16, 92, 169, 180 | 0 |
| 9 | CJ | 98/103 (95%) | 0.30 | 5 (5%) 29 23 | 26, 87, 153, 180 | 0 |
| 10 | AK | 117/128 (91%) | -0.16 | 0 100 100 | 7, 59, 119, 180 | 0 |
| 10 | CK | 117/128 (91%) | -0.19 | 2 (1%) 70 61 | 5, 52, 120, 180 | 0 |
| 11 | AL | 123/123 (100%) | 0.10 | 3 (2%) 59 49 | 14, 78, 152, 180 | 0 |
| 11 | CL | 123/123 (100%) | -0.05 | 0 100 100 | 5, 46, 127, 170 | 0 |
| 12 | AM | 114/117 (97%) | -0.18 | 0 100 100 | 40, 114, 180, 180 | 0 |
| 12 | CM | 113/117 (96%) | -0.23 | 0 100 100 | 27, 100, 173, 180 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AN | 96/100 (96%) | -0.01 | 0 100 100 | 8, 86, 158, 180 | 0 |
| 13 | CN | 96/100 (96%) | 0.08 | 1 (1%) 82 74 | 14, 87, 147, 178 | 0 |
| 14 | AO | 88/89 (98%) | -0.35 | 0 100 100 | 5, 76, 128, 180 | 0 |
| 14 | CO | 88/89 (98%) | -0.20 | 0 100 100 | 10, 63, 132, 159 | 0 |
| 15 | AP | 82/82 (100%) | 0.67 | 3 (3%) 42 33 | 24, 94, 154, 180 | 0 |
| 15 | CP | 80/82 (97%) | 0.43 | 5 (6%) 21 15 | 5, 46, 128, 180 | 0 |
| 16 | AQ | 80/83 (96%) | 0.02 | 0 100 100 | 36, 96, 168, 180 | 0 |
| 16 | CQ | 81/83 (97%) | 0.01 | 0 100 100 | 5, 52, 135, 180 | 0 |
| 17 | AR | 55/74 (74%) | -0.05 | 1 (1%) 69 60 | 14, 70, 148, 180 | 0 |
| 17 | CR | 55/74 (74%) | 0.39 | 3 (5%) 26 20 | 12, 64, 136, 180 | 0 |
| 18 | AS | 79/91 (86%) | 0.40 | 6 (7%) 15 11 | 44, 120, 176, 180 | 0 |
| 18 | CS | 80/91 (87%) | -0.18 | 0 100 100 | 34, 107, 180, 180 | 0 |
| 19 | AT | 85/86 (98%) | -0.20 | 0 100 100 | 34, 101, 168, 180 | 0 |
| 19 | CT | 85/86 (98%) | -0.40 | 0 100 100 | 5, 62, 140, 180 | 0 |
| 20 | AB | 218/240 (90%) | 0.13 | 8 (3%) 42 33 | 18, 97, 160, 180 | 0 |
| 20 | CB | 218/240 (90%) | 0.11 | 6 (2%) 53 43 | 16, 93, 160, 180 | 0 |
| 21 | AU | 51/70 (72%) | 0.00 | 1 (1%) 65 56 | 27, 89, 171, 180 | 0 |
| 21 | CU | 51/70 (72%) | -0.11 | 0 100 100 | 23, 81, 137, 180 | 0 |
| 22 | BA | 117/120 (97%) | -0.42 | 0 100 100 | 49, 85, 136, 180 | 0 |
| 22 | DA | 117/120 (97%) | -0.35 | 2 (1%) 70 61 | 36, 88, 148, 180 | 0 |
| 23 | BB | 2841/2904 (97%) | -0.16 | 14 (0%) 90 86 | 6, 60, 150, 180 | 0 |
| 23 | DB | 2841/2904 (97%) | -0.20 | 8 (0%) 93 91 | 5, 46, 154, 180 | 0 |
| 24 | BI | 141/141 (100%) | 0.97 | 24 (17%) 2 3 | 72, 166, 180, 180 | 0 |
| 24 | DI | 141/141 (100%) | 0.58 | 12 (8%) 11 10 | 63, 162, 180, 180 | 0 |
| 25 | BC | 271/272 (99%) | 0.09 | 2 (0%) 87 82 | 5, 47, 107, 156 | 0 |
| 25 | DC | 271/272 (99%) | 0.03 | 0 100 100 | 5, 38, 99, 145 | 0 |
| 26 | BD | 209/209 (100%) | 0.38 | 16 (7%) 14 11 | 8, 72, 145, 180 | 0 |
| 26 | DD | 209/209 (100%) | 0.10 | 1 (0%) 90 86 | 5, 51, 131, 180 | 0 |
| 27 | BK | 121/123 (98%) | 0.62 | 5 (4%) 38 29 | 16, 62, 142, 180 | 0 |
| 27 | DK | 121/123 (98%) | 0.23 | 0 100 100 | 5, 42, 103, 180 | 0 |
| 28 | BP | 114/114 (100%) | 1.10 | 18 (15%) 2 3 | 28, 86, 155, 173 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28 | DP | 114/114 (100%) | -0.22 | 0 100 100 | 5, 52, 119, 161 | 0 |
| 29 | BE | 201/201 (100%) | 0.34 | 14 (6%) 17 13 | 5, 76, 143, 180 | 0 |
| 29 | DE | 201/201 (100%) | 0.08 | 5 (2%) 58 47 | 5, 66, 138, 180 | 0 |
| 30 | BY | 58/58 (100%) | 0.28 | 2 (3%) 46 36 | 22, 84, 137, 180 | 0 |
| 30 | DY | 58/58 (100%) | -0.05 | 1 (1%) 70 61 | 10, 66, 149, 158 | 0 |
| 31 | B0 | 56/56 (100%) | 0.16 | 2 (3%) 43 34 | 5, 81, 149, 180 | 0 |
| 31 | D0 | 56/56 (100%) | -0.25 | 0 100 100 | 9, 54, 119, 180 | 0 |
| 32 | B4 | 38/38 (100%) | 0.07 | 1 (2%) 56 46 | 5, 71, 153, 168 | 0 |
| 32 | D4 | 38/38 (100%) | -0.01 | 0 100 100 | 17, 62, 132, 171 | 0 |
| 33 | B1 | 50/54 (92%) | 0.40 | 3 (6%) 23 16 | 32, 87, 132, 174 | 0 |
| 33 | D1 | 50/54 (92%) | 0.17 | 2 (4%) 39 30 | 24, 73, 125, 155 | 0 |
| 34 | B3 | 64/64 (100%) | 0.59 | 4 (6%) 21 15 | 19, 64, 105, 133 | 0 |
| 34 | D3 | 64/64 (100%) | 0.14 | 1 (1%) 72 63 | 6, 49, 107, 180 | 0 |
| 35 | BV | 94/94 (100%) | -0.11 | 1 (1%) 80 72 | 37, 92, 143, 180 | 0 |
