



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:17 am GMT

PDB ID : 4V9P
Title : Control of ribosomal subunit rotation by elongation factor G
Authors : Pulk, A.; Cate, J.H.D.
Deposited on : 2013-05-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

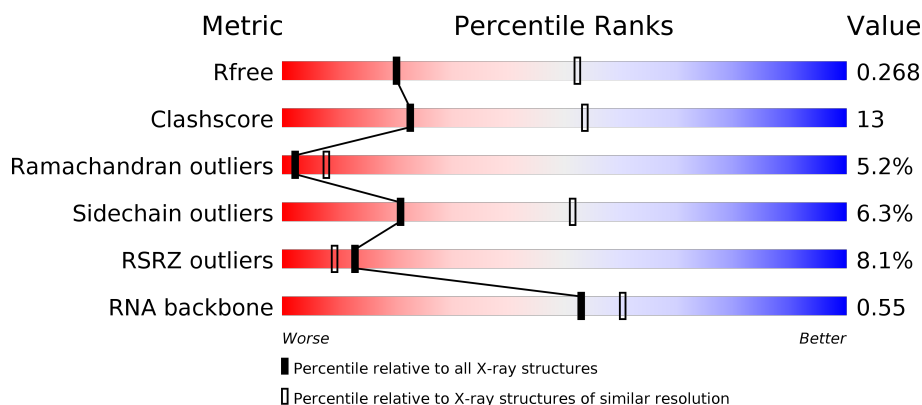
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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

















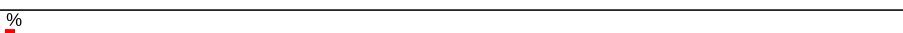




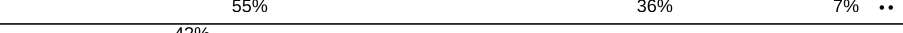





| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1586 (2.90-2.90) |
| Clashscore | 112137 | 1807 (2.90-2.90) |
| Ramachandran outliers | 110173 | 1768 (2.90-2.90) |
| Sidechain outliers | 110143 | 1770 (2.90-2.90) |
| RSRZ outliers | 101464 | 1596 (2.90-2.90) |
| RNA backbone | 2435 | 1004 (3.20-2.60) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | AA | 2904 | <div> <div>2%</div> <div>47% 38% 11% ..</div> </div> |
| 1 | CA | 2904 | <div> <div>2%</div> <div>53% 33% 11% ..</div> </div> |
| 1 | EA | 2904 | <div> <div>2%</div> <div>50% 34% 12% ..</div> </div> |
| 1 | GA | 2904 | <div> <div>2%</div> <div>54% 33% 11% ..</div> </div> |





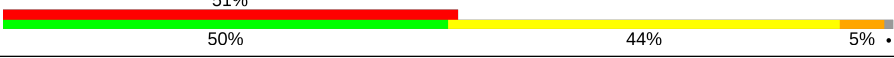
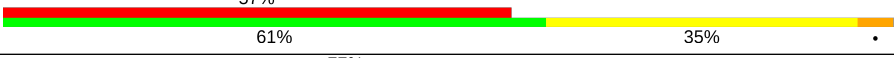
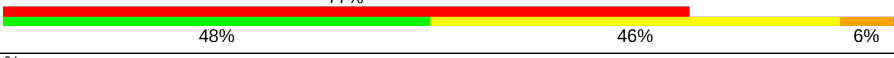
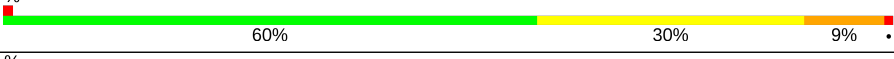

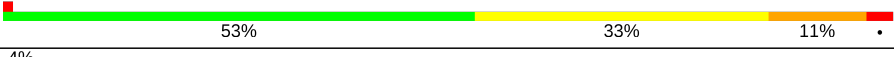

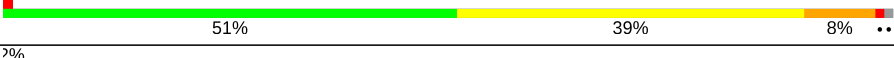








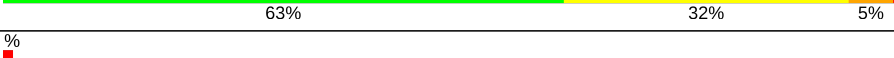
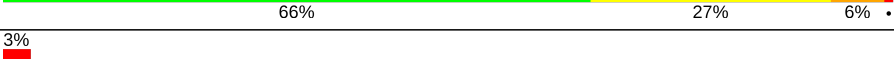

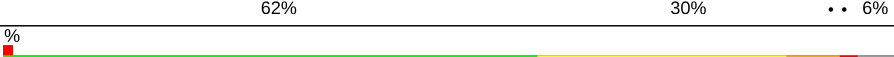

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | AB | 120 |  |
| 2 | CB | 120 |  |
| 2 | EB | 120 |  |
| 2 | GB | 120 |  |
| 3 | AC | 273 |  |
| 3 | CC | 273 |  |
| 3 | EC | 273 |  |
| 3 | GC | 273 |  |
| 4 | AD | 209 |  |
| 4 | CD | 209 |  |
| 4 | ED | 209 |  |
| 4 | GD | 209 |  |
| 5 | AE | 201 |  |
| 5 | CE | 201 |  |
| 5 | EE | 201 |  |
| 5 | GE | 201 |  |
| 6 | AF | 179 |  |
| 6 | CF | 179 |  |
| 6 | EF | 179 |  |
| 6 | GF | 179 |  |
| 7 | AG | 177 |  |
| 7 | CG | 177 |  |
| 7 | EG | 177 |  |
| 7 | GG | 177 |  |
| 8 | AH | 50 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 8 | CH | 50 |  |
| 8 | EH | 50 |  |
| 8 | GH | 50 |  |
| 9 | AI | 142 |  |
| 9 | CI | 142 |  |
| 9 | EI | 142 |  |
| 9 | GI | 142 |  |
| 10 | AJ | 142 |  |
| 10 | CJ | 142 |  |
| 10 | EJ | 142 |  |
| 10 | GJ | 142 |  |
| 11 | AK | 123 |  |
| 11 | CK | 123 |  |
| 11 | EK | 123 |  |
| 11 | GK | 123 |  |
| 12 | AL | 144 |  |
| 12 | CL | 144 |  |
| 12 | EL | 144 |  |
| 12 | GL | 144 |  |
| 13 | AM | 136 |  |
| 13 | CM | 136 |  |
| 13 | EM | 136 |  |
| 13 | GM | 136 |  |
| 14 | AN | 127 |  |
| 14 | CN | 127 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14 | EN | 127 | |
| 14 | GN | 127 | |
| 15 | AO | 117 | |
| 15 | CO | 117 | |
| 15 | EO | 117 | |
| 15 | GO | 117 | |
| 16 | AP | 115 | |
| 16 | CP | 115 | |
| 16 | EP | 115 | |
| 16 | GP | 115 | |
| 17 | AQ | 118 | |
| 17 | CQ | 118 | |
| 17 | EQ | 118 | |
| 17 | GQ | 118 | |
| 18 | AR | 103 | |
| 18 | CR | 103 | |
| 18 | ER | 103 | |
| 18 | GR | 103 | |
| 19 | AS | 110 | |
| 19 | CS | 110 | |
| 19 | ES | 110 | |
| 19 | GS | 110 | |
| 20 | AT | 100 | |
| 20 | CT | 100 | |
| 20 | ET | 100 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 20 | GT | 100 | |
| 21 | AU | 104 | |
| 21 | CU | 104 | |
| 21 | EU | 104 | |
| 21 | GU | 104 | |
| 22 | AV | 94 | |
| 22 | CV | 94 | |
| 22 | EV | 94 | |
| 22 | GV | 94 | |
| 23 | AW | 85 | |
| 23 | CW | 85 | |
| 23 | EW | 85 | |
| 23 | GW | 85 | |
| 24 | AX | 78 | |
| 24 | CX | 78 | |
| 24 | EX | 78 | |
| 24 | GX | 78 | |
| 25 | AY | 63 | |
| 25 | CY | 63 | |
| 25 | EY | 63 | |
| 25 | GY | 63 | |
| 26 | AZ | 59 | |
| 26 | CZ | 59 | |
| 26 | EZ | 59 | |
| 26 | GZ | 59 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27 | A0 | 57 | |
| 27 | C0 | 57 | |
| 27 | E0 | 57 | |
| 27 | G0 | 57 | |
| 28 | A1 | 55 | |
| 28 | C1 | 55 | |
| 28 | E1 | 55 | |
| 28 | G1 | 55 | |
| 29 | A2 | 46 | |
| 29 | C2 | 46 | |
| 29 | E2 | 46 | |
| 29 | G2 | 46 | |
| 30 | A3 | 65 | |
| 30 | C3 | 65 | |
| 30 | E3 | 65 | |
| 30 | G3 | 65 | |
| 31 | A4 | 38 | |
| 31 | C4 | 38 | |
| 31 | E4 | 38 | |
| 31 | G4 | 38 | |
| 32 | A5 | 165 | |
| 32 | E5 | 165 | |
| 33 | BA | 1542 | |
| 33 | DA | 1542 | |
| 33 | FA | 1542 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 33 | HA | 1542 | |
| 34 | BB | 241 | |
| 34 | DB | 241 | |
| 34 | FB | 241 | |
| 34 | HB | 241 | |
| 35 | BC | 233 | |
| 35 | DC | 233 | |
| 35 | FC | 233 | |
| 35 | HC | 233 | |
| 36 | BD | 206 | |
| 36 | DD | 206 | |
| 36 | FD | 206 | |
| 36 | HD | 206 | |
| 37 | BE | 167 | |
| 37 | DE | 167 | |
| 37 | FE | 167 | |
| 37 | HE | 167 | |
| 38 | BF | 135 | |
| 38 | DF | 135 | |
| 38 | FF | 135 | |
| 38 | HF | 135 | |
| 39 | BG | 179 | |
| 39 | DG | 179 | |
| 39 | FG | 179 | |
| 39 | HG | 179 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | BH | 130 | |
| 40 | DH | 130 | |
| 40 | FH | 130 | |
| 40 | HH | 130 | |
| 41 | BI | 130 | |
| 41 | DI | 130 | |
| 41 | FI | 130 | |
| 41 | HI | 130 | |
| 42 | BJ | 103 | |
| 42 | DJ | 103 | |
| 42 | FJ | 103 | |
| 42 | HJ | 103 | |
| 43 | BK | 129 | |
| 43 | DK | 129 | |
| 43 | FK | 129 | |
| 43 | HK | 129 | |
| 44 | BL | 124 | |
| 44 | DL | 124 | |
| 44 | FL | 124 | |
| 44 | HL | 124 | |
| 45 | BM | 118 | |
| 45 | DM | 118 | |
| 45 | FM | 118 | |
| 45 | HM | 118 | |
| 46 | BN | 101 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 46 | DN | 101 | |
| 46 | FN | 101 | |
| 46 | HN | 101 | |
| 47 | BO | 89 | |
| 47 | DO | 89 | |
| 47 | FO | 89 | |
| 47 | HO | 89 | |
| 48 | BP | 82 | |
| 48 | DP | 82 | |
| 48 | FP | 82 | |
| 48 | HP | 82 | |
| 49 | BQ | 84 | |
| 49 | DQ | 84 | |
| 49 | FQ | 84 | |
| 49 | HQ | 84 | |
| 50 | BR | 75 | |
| 50 | DR | 75 | |
| 50 | FR | 75 | |
| 50 | HR | 75 | |
| 51 | BS | 92 | |
| 51 | DS | 92 | |
| 51 | FS | 92 | |
| 51 | HS | 92 | |
| 52 | BT | 87 | |
| 52 | DT | 87 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52 | FT | 87 | |
| 52 | HT | 87 | |
| 53 | BU | 71 | |
| 53 | DU | 71 | |
| 53 | FU | 71 | |
| 53 | HU | 71 | |
| 54 | BV | 704 | |
| 54 | DV | 704 | |
| 54 | FV | 704 | |
| 54 | HV | 704 | |
| 55 | BW | 6 | |
| 55 | DW | 6 | |
| 55 | FW | 6 | |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | AA | 3009 | - | - | - | X |
| 56 | MG | AA | 3017 | - | - | - | X |
| 56 | MG | AA | 3028 | - | - | - | X |
| 56 | MG | AA | 3083 | - | - | - | X |
| 56 | MG | AA | 3098 | - | - | - | X |
| 56 | MG | AA | 3102 | - | - | - | X |
| 56 | MG | AA | 3107 | - | - | - | X |
| 56 | MG | AA | 3109 | - | - | - | X |
| 56 | MG | AC | 301 | - | - | - | X |
| 56 | MG | AC | 303 | - | - | - | X |
| 56 | MG | BA | 1606 | - | - | - | X |
| 56 | MG | BA | 1612 | - | - | - | X |
| 56 | MG | BA | 1614 | - | - | - | X |
| 56 | MG | BA | 1615 | - | - | - | X |
| 56 | MG | BA | 1619 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | BA | 1622 | - | - | - | X |
| 56 | MG | CA | 3028 | - | - | - | X |
| 56 | MG | CA | 3037 | - | - | - | X |
| 56 | MG | CA | 3040 | - | - | - | X |
| 56 | MG | CA | 3073 | - | - | - | X |
| 56 | MG | CA | 3077 | - | - | - | X |
| 56 | MG | CA | 3079 | - | - | - | X |
| 56 | MG | CA | 3119 | - | - | - | X |
| 56 | MG | DA | 1616 | - | - | - | X |
| 56 | MG | DA | 1621 | - | - | - | X |
| 56 | MG | DA | 1628 | - | - | - | X |
| 56 | MG | DA | 1640 | - | - | - | X |
| 56 | MG | EA | 3009 | - | - | - | X |
| 56 | MG | EA | 3025 | - | - | - | X |
| 56 | MG | EA | 3042 | - | - | - | X |
| 56 | MG | EA | 3049 | - | - | - | X |
| 56 | MG | EA | 3064 | - | - | - | X |
| 56 | MG | EA | 3078 | - | - | - | X |
| 56 | MG | EA | 3099 | - | - | - | X |
| 56 | MG | EA | 3114 | - | - | - | X |
| 56 | MG | EA | 3118 | - | - | - | X |
| 56 | MG | EA | 3129 | - | - | - | X |
| 56 | MG | EA | 3131 | - | - | - | X |
| 56 | MG | EQ | 201 | - | - | - | X |
| 56 | MG | FA | 1609 | - | - | - | X |
| 56 | MG | FA | 1621 | - | - | - | X |
| 56 | MG | FA | 1623 | - | - | - | X |
| 56 | MG | FA | 1627 | - | - | - | X |
| 56 | MG | GA | 3004 | - | - | - | X |
| 56 | MG | GA | 3014 | - | - | - | X |
| 56 | MG | GA | 3030 | - | - | - | X |
| 56 | MG | GA | 3040 | - | - | - | X |
| 56 | MG | GA | 3060 | - | - | - | X |
| 56 | MG | GA | 3063 | - | - | - | X |
| 56 | MG | GA | 3078 | - | - | - | X |
| 56 | MG | GA | 3083 | - | - | - | X |
| 56 | MG | GA | 3102 | - | - | - | X |
| 56 | MG | GA | 3103 | - | - | - | X |
| 56 | MG | GA | 3108 | - | - | - | X |
| 56 | MG | GA | 3110 | - | - | - | X |
| 56 | MG | GA | 3114 | - | - | - | X |
| 56 | MG | GA | 3129 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | HA | 1610 | - | - | - | X |
| 56 | MG | HA | 1612 | - | - | - | X |
| 56 | MG | HA | 1626 | - | - | - | X |
| 56 | MG | HA | 1632 | - | - | - | X |

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 590573 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 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1 | AA | 2854 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61274 | 27334 | 11279 | 19807 | 2854 | | | |
| 1 | CA | 2854 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61274 | 27334 | 11279 | 19807 | 2854 | | | |
| 1 | EA | 2854 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61274 | 27334 | 11279 | 19807 | 2854 | | | |
| 1 | GA | 2854 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61274 | 27334 | 11279 | 19807 | 2854 | | | |

- Molecule 2 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2 | AB | 118 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | | |
| 2 | CB | 118 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | | |
| 2 | EB | 118 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | | |
| 2 | GB | 118 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | | |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |
| 3 | CC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |
| 3 | EC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |
| 3 | GC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2082 | 1288 | 423 | 364 | 7 | | | |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4 | AD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |
| 4 | CD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |
| 4 | ED | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |
| 4 | GD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 5 | CE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 5 | EE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 5 | GE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | | |
| 6 | CF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | | |
| 6 | EF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | | |
| 6 | GF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1410 | 899 | 249 | 256 | 6 | | | |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 7 | CG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 7 | EG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | GG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | AH | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 247 | 68 | 68 | 1 | | | |
| 8 | CH | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 247 | 68 | 68 | 1 | | | |
| 8 | EH | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 247 | 68 | 68 | 1 | | | |
| 8 | GH | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 384 | 247 | 68 | 68 | 1 | | | |

- Molecule 9 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | AI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 9 | CI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 9 | EI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |
| 9 | GI | 141 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1032 | 651 | 179 | 196 | 6 | | | |

- Molecule 10 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |
| 10 | CJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |
| 10 | EJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |
| 10 | GJ | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

- Molecule 11 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | | |
| 11 | CK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | | |
| 11 | EK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | | |
| 11 | GK | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | | |

- Molecule 12 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |
| 12 | CL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |
| 12 | EL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |
| 12 | GL | 143 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1045 | 649 | 206 | 189 | 1 | | | |

- Molecule 13 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |
| 13 | CM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |
| 13 | EM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |
| 13 | GM | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1074 | 686 | 205 | 177 | 6 | | | |

- Molecule 14 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | AN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |
| 14 | CN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |
| 14 | EN | 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 |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | GN | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |

- Molecule 15 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 15 | AO | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |
| 15 | CO | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |
| 15 | EO | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |
| 15 | GO | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |

- Molecule 16 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |
| 16 | CP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |
| 16 | EP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |
| 16 | GP | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |

- Molecule 17 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 17 | AQ | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |
| 17 | CQ | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |
| 17 | EQ | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |
| 17 | GQ | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |

- Molecule 18 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18 | AR | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |
| 18 | CR | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |
| 18 | ER | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |
| 18 | GR | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |

- Molecule 19 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |
| 19 | CS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |
| 19 | ES | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |
| 19 | GS | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |

- Molecule 20 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |
| 20 | CT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |
| 20 | ET | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |
| 20 | GT | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 738 | 466 | 139 | 131 | 2 | | | |

- Molecule 21 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 21 | AU | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | |
| 21 | CU | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | |
| 21 | EU | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 21 | GU | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 779 | 492 | 146 | 141 | | | |

- Molecule 22 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | AV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 22 | CV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 22 | EV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 22 | GV | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- Molecule 23 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | AW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |
| 23 | CW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |
| 23 | EW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |
| 23 | GW | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 596 | 367 | 120 | 108 | 1 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24 | AX | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 24 | CX | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 24 | EX | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 24 | GX | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 25 | AY | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |
| 25 | CY | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |
| 25 | EY | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |
| 25 | GY | 63 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 509 | 313 | 99 | 95 | 2 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | AZ | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |
| 26 | CZ | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |
| 26 | EZ | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |
| 26 | GZ | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27 | A0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 27 | C0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 27 | E0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 27 | G0 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 28 | A1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |
| 28 | C1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |
| 28 | E1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 28 | G1 | 50 | Total | C | N | O | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 29 | A2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 29 | C2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 29 | E2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 29 | G2 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30 | A3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 30 | C3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 30 | E3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 30 | G3 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31 | A4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 31 | C4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 31 | E4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 31 | G4 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | A5 | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 705 | 196 | 209 | 7 | | | |
| 32 | E5 | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1092 | 691 | 192 | 202 | 7 | | | |

- Molecule 33 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 33 | BA | 1533 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32895 | 14671 | 6036 | 10655 | 1533 | | | |
| 33 | DA | 1533 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32895 | 14671 | 6036 | 10655 | 1533 | | | |
| 33 | FA | 1533 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32895 | 14671 | 6036 | 10655 | 1533 | | | |
| 33 | HA | 1533 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32895 | 14671 | 6036 | 10655 | 1533 | | | |

- Molecule 34 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 34 | BB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |
| 34 | DB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |
| 34 | FB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |
| 34 | HB | 218 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1704 | 1081 | 305 | 311 | 7 | | | |

- Molecule 35 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35 | BC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | | |
| 35 | DC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | | |
| 35 | FC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | | |
| 35 | HC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1028 | 305 | 288 | 3 | | | |

- Molecule 36 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 36 | BD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |
| 36 | DD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |
| 36 | FD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |
| 36 | HD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |

- Molecule 37 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | BE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |
| 37 | DE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |
| 37 | FE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |
| 37 | HE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |

- Molecule 38 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38 | BF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |
| 38 | DF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |
| 38 | FF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |
| 38 | HF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |

- Molecule 39 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | BG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | | |
| 39 | DG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | | |
| 39 | FG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | HG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1181 | 735 | 227 | 215 | 4 | | | |

- Molecule 40 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | BH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |
| 40 | DH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |
| 40 | FH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |
| 40 | HH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |

- Molecule 41 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | BI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 41 | DI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 41 | FI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 41 | HI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |

- Molecule 42 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42 | BJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |
| 42 | DJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |
| 42 | FJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |
| 42 | HJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 786 | 493 | 150 | 142 | 1 | | | |

- Molecule 43 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | BK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |
| 43 | DK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |
| 43 | FK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |
| 43 | HK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

- Molecule 44 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | BL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |
| 44 | DL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |
| 44 | FL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |
| 44 | HL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 955 | 590 | 196 | 165 | 4 | | | |

- Molecule 45 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | BM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | | |
| 45 | DM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | | |
| 45 | FM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | | |
| 45 | HM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 883 | 546 | 178 | 156 | 3 | | | |

- Molecule 46 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | BN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |
| 46 | DN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |
| 46 | FN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46 | HN | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 774 | 483 | 160 | 128 | 3 | | | |

- Molecule 47 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47 | BO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |
| 47 | DO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |
| 47 | FO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |
| 47 | HO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |

- Molecule 48 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48 | BP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 48 | DP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 48 | FP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 48 | HP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |

- Molecule 49 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49 | BQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | | |
| 49 | DQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | | |
| 49 | FQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | | |
| 49 | HQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 648 | 411 | 121 | 113 | 3 | | | |

- Molecule 50 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 50 | BR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |
| 50 | DR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |
| 50 | FR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |
| 50 | HR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 455 | 288 | 86 | 81 | | | |

- Molecule 51 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51 | BS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 637 | 408 | 120 | 107 | 2 | | | |
| 51 | DS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 637 | 408 | 120 | 107 | 2 | | | |
| 51 | FS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 637 | 408 | 120 | 107 | 2 | | | |
| 51 | HS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 637 | 408 | 120 | 107 | 2 | | | |

- Molecule 52 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 52 | BT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |
| 52 | DT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |
| 52 | FT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |
| 52 | HT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |

- Molecule 53 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | BU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |
| 53 | DU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |
| 53 | FU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 53 | HU | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 425 | 265 | 86 | 73 | 1 | | | |

- Molecule 54 is a protein called elongation factor G.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 54 | BV | 689 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5319 | 3345 | 919 | 1030 | 25 | | | |
| 54 | DV | 689 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5319 | 3345 | 919 | 1030 | 25 | | | |
| 54 | FV | 689 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5319 | 3345 | 919 | 1030 | 25 | | | |
| 54 | HV | 689 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5319 | 3345 | 919 | 1030 | 25 | | | |

- Molecule 55 is a protein called Viomycin.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 55 | BW | 6 | Total | C | N | O | 0 | 0 | 0 |
| | | | 48 | 25 | 13 | 10 | | | |
| 55 | DW | 6 | Total | C | N | O | 0 | 0 | 0 |
| | | | 48 | 25 | 13 | 10 | | | |
| 55 | FW | 6 | Total | C | N | O | 0 | 0 | 0 |
| | | | 48 | 25 | 13 | 10 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | FA | 41 | Total | Mg | 0 | 0 |
| | | | 41 | 41 | | |
| 56 | BA | 40 | Total | Mg | 0 | 0 |
| | | | 40 | 40 | | |
| 56 | CA | 134 | Total | Mg | 0 | 0 |
| | | | 134 | 134 | | |
| 56 | HE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | AB | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | BL | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | BE | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | GA | 134 | Total 134 | Mg 134 | 0 | 0 |
| 56 | DU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | EB | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | FU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | FV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | C4 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AA | 130 | Total 130 | Mg 130 | 0 | 0 |
| 56 | FE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | GB | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | DV | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | EA | 133 | Total 133 | Mg 133 | 0 | 0 |
| 56 | BU | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | GC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | HT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | GL | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | DA | 42 | Total 42 | Mg 42 | 0 | 0 |
| 56 | EC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | HC | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | BV | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 56 | CB | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | GS | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AC | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | EQ | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | ED | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | CD | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | AT | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | CE | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | A3 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | HA | 40 | Total 40 | Mg 40 | 0 | 0 |
| 56 | HV | 1 | Total 1 | Mg 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57 | E4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | G4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | A4 | 1 | Total 1 | Zn 1 | 0 | 0 |
| 57 | C4 | 1 | Total 1 | Zn 1 | 0 | 0 |

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



- Molecule 59 is water.

