



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 02:53 pm BST

PDB ID : 4V54
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with 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 : 2007-06-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

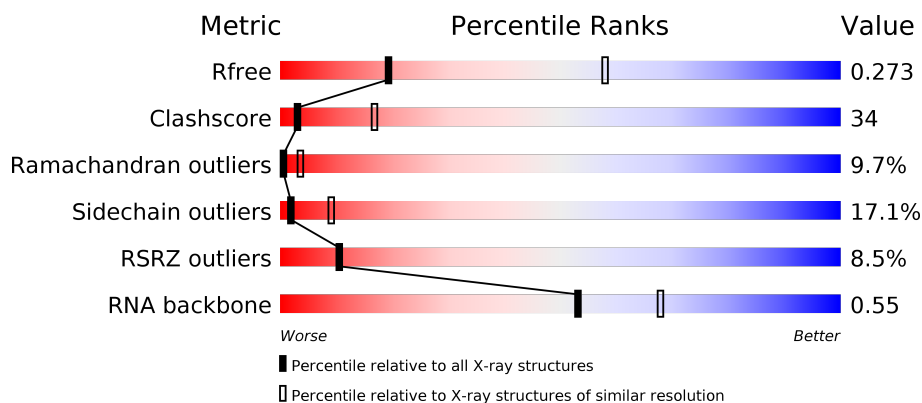
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1149 (3.34-3.26) |
| Clashscore | 141614 | 1205 (3.34-3.26) |
| Ramachandran outliers | 138981 | 1183 (3.34-3.26) |
| Sidechain outliers | 138945 | 1182 (3.34-3.26) |
| RSRZ outliers | 127900 | 1115 (3.34-3.26) |
| RNA backbone | 3102 | 1117 (3.70-2.90) |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>27%</div> <div>60%</div> <div>13%</div> <div>•</div> </div> |
| 1 | CA | 1542 | <div> <div>26%</div> <div>61%</div> <div>12%</div> <div>••</div> </div> |
| 2 | AC | 232 | <div> <div>3%</div> <div>30%</div> <div>47%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> |
| 2 | CC | 232 | <div> <div>2%</div> <div>31%</div> <div>45%</div> <div>12%</div> <div>•</div> <div>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 | AA | 2025 | - | - | - | X |
| 54 | MG | AA | 2037 | - | - | - | X |
| 54 | MG | AA | 2059 | - | - | - | X |
| 54 | MG | BB | 3093 | - | - | - | X |
| 54 | MG | BB | 3100 | - | - | - | X |
| 54 | MG | DB | 3058 | - | - | - | X |

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286960 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 |
| | | | 1022 | 634 | 206 | 179 | 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 ribosome recycling factor.

| 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 ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 55 | B4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 55 | D4 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 56 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | AA | 289 | Total | O | 0 | 0 |
| | | | 289 | 289 | | |
| 56 | AE | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | AK | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | AL | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | AN | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | AP | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

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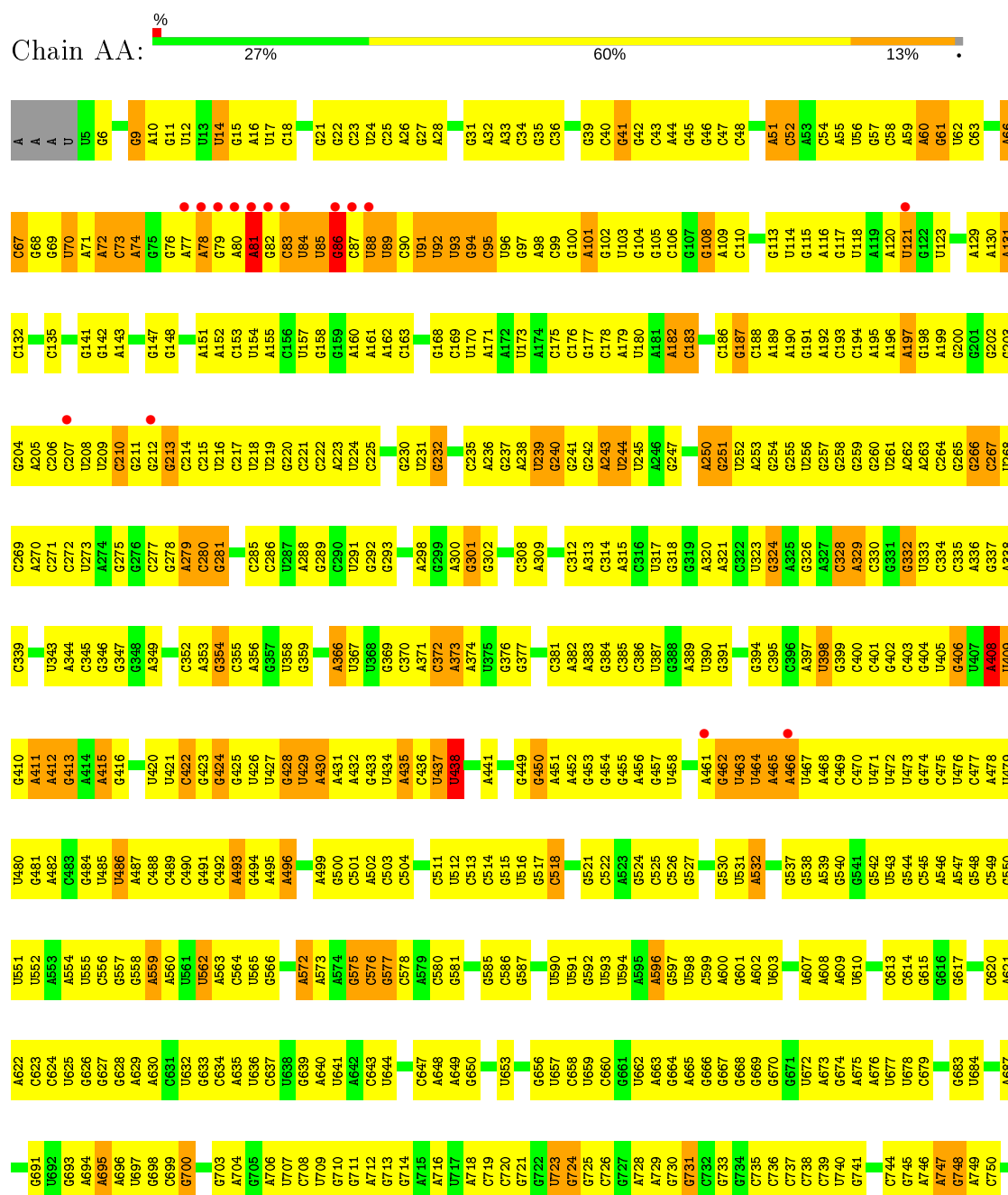
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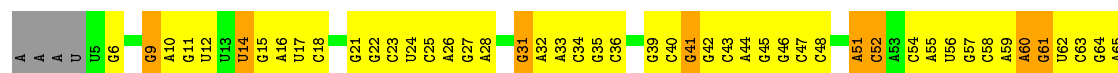
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 56 | AT | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | BB | 495 | Total 495 | O 495 | 0 | 0 |
| 56 | BC | 4 | Total 4 | O 4 | 0 | 0 |
| 56 | BD | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | BE | 3 | Total 3 | O 3 | 0 | 0 |
| 56 | B2 | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | BL | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | BT | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CE | 2 | Total 2 | O 2 | 0 | 0 |
| 56 | CK | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CL | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CN | 4 | Total 4 | O 4 | 0 | 0 |
| 56 | CT | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | CA | 300 | Total 300 | O 300 | 0 | 0 |
| 56 | DB | 505 | Total 505 | O 505 | 0 | 0 |
| 56 | DC | 4 | Total 4 | O 4 | 0 | 0 |
| 56 | DD | 1 | Total 1 | O 1 | 0 | 0 |
| 56 | DE | 2 | Total 2 | O 2 | 0 | 0 |

3 Residue-property plots

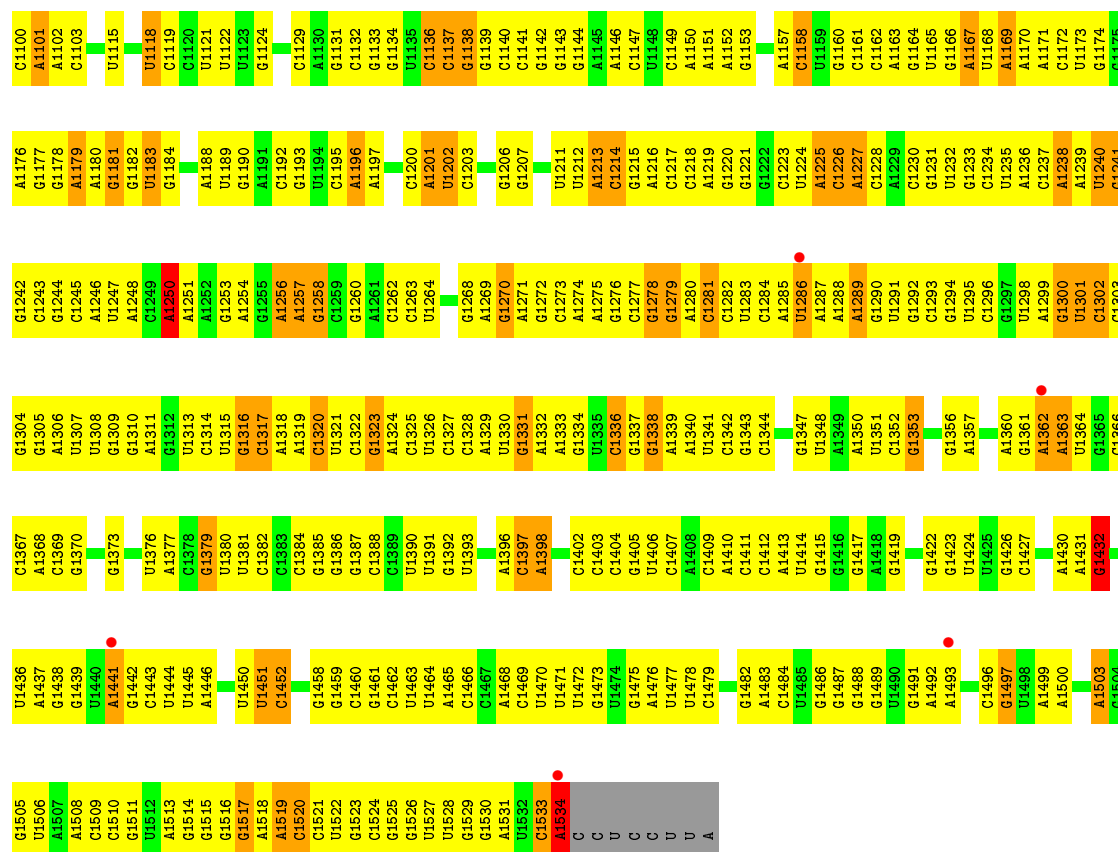
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

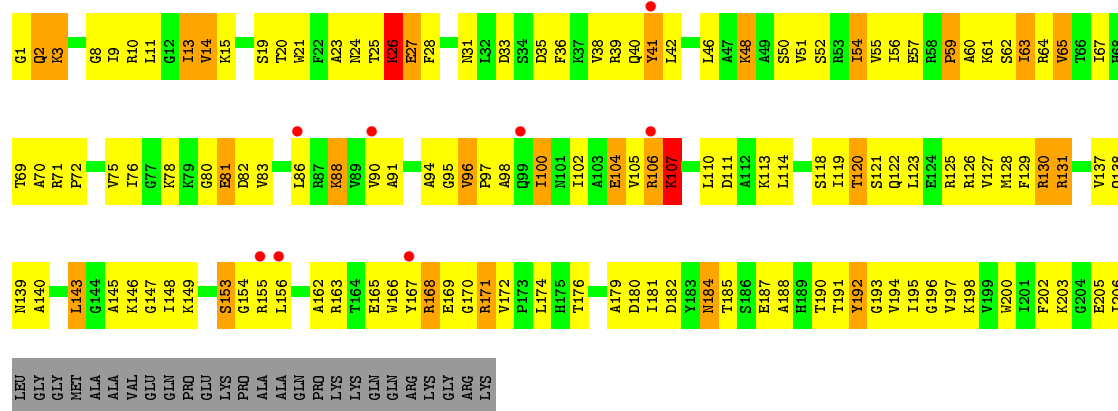


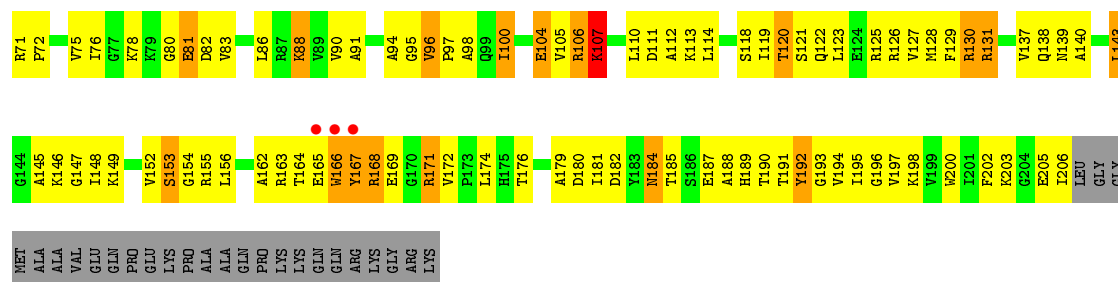


| | | | | | | | | | | | | |
|-------|------|------|------|------|------|------|------|------|------|------|------|------|
| A1036 | G976 | G830 | G683 | G617 | G548 | U476 | G406 | A336 | G266 | G202 | A130 | G69 |
| C1037 | A977 | A831 | U684 | G620 | C549 | C477 | U407 | G337 | C267 | G203 | A131 | U70 |
| G1038 | A978 | G832 | A687 | G621 | G550 | A478 | A403 | A338 | U268 | G204 | C132 | A71 |
| G1039 | C979 | G833 | G687 | A621 | U551 | U479 | U409 | C339 | C269 | A205 | C135 | A72 |
| U1040 | C980 | U834 | G755 | G622 | U552 | U480 | A410 | C340 | C270 | C206 | G141 | C73 |
| G1041 | A981 | U835 | G756 | A623 | A553 | G481 | A411 | U343 | A271 | C207 | G142 | A74 |
| A1042 | U982 | G836 | G757 | G624 | A554 | A482 | A412 | A344 | C272 | U208 | A143 | G75 |
| G1043 | A983 | U837 | G758 | G625 | U555 | C483 | G413 | G345 | U273 | U209 | G143 | G76 |
| A1044 | A984 | G838 | A695 | G626 | C556 | U485 | A414 | G346 | A274 | C210 | G147 | A77 |
| C1045 | U916 | C839 | A696 | G627 | G557 | U486 | A415 | A349 | G275 | G211 | G148 | A78 |
| C1046 | A917 | C840 | U697 | G628 | G558 | A487 | A416 | C352 | G276 | G212 | G149 | A79 |
| G1047 | A918 | C841 | U698 | A629 | A559 | A488 | U420 | A353 | C277 | G213 | A151 | A80 |
| G1048 | U920 | U842 | C699 | A630 | A560 | C489 | U421 | A354 | A279 | C214 | A152 | A81 |
| U1049 | U921 | U843 | G700 | G631 | U561 | C490 | U422 | C355 | C280 | C215 | A153 | A82 |
| G1050 | G922 | G844 | G703 | U632 | U562 | C491 | C423 | C356 | C281 | U216 | C153 | C83 |
| C1051 | A923 | A845 | A704 | G633 | A563 | G491 | C424 | C357 | G289 | A223 | U154 | U84 |
| U1052 | C924 | G846 | G705 | C634 | C564 | C492 | G425 | A356 | C290 | U224 | U155 | U85 |
| G993 | G925 | G847 | G706 | A635 | U565 | A493 | U426 | G357 | C285 | G220 | C156 | G86 |
| A994 | G926 | C848 | U707 | U636 | G566 | C494 | U427 | U358 | C286 | C221 | U157 | C87 |
| C995 | G927 | G849 | U708 | C637 | A572 | A496 | G428 | G359 | U287 | C222 | U158 | U88 |
| A996 | G928 | G850 | G709 | U638 | A573 | C497 | U429 | A363 | A288 | A223 | G159 | U89 |
| U997 | G929 | G852 | U710 | G639 | A574 | G500 | A430 | A364 | C289 | A224 | A160 | C90 |
| C998 | C930 | C853 | G711 | A640 | G575 | C501 | A431 | U365 | C291 | C225 | A161 | U91 |
| A1000 | C931 | C854 | A712 | U641 | C576 | A502 | A432 | C366 | U291 | G225 | A162 | U92 |
| C1001 | C934 | C857 | G713 | C643 | G577 | C503 | G433 | U367 | G292 | G230 | U163 | U93 |
| G1002 | A935 | G858 | G714 | U644 | C578 | C504 | U434 | C370 | A298 | U231 | C168 | C95 |
| G1003 | A936 | G859 | A715 | G645 | A579 | C511 | U435 | C371 | G299 | G232 | G169 | U96 |
| U1004 | G939 | A860 | A716 | C647 | A580 | U512 | C436 | A372 | A300 | C233 | C170 | G97 |
| C1005 | C940 | G861 | U717 | A648 | G581 | U513 | U437 | C373 | G301 | C234 | G177 | U103 |
| A1006 | G941 | C862 | A718 | A649 | G582 | C514 | U438 | A374 | G302 | C235 | C178 | G104 |
| U1007 | G942 | U863 | C719 | G650 | G585 | C515 | U439 | A303 | A303 | A236 | A172 | C99 |
| U1008 | A946 | A864 | C720 | U653 | C586 | G516 | G441 | U375 | G237 | G237 | U173 | G100 |
| G947 | G947 | A865 | G721 | U654 | G587 | U517 | G442 | C376 | A308 | A238 | A174 | A101 |
| U1009 | C948 | C866 | G722 | G656 | C518 | C518 | G443 | G377 | C309 | U239 | C175 | G102 |
| C1010 | A949 | G867 | U723 | U657 | U591 | A451 | A451 | C381 | G312 | G241 | G176 | U103 |
| U1011 | C950 | G868 | G724 | U658 | G592 | A452 | A452 | A382 | A313 | G242 | C178 | G105 |
| A1012 | U950 | C869 | G725 | C658 | G593 | A453 | G454 | A383 | C314 | A243 | U180 | C106 |
| G1013 | G951 | G869 | G726 | U659 | U594 | G454 | A455 | G384 | A315 | U244 | A181 | G108 |
| U1014 | G952 | U875 | G727 | C660 | U595 | G455 | A456 | C385 | C316 | U245 | A182 | A109 |
| G1015 | U955 | C876 | A728 | U662 | A596 | C525 | A457 | C386 | U317 | A246 | C183 | C110 |
| U956 | U956 | G877 | U729 | A663 | A597 | C526 | G457 | U387 | G318 | G247 | C186 | G113 |
| U957 | U957 | A878 | G730 | G664 | U598 | G527 | U458 | G388 | C319 | G247 | C187 | U114 |
| A958 | A958 | A879 | G731 | G665 | C599 | G530 | A461 | A389 | A320 | A250 | C188 | G115 |
| U959 | A959 | C882 | C732 | A666 | A600 | U531 | A462 | U390 | A321 | G251 | C189 | A116 |
| U960 | U960 | C883 | G733 | G667 | G601 | A532 | A463 | G391 | C322 | U252 | A190 | G117 |
| A1022 | U961 | U884 | A816 | G667 | A602 | A532 | U464 | G392 | U323 | G254 | G191 | U118 |
| U1023 | C962 | G885 | C735 | G668 | U603 | A532 | U465 | G393 | G324 | G255 | A192 | A119 |
| G1024 | G963 | G886 | G736 | G669 | U604 | A532 | A466 | G394 | A325 | U256 | C193 | A120 |
| A964 | A964 | A892 | C737 | G670 | U605 | G537 | A467 | C395 | G326 | G257 | A194 | G122 |
| U1025 | U965 | A893 | A818 | G671 | A607 | U538 | A468 | C396 | A327 | C258 | A195 | U123 |
| G1026 | U966 | C893 | G739 | U672 | A608 | A539 | U469 | C397 | A328 | G259 | A196 | C124 |
| C1027 | C967 | G894 | U740 | A673 | A609 | G540 | A469 | U398 | A329 | C330 | A197 | U125 |
| U1028 | A968 | U895 | G741 | G674 | U610 | G541 | C469 | C399 | A330 | U261 | G198 | G126 |
| U1029 | U969 | A901 | C823 | A675 | G511 | G542 | C470 | C400 | C331 | A262 | A199 | G200 |
| C1030 | A970 | G902 | A825 | A676 | C512 | U543 | U471 | C401 | G332 | A263 | G201 | A129 |
| U1031 | A971 | G903 | A826 | U677 | C513 | G544 | U472 | C402 | U333 | G264 | | |
| G1032 | C972 | G904 | G745 | U678 | C514 | G545 | U473 | G403 | U334 | A265 | | |
| C1033 | A973 | U904 | A746 | C679 | C515 | A546 | G474 | C404 | C335 | | | |
| G1034 | A974 | U905 | A747 | U679 | G516 | A547 | C475 | U405 | | | | |
| U1035 | A975 | A906 | G748 | | G616 | | | | | | | |

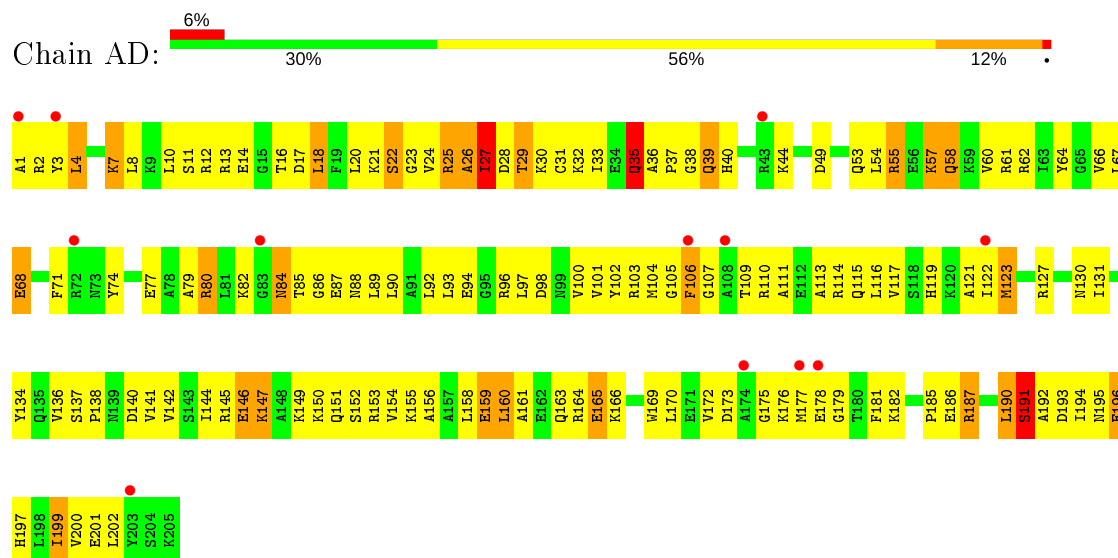


• Molecule 2: 30S ribosomal protein S3

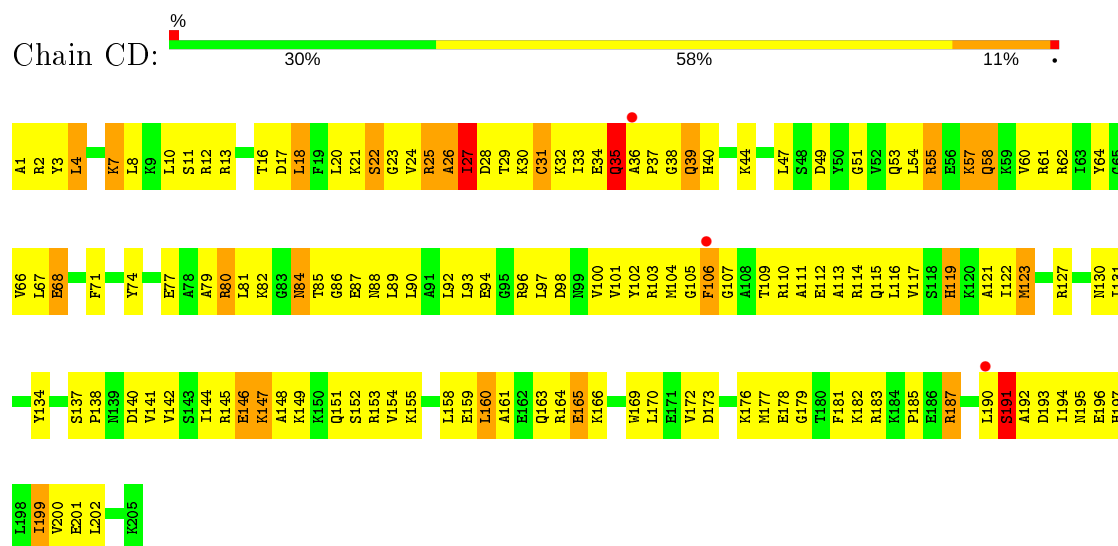




• Molecule 3: 30S ribosomal protein S4

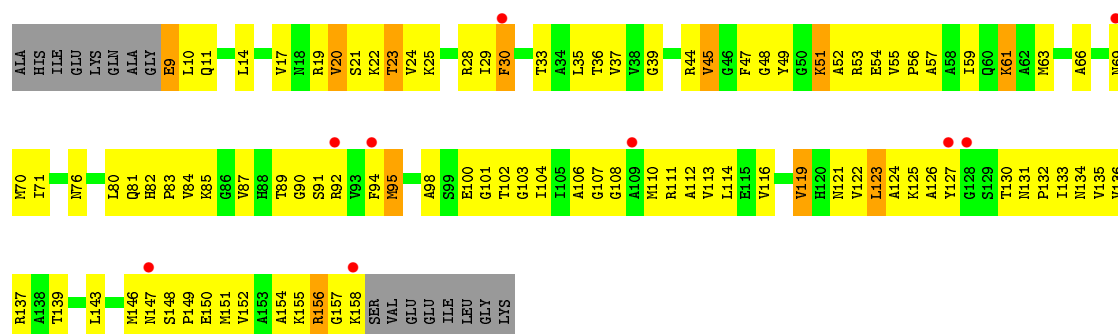


• Molecule 3: 30S ribosomal protein S4

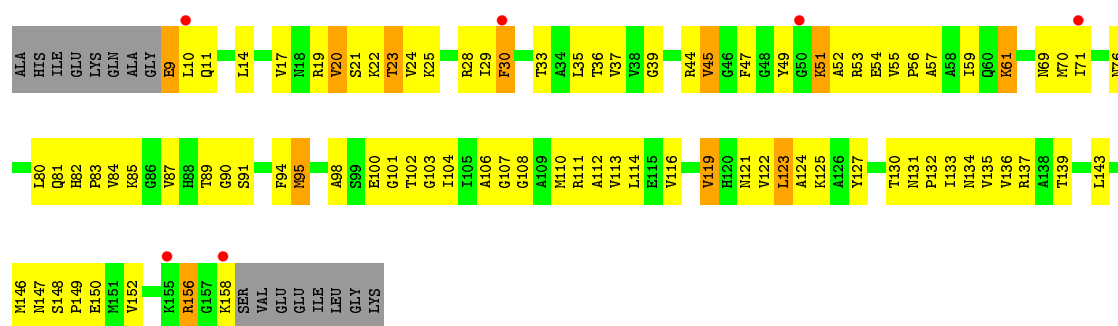


• Molecule 4: 30S ribosomal protein S5

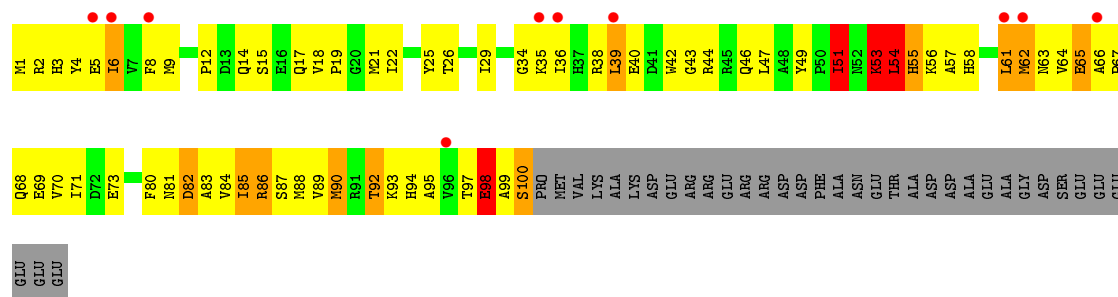
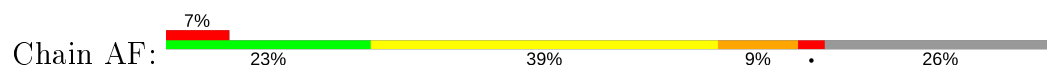