| 35 | DV | 94/94 (100%) | -0.09 | 0 100 100 | 27, 94, 160, 180 | 0 |
| 36 | B2 | 46/46 (100%) | 0.00 | 0 100 100 | 5, 50, 123, 143 | 0 |
| 36 | D2 | 46/46 (100%) | -0.12 | 0 100 100 | 7, 43, 103, 180 | 0 |
| 37 | BL | 143/144 (99%) | 0.24 | 1 (0%) 87 82 | 7, 72, 131, 180 | 0 |
| 37 | DL | 143/144 (99%) | 0.12 | 0 100 100 | 5, 61, 128, 162 | 0 |
| 38 | BM | 136/136 (100%) | 0.08 | 4 (2%) 52 42 | 16, 68, 144, 165 | 0 |
| 38 | DM | 136/136 (100%) | 0.22 | 4 (2%) 52 42 | 5, 63, 134, 171 | 0 |
| 39 | BX | 63/63 (100%) | 0.26 | 2 (3%) 48 38 | 24, 92, 169, 180 | 0 |
| 39 | DX | 63/63 (100%) | -0.09 | 2 (3%) 48 38 | 38, 94, 166, 180 | 0 |
| 40 | BH | 149/149 (100%) | 1.22 | 28 (18%) 1 3 | 13, 125, 180, 180 | 0 |
| 40 | DH | 149/149 (100%) | 0.38 | 6 (4%) 39 30 | 5, 109, 171, 180 | 0 |
| 41 | BJ | 142/142 (100%) | 0.03 | 2 (1%) 75 66 | 13, 77, 132, 166 | 0 |
| 41 | DJ | 142/142 (100%) | -0.13 | 1 (0%) 87 82 | 5, 65, 128, 180 | 0 |
| 42 | BN | 120/127 (94%) | 0.06 | 1 (0%) 86 79 | 5, 68, 136, 180 | 0 |
| 42 | DN | 120/127 (94%) | -0.38 | 0 100 100 | 5, 44, 116, 141 | 0 |
| 43 | BO | 116/117 (99%) | 0.39 | 8 (6%) 18 13 | 29, 94, 144, 180 | 0 |
| 43 | DO | 116/117 (99%) | -0.10 | 2 (1%) 70 61 | 5, 93, 156, 180 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44 | BQ | 117/117 (100%) | -0.37 | 0 100 100 | 5, 72, 134, 171 | 0 |
| 44 | DQ | 117/117 (100%) | 0.05 | 1 (0%) 84 77 | 5, 50, 131, 156 | 0 |
| 45 | BS | 110/110 (100%) | 0.44 | 2 (1%) 69 60 | 5, 67, 129, 180 | 0 |
| 45 | DS | 110/110 (100%) | 0.29 | 0 100 100 | 5, 50, 120, 157 | 0 |
| 46 | BU | 102/103 (99%) | 0.71 | 6 (5%) 23 17 | 13, 88, 148, 177 | 0 |
| 46 | DU | 102/103 (99%) | -0.00 | 1 (0%) 82 74 | 26, 93, 154, 180 | 0 |
| 47 | BF | 178/178 (100%) | 0.29 | 2 (1%) 80 72 | 39, 115, 174, 180 | 0 |
| 47 | DF | 178/178 (100%) | 0.60 | 13 (7%) 16 12 | 22, 106, 175, 180 | 0 |
| 48 | BG | 176/176 (100%) | 0.23 | 2 (1%) 80 72 | 8, 102, 172, 180 | 0 |
| 48 | DG | 176/176 (100%) | 0.03 | 3 (1%) 70 61 | 32, 104, 164, 180 | 0 |
| 49 | BR | 103/103 (100%) | 0.14 | 3 (2%) 52 42 | 18, 99, 151, 173 | 0 |
| 49 | DR | 103/103 (100%) | 0.29 | 4 (3%) 40 31 | 5, 85, 144, 180 | 0 |
| 50 | BT | 93/100 (93%) | 0.22 | 2 (2%) 62 53 | 13, 83, 160, 180 | 0 |
| 50 | DT | 93/100 (93%) | 0.31 | 3 (3%) 48 38 | 15, 79, 167, 180 | 0 |
| 51 | BZ | 77/78 (98%) | 0.29 | 3 (3%) 40 31 | 12, 57, 112, 152 | 0 |
| 51 | DZ | 77/78 (98%) | -0.13 | 1 (1%) 77 68 | 5, 56, 101, 131 | 0 |
| 52 | BW | 79/84 (94%) | 0.60 | 7 (8%) 10 9 | 19, 88, 139, 180 | 0 |
| 52 | DW | 79/84 (94%) | 0.03 | 3 (3%) 41 32 | 5, 79, 143, 180 | 0 |
| 53 | B6 | 185/185 (100%) | 2.72 | 83 (44%) 0 1 | 23, 123, 180, 180 | 0 |
| 53 | D6 | 185/185 (100%) | 1.06 | 49 (26%) 1 2 | 5, 104, 180, 180 | 0 |
| All | All | 20787/21416 (97%) | 0.00 | 483 (2%) 61 52 | 5, 69, 159, 180 | 0 |

The worst 5 of 483 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 53 | B6 | 96 | GLY | 15.3 |
| 53 | B6 | 97 | ASP | 15.0 |
| 53 | B6 | 98 | ALA | 13.2 |
| 53 | B6 | 88 | LEU | 10.7 |
| 53 | B6 | 94 | ASN | 10.0 |

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 55 | LLL | DB | 3112 | 31/31 | 0.84 | 0.34 | 7.10 | 121,121,121,121 | 0 |
| 55 | LLL | BB | 3111 | 31/31 | 0.87 | 0.26 | 3.45 | 107,107,107,107 | 0 |
| 54 | MG | DB | 3059 | 1/1 | 0.69 | 0.23 | 2.64 | 166,166,166,166 | 0 |
| 55 | LLL | CA | 1662 | 31/31 | 0.94 | 0.22 | 1.74 | 14,14,14,14 | 0 |
| 54 | MG | CA | 1604 | 1/1 | 0.97 | 0.27 | 1.54 | 16,16,16,16 | 0 |
| 54 | MG | BB | 3087 | 1/1 | 0.98 | 0.22 | 1.50 | 114,114,114,114 | 0 |
| 54 | MG | BB | 3013 | 1/1 | 0.81 | 0.18 | 1.49 | 92,92,92,92 | 0 |
| 54 | MG | DB | 3089 | 1/1 | 0.95 | 0.19 | 1.20 | 61,61,61,61 | 0 |
| 54 | MG | BB | 3108 | 1/1 | 0.92 | 0.22 | 1.14 | 44,44,44,44 | 0 |
| 54 | MG | AA | 1653 | 1/1 | 0.97 | 0.18 | 0.74 | 87,87,87,87 | 0 |
| 54 | MG | DB | 3099 | 1/1 | 0.98 | 0.20 | 0.55 | 5,5,5,5 | 0 |