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 59 | AP | 1 | Total O 1 1 | 0 | 0 |
| 59 | AQ | 1 | Total O 1 1 | 0 | 0 |
| 59 | AS | 1 | Total O 1 1 | 0 | 0 |
| 59 | AU | 1 | Total O 1 1 | 0 | 0 |
| 59 | A0 | 1 | Total O 1 1 | 0 | 0 |
| 59 | A3 | 1 | Total O 1 1 | 0 | 0 |
| 59 | A4 | 2 | Total O 2 2 | 0 | 0 |
| 59 | BA | 197 | Total O 197 197 | 0 | 0 |
| 59 | BC | 1 | Total O 1 1 | 0 | 0 |
| 59 | BD | 1 | Total O 1 1 | 0 | 0 |
| 59 | BI | 1 | Total O 1 1 | 0 | 0 |
| 59 | BK | 1 | Total O 1 1 | 0 | 0 |
| 59 | BN | 3 | Total O 3 3 | 0 | 0 |
| 59 | BT | 2 | Total O 2 2 | 0 | 0 |
| 59 | BU | 1 | Total O 1 1 | 0 | 0 |
| 59 | BV | 1 | Total O 1 1 | 0 | 0 |
| 59 | CA | 604 | Total O 604 604 | 0 | 0 |
| 59 | CB | 20 | Total O 20 20 | 0 | 0 |
| 59 | CC | 11 | Total O 11 11 | 0 | 0 |
| 59 | CD | 3 | Total O 3 3 | 0 | 0 |
| 59 | CE | 1 | Total O 1 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 59 | CF | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | CJ | 3 | Total 3 | O 3 | 0 | 0 |
| 59 | CL | 6 | Total 6 | O 6 | 0 | 0 |
| 59 | CN | 4 | Total 4 | O 4 | 0 | 0 |
| 59 | CS | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | CT | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | C2 | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | C3 | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | C4 | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | DA | 193 | Total 193 | O 193 | 0 | 0 |
| 59 | DC | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | DE | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | DG | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | DK | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | DL | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | DN | 6 | Total 6 | O 6 | 0 | 0 |
| 59 | DQ | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | DT | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | DU | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | DV | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | EA | 617 | Total 617 | O 617 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 59 | EB | 20 | Total 20 | O 20 | 0 | 0 |
| 59 | EC | 8 | Total 8 | O 8 | 0 | 0 |
| 59 | ED | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | EL | 4 | Total 4 | O 4 | 0 | 0 |
| 59 | EN | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | ER | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | ET | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | EU | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | E0 | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | E3 | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | E4 | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | FA | 198 | Total 198 | O 198 | 0 | 0 |
| 59 | FE | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | FK | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | FN | 3 | Total 3 | O 3 | 0 | 0 |
| 59 | FQ | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | FT | 4 | Total 4 | O 4 | 0 | 0 |
| 59 | FV | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | GA | 607 | Total 607 | O 607 | 0 | 0 |
| 59 | GB | 19 | Total 19 | O 19 | 0 | 0 |
| 59 | GC | 9 | Total 9 | O 9 | 0 | 0 |

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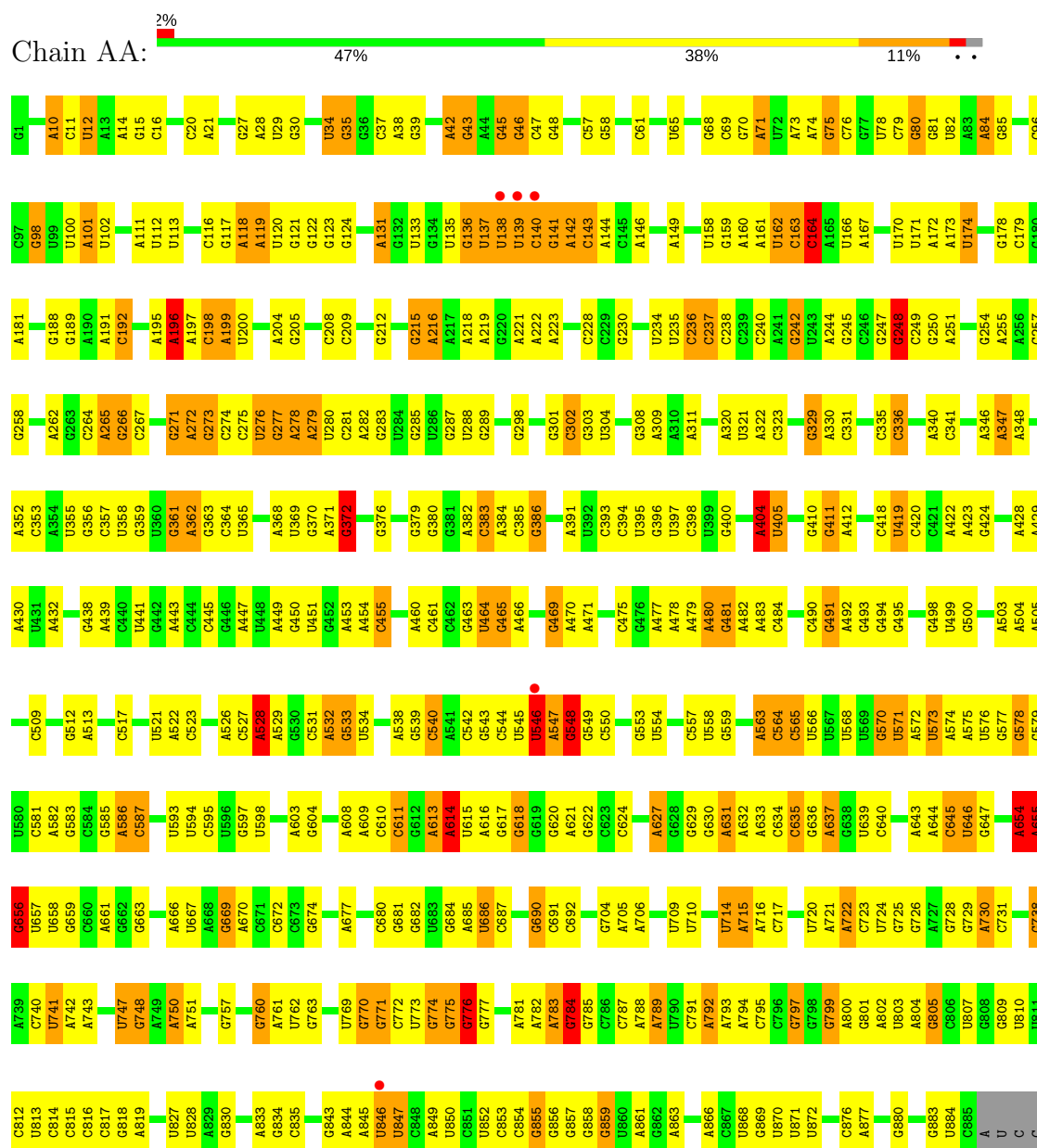
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 59 | GD | 4 | Total 4 | O 4 | 0 | 0 |
| 59 | GE | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | GL | 4 | Total 4 | O 4 | 0 | 0 |
| 59 | GN | 3 | Total 3 | O 3 | 0 | 0 |
| 59 | GQ | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | GR | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | GS | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | GT | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | GU | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | GV | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | G2 | 2 | Total 2 | O 2 | 0 | 0 |
| 59 | G3 | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | G4 | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | HA | 197 | Total 197 | O 197 | 0 | 0 |
| 59 | HD | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | HE | 3 | Total 3 | O 3 | 0 | 0 |
| 59 | HN | 5 | Total 5 | O 5 | 0 | 0 |
| 59 | HT | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | HU | 1 | Total 1 | O 1 | 0 | 0 |
| 59 | HV | 1 | Total 1 | O 1 | 0 | 0 |

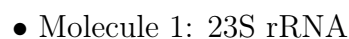
3 Residue-property plots

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: 23S rRNA

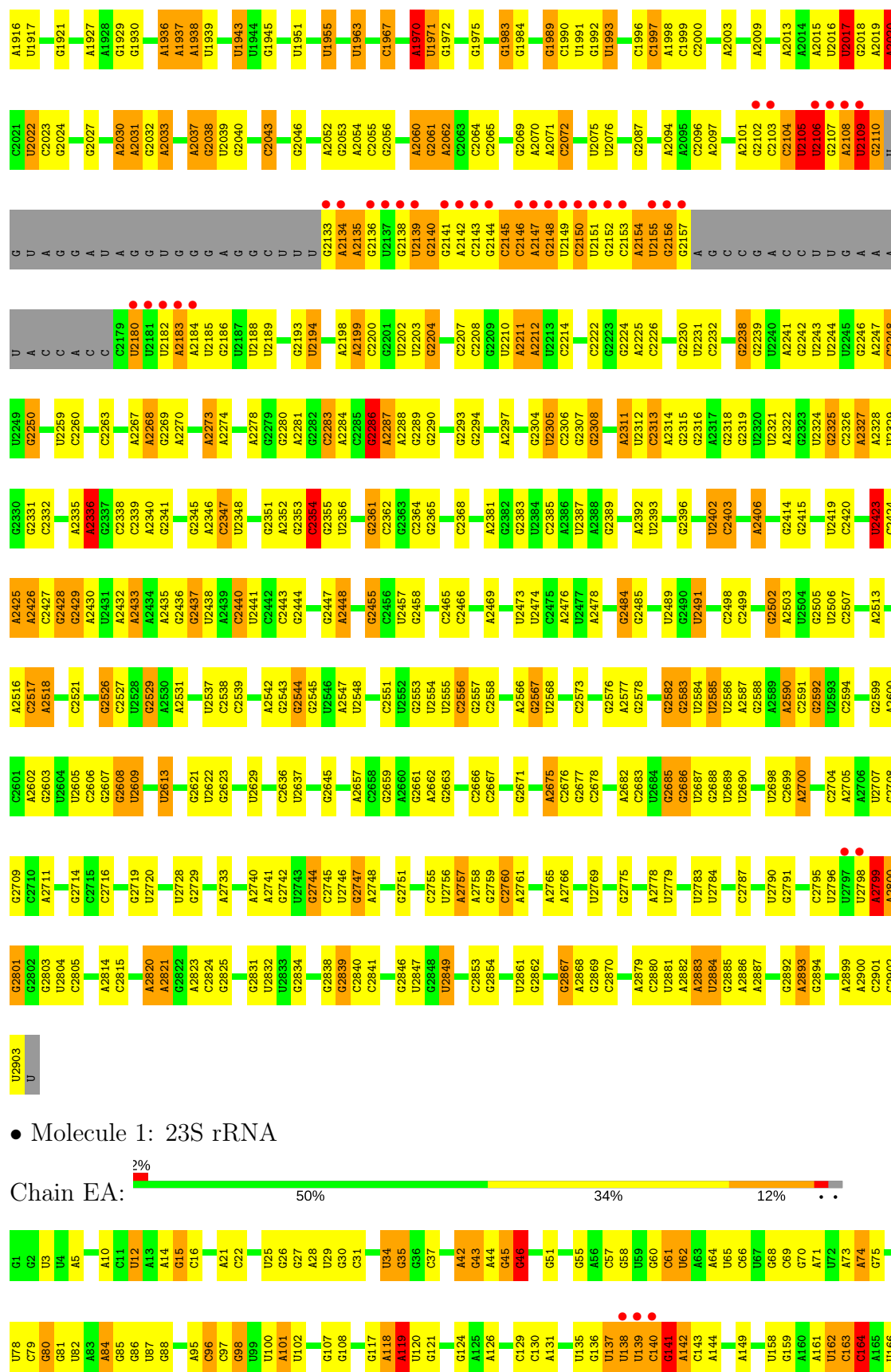


| | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A2108 | C2024 | G1924 | G1805 | C1726 | G1645 | A1548 | U1474 | U1390 | G1300 | G1227 | G1139 | G1063 | A984 | C |
| U2109 | C2025 | C1924 | C1806 | C1727 | C1646 | A1548 | U1475 | U1394 | A1301 | U1231 | C1140 | C1064 | C985 | G |
| G | U2026 | A1927 | G1807 | U1729 | U1647 | A1551 | U1476 | A1395 | C1305 | U1232 | A1141 | U1065 | C989 | A892 |
| U | G2027 | G1928 | A1808 | C1730 | G1649 | G1555 | U1477 | U1396 | C1306 | C1233 | A1142 | U1066 | C991 | C893 |
| A | A2030 | G1929 | G1811 | G1731 | A1650 | G1555 | U1478 | U1397 | A1307 | U1234 | G1146 | G1067 | A896 | A896 |
| A | A2031 | G1930 | G1812 | C1732 | G1651 | C1556 | G1479 | U1398 | A1308 | G1235 | C1150 | A1068 | C897 | C897 |
| G | G2032 | G1935 | U1813 | G1733 | A1652 | C1565 | U1480 | C1399 | G1309 | A1237 | A1151 | G1070 | C898 | C898 |
| G | A2033 | G1813 | G1813 | G1734 | G1653 | C1566 | U1481 | U1400 | C1315 | G1238 | C1151 | C1072 | A910 | A910 |
| A | A2034 | A1936 | A1814 | U1735 | A1654 | A1566 | G1482 | G1401 | G1316 | U1239 | C1161 | C1073 | A911 | A911 |
| U | G2038 | A1937 | A1815 | U1736 | A1655 | G1567 | G1483 | U1402 | U1316 | U1240 | C1161 | C1074 | A1000 | A1000 |
| A | U2039 | A1938 | C1816 | U1737 | C1656 | G1568 | G1484 | A1403 | G1317 | U1240 | C1161 | C1075 | A1001 | A1001 |
| C | A2040 | A1939 | G1817 | G1738 | U1657 | A1569 | U1486 | C1404 | U1318 | U1241 | C1161 | C1076 | A1002 | A1002 |
| G | C2043 | U1943 | U1818 | A1739 | C1658 | C1574 | U1487 | U1405 | C1319 | U1242 | C1161 | C1077 | A1003 | A1003 |
| U | G2047 | U1944 | A1819 | G1740 | A1665 | C1574 | U1488 | U1406 | C1320 | U1243 | C1161 | C1078 | A1004 | A1004 |
| G | C2048 | G1945 | U1820 | U1741 | A1666 | U1578 | C1493 | U1407 | A1321 | U1244 | C1161 | C1079 | A1005 | A1005 |
| G | C2049 | G1946 | U1821 | U1742 | G1667 | U1578 | A1495 | U1408 | A1322 | U1245 | C1161 | C1080 | A1006 | A1006 |
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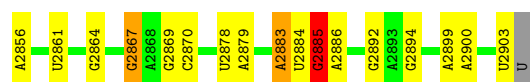
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| C491 | C387 | | G117 | G15 |
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| C494 | U390 | G298 | U120 | |
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| | G400 | G301 | A199 | |
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
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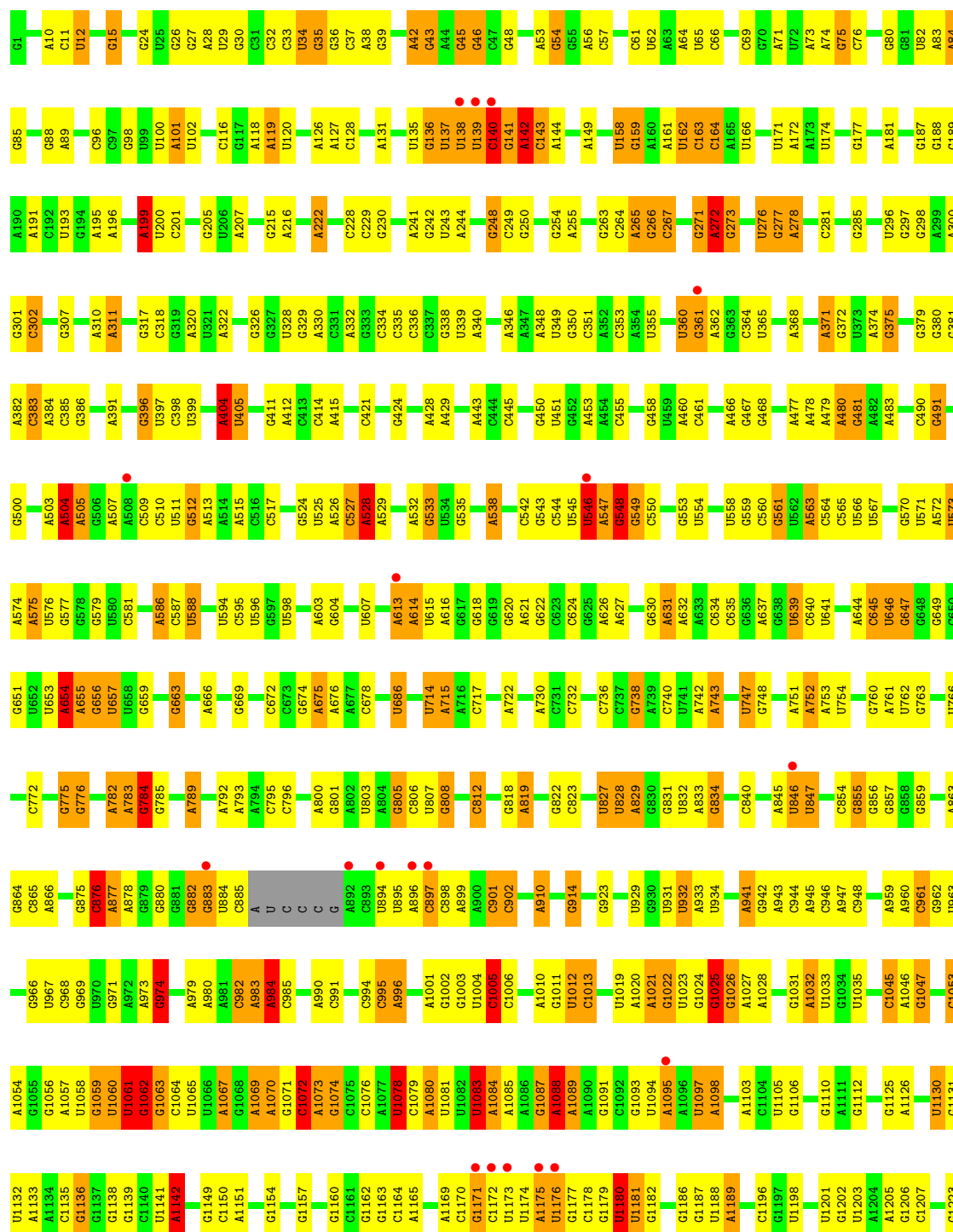




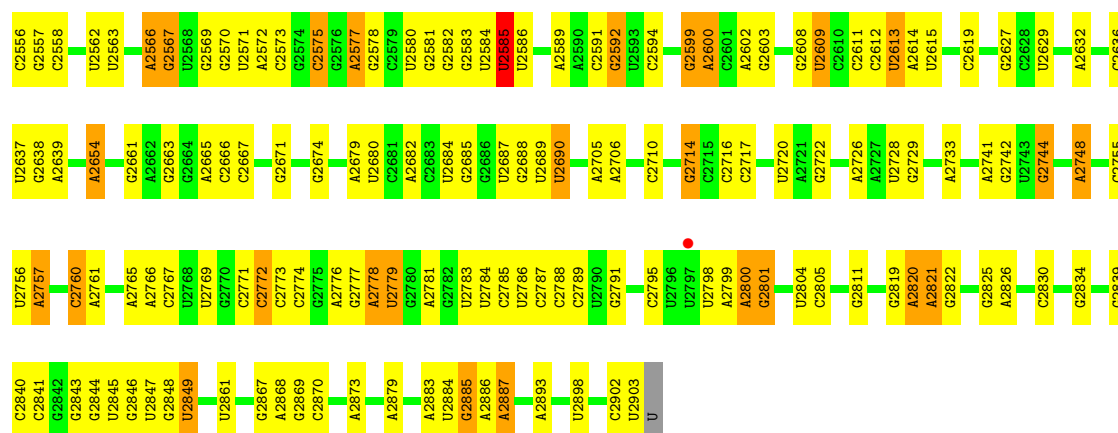




• Molecule 1: 23S rRNA

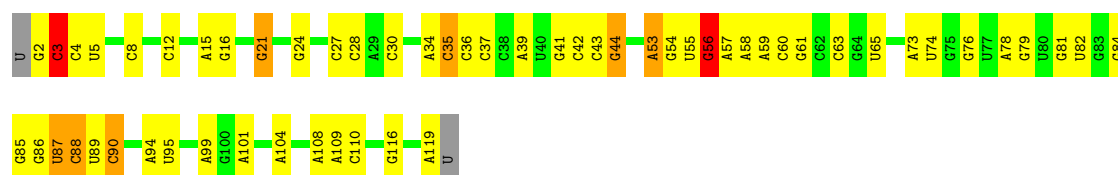


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| U2505 | C2336 | A2336 | C2254 | A | U2109 | G2029 | U1928 | G1826 | A1744 | G1628 | U1515 | A1329 | C1330 | U1255 |
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| C2507 | A2267 | C2339 | A2267 | A | U | A2031 | G1930 | G1828 | A1746 | U1636 | G1524 | A1427 | G1331 | G1256 |
| G2508 | A2268 | A2340 | A2268 | U | G | G2032 | U1931 | G1829 | A1747 | U1636 | G1524 | A1427 | G1331 | G1256 |
| G2509 | G2269 | G2341 | A2269 | A | U | A2033 | U1931 | G1829 | A1747 | U1636 | G1524 | A1427 | G1331 | G1256 |
| C2510 | C2270 | C | A2270 | C | A | U2034 | A1936 | G1831 | A1748 | U1647 | A1532 | A1430 | A1336 | U1258 |
| U2511 | G2271 | C | G2271 | C | A | G | A1937 | G1832 | U1758 | U1648 | U1533 | A1431 | A1360 | U1260 |
| G2512 | G2272 | C | G2272 | C | A | G | A1938 | G1833 | U1759 | U1649 | U1534 | A1432 | G1341 | C1261 |
| A2430 | A2273 | C | A2273 | C | U | U2039 | U1939 | U1834 | C1760 | A1652 | A1535 | A1434 | A1342 | A1262 |
| U2519 | A2274 | C | A2274 | C | U | G2040 | U1940 | U1835 | C1761 | G1653 | G1537 | G1436 | G1343 | U1263 |
| C2520 | C2275 | U2180 | G2275 | U2179 | A | U2041 | U1943 | C1838 | A1762 | A1654 | U1545 | U1437 | A1347 | A1265 |
| G2526 | G2276 | G | G2276 | U2181 | G | C2042 | U1944 | G1839 | G1763 | A1655 | A1548 | U1438 | U1352 | G1266 |
| C2527 | G2277 | U2182 | G2277 | U2182 | U | C2043 | G1945 | G1840 | C1764 | A1656 | A1549 | U1440 | A1353 | A1267 |
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| G2529 | A2281 | A2184 | A2281 | A2184 | G | C2055 | G1954 | C1843 | A1773 | A1664 | G1555 | U1442 | G1355 | C1270 |
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| U2534 | A2284 | U2187 | A2284 | U2187 | G | A2058 | C1967 | A1848 | U1779 | A1669 | C1565 | G1448 | C1362 | U1273 |
| G2447 | C2285 | C | C2285 | C | C | A2059 | A1970 | G1857 | U1780 | U1679 | A1566 | G1449 | A1365 | G1277 |
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| G2550 | G2305 | G2140 | G2305 | G2140 | G | C2073 | U1991 | A1871 | A1791 | C1685 | C1582 | G1471 | A1382 | C1290 |
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| G2553 | G2307 | C2143 | G2307 | C2143 | G | U2077 | C1996 | G1875 | U1796 | G1703 | U1474 | G1473 | A1385 | G1293 |
| U2554 | U2212 | U2144 | U2212 | U2144 | G | C2078 | C1997 | G1875 | G1797 | G1703 | A1597 | U1475 | A1387 | C1293 |
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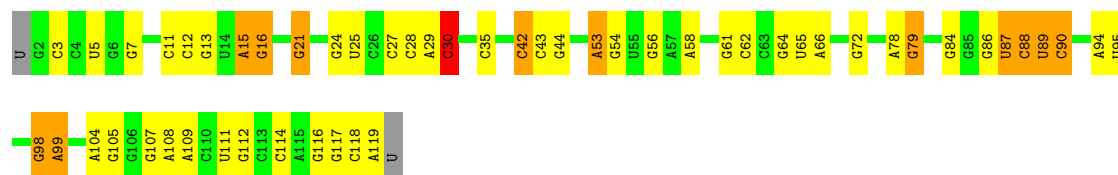
• Molecule 2: 5S rRNA

Chain AB: 51% 40% 6% ..



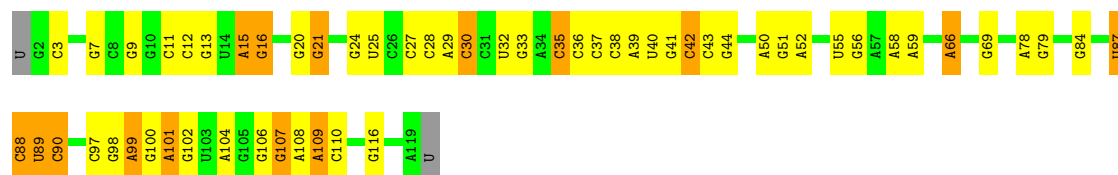
• Molecule 2: 5S rRNA

Chain CB: 54% 33% 10% ..



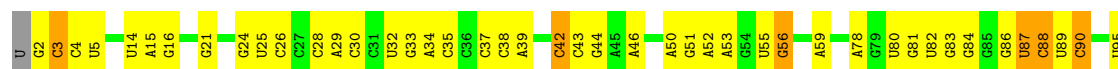
• Molecule 2: 5S rRNA

Chain EB: 51% 35% 13% .