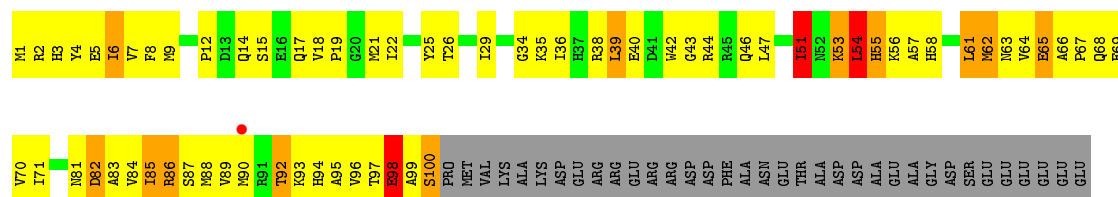
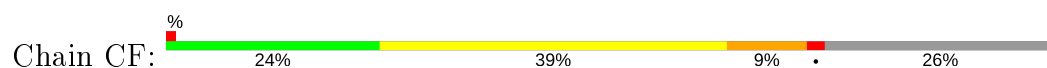
• Molecule 4: 30S ribosomal protein S5



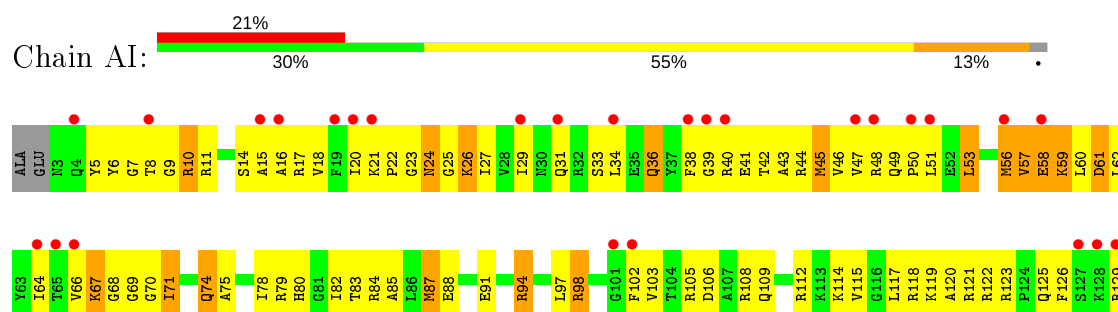
• Molecule 5: 30S ribosomal protein S6



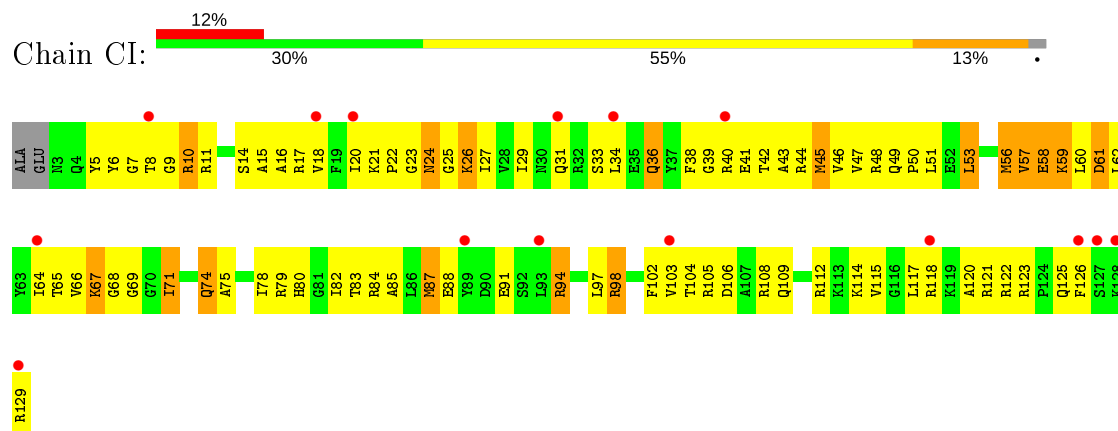
• Molecule 5: 30S ribosomal protein S6



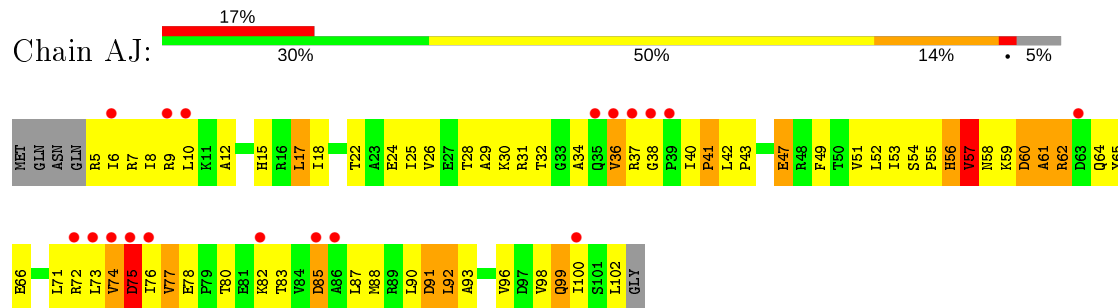
• Molecule 6: 30S ribosomal protein S7



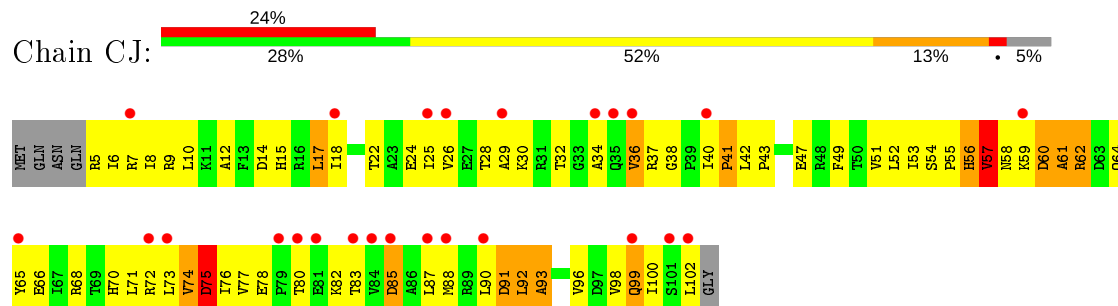
- Molecule 8: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S10



- Molecule 9: 30S ribosomal protein S10



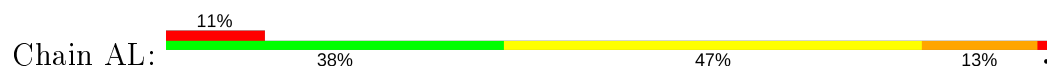
- Molecule 10: 30S ribosomal protein S11



- Molecule 10: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S12



- Molecule 11: 30S ribosomal protein S12

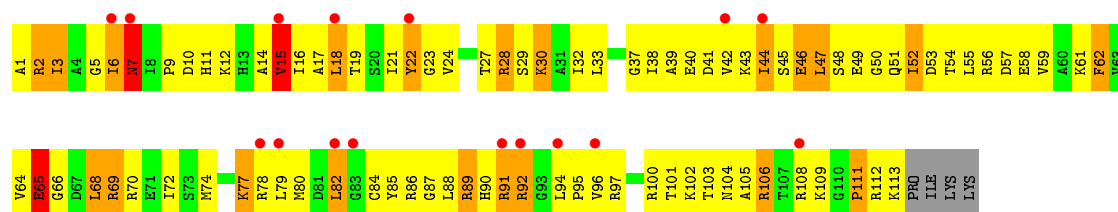


- Molecule 12: 30S ribosomal protein S13



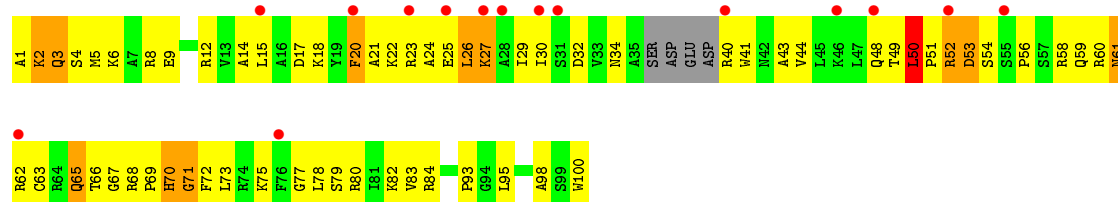
- Molecule 12: 30S ribosomal protein S13

Chain CM: 



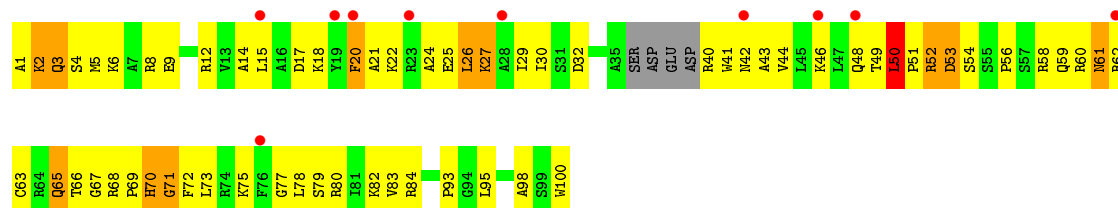
- Molecule 13: 30S ribosomal protein S14

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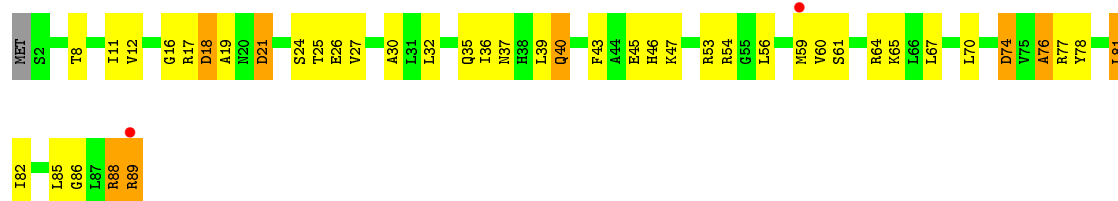
- Molecule 13: 30S ribosomal protein S14

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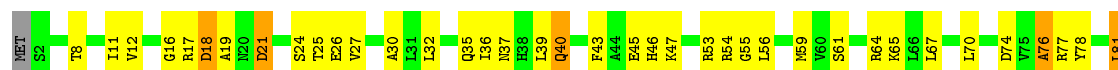
- Molecule 14: 30S ribosomal protein S15

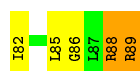
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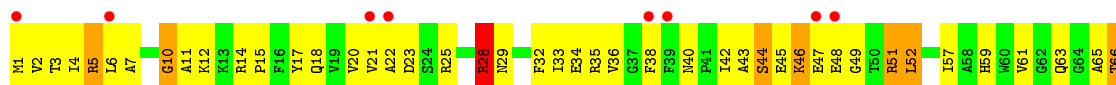
- Molecule 14: 30S ribosomal protein S15

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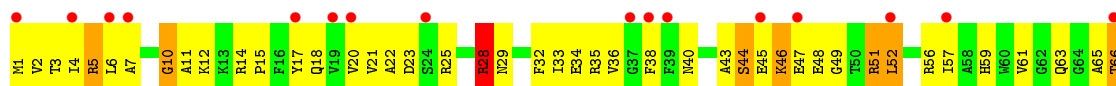




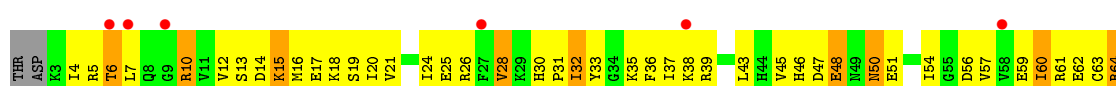
- Molecule 15: 30S ribosomal protein S16



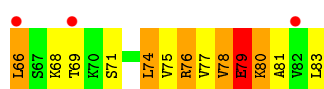
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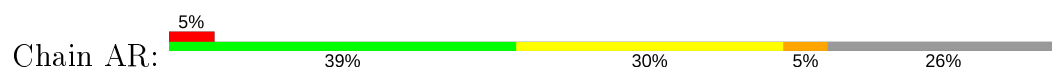
- Molecule 16: 30S ribosomal protein S17

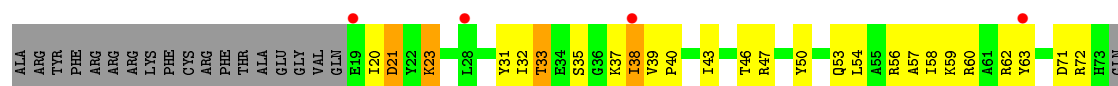


- Molecule 16: 30S ribosomal protein S17

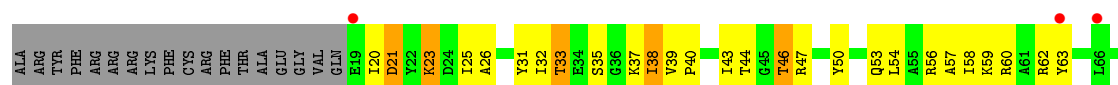


- Molecule 17: 30S ribosomal protein S18

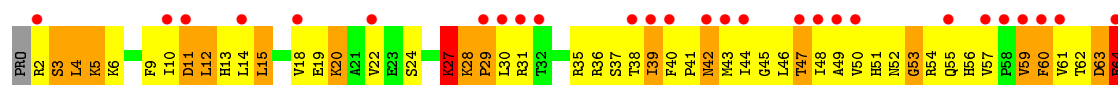
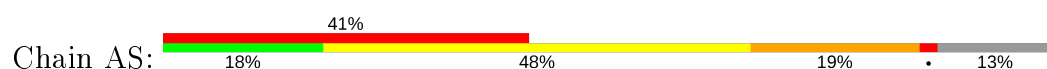




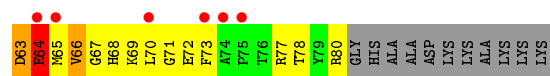
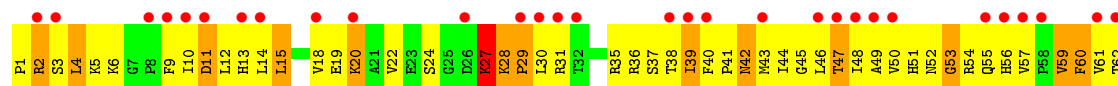
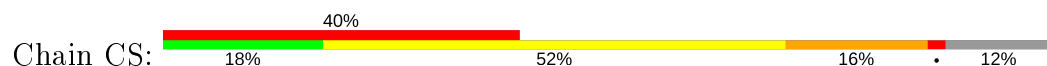
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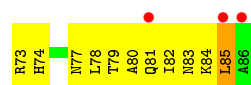
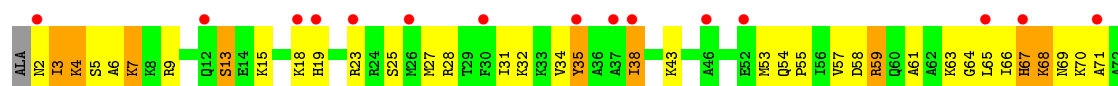
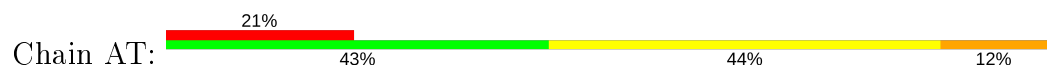
- Molecule 18: 30S ribosomal protein S19



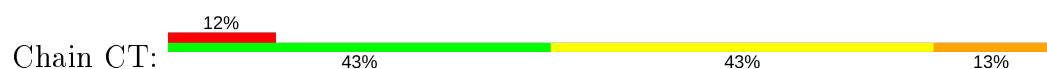
- Molecule 18: 30S ribosomal protein S19

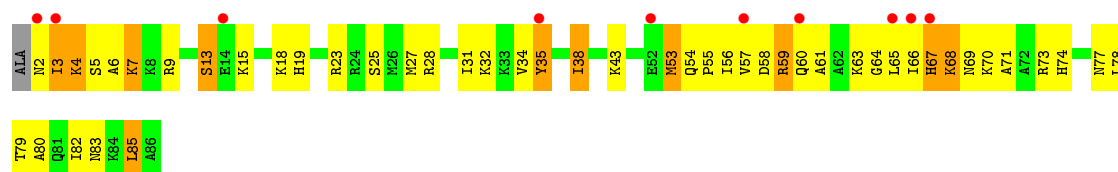


- Molecule 19: 30S ribosomal protein S20

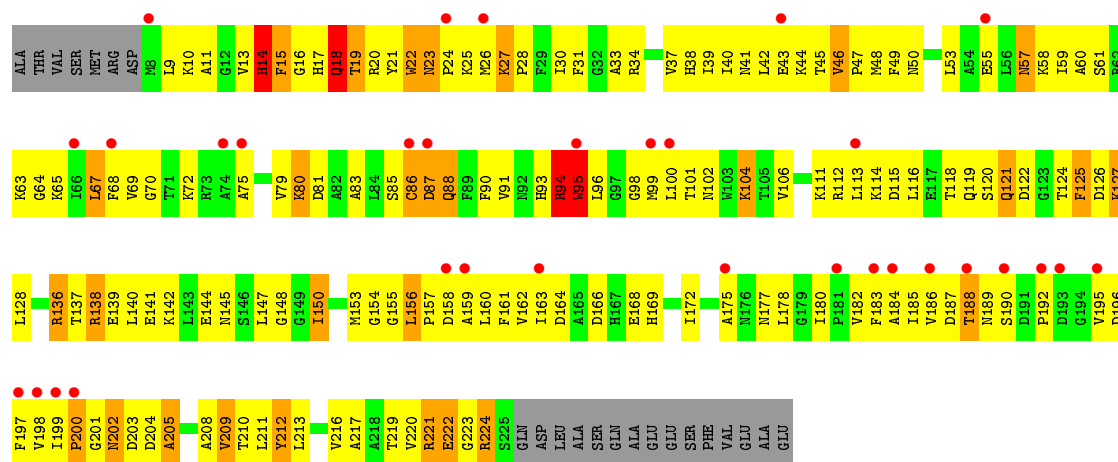


- Molecule 19: 30S ribosomal protein S20

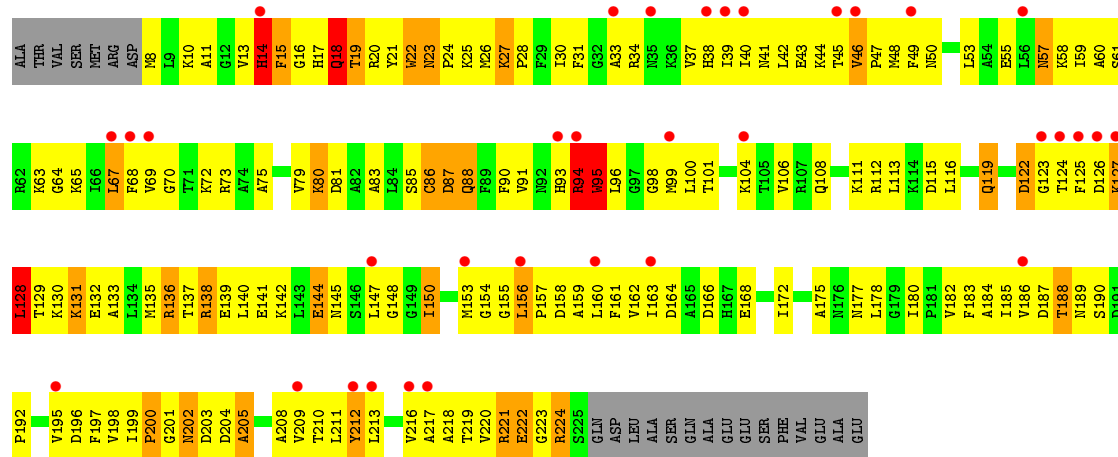




• Molecule 20: 30S ribosomal protein S2



• Molecule 20: 30S ribosomal protein S2

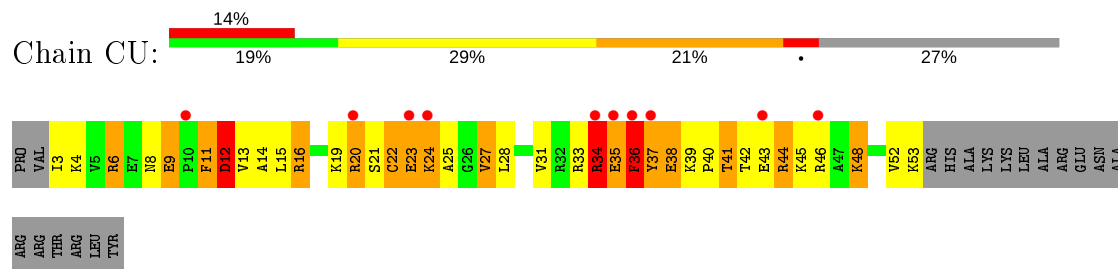


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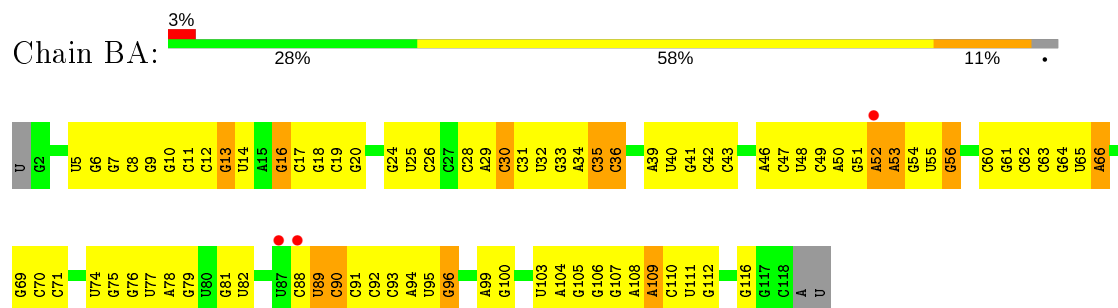


ALA
ARG
ARG
THR
ARG
LEU
TYR

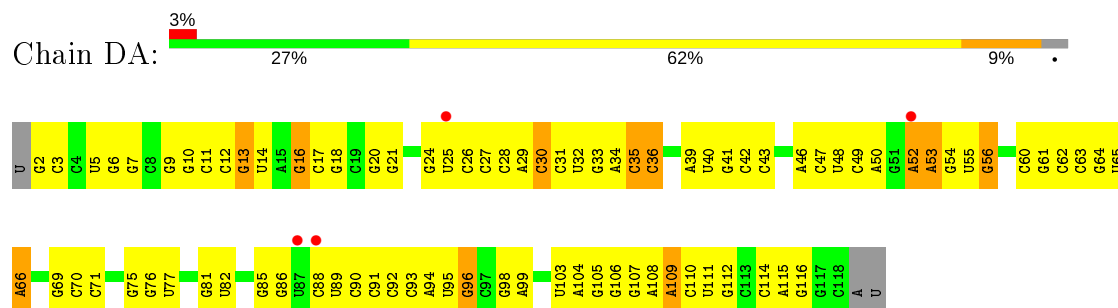
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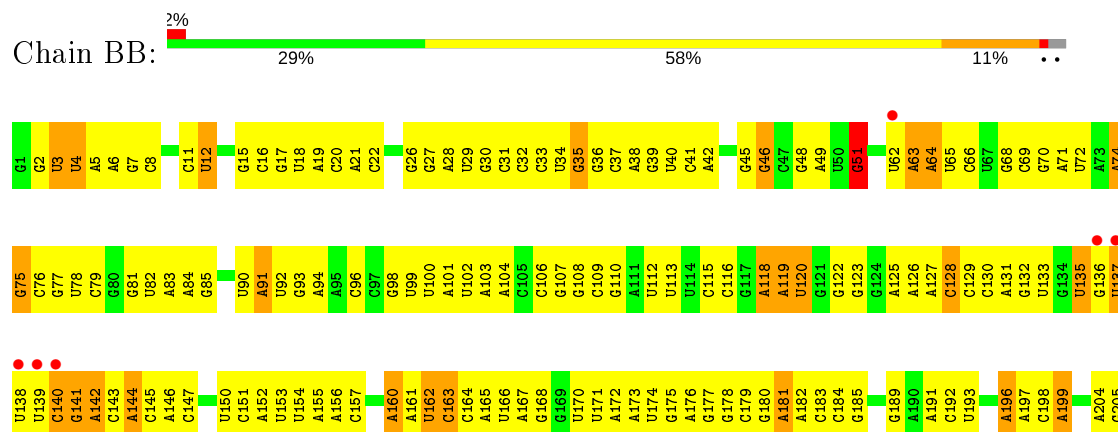
- Molecule 22: 5S rRNA