| 54 | MG | DB | 3092 | 1/1 | 0.96 | 0.15 | 0.48 | 56,56,56,56 | 0 |
| 54 | MG | DB | 3090 | 1/1 | 0.96 | 0.30 | 0.45 | 64,64,64,64 | 0 |
| 55 | LLL | AA | 1661 | 31/31 | 0.95 | 0.21 | 0.21 | 21,21,21,21 | 0 |
| 54 | MG | DB | 3051 | 1/1 | 0.98 | 0.20 | 0.20 | 32,32,32,32 | 0 |
| 54 | MG | CA | 1638 | 1/1 | 0.86 | 0.11 | 0.13 | 98,98,98,98 | 0 |
| 54 | MG | DB | 3035 | 1/1 | 0.93 | 0.19 | -0.09 | 75,75,75,75 | 0 |
| 54 | MG | AA | 1615 | 1/1 | 0.92 | 0.23 | -0.12 | 106,106,106,106 | 0 |
| 54 | MG | CA | 1614 | 1/1 | 0.71 | 0.16 | -0.19 | 90,90,90,90 | 0 |
| 54 | MG | BB | 3011 | 1/1 | 0.99 | 0.21 | -0.30 | 29,29,29,29 | 0 |
| 54 | MG | BB | 3079 | 1/1 | 0.79 | 0.20 | -0.31 | 63,63,63,63 | 0 |
| 54 | MG | DB | 3110 | 1/1 | 0.94 | 0.17 | -0.34 | 38,38,38,38 | 0 |
| 54 | MG | AA | 1635 | 1/1 | 0.52 | 0.09 | -0.36 | 103,103,103,103 | 0 |
| 54 | MG | BB | 3098 | 1/1 | 0.98 | 0.16 | -0.45 | 16,16,16,16 | 0 |
| 54 | MG | BB | 3032 | 1/1 | 0.97 | 0.20 | -0.47 | 49,49,49,49 | 0 |
| 54 | MG | BB | 3083 | 1/1 | 0.98 | 0.21 | -0.51 | 28,28,28,28 | 0 |
| 54 | MG | CA | 1616 | 1/1 | 0.83 | 0.14 | -0.58 | 88,88,88,88 | 0 |
| 54 | MG | CA | 1601 | 1/1 | 0.98 | 0.17 | -0.58 | 5,5,5,5 | 0 |
| 54 | MG | DB | 3003 | 1/1 | 0.93 | 0.16 | -0.59 | 33,33,33,33 | 0 |
| 54 | MG | DB | 3100 | 1/1 | 0.84 | 0.21 | -0.61 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | DB | 3014 | 1/1 | 0.99 | 0.12 | -0.64 | 43,43,43,43 | 0 |
| 54 | MG | BB | 3023 | 1/1 | 0.97 | 0.20 | -0.71 | 11,11,11,11 | 0 |
| 54 | MG | DB | 3069 | 1/1 | 0.98 | 0.20 | -0.77 | 14,14,14,14 | 0 |
| 54 | MG | DB | 3088 | 1/1 | 0.98 | 0.16 | -0.78 | 46,46,46,46 | 0 |
| 54 | MG | CA | 1633 | 1/1 | 0.96 | 0.14 | -0.84 | 50,50,50,50 | 0 |
| 54 | MG | AA | 1613 | 1/1 | 0.81 | 0.08 | -0.84 | 71,71,71,71 | 0 |
| 54 | MG | BB | 3082 | 1/1 | 0.98 | 0.19 | -0.87 | 5,5,5,5 | 0 |
| 54 | MG | CA | 1618 | 1/1 | 0.98 | 0.12 | -0.88 | 30,30,30,30 | 0 |
| 54 | MG | DB | 3009 | 1/1 | 0.98 | 0.17 | -0.92 | 18,18,18,18 | 0 |
| 54 | MG | DB | 3098 | 1/1 | 0.99 | 0.17 | -0.98 | 28,28,28,28 | 0 |
| 54 | MG | BB | 3005 | 1/1 | 0.97 | 0.19 | -1.03 | 20,20,20,20 | 0 |
| 54 | MG | AA | 1636 | 1/1 | 0.95 | 0.06 | -1.04 | 93,93,93,93 | 0 |
| 54 | MG | BB | 3021 | 1/1 | 0.97 | 0.10 | -1.06 | 51,51,51,51 | 0 |
| 54 | MG | CA | 1636 | 1/1 | 0.93 | 0.05 | -1.10 | 92,92,92,92 | 0 |
| 54 | MG | DB | 3026 | 1/1 | 0.88 | 0.18 | -1.10 | 54,54,54,54 | 0 |
| 54 | MG | CA | 1645 | 1/1 | 0.98 | 0.10 | -1.12 | 66,66,66,66 | 0 |
| 54 | MG | DB | 3096 | 1/1 | 0.99 | 0.16 | -1.13 | 20,20,20,20 | 0 |
| 54 | MG | BB | 3040 | 1/1 | 0.99 | 0.12 | -1.15 | 27,27,27,27 | 0 |
| 54 | MG | BB | 3092 | 1/1 | 0.89 | 0.08 | -1.19 | 45,45,45,45 | 0 |
| 54 | MG | DB | 3087 | 1/1 | 0.99 | 0.15 | -1.22 | 75,75,75,75 | 0 |
| 54 | MG | DB | 3006 | 1/1 | 0.92 | 0.15 | -1.23 | 15,15,15,15 | 0 |
| 54 | MG | DB | 3030 | 1/1 | 0.86 | 0.17 | -1.26 | 10,10,10,10 | 0 |
| 54 | MG | CA | 1605 | 1/1 | 0.97 | 0.12 | -1.38 | 18,18,18,18 | 0 |
| 54 | MG | BB | 3096 | 1/1 | 0.98 | 0.15 | -1.40 | 67,67,67,67 | 0 |
| 56 | ZN | D4 | 101 | 1/1 | 0.94 | 0.07 | -1.51 | 45,45,45,45 | 0 |
| 54 | MG | AA | 1607 | 1/1 | 0.96 | 0.07 | -1.52 | 42,42,42,42 | 0 |
| 54 | MG | AA | 1630 | 1/1 | 0.92 | 0.11 | -1.64 | 88,88,88,88 | 0 |
| 56 | ZN | B4 | 101 | 1/1 | 0.95 | 0.09 | -1.64 | 64,64,64,64 | 0 |
| 54 | MG | BB | 3019 | 1/1 | 0.86 | 0.09 | -1.83 | 40,40,40,40 | 0 |
| 54 | MG | BB | 3086 | 1/1 | 0.95 | 0.17 | -1.83 | 18,18,18,18 | 0 |
| 54 | MG | AA | 1609 | 1/1 | 0.99 | 0.11 | -1.87 | 5,5,5,5 | 0 |
| 54 | MG | CA | 1617 | 1/1 | 0.98 | 0.08 | -1.91 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3037 | 1/1 | 0.90 | 0.11 | -1.92 | 44,44,44,44 | 0 |
| 54 | MG | AA | 1601 | 1/1 | 0.91 | 0.12 | -1.93 | 41,41,41,41 | 0 |
| 54 | MG | DB | 3068 | 1/1 | 0.96 | 0.17 | -1.94 | 22,22,22,22 | 0 |
| 54 | MG | DB | 3055 | 1/1 | 0.88 | 0.13 | -1.97 | 41,41,41,41 | 0 |