• Molecule 2: 5S rRNA

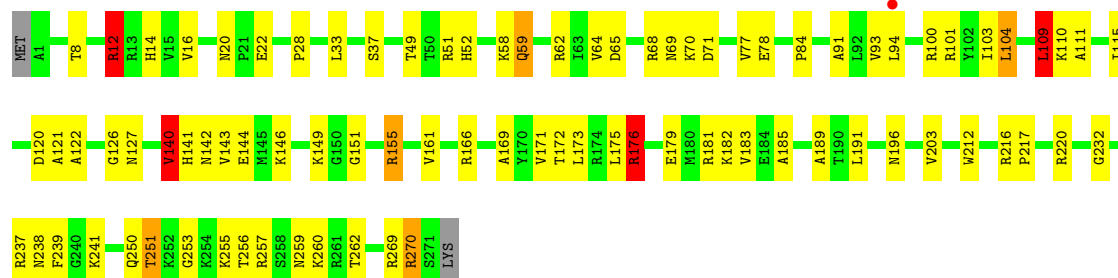
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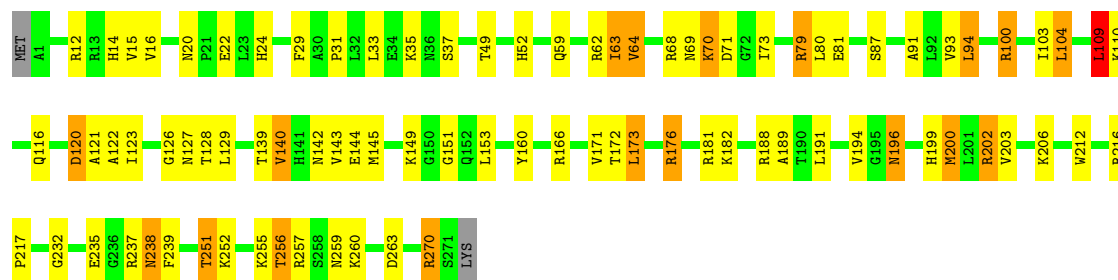
- Molecule 3: 50S ribosomal protein L2

Chain AC: 68% 28%



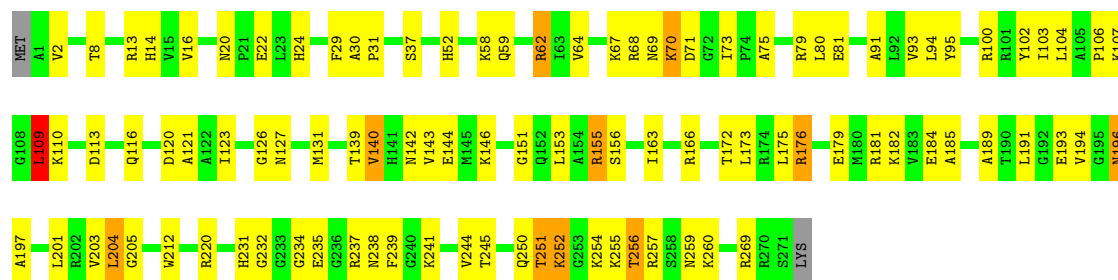
- Molecule 3: 50S ribosomal protein L2

Chain CC: 67% 25% 7%



- Molecule 3: 50S ribosomal protein L2

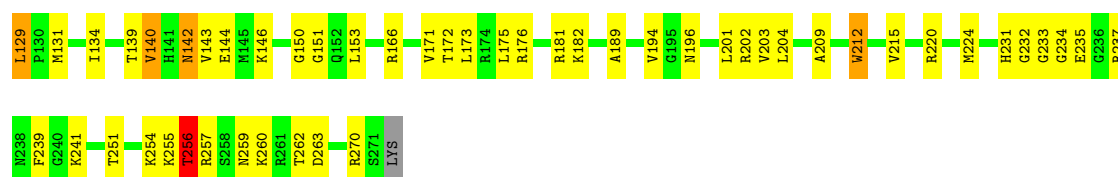
Chain EC: 63% 33%



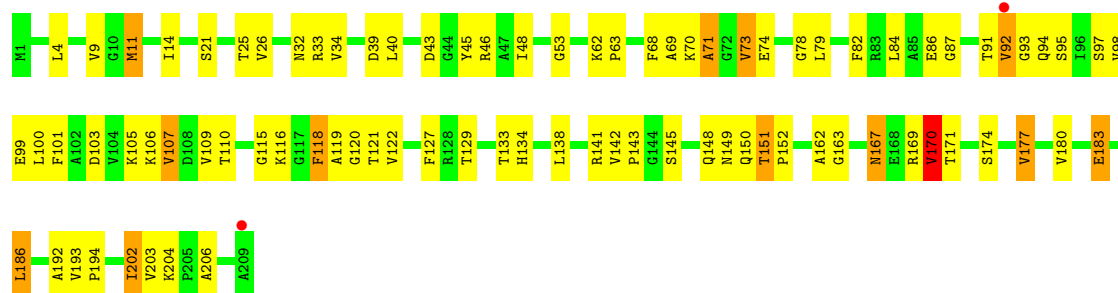
- Molecule 3: 50S ribosomal protein L2

Chain GC: 68% 28%

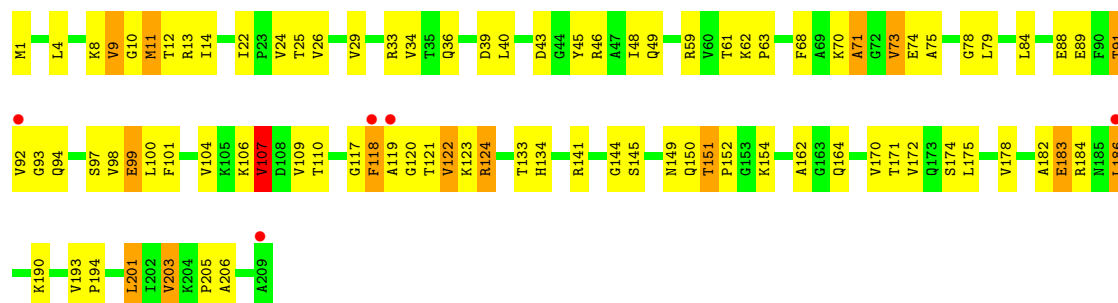




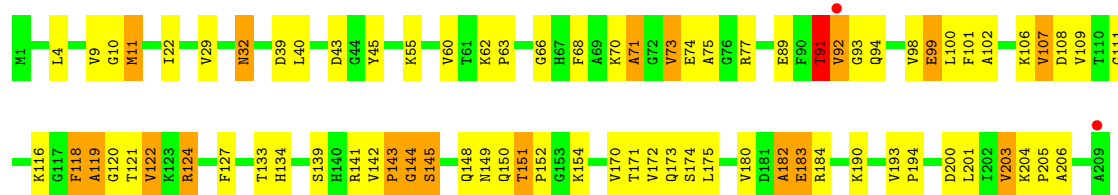
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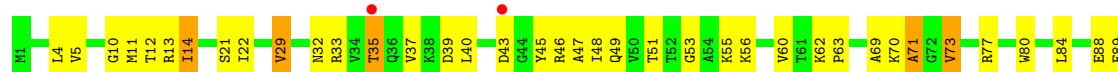
• Molecule 4: 50S ribosomal protein L3

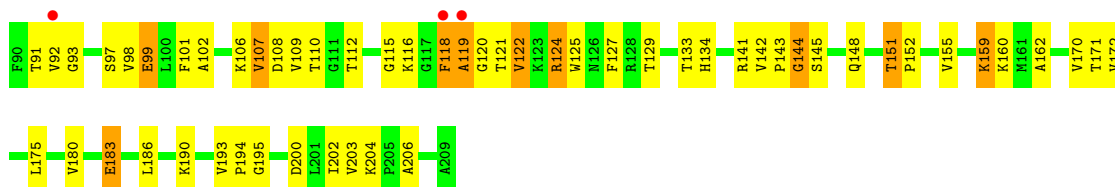


• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

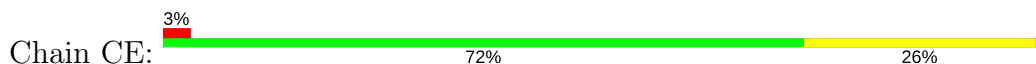




• Molecule 5: 50S ribosomal protein L4



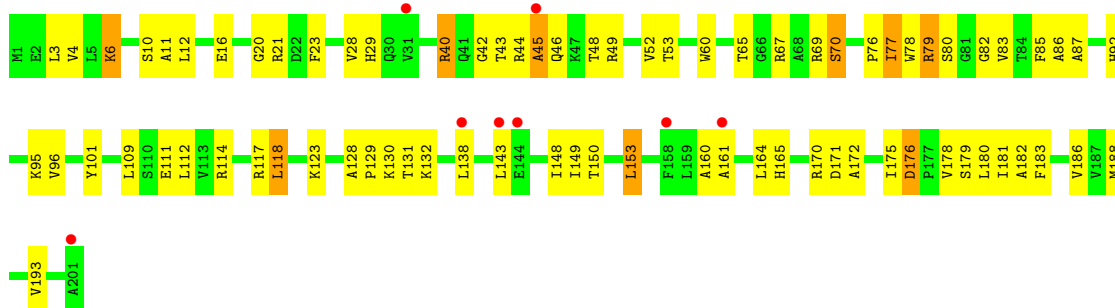
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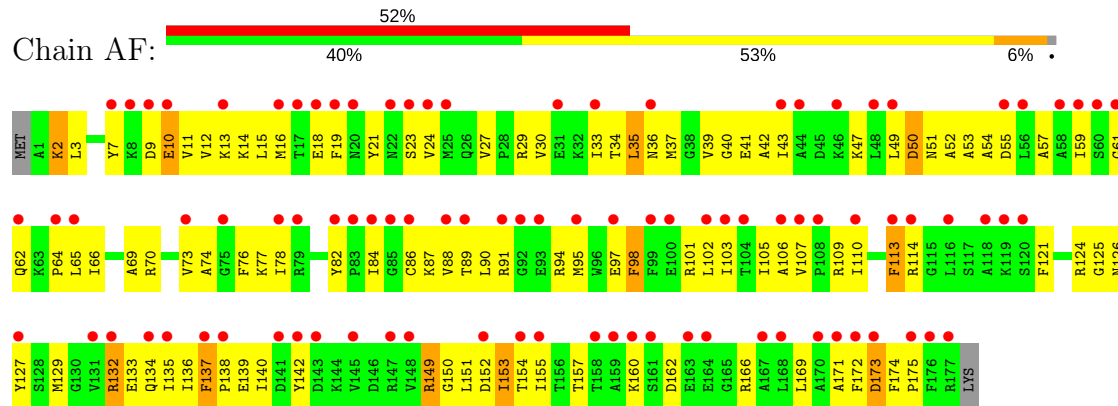
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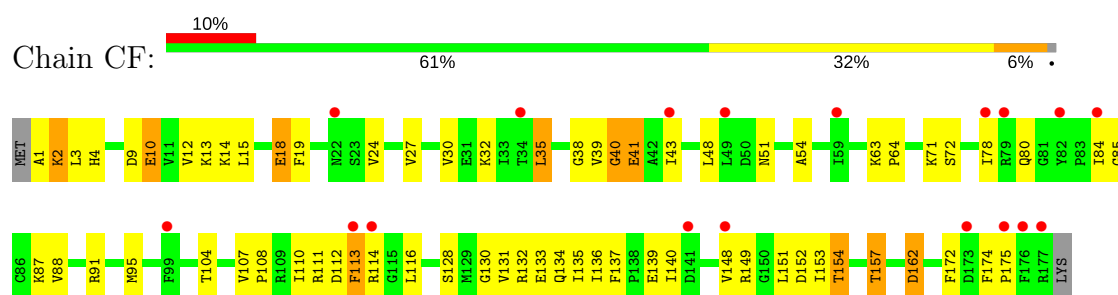
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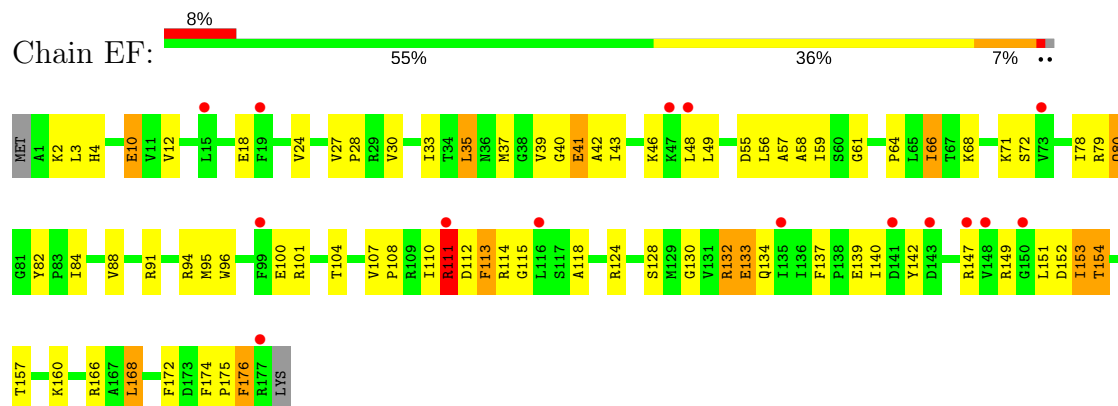
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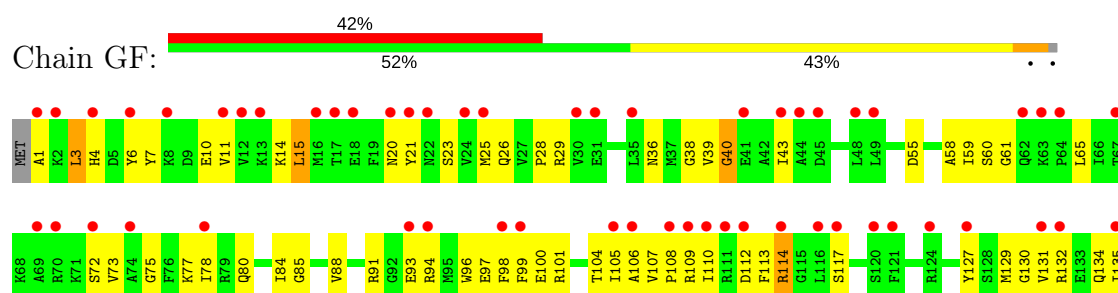
- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

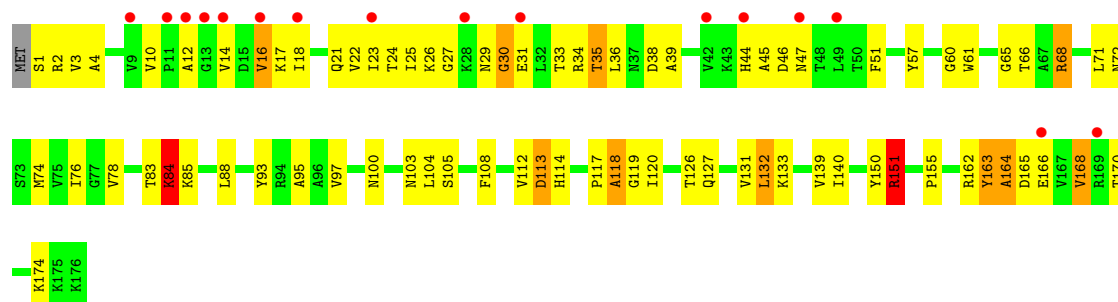


- Molecule 6: 50S ribosomal protein L5

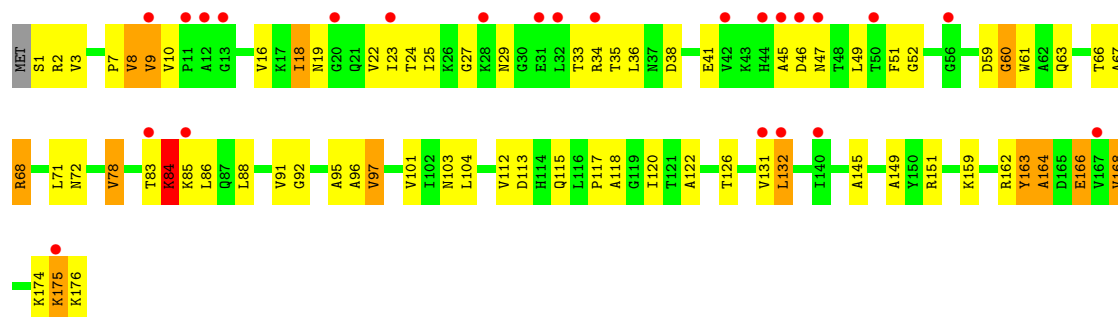




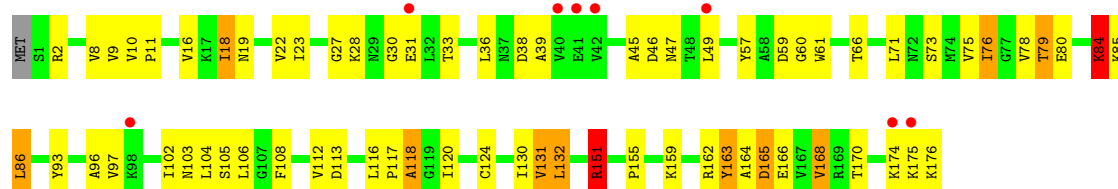
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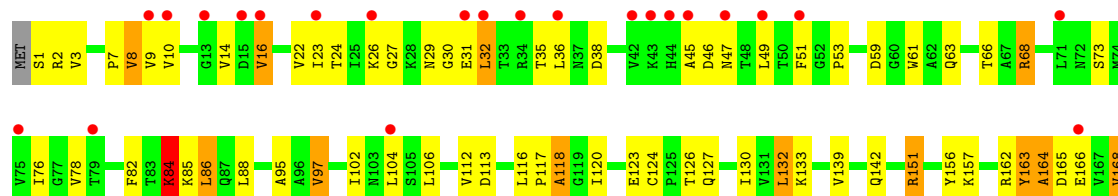
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

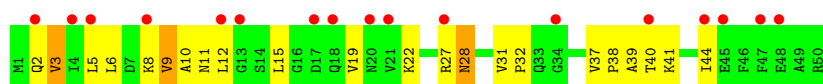




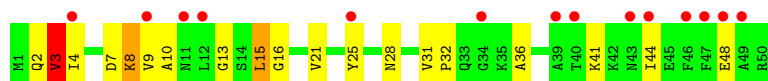
- Molecule 8: 50S ribosomal protein L9



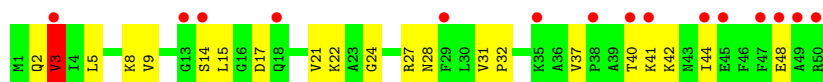
- Molecule 8: 50S ribosomal protein L9



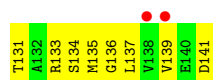
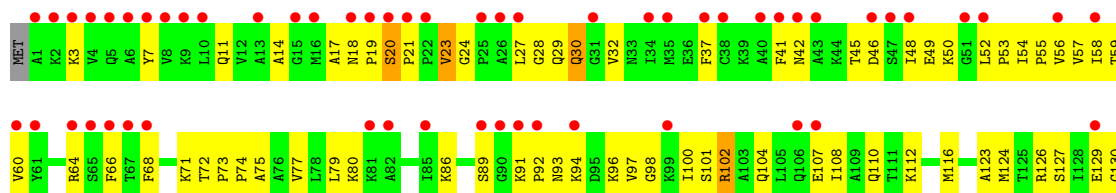
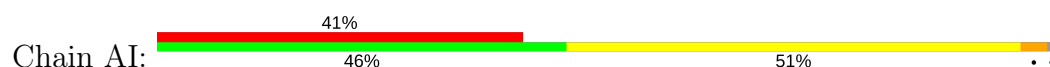
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- Molecule 8: 50S ribosomal protein L9

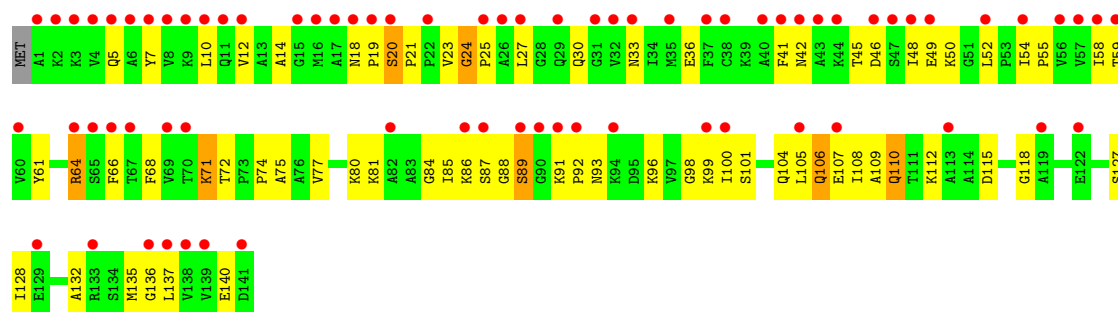


- Molecule 9: 50S ribosomal protein L11

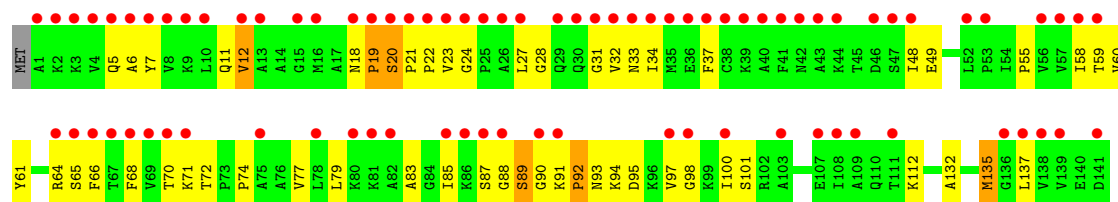


- Molecule 9: 50S ribosomal protein L11

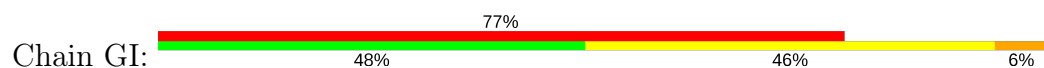




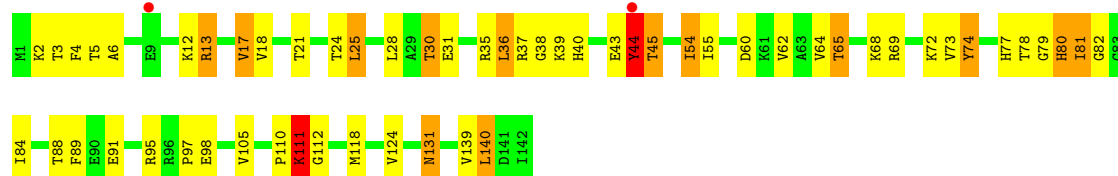
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• Molecule 9: 50S ribosomal protein L11

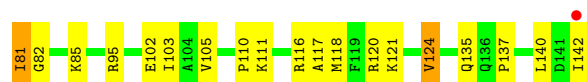


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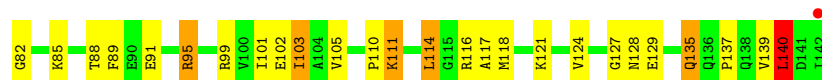
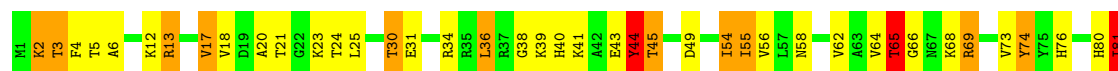


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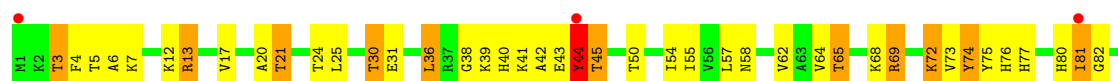




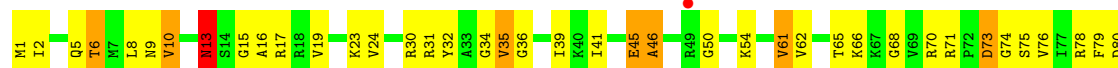
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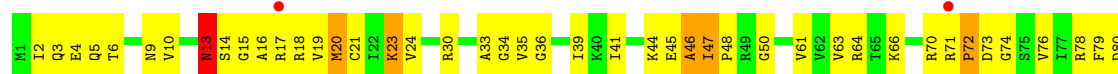
- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L14

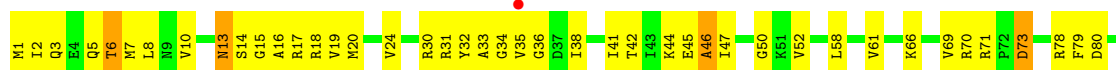


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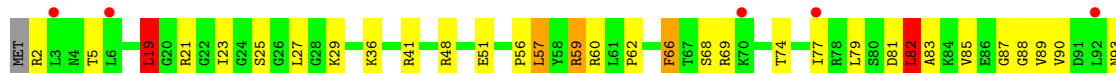




- Molecule 11: 50S ribosomal protein L14



- Molecule 12: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L15

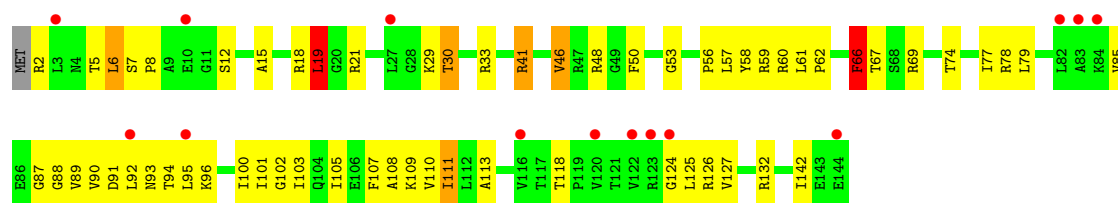


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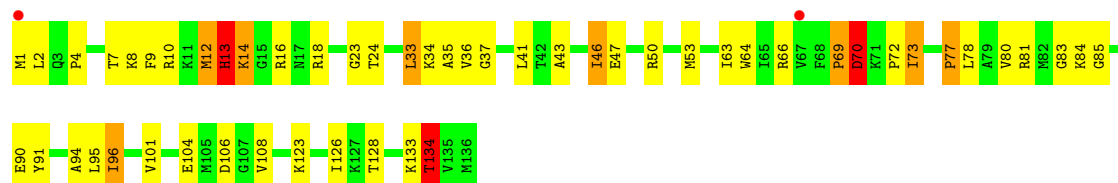


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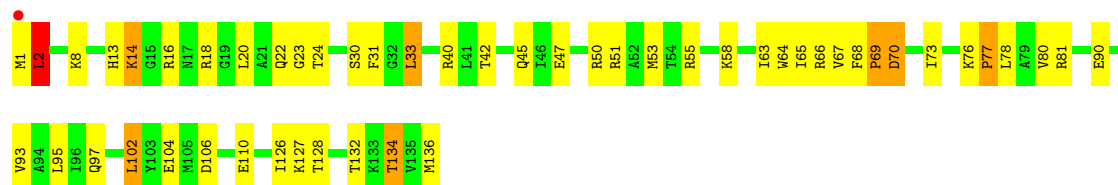




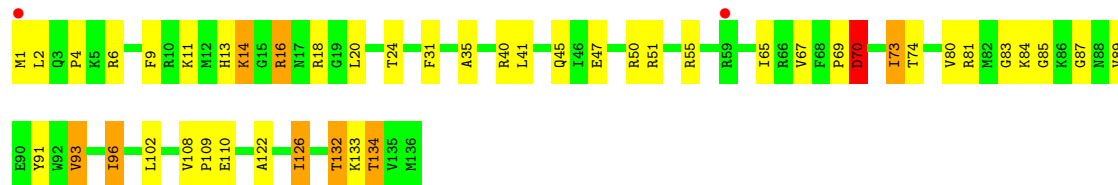
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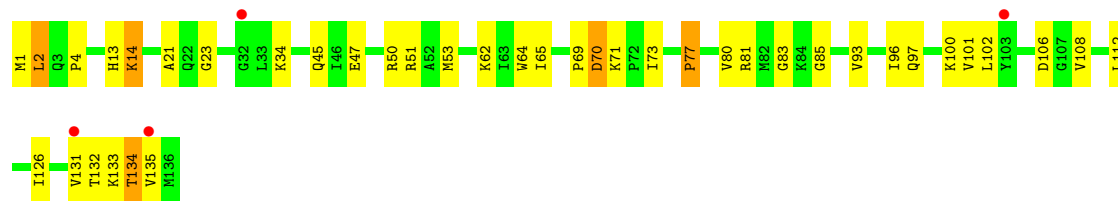
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• Molecule 13: 50S ribosomal protein L16