- Molecule 22: 5S rRNA



- Molecule 23: 23S rRNA



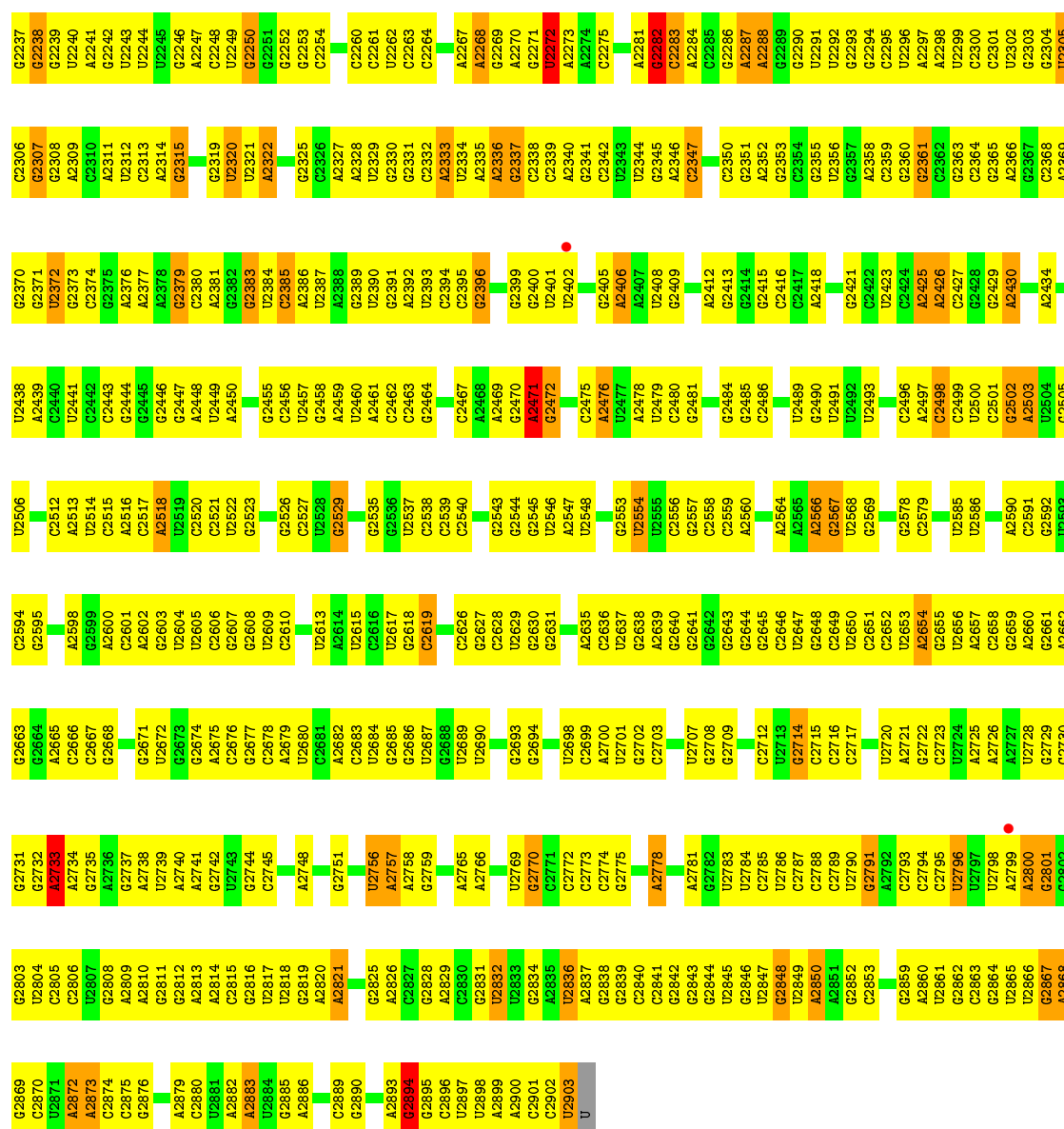
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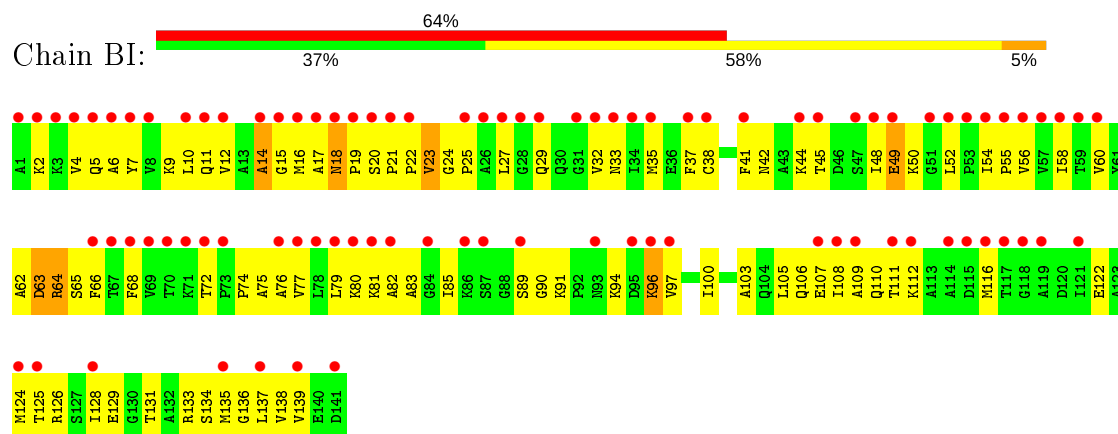
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------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| G2237 | G2238 | G2239 | U2240 | G2241 | G2242 | U2243 | U2244 | G2245 | G2246 | A2247 | U2248 | U2249 | G2250 | G2251 | G2254 | G2260 | G2261 | U2262 | G2263 | G2264 | U2265 | A2266 | A2267 | A2268 | G2269 | A2270 | G2271 | U2272 | G2275 | A2281 | G2282 | G2283 | A2284 | G2285 | A2287 | A2288 | G2289 | G2290 | U2291 | U2292 | G2293 | G2294 | G2295 | G2296 | A2297 | A2298 | U2299 | G2300 | G2301 | U2302 | G2303 | U2304 | G2306 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2307 | G2308 | G2309 | G2310 | G2311 | U2312 | G2313 | G2314 | G2315 | G2319 | U2320 | U2321 | A2322 | G2325 | G2326 | G2327 | U2328 | U2329 | G2330 | G2331 | G2332 | G2333 | U2334 | A2335 | A2336 | G2337 | U2401 | U2402 | G2405 | A2406 | A2407 | U2408 | G2409 | A2412 | G2413 | G2414 | C2415 | C2416 | U2419 | C2420 | U2423 | C2424 | G2425 | A2426 | C2427 | G2428 | G2429 | A2430 | A2434 | U2438 | A2439 | C2440 | U2441 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2443 | G2444 | G2445 | G2446 | G2447 | A2448 | U2449 | A2450 | G2455 | G2456 | U2457 | G2458 | U2459 | A2461 | C2462 | C2463 | G2464 | A2471 | G2472 | C2475 | A2476 | U2477 | A2478 | U2479 | C2480 | G2481 | C2483 | C2484 | G2485 | C2486 | U2489 | G2490 | U2491 | G2496 | A2497 | C2498 | C2499 | U2500 | U2501 | G2502 | A2503 | U2504 | G2505 | U2506 | C2512 | A2513 | U2514 | G2515 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A2516 | G2517 | A2518 | G2519 | G2520 | G2521 | U2522 | G2523 | G2526 | G2527 | U2528 | G2529 | A2530 | A2531 | G2532 | G2535 | G2536 | U2537 | G2538 | U2543 | G2544 | U2546 | A2547 | U2548 | G2553 | U2554 | G2555 | G2556 | G2557 | C2558 | A2564 | A2565 | A2566 | G2567 | U2568 | G2569 | G2578 | G2579 | U2585 | U2586 | A2590 | C2591 | G2592 | U2593 | G2594 | G2595 | A2598 | G2599 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A2600 | G2601 | A2602 | G2603 | U2604 | G2605 | G2606 | G2607 | U2608 | U2609 | G2610 | U2613 | A2614 | U2615 | U2616 | U2617 | G2618 | C2619 | C2626 | G2627 | G2628 | U2629 | G2630 | G2631 | A2635 | G2636 | U2637 | G2638 | A2639 | G2640 | G2642 | G2643 | G2644 | G2645 | U2646 | G2647 | G2648 | C2649 | U2650 | C2651 | G2652 | U2653 | A2654 | A2657 | A2660 | G2661 | U2662 | G2663 | G2664 | A2665 | G2666 | C2667 | G2668 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2671 | U2672 | G2673 | G2674 | U2675 | G2676 | G2677 | G2678 | U2679 | U2680 | G2681 | G2682 | C2683 | U2684 | G2685 | U2686 | U2687 | G2688 | U2689 | U2698 | G2699 | A2700 | U2701 | G2702 | C2703 | U2707 | G2708 | G2709 | U2712 | U2713 | G2714 | G2715 | C2716 | G2717 | G2718 | G2719 | U2720 | A2721 | G2722 | C2723 | U2724 | A2725 | A2726 | U2727 | U2728 | G2729 | C2730 | G2731 | A2732 | U2733 | A2734 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2735 | A2736 | G2737 | A2738 | U2739 | A2740 | G2741 | G2742 | U2743 | G2744 | C2745 | U2746 | G2747 | A2748 | A2749 | A2750 | G2751 | C2752 | A2753 | U2754 | C2755 | U2756 | A2757 | A2758 | G2759 | C2760 | A2761 | A2765 | U2769 | G2770 | G2771 | C2772 | C2773 | C2774 | G2775 | A2778 | A2781 | G2782 | U2783 | U2784 | C2785 | U2786 | C2787 | C2788 | C2789 | U2790 | G2791 | A2792 | C2793 | C2794 | G2795 | U2796 | U2797 | U2798 | A2800 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2801 | G2802 | U2803 | U2804 | C2805 | G2806 | U2807 | G2808 | A2809 | U2810 | G2811 | G2812 | A2813 | A2814 | G2815 | G2816 | G2819 | A2820 | A2821 | G2822 | A2823 | G2824 | G2825 | A2826 | G2827 | G2828 | A2829 | G2830 | G2831 | U2832 | U2833 | G2834 | A2835 | U2836 | A2837 | G2838 | G2839 | C2840 | C2841 | G2842 | G2843 | U2844 | U2845 | G2846 | U2847 | U2848 | U2849 | A2850 | A2851 | G2852 | G2853 | G2854 | G2855 | A2856 | G2859 | A2860 | U2861 | G2862 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| C2863 | G2864 | U2865 | U2866 | G2867 | A2868 | G2869 | U2870 | G2871 | U2872 | A2873 | G2874 | C2875 | G2876 | A2879 | C2880 | U2881 | A2882 | A2883 | U2884 | G2885 | A2886 | A2887 | G2888 | G2889 | A2893 | G2894 | G2895 | C2896 | U2897 | U2898 | A2899 | A2900 | C2901 | C2902 | U2903 | U | G2904 | G2905 | G2906 | G2907 | G2908 | G2909 | G2910 | G2911 | G2912 | G2913 | G2914 | G2915 | G2916 | G2917 | G2918 | G2919 | G2920 | G2921 | G2922 | G2923 | G2924 | G2925 | G2926 | G2927 | G2928 | G2929 | G2930 | G2931 | G2932 | G2933 | G2934 | G2935 | G2936 | G2937 | G2938 | G2939 | G2940 | G2941 | G2942 | G2943 | G2944 | G2945 | G2946 | G2947 | G2948 | G2949 | G2950 | G2951 | G2952 | G2953 | G2954 | G2955 | G2956 | G2957 | G2958 | G2959 | G2960 | G2961 | G2962 | G2963 | G2964 | G2965 | G2966 | G2967 | G2968 | G2969 | G2970 | G2971 | G2972 | G2973 | G2974 | G2975 | G2976 | G2977 | G2978 | G2979 | G2980 | G2981 | G2982 | G2983 | G2984 | G2985 | G2986 | G2987 | G2988 | G2989 | G2990 | G2991 | 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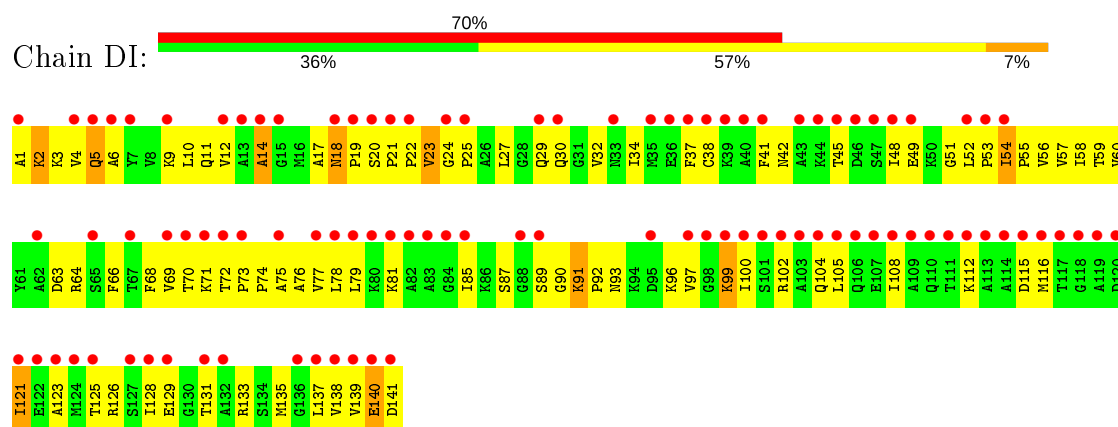




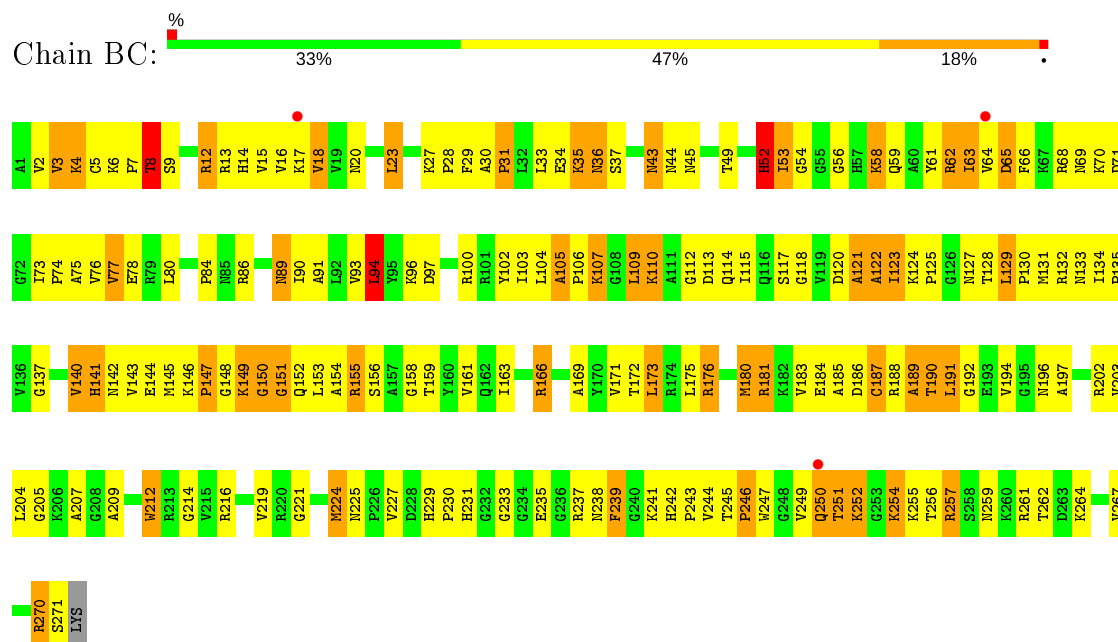
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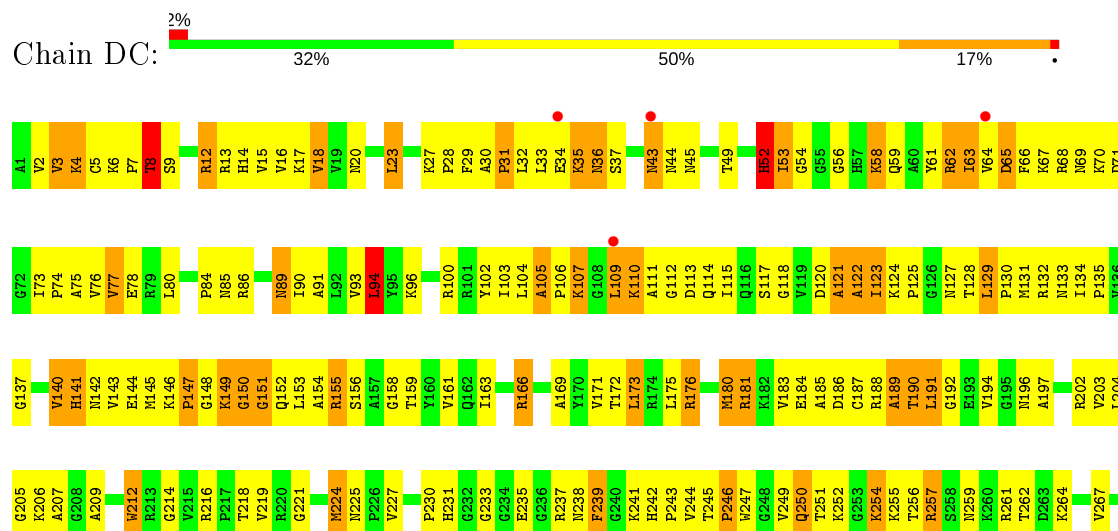
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• Molecule 25: 50S ribosomal protein L2

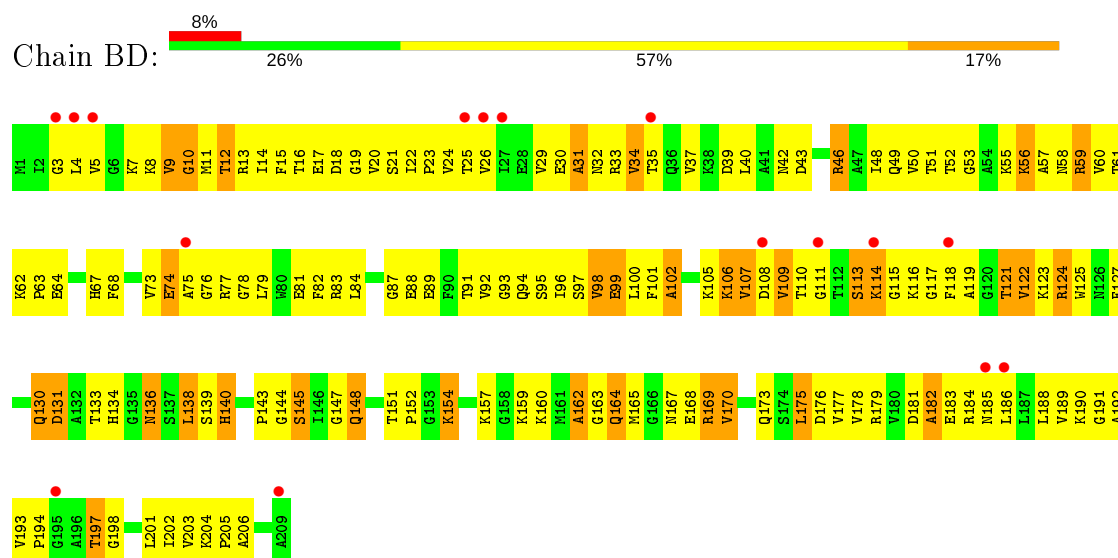


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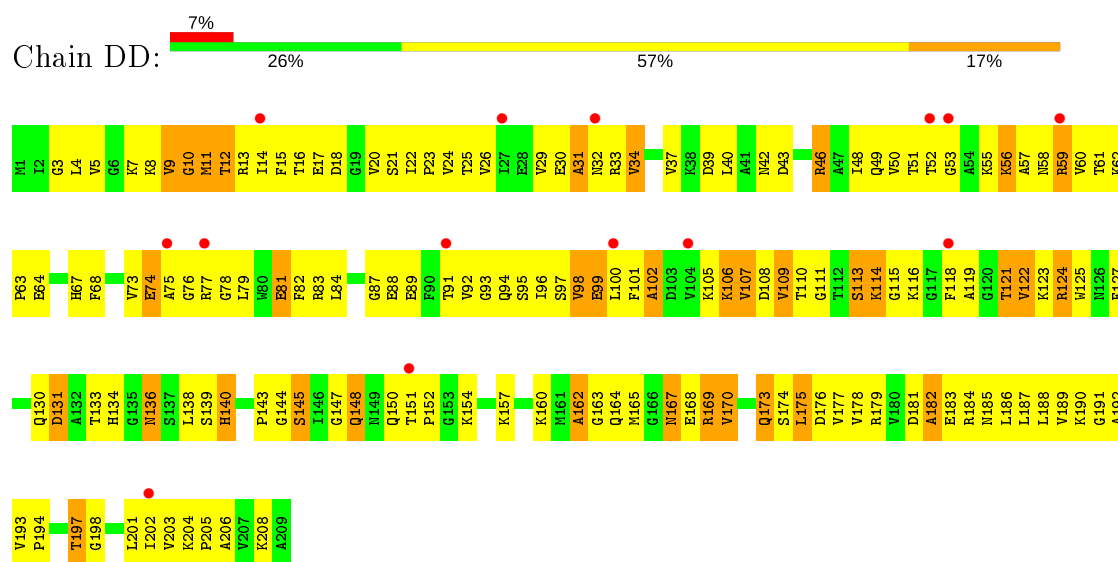