| 54 | MG | BB | 3029 | 1/1 | 0.96 | 0.11 | -1.98 | 17,17,17,17 | 0 |
| 54 | MG | BB | 3048 | 1/1 | 0.95 | 0.10 | -2.03 | 7,7,7,7 | 0 |
| 54 | MG | BB | 3090 | 1/1 | 0.98 | 0.10 | -2.14 | 91,91,91,91 | 0 |
| 54 | MG | DB | 3085 | 1/1 | 0.96 | 0.13 | -2.24 | 49,49,49,49 | 0 |
| 54 | MG | AA | 1610 | 1/1 | 0.98 | 0.06 | -2.31 | 62,62,62,62 | 0 |
| 54 | MG | BB | 3074 | 1/1 | 0.97 | 0.14 | -2.41 | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 54 | MG | BB | 3077 | 1/1 | 0.96 | 0.07 | -2.48 | 83,83,83,83 | 0 |
| 54 | MG | CA | 1612 | 1/1 | 0.98 | 0.07 | -2.55 | 72,72,72,72 | 0 |
| 54 | MG | AA | 1638 | 1/1 | 0.98 | 0.07 | -2.55 | 20,20,20,20 | 0 |
| 54 | MG | DB | 3078 | 1/1 | 0.99 | 0.08 | -2.56 | 32,32,32,32 | 0 |
| 54 | MG | BB | 3110 | 1/1 | 0.95 | 0.09 | -2.59 | 40,40,40,40 | 0 |
| 54 | MG | DB | 3070 | 1/1 | 0.98 | 0.10 | -2.72 | 38,38,38,38 | 0 |
| 54 | MG | DB | 3007 | 1/1 | 0.97 | 0.11 | -2.87 | 13,13,13,13 | 0 |
| 54 | MG | BB | 3085 | 1/1 | 0.99 | 0.11 | -2.88 | 43,43,43,43 | 0 |
| 54 | MG | AA | 1629 | 1/1 | 0.99 | 0.05 | -2.94 | 26,26,26,26 | 0 |
| 54 | MG | BB | 3016 | 1/1 | 0.99 | 0.13 | -2.94 | 91,91,91,91 | 0 |
| 54 | MG | DB | 3103 | 1/1 | 0.98 | 0.11 | -3.05 | 42,42,42,42 | 0 |
| 54 | MG | BB | 3081 | 1/1 | 0.88 | 0.17 | -3.07 | 16,16,16,16 | 0 |
| 54 | MG | BB | 3012 | 1/1 | 0.98 | 0.09 | -3.07 | 53,53,53,53 | 0 |
| 54 | MG | DB | 3072 | 1/1 | 0.90 | 0.09 | -3.08 | 54,54,54,54 | 0 |
| 54 | MG | BB | 3062 | 1/1 | 0.98 | 0.05 | -3.15 | 27,27,27,27 | 0 |
| 54 | MG | DB | 3047 | 1/1 | 0.98 | 0.11 | -3.16 | 19,19,19,19 | 0 |
| 54 | MG | DB | 3074 | 1/1 | 0.92 | 0.09 | -3.17 | 17,17,17,17 | 0 |
| 54 | MG | BB | 3002 | 1/1 | 0.96 | 0.08 | -3.32 | 30,30,30,30 | 0 |
| 54 | MG | BB | 3001 | 1/1 | 0.95 | 0.07 | -3.34 | 29,29,29,29 | 0 |
| 54 | MG | DB | 3108 | 1/1 | 0.97 | 0.10 | -3.54 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3069 | 1/1 | 0.98 | 0.14 | -3.63 | 10,10,10,10 | 0 |
| 54 | MG | AA | 1603 | 1/1 | 0.96 | 0.10 | -3.71 | 14,14,14,14 | 0 |
| 54 | MG | BB | 3035 | 1/1 | 0.93 | 0.13 | -3.77 | 82,82,82,82 | 0 |
| 54 | MG | AA | 1654 | 1/1 | 0.95 | 0.07 | -3.77 | 82,82,82,82 | 0 |
| 54 | MG | DB | 3012 | 1/1 | 0.98 | 0.09 | -3.84 | 12,12,12,12 | 0 |
| 54 | MG | BB | 3088 | 1/1 | 0.92 | 0.08 | -4.09 | 36,36,36,36 | 0 |
| 54 | MG | DB | 3001 | 1/1 | 0.97 | 0.09 | -4.26 | 6,6,6,6 | 0 |
| 54 | MG | BB | 3094 | 1/1 | 0.98 | 0.13 | -4.39 | 47,47,47,47 | 0 |
| 54 | MG | DB | 3056 | 1/1 | 0.99 | 0.12 | -4.40 | 12,12,12,12 | 0 |
| 54 | MG | CA | 1632 | 1/1 | 0.98 | 0.08 | -4.61 | 18,18,18,18 | 0 |
| 54 | MG | CA | 1643 | 1/1 | 0.84 | 0.07 | -4.67 | 32,32,32,32 | 0 |
| 54 | MG | DB | 3010 | 1/1 | 0.98 | 0.09 | -4.76 | 16,16,16,16 | 0 |
| 54 | MG | BB | 3103 | 1/1 | 0.96 | 0.09 | -4.84 | 20,20,20,20 | 0 |
| 54 | MG | AA | 1641 | 1/1 | 0.92 | 0.04 | -4.99 | 69,69,69,69 | 0 |
| 54 | MG | DB | 3080 | 1/1 | 0.93 | 0.08 | -5.03 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3065 | 1/1 | 0.94 | 0.06 | -5.07 | 5,5,5,5 | 0 |
| 54 | MG | CA | 1656 | 1/1 | 0.97 | 0.05 | -5.08 | 11,11,11,11 | 0 |
| 54 | MG | CA | 1640 | 1/1 | 0.97 | 0.08 | -5.13 | 5,5,5,5 | 0 |
| 54 | MG | BB | 3052 | 1/1 | 0.97 | 0.08 | -5.16 | 36,36,36,36 | 0 |
| 54 | MG | BB | 3056 | 1/1 | 0.97 | 0.06 | -5.43 | 31,31,31,31 | 0 |
| 54 | MG | CA | 1653 | 1/1 | 0.98 | 0.04 | -5.51 | 51,51,51,51 | 0 |
| 54 | MG | DB | 3002 | 1/1 | 0.98 | 0.08 | -6.04 | 6,6,6,6 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 54 | MG | CA | 1655 | 1/1 | 0.99 | 0.07 | -8.77 | 25,25,25,25 | 0 |
| 54 | MG | AA | 1643 | 1/1 | 0.97 | 0.03 | -8.90 | 29,29,29,29 | 0 |
| 54 | MG | CA | 1651 | 1/1 | 0.95 | 0.11 | - | 38,38,38,38 | 0 |
| 54 | MG | DB | 3041 | 1/1 | 0.98 | 0.08 | - | 34,34,34,34 | 0 |
| 54 | MG | AA | 1649 | 1/1 | 0.91 | 0.06 | - | 82,82,82,82 | 0 |
| 54 | MG | CA | 1630 | 1/1 | 0.97 | 0.29 | - | 52,52,52,52 | 0 |