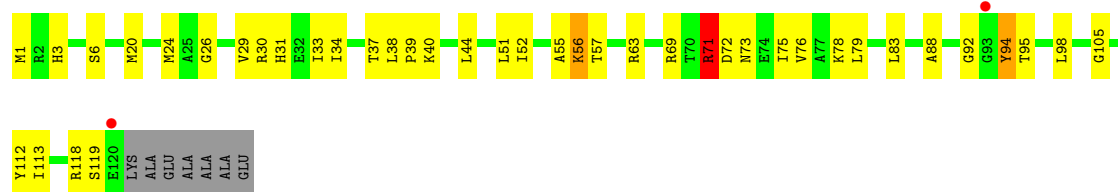


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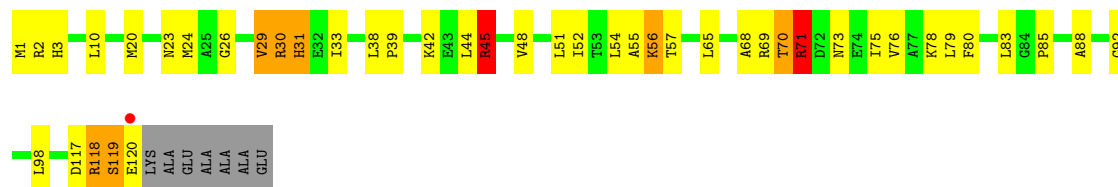


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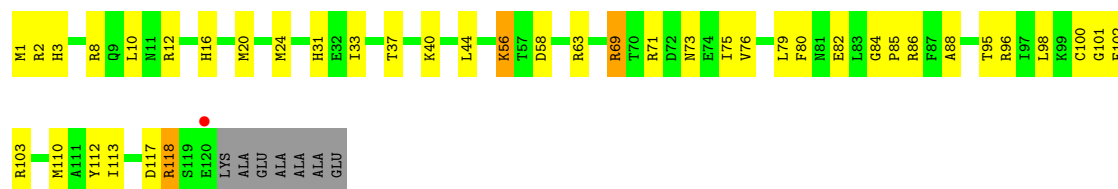




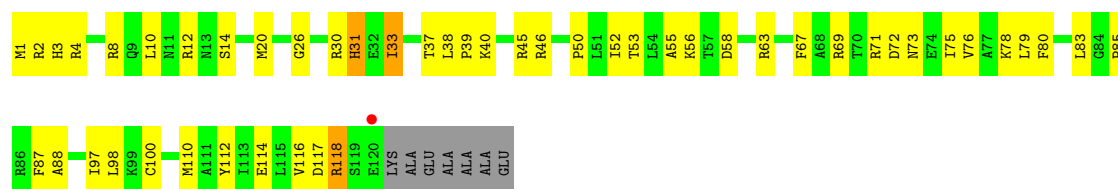
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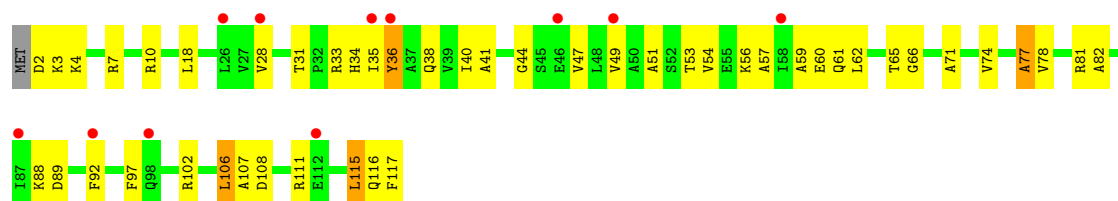
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• Molecule 14: 50S ribosomal protein L17

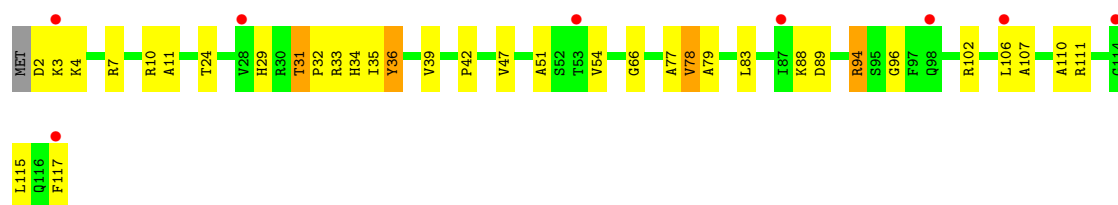


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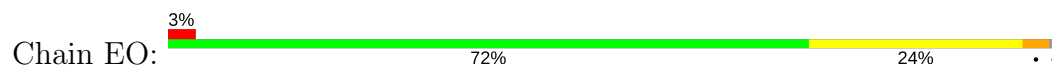


• Molecule 15: 50S ribosomal protein L18





- Molecule 15: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19

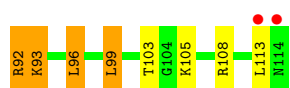


- Molecule 16: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L19





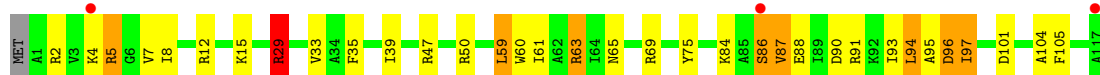
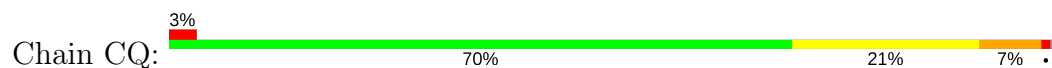
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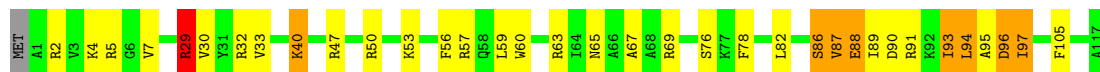
- Molecule 17: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L20

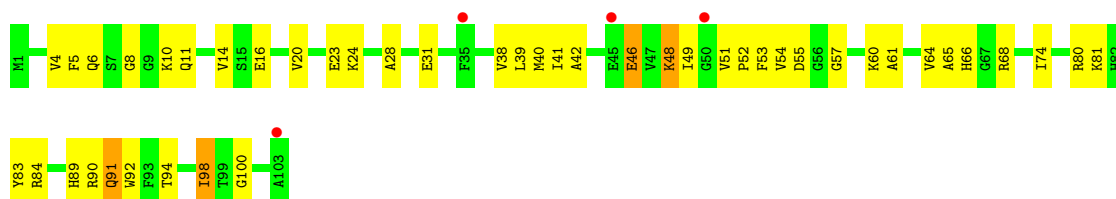


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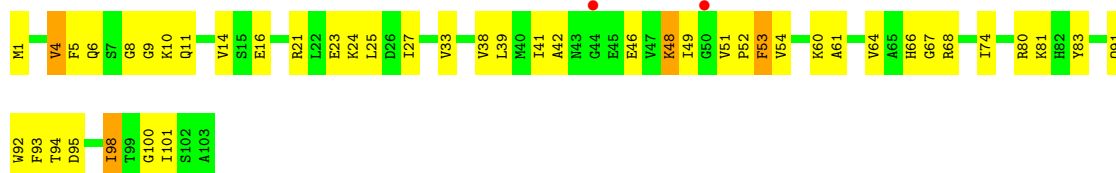


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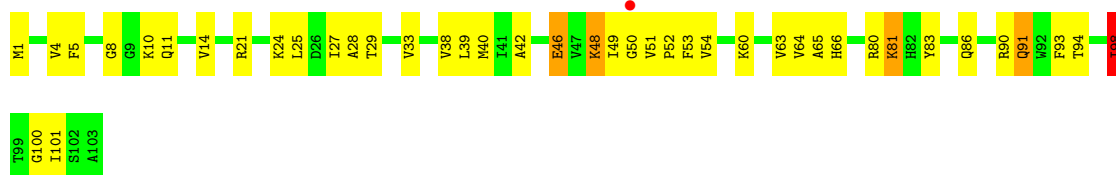




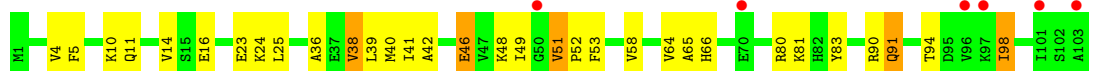
• Molecule 18: 50S ribosomal protein L21



• Molecule 18: 50S ribosomal protein L21



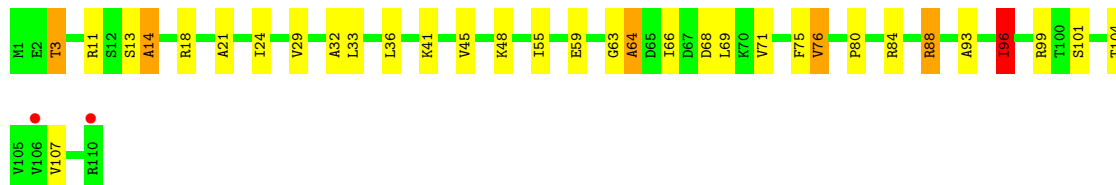
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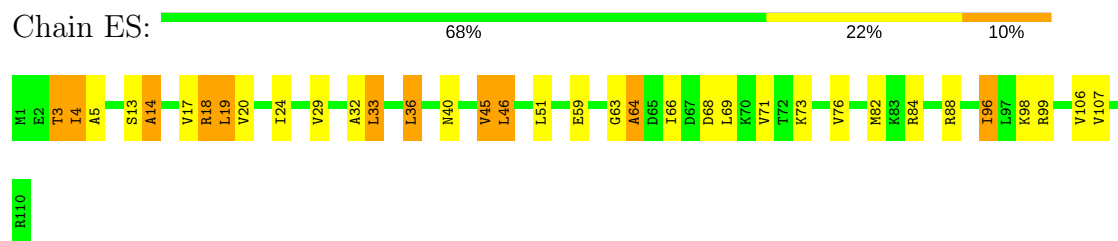
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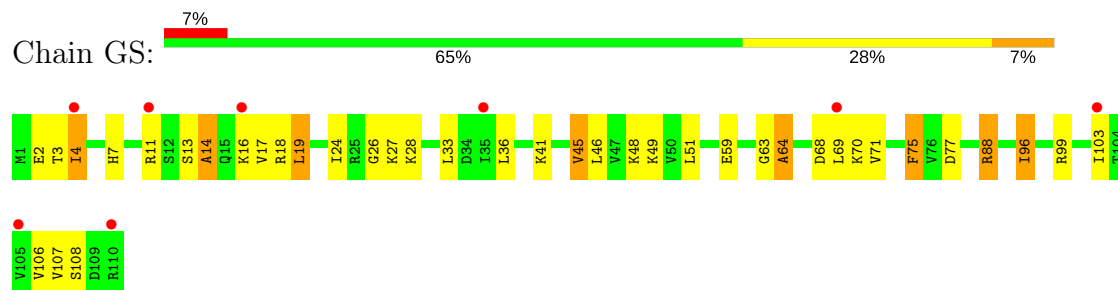
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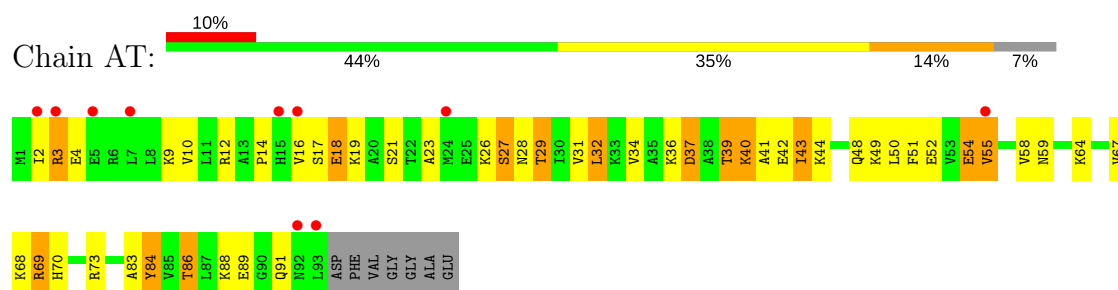
- Molecule 19: 50S ribosomal protein L22



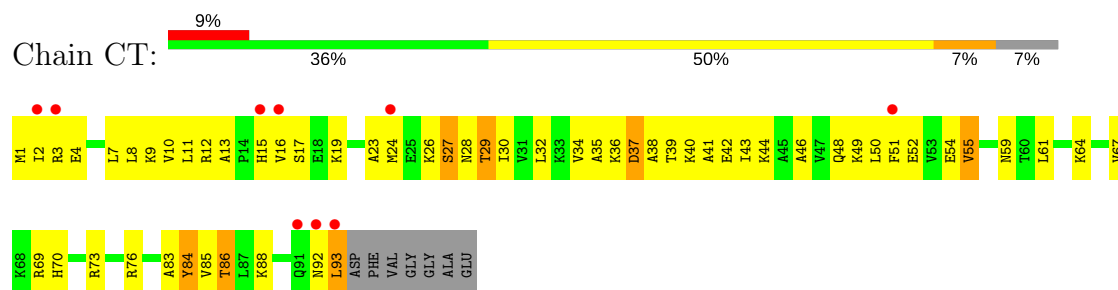
- Molecule 19: 50S ribosomal protein L22



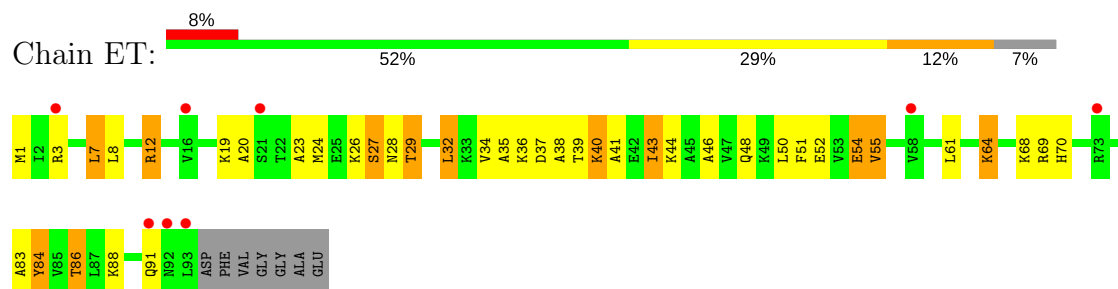
- Molecule 20: 50S ribosomal protein L23



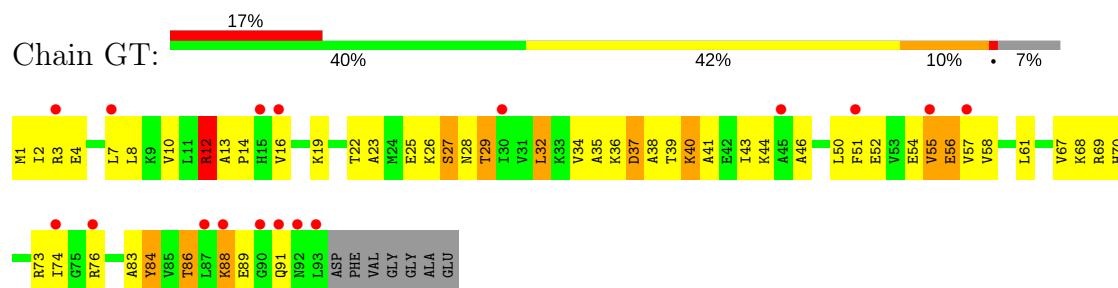
- Molecule 20: 50S ribosomal protein L23



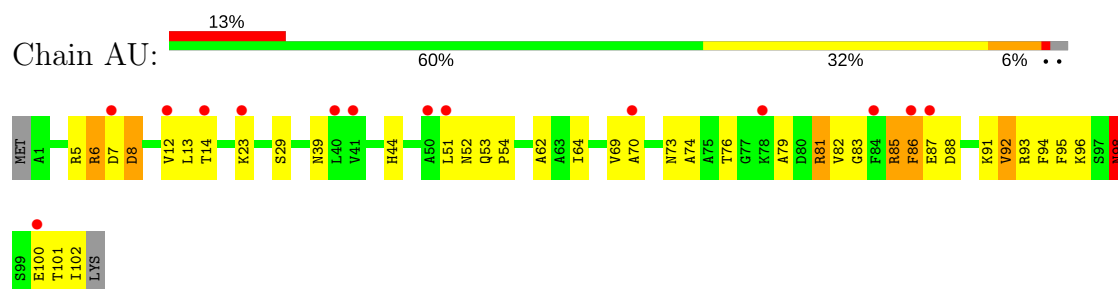
- Molecule 20: 50S ribosomal protein L23



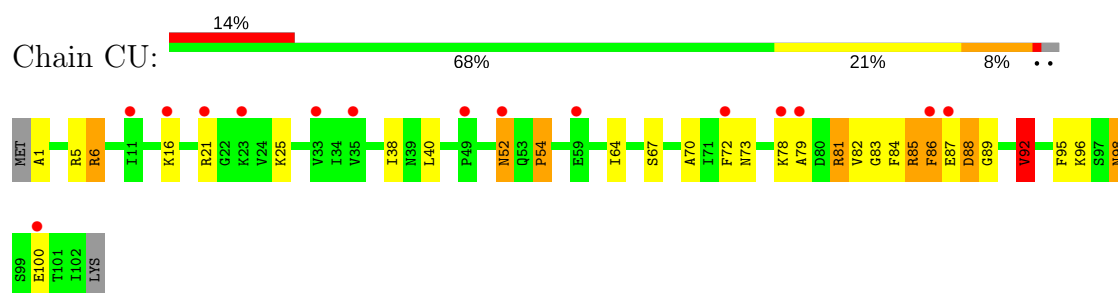
- Molecule 20: 50S ribosomal protein L23



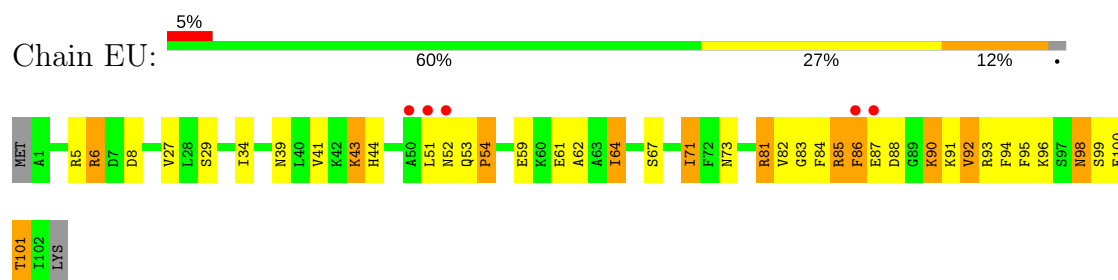
- Molecule 21: 50S ribosomal protein L24



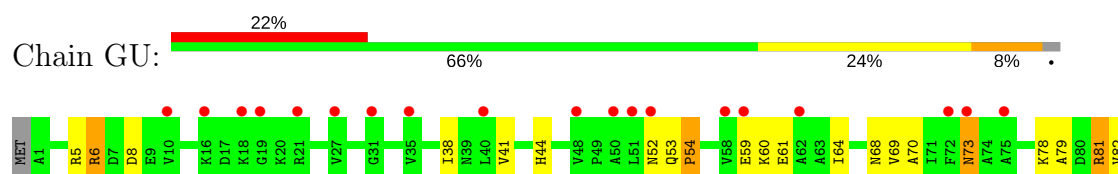
- Molecule 21: 50S ribosomal protein L24

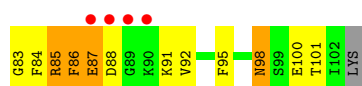


- Molecule 21: 50S ribosomal protein L24

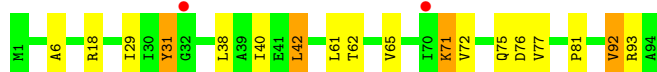
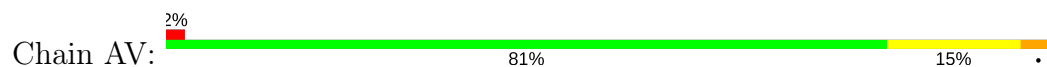


- Molecule 21: 50S ribosomal protein L24

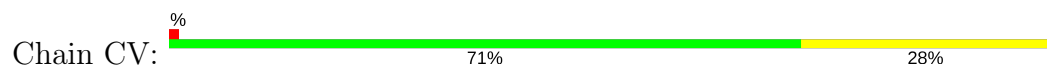




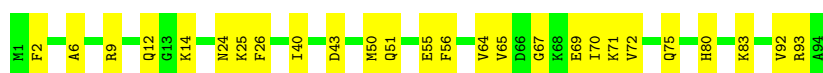
- Molecule 22: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L25



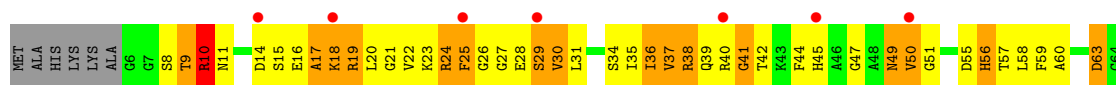
- Molecule 22: 50S ribosomal protein L25



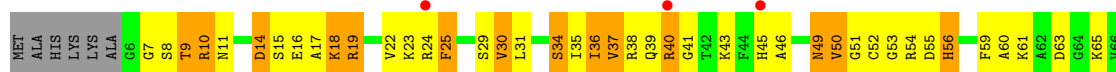
- Molecule 22: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L27

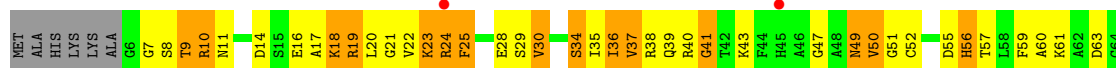


- Molecule 23: 50S ribosomal protein L27

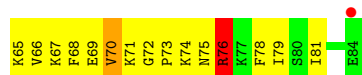
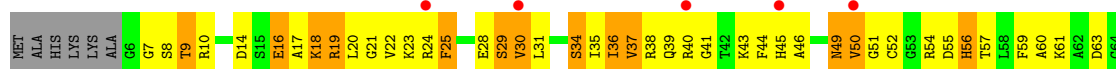




- Molecule 23: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L28

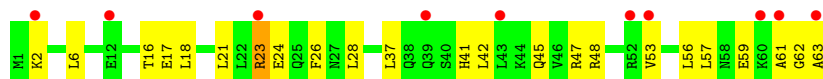


- Molecule 24: 50S ribosomal protein L28





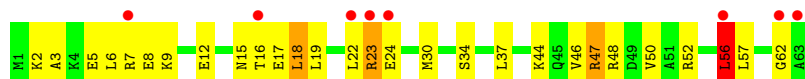
- Molecule 25: 50S ribosomal protein L29



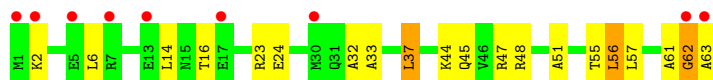
- Molecule 25: 50S ribosomal protein L29



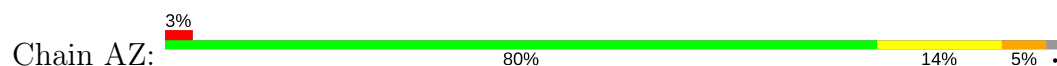
- Molecule 25: 50S ribosomal protein L29



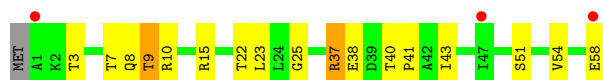
- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L30

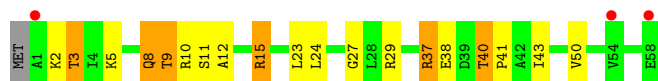


- Molecule 26: 50S ribosomal protein L30

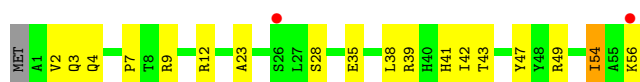




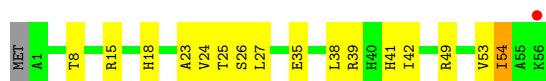
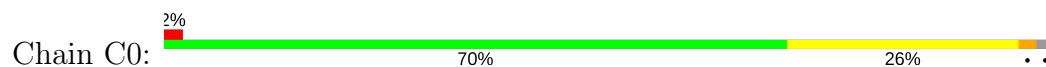
- Molecule 26: 50S ribosomal protein L30



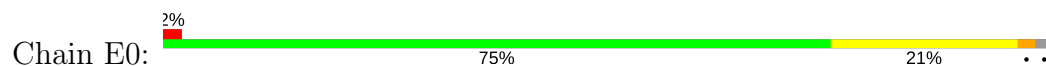
- Molecule 27: 50S ribosomal protein L32



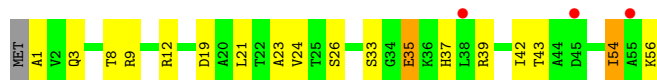
- Molecule 27: 50S ribosomal protein L32



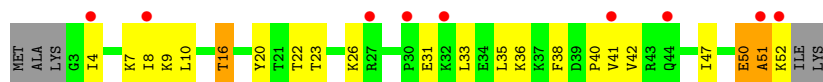
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

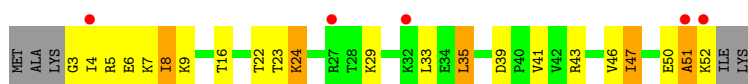


- Molecule 28: 50S ribosomal protein L33

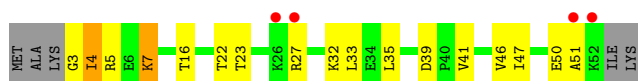


- Molecule 28: 50S ribosomal protein L33

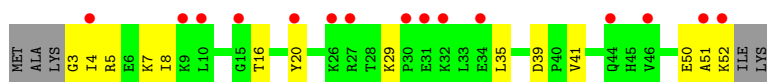




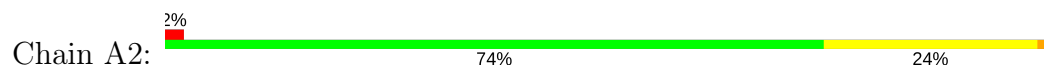
- Molecule 28: 50S ribosomal protein L33



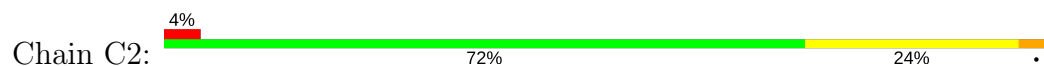
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34

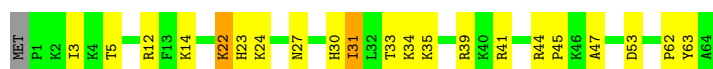


- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35





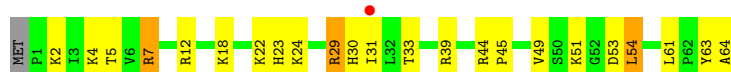
- Molecule 30: 50S ribosomal protein L35