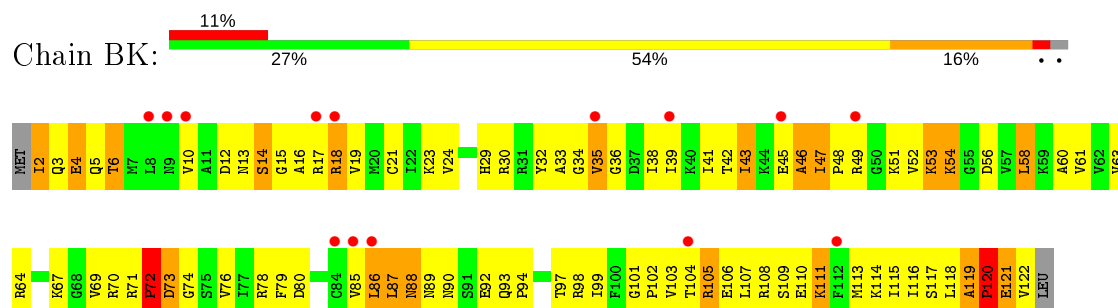
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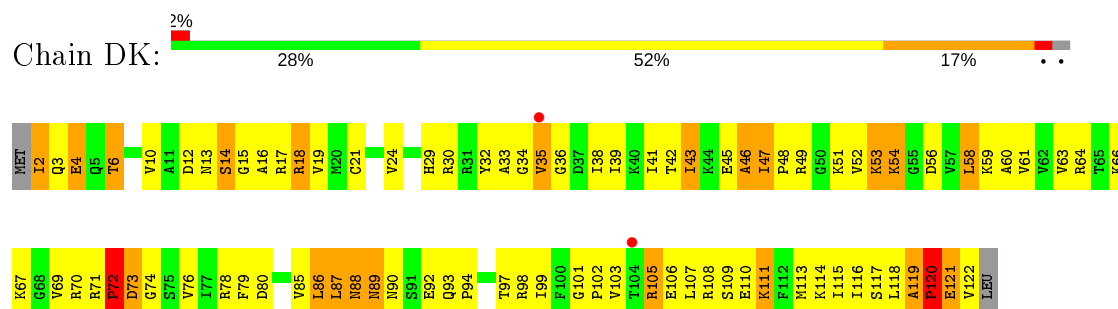
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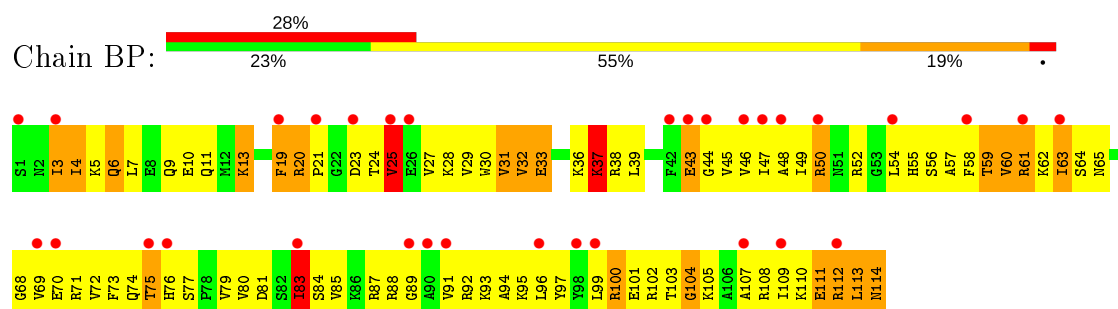
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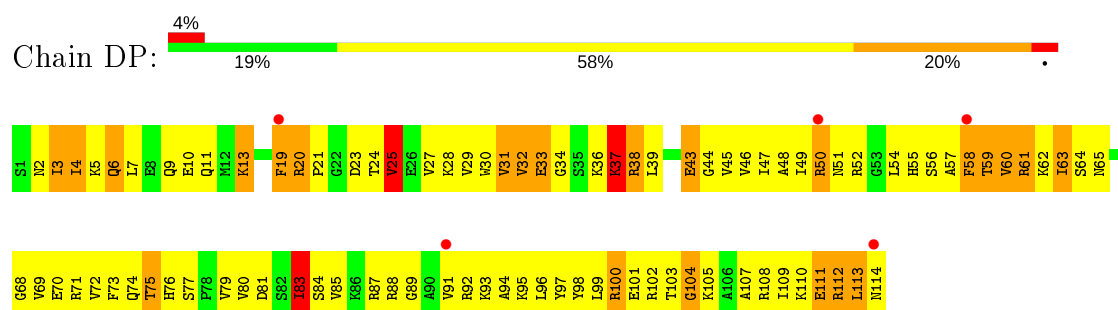
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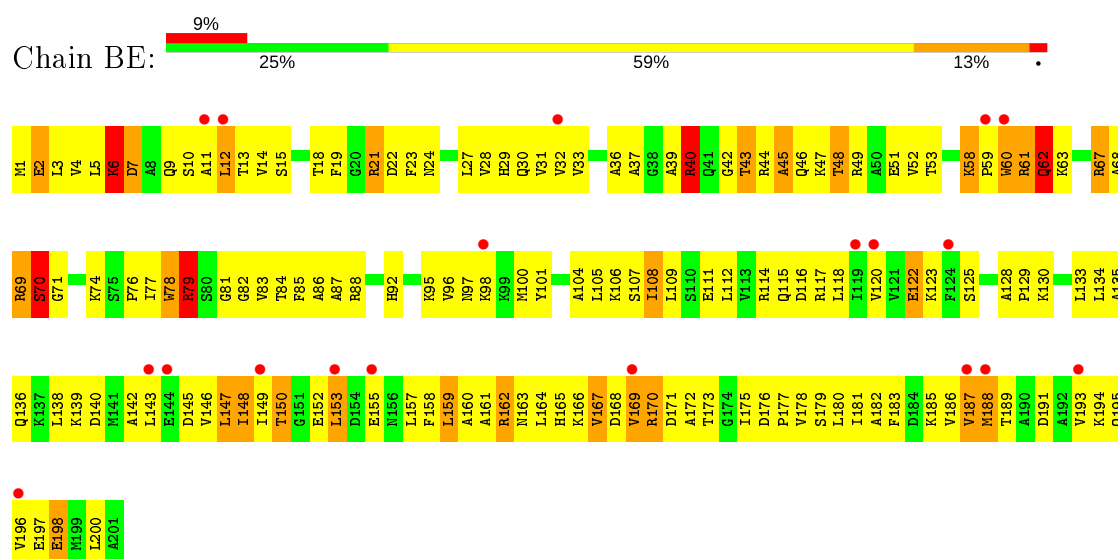
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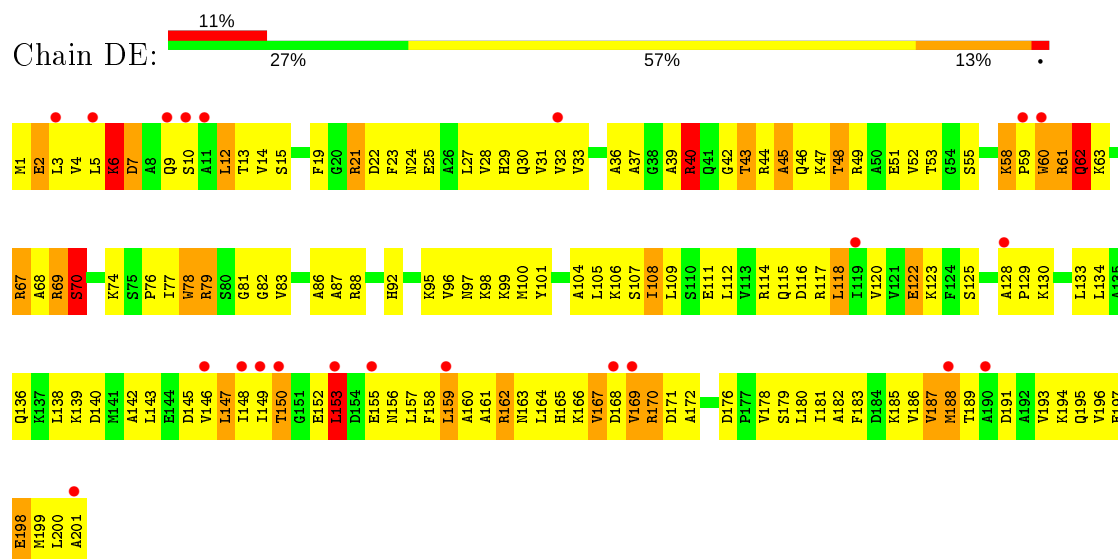
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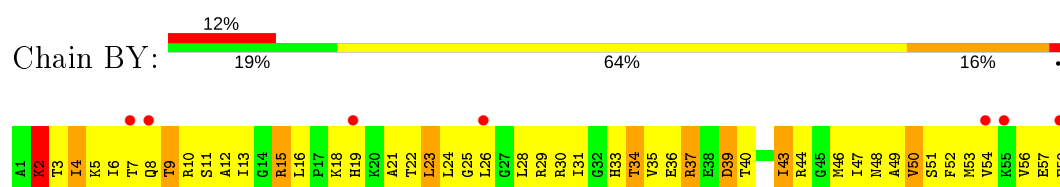
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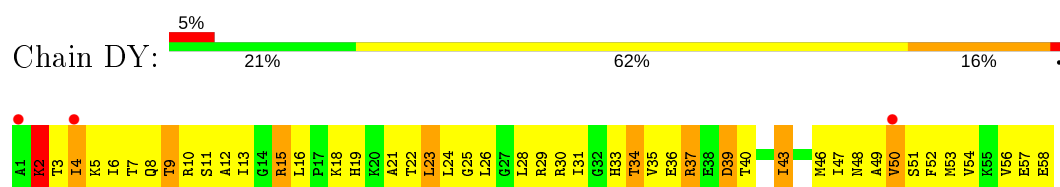
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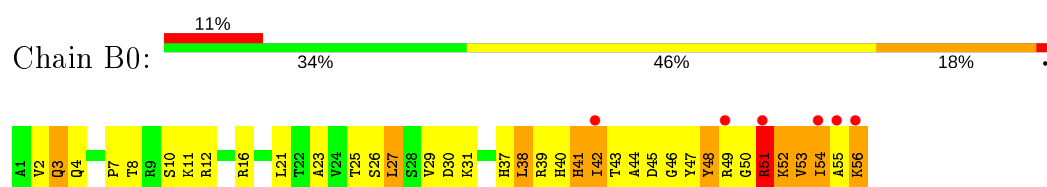
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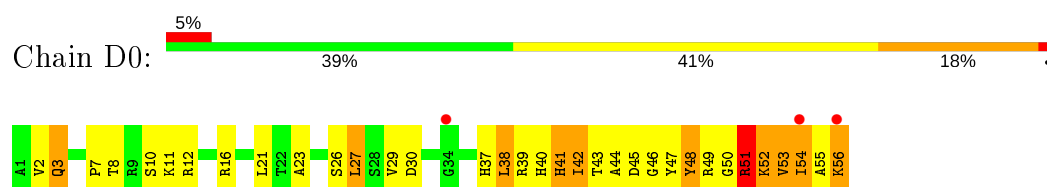
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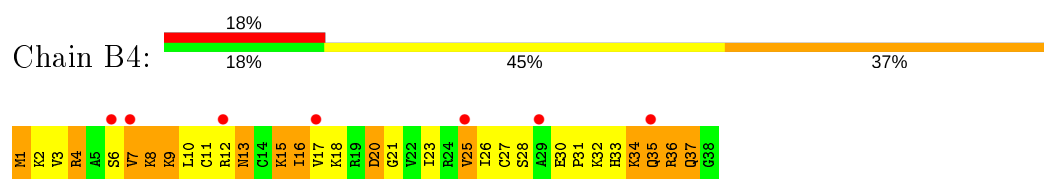
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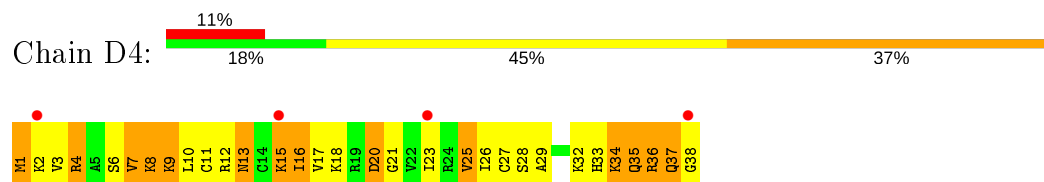
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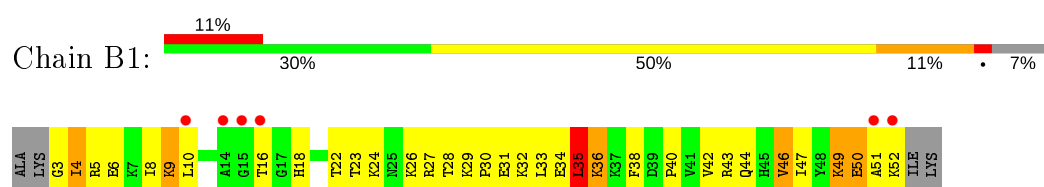
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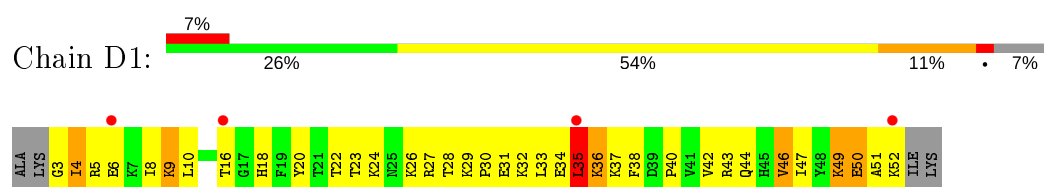
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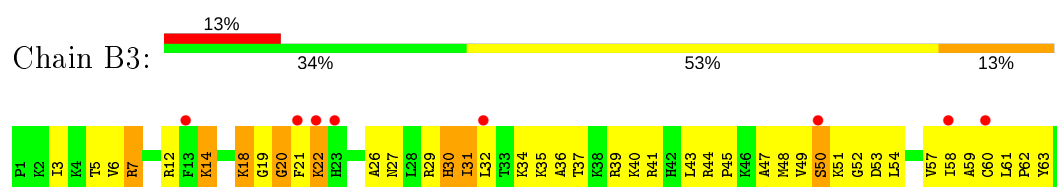
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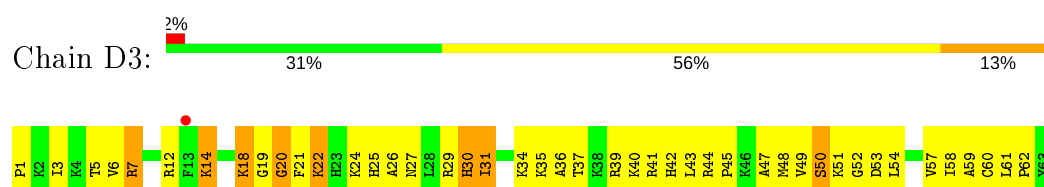
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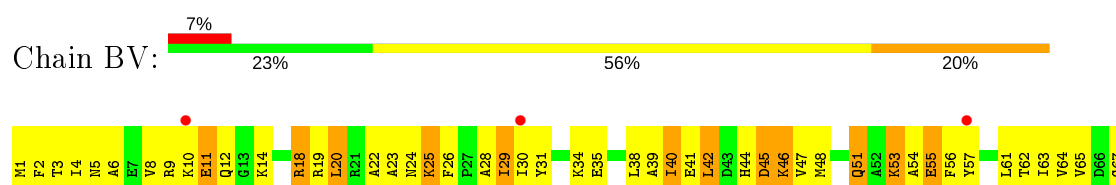
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- Molecule 34: 50S ribosomal protein L35

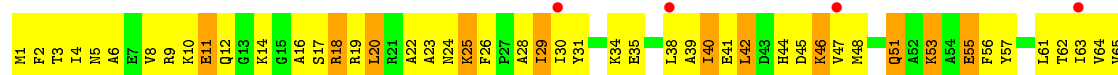


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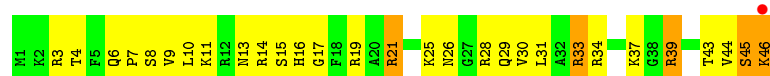




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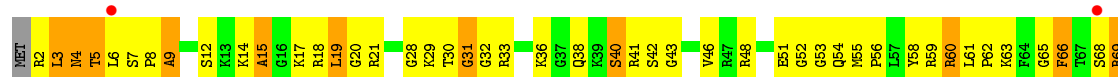
- Molecule 36: 50S ribosomal protein L34



- Molecule 36: 50S ribosomal protein L34

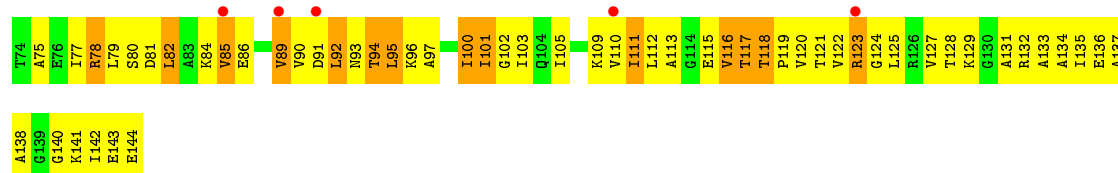


- Molecule 37: 50S ribosomal protein L15

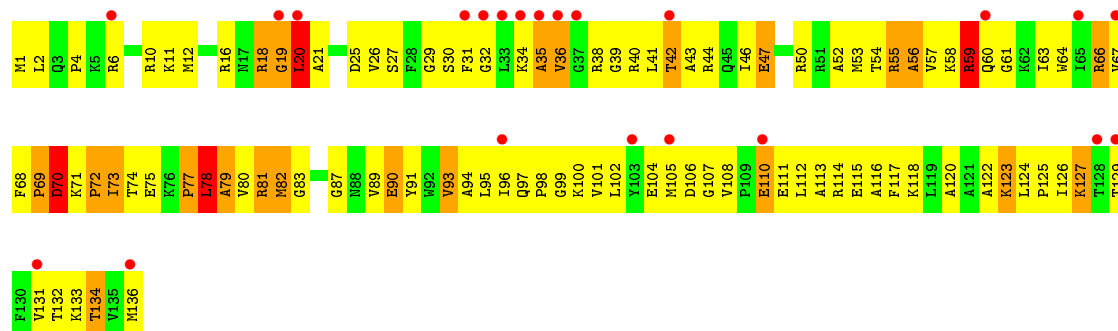


- Molecule 37: 50S ribosomal protein L15

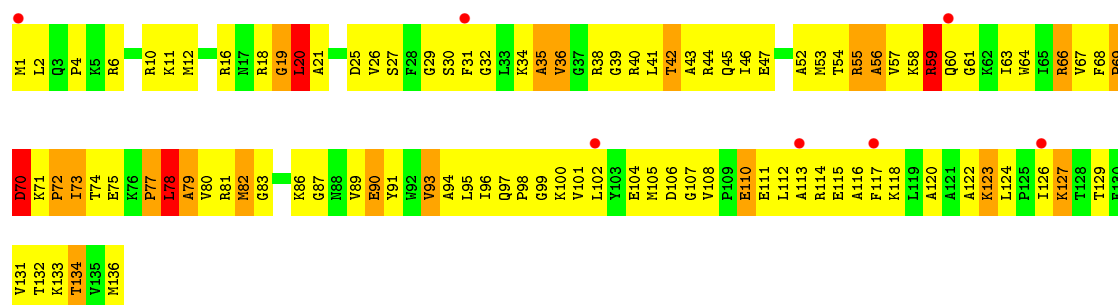




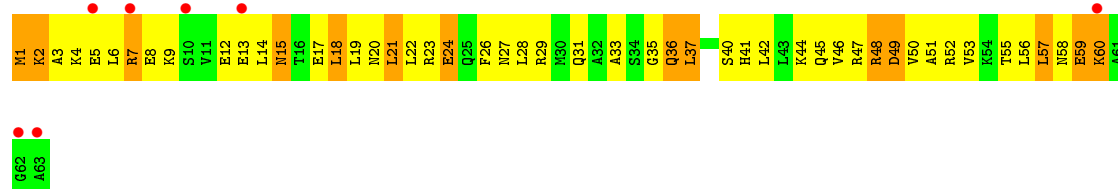
• Molecule 38: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L16



• Molecule 39: 50S ribosomal protein L29

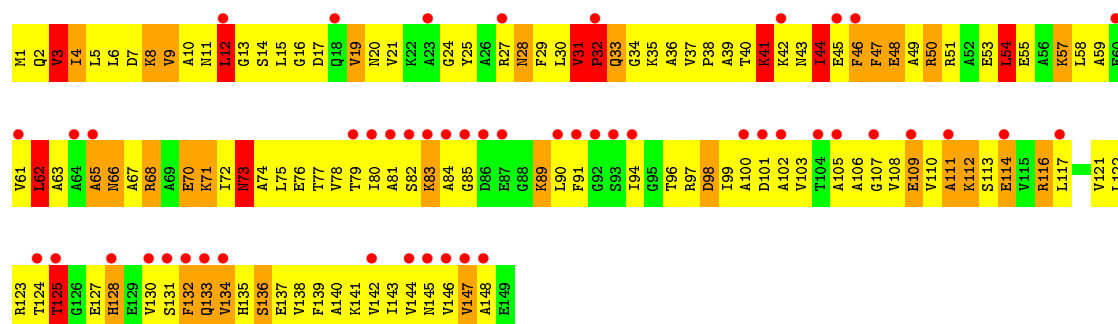
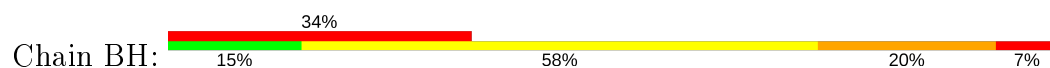


• Molecule 39: 50S ribosomal protein L29

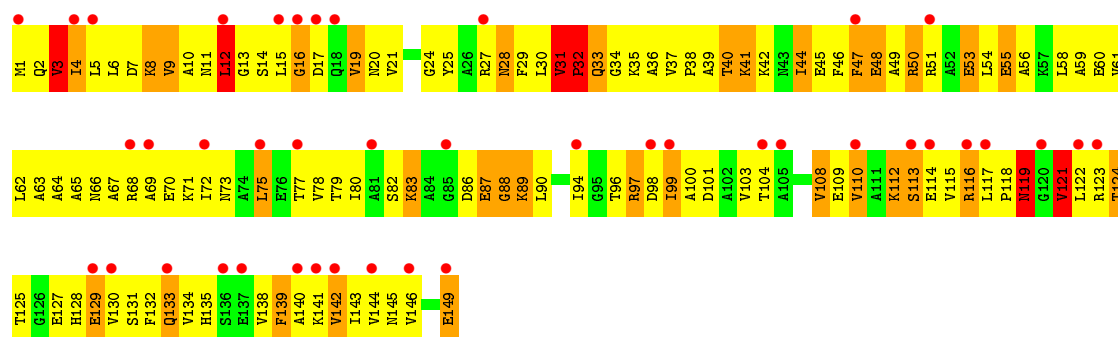




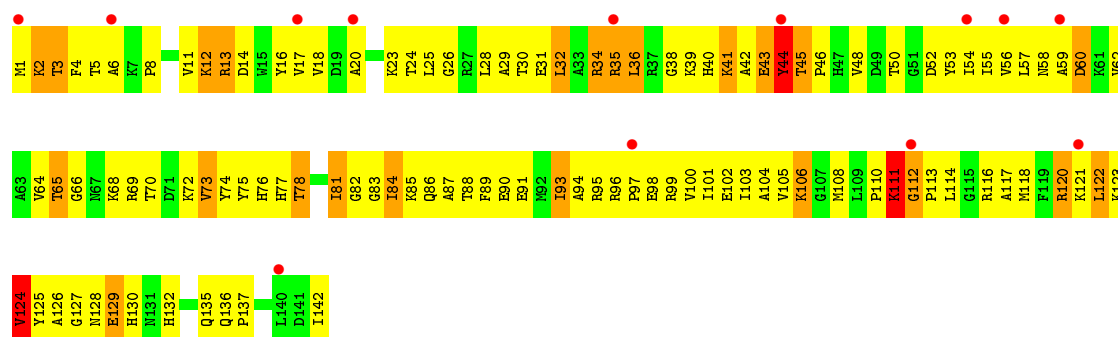
• Molecule 40: 50S ribosomal protein L9



• Molecule 40: 50S ribosomal protein L9



• Molecule 41: 50S ribosomal protein L13

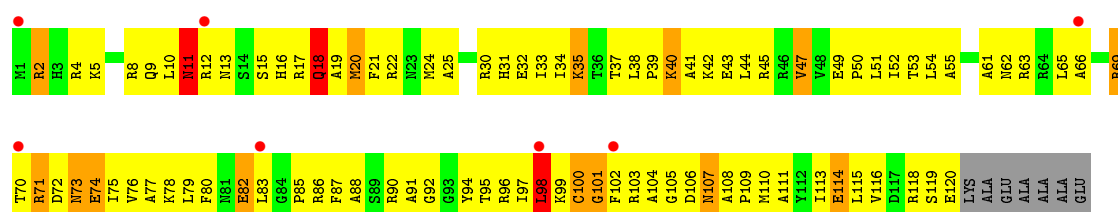


• Molecule 41: 50S ribosomal protein L13

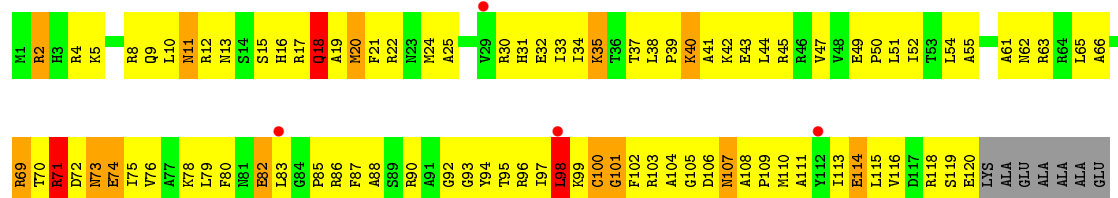




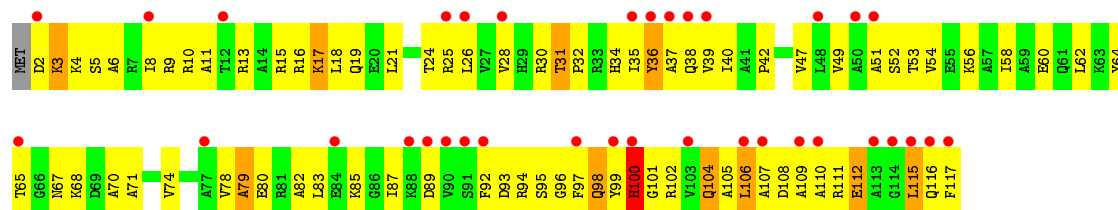
• Molecule 42: 50S ribosomal protein L17



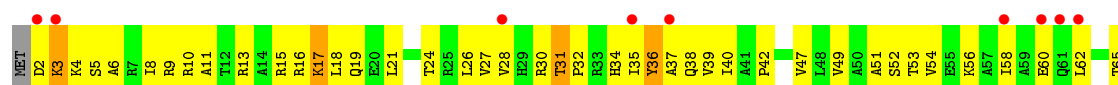
• Molecule 42: 50S ribosomal protein L17

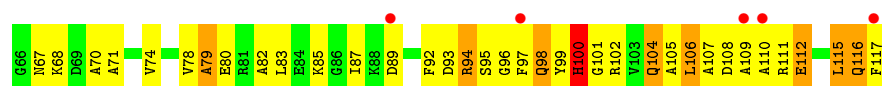


• Molecule 43: 50S ribosomal protein L18

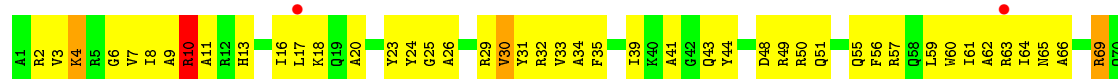


• Molecule 43: 50S ribosomal protein L18

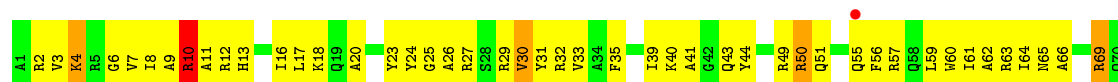




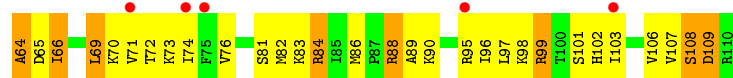
- Molecule 44: 50S ribosomal protein L20



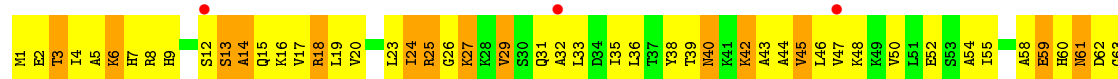
- Molecule 44: 50S ribosomal protein L20



- Molecule 45: 50S ribosomal protein L22

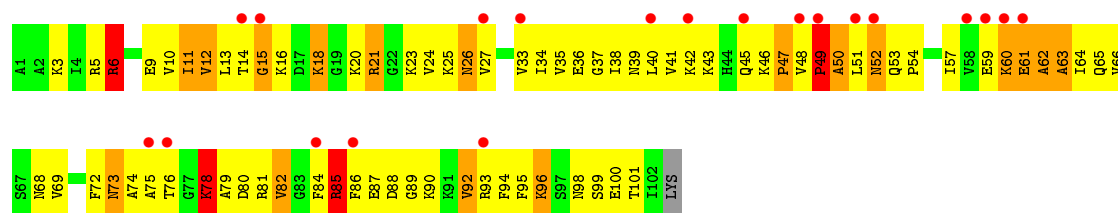


- Molecule 45: 50S ribosomal protein L22

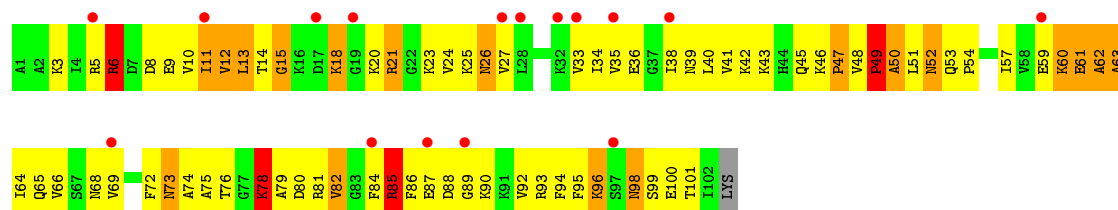


- Molecule 46: 50S ribosomal protein L24

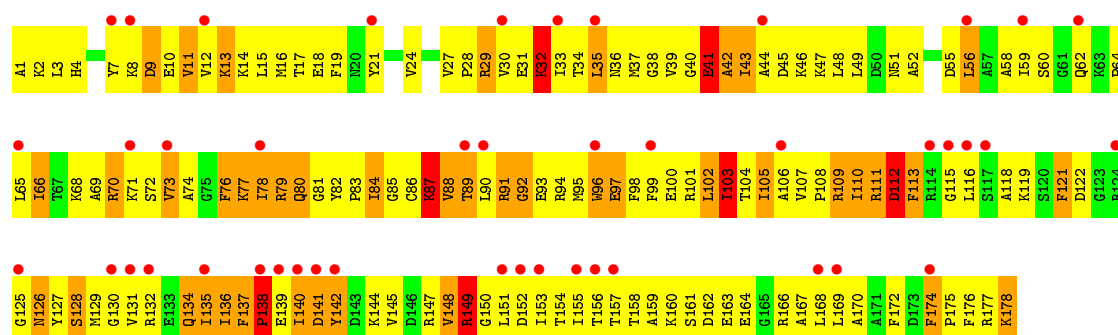
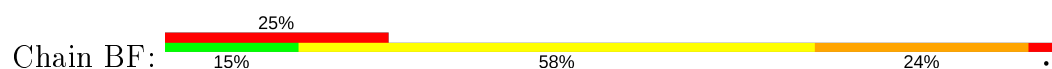