| 54 | MG | BB | 3101 | 1/1 | 0.98 | 0.05 | - | 5,5,5,5 | 0 |
| 54 | MG | BB | 3102 | 1/1 | 0.98 | 0.04 | - | 31,31,31,31 | 0 |
| 54 | MG | CA | 1658 | 1/1 | 0.83 | 0.34 | - | 53,53,53,53 | 0 |
| 54 | MG | BB | 3063 | 1/1 | 0.98 | 0.14 | - | 28,28,28,28 | 0 |
| 54 | MG | DB | 3066 | 1/1 | 0.68 | 0.30 | - | 158,158,158,158 | 0 |
| 54 | MG | CA | 1647 | 1/1 | 0.97 | 0.07 | - | 65,65,65,65 | 0 |
| 54 | MG | DB | 3022 | 1/1 | 0.94 | 0.08 | - | 71,71,71,71 | 0 |
| 54 | MG | DB | 3033 | 1/1 | 0.90 | 0.12 | - | 43,43,43,43 | 0 |
| 54 | MG | DB | 3019 | 1/1 | 0.98 | 0.06 | - | 5,5,5,5 | 0 |
| 54 | MG | BB | 3105 | 1/1 | 0.99 | 0.05 | - | 60,60,60,60 | 0 |
| 54 | MG | DB | 3048 | 1/1 | 0.99 | 0.08 | - | 34,34,34,34 | 0 |
| 54 | MG | BB | 3055 | 1/1 | 0.98 | 0.19 | - | 53,53,53,53 | 0 |
| 54 | MG | BB | 3042 | 1/1 | 0.56 | 0.12 | - | 135,135,135,135 | 0 |
| 54 | MG | AA | 1640 | 1/1 | 0.98 | 0.09 | - | 56,56,56,56 | 0 |
| 54 | MG | DB | 3097 | 1/1 | 0.94 | 0.18 | - | 64,64,64,64 | 0 |
| 54 | MG | BB | 3066 | 1/1 | 0.98 | 0.14 | - | 25,25,25,25 | 0 |
| 54 | MG | CA | 1607 | 1/1 | 0.96 | 0.07 | - | 83,83,83,83 | 0 |
| 54 | MG | CA | 1652 | 1/1 | 0.94 | 0.16 | - | 65,65,65,65 | 0 |
| 54 | MG | AA | 1650 | 1/1 | 0.69 | 0.14 | - | 122,122,122,122 | 0 |
| 54 | MG | CA | 1606 | 1/1 | 0.93 | 0.13 | - | 138,138,138,138 | 0 |
| 54 | MG | BB | 3106 | 1/1 | 0.98 | 0.11 | - | 39,39,39,39 | 0 |
| 54 | MG | BB | 3009 | 1/1 | 0.96 | 0.14 | - | 96,96,96,96 | 0 |
| 54 | MG | AA | 1616 | 1/1 | 0.97 | 0.06 | - | 42,42,42,42 | 0 |
| 54 | MG | DB | 3024 | 1/1 | 0.95 | 0.14 | - | 45,45,45,45 | 0 |
| 54 | MG | CA | 1609 | 1/1 | 0.91 | 0.04 | - | 84,84,84,84 | 0 |
| 54 | MG | BB | 3104 | 1/1 | 0.99 | 0.16 | - | 28,28,28,28 | 0 |
| 54 | MG | AA | 1617 | 1/1 | 0.97 | 0.12 | - | 100,100,100,100 | 0 |
| 54 | MG | BB | 3044 | 1/1 | 0.97 | 0.08 | - | 52,52,52,52 | 0 |
| 54 | MG | DB | 3046 | 1/1 | 0.97 | 0.07 | - | 11,11,11,11 | 0 |
| 54 | MG | CE | 201 | 1/1 | 0.80 | 0.22 | - | 113,113,113,113 | 0 |
| 54 | MG | CA | 1642 | 1/1 | 0.93 | 0.13 | - | 108,108,108,108 | 0 |
| 54 | MG | CA | 1657 | 1/1 | 0.92 | 0.24 | - | 89,89,89,89 | 0 |
| 54 | MG | BB | 3022 | 1/1 | 0.95 | 0.29 | - | 37,37,37,37 | 0 |
| 54 | MG | AA | 1622 | 1/1 | 0.53 | 0.39 | - | 163,163,163,163 | 0 |
| 54 | MG | DB | 3079 | 1/1 | 0.98 | 0.12 | - | 34,34,34,34 | 0 |
| 54 | MG | AA | 1606 | 1/1 | 0.87 | 0.08 | - | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DB | 3038 | 1/1 | 0.95 | 0.15 | - | 37,37,37,37 | 0 |
| 54 | MG | DB | 3028 | 1/1 | 0.98 | 0.18 | - | 58,58,58,58 | 0 |
| 54 | MG | DB | 3101 | 1/1 | 0.99 | 0.25 | - | 25,25,25,25 | 0 |
| 54 | MG | DB | 3005 | 1/1 | 0.98 | 0.16 | - | 45,45,45,45 | 0 |
| 54 | MG | DB | 3029 | 1/1 | 0.88 | 0.14 | - | 59,59,59,59 | 0 |
| 54 | MG | BB | 3050 | 1/1 | 0.95 | 0.10 | - | 33,33,33,33 | 0 |
| 54 | MG | DB | 3008 | 1/1 | 0.96 | 0.14 | - | 17,17,17,17 | 0 |
| 54 | MG | BB | 3030 | 1/1 | 0.98 | 0.04 | - | 70,70,70,70 | 0 |
| 54 | MG | DB | 3077 | 1/1 | 0.98 | 0.08 | - | 15,15,15,15 | 0 |
| 54 | MG | DB | 3043 | 1/1 | 0.99 | 0.08 | - | 32,32,32,32 | 0 |
| 54 | MG | CA | 1660 | 1/1 | 0.92 | 0.10 | - | 63,63,63,63 | 0 |
| 54 | MG | DB | 3004 | 1/1 | 0.99 | 0.13 | - | 69,69,69,69 | 0 |
| 54 | MG | DB | 3044 | 1/1 | 0.98 | 0.07 | - | 21,21,21,21 | 0 |
| 54 | MG | BB | 3093 | 1/1 | 0.70 | 0.37 | - | 131,131,131,131 | 0 |
| 54 | MG | AA | 1645 | 1/1 | 0.89 | 0.09 | - | 95,95,95,95 | 0 |
| 54 | MG | CA | 1641 | 1/1 | 0.81 | 0.17 | - | 42,42,42,42 | 0 |
| 54 | MG | BB | 3046 | 1/1 | 0.98 | 0.08 | - | 64,64,64,64 | 0 |
| 54 | MG | AA | 1639 | 1/1 | 0.60 | 0.34 | - | 134,134,134,134 | 0 |
| 54 | MG | AA | 1659 | 1/1 | 0.68 | 0.45 | - | 180,180,180,180 | 0 |
| 54 | MG | BB | 3036 | 1/1 | 0.96 | 0.13 | - | 62,62,62,62 | 0 |
| 54 | MG | AA | 1602 | 1/1 | 0.73 | 0.18 | - | 147,147,147,147 | 0 |