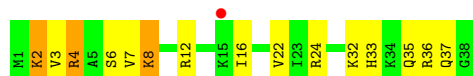
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36

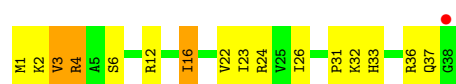


- Molecule 31: 50S ribosomal protein L36

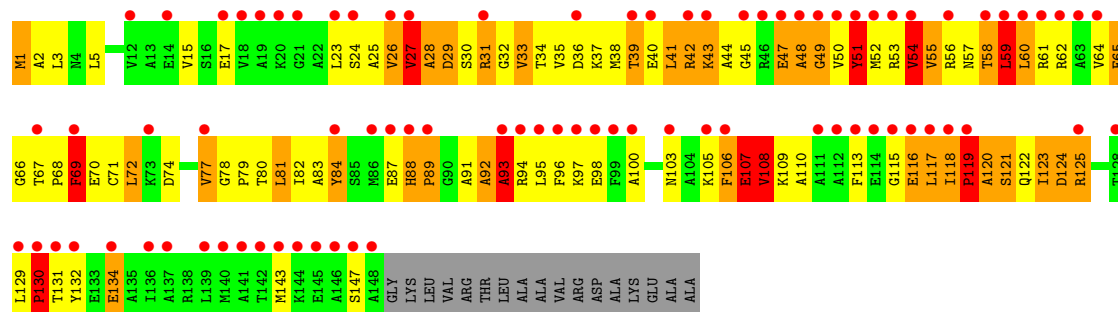
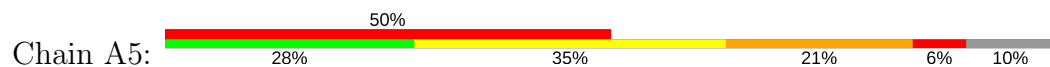


- Molecule 31: 50S ribosomal protein L36

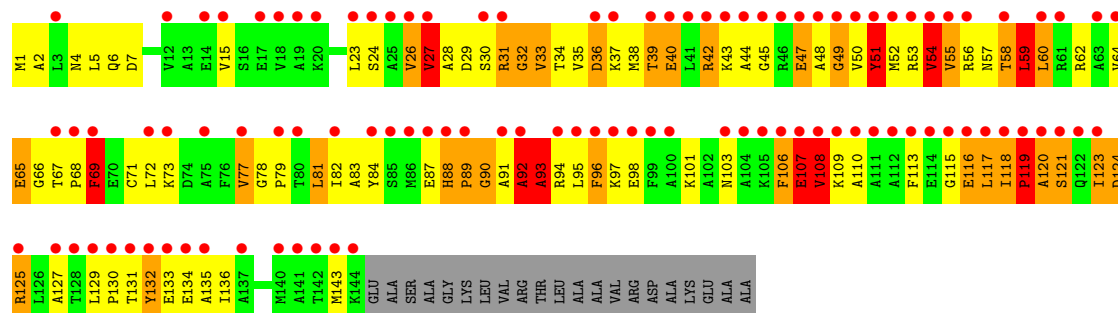
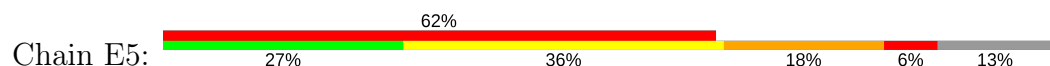




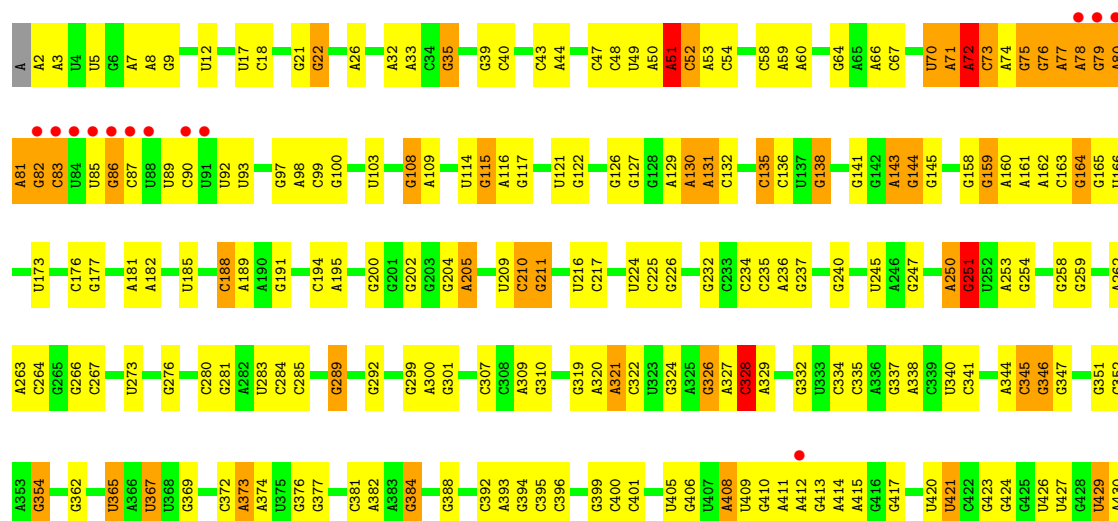
• Molecule 32: 50S ribosomal protein L10



• Molecule 32: 50S ribosomal protein L10

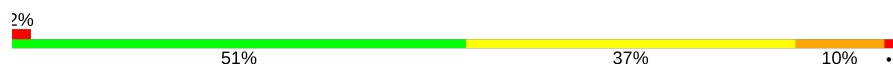


• Molecule 33: 16S rRNA

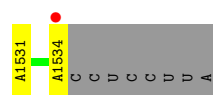




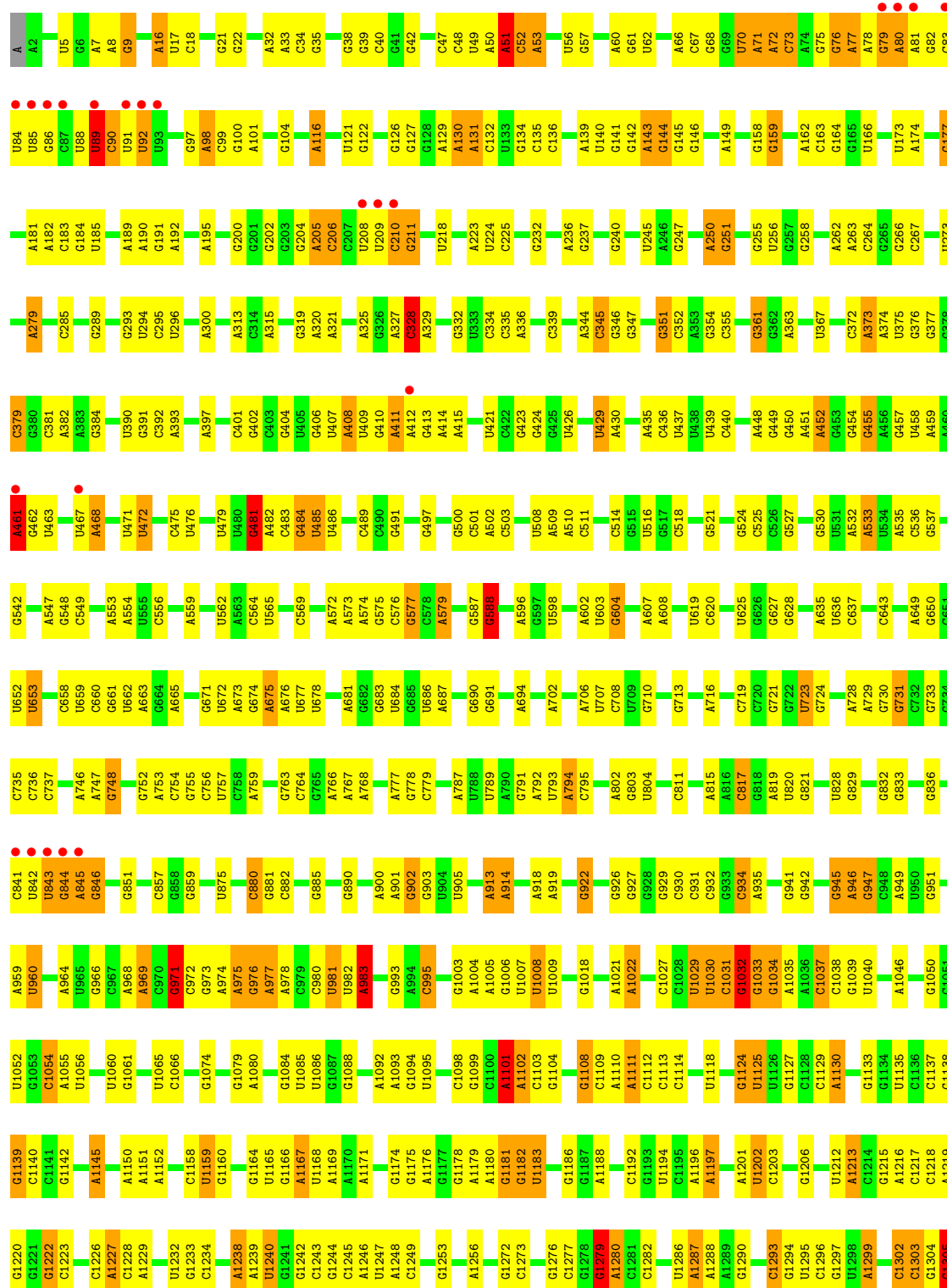
- Chain DA:

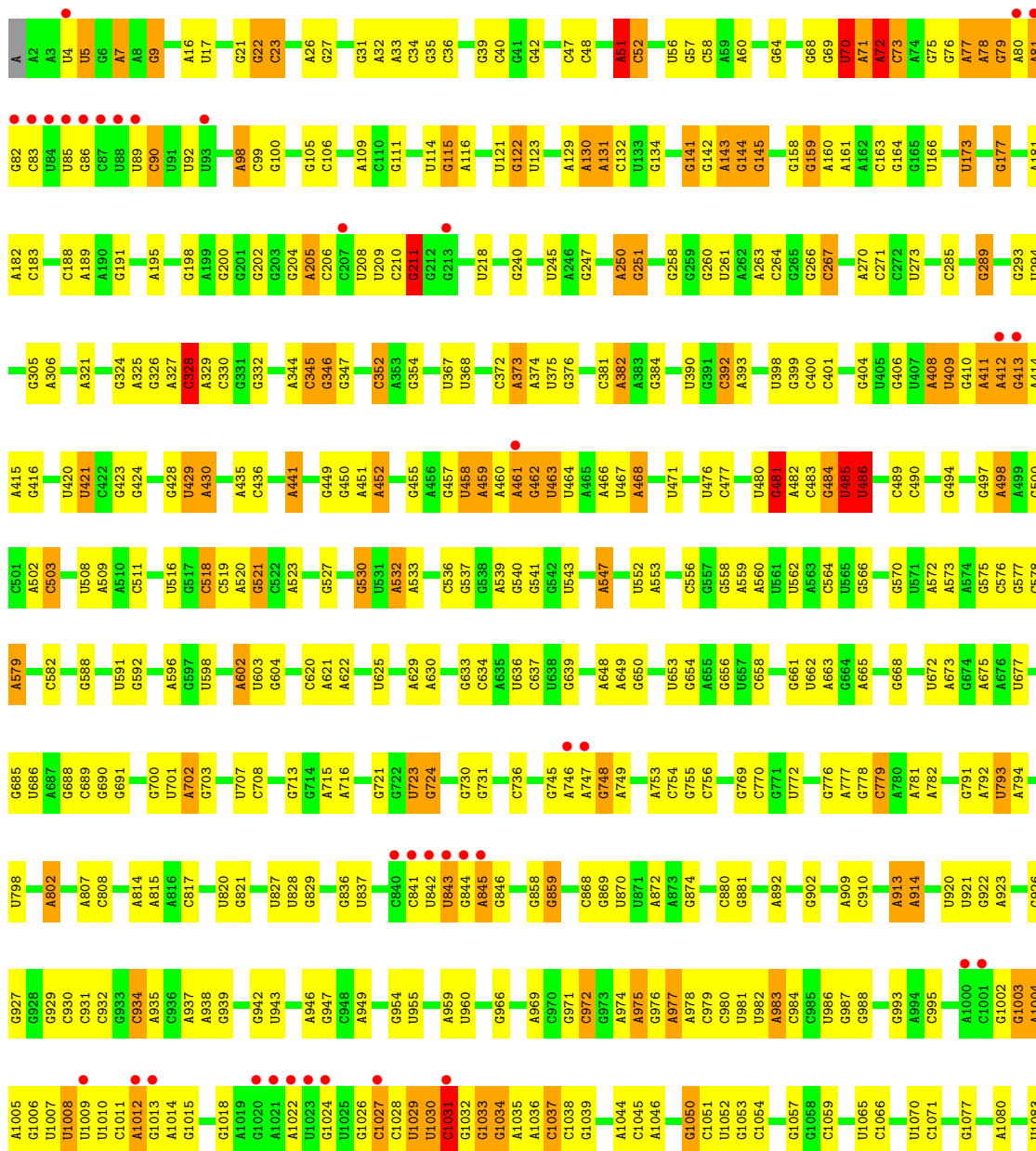


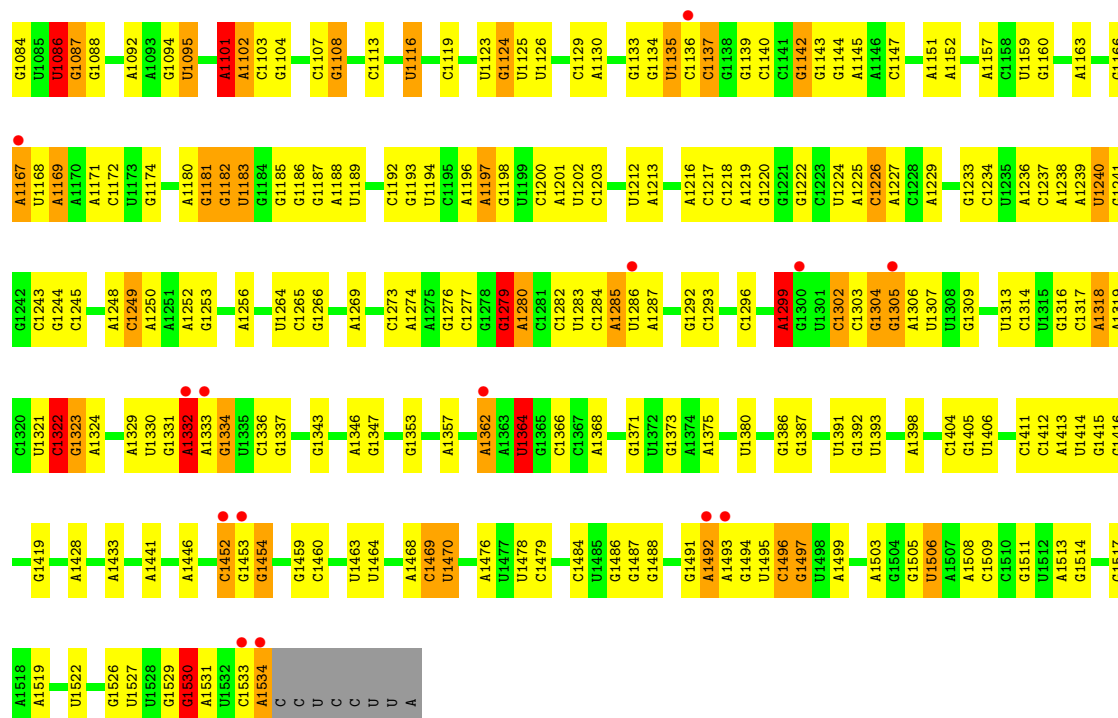
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| A1446 | A1367 | G1272 | U1159 | G1077 | G890 | G775 | U653 | U561 | C489 | U426 | C355 | A263 | U174 | G79 |
| U1451 | U1364 | G1273 | G1160 | U1078 | U891 | G776 | G656 | A563 | C490 | U427 | C359 | G265 | A174 | A80 |
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| G1458 | G1370 | G1279 | U1168 | G1084 | A900 | G780 | G661 | A572 | A495 | A431 | U367 | A270 | A182 | U84 |
| U1464 | A1371 | A1280 | G1178 | U1085 | A901 | A781 | G662 | A573 | A496 | A432 | A372 | C271 | A187 | U85 |
| U1468 | U1375 | U1283 | G1179 | U1086 | G902 | A782 | G665 | A574 | A497 | A433 | C372 | U273 | G187 | U86 |
| C1469 | U1376 | C1284 | U1087 | U1087 | A906 | U793 | A664 | G575 | A498 | U434 | A373 | U274 | C188 | U87 |
| U1470 | A1377 | A1285 | G1088 | G1088 | A913 | A794 | G674 | C576 | G500 | A435 | A374 | G276 | A189 | U88 |
| G1475 | U1380 | U1286 | G1182 | U1009 | A914 | C796 | U677 | C577 | A502 | U436 | U375 | C277 | A190 | U89 |
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| U1477 | C1193 | U1288 | U1183 | C1011 | A920 | A802 | U684 | G588 | G505 | A442 | G377 | A279 | A195 | C95 |
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| G1489 | U1201 | U1296 | U1183 | G1021 | G928 | U820 | A703 | U598 | G515 | A452 | A389 | C292 | U208 | U114 |
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| G1504 | U1212 | U1307 | U1183 | G1032 | G942 | C831 | A728 | C618 | A533 | U464 | C401 | C322 | C235 | C132 |
| U1505 | U1213 | U1308 | U1183 | G1033 | G943 | C832 | G731 | U619 | U534 | A465 | C402 | U323 | A236 | U133 |
| U1506 | U1214 | U1309 | U1183 | G1034 | G944 | C833 | G732 | C620 | U535 | A466 | C403 | G324 | G237 | G134 |
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| G1524 | U1224 | U1319 | U1183 | G1044 | G954 | C843 | G750 | U637 | G545 | U477 | A415 | A344 | G254 | A149 |
| C1525 | U1225 | U1320 | U1183 | G1045 | G955 | C844 | G751 | C643 | A546 | U480 | A416 | C345 | G255 | G158 |
| G1526 | U1226 | U1321 | U1183 | G1046 | G956 | C845 | G752 | U644 | A547 | G481 | C419 | G346 | U256 | G159 |
| U1529 | U1227 | U1322 | U1183 | G1047 | G957 | C846 | G753 | U645 | A548 | G482 | C420 | G347 | G257 | C163 |
| G1530 | U1228 | U1323 | U1183 | G1048 | G958 | C847 | G754 | U646 | A549 | G483 | C421 | G348 | G258 | G164 |
| | U1229 | U1324 | U1183 | G1049 | G959 | C848 | G755 | U647 | A550 | G484 | C422 | G349 | G259 | U166 |
| | U1230 | U1325 | U1183 | G1050 | G960 | C849 | G756 | U648 | A551 | G485 | G423 | G350 | G260 | |
| | U1231 | U1326 | U1183 | G1051 | G961 | C850 | G757 | U649 | A552 | G486 | G424 | G351 | U261 | |
| | U1232 | U1327 | U1183 | G1052 | G962 | C851 | G758 | U650 | A553 | G487 | | G352 | | |
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| | U1245 | U1340 | U1183 | G1065 | G975 | C864 | G771 | U663 | A566 | G500 | | G365 | | |
| | U1246 | U1341 | U1183 | G1066 | G976 | C865 | G772 | U664 | A567 | G501 | | G366 | | |
| | U1247 | U1342 | U1183 | G1067 | G977 | C866 | G773 | U665 | A568 | G502 | | G367 | | |
| | U1248 | U1343 | U1183 | G1068 | G978 | C867 | G774 | U666 | A569 | G503 | | G368 | | |
| | U1249 | U1344 | U1183 | G1069 | G979 | C868 | G775 | U667 | A570 | G504 | | G369 | | |
| | U1250 | U1345 | U1183 | G1070 | G980 | C869 | G776 | U668 | A571 | G505 | | G370 | | |
| | U1251 | U1346 | U1183 | G1071 | G981 | C870 | G777 | U669 | A572 | G506 | | G371 | | |
| | U1252 | U1347 | U1183 | G1072 | G982 | C871 | G778 | U670 | A573 | G507 | | G372 | | |
| | U1253 | U1348 | U1183 | G1073 | G983 | C872 | G779 | U671 | A574 | G508 | | G373 | | |
| | U1254 | U1349 | U1183 | G1074 | G984 | C873 | G780 | U672 | A575 | G509 | | G374 | | |
| | U1255 | U1350 | U1183 | G1075 | G985 | C874 | G781 | U673 | A576 | G510 | | G375 | | |
| | U1256 | U1351 | U1183 | G1076 | G986 | C875 | G782 | U674 | A577 | G511 | | G376 | | |
| | U1257 | U1352 | U1183 | G1077 | G987 | C876 | G783 | U675 | A578 | G512 | | G377 | | |
| | U1258 | U1353 | U1183 | G1078 | G988 | C877 | G784 | U676 | A579 | G513 | | G378 | | |
| | U1259 | U1354 | U1183 | G1079 | G989 | C878 | G785 | U677 | A580 | G514 | | G379 | | |
| | U1260 | U1355 | U1183 | G1080 | G990 | C879 | G786 | U678 | A581 | G515 | | G380 | | |
| | U1261 | U1356 | U1183 | G1081 | G991 | C880 | G787 | U679 | A582 | G516 | | G381 | | |
| | U1262 | U1357 | U1183 | G1082 | G992 | C881 | G788 | U680 | A583 | G517 | | G382 | | |
| | U1263 | U1358 | U1183 | G1083 | G993 | C882 | G789 | U681 | A584 | G518 | | G383 | | |
| | U1264 | U1359 | U1183 | G1084 | G994 | C883 | G790 | U682 | A585 | G519 | | G384 | | |
| | U1265 | U1360 | U1183 | G1085 | G995 | C884 | G791 | U683 | A586 | G520 | | G385 | | |
| | U1266 | U1361 | U1183 | G1086 | G996 | C885 | G792 | U684 | A587 | G521 | | G386 | | |
| | U1267 | U1362 | U1183 | G1087 | G997 | C886 | G793 | U685 | A588 | G522 | | G387 | | |
| | U1268 | U1363 | U1183 | G1088 | G998 | C887 | G794 | U686 | A589 | G523 | | G388 | | |
| | U1269 | U1364 | U1183 | G1089 | G999 | C888 | G795 | U687 | A590 | G524 | | G389 | | |
| | U1270 | U1365 | U1183 | G1090 | G1000 | C889 | G796 | U688 | A591 | G525 | | G390 | | |
| | U1271 | U1366 | U1183 | G1091 | G1001 | C890 | G797 | U689 | A592 | G526 | | G391 | | |
| | U1272 | U1367 | U1183 | G1092 | G1002 | C891 | G798 | U690 | A593 | G527 | | G392 | | |
| | U1273 | U1368 | U1183 | G1093 | G1003 | C892 | G799 | U691 | A594 | G528 | | G393 | | |
| | U1274 | U1369 | U1183 | G1094 | G1004 | C893 | G800 | U692 | A595 | G529 | | G394 | | |
| | U1275 | U1370 | U1183 | G1095 | G1005 | C894 | G801 | U693 | A596 | G530 | | G395 | | |
| | U1276 | U1371 | U1183 | G1096 | G1006 | C895 | G802 | U694 | A597 | G531 | | G396 | | |
| | U1277 | U1372 | U1183 | G1097 | G1007 | C896 | G803 | U695 | A598 | G532 | | G397 | | |
| | U1278 | U1373</ | | | | | | | | | | | | |