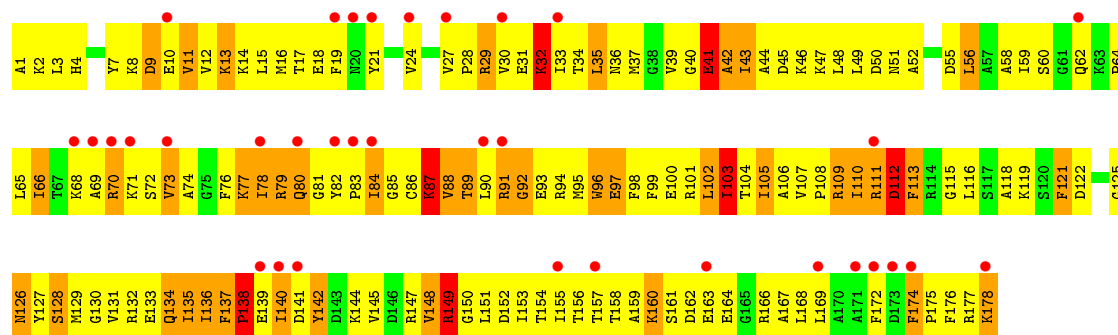
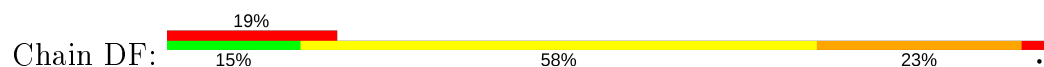
• Molecule 46: 50S ribosomal protein L24



• Molecule 47: 50S ribosomal protein L5

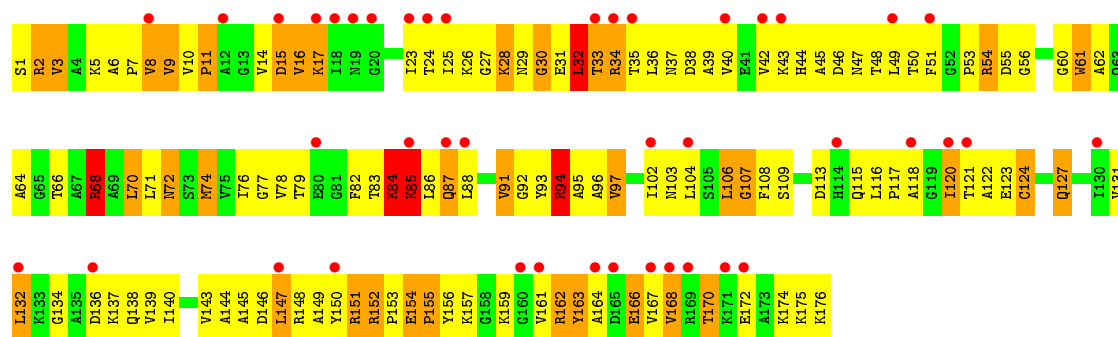


• Molecule 47: 50S ribosomal protein L5

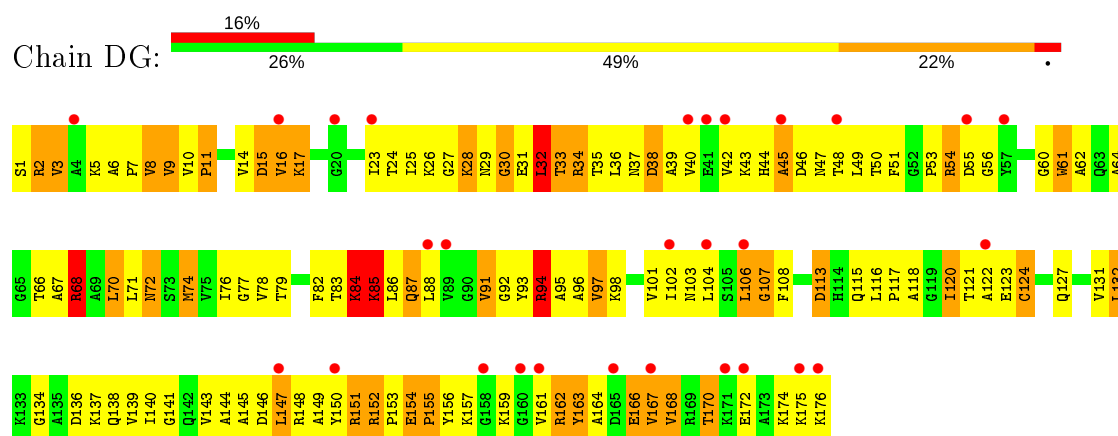


• Molecule 48: 50S ribosomal protein L6

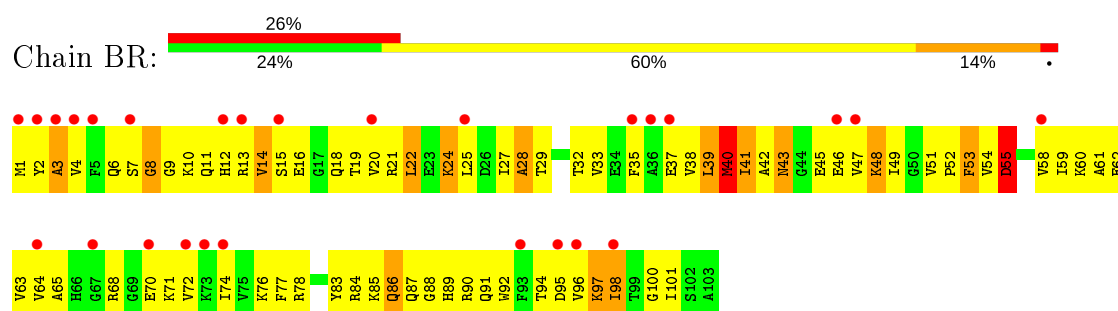




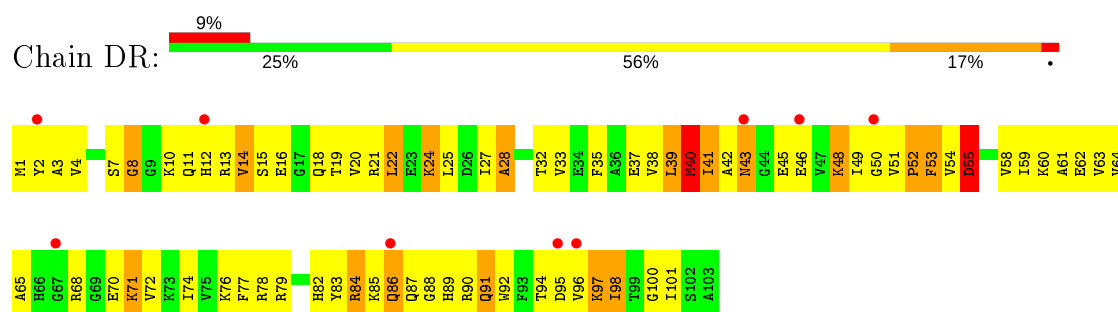
• Molecule 48: 50S ribosomal protein L6



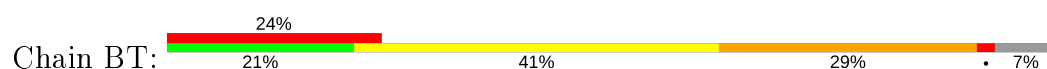
• Molecule 49: 50S ribosomal protein L21

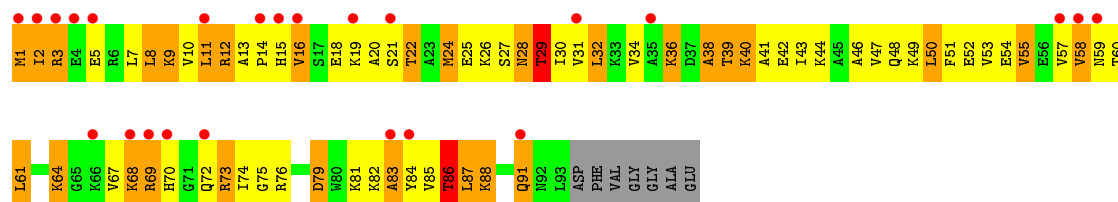


• Molecule 49: 50S ribosomal protein L21

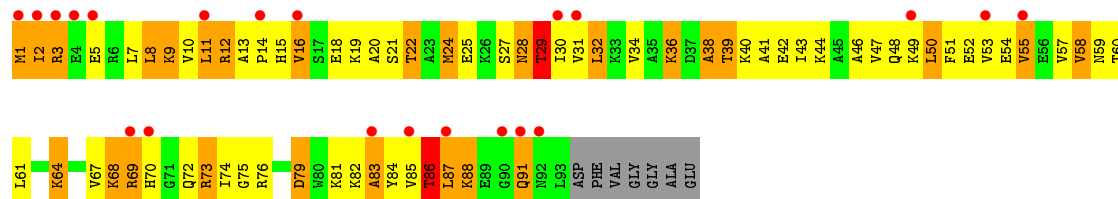
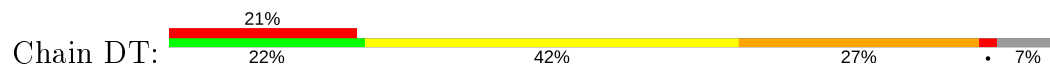


• Molecule 50: 50S ribosomal protein L23

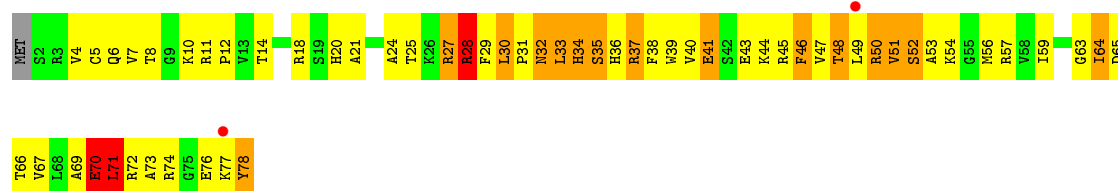




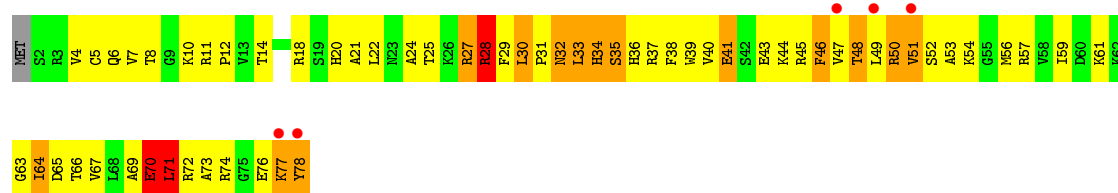
• Molecule 50: 50S ribosomal protein L23



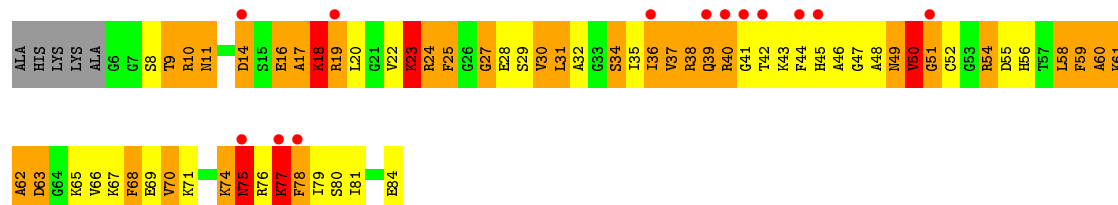
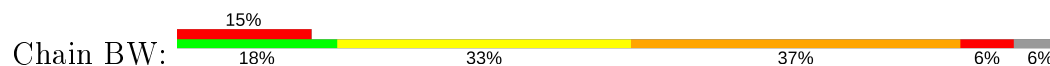
• Molecule 51: 50S ribosomal protein L28



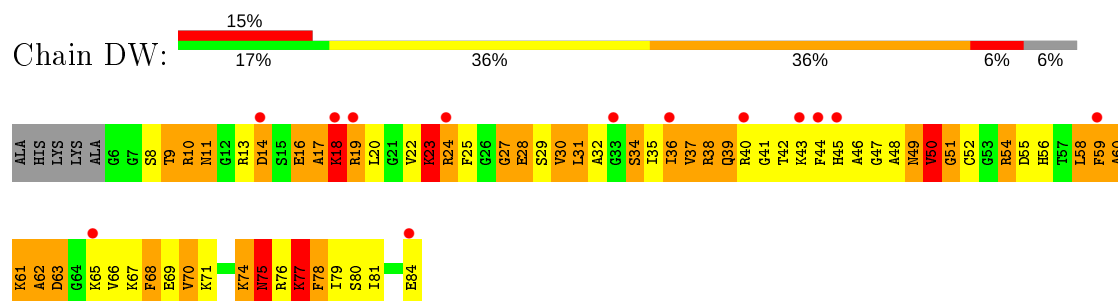
• Molecule 51: 50S ribosomal protein L28



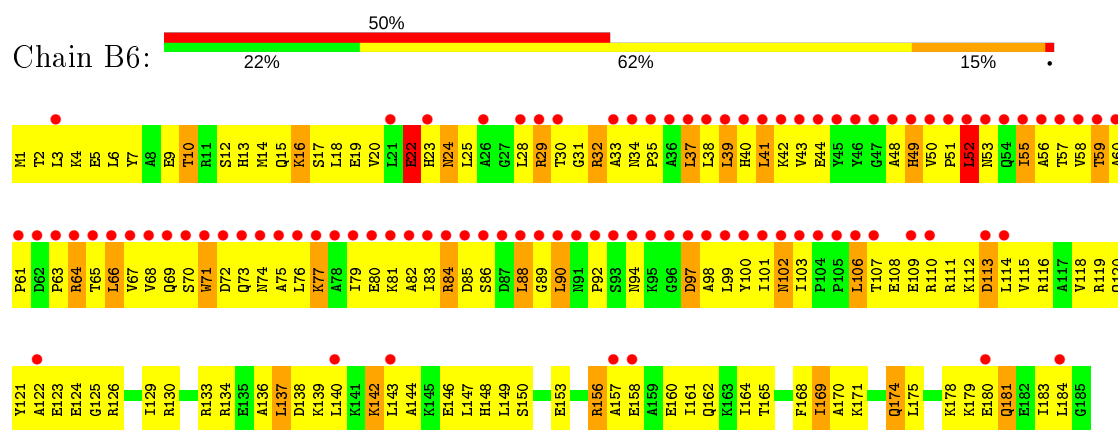
• Molecule 52: 50S ribosomal protein L27



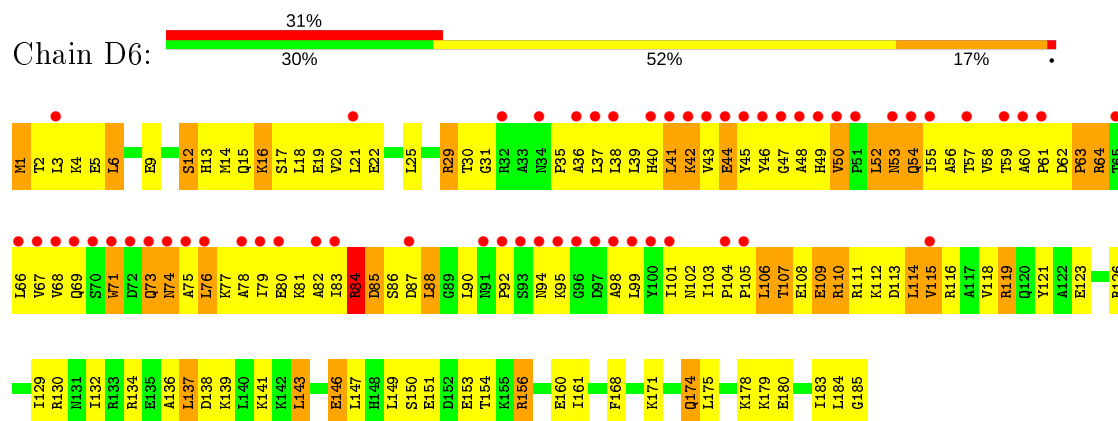
- Molecule 52: 50S ribosomal protein L27



- Molecule 53: ribosome recycling factor



- Molecule 53: ribosome recycling factor



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 207.90 Å 378.20 Å 736.30 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 3.30 82.86 – 3.32 | Depositor EDS |
| % Data completeness (in resolution range) | 85.8 (40.00-3.30) 87.2 (82.86-3.32) | Depositor EDS |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.17 (at 3.33 Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.275 , 0.304 0.248 , 0.273 | Depositor DCC |
| R_{free} test set | 35399 reflections (4.79%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 83.9 | Xtriage |
| Anisotropy | 0.393 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.25 , 57.6 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 286960 | wwPDB-VP |
| Average B, all atoms (Å ²) | 67.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% 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

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 | 0.26 | 0/36762 | 0.75 | 11/57350 (0.0%) |
| 1 | CA | 0.26 | 0/36762 | 0.75 | 18/57350 (0.0%) |
| 2 | AC | 0.23 | 0/1651 | 0.44 | 0/2225 |
| 2 | CC | 0.23 | 0/1651 | 0.45 | 0/2225 |
| 3 | AD | 0.23 | 0/1665 | 0.44 | 0/2227 |
| 3 | CD | 0.23 | 0/1665 | 0.43 | 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 | 0.45 | 0/1591 |
| 6 | CG | 0.23 | 0/1211 | 0.45 | 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 | 0/1034 | 0.46 | 0/1375 |
| 9 | AJ | 0.22 | 0/796 | 0.49 | 0/1077 |
| 9 | CJ | 0.22 | 0/796 | 0.49 | 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 | 0.48 | 0/1300 |
| 11 | CL | 0.22 | 0/969 | 0.49 | 0/1300 |
| 12 | AM | 0.21 | 0/892 | 0.46 | 0/1193 |
| 12 | CM | 0.21 | 0/884 | 0.45 | 0/1181 |
| 13 | AN | 0.24 | 0/785 | 0.44 | 0/1043 |
| 13 | CN | 0.24 | 0/785 | 0.44 | 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 | 0.45 | 0/884 |
| 15 | CP | 0.25 | 0/648 | 0.45 | 0/870 |
| 16 | AQ | 0.23 | 0/657 | 0.47 | 0/881 |
| 16 | CQ | 0.24 | 0/666 | 0.48 | 0/892 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | AR | 0.23 | 0/462 | 0.45 | 0/621 |
| 17 | CR | 0.23 | 0/462 | 0.45 | 0/621 |
| 18 | AS | 0.25 | 0/652 | 0.46 | 0/877 |
| 18 | CS | 0.25 | 0/660 | 0.48 | 0/888 |
| 19 | AT | 0.23 | 0/671 | 0.40 | 0/888 |
| 19 | CT | 0.23 | 0/671 | 0.40 | 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 | 0.25 | 0/2803 | 0.74 | 1/4371 (0.0%) |
| 22 | DA | 0.25 | 0/2803 | 0.74 | 1/4371 (0.0%) |
| 23 | BB | 0.28 | 6/68314 (0.0%) | 0.77 | 55/106569 (0.1%) |
| 23 | DB | 0.28 | 8/68314 (0.0%) | 0.78 | 51/106569 (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 | 0.25 | 0/929 | 0.50 | 0/1242 |
| 28 | DP | 0.24 | 0/929 | 0.50 | 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 | 0.50 | 0/605 |
| 30 | DY | 0.23 | 0/453 | 0.50 | 0/605 |
| 31 | B0 | 0.22 | 0/450 | 0.56 | 0/599 |
| 31 | D0 | 0.22 | 0/450 | 0.56 | 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 | 0.47 | 0/676 |
| 34 | D3 | 0.24 | 0/513 | 0.47 | 0/676 |
| 35 | BV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 35 | DV | 0.25 | 0/766 | 0.43 | 0/1025 |
| 36 | B2 | 0.26 | 0/380 | 0.48 | 0/498 |
| 36 | D2 | 0.26 | 0/380 | 0.48 | 0/498 |
| 37 | BL | 0.23 | 0/1054 | 0.49 | 0/1403 |
| 37 | DL | 0.23 | 0/1054 | 0.49 | 0/1403 |
| 38 | BM | 0.25 | 0/1093 | 0.49 | 0/1460 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | DM | 0.25 | 0/1093 | 0.49 | 0/1460 |
| 39 | BX | 0.24 | 0/510 | 0.52 | 0/677 |
| 39 | DX | 0.24 | 0/510 | 0.52 | 0/677 |
| 40 | BH | 0.25 | 0/1122 | 0.48 | 0/1515 |
| 40 | DH | 0.25 | 0/1122 | 0.49 | 0/1515 |
| 41 | BJ | 0.23 | 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 | 0.25 | 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 | 0.48 | 0/1816 |
| 48 | DG | 0.23 | 0/1343 | 0.47 | 0/1816 |
| 49 | BR | 0.25 | 0/829 | 0.49 | 0/1107 |
| 49 | DR | 0.25 | 0/829 | 0.49 | 0/1107 |
| 50 | BT | 0.23 | 0/744 | 0.55 | 0/994 |
| 50 | DT | 0.23 | 0/744 | 0.55 | 0/994 |
| 51 | BZ | 0.25 | 0/635 | 0.52 | 0/848 |
| 51 | DZ | 0.25 | 0/635 | 0.52 | 0/848 |
| 52 | BW | 0.28 | 0/603 | 0.52 | 0/797 |
| 52 | DW | 0.28 | 0/603 | 0.52 | 0/797 |
| 53 | B6 | 0.24 | 0/1497 | 0.48 | 0/2017 |
| 53 | D6 | 0.23 | 0/1497 | 0.48 | 0/2017 |
| All | All | 0.26 | 14/309354 (0.0%) | 0.70 | 137/462003 (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 | 14 |
| 1 | CA | 0 | 13 |
| 23 | BB | 0 | 29 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 23 | DB | 0 | 29 |
| All | All | 0 | 85 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 23 | BB | 1086 | A | C5-C6 | -16.41 | 1.26 | 1.41 |
| 23 | DB | 1086 | A | C5-C6 | -16.29 | 1.26 | 1.41 |
| 23 | DB | 1088 | A | C6-N1 | -10.64 | 1.28 | 1.35 |
| 23 | BB | 1088 | A | C6-N1 | -10.54 | 1.28 | 1.35 |
| 23 | DB | 1060 | U | C2-N3 | 7.91 | 1.43 | 1.37 |

The worst 5 of 137 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 23 | DB | 2204 | G | O5'-P-OP1 | -29.30 | 75.55 | 110.70 |
| 23 | BB | 2204 | G | O5'-P-OP2 | -27.99 | 77.11 | 110.70 |
| 23 | BB | 2791 | G | O5'-P-OP1 | -27.68 | 77.49 | 110.70 |
| 23 | DB | 2791 | G | O5'-P-OP2 | -27.63 | 77.54 | 110.70 |
| 23 | DB | 2791 | G | O5'-P-OP1 | 18.08 | 132.40 | 110.70 |

There are no chirality outliers.

5 of 85 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 | 81 | A | 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 | 1174 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | CA | 32831 | 0 | 16521 | 1151 | 0 |
| 2 | AC | 1624 | 0 | 1699 | 141 | 0 |
| 2 | CC | 1624 | 0 | 1699 | 138 | 0 |
| 3 | AD | 1643 | 0 | 1710 | 151 | 0 |
| 3 | CD | 1643 | 0 | 1710 | 155 | 0 |
| 4 | AE | 1105 | 0 | 1148 | 107 | 0 |
| 4 | CE | 1105 | 0 | 1148 | 102 | 0 |
| 5 | AF | 817 | 0 | 808 | 85 | 0 |
| 5 | CF | 817 | 0 | 808 | 82 | 0 |
| 6 | AG | 1174 | 0 | 1230 | 102 | 0 |
| 6 | CG | 1196 | 0 | 1246 | 91 | 0 |
| 7 | AH | 979 | 0 | 1034 | 62 | 0 |
| 7 | CH | 979 | 0 | 1034 | 62 | 0 |
| 8 | AI | 1022 | 0 | 1070 | 123 | 0 |
| 8 | CI | 1022 | 0 | 1070 | 126 | 0 |
| 9 | AJ | 786 | 0 | 828 | 76 | 0 |
| 9 | CJ | 786 | 0 | 828 | 76 | 0 |
| 10 | AK | 877 | 0 | 887 | 84 | 0 |
| 10 | CK | 877 | 0 | 887 | 73 | 0 |
| 11 | AL | 955 | 0 | 1019 | 85 | 0 |
| 11 | CL | 955 | 0 | 1019 | 92 | 0 |
| 12 | AM | 883 | 0 | 944 | 104 | 0 |
| 12 | CM | 876 | 0 | 937 | 109 | 0 |
| 13 | AN | 774 | 0 | 827 | 96 | 0 |
| 13 | CN | 774 | 0 | 827 | 95 | 0 |
| 14 | AO | 714 | 0 | 734 | 46 | 0 |
| 14 | CO | 714 | 0 | 734 | 51 | 0 |
| 15 | AP | 649 | 0 | 666 | 60 | 0 |
| 15 | CP | 638 | 0 | 656 | 60 | 0 |
| 16 | AQ | 648 | 0 | 691 | 64 | 0 |
| 16 | CQ | 657 | 0 | 702 | 65 | 0 |
| 17 | AR | 455 | 0 | 478 | 36 | 0 |
| 17 | CR | 455 | 0 | 478 | 37 | 0 |
| 18 | AS | 637 | 0 | 665 | 89 | 0 |
| 18 | CS | 644 | 0 | 675 | 91 | 0 |
| 19 | AT | 665 | 0 | 714 | 45 | 0 |
| 19 | CT | 665 | 0 | 714 | 44 | 0 |
| 20 | AB | 1704 | 0 | 1732 | 195 | 0 |
| 20 | CB | 1704 | 0 | 1732 | 198 | 0 |
| 21 | AU | 425 | 0 | 449 | 69 | 0 |
| 21 | CU | 425 | 0 | 449 | 68 | 0 |
| 22 | BA | 2507 | 0 | 1270 | 89 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 22 | DA | 2507 | 0 | 1270 | 83 | 0 |
| 23 | BB | 60995 | 0 | 30679 | 2163 | 0 |
| 23 | DB | 60995 | 0 | 30677 | 2184 | 0 |
| 24 | BI | 1032 | 0 | 1088 | 112 | 0 |
| 24 | DI | 1032 | 0 | 1088 | 183 | 0 |
| 25 | BC | 2082 | 0 | 2157 | 232 | 0 |
| 25 | DC | 2082 | 0 | 2157 | 232 | 0 |
| 26 | BD | 1565 | 0 | 1616 | 186 | 0 |
| 26 | DD | 1565 | 0 | 1616 | 184 | 0 |
| 27 | BK | 930 | 0 | 1000 | 110 | 0 |
| 27 | DK | 930 | 0 | 1000 | 113 | 0 |
| 28 | BP | 917 | 0 | 965 | 136 | 0 |
| 28 | DP | 917 | 0 | 965 | 145 | 0 |
| 29 | BE | 1552 | 0 | 1619 | 188 | 0 |
| 29 | DE | 1552 | 0 | 1619 | 191 | 0 |
| 30 | BY | 449 | 0 | 491 | 52 | 0 |
| 30 | DY | 449 | 0 | 491 | 52 | 0 |
| 31 | B0 | 444 | 0 | 461 | 39 | 0 |
| 31 | D0 | 444 | 0 | 461 | 31 | 0 |
| 32 | B4 | 302 | 0 | 340 | 50 | 0 |
| 32 | D4 | 302 | 0 | 340 | 53 | 0 |
| 33 | B1 | 409 | 0 | 440 | 51 | 0 |
| 33 | D1 | 409 | 0 | 440 | 43 | 0 |
| 34 | B3 | 504 | 0 | 574 | 54 | 0 |
| 34 | D3 | 504 | 0 | 574 | 57 | 0 |
| 35 | BV | 753 | 0 | 780 | 86 | 0 |
| 35 | DV | 753 | 0 | 780 | 84 | 0 |
| 36 | B2 | 377 | 0 | 418 | 34 | 0 |
| 36 | D2 | 377 | 0 | 418 | 32 | 0 |
| 37 | BL | 1045 | 0 | 1117 | 138 | 0 |
| 37 | DL | 1045 | 0 | 1117 | 144 | 0 |
| 38 | BM | 1074 | 0 | 1157 | 120 | 0 |
| 38 | DM | 1074 | 0 | 1157 | 118 | 0 |
| 39 | BX | 509 | 0 | 543 | 56 | 0 |
| 39 | DX | 509 | 0 | 543 | 58 | 0 |
| 40 | BH | 1111 | 0 | 1148 | 220 | 0 |
| 40 | DH | 1111 | 0 | 1148 | 161 | 0 |
| 41 | BJ | 1129 | 0 | 1162 | 156 | 0 |
| 41 | DJ | 1129 | 0 | 1162 | 161 | 0 |
| 42 | BN | 960 | 0 | 1000 | 111 | 0 |
| 42 | DN | 960 | 0 | 1000 | 108 | 0 |
| 43 | BO | 892 | 0 | 923 | 76 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43 | DO | 892 | 0 | 923 | 81 | 0 |
| 44 | BQ | 947 | 0 | 1022 | 125 | 0 |
| 44 | DQ | 947 | 0 | 1022 | 136 | 0 |
| 45 | BS | 857 | 0 | 922 | 94 | 0 |
| 45 | DS | 857 | 0 | 922 | 93 | 0 |
| 46 | BU | 779 | 0 | 834 | 111 | 0 |
| 46 | DU | 779 | 0 | 834 | 111 | 0 |
| 47 | BF | 1420 | 0 | 1460 | 242 | 0 |
| 47 | DF | 1420 | 0 | 1460 | 233 | 0 |
| 48 | BG | 1323 | 0 | 1374 | 158 | 0 |
| 48 | DG | 1323 | 0 | 1374 | 159 | 0 |
| 49 | BR | 816 | 0 | 839 | 85 | 0 |
| 49 | DR | 816 | 0 | 839 | 96 | 0 |
| 50 | BT | 738 | 0 | 807 | 120 | 0 |
| 50 | DT | 738 | 0 | 807 | 115 | 0 |
| 51 | BZ | 625 | 0 | 652 | 63 | 0 |
| 51 | DZ | 625 | 0 | 652 | 61 | 0 |
| 52 | BW | 596 | 0 | 610 | 138 | 0 |
| 52 | DW | 596 | 0 | 610 | 152 | 0 |
| 53 | B6 | 1478 | 0 | 1526 | 204 | 0 |
| 53 | D6 | 1478 | 0 | 1526 | 177 | 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 | B4 | 1 | 0 | 0 | 0 | 0 |
| 55 | D4 | 1 | 0 | 0 | 0 | 0 |
| 56 | AA | 289 | 0 | 0 | 1 | 0 |
| 56 | AE | 4 | 0 | 0 | 0 | 0 |
| 56 | AK | 1 | 0 | 0 | 0 | 0 |
| 56 | AL | 1 | 0 | 0 | 0 | 0 |
| 56 | AN | 3 | 0 | 0 | 0 | 0 |
| 56 | AP | 1 | 0 | 0 | 0 | 0 |
| 56 | AT | 1 | 0 | 0 | 0 | 0 |
| 56 | B2 | 1 | 0 | 0 | 0 | 0 |
| 56 | BB | 495 | 0 | 0 | 5 | 0 |
| 56 | BC | 4 | 0 | 0 | 0 | 0 |
| 56 | BD | 1 | 0 | 0 | 0 | 0 |
| 56 | BE | 3 | 0 | 0 | 0 | 0 |
| 56 | BL | 1 | 0 | 0 | 0 | 0 |
| 56 | BT | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 56 | CA | 300 | 0 | 0 | 0 | 0 |
| 56 | CE | 2 | 0 | 0 | 0 | 0 |
| 56 | CK | 1 | 0 | 0 | 0 | 0 |
| 56 | CL | 1 | 0 | 0 | 0 | 0 |
| 56 | CN | 4 | 0 | 0 | 0 | 0 |
| 56 | CT | 1 | 0 | 0 | 0 | 0 |
| 56 | DB | 505 | 0 | 0 | 7 | 0 |
| 56 | DC | 4 | 0 | 0 | 1 | 0 |
| 56 | DD | 1 | 0 | 0 | 0 | 0 |
| 56 | DE | 2 | 0 | 0 | 0 | 0 |
| All | All | 286960 | 0 | 193714 | 16198 | 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 34.