| 54 | MG | CA | 1650 | 1/1 | 0.99 | 0.07 | - | 33,33,33,33 | 0 |
| 54 | MG | CA | 1661 | 1/1 | 0.96 | 0.10 | - | 48,48,48,48 | 0 |
| 54 | MG | DB | 3082 | 1/1 | 0.98 | 0.08 | - | 57,57,57,57 | 0 |
| 54 | MG | DB | 3013 | 1/1 | 0.88 | 0.14 | - | 41,41,41,41 | 0 |
| 54 | MG | CA | 1626 | 1/1 | 0.96 | 0.23 | - | 41,41,41,41 | 1 |
| 54 | MG | BB | 3076 | 1/1 | 0.99 | 0.06 | - | 20,20,20,20 | 0 |
| 54 | MG | AA | 1620 | 1/1 | 0.85 | 0.06 | - | 113,113,113,113 | 0 |
| 54 | MG | AA | 1637 | 1/1 | 0.66 | 2.40 | - | 151,151,151,151 | 0 |
| 54 | MG | CA | 1659 | 1/1 | 0.92 | 0.09 | - | 90,90,90,90 | 0 |
| 54 | MG | CA | 1654 | 1/1 | 0.94 | 0.10 | - | 59,59,59,59 | 0 |
| 54 | MG | DB | 3063 | 1/1 | 0.96 | 0.06 | - | 19,19,19,19 | 0 |
| 54 | MG | AA | 1644 | 1/1 | 0.94 | 0.13 | - | 98,98,98,98 | 0 |
| 54 | MG | BB | 3018 | 1/1 | 0.92 | 0.18 | - | 50,50,50,50 | 0 |
| 54 | MG | BB | 3057 | 1/1 | 0.90 | 0.36 | - | 65,65,65,65 | 0 |
| 54 | MG | BB | 3089 | 1/1 | 0.98 | 0.19 | - | 25,25,25,25 | 0 |
| 54 | MG | AA | 1625 | 1/1 | 0.26 | 0.88 | - | 84,84,84,84 | 1 |
| 54 | MG | DB | 3023 | 1/1 | 0.97 | 0.10 | - | 17,17,17,17 | 0 |
| 54 | MG | BB | 3031 | 1/1 | 0.95 | 0.13 | - | 63,63,63,63 | 0 |
| 54 | MG | CA | 1625 | 1/1 | 0.95 | 0.18 | - | 6,6,6,6 | 0 |
| 54 | MG | BB | 3078 | 1/1 | 0.91 | 0.21 | - | 101,101,101,101 | 0 |
| 54 | MG | BB | 3033 | 1/1 | 0.47 | 0.64 | - | 141,141,141,141 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DB | 3021 | 1/1 | 0.99 | 0.08 | - | 51,51,51,51 | 0 |
| 54 | MG | BB | 3049 | 1/1 | 0.88 | 0.15 | - | 35,35,35,35 | 0 |
| 54 | MG | AA | 1628 | 1/1 | 0.97 | 0.12 | - | 59,59,59,59 | 0 |
| 54 | MG | BB | 3043 | 1/1 | 0.82 | 0.08 | - | 122,122,122,122 | 0 |
| 54 | MG | BB | 3071 | 1/1 | 0.96 | 0.09 | - | 89,89,89,89 | 0 |
| 54 | MG | DB | 3039 | 1/1 | 0.97 | 0.08 | - | 69,69,69,69 | 0 |
| 54 | MG | AA | 1658 | 1/1 | 0.86 | 0.09 | - | 85,85,85,85 | 0 |
| 54 | MG | DB | 3083 | 1/1 | 0.95 | 0.17 | - | 83,83,83,83 | 0 |
| 54 | MG | BB | 3020 | 1/1 | 0.95 | 0.09 | - | 36,36,36,36 | 0 |
| 54 | MG | AA | 1656 | 1/1 | 0.71 | 0.79 | - | 161,161,161,161 | 0 |
| 54 | MG | CA | 1634 | 1/1 | 0.96 | 0.10 | - | 23,23,23,23 | 0 |
| 54 | MG | CA | 1613 | 1/1 | 0.98 | 0.11 | - | 40,40,40,40 | 0 |
| 54 | MG | DB | 3075 | 1/1 | 0.98 | 0.12 | - | 35,35,35,35 | 0 |
| 54 | MG | AA | 1632 | 1/1 | 0.65 | 0.26 | - | 62,62,62,62 | 0 |
| 54 | MG | CA | 1623 | 1/1 | 0.76 | 0.08 | - | 173,173,173,173 | 0 |
| 54 | MG | BB | 3067 | 1/1 | 0.95 | 0.13 | - | 24,24,24,24 | 0 |
| 54 | MG | BB | 3061 | 1/1 | 0.91 | 0.10 | - | 56,56,56,56 | 0 |
| 54 | MG | BB | 3060 | 1/1 | 0.99 | 0.08 | - | 22,22,22,22 | 0 |
| 54 | MG | DB | 3076 | 1/1 | 0.98 | 0.14 | - | 104,104,104,104 | 0 |
| 54 | MG | CA | 1603 | 1/1 | 0.97 | 0.09 | - | 29,29,29,29 | 0 |
| 54 | MG | AA | 1611 | 1/1 | 0.98 | 0.09 | - | 77,77,77,77 | 0 |
| 54 | MG | BB | 3107 | 1/1 | 0.96 | 0.08 | - | 30,30,30,30 | 0 |
| 54 | MG | DB | 3036 | 1/1 | 0.95 | 0.08 | - | 20,20,20,20 | 0 |
| 54 | MG | CA | 1624 | 1/1 | 0.93 | 0.12 | - | 56,56,56,56 | 0 |
| 54 | MG | AA | 1624 | 1/1 | 0.93 | 0.10 | - | 77,77,77,77 | 0 |
| 54 | MG | BB | 3025 | 1/1 | 0.99 | 0.06 | - | 42,42,42,42 | 0 |
| 54 | MG | CA | 1648 | 1/1 | 0.97 | 0.19 | - | 14,14,14,14 | 0 |
| 54 | MG | CA | 1611 | 1/1 | 0.97 | 0.06 | - | 57,57,57,57 | 0 |
| 54 | MG | AA | 1626 | 1/1 | 0.54 | 0.18 | - | 49,49,49,49 | 1 |
| 54 | MG | BB | 3100 | 1/1 | 0.94 | 0.21 | - | 151,151,151,151 | 0 |
| 54 | MG | DB | 3084 | 1/1 | 0.98 | 0.14 | - | 16,16,16,16 | 0 |
| 54 | MG | DB | 3016 | 1/1 | 0.95 | 0.07 | - | 25,25,25,25 | 0 |
| 54 | MG | DB | 3093 | 1/1 | 0.94 | 0.17 | - | 10,10,10,10 | 0 |
| 54 | MG | DB | 3015 | 1/1 | 0.89 | 0.10 | - | 24,24,24,24 | 0 |
| 54 | MG | DB | 3027 | 1/1 | 0.96 | 0.17 | - | 28,28,28,28 | 0 |
| 54 | MG | BB | 3038 | 1/1 | 0.95 | 0.23 | - | 152,152,152,152 | 0 |
| 54 | MG | BB | 3034 | 1/1 | 0.96 | 0.24 | - | 59,59,59,59 | 0 |