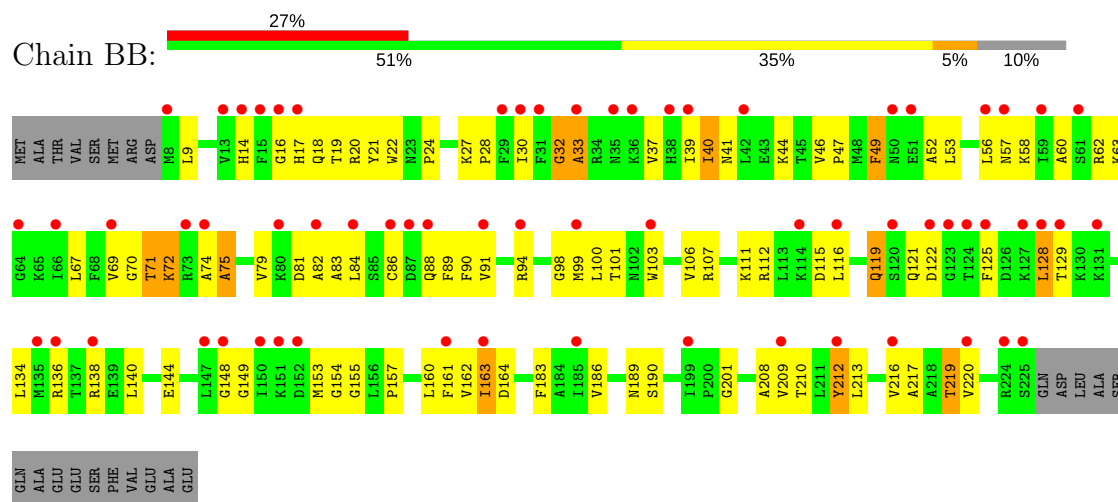
● Molecule 33: 16S rRNA



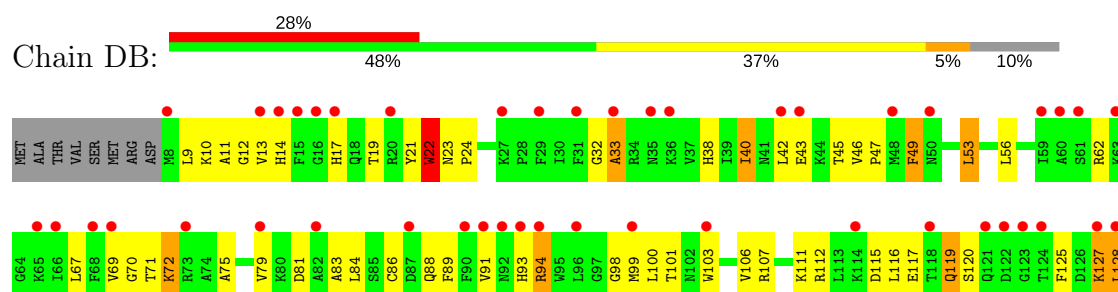


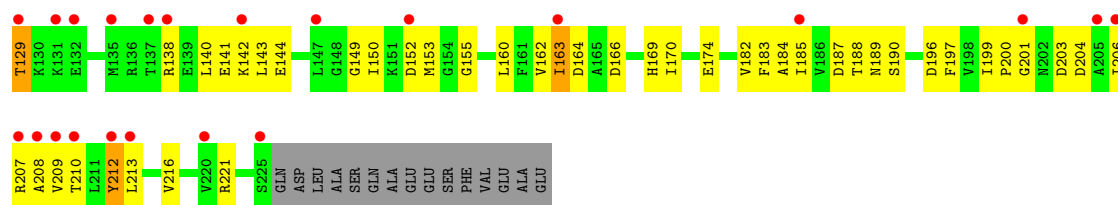


• Molecule 34: 30S ribosomal protein S2

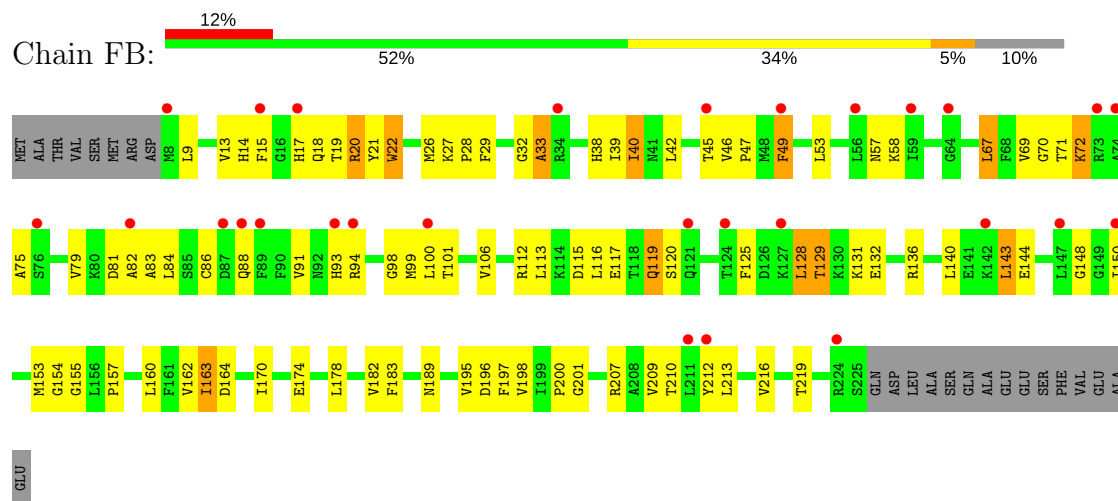


• Molecule 34: 30S ribosomal protein S2

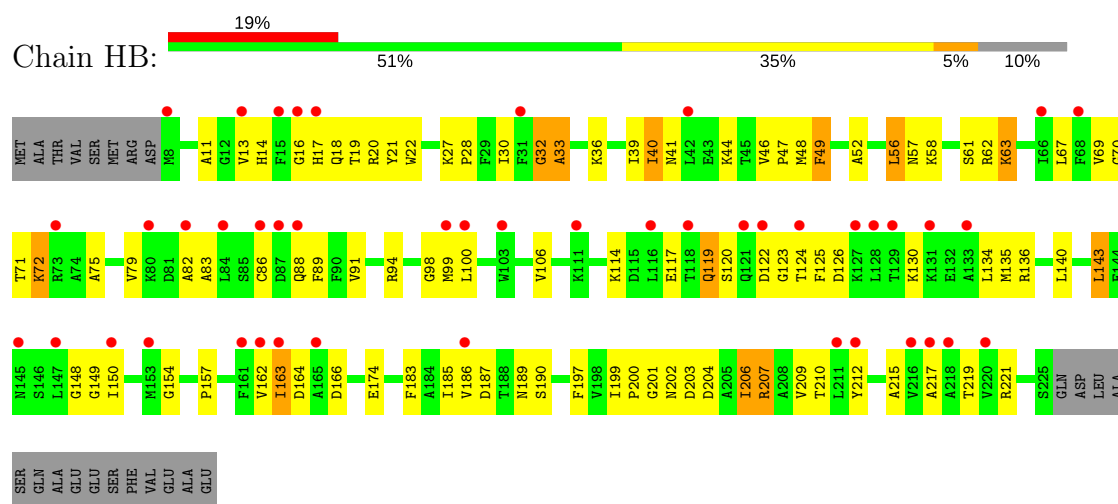




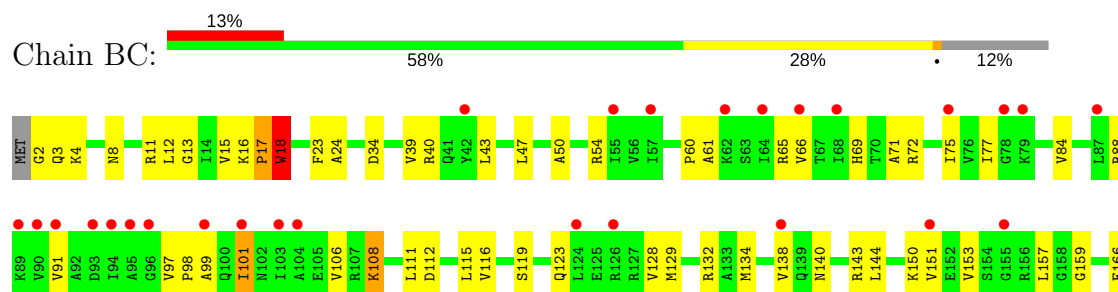
• Molecule 34: 30S ribosomal protein S2

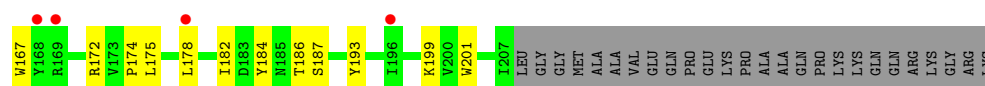


• Molecule 34: 30S ribosomal protein S2

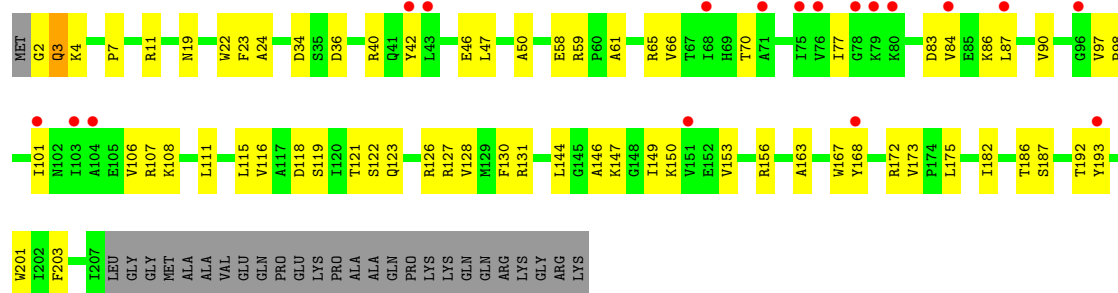


• Molecule 35: 30S ribosomal protein S3

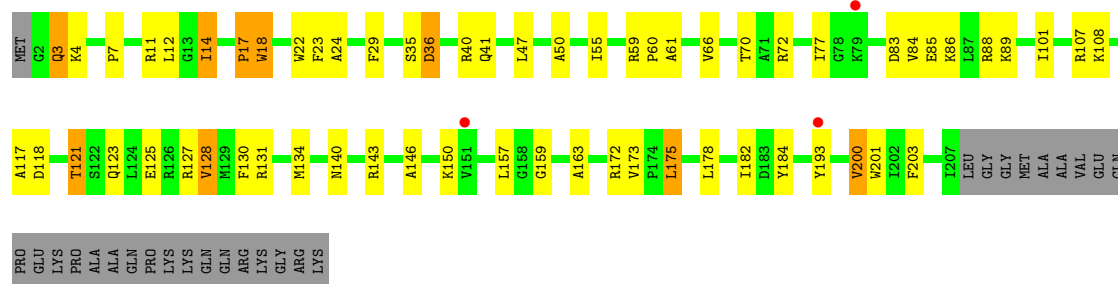




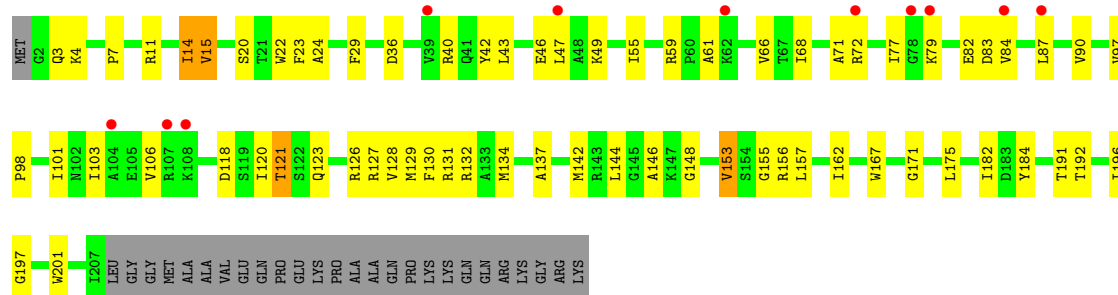
- Molecule 35: 30S ribosomal protein S3



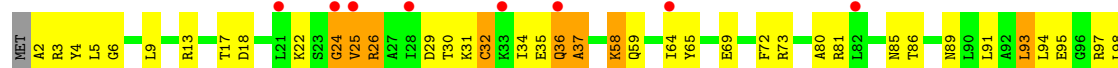
- Molecule 35: 30S ribosomal protein S3

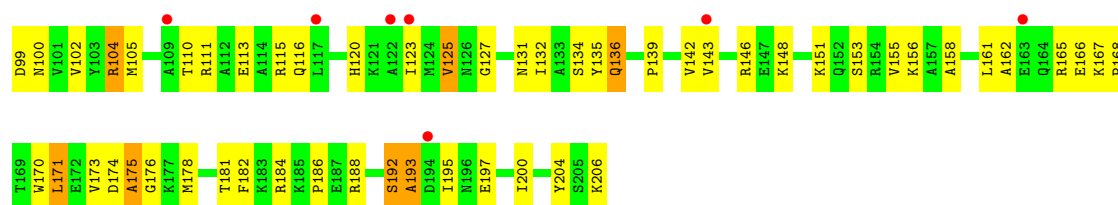


- Molecule 35: 30S ribosomal protein S3

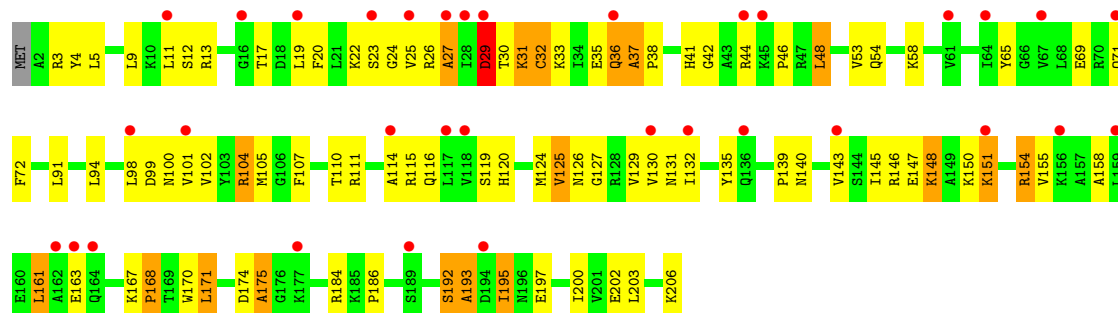


- Molecule 36: 30S ribosomal protein S4

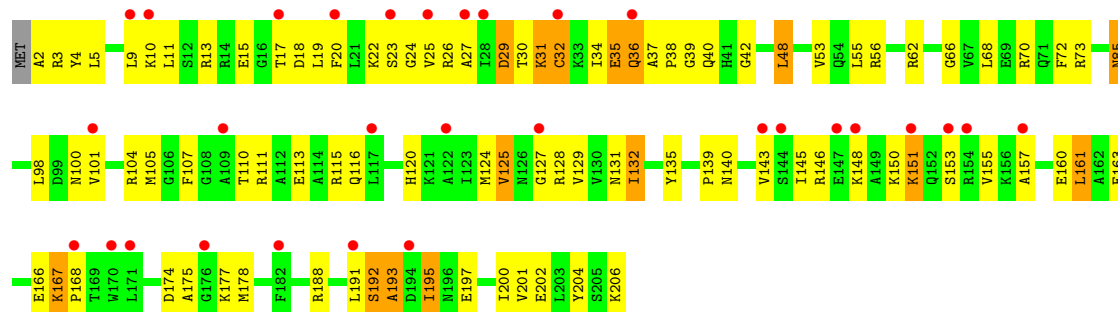




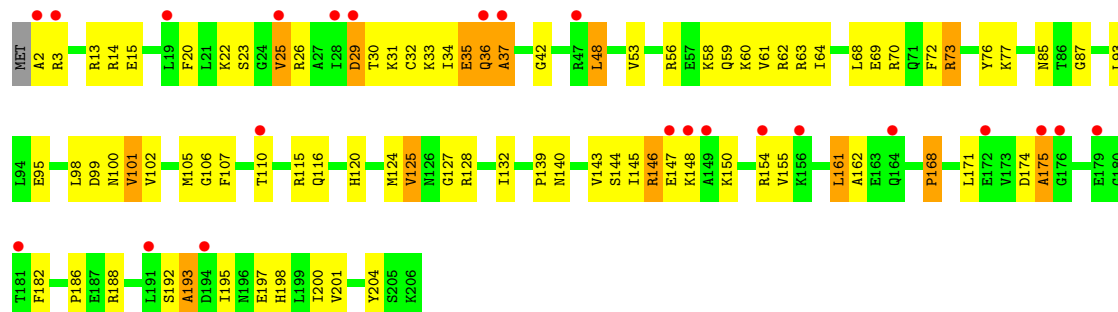
• Molecule 36: 30S ribosomal protein S4



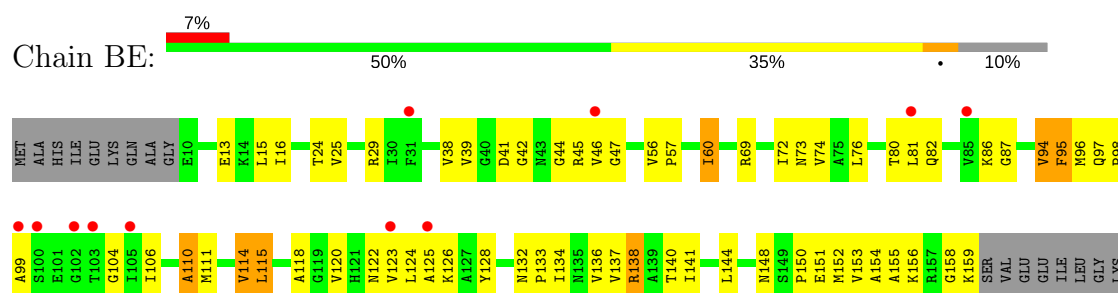
• Molecule 36: 30S ribosomal protein S4



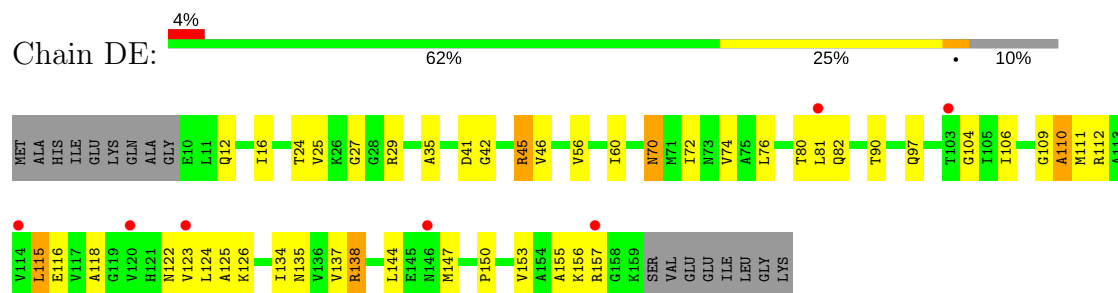
• Molecule 36: 30S ribosomal protein S4



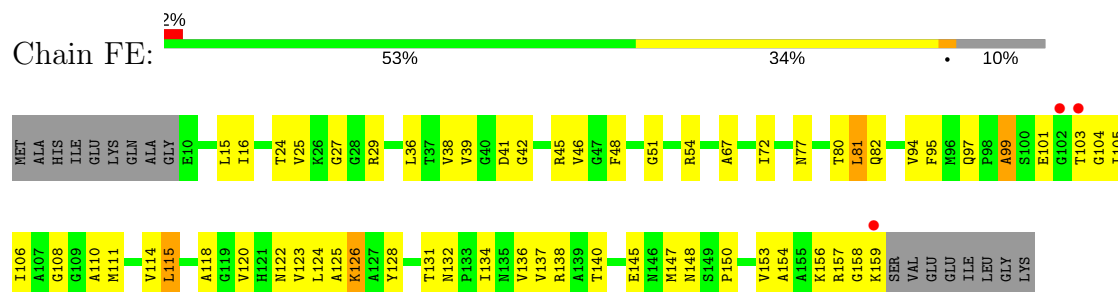
• Molecule 37: 30S ribosomal protein S5



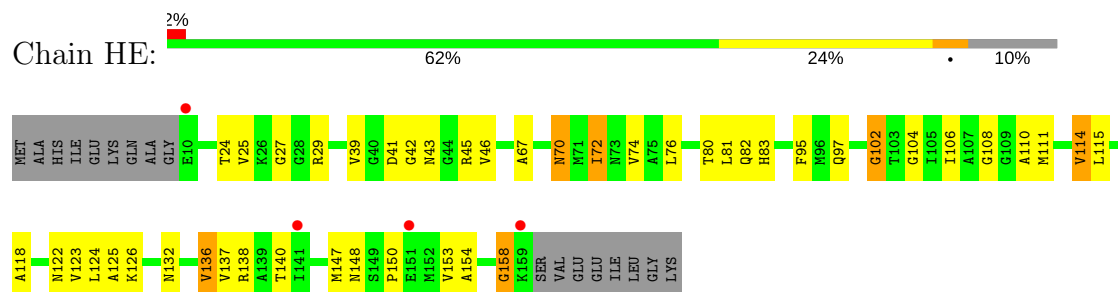
- Molecule 37: 30S ribosomal protein S5



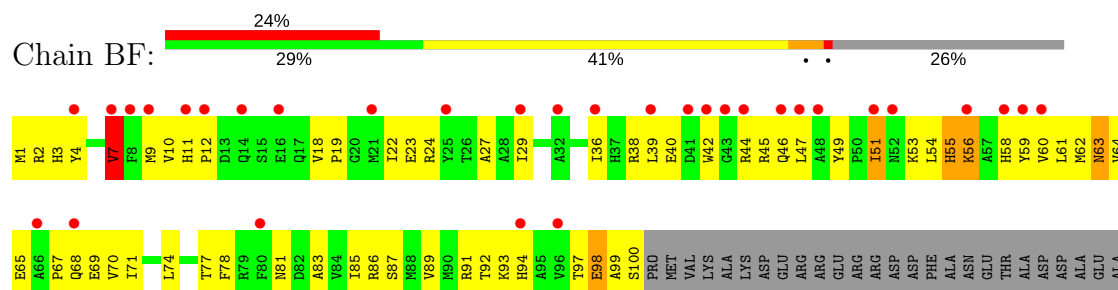
- Molecule 37: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S5

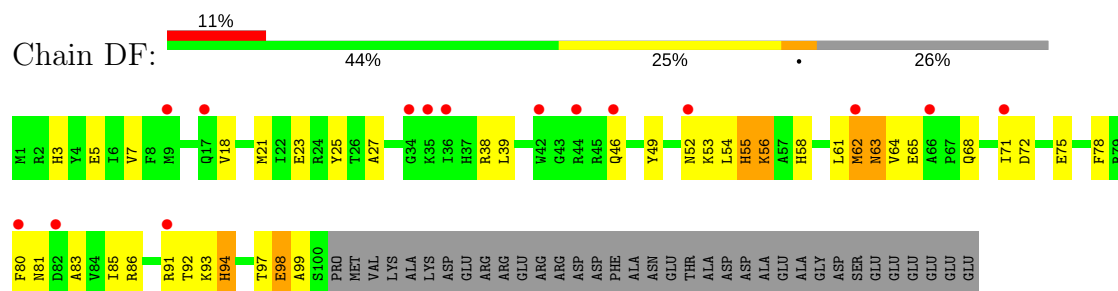


- Molecule 38: 30S ribosomal protein S6

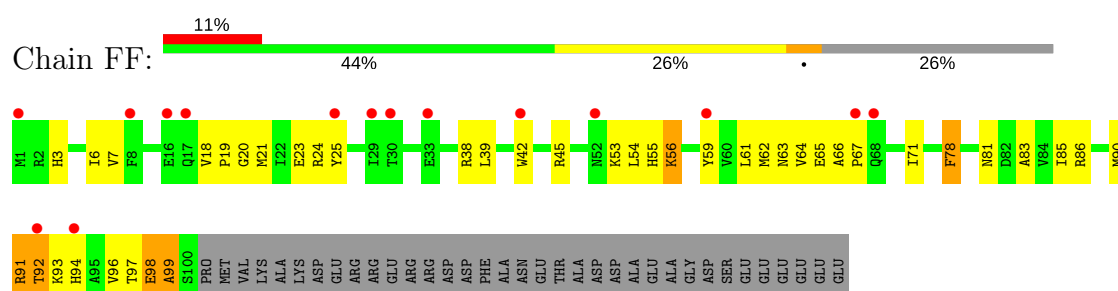


GLY
ASP
SER
GLU
GLU
GLU
GLU

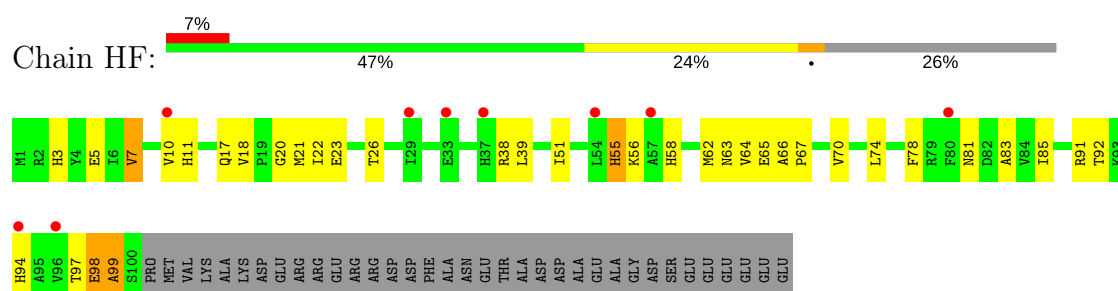
• Molecule 38: 30S ribosomal protein S6



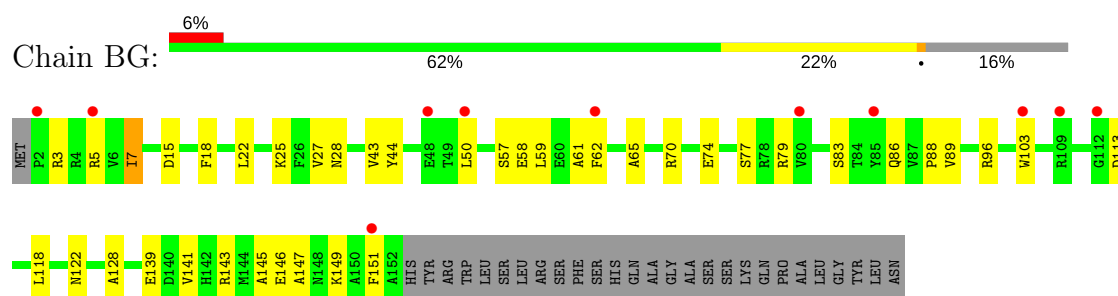
• Molecule 38: 30S ribosomal protein S6



• Molecule 38: 30S ribosomal protein S6

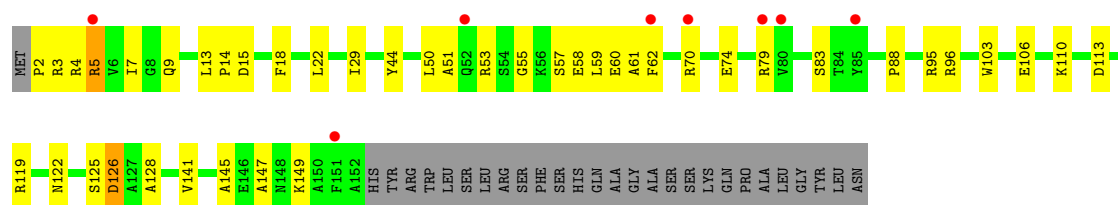


• Molecule 39: 30S ribosomal protein S7

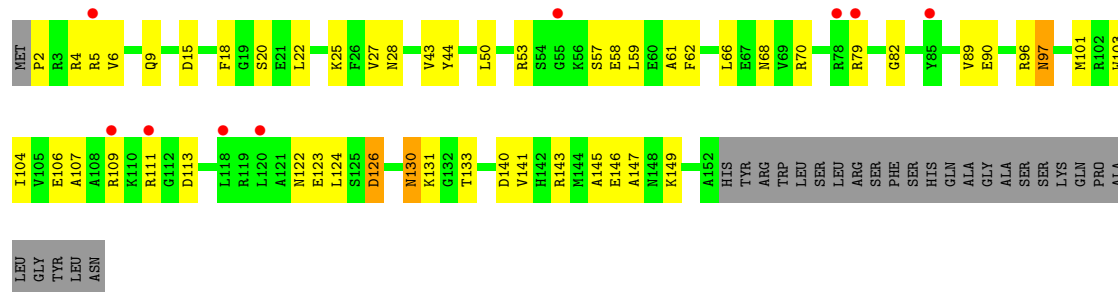


• Molecule 39: 30S ribosomal protein S7

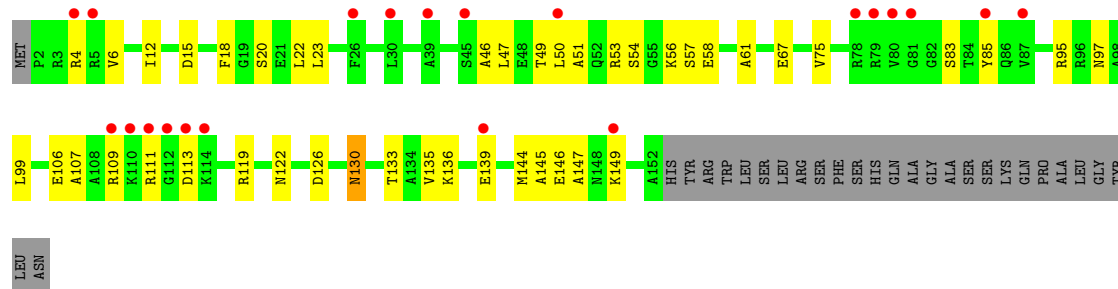




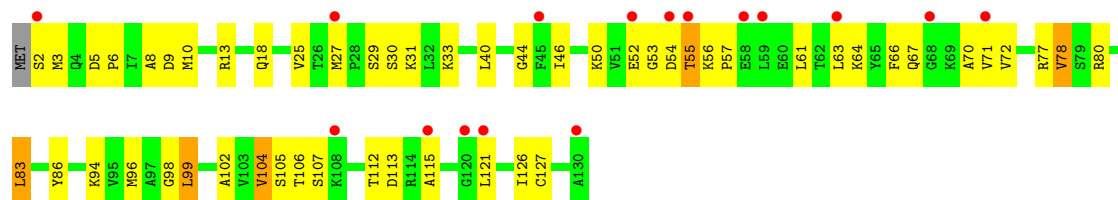
• Molecule 39: 30S ribosomal protein S7



• Molecule 39: 30S ribosomal protein S7



• Molecule 40: 30S ribosomal protein S8

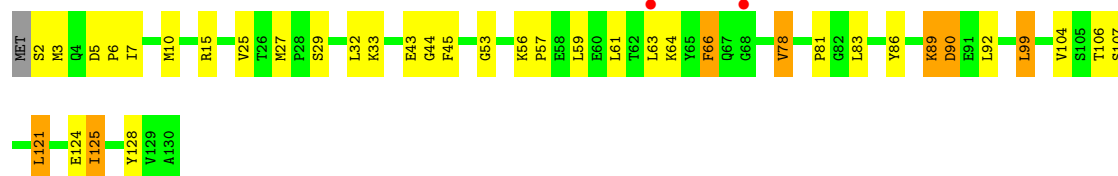
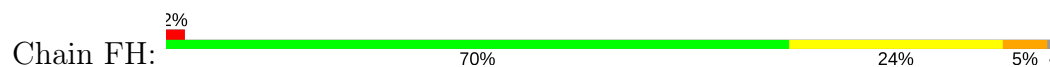