The worst 5 of 16198 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 | 1.39 | 1.17 |
| 13:CN:63:CYS:HB3 | 13:CN:67:GLY:H | 1.09 | 1.16 |
| 13:AN:63:CYS:HB3 | 13:AN:67:GLY:H | 1.05 | 1.15 |
| 10:AK:124:LYS:HA | 21:AU:34:ARG:HB3 | 1.27 | 1.14 |
| 29:DE:21:ARG:HD2 | 29:DE:107:SER:HB3 | 1.30 | 1.13 |

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%) | 152 (74%) | 36 (18%) | 16 (8%) | 1 | 6 |
| 2 | CC | 204/232 (88%) | 151 (74%) | 37 (18%) | 16 (8%) | 1 | 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | AD | 203/205 (99%) | 151 (74%) | 39 (19%) | 13 (6%) | 1 | 9 |
| 3 | CD | 203/205 (99%) | 150 (74%) | 41 (20%) | 12 (6%) | 1 | 10 |
| 4 | AE | 148/166 (89%) | 125 (84%) | 20 (14%) | 3 (2%) | 7 | 32 |
| 4 | CE | 148/166 (89%) | 125 (84%) | 20 (14%) | 3 (2%) | 7 | 32 |
| 5 | AF | 98/135 (73%) | 71 (72%) | 18 (18%) | 9 (9%) | 1 | 4 |
| 5 | CF | 98/135 (73%) | 69 (70%) | 21 (21%) | 8 (8%) | 1 | 5 |
| 6 | AG | 148/178 (83%) | 114 (77%) | 28 (19%) | 6 (4%) | 3 | 17 |
| 6 | CG | 150/178 (84%) | 118 (79%) | 25 (17%) | 7 (5%) | 2 | 14 |
| 7 | AH | 127/129 (98%) | 106 (84%) | 17 (13%) | 4 (3%) | 4 | 23 |
| 7 | CH | 127/129 (98%) | 105 (83%) | 18 (14%) | 4 (3%) | 4 | 23 |
| 8 | AI | 125/129 (97%) | 92 (74%) | 28 (22%) | 5 (4%) | 3 | 18 |
| 8 | CI | 125/129 (97%) | 93 (74%) | 28 (22%) | 4 (3%) | 4 | 22 |
| 9 | AJ | 96/103 (93%) | 73 (76%) | 13 (14%) | 10 (10%) | 0 | 3 |
| 9 | CJ | 96/103 (93%) | 74 (77%) | 12 (12%) | 10 (10%) | 0 | 3 |
| 10 | AK | 115/128 (90%) | 85 (74%) | 25 (22%) | 5 (4%) | 2 | 16 |
| 10 | CK | 115/128 (90%) | 84 (73%) | 25 (22%) | 6 (5%) | 2 | 13 |
| 11 | AL | 121/123 (98%) | 84 (69%) | 28 (23%) | 9 (7%) | 1 | 7 |
| 11 | CL | 121/123 (98%) | 86 (71%) | 25 (21%) | 10 (8%) | 1 | 5 |
| 12 | AM | 112/117 (96%) | 85 (76%) | 16 (14%) | 11 (10%) | 0 | 3 |
| 12 | CM | 111/117 (95%) | 83 (75%) | 17 (15%) | 11 (10%) | 0 | 3 |
| 13 | AN | 92/100 (92%) | 65 (71%) | 19 (21%) | 8 (9%) | 1 | 5 |
| 13 | CN | 92/100 (92%) | 66 (72%) | 18 (20%) | 8 (9%) | 1 | 5 |
| 14 | AO | 86/89 (97%) | 68 (79%) | 15 (17%) | 3 (4%) | 3 | 21 |
| 14 | CO | 86/89 (97%) | 70 (81%) | 14 (16%) | 2 (2%) | 6 | 29 |
| 15 | AP | 80/82 (98%) | 62 (78%) | 10 (12%) | 8 (10%) | 0 | 3 |
| 15 | CP | 78/82 (95%) | 61 (78%) | 11 (14%) | 6 (8%) | 1 | 6 |
| 16 | AQ | 78/83 (94%) | 59 (76%) | 15 (19%) | 4 (5%) | 2 | 13 |
| 16 | CQ | 79/83 (95%) | 60 (76%) | 15 (19%) | 4 (5%) | 2 | 13 |
| 17 | AR | 53/74 (72%) | 48 (91%) | 5 (9%) | 0 | 100 | 100 |
| 17 | CR | 53/74 (72%) | 48 (91%) | 5 (9%) | 0 | 100 | 100 |
| 18 | AS | 77/91 (85%) | 59 (77%) | 12 (16%) | 6 (8%) | 1 | 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 18 | CS | 78/91 (86%) | 61 (78%) | 11 (14%) | 6 (8%) | 1 | 6 |
| 19 | AT | 83/86 (96%) | 64 (77%) | 15 (18%) | 4 (5%) | 2 | 14 |
| 19 | CT | 83/86 (96%) | 65 (78%) | 14 (17%) | 4 (5%) | 2 | 14 |
| 20 | AB | 216/240 (90%) | 153 (71%) | 48 (22%) | 15 (7%) | 1 | 8 |
| 20 | CB | 216/240 (90%) | 150 (69%) | 49 (23%) | 17 (8%) | 1 | 6 |
| 21 | AU | 49/70 (70%) | 31 (63%) | 10 (20%) | 8 (16%) | 0 | 1 |
| 21 | CU | 49/70 (70%) | 31 (63%) | 10 (20%) | 8 (16%) | 0 | 1 |
| 24 | BI | 139/141 (99%) | 119 (86%) | 15 (11%) | 5 (4%) | 3 | 20 |
| 24 | DI | 139/141 (99%) | 114 (82%) | 21 (15%) | 4 (3%) | 4 | 24 |
| 25 | BC | 269/272 (99%) | 176 (65%) | 61 (23%) | 32 (12%) | 0 | 2 |
| 25 | DC | 269/272 (99%) | 177 (66%) | 59 (22%) | 33 (12%) | 0 | 1 |
| 26 | BD | 207/209 (99%) | 123 (59%) | 56 (27%) | 28 (14%) | 0 | 1 |
| 26 | DD | 207/209 (99%) | 122 (59%) | 55 (27%) | 30 (14%) | 0 | 1 |
| 27 | BK | 119/123 (97%) | 80 (67%) | 25 (21%) | 14 (12%) | 0 | 2 |
| 27 | DK | 119/123 (97%) | 81 (68%) | 24 (20%) | 14 (12%) | 0 | 2 |
| 28 | BP | 112/114 (98%) | 68 (61%) | 29 (26%) | 15 (13%) | 0 | 1 |
| 28 | DP | 112/114 (98%) | 69 (62%) | 28 (25%) | 15 (13%) | 0 | 1 |
| 29 | BE | 199/201 (99%) | 126 (63%) | 54 (27%) | 19 (10%) | 0 | 4 |
| 29 | DE | 199/201 (99%) | 127 (64%) | 52 (26%) | 20 (10%) | 0 | 3 |
| 30 | BY | 56/58 (97%) | 39 (70%) | 11 (20%) | 6 (11%) | 0 | 3 |
| 30 | DY | 56/58 (97%) | 39 (70%) | 11 (20%) | 6 (11%) | 0 | 3 |
| 31 | B0 | 54/56 (96%) | 40 (74%) | 5 (9%) | 9 (17%) | 0 | 1 |
| 31 | D0 | 54/56 (96%) | 40 (74%) | 5 (9%) | 9 (17%) | 0 | 1 |
| 32 | B4 | 36/38 (95%) | 22 (61%) | 5 (14%) | 9 (25%) | 0 | 0 |
| 32 | D4 | 36/38 (95%) | 22 (61%) | 5 (14%) | 9 (25%) | 0 | 0 |
| 33 | B1 | 48/54 (89%) | 37 (77%) | 6 (12%) | 5 (10%) | 0 | 3 |
| 33 | D1 | 48/54 (89%) | 36 (75%) | 7 (15%) | 5 (10%) | 0 | 3 |
| 34 | B3 | 62/64 (97%) | 42 (68%) | 14 (23%) | 6 (10%) | 0 | 3 |
| 34 | D3 | 62/64 (97%) | 42 (68%) | 14 (23%) | 6 (10%) | 0 | 3 |
| 35 | BV | 92/94 (98%) | 71 (77%) | 18 (20%) | 3 (3%) | 4 | 22 |
| 35 | DV | 92/94 (98%) | 71 (77%) | 18 (20%) | 3 (3%) | 4 | 22 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 36 | B2 | 44/46 (96%) | 36 (82%) | 7 (16%) | 1 (2%) | 6 | 29 |
| 36 | D2 | 44/46 (96%) | 35 (80%) | 7 (16%) | 2 (4%) | 2 | 15 |
| 37 | BL | 141/144 (98%) | 92 (65%) | 31 (22%) | 18 (13%) | 0 | 1 |
| 37 | DL | 141/144 (98%) | 94 (67%) | 28 (20%) | 19 (14%) | 0 | 1 |
| 38 | BM | 134/136 (98%) | 90 (67%) | 24 (18%) | 20 (15%) | 0 | 1 |
| 38 | DM | 134/136 (98%) | 90 (67%) | 24 (18%) | 20 (15%) | 0 | 1 |
| 39 | BX | 61/63 (97%) | 40 (66%) | 17 (28%) | 4 (7%) | 1 | 8 |
| 39 | DX | 61/63 (97%) | 39 (64%) | 18 (30%) | 4 (7%) | 1 | 8 |
| 40 | BH | 147/149 (99%) | 74 (50%) | 50 (34%) | 23 (16%) | 0 | 1 |
| 40 | DH | 147/149 (99%) | 92 (63%) | 38 (26%) | 17 (12%) | 0 | 2 |
| 41 | BJ | 140/142 (99%) | 96 (69%) | 31 (22%) | 13 (9%) | 0 | 4 |
| 41 | DJ | 140/142 (99%) | 95 (68%) | 32 (23%) | 13 (9%) | 0 | 4 |
| 42 | BN | 118/127 (93%) | 84 (71%) | 25 (21%) | 9 (8%) | 1 | 6 |
| 42 | DN | 118/127 (93%) | 82 (70%) | 25 (21%) | 11 (9%) | 0 | 4 |
| 43 | BO | 114/117 (97%) | 87 (76%) | 21 (18%) | 6 (5%) | 2 | 12 |
| 43 | DO | 114/117 (97%) | 86 (75%) | 21 (18%) | 7 (6%) | 1 | 10 |
| 44 | BQ | 115/117 (98%) | 81 (70%) | 21 (18%) | 13 (11%) | 0 | 2 |
| 44 | DQ | 115/117 (98%) | 81 (70%) | 22 (19%) | 12 (10%) | 0 | 3 |
| 45 | BS | 108/110 (98%) | 72 (67%) | 21 (19%) | 15 (14%) | 0 | 1 |
| 45 | DS | 108/110 (98%) | 73 (68%) | 20 (18%) | 15 (14%) | 0 | 1 |
| 46 | BU | 100/103 (97%) | 58 (58%) | 27 (27%) | 15 (15%) | 0 | 1 |
| 46 | DU | 100/103 (97%) | 58 (58%) | 27 (27%) | 15 (15%) | 0 | 1 |
| 47 | BF | 176/178 (99%) | 106 (60%) | 36 (20%) | 34 (19%) | 0 | 1 |
| 47 | DF | 176/178 (99%) | 106 (60%) | 36 (20%) | 34 (19%) | 0 | 1 |
| 48 | BG | 174/176 (99%) | 108 (62%) | 41 (24%) | 25 (14%) | 0 | 1 |
| 48 | DG | 174/176 (99%) | 109 (63%) | 39 (22%) | 26 (15%) | 0 | 1 |
| 49 | BR | 101/103 (98%) | 74 (73%) | 16 (16%) | 11 (11%) | 0 | 2 |
| 49 | DR | 101/103 (98%) | 73 (72%) | 17 (17%) | 11 (11%) | 0 | 2 |
| 50 | BT | 91/100 (91%) | 52 (57%) | 23 (25%) | 16 (18%) | 0 | 1 |
| 50 | DT | 91/100 (91%) | 52 (57%) | 24 (26%) | 15 (16%) | 0 | 1 |
| 51 | BZ | 75/78 (96%) | 50 (67%) | 16 (21%) | 9 (12%) | 0 | 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|------------|------------|------------|-------------|----|
| 51 | DZ | 75/78 (96%) | 50 (67%) | 17 (23%) | 8 (11%) | 0 | 3 |
| 52 | BW | 77/84 (92%) | 32 (42%) | 20 (26%) | 25 (32%) | 0 | 0 |
| 52 | DW | 77/84 (92%) | 33 (43%) | 18 (23%) | 26 (34%) | 0 | 0 |
| 53 | B6 | 183/185 (99%) | 140 (76%) | 36 (20%) | 7 (4%) | 3 | 19 |
| 53 | D6 | 183/185 (99%) | 146 (80%) | 28 (15%) | 9 (5%) | 2 | 14 |
| All | All | 11607/12284 (94%) | 8146 (70%) | 2335 (20%) | 1126 (10%) | 0 | 3 |

5 of 1126 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AC | 14 | VAL |
| 2 | AC | 25 | THR |
| 2 | AC | 54 | ILE |
| 2 | AC | 100 | ILE |
| 2 | AC | 104 | GLU |

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%) | 145 (85%) | 25 (15%) | 3 | 14 |
| 2 | CC | 170/189 (90%) | 145 (85%) | 25 (15%) | 3 | 14 |
| 3 | AD | 172/172 (100%) | 138 (80%) | 34 (20%) | 1 | 5 |
| 3 | CD | 172/172 (100%) | 138 (80%) | 34 (20%) | 1 | 5 |
| 4 | AE | 113/125 (90%) | 99 (88%) | 14 (12%) | 4 | 19 |
| 4 | CE | 113/125 (90%) | 99 (88%) | 14 (12%) | 4 | 19 |
| 5 | AF | 87/116 (75%) | 70 (80%) | 17 (20%) | 1 | 5 |
| 5 | CF | 87/116 (75%) | 70 (80%) | 17 (20%) | 1 | 5 |
| 6 | AG | 123/146 (84%) | 101 (82%) | 22 (18%) | 2 | 8 |
| 6 | CG | 125/146 (86%) | 103 (82%) | 22 (18%) | 2 | 8 |
| 7 | AH | 104/104 (100%) | 95 (91%) | 9 (9%) | 10 | 34 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 7 | CH | 104/104 (100%) | 96 (92%) | 8 (8%) | 13 | 38 |
| 8 | AI | 105/106 (99%) | 86 (82%) | 19 (18%) | 1 | 7 |
| 8 | CI | 105/106 (99%) | 86 (82%) | 19 (18%) | 1 | 7 |
| 9 | AJ | 86/90 (96%) | 75 (87%) | 11 (13%) | 4 | 18 |
| 9 | CJ | 86/90 (96%) | 76 (88%) | 10 (12%) | 5 | 22 |
| 10 | AK | 90/98 (92%) | 74 (82%) | 16 (18%) | 2 | 8 |
| 10 | CK | 90/98 (92%) | 74 (82%) | 16 (18%) | 2 | 8 |
| 11 | AL | 103/103 (100%) | 87 (84%) | 16 (16%) | 2 | 12 |
| 11 | CL | 103/103 (100%) | 87 (84%) | 16 (16%) | 2 | 12 |
| 12 | AM | 92/95 (97%) | 71 (77%) | 21 (23%) | 1 | 3 |
| 12 | CM | 91/95 (96%) | 69 (76%) | 22 (24%) | 0 | 2 |
| 13 | AN | 79/83 (95%) | 71 (90%) | 8 (10%) | 7 | 27 |
| 13 | CN | 79/83 (95%) | 71 (90%) | 8 (10%) | 7 | 27 |
| 14 | AO | 76/77 (99%) | 70 (92%) | 6 (8%) | 12 | 37 |
| 14 | CO | 76/77 (99%) | 70 (92%) | 6 (8%) | 12 | 37 |
| 15 | AP | 65/65 (100%) | 57 (88%) | 8 (12%) | 4 | 20 |
| 15 | CP | 65/65 (100%) | 56 (86%) | 9 (14%) | 3 | 16 |
| 16 | AQ | 74/77 (96%) | 59 (80%) | 15 (20%) | 1 | 5 |
| 16 | CQ | 75/77 (97%) | 60 (80%) | 15 (20%) | 1 | 5 |
| 17 | AR | 48/64 (75%) | 43 (90%) | 5 (10%) | 7 | 25 |
| 17 | CR | 48/64 (75%) | 43 (90%) | 5 (10%) | 7 | 25 |
| 18 | AS | 70/78 (90%) | 53 (76%) | 17 (24%) | 0 | 2 |
| 18 | CS | 71/78 (91%) | 55 (78%) | 16 (22%) | 1 | 3 |
| 19 | AT | 65/65 (100%) | 54 (83%) | 11 (17%) | 2 | 9 |
| 19 | CT | 65/65 (100%) | 54 (83%) | 11 (17%) | 2 | 9 |
| 20 | AB | 180/198 (91%) | 145 (81%) | 35 (19%) | 1 | 5 |
| 20 | CB | 180/198 (91%) | 144 (80%) | 36 (20%) | 1 | 5 |
| 21 | AU | 44/60 (73%) | 28 (64%) | 16 (36%) | 0 | 0 |
| 21 | CU | 44/60 (73%) | 27 (61%) | 17 (39%) | 0 | 0 |
| 24 | BI | 109/109 (100%) | 107 (98%) | 2 (2%) | 59 | 78 |
| 24 | DI | 109/109 (100%) | 103 (94%) | 6 (6%) | 21 | 52 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 25 | BC | 216/217 (100%) | 186 (86%) | 30 (14%) | 3 | 16 |
| 25 | DC | 216/217 (100%) | 187 (87%) | 29 (13%) | 4 | 16 |
| 26 | BD | 164/164 (100%) | 146 (89%) | 18 (11%) | 6 | 24 |
| 26 | DD | 164/164 (100%) | 148 (90%) | 16 (10%) | 8 | 29 |
| 27 | BK | 102/104 (98%) | 84 (82%) | 18 (18%) | 2 | 8 |
| 27 | DK | 102/104 (98%) | 84 (82%) | 18 (18%) | 2 | 8 |
| 28 | BP | 99/99 (100%) | 78 (79%) | 21 (21%) | 1 | 4 |
| 28 | DP | 99/99 (100%) | 78 (79%) | 21 (21%) | 1 | 4 |
| 29 | BE | 165/165 (100%) | 136 (82%) | 29 (18%) | 2 | 8 |
| 29 | DE | 165/165 (100%) | 137 (83%) | 28 (17%) | 2 | 9 |
| 30 | BY | 48/48 (100%) | 41 (85%) | 7 (15%) | 3 | 14 |
| 30 | DY | 48/48 (100%) | 41 (85%) | 7 (15%) | 3 | 14 |
| 31 | B0 | 47/47 (100%) | 37 (79%) | 10 (21%) | 1 | 4 |
| 31 | D0 | 47/47 (100%) | 37 (79%) | 10 (21%) | 1 | 4 |
| 32 | B4 | 34/34 (100%) | 26 (76%) | 8 (24%) | 1 | 3 |
| 32 | D4 | 34/34 (100%) | 26 (76%) | 8 (24%) | 1 | 3 |
| 33 | B1 | 45/48 (94%) | 39 (87%) | 6 (13%) | 4 | 17 |
| 33 | D1 | 45/48 (94%) | 39 (87%) | 6 (13%) | 4 | 17 |
| 34 | B3 | 51/51 (100%) | 47 (92%) | 4 (8%) | 12 | 38 |
| 34 | D3 | 51/51 (100%) | 47 (92%) | 4 (8%) | 12 | 38 |
| 35 | BV | 78/78 (100%) | 59 (76%) | 19 (24%) | 0 | 2 |
| 35 | DV | 78/78 (100%) | 59 (76%) | 19 (24%) | 0 | 2 |
| 36 | B2 | 38/38 (100%) | 32 (84%) | 6 (16%) | 2 | 11 |
| 36 | D2 | 38/38 (100%) | 32 (84%) | 6 (16%) | 2 | 11 |
| 37 | BL | 102/103 (99%) | 92 (90%) | 10 (10%) | 8 | 29 |
| 37 | DL | 102/103 (99%) | 92 (90%) | 10 (10%) | 8 | 29 |
| 38 | BM | 109/109 (100%) | 90 (83%) | 19 (17%) | 2 | 8 |
| 38 | DM | 109/109 (100%) | 90 (83%) | 19 (17%) | 2 | 8 |
| 39 | BX | 55/55 (100%) | 43 (78%) | 12 (22%) | 1 | 4 |
| 39 | DX | 55/55 (100%) | 43 (78%) | 12 (22%) | 1 | 4 |
| 40 | BH | 114/114 (100%) | 79 (69%) | 35 (31%) | 0 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 40 | DH | 114/114 (100%) | 82 (72%) | 32 (28%) | 0 | 1 |
| 41 | BJ | 116/116 (100%) | 96 (83%) | 20 (17%) | 2 | 9 |
| 41 | DJ | 116/116 (100%) | 98 (84%) | 18 (16%) | 2 | 12 |
| 42 | BN | 100/103 (97%) | 84 (84%) | 16 (16%) | 2 | 11 |
| 42 | DN | 100/103 (97%) | 84 (84%) | 16 (16%) | 2 | 11 |
| 43 | BO | 86/87 (99%) | 74 (86%) | 12 (14%) | 3 | 16 |
| 43 | DO | 86/87 (99%) | 72 (84%) | 14 (16%) | 2 | 10 |
| 44 | BQ | 89/89 (100%) | 78 (88%) | 11 (12%) | 4 | 19 |
| 44 | DQ | 89/89 (100%) | 78 (88%) | 11 (12%) | 4 | 19 |
| 45 | BS | 93/93 (100%) | 82 (88%) | 11 (12%) | 5 | 21 |
| 45 | DS | 93/93 (100%) | 82 (88%) | 11 (12%) | 5 | 21 |
| 46 | BU | 83/84 (99%) | 71 (86%) | 12 (14%) | 3 | 14 |
| 46 | DU | 83/84 (99%) | 70 (84%) | 13 (16%) | 2 | 12 |
| 47 | BF | 149/149 (100%) | 114 (76%) | 35 (24%) | 1 | 3 |
| 47 | DF | 149/149 (100%) | 115 (77%) | 34 (23%) | 1 | 3 |
| 48 | BG | 137/137 (100%) | 106 (77%) | 31 (23%) | 1 | 3 |
| 48 | DG | 137/137 (100%) | 105 (77%) | 32 (23%) | 1 | 3 |
| 49 | BR | 84/84 (100%) | 71 (84%) | 13 (16%) | 2 | 12 |
| 49 | DR | 84/84 (100%) | 71 (84%) | 13 (16%) | 2 | 12 |
| 50 | BT | 80/84 (95%) | 59 (74%) | 21 (26%) | 0 | 2 |
| 50 | DT | 80/84 (95%) | 59 (74%) | 21 (26%) | 0 | 2 |
| 51 | BZ | 67/68 (98%) | 52 (78%) | 15 (22%) | 1 | 3 |
| 51 | DZ | 67/68 (98%) | 52 (78%) | 15 (22%) | 1 | 3 |
| 52 | BW | 59/62 (95%) | 42 (71%) | 17 (29%) | 0 | 1 |
| 52 | DW | 59/62 (95%) | 43 (73%) | 16 (27%) | 0 | 1 |
| 53 | B6 | 157/157 (100%) | 126 (80%) | 31 (20%) | 1 | 5 |
| 53 | D6 | 157/157 (100%) | 121 (77%) | 36 (23%) | 1 | 3 |
| All | All | 9647/10014 (96%) | 7996 (83%) | 1651 (17%) | 2 | 9 |