| 54 | MG | BB | 3095 | 1/1 | 0.95 | 0.11 | - | 81,81,81,81 | 0 |
| 54 | MG | DB | 3102 | 1/1 | 0.97 | 0.09 | - | 22,22,22,22 | 0 |
| 54 | MG | BB | 3070 | 1/1 | 0.98 | 0.19 | - | 59,59,59,59 | 0 |
| 54 | MG | BB | 3028 | 1/1 | 0.97 | 0.15 | - | 61,61,61,61 | 0 |
| 54 | MG | DB | 3058 | 1/1 | 0.83 | 0.85 | - | 162,162,162,162 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1635 | 1/1 | 0.83 | 0.14 | - | 98,98,98,98 | 0 |
| 54 | MG | CA | 1627 | 1/1 | 0.52 | 0.33 | - | 69,69,69,69 | 1 |
| 54 | MG | DB | 3109 | 1/1 | 0.95 | 0.09 | - | 83,83,83,83 | 0 |
| 54 | MG | BB | 3010 | 1/1 | 0.84 | 0.13 | - | 40,40,40,40 | 0 |
| 54 | MG | BB | 3045 | 1/1 | 0.99 | 0.04 | - | 38,38,38,38 | 0 |
| 54 | MG | AA | 1618 | 1/1 | 0.95 | 0.13 | - | 93,93,93,93 | 0 |
| 54 | MG | CA | 1602 | 1/1 | 0.99 | 0.12 | - | 11,11,11,11 | 0 |
| 54 | MG | BB | 3058 | 1/1 | 0.97 | 0.09 | - | 11,11,11,11 | 0 |
| 54 | MG | DB | 3060 | 1/1 | 0.55 | 0.10 | - | 104,104,104,104 | 0 |
| 54 | MG | BB | 3073 | 1/1 | 0.99 | 0.23 | - | 38,38,38,38 | 0 |
| 54 | MG | AA | 1621 | 1/1 | 0.97 | 0.17 | - | 26,26,26,26 | 0 |
| 54 | MG | DB | 3111 | 1/1 | 0.97 | 0.18 | - | 32,32,32,32 | 0 |
| 54 | MG | AA | 1646 | 1/1 | 0.73 | 0.18 | - | 104,104,104,104 | 0 |
| 54 | MG | BB | 3051 | 1/1 | 0.96 | 0.18 | - | 65,65,65,65 | 0 |
| 54 | MG | BB | 3026 | 1/1 | 0.95 | 0.21 | - | 43,43,43,43 | 0 |
| 54 | MG | DB | 3107 | 1/1 | 0.98 | 0.07 | - | 11,11,11,11 | 0 |
| 54 | MG | DB | 3061 | 1/1 | 0.94 | 0.09 | - | 69,69,69,69 | 0 |
| 54 | MG | CA | 1639 | 1/1 | 0.98 | 0.07 | - | 7,7,7,7 | 0 |
| 54 | MG | DB | 3105 | 1/1 | 0.97 | 0.08 | - | 30,30,30,30 | 0 |
| 54 | MG | CA | 1629 | 1/1 | 0.89 | 0.12 | - | 65,65,65,65 | 1 |
| 54 | MG | DB | 3037 | 1/1 | 0.93 | 0.17 | - | 54,54,54,54 | 0 |
| 54 | MG | AA | 1612 | 1/1 | 0.96 | 0.12 | - | 88,88,88,88 | 0 |
| 54 | MG | DB | 3095 | 1/1 | 0.96 | 0.12 | - | 88,88,88,88 | 0 |
| 54 | MG | BB | 3109 | 1/1 | 0.98 | 0.07 | - | 59,59,59,59 | 0 |
| 54 | MG | BB | 3059 | 1/1 | 0.99 | 0.11 | - | 60,60,60,60 | 0 |
| 54 | MG | DB | 3034 | 1/1 | 0.81 | 0.20 | - | 69,69,69,69 | 0 |
| 54 | MG | DB | 3094 | 1/1 | 0.98 | 0.10 | - | 55,55,55,55 | 0 |
| 54 | MG | BB | 3003 | 1/1 | 0.92 | 0.09 | - | 51,51,51,51 | 0 |
| 54 | MG | BB | 3027 | 1/1 | 0.95 | 0.13 | - | 42,42,42,42 | 0 |
| 54 | MG | CA | 1644 | 1/1 | 0.98 | 0.07 | - | 68,68,68,68 | 0 |
| 54 | MG | BB | 3041 | 1/1 | 0.96 | 0.15 | - | 8,8,8,8 | 0 |
| 54 | MG | AA | 1633 | 1/1 | 0.97 | 0.03 | - | 48,48,48,48 | 0 |
| 54 | MG | BB | 3008 | 1/1 | 0.89 | 0.20 | - | 75,75,75,75 | 0 |
| 54 | MG | DB | 3062 | 1/1 | 0.97 | 0.04 | - | 67,67,67,67 | 0 |
| 54 | MG | DB | 3073 | 1/1 | 0.98 | 0.21 | - | 67,67,67,67 | 0 |
| 54 | MG | AA | 1651 | 1/1 | 0.86 | 0.09 | - | 112,112,112,112 | 0 |
| 54 | MG | DB | 3042 | 1/1 | 0.94 | 0.07 | - | 23,23,23,23 | 0 |
| 54 | MG | CA | 1649 | 1/1 | 0.91 | 0.14 | - | 127,127,127,127 | 0 |
| 54 | MG | DB | 3054 | 1/1 | 0.96 | 0.06 | - | 29,29,29,29 | 0 |
| 54 | MG | DB | 3017 | 1/1 | 0.96 | 0.10 | - | 5,5,5,5 | 0 |
| 54 | MG | BB | 3097 | 1/1 | 0.80 | 0.07 | - | 88,88,88,88 | 0 |
| 54 | MG | DB | 3025 | 1/1 | 0.97 | 0.17 | - | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DB | 3053 | 1/1 | 0.92 | 0.09 | - | 80,80,80,80 | 0 |
| 54 | MG | AA | 1619 | 1/1 | 0.64 | 0.25 | - | 180,180,180,180 | 0 |
| 54 | MG | AA | 1655 | 1/1 | 0.95 | 0.06 | - | 54,54,54,54 | 0 |
| 54 | MG | BB | 3039 | 1/1 | 0.97 | 0.07 | - | 5,5,5,5 | 0 |
| 54 | MG | BB | 3064 | 1/1 | 0.98 | 0.08 | - | 37,37,37,37 | 0 |
| 54 | MG | DB | 3049 | 1/1 | 0.98 | 0.07 | - | 9,9,9,9 | 0 |
| 54 | MG | CA | 1619 | 1/1 | 0.70 | 0.19 | - | 70,70,70,70 | 0 |
| 54 | MG | BB | 3075 | 1/1 | 0.97 | 0.16 | - | 29,29,29,29 | 0 |
| 54 | MG | DB | 3057 | 1/1 | 0.80 | 0.10 | - | 77,77,77,77 | 0 |
| 54 | MG | BB | 3017 | 1/1 | 0.93 | 0.17 | - | 73,73,73,73 | 0 |