• Molecule 40: 30S ribosomal protein S8

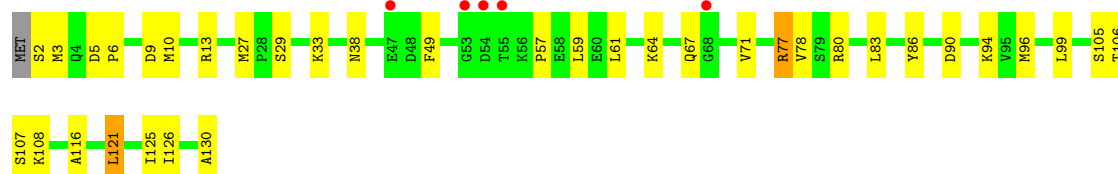




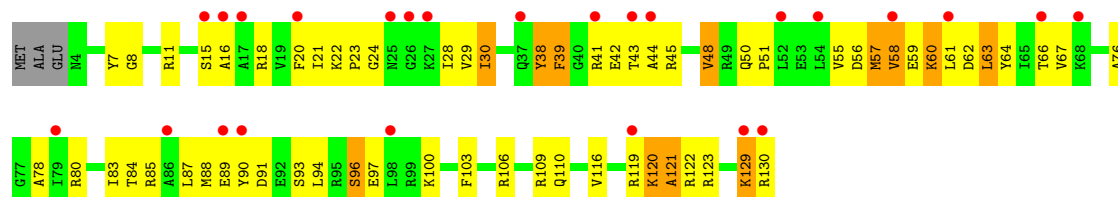
- Molecule 40: 30S ribosomal protein S8



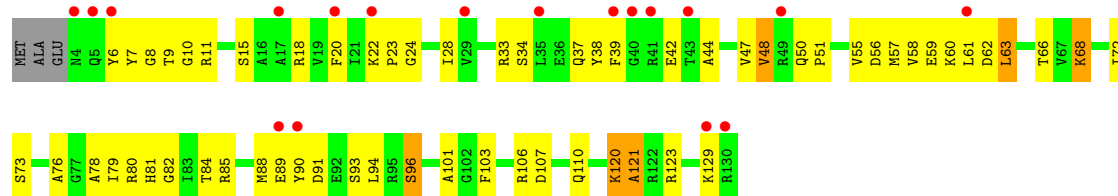
- Molecule 40: 30S ribosomal protein S8



- Molecule 41: 30S ribosomal protein S9

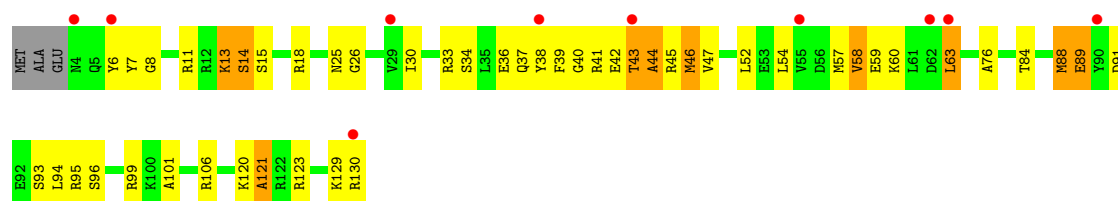


- Molecule 41: 30S ribosomal protein S9

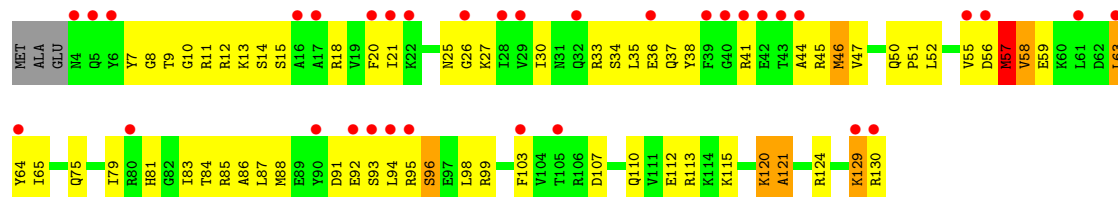


- Molecule 41: 30S ribosomal protein S9

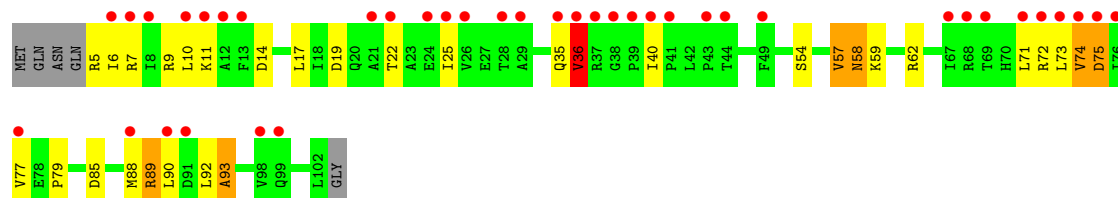
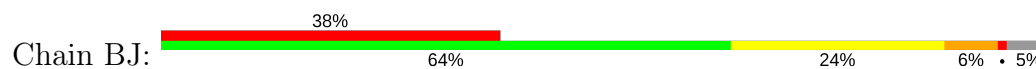




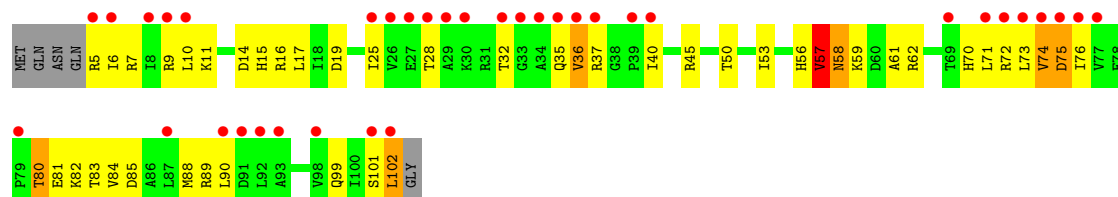
- Molecule 41: 30S ribosomal protein S9



- Molecule 42: 30S ribosomal protein S10



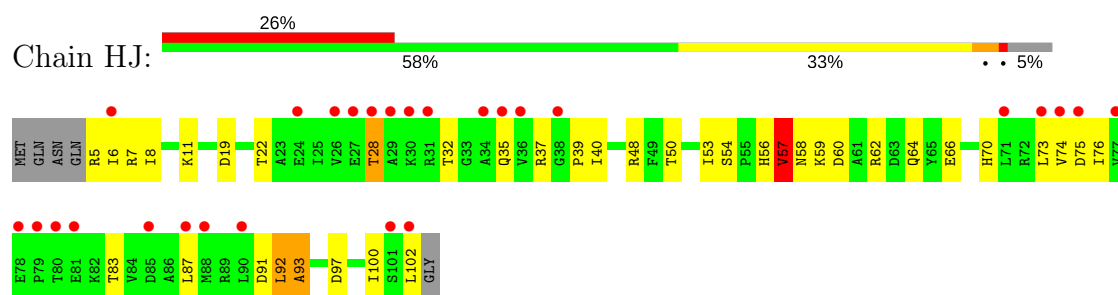
- Molecule 42: 30S ribosomal protein S10



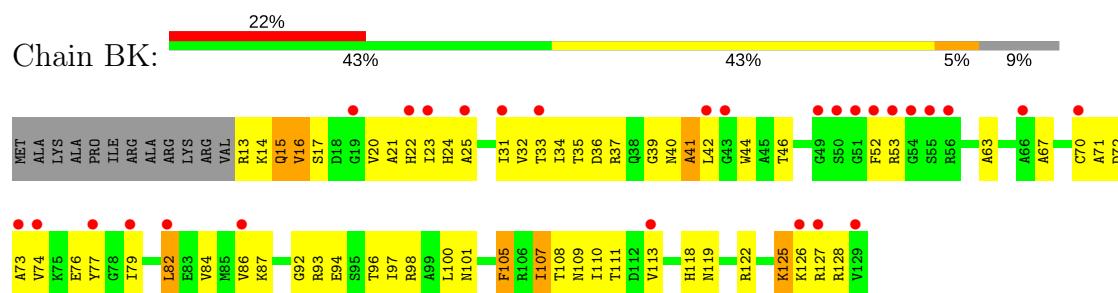
- Molecule 42: 30S ribosomal protein S10



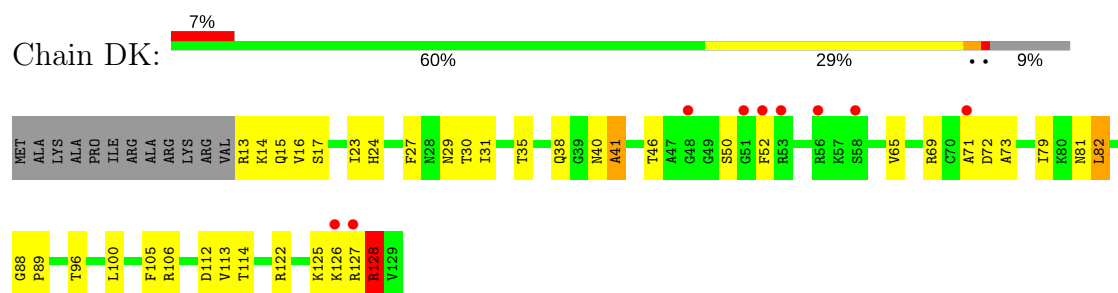
- Molecule 42: 30S ribosomal protein S10



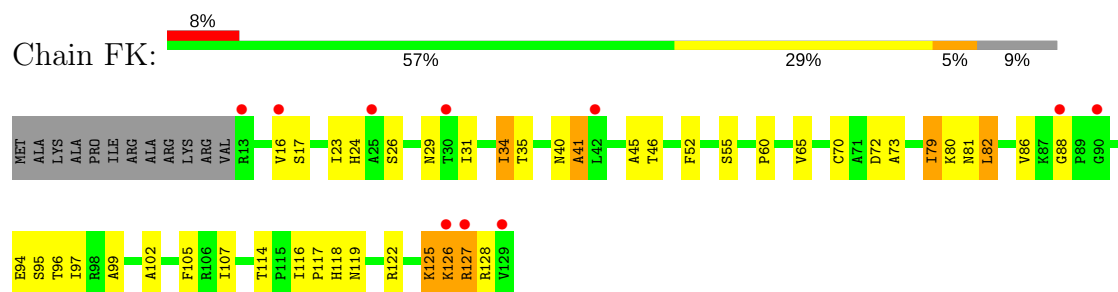
- Molecule 43: 30S ribosomal protein S11



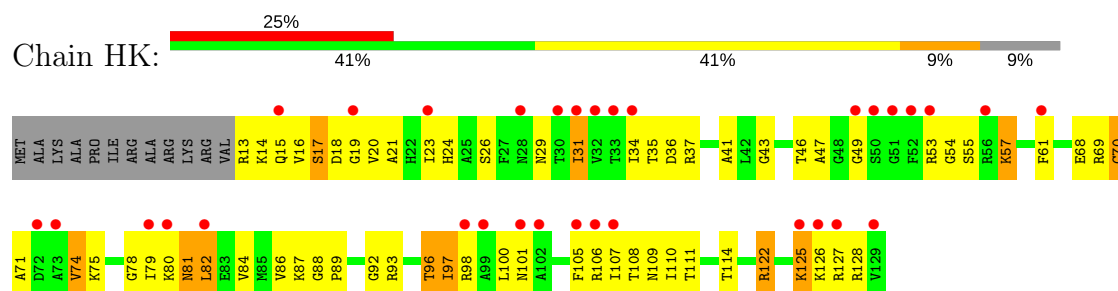
- Molecule 43: 30S ribosomal protein S11





- Molecule 43: 30S ribosomal protein S11



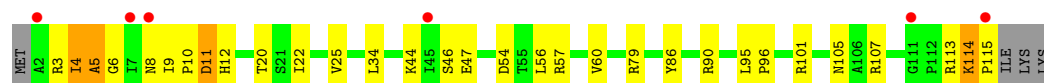
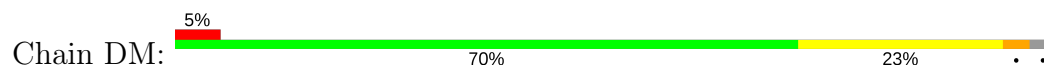
- Molecule 43: 30S ribosomal protein S11



- Chain BM: 
- 
- | Model | Performance (approx.) | Significance |
|-------|-----------------------|--------------|
| MET | 0.00 | |
| A2 | 0.05 | |
| R3 | 0.10 | |
| A4 | 0.15 | |
| A5 | 0.20 | |
| G6 | 0.25 | |
| I7 | 0.30 | |
| N8 | 0.35 | |
| I9 | 0.40 | |
| P10 | 0.45 | |
| D11 | 0.50 | |
| H12 | 0.55 | |
| K13 | 0.60 | |
| H14 | 0.65 | |
| A15 | 0.70 | |
| V16 | 0.75 | |
| I17 | 0.80 | |
| A18 | 0.85 | |
| L19 | 0.90 | |
| T20 | 0.95 | |
| S21 | 1.00 | |
| I22 | 1.05 | |
| V25 | 1.10 | |
| R29 | 1.15 | |
| I39 | 1.20 | |
| A40 | 1.25 | |
| E41 | 1.30 | |
| V43 | 1.35 | |
| K44 | 1.40 | |
| I45 | 1.45 | |
| S46 | 1.50 | |
| E47 | 1.55 | |
| L48 | 1.60 | |
| S49 | 1.65 | |
| Q52 | 1.70 | |
| I53 | 1.75 | |
| D54 | 1.80 | |
| I55 | 1.85 | |
| L56 | 1.90 | |
| R57 | 1.95 | |
| V60 | 2.00 | |
| F63 | 2.05 | |
| E66 | 2.10 | |
| R67 | 2.15 | |
| L95 | 2.20 | |
| N105 | 2.25 | |
| R109 | 2.30 | |



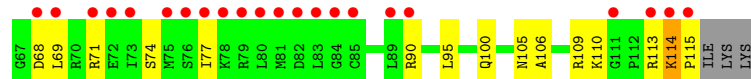
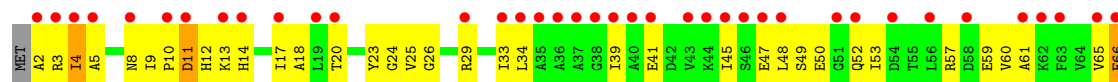
- Molecule 45: 30S ribosomal protein S13



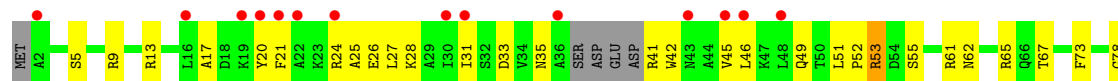
- Molecule 45: 30S ribosomal protein S13



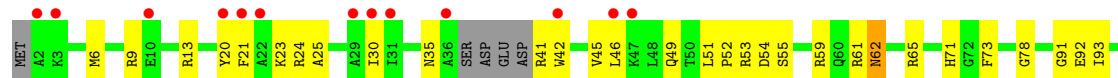
- Molecule 45: 30S ribosomal protein S13



- Molecule 46: 30S ribosomal protein S14



- Molecule 46: 30S ribosomal protein S14



W101

- Molecule 46: 30S ribosomal protein S14

Chain FN: 2% 60% 31% 5%



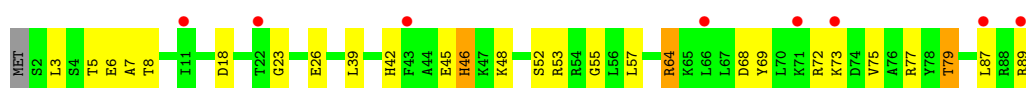
- Molecule 46: 30S ribosomal protein S14

Chain HN: 15% 58% 34% 5%



- Molecule 47: 30S ribosomal protein S15

Chain BO: 9% 69% 27% 5%



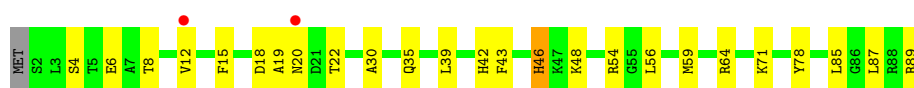
- Molecule 47: 30S ribosomal protein S15

Chain DO: 7% 74% 22% 5%



- Molecule 47: 30S ribosomal protein S15

Chain FO: 2% 71% 27% 5%

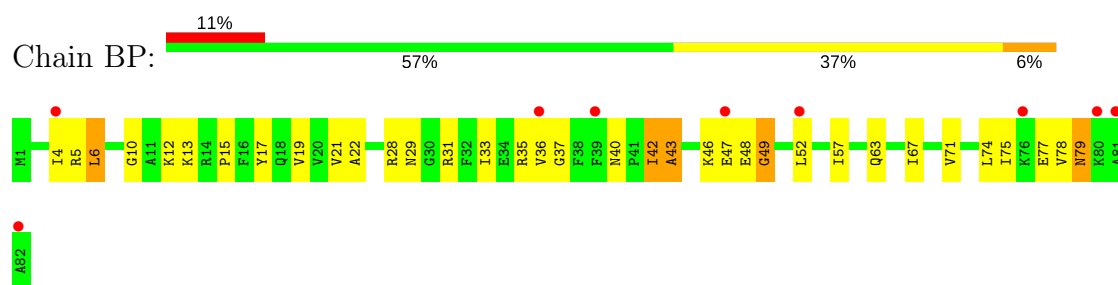


- Molecule 47: 30S ribosomal protein S15

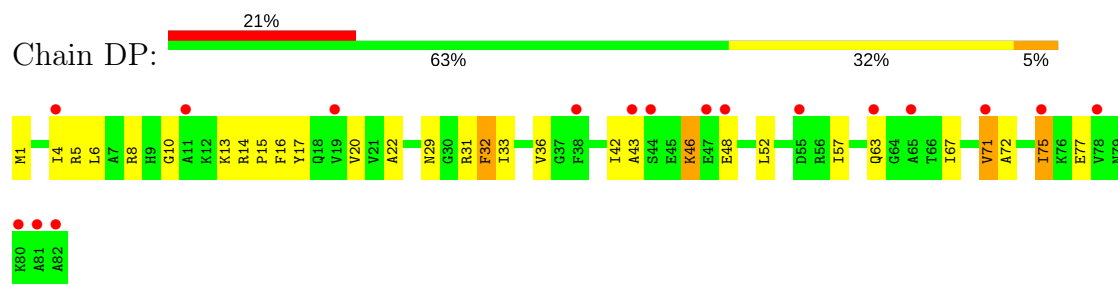
Chain HO: 3% 67% 28% 5%



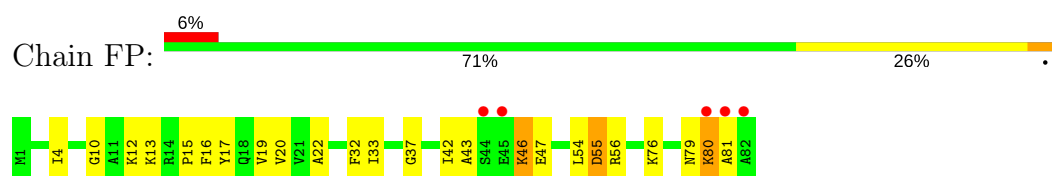
- Molecule 48: 30S ribosomal protein S16



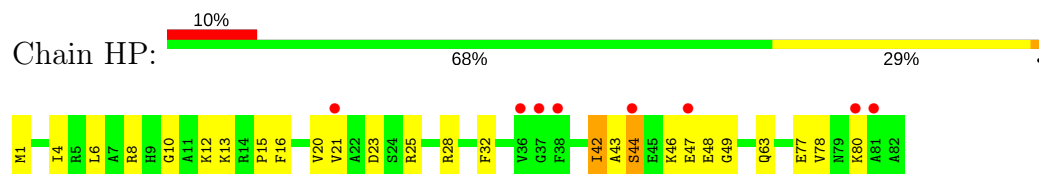
- Molecule 48: 30S ribosomal protein S16



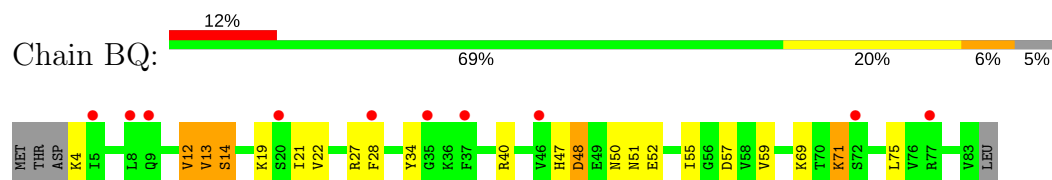
- Molecule 48: 30S ribosomal protein S16



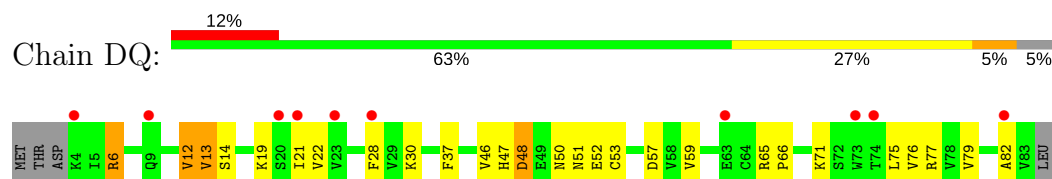
- Molecule 48: 30S ribosomal protein S16



- Molecule 49: 30S ribosomal protein S17



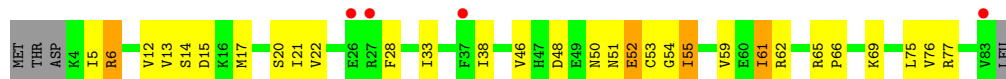
- Molecule 49: 30S ribosomal protein S17



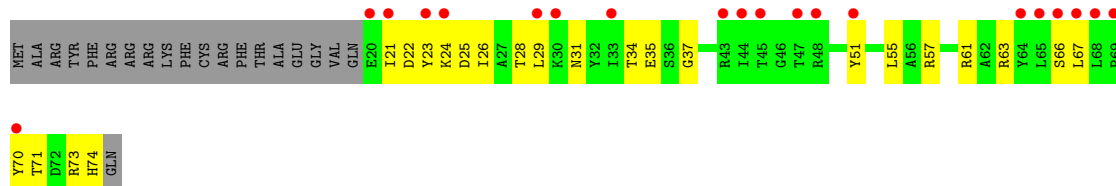
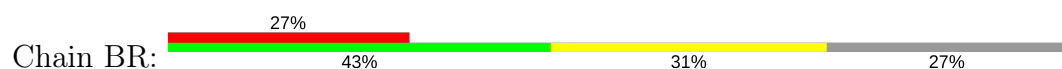
- Molecule 49: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S17



- Molecule 50: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S18



- Molecule 51: 30S ribosomal protein S19

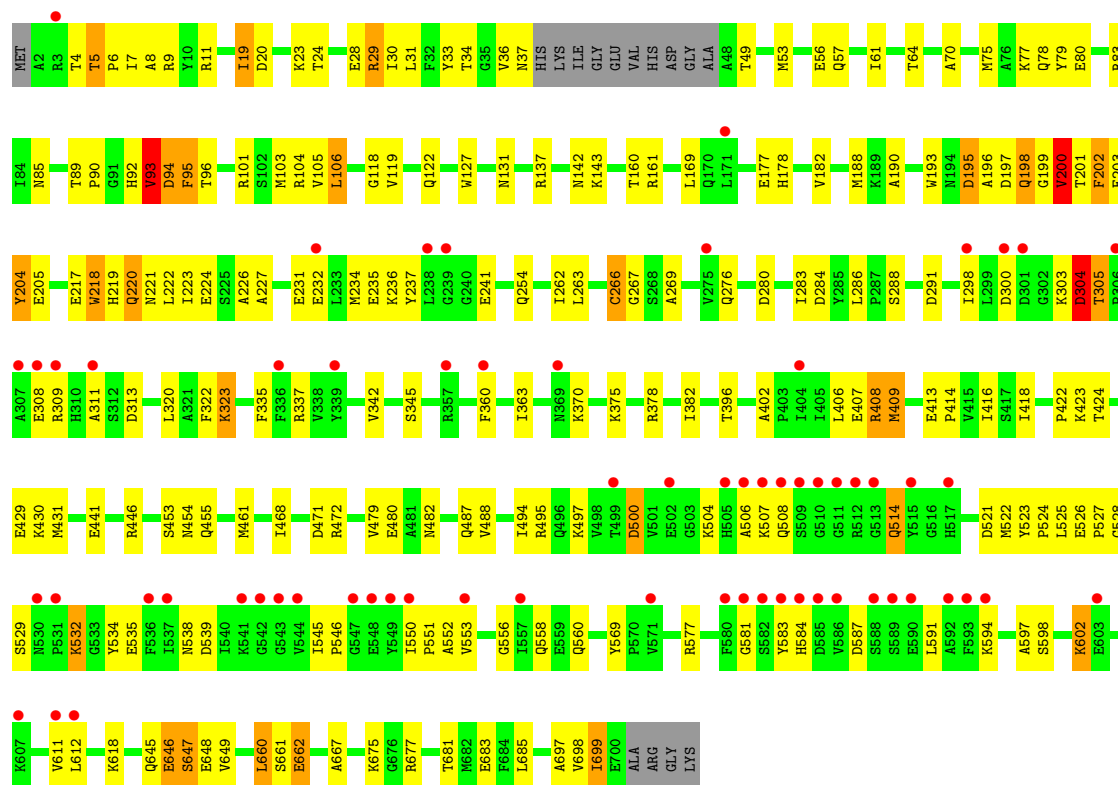


- [illegible]

ASN
ALA
ARG
THR
ARG
LEU
TYR

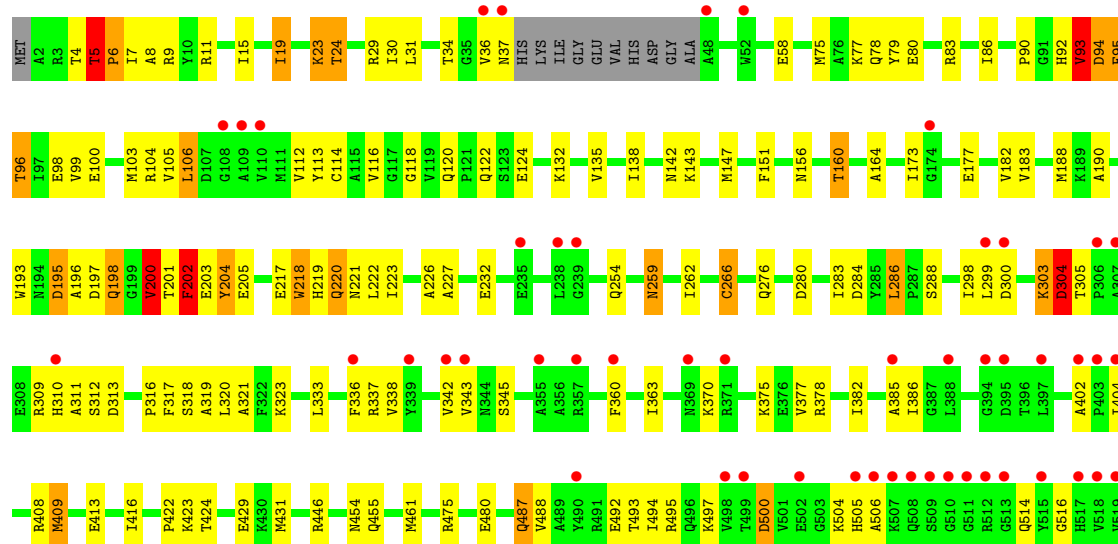
• Molecule 54: elongation factor G

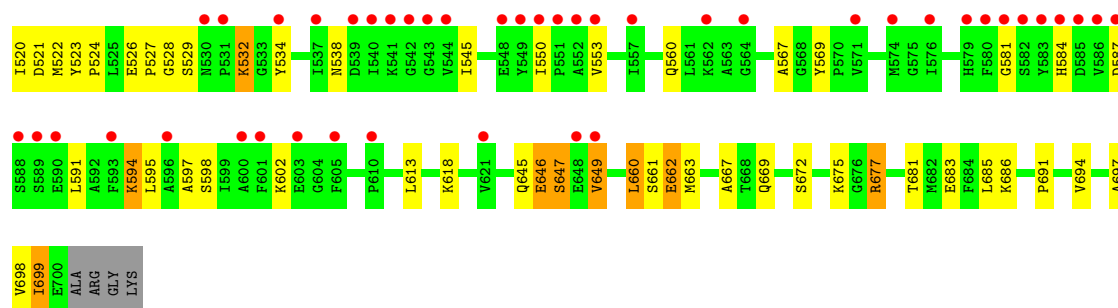
Chain BV: 



• Molecule 54: elongation factor G

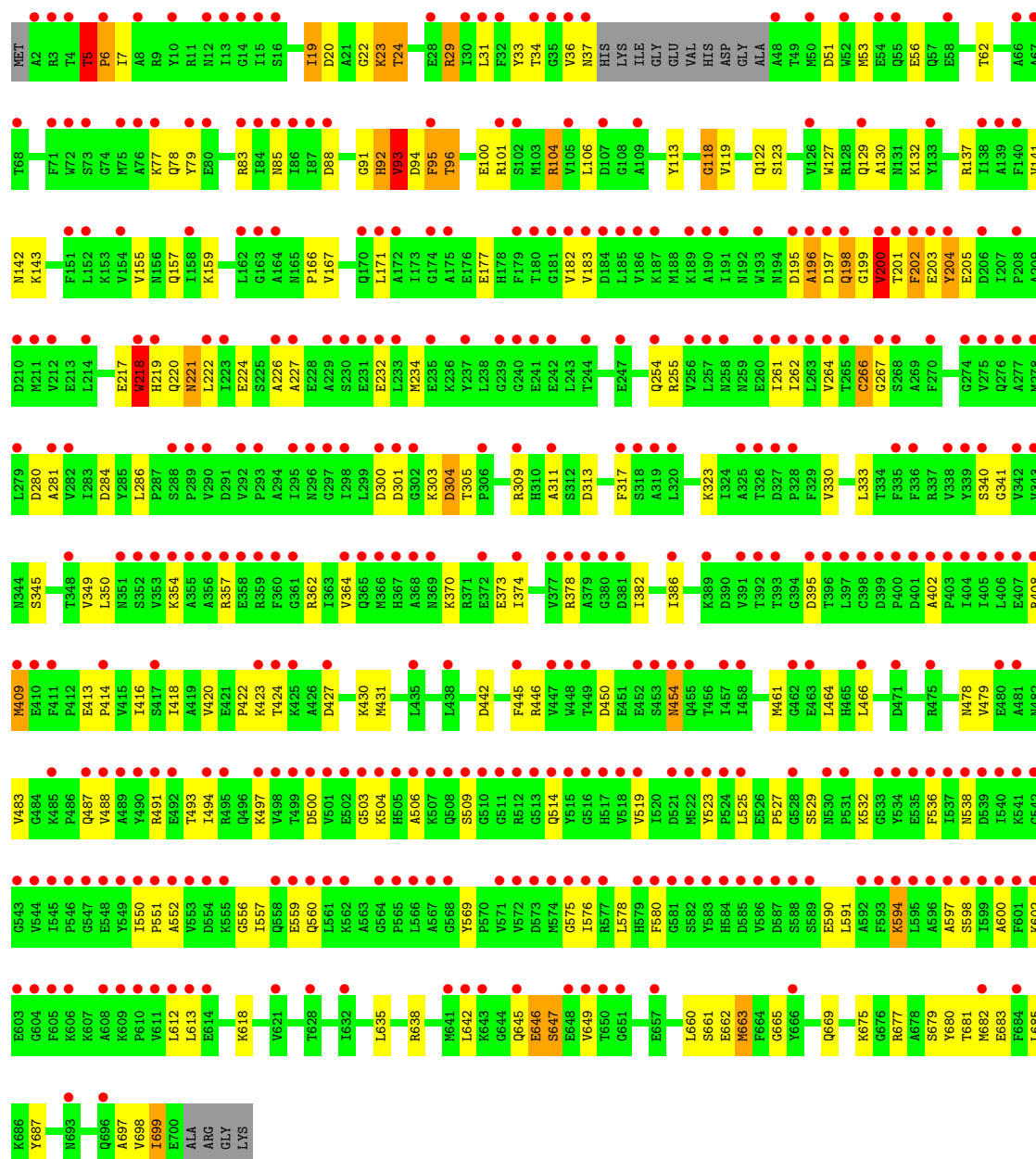
Chain DV: 



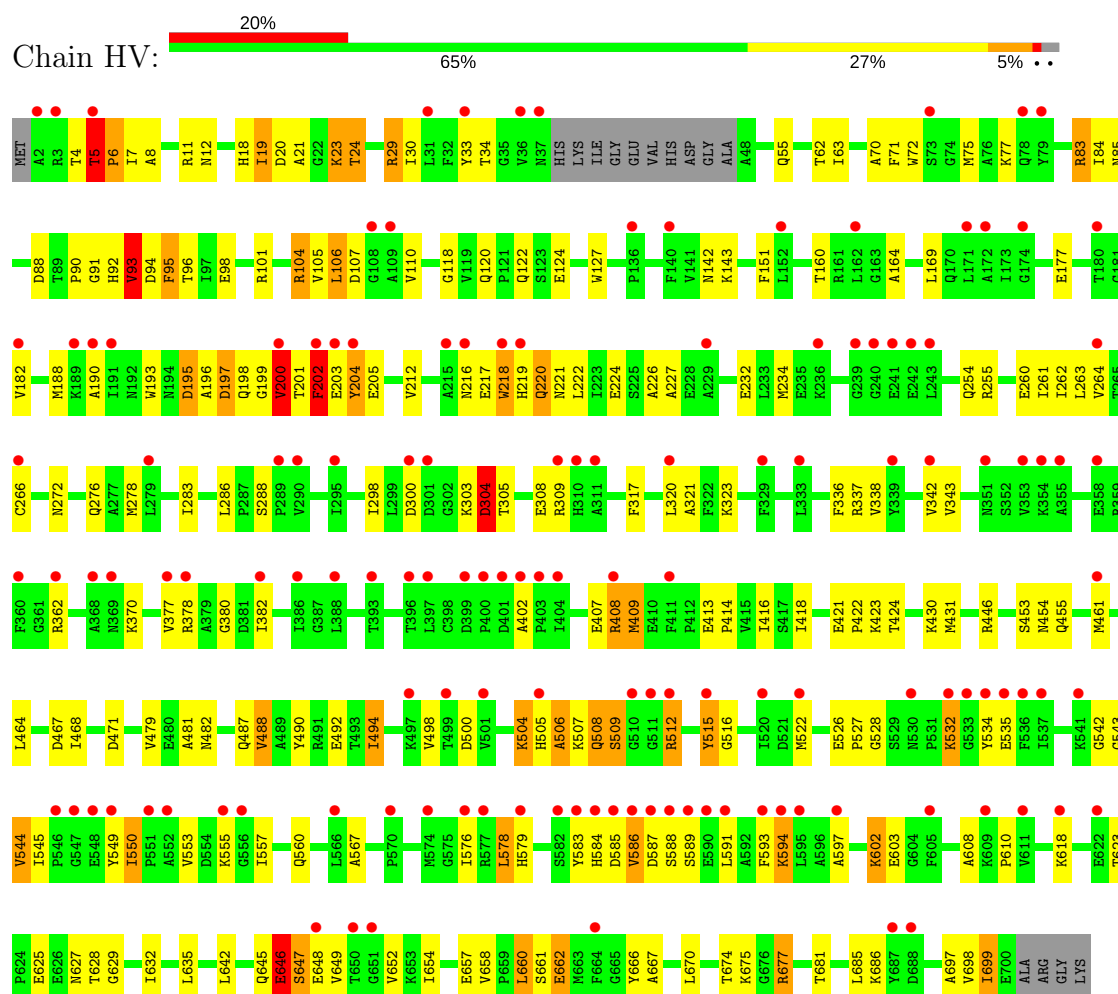


- Molecule 54: elongation factor G

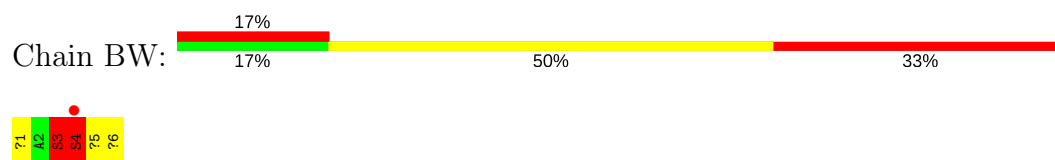
Chain FV: 52% 68% 26%



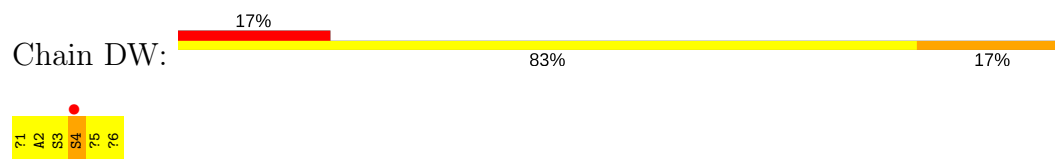
- Molecule 54: elongation factor G



• Molecule 55: Viomycin



• Molecule 55: Viomycin



• Molecule 55: Viomycin



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 361.14Å 360.51Å 429.73Å 90.00° 103.22° 90.00° | Depositor |
| Resolution (Å) | 70.00 – 2.90 69.13 – 2.80 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (70.00-2.90) 77.4 (69.13-2.80) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.24 (at 2.81Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.215 , 0.267 0.215 , 0.268 | Depositor DCC |
| R_{free} test set | 3890 reflections (0.43%) | DCC |
| Wilson B-factor (Å ²) | 54.5 | Xtriage |
| Anisotropy | 0.324 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 39.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 590573 | wwPDB-VP |
| Average B, all atoms (Å ²) | 35.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.8072e-03.*

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, DPP, MG, KBE, GCP, UAL, 5OH

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 | 0.74 | 9/68626 (0.0%) | 1.28 | 446/107056 (0.4%) |
| 1 | CA | 0.76 | 7/68626 (0.0%) | 1.27 | 404/107056 (0.4%) |
| 1 | EA | 0.90 | 29/68626 (0.0%) | 1.41 | 729/107056 (0.7%) |
| 1 | GA | 0.72 | 11/68626 (0.0%) | 1.25 | 345/107056 (0.3%) |
| 2 | AB | 0.67 | 0/2828 | 1.20 | 13/4410 (0.3%) |
| 2 | CB | 0.61 | 0/2828 | 1.15 | 11/4410 (0.2%) |
| 2 | EB | 0.75 | 1/2828 (0.0%) | 1.38 | 18/4410 (0.4%) |
| 2 | GB | 0.62 | 0/2828 | 1.09 | 2/4410 (0.0%) |
| 3 | AC | 0.55 | 0/2121 | 0.83 | 3/2852 (0.1%) |
| 3 | CC | 0.60 | 0/2121 | 0.81 | 0/2852 |
| 3 | EC | 0.62 | 0/2121 | 0.83 | 1/2852 (0.0%) |
| 3 | GC | 0.59 | 0/2121 | 0.84 | 1/2852 (0.0%) |
| 4 | AD | 0.60 | 0/1586 | 0.81 | 1/2134 (0.0%) |
| 4 | CD | 0.55 | 0/1586 | 0.75 | 1/2134 (0.0%) |
| 4 | ED | 0.63 | 0/1586 | 0.81 | 0/2134 |
| 4 | GD | 0.54 | 0/1586 | 0.78 | 1/2134 (0.0%) |
| 5 | AE | 0.50 | 0/1571 | 0.76 | 1/2113 (0.0%) |
| 5 | CE | 0.53 | 0/1571 | 0.71 | 0/2113 |
| 5 | EE | 0.59 | 0/1571 | 0.79 | 2/2113 (0.1%) |
| 5 | GE | 0.49 | 0/1571 | 0.68 | 0/2113 |
| 6 | AF | 0.69 | 0/1434 | 0.89 | 0/1926 |
| 6 | CF | 0.52 | 0/1434 | 0.70 | 0/1926 |
| 6 | EF | 0.51 | 0/1434 | 0.73 | 0/1926 |
| 6 | GF | 0.58 | 0/1434 | 0.77 | 1/1926 (0.1%) |
| 7 | AG | 0.54 | 0/1343 | 0.72 | 0/1816 |
| 7 | CG | 0.52 | 0/1343 | 0.73 | 0/1816 |
| 7 | EG | 0.53 | 0/1343 | 0.74 | 0/1816 |
| 7 | GG | 0.52 | 0/1343 | 0.72 | 0/1816 |
| 8 | AH | 0.54 | 0/389 | 0.71 | 0/523 |
| 8 | CH | 0.60 | 0/389 | 0.76 | 0/523 |
| 8 | EH | 0.57 | 0/389 | 0.73 | 0/523 |
| 8 | GH | 0.57 | 0/389 | 0.74 | 0/523 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 9 | AI | 0.58 | 0/1046 | 0.77 | 0/1410 |
| 9 | CI | 0.58 | 0/1046 | 0.74 | 0/1410 |
| 9 | EI | 0.61 | 0/1046 | 0.75 | 0/1410 |
| 9 | GI | 0.71 | 0/1046 | 0.84 | 0/1410 |
| 10 | AJ | 0.53 | 0/1152 | 0.77 | 0/1551 |
| 10 | CJ | 0.57 | 1/1152 (0.1%) | 0.78 | 0/1551 |
| 10 | EJ | 0.70 | 1/1152 (0.1%) | 0.82 | 1/1551 (0.1%) |
| 10 | GJ | 0.55 | 1/1152 (0.1%) | 0.71 | 0/1551 |
| 11 | AK | 0.62 | 0/947 | 0.79 | 0/1268 |
| 11 | CK | 0.63 | 0/947 | 0.78 | 0/1268 |
| 11 | EK | 0.59 | 0/947 | 0.83 | 0/1268 |
| 11 | GK | 0.55 | 0/947 | 0.80 | 0/1268 |
| 12 | AL | 0.53 | 0/1054 | 0.78 | 2/1403 (0.1%) |
| 12 | CL | 0.53 | 0/1054 | 0.81 | 2/1403 (0.1%) |
| 12 | EL | 0.61 | 0/1054 | 0.81 | 0/1403 |
| 12 | GL | 0.52 | 0/1054 | 0.78 | 0/1403 |
| 13 | AM | 0.61 | 1/1093 (0.1%) | 0.81 | 1/1460 (0.1%) |
| 13 | CM | 0.53 | 0/1093 | 0.75 | 0/1460 |
| 13 | EM | 0.62 | 0/1093 | 0.87 | 2/1460 (0.1%) |
| 13 | GM | 0.52 | 0/1093 | 0.73 | 0/1460 |
| 14 | AN | 0.51 | 0/973 | 0.75 | 1/1301 (0.1%) |
| 14 | CN | 0.46 | 0/973 | 0.77 | 4/1301 (0.3%) |
| 14 | EN | 0.57 | 0/973 | 0.74 | 0/1301 |
| 14 | GN | 0.49 | 0/973 | 0.69 | 0/1301 |
| 15 | AO | 0.48 | 0/902 | 0.72 | 0/1209 |
| 15 | CO | 0.47 | 0/902 | 0.70 | 0/1209 |
| 15 | EO | 0.48 | 0/902 | 0.75 | 0/1209 |
| 15 | GO | 0.48 | 0/902 | 0.74 | 0/1209 |
| 16 | AP | 0.56 | 0/929 | 0.87 | 2/1242 (0.2%) |
| 16 | CP | 0.56 | 0/929 | 0.85 | 2/1242 (0.2%) |
| 16 | EP | 0.63 | 1/929 (0.1%) | 0.89 | 1/1242 (0.1%) |
| 16 | GP | 0.58 | 0/929 | 0.80 | 0/1242 |
| 17 | AQ | 0.56 | 0/960 | 0.75 | 1/1278 (0.1%) |
| 17 | CQ | 0.60 | 0/960 | 0.78 | 1/1278 (0.1%) |
| 17 | EQ | 0.70 | 0/960 | 0.88 | 2/1278 (0.2%) |
| 17 | GQ | 0.53 | 0/960 | 0.74 | 0/1278 |
| 18 | AR | 0.59 | 0/829 | 0.75 | 0/1107 |
| 18 | CR | 0.59 | 0/829 | 0.75 | 0/1107 |
| 18 | ER | 0.68 | 2/829 (0.2%) | 0.79 | 0/1107 |
| 18 | GR | 0.56 | 0/829 | 0.75 | 0/1107 |
| 19 | AS | 0.52 | 0/864 | 0.76 | 0/1156 |
| 19 | CS | 0.52 | 0/864 | 0.73 | 0/1156 |
| 19 | ES | 0.62 | 0/864 | 0.84 | 1/1156 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------|-------------|--------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 19 | GS | 0.49 | 0/864 | 0.72 | 0/1156 |
| 20 | AT | 0.60 | 0/744 | 0.84 | 0/994 |
| 20 | CT | 0.56 | 0/744 | 0.89 | 0/994 |
| 20 | ET | 0.65 | 0/744 | 0.92 | 1/994 (0.1%) |
| 20 | GT | 0.57 | 0/744 | 0.91 | 1/994 (0.1%) |
| 21 | AU | 0.56 | 0/787 | 0.76 | 0/1051 |
| 21 | CU | 0.52 | 0/787 | 0.75 | 0/1051 |
| 21 | EU | 0.61 | 0/787 | 0.81 | 0/1051 |
| 21 | GU | 0.52 | 0/787 | 0.77 | 0/1051 |
| 22 | AV | 0.48 | 0/766 | 0.67 | 0/1025 |
| 22 | CV | 0.55 | 1/766 (0.1%) | 0.67 | 0/1025 |
| 22 | EV | 0.57 | 0/766 | 0.72 | 0/1025 |
| 22 | GV | 0.47 | 0/766 | 0.65 | 0/1025 |
| 23 | AW | 0.63 | 0/603 | 0.93 | 1/797 (0.1%) |
| 23 | CW | 0.70 | 0/603 | 0.94 | 1/797 (0.1%) |
| 23 | EW | 0.78 | 0/603 | 0.97 | 1/797 (0.1%) |
| 23 | GW | 0.66 | 0/603 | 0.92 | 0/797 |
| 24 | AX | 0.52 | 0/635 | 0.83 | 1/848 (0.1%) |
| 24 | CX | 0.58 | 0/635 | 0.80 | 2/848 (0.2%) |
| 24 | EX | 0.56 | 0/635 | 0.79 | 1/848 (0.1%) |
| 24 | GX | 0.51 | 0/635 | 0.79 | 0/848 |
| 25 | AY | 0.47 | 0/510 | 0.75 | 0/677 |
| 25 | CY | 0.51 | 0/510 | 0.76 | 0/677 |
| 25 | EY | 0.54 | 0/510 | 0.85 | 1/677 (0.1%) |
| 25 | GY | 0.55 | 0/510 | 0.79 | 1/677 (0.1%) |
| 26 | AZ | 0.53 | 0/453 | 0.65 | 0/605 |
| 26 | CZ | 0.49 | 0/453 | 0.75 | 0/605 |
| 26 | EZ | 0.58 | 0/453 | 0.82 | 0/605 |
| 26 | GZ | 0.48 | 0/453 | 0.73 | 0/605 |
| 27 | A0 | 0.50 | 0/450 | 0.77 | 0/599 |
| 27 | C0 | 0.49 | 0/450 | 0.72 | 0/599 |
| 27 | E0 | 0.68 | 1/450 (0.2%) | 0.80 | 1/599 (0.2%) |
| 27 | G0 | 0.52 | 1/450 (0.2%) | 0.69 | 0/599 |
| 28 | A1 | 0.54 | 0/416 | 0.78 | 0/554 |
| 28 | C1 | 0.51 | 0/416 | 0.76 | 0/554 |
| 28 | E1 | 0.54 | 0/416 | 0.72 | 0/554 |
| 28 | G1 | 0.54 | 0/416 | 0.73 | 0/554 |
| 29 | A2 | 0.52 | 0/380 | 0.77 | 0/498 |
| 29 | C2 | 0.56 | 0/380 | 0.73 | 0/498 |
| 29 | E2 | 0.75 | 1/380 (0.3%) | 0.84 | 1/498 (0.2%) |
| 29 | G2 | 0.59 | 0/380 | 0.75 | 0/498 |
| 30 | A3 | 0.51 | 0/513 | 0.74 | 0/676 |
| 30 | C3 | 0.54 | 0/513 | 0.68 | 0/676 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 30 | E3 | 0.64 | 0/513 | 0.81 | 0/676 |
| 30 | G3 | 0.50 | 0/513 | 0.70 | 0/676 |
| 31 | A4 | 0.61 | 0/303 | 0.78 | 0/397 |
| 31 | C4 | 0.60 | 0/303 | 0.81 | 0/397 |
| 31 | E4 | 0.60 | 0/303 | 0.82 | 0/397 |
| 31 | G4 | 0.53 | 0/303 | 0.77 | 0/397 |
| 32 | A5 | 0.83 | 0/1131 | 1.34 | 28/1524 (1.8%) |
| 32 | E5 | 0.74 | 0/1106 | 1.34 | 26/1490 (1.7%) |
| 33 | BA | 0.64 | 0/36834 | 1.15 | 99/57462 (0.2%) |
| 33 | DA | 0.63 | 0/36834 | 1.13 | 95/57462 (0.2%) |
| 33 | FA | 0.65 | 1/36834 (0.0%) | 1.18 | 114/57462 (0.2%) |
| 33 | HA | 0.64 | 0/36834 | 1.13 | 101/57462 (0.2%) |
| 34 | BB | 0.53 | 0/1735 | 0.72 | 0/2338 |
| 34 | DB | 0.49 | 0/1735 | 0.70 | 0/2338 |
| 34 | FB | 0.54 | 0/1735 | 0.73 | 0/2338 |
| 34 | HB | 0.52 | 0/1735 | 0.72 | 0/2338 |
| 35 | BC | 0.47 | 0/1651 | 0.64 | 0/2225 |
| 35 | DC | 0.47 | 0/1651 | 0.61 | 0/2225 |
| 35 | FC | 0.50 | 0/1651 | 0.71 | 0/2225 |
| 35 | HC | 0.48 | 0/1651 | 0.67 | 0/2225 |
| 36 | BD | 0.52 | 0/1665 | 0.74 | 0/2227 |
| 36 | DD | 0.54 | 0/1665 | 0.76 | 0/2227 |
| 36 | FD | 0.49 | 0/1665 | 0.71 | 0/2227 |
| 36 | HD | 0.52 | 0/1665 | 0.73 | 0/2227 |
| 37 | BE | 0.56 | 1/1118 (0.1%) | 0.77 | 0/1504 |
| 37 | DE | 0.50 | 0/1118 | 0.74 | 0/1504 |
| 37 | FE | 0.54 | 0/1118 | 0.78 | 0/1504 |
| 37 | HE | 0.52 | 0