5 of 1651 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50 | BT | 12 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | CG | 75 | LYS |
| 48 | DG | 37 | ASN |
| 51 | BZ | 41 | GLU |
| 2 | CC | 120 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 342 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | BR | 43 | ASN |
| 5 | CF | 46 | GLN |
| 47 | DF | 51 | ASN |
| 50 | BT | 92 | ASN |
| 53 | B6 | 102 | ASN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1529/1542 (99%) | 248 (16%) | 28 (1%) |
| 1 | CA | 1529/1542 (99%) | 239 (15%) | 25 (1%) |
| 22 | BA | 116/120 (96%) | 18 (15%) | 0 |
| 22 | DA | 116/120 (96%) | 19 (16%) | 0 |
| 23 | BB | 2837/2904 (97%) | 448 (15%) | 20 (0%) |
| 23 | DB | 2837/2904 (97%) | 432 (15%) | 19 (0%) |
| All | All | 8964/9132 (98%) | 1404 (15%) | 92 (1%) |

5 of 1404 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 9 | G |
| 1 | AA | 14 | U |
| 1 | AA | 15 | G |
| 1 | AA | 31 | G |
| 1 | AA | 32 | A |

5 of 92 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 2213 | U |
| 1 | CA | 243 | A |
| 23 | DB | 2213 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 23 | BB | 2282 | G |
| 23 | BB | 2873 | A |

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 345 ligands modelled in this entry, 345 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%) | -0.10 | 22 (1%) 75 75 | 20, 68, 149, 180 | 0 |
| 1 | CA | 1530/1542 (99%) | -0.20 | 9 (0%) 89 90 | 10, 51, 126, 180 | 0 |
| 2 | AC | 206/232 (88%) | 0.45 | 8 (3%) 39 37 | 24, 58, 114, 180 | 0 |
| 2 | CC | 206/232 (88%) | 0.36 | 5 (2%) 59 56 | 28, 67, 117, 175 | 0 |
| 3 | AD | 205/205 (100%) | 0.51 | 12 (5%) 22 22 | 22, 77, 137, 154 | 0 |
| 3 | CD | 205/205 (100%) | 0.19 | 3 (1%) 73 72 | 15, 53, 129, 160 | 0 |
| 4 | AE | 150/166 (90%) | 0.41 | 9 (6%) 21 21 | 16, 62, 116, 154 | 0 |
| 4 | CE | 150/166 (90%) | 0.40 | 6 (4%) 38 36 | 20, 50, 105, 159 | 0 |
| 5 | AF | 100/135 (74%) | 0.58 | 10 (10%) 7 7 | 33, 73, 126, 163 | 0 |
| 5 | CF | 100/135 (74%) | 0.24 | 1 (1%) 82 82 | 20, 63, 115, 146 | 0 |
| 6 | AG | 150/178 (84%) | 0.76 | 25 (16%) 1 1 | 40, 87, 140, 168 | 0 |
| 6 | CG | 152/178 (85%) | 0.74 | 20 (13%) 3 3 | 21, 80, 132, 169 | 0 |
| 7 | AH | 129/129 (100%) | 0.90 | 22 (17%) 1 1 | 34, 71, 116, 137 | 0 |
| 7 | CH | 129/129 (100%) | 0.46 | 8 (6%) 20 20 | 18, 50, 96, 131 | 0 |
| 8 | AI | 127/129 (98%) | 1.01 | 27 (21%) 0 1 | 23, 81, 151, 180 | 0 |
| 8 | CI | 127/129 (98%) | 0.73 | 15 (11%) 4 4 | 26, 82, 135, 180 | 0 |
| 9 | AJ | 98/103 (95%) | 1.13 | 18 (18%) 1 1 | 21, 74, 134, 180 | 0 |
| 9 | CJ | 98/103 (95%) | 1.30 | 25 (25%) 0 0 | 34, 83, 136, 163 | 0 |
| 10 | AK | 117/128 (91%) | 0.39 | 7 (5%) 21 21 | 19, 57, 100, 155 | 0 |
| 10 | CK | 117/128 (91%) | 0.20 | 2 (1%) 70 68 | 18, 48, 100, 142 | 0 |
| 11 | AL | 123/123 (100%) | 0.92 | 14 (11%) 5 4 | 29, 68, 124, 169 | 0 |
| 11 | CL | 123/123 (100%) | 0.46 | 4 (3%) 46 44 | 10, 44, 107, 159 | 0 |
| 12 | AM | 114/117 (97%) | 1.10 | 23 (20%) 1 1 | 48, 105, 157, 171 | 0 |
| 12 | CM | 113/117 (96%) | 0.86 | 16 (14%) 2 2 | 44, 98, 149, 166 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13 | AN | 96/100 (96%) | 0.93 | 15 (15%) 2 2 | 31, 77, 136, 171 | 0 |
| 13 | CN | 96/100 (96%) | 0.82 | 10 (10%) 6 6 | 31, 78, 137, 161 | 0 |
| 14 | AO | 88/89 (98%) | 0.35 | 2 (2%) 60 59 | 33, 67, 119, 173 | 0 |
| 14 | CO | 88/89 (98%) | 0.05 | 0 100 100 | 18, 53, 105, 133 | 0 |
| 15 | AP | 82/82 (100%) | 1.16 | 13 (15%) 1 2 | 38, 78, 140, 157 | 0 |
| 15 | CP | 80/82 (97%) | 1.29 | 18 (22%) 0 1 | 16, 44, 124, 180 | 0 |
| 16 | AQ | 80/83 (96%) | 0.78 | 6 (7%) 14 13 | 47, 86, 139, 155 | 0 |
| 16 | CQ | 81/83 (97%) | 0.63 | 6 (7%) 14 14 | 25, 56, 117, 151 | 0 |
| 17 | AR | 55/74 (74%) | 0.78 | 4 (7%) 15 15 | 27, 66, 125, 149 | 0 |
| 17 | CR | 55/74 (74%) | 0.57 | 3 (5%) 25 23 | 24, 51, 105, 154 | 0 |
| 18 | AS | 79/91 (86%) | 1.98 | 37 (46%) 0 0 | 61, 116, 158, 179 | 0 |
| 18 | CS | 80/91 (87%) | 1.96 | 36 (45%) 0 0 | 54, 107, 165, 177 | 0 |
| 19 | AT | 85/86 (98%) | 1.22 | 18 (21%) 0 1 | 52, 92, 133, 180 | 0 |
| 19 | CT | 85/86 (98%) | 0.77 | 10 (11%) 4 4 | 24, 52, 103, 156 | 0 |
| 20 | AB | 218/240 (90%) | 0.83 | 32 (14%) 2 2 | 29, 88, 139, 180 | 0 |
| 20 | CB | 218/240 (90%) | 0.75 | 34 (15%) 2 2 | 40, 92, 143, 161 | 0 |
| 21 | AU | 51/70 (72%) | 0.98 | 8 (15%) 2 2 | 36, 90, 150, 153 | 0 |
| 21 | CU | 51/70 (72%) | 0.97 | 10 (19%) 1 1 | 26, 74, 136, 174 | 0 |
| 22 | BA | 117/120 (97%) | -0.26 | 3 (2%) 56 53 | 46, 80, 115, 168 | 0 |
| 22 | DA | 117/120 (97%) | -0.10 | 4 (3%) 45 43 | 35, 69, 110, 178 | 0 |
| 23 | BB | 2841/2904 (97%) | -0.04 | 51 (1%) 68 67 | 16, 56, 145, 180 | 0 |
| 23 | DB | 2841/2904 (97%) | -0.07 | 35 (1%) 79 78 | 7, 45, 142, 180 | 0 |
| 24 | BI | 141/141 (100%) | 2.92 | 90 (63%) 0 0 | 62, 152, 180, 180 | 0 |
| 24 | DI | 141/141 (100%) | 3.47 | 98 (69%) 0 0 | 85, 155, 180, 180 | 0 |
| 25 | BC | 271/272 (99%) | 0.43 | 3 (1%) 80 81 | 9, 45, 87, 170 | 0 |
| 25 | DC | 271/272 (99%) | 0.37 | 5 (1%) 68 67 | 5, 37, 75, 125 | 0 |
| 26 | BD | 209/209 (100%) | 0.62 | 16 (7%) 13 12 | 22, 66, 124, 167 | 0 |
| 26 | DD | 209/209 (100%) | 0.49 | 14 (6%) 17 17 | 10, 44, 112, 139 | 0 |
| 27 | BK | 121/123 (98%) | 0.84 | 14 (11%) 4 4 | 16, 67, 120, 154 | 0 |
| 27 | DK | 121/123 (98%) | 0.35 | 2 (1%) 70 68 | 8, 39, 93, 152 | 0 |
| 28 | BP | 114/114 (100%) | 1.17 | 32 (28%) 0 0 | 27, 77, 122, 160 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 28 | DP | 114/114 (100%) | 0.43 | 5 (4%) 34 33 | 5, 42, 104, 160 | 0 |
| 29 | BE | 201/201 (100%) | 0.64 | 19 (9%) 8 8 | 16, 67, 132, 148 | 0 |
| 29 | DE | 201/201 (100%) | 0.56 | 22 (10%) 5 5 | 5, 65, 124, 156 | 0 |
| 30 | BY | 58/58 (100%) | 0.78 | 7 (12%) 4 3 | 42, 73, 129, 143 | 0 |
| 30 | DY | 58/58 (100%) | 0.58 | 3 (5%) 27 25 | 9, 58, 127, 150 | 0 |
| 31 | B0 | 56/56 (100%) | 0.61 | 6 (10%) 6 5 | 33, 71, 126, 141 | 0 |
| 31 | D0 | 56/56 (100%) | 0.53 | 3 (5%) 25 24 | 11, 45, 122, 170 | 0 |
| 32 | B4 | 38/38 (100%) | 1.04 | 7 (18%) 1 1 | 23, 75, 134, 149 | 0 |
| 32 | D4 | 38/38 (100%) | 0.82 | 4 (10%) 6 6 | 29, 54, 106, 125 | 0 |
| 33 | B1 | 50/54 (92%) | 0.97 | 6 (12%) 4 3 | 43, 79, 117, 132 | 0 |
| 33 | D1 | 50/54 (92%) | 0.82 | 4 (8%) 12 11 | 34, 66, 111, 135 | 0 |
| 34 | B3 | 64/64 (100%) | 0.73 | 8 (12%) 3 3 | 31, 51, 91, 115 | 0 |
| 34 | D3 | 64/64 (100%) | 0.47 | 1 (1%) 72 70 | 20, 40, 75, 110 | 0 |
| 35 | BV | 94/94 (100%) | 0.72 | 7 (7%) 14 14 | 32, 90, 135, 169 | 0 |
| 35 | DV | 94/94 (100%) | 0.52 | 7 (7%) 14 14 | 28, 74, 131, 167 | 0 |
| 36 | B2 | 46/46 (100%) | 0.52 | 1 (2%) 62 60 | 13, 40, 87, 121 | 0 |
| 36 | D2 | 46/46 (100%) | 0.28 | 0 100 100 | 11, 32, 67, 131 | 0 |
| 37 | BL | 143/144 (99%) | 0.58 | 8 (5%) 24 23 | 13, 64, 117, 161 | 0 |
| 37 | DL | 143/144 (99%) | 0.41 | 5 (3%) 44 42 | 13, 54, 108, 133 | 0 |
| 38 | BM | 136/136 (100%) | 0.88 | 22 (16%) 1 2 | 24, 68, 124, 174 | 0 |
| 38 | DM | 136/136 (100%) | 0.57 | 7 (5%) 28 26 | 13, 46, 109, 131 | 0 |
| 39 | BX | 63/63 (100%) | 0.74 | 7 (11%) 5 5 | 20, 86, 141, 171 | 0 |
| 39 | DX | 63/63 (100%) | 0.48 | 4 (6%) 20 20 | 38, 84, 134, 172 | 0 |
| 40 | BH | 149/149 (100%) | 1.73 | 50 (33%) 0 0 | 37, 121, 160, 180 | 0 |
| 40 | DH | 149/149 (100%) | 1.42 | 42 (28%) 0 0 | 20, 108, 147, 180 | 0 |
| 41 | BJ | 142/142 (100%) | 0.76 | 13 (9%) 9 9 | 25, 73, 126, 137 | 0 |
| 41 | DJ | 142/142 (100%) | 0.68 | 13 (9%) 9 9 | 19, 55, 104, 167 | 0 |
| 42 | BN | 120/127 (94%) | 0.45 | 7 (5%) 23 22 | 20, 65, 117, 173 | 0 |
| 42 | DN | 120/127 (94%) | 0.42 | 4 (3%) 46 44 | 8, 40, 80, 125 | 0 |
| 43 | BO | 116/117 (99%) | 1.40 | 35 (30%) 0 0 | 27, 82, 128, 179 | 0 |
| 43 | DO | 116/117 (99%) | 0.87 | 14 (12%) 4 3 | 19, 68, 119, 144 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | BQ | 117/117 (100%) | 0.53 | 7 (5%) 21 21 | 5, 64, 111, 163 | 0 |
| 44 | DQ | 117/117 (100%) | 0.42 | 8 (6%) 17 17 | 14, 48, 96, 180 | 0 |
| 45 | BS | 110/110 (100%) | 0.62 | 9 (8%) 11 11 | 15, 58, 112, 161 | 0 |
| 45 | DS | 110/110 (100%) | 0.56 | 3 (2%) 54 52 | 8, 42, 101, 132 | 0 |
| 46 | BU | 102/103 (99%) | 1.08 | 20 (19%) 1 1 | 26, 75, 130, 171 | 0 |
| 46 | DU | 102/103 (99%) | 0.99 | 16 (15%) 2 2 | 27, 83, 143, 180 | 0 |
| 47 | BF | 178/178 (100%) | 1.30 | 44 (24%) 0 0 | 42, 113, 160, 180 | 0 |
| 47 | DF | 178/178 (100%) | 1.06 | 34 (19%) 1 1 | 38, 97, 155, 180 | 0 |
| 48 | BG | 176/176 (100%) | 1.13 | 42 (23%) 0 0 | 51, 103, 141, 162 | 0 |
| 48 | DG | 176/176 (100%) | 0.87 | 28 (15%) 1 2 | 34, 91, 142, 169 | 0 |
| 49 | BR | 103/103 (100%) | 1.43 | 27 (26%) 0 0 | 27, 86, 128, 157 | 0 |
| 49 | DR | 103/103 (100%) | 0.71 | 9 (8%) 10 10 | 18, 76, 122, 148 | 0 |
| 50 | BT | 93/100 (93%) | 1.24 | 24 (25%) 0 0 | 31, 70, 134, 164 | 0 |
| 50 | DT | 93/100 (93%) | 1.25 | 21 (22%) 0 1 | 21, 66, 136, 173 | 0 |
| 51 | BZ | 77/78 (98%) | 0.68 | 2 (2%) 56 53 | 22, 50, 93, 129 | 0 |
| 51 | DZ | 77/78 (98%) | 0.38 | 5 (6%) 18 18 | 17, 46, 95, 130 | 0 |
| 52 | BW | 79/84 (94%) | 1.05 | 13 (16%) 1 2 | 29, 81, 126, 153 | 0 |
| 52 | DW | 79/84 (94%) | 1.14 | 13 (16%) 1 2 | 20, 59, 119, 135 | 0 |
| 53 | B6 | 185/185 (100%) | 2.71 | 93 (50%) 0 0 | 33, 116, 167, 180 | 0 |
| 53 | D6 | 185/185 (100%) | 1.65 | 58 (31%) 0 0 | 19, 88, 157, 180 | 0 |
| All | All | 20787/21416 (97%) | 0.44 | 1757 (8%) 10 10 | 5, 63, 142, 180 | 0 |

The worst 5 of 1757 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 15 | AP | 81 | ALA | 13.1 |
| 53 | D6 | 72 | ASP | 11.6 |
| 24 | BI | 1 | ALA | 11.3 |
| 24 | DI | 85 | ILE | 10.8 |
| 24 | DI | 99 | LYS | 10.6 |

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. 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 | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | BB | 3093 | 1/1 | 0.21 | 0.64 | 38,38,38,38 | 1 |
| 54 | MG | DB | 3059 | 1/1 | 0.39 | 0.15 | 65,65,65,65 | 1 |
| 54 | MG | AA | 2025 | 1/1 | 0.42 | 0.70 | 54,54,54,54 | 1 |
| 54 | MG | DB | 3060 | 1/1 | 0.48 | 0.10 | 89,89,89,89 | 0 |
| 54 | MG | AA | 2059 | 1/1 | 0.51 | 2.00 | 127,127,127,127 | 0 |
| 54 | MG | BB | 3100 | 1/1 | 0.51 | 0.58 | 75,75,75,75 | 1 |
| 54 | MG | AA | 2039 | 1/1 | 0.52 | 0.37 | 108,108,108,108 | 0 |
| 54 | MG | DB | 3052 | 1/1 | 0.55 | 0.35 | 114,114,114,114 | 0 |
| 54 | MG | BB | 3010 | 1/1 | 0.61 | 0.15 | 70,70,70,70 | 0 |
| 54 | MG | BB | 3081 | 1/1 | 0.62 | 0.23 | 35,35,35,35 | 0 |
| 54 | MG | BB | 3042 | 1/1 | 0.63 | 0.10 | 123,123,123,123 | 0 |
| 54 | MG | DB | 3066 | 1/1 | 0.65 | 0.28 | 63,63,63,63 | 1 |
| 54 | MG | BB | 3097 | 1/1 | 0.65 | 0.13 | 101,101,101,101 | 0 |
| 54 | MG | BB | 3037 | 1/1 | 0.68 | 0.10 | 23,23,23,23 | 0 |
| 54 | MG | AA | 2037 | 1/1 | 0.69 | 1.61 | 139,139,139,139 | 0 |
| 54 | MG | AA | 2014 | 1/1 | 0.69 | 0.13 | 101,101,101,101 | 0 |
| 54 | MG | DB | 3030 | 1/1 | 0.69 | 0.35 | 47,47,47,47 | 0 |
| 55 | ZN | B4 | 101 | 1/1 | 0.70 | 0.09 | 55,55,55,55 | 0 |
| 54 | MG | BB | 3046 | 1/1 | 0.70 | 0.17 | 69,69,69,69 | 0 |
| 54 | MG | AA | 2023 | 1/1 | 0.71 | 0.30 | 32,32,32,32 | 1 |
| 54 | MG | AA | 2043 | 1/1 | 0.71 | 0.11 | 42,42,42,42 | 0 |
| 54 | MG | DB | 3058 | 1/1 | 0.71 | 2.01 | 145,145,145,145 | 0 |
| 54 | MG | BB | 3008 | 1/1 | 0.72 | 0.24 | 93,93,93,93 | 0 |
| 54 | MG | CA | 1634 | 1/1 | 0.72 | 0.11 | 32,32,32,32 | 0 |
| 54 | MG | BB | 3049 | 1/1 | 0.73 | 0.14 | 26,26,26,26 | 0 |
| 54 | MG | AA | 2026 | 1/1 | 0.75 | 0.16 | 5,5,5,5 | 1 |
| 54 | MG | DB | 3015 | 1/1 | 0.75 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | CA | 1623 | 1/1 | 0.75 | 0.18 | 101,101,101,101 | 0 |
| 54 | MG | DB | 3022 | 1/1 | 0.76 | 0.17 | 32,32,32,32 | 0 |
| 54 | MG | BB | 3090 | 1/1 | 0.76 | 0.18 | 78,78,78,78 | 0 |
| 54 | MG | CA | 1615 | 1/1 | 0.77 | 0.14 | 121,121,121,121 | 0 |
| 54 | MG | CA | 1641 | 1/1 | 0.77 | 0.21 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1654 | 1/1 | 0.78 | 0.15 | 52,52,52,52 | 0 |
| 54 | MG | CA | 1633 | 1/1 | 0.78 | 0.12 | 42,42,42,42 | 0 |
| 54 | MG | DB | 3064 | 1/1 | 0.78 | 0.15 | 37,37,37,37 | 0 |
| 54 | MG | AA | 2042 | 1/1 | 0.78 | 0.12 | 32,32,32,32 | 0 |
| 54 | MG | AA | 2022 | 1/1 | 0.79 | 0.29 | 77,77,77,77 | 0 |
| 54 | MG | AA | 2053 | 1/1 | 0.79 | 0.17 | 46,46,46,46 | 0 |
| 54 | MG | CA | 1622 | 1/1 | 0.80 | 0.08 | 46,46,46,46 | 0 |
| 54 | MG | CA | 1619 | 1/1 | 0.80 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | BB | 3073 | 1/1 | 0.80 | 0.17 | 70,70,70,70 | 0 |
| 54 | MG | DB | 3085 | 1/1 | 0.81 | 0.12 | 5,5,5,5 | 0 |
| 54 | MG | CA | 1608 | 1/1 | 0.82 | 0.11 | 106,106,106,106 | 0 |
| 54 | MG | BB | 3079 | 1/1 | 0.82 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | BB | 3094 | 1/1 | 0.83 | 0.09 | 21,21,21,21 | 0 |
| 54 | MG | DB | 3034 | 1/1 | 0.83 | 0.19 | 82,82,82,82 | 0 |
| 54 | MG | CA | 1635 | 1/1 | 0.83 | 0.07 | 55,55,55,55 | 0 |
| 54 | MG | AA | 2002 | 1/1 | 0.83 | 0.14 | 85,85,85,85 | 0 |
| 54 | MG | DB | 3074 | 1/1 | 0.83 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | AA | 2008 | 1/1 | 0.84 | 0.16 | 94,94,94,94 | 0 |
| 54 | MG | DB | 3013 | 1/1 | 0.84 | 0.22 | 47,47,47,47 | 0 |
| 54 | MG | BB | 3047 | 1/1 | 0.84 | 0.11 | 70,70,70,70 | 0 |
| 54 | MG | AA | 2050 | 1/1 | 0.84 | 0.12 | 101,101,101,101 | 0 |
| 54 | MG | AA | 2012 | 1/1 | 0.84 | 0.06 | 63,63,63,63 | 0 |
| 54 | MG | DB | 3110 | 1/1 | 0.84 | 0.26 | 40,40,40,40 | 0 |
| 54 | MG | CA | 1648 | 1/1 | 0.84 | 0.15 | 47,47,47,47 | 0 |
| 54 | MG | AA | 2030 | 1/1 | 0.84 | 0.09 | 102,102,102,102 | 0 |
| 54 | MG | DB | 3100 | 1/1 | 0.84 | 0.11 | 17,17,17,17 | 0 |
| 54 | MG | BB | 3031 | 1/1 | 0.84 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | BB | 3051 | 1/1 | 0.84 | 0.11 | 35,35,35,35 | 0 |
| 54 | MG | AA | 2018 | 1/1 | 0.84 | 0.07 | 78,78,78,78 | 0 |
| 54 | MG | BB | 3017 | 1/1 | 0.84 | 0.15 | 59,59,59,59 | 0 |
| 54 | MG | DB | 3063 | 1/1 | 0.85 | 0.15 | 28,28,28,28 | 0 |
| 54 | MG | AA | 2019 | 1/1 | 0.85 | 0.13 | 120,120,120,120 | 0 |
| 54 | MG | BB | 3014 | 1/1 | 0.85 | 0.14 | 58,58,58,58 | 0 |
| 54 | MG | AA | 2032 | 1/1 | 0.85 | 0.43 | 64,64,64,64 | 0 |
| 54 | MG | AA | 2045 | 1/1 | 0.85 | 0.07 | 63,63,63,63 | 0 |
| 54 | MG | AA | 2049 | 1/1 | 0.85 | 0.08 | 90,90,90,90 | 0 |
| 54 | MG | BB | 3102 | 1/1 | 0.86 | 0.09 | 38,38,38,38 | 0 |
| 54 | MG | CA | 1627 | 1/1 | 0.86 | 0.37 | 5,5,5,5 | 1 |
| 54 | MG | BB | 3053 | 1/1 | 0.86 | 0.07 | 61,61,61,61 | 0 |
| 54 | MG | BB | 3028 | 1/1 | 0.86 | 0.17 | 46,46,46,46 | 0 |
| 54 | MG | CA | 1652 | 1/1 | 0.86 | 0.09 | 54,54,54,54 | 0 |
| 54 | MG | AA | 2047 | 1/1 | 0.86 | 0.48 | 126,126,126,126 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | DB | 3025 | 1/1 | 0.87 | 0.13 | 28,28,28,28 | 0 |
| 54 | MG | BB | 3099 | 1/1 | 0.87 | 0.12 | 51,51,51,51 | 0 |
| 54 | MG | BB | 3054 | 1/1 | 0.87 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | DB | 3048 | 1/1 | 0.87 | 0.11 | 41,41,41,41 | 0 |
| 54 | MG | DB | 3083 | 1/1 | 0.87 | 0.14 | 72,72,72,72 | 0 |
| 54 | MG | BB | 3087 | 1/1 | 0.87 | 0.25 | 100,100,100,100 | 0 |
| 54 | MG | DB | 3068 | 1/1 | 0.87 | 0.16 | 8,8,8,8 | 0 |
| 54 | MG | BB | 3044 | 1/1 | 0.87 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | BB | 3061 | 1/1 | 0.87 | 0.07 | 38,38,38,38 | 0 |
| 54 | MG | CA | 1660 | 1/1 | 0.88 | 0.08 | 96,96,96,96 | 0 |
| 54 | MG | BB | 3104 | 1/1 | 0.88 | 0.14 | 20,20,20,20 | 0 |
| 54 | MG | BB | 3077 | 1/1 | 0.88 | 0.07 | 36,36,36,36 | 0 |
| 54 | MG | DB | 3045 | 1/1 | 0.88 | 0.08 | 61,61,61,61 | 0 |
| 54 | MG | DB | 3097 | 1/1 | 0.88 | 0.13 | 32,32,32,32 | 0 |
| 54 | MG | CA | 1611 | 1/1 | 0.88 | 0.11 | 81,81,81,81 | 0 |
| 54 | MG | AA | 2035 | 1/1 | 0.88 | 0.10 | 102,102,102,102 | 0 |
| 54 | MG | BB | 3052 | 1/1 | 0.89 | 0.09 | 25,25,25,25 | 0 |
| 54 | MG | CA | 1616 | 1/1 | 0.89 | 0.09 | 42,42,42,42 | 0 |
| 54 | MG | DB | 3029 | 1/1 | 0.89 | 0.15 | 67,67,67,67 | 0 |
| 54 | MG | BB | 3038 | 1/1 | 0.89 | 0.10 | 98,98,98,98 | 0 |
| 54 | MG | DB | 3057 | 1/1 | 0.89 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | DB | 3003 | 1/1 | 0.89 | 0.16 | 29,29,29,29 | 0 |
| 54 | MG | AA | 2044 | 1/1 | 0.89 | 0.09 | 47,47,47,47 | 0 |
| 54 | MG | AA | 2046 | 1/1 | 0.89 | 0.09 | 46,46,46,46 | 0 |
| 54 | MG | CA | 1638 | 1/1 | 0.89 | 0.12 | 90,90,90,90 | 0 |
| 54 | MG | BB | 3009 | 1/1 | 0.89 | 0.14 | 87,87,87,87 | 0 |
| 54 | MG | BB | 3016 | 1/1 | 0.89 | 0.18 | 34,34,34,34 | 0 |
| 54 | MG | CA | 1644 | 1/1 | 0.89 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | BB | 3033 | 1/1 | 0.89 | 0.19 | 94,94,94,94 | 0 |
| 54 | MG | DB | 3033 | 1/1 | 0.89 | 0.12 | 20,20,20,20 | 0 |
| 54 | MG | CA | 1643 | 1/1 | 0.89 | 0.08 | 20,20,20,20 | 0 |
| 54 | MG | DB | 3032 | 1/1 | 0.89 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | BB | 3032 | 1/1 | 0.89 | 0.12 | 34,34,34,34 | 0 |
| 54 | MG | BB | 3110 | 1/1 | 0.90 | 0.14 | 56,56,56,56 | 0 |
| 54 | MG | DB | 3055 | 1/1 | 0.90 | 0.12 | 17,17,17,17 | 0 |
| 54 | MG | BB | 3068 | 1/1 | 0.90 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | BB | 3056 | 1/1 | 0.90 | 0.07 | 31,31,31,31 | 0 |
| 54 | MG | AA | 2006 | 1/1 | 0.90 | 0.06 | 71,71,71,71 | 0 |
| 54 | MG | AA | 2057 | 1/1 | 0.90 | 0.62 | 93,93,93,93 | 0 |
| 54 | MG | AA | 2028 | 1/1 | 0.90 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | CA | 1637 | 1/1 | 0.90 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | BB | 3070 | 1/1 | 0.90 | 0.10 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | BB | 3007 | 1/1 | 0.91 | 0.11 | 74,74,74,74 | 0 |
| 54 | MG | DB | 3090 | 1/1 | 0.91 | 0.07 | 49,49,49,49 | 0 |
| 54 | MG | CE | 201 | 1/1 | 0.91 | 0.20 | 102,102,102,102 | 0 |
| 54 | MG | DB | 3050 | 1/1 | 0.91 | 0.05 | 70,70,70,70 | 0 |
| 54 | MG | BB | 3059 | 1/1 | 0.91 | 0.11 | 32,32,32,32 | 0 |
| 54 | MG | BB | 3076 | 1/1 | 0.91 | 0.07 | 43,43,43,43 | 0 |
| 54 | MG | BB | 3062 | 1/1 | 0.91 | 0.18 | 41,41,41,41 | 0 |
| 54 | MG | AA | 2027 | 1/1 | 0.91 | 0.21 | 62,62,62,62 | 0 |
| 54 | MG | DB | 3017 | 1/1 | 0.91 | 0.13 | 18,18,18,18 | 0 |
| 54 | MG | AA | 2060 | 1/1 | 0.91 | 0.05 | 75,75,75,75 | 0 |
| 54 | MG | BB | 3034 | 1/1 | 0.91 | 0.13 | 35,35,35,35 | 0 |
| 54 | MG | DB | 3018 | 1/1 | 0.91 | 0.12 | 23,23,23,23 | 0 |
| 54 | MG | CA | 1658 | 1/1 | 0.91 | 0.19 | 33,33,33,33 | 0 |
| 54 | MG | DB | 3095 | 1/1 | 0.91 | 0.38 | 19,19,19,19 | 1 |
| 54 | MG | BB | 3039 | 1/1 | 0.91 | 0.15 | 43,43,43,43 | 0 |
| 54 | MG | CA | 1628 | 1/1 | 0.91 | 0.11 | 38,38,38,38 | 0 |
| 54 | MG | CA | 1657 | 1/1 | 0.91 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | BB | 3063 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 54 | MG | AA | 2056 | 1/1 | 0.91 | 0.32 | 46,46,46,46 | 0 |
| 54 | MG | BB | 3015 | 1/1 | 0.92 | 0.10 | 40,40,40,40 | 0 |
| 54 | MG | BB | 3005 | 1/1 | 0.92 | 0.10 | 24,24,24,24 | 0 |
| 54 | MG | DB | 3108 | 1/1 | 0.92 | 0.11 | 11,11,11,11 | 0 |
| 54 | MG | CA | 1624 | 1/1 | 0.92 | 0.10 | 22,22,22,22 | 0 |
| 54 | MG | CA | 1621 | 1/1 | 0.92 | 0.41 | 110,110,110,110 | 0 |
| 54 | MG | BB | 3003 | 1/1 | 0.92 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | CA | 1661 | 1/1 | 0.92 | 0.06 | 49,49,49,49 | 0 |
| 54 | MG | AA | 2031 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | DB | 3073 | 1/1 | 0.92 | 0.10 | 29,29,29,29 | 0 |
| 54 | MG | DB | 3079 | 1/1 | 0.92 | 0.08 | 34,34,34,34 | 0 |
| 54 | MG | BB | 3085 | 1/1 | 0.92 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | AA | 2051 | 1/1 | 0.92 | 0.11 | 80,80,80,80 | 0 |
| 54 | MG | DB | 3054 | 1/1 | 0.92 | 0.08 | 25,25,25,25 | 0 |
| 54 | MG | CA | 1659 | 1/1 | 0.92 | 0.11 | 64,64,64,64 | 0 |
| 54 | MG | CA | 1620 | 1/1 | 0.92 | 0.06 | 58,58,58,58 | 0 |
| 54 | MG | AA | 2058 | 1/1 | 0.92 | 0.06 | 88,88,88,88 | 0 |
| 54 | MG | BB | 3025 | 1/1 | 0.92 | 0.13 | 49,49,49,49 | 0 |
| 54 | MG | DB | 3056 | 1/1 | 0.92 | 0.10 | 11,11,11,11 | 0 |
| 54 | MG | CA | 1629 | 1/1 | 0.92 | 0.07 | 20,20,20,20 | 1 |
| 54 | MG | CA | 1626 | 1/1 | 0.93 | 0.30 | 42,42,42,42 | 1 |
| 54 | MG | DB | 3109 | 1/1 | 0.93 | 0.09 | 35,35,35,35 | 0 |
| 54 | MG | CA | 1610 | 1/1 | 0.93 | 0.07 | 56,56,56,56 | 0 |
| 54 | MG | BB | 3078 | 1/1 | 0.93 | 0.10 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | DB | 3037 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 54 | MG | AA | 2021 | 1/1 | 0.93 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | AA | 2038 | 1/1 | 0.93 | 0.11 | 63,63,63,63 | 0 |
| 54 | MG | DB | 3024 | 1/1 | 0.93 | 0.13 | 30,30,30,30 | 0 |
| 54 | MG | DB | 3082 | 1/1 | 0.93 | 0.10 | 21,21,21,21 | 0 |
| 54 | MG | BB | 3108 | 1/1 | 0.93 | 0.11 | 37,37,37,37 | 0 |
| 54 | MG | CA | 1636 | 1/1 | 0.93 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | DB | 3080 | 1/1 | 0.93 | 0.15 | 29,29,29,29 | 0 |
| 54 | MG | BB | 3057 | 1/1 | 0.93 | 0.27 | 37,37,37,37 | 0 |
| 54 | MG | DB | 3102 | 1/1 | 0.93 | 0.13 | 15,15,15,15 | 0 |
| 54 | MG | AA | 2011 | 1/1 | 0.93 | 0.08 | 45,45,45,45 | 0 |
| 54 | MG | BB | 3089 | 1/1 | 0.93 | 0.08 | 38,38,38,38 | 0 |
| 54 | MG | BB | 3084 | 1/1 | 0.93 | 0.14 | 38,38,38,38 | 0 |
| 54 | MG | DB | 3062 | 1/1 | 0.93 | 0.08 | 41,41,41,41 | 0 |
| 54 | MG | DB | 3099 | 1/1 | 0.93 | 0.18 | 15,15,15,15 | 0 |
| 54 | MG | AA | 2020 | 1/1 | 0.93 | 0.09 | 84,84,84,84 | 0 |
| 54 | MG | DB | 3077 | 1/1 | 0.93 | 0.17 | 51,51,51,51 | 0 |
| 54 | MG | BB | 3024 | 1/1 | 0.93 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | BB | 3030 | 1/1 | 0.93 | 0.07 | 40,40,40,40 | 0 |
| 54 | MG | DB | 3006 | 1/1 | 0.93 | 0.15 | 26,26,26,26 | 0 |
| 54 | MG | BB | 3029 | 1/1 | 0.93 | 0.11 | 28,28,28,28 | 0 |
| 54 | MG | CA | 1656 | 1/1 | 0.93 | 0.10 | 22,22,22,22 | 0 |
| 54 | MG | BB | 3101 | 1/1 | 0.94 | 0.10 | 22,22,22,22 | 0 |
| 54 | MG | AA | 2015 | 1/1 | 0.94 | 0.13 | 86,86,86,86 | 0 |
| 54 | MG | BB | 3095 | 1/1 | 0.94 | 0.07 | 25,25,25,25 | 0 |
| 54 | MG | BB | 3027 | 1/1 | 0.94 | 0.14 | 34,34,34,34 | 0 |
| 54 | MG | BB | 3045 | 1/1 | 0.94 | 0.05 | 41,41,41,41 | 0 |
| 54 | MG | DB | 3011 | 1/1 | 0.94 | 0.17 | 16,16,16,16 | 0 |
| 54 | MG | BB | 3072 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 54 | MG | AA | 2034 | 1/1 | 0.94 | 0.11 | 40,40,40,40 | 0 |
| 54 | MG | AA | 2052 | 1/1 | 0.94 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | DB | 3012 | 1/1 | 0.94 | 0.18 | 23,23,23,23 | 0 |
| 54 | MG | CA | 1606 | 1/1 | 0.94 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | DB | 3051 | 1/1 | 0.94 | 0.17 | 25,25,25,25 | 0 |
| 54 | MG | DB | 3088 | 1/1 | 0.94 | 0.12 | 28,28,28,28 | 0 |
| 54 | MG | DB | 3091 | 1/1 | 0.94 | 0.12 | 29,29,29,29 | 0 |
| 54 | MG | DB | 3016 | 1/1 | 0.94 | 0.09 | 28,28,28,28 | 0 |
| 54 | MG | BB | 3018 | 1/1 | 0.94 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | AA | 2013 | 1/1 | 0.94 | 0.10 | 85,85,85,85 | 0 |
| 54 | MG | BB | 3002 | 1/1 | 0.94 | 0.11 | 12,12,12,12 | 0 |
| 54 | MG | BB | 3006 | 1/1 | 0.94 | 0.08 | 28,28,28,28 | 0 |
| 54 | MG | BB | 3069 | 1/1 | 0.94 | 0.08 | 17,17,17,17 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | CA | 1601 | 1/1 | 0.94 | 0.11 | 9,9,9,9 | 0 |
| 54 | MG | BB | 3040 | 1/1 | 0.94 | 0.19 | 60,60,60,60 | 0 |
| 54 | MG | BB | 3092 | 1/1 | 0.94 | 0.05 | 51,51,51,51 | 0 |
| 54 | MG | AA | 2016 | 1/1 | 0.94 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | DB | 3039 | 1/1 | 0.94 | 0.07 | 34,34,34,34 | 0 |
| 54 | MG | CA | 1605 | 1/1 | 0.94 | 0.13 | 38,38,38,38 | 0 |
| 54 | MG | DB | 3092 | 1/1 | 0.94 | 0.11 | 65,65,65,65 | 0 |
| 54 | MG | AA | 2024 | 1/1 | 0.94 | 0.08 | 61,61,61,61 | 0 |
| 54 | MG | DB | 3106 | 1/1 | 0.94 | 0.10 | 9,9,9,9 | 0 |
| 54 | MG | BB | 3106 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |
| 54 | MG | BB | 3096 | 1/1 | 0.94 | 0.07 | 37,37,37,37 | 0 |
| 54 | MG | AA | 2041 | 1/1 | 0.94 | 0.04 | 40,40,40,40 | 0 |
| 54 | MG | DB | 3026 | 1/1 | 0.94 | 0.14 | 41,41,41,41 | 0 |
| 54 | MG | AA | 2055 | 1/1 | 0.94 | 0.11 | 54,54,54,54 | 0 |
| 54 | MG | DB | 3104 | 1/1 | 0.94 | 0.09 | 28,28,28,28 | 0 |
| 54 | MG | BB | 3019 | 1/1 | 0.94 | 0.07 | 37,37,37,37 | 0 |
| 54 | MG | BB | 3080 | 1/1 | 0.94 | 0.09 | 57,57,57,57 | 0 |
| 54 | MG | DB | 3020 | 1/1 | 0.95 | 0.20 | 14,14,14,14 | 0 |
| 54 | MG | BB | 3013 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | CA | 1647 | 1/1 | 0.95 | 0.09 | 102,102,102,102 | 0 |
| 54 | MG | DB | 3096 | 1/1 | 0.95 | 0.16 | 30,30,30,30 | 0 |
| 54 | MG | AA | 2017 | 1/1 | 0.95 | 0.29 | 75,75,75,75 | 0 |
| 54 | MG | BB | 3035 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 54 | MG | DB | 3094 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |
| 54 | MG | AA | 2029 | 1/1 | 0.95 | 0.08 | 40,40,40,40 | 0 |
| 54 | MG | CA | 1603 | 1/1 | 0.95 | 0.10 | 29,29,29,29 | 0 |
| 54 | MG | DB | 3061 | 1/1 | 0.95 | 0.05 | 51,51,51,51 | 0 |
| 54 | MG | CA | 1614 | 1/1 | 0.95 | 0.12 | 58,58,58,58 | 0 |
| 54 | MG | DB | 3028 | 1/1 | 0.95 | 0.14 | 29,29,29,29 | 0 |
| 54 | MG | BB | 3050 | 1/1 | 0.95 | 0.11 | 28,28,28,28 | 0 |
| 54 | MG | DB | 3004 | 1/1 | 0.95 | 0.15 | 17,17,17,17 | 0 |
| 54 | MG | BB | 3048 | 1/1 | 0.95 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | BB | 3055 | 1/1 | 0.95 | 0.18 | 41,41,41,41 | 0 |
| 54 | MG | AA | 2005 | 1/1 | 0.95 | 0.07 | 36,36,36,36 | 0 |
| 54 | MG | CA | 1640 | 1/1 | 0.95 | 0.11 | 43,43,43,43 | 0 |
| 54 | MG | AA | 2010 | 1/1 | 0.95 | 0.07 | 36,36,36,36 | 0 |
| 54 | MG | BB | 3026 | 1/1 | 0.95 | 0.09 | 28,28,28,28 | 0 |
| 54 | MG | DB | 3070 | 1/1 | 0.95 | 0.12 | 26,26,26,26 | 0 |
| 54 | MG | DB | 3049 | 1/1 | 0.95 | 0.11 | 26,26,26,26 | 0 |
| 54 | MG | CA | 1617 | 1/1 | 0.95 | 0.12 | 21,21,21,21 | 0 |
| 54 | MG | BB | 3065 | 1/1 | 0.95 | 0.06 | 40,40,40,40 | 0 |
| 54 | MG | CA | 1609 | 1/1 | 0.95 | 0.11 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | BB | 3001 | 1/1 | 0.95 | 0.08 | 35,35,35,35 | 0 |
| 54 | MG | DB | 3023 | 1/1 | 0.95 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | BB | 3004 | 1/1 | 0.95 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | BB | 3071 | 1/1 | 0.96 | 0.07 | 25,25,25,25 | 0 |
| 54 | MG | CA | 1613 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 54 | MG | DB | 3053 | 1/1 | 0.96 | 0.09 | 28,28,28,28 | 0 |
| 54 | MG | CA | 1642 | 1/1 | 0.96 | 0.04 | 63,63,63,63 | 0 |
| 54 | MG | BB | 3109 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 54 | MG | BB | 3088 | 1/1 | 0.96 | 0.09 | 75,75,75,75 | 0 |
| 54 | MG | CA | 1607 | 1/1 | 0.96 | 0.06 | 37,37,37,37 | 0 |
| 54 | MG | DB | 3019 | 1/1 | 0.96 | 0.07 | 21,21,21,21 | 0 |
| 54 | MG | BB | 3011 | 1/1 | 0.96 | 0.09 | 30,30,30,30 | 0 |
| 54 | MG | AA | 2048 | 1/1 | 0.96 | 0.11 | 27,27,27,27 | 0 |
| 54 | MG | CA | 1650 | 1/1 | 0.96 | 0.16 | 41,41,41,41 | 0 |
| 54 | MG | DB | 3093 | 1/1 | 0.96 | 0.12 | 6,6,6,6 | 0 |
| 54 | MG | CA | 1630 | 1/1 | 0.96 | 0.10 | 39,39,39,39 | 0 |
| 54 | MG | DB | 3071 | 1/1 | 0.96 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | BB | 3022 | 1/1 | 0.96 | 0.05 | 44,44,44,44 | 0 |
| 54 | MG | CA | 1632 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 54 | MG | CA | 1651 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | CA | 1612 | 1/1 | 0.96 | 0.08 | 46,46,46,46 | 0 |
| 54 | MG | BB | 3103 | 1/1 | 0.96 | 0.09 | 20,20,20,20 | 0 |
| 54 | MG | BB | 3021 | 1/1 | 0.96 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | DB | 3078 | 1/1 | 0.96 | 0.11 | 45,45,45,45 | 0 |
| 54 | MG | DB | 3008 | 1/1 | 0.96 | 0.14 | 33,33,33,33 | 0 |
| 54 | MG | CA | 1646 | 1/1 | 0.96 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | DB | 3084 | 1/1 | 0.96 | 0.20 | 34,34,34,34 | 0 |
| 54 | MG | BB | 3064 | 1/1 | 0.96 | 0.10 | 31,31,31,31 | 0 |
| 54 | MG | DB | 3072 | 1/1 | 0.96 | 0.10 | 23,23,23,23 | 0 |
| 54 | MG | BB | 3075 | 1/1 | 0.96 | 0.14 | 37,37,37,37 | 0 |
| 54 | MG | DB | 3107 | 1/1 | 0.96 | 0.06 | 34,34,34,34 | 0 |
| 54 | MG | AA | 2040 | 1/1 | 0.96 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | DB | 3065 | 1/1 | 0.96 | 0.09 | 12,12,12,12 | 0 |
| 54 | MG | DB | 3101 | 1/1 | 0.96 | 0.16 | 5,5,5,5 | 0 |
| 54 | MG | DB | 3046 | 1/1 | 0.96 | 0.06 | 22,22,22,22 | 0 |
| 54 | MG | BB | 3082 | 1/1 | 0.96 | 0.15 | 38,38,38,38 | 0 |
| 54 | MG | BB | 3107 | 1/1 | 0.96 | 0.08 | 31,31,31,31 | 0 |
| 54 | MG | DB | 3005 | 1/1 | 0.96 | 0.05 | 56,56,56,56 | 0 |
| 54 | MG | AA | 2054 | 1/1 | 0.96 | 0.05 | 49,49,49,49 | 0 |
| 54 | MG | BB | 3067 | 1/1 | 0.96 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | BB | 3074 | 1/1 | 0.96 | 0.14 | 21,21,21,21 | 0 |
| 54 | MG | DB | 3042 | 1/1 | 0.96 | 0.11 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | DB | 3044 | 1/1 | 0.97 | 0.06 | 12,12,12,12 | 0 |
| 54 | MG | BB | 3036 | 1/1 | 0.97 | 0.08 | 39,39,39,39 | 0 |
| 54 | MG | AA | 2004 | 1/1 | 0.97 | 0.19 | 36,36,36,36 | 0 |
| 54 | MG | DB | 3086 | 1/1 | 0.97 | 0.19 | 26,26,26,26 | 0 |
| 54 | MG | BB | 3105 | 1/1 | 0.97 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | DB | 3089 | 1/1 | 0.97 | 0.21 | 50,50,50,50 | 0 |
| 54 | MG | AA | 2009 | 1/1 | 0.97 | 0.12 | 21,21,21,21 | 0 |
| 54 | MG | DB | 3111 | 1/1 | 0.97 | 0.19 | 51,51,51,51 | 0 |
| 54 | MG | CA | 1625 | 1/1 | 0.97 | 0.10 | 19,19,19,19 | 0 |
| 54 | MG | BB | 3083 | 1/1 | 0.97 | 0.10 | 30,30,30,30 | 0 |
| 55 | ZN | D4 | 101 | 1/1 | 0.97 | 0.07 | 55,55,55,55 | 0 |
| 54 | MG | BB | 3066 | 1/1 | 0.97 | 0.07 | 21,21,21,21 | 0 |
| 54 | MG | DB | 3103 | 1/1 | 0.97 | 0.09 | 26,26,26,26 | 0 |
| 54 | MG | AA | 2033 | 1/1 | 0.97 | 0.07 | 40,40,40,40 | 0 |
| 54 | MG | BB | 3043 | 1/1 | 0.97 | 0.16 | 53,53,53,53 | 0 |
| 54 | MG | BB | 3023 | 1/1 | 0.97 | 0.07 | 23,23,23,23 | 0 |
| 54 | MG | DB | 3014 | 1/1 | 0.97 | 0.07 | 21,21,21,21 | 0 |
| 54 | MG | DB | 3038 | 1/1 | 0.97 | 0.15 | 26,26,26,26 | 0 |
| 54 | MG | CA | 1645 | 1/1 | 0.97 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | DB | 3067 | 1/1 | 0.97 | 0.09 | 18,18,18,18 | 0 |
| 54 | MG | BB | 3091 | 1/1 | 0.97 | 0.11 | 31,31,31,31 | 0 |
| 54 | MG | DB | 3069 | 1/1 | 0.97 | 0.13 | 21,21,21,21 | 0 |
| 54 | MG | CA | 1631 | 1/1 | 0.97 | 0.09 | 38,38,38,38 | 0 |
| 54 | MG | BB | 3020 | 1/1 | 0.97 | 0.12 | 20,20,20,20 | 0 |
| 54 | MG | DB | 3031 | 1/1 | 0.97 | 0.09 | 17,17,17,17 | 0 |
| 54 | MG | BB | 3086 | 1/1 | 0.97 | 0.20 | 45,45,45,45 | 0 |
| 54 | MG | BB | 3041 | 1/1 | 0.97 | 0.10 | 22,22,22,22 | 0 |
| 54 | MG | BB | 3058 | 1/1 | 0.97 | 0.14 | 33,33,33,33 | 0 |
| 54 | MG | AA | 2007 | 1/1 | 0.97 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | CA | 1618 | 1/1 | 0.97 | 0.07 | 18,18,18,18 | 0 |
| 54 | MG | DB | 3010 | 1/1 | 0.97 | 0.10 | 19,19,19,19 | 0 |
| 54 | MG | CA | 1655 | 1/1 | 0.97 | 0.09 | 28,28,28,28 | 0 |
| 54 | MG | CA | 1653 | 1/1 | 0.97 | 0.04 | 55,55,55,55 | 0 |
| 54 | MG | DB | 3040 | 1/1 | 0.98 | 0.09 | 9,9,9,9 | 0 |
| 54 | MG | DB | 3041 | 1/1 | 0.98 | 0.13 | 36,36,36,36 | 0 |
| 54 | MG | BB | 3012 | 1/1 | 0.98 | 0.09 | 32,32,32,32 | 0 |
| 54 | MG | DB | 3105 | 1/1 | 0.98 | 0.08 | 32,32,32,32 | 0 |
| 54 | MG | CA | 1602 | 1/1 | 0.98 | 0.20 | 34,34,34,34 | 0 |
| 54 | MG | DB | 3087 | 1/1 | 0.98 | 0.11 | 54,54,54,54 | 0 |
| 54 | MG | CA | 1649 | 1/1 | 0.98 | 0.07 | 80,80,80,80 | 0 |
| 54 | MG | BB | 3098 | 1/1 | 0.98 | 0.13 | 30,30,30,30 | 0 |
| 54 | MG | AA | 2036 | 1/1 | 0.98 | 0.10 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | AA | 2003 | 1/1 | 0.98 | 0.13 | 31,31,31,31 | 0 |
| 54 | MG | DB | 3001 | 1/1 | 0.98 | 0.11 | 9,9,9,9 | 0 |
| 54 | MG | DB | 3002 | 1/1 | 0.98 | 0.06 | 11,11,11,11 | 0 |
| 54 | MG | DB | 3043 | 1/1 | 0.98 | 0.10 | 8,8,8,8 | 0 |
| 54 | MG | DB | 3027 | 1/1 | 0.98 | 0.19 | 27,27,27,27 | 0 |
| 54 | MG | DB | 3035 | 1/1 | 0.98 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | DB | 3021 | 1/1 | 0.98 | 0.12 | 21,21,21,21 | 0 |
| 54 | MG | AA | 2001 | 1/1 | 0.98 | 0.07 | 29,29,29,29 | 0 |
| 54 | MG | DB | 3081 | 1/1 | 0.99 | 0.11 | 17,17,17,17 | 0 |
| 54 | MG | DB | 3098 | 1/1 | 0.99 | 0.10 | 29,29,29,29 | 0 |
| 54 | MG | DB | 3047 | 1/1 | 0.99 | 0.15 | 13,13,13,13 | 0 |
| 54 | MG | BB | 3060 | 1/1 | 0.99 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | DB | 3075 | 1/1 | 0.99 | 0.06 | 33,33,33,33 | 0 |
| 54 | MG | DB | 3009 | 1/1 | 0.99 | 0.15 | 17,17,17,17 | 0 |
| 54 | MG | DB | 3007 | 1/1 | 0.99 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | CA | 1604 | 1/1 | 0.99 | 0.10 | 36,36,36,36 | 0 |
| 54 | MG | CA | 1639 | 1/1 | 0.99 | 0.12 | 24,24,24,24 | 0 |
| 54 | MG | DB | 3036 | 1/1 | 0.99 | 0.12 | 25,25,25,25 | 0 |
| 54 | MG | DB | 3076 | 1/1 | 0.99 | 0.07 | 17,17,17,17 | 0 |

6.5 Other polymers

There are no such residues in this entry.