| 54 | MG | DB | 3040 | 1/1 | 0.98 | 0.09 | - | 18,18,18,18 | 0 |
| 54 | MG | BB | 3007 | 1/1 | 0.98 | 0.07 | - | 53,53,53,53 | 0 |
| 54 | MG | BB | 3072 | 1/1 | 0.90 | 0.14 | - | 79,79,79,79 | 0 |
| 54 | MG | AA | 1604 | 1/1 | 0.98 | 0.09 | - | 19,19,19,19 | 0 |
| 54 | MG | BB | 3015 | 1/1 | 0.99 | 0.08 | - | 42,42,42,42 | 0 |
| 54 | MG | AA | 1652 | 1/1 | 0.97 | 0.08 | - | 90,90,90,90 | 0 |
| 54 | MG | AA | 1642 | 1/1 | 0.97 | 0.12 | - | 41,41,41,41 | 0 |
| 54 | MG | BB | 3053 | 1/1 | 0.89 | 0.07 | - | 79,79,79,79 | 0 |
| 54 | MG | DB | 3071 | 1/1 | 0.98 | 0.05 | - | 37,37,37,37 | 0 |
| 54 | MG | DB | 3065 | 1/1 | 0.97 | 0.06 | - | 45,45,45,45 | 0 |
| 54 | MG | DB | 3020 | 1/1 | 0.94 | 0.20 | - | 13,13,13,13 | 0 |
| 54 | MG | DB | 3011 | 1/1 | 0.97 | 0.27 | - | 33,33,33,33 | 0 |
| 54 | MG | AA | 1648 | 1/1 | 0.95 | 0.07 | - | 40,40,40,40 | 0 |
| 54 | MG | DB | 3086 | 1/1 | 0.98 | 0.20 | - | 52,52,52,52 | 0 |
| 54 | MG | AA | 1605 | 1/1 | 0.97 | 0.09 | - | 47,47,47,47 | 0 |
| 54 | MG | CA | 1621 | 1/1 | 0.92 | 0.53 | - | 110,110,110,110 | 0 |
| 54 | MG | CA | 1608 | 1/1 | 0.96 | 0.09 | - | 139,139,139,139 | 0 |
| 54 | MG | AA | 1634 | 1/1 | 0.97 | 0.07 | - | 67,67,67,67 | 0 |
| 54 | MG | BB | 3080 | 1/1 | 0.79 | 0.20 | - | 77,77,77,77 | 0 |
| 54 | MG | CA | 1646 | 1/1 | 0.91 | 0.08 | - | 99,99,99,99 | 0 |
| 54 | MG | DB | 3045 | 1/1 | 0.92 | 0.07 | - | 68,68,68,68 | 0 |
| 54 | MG | CA | 1637 | 1/1 | 0.98 | 0.07 | - | 92,92,92,92 | 0 |
| 54 | MG | BB | 3054 | 1/1 | 0.96 | 0.14 | - | 46,46,46,46 | 0 |
| 54 | MG | BB | 3004 | 1/1 | 0.93 | 0.19 | - | 73,73,73,73 | 0 |
| 54 | MG | AA | 1608 | 1/1 | 0.49 | 0.29 | - | 147,147,147,147 | 0 |
| 54 | MG | DB | 3104 | 1/1 | 0.96 | 0.19 | - | 71,71,71,71 | 0 |
| 54 | MG | AA | 1657 | 1/1 | 0.75 | 0.42 | - | 124,124,124,124 | 0 |
| 54 | MG | AA | 1627 | 1/1 | 0.79 | 0.19 | - | 68,68,68,68 | 0 |
| 54 | MG | AA | 1660 | 1/1 | 0.94 | 0.08 | - | 37,37,37,37 | 0 |
| 54 | MG | DB | 3031 | 1/1 | 0.98 | 0.07 | - | 24,24,24,24 | 0 |
| 54 | MG | BB | 3006 | 1/1 | 0.99 | 0.08 | - | 20,20,20,20 | 0 |
| 54 | MG | DB | 3064 | 1/1 | 0.92 | 0.10 | - | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 54 | MG | DB | 3091 | 1/1 | 0.99 | 0.14 | - | 5,5,5,5 | 0 |
| 54 | MG | DB | 3067 | 1/1 | 0.97 | 0.13 | - | 16,16,16,16 | 0 |
| 54 | MG | AA | 1631 | 1/1 | 0.94 | 0.12 | - | 88,88,88,88 | 0 |
| 54 | MG | DB | 3018 | 1/1 | 0.97 | 0.10 | - | 22,22,22,22 | 0 |
| 54 | MG | DB | 3081 | 1/1 | 0.95 | 0.11 | - | 19,19,19,19 | 0 |
| 54 | MG | DB | 3106 | 1/1 | 0.94 | 0.18 | - | 64,64,64,64 | 0 |
| 54 | MG | CA | 1622 | 1/1 | 0.98 | 0.10 | - | 18,18,18,18 | 0 |
| 54 | MG | CA | 1610 | 1/1 | 0.96 | 0.07 | - | 75,75,75,75 | 0 |
| 54 | MG | CA | 1620 | 1/1 | 0.93 | 0.14 | - | 37,37,37,37 | 0 |
| 54 | MG | BB | 3024 | 1/1 | 0.95 | 0.06 | - | 44,44,44,44 | 0 |
| 54 | MG | CA | 1615 | 1/1 | 0.93 | 0.09 | - | 180,180,180,180 | 0 |
| 54 | MG | BB | 3047 | 1/1 | 0.96 | 0.13 | - | 116,116,116,116 | 0 |
| 54 | MG | DB | 3050 | 1/1 | 0.97 | 0.14 | - | 123,123,123,123 | 0 |
| 54 | MG | BB | 3014 | 1/1 | 0.96 | 0.13 | - | 58,58,58,58 | 0 |
| 54 | MG | BB | 3084 | 1/1 | 0.98 | 0.20 | - | 77,77,77,77 | 0 |
| 54 | MG | AA | 1623 | 1/1 | 0.83 | 0.66 | - | 73,73,73,73 | 1 |
| 54 | MG | CA | 1631 | 1/1 | 0.98 | 0.10 | - | 40,40,40,40 | 0 |
| 54 | MG | AA | 1614 | 1/1 | 0.71 | 0.11 | - | 113,113,113,113 | 0 |
| 54 | MG | BB | 3091 | 1/1 | 0.97 | 0.10 | - | 37,37,37,37 | 0 |
| 54 | MG | DB | 3052 | 1/1 | 0.91 | 0.24 | - | 113,113,113,113 | 0 |
| 54 | MG | AA | 1647 | 1/1 | 0.55 | 0.99 | - | 180,180,180,180 | 0 |
| 54 | MG | CA | 1628 | 1/1 | 0.94 | 0.07 | - | 44,44,44,44 | 0 |
| 54 | MG | BB | 3068 | 1/1 | 1.00 | 0.05 | - | 61,61,61,61 | 0 |
| 54 | MG | DB | 3032 | 1/1 | 0.96 | 0.09 | - | 51,51,51,51 | 0 |
| 54 | MG | BB | 3099 | 1/1 | 0.95 | 0.15 | - | 56,56,56,56 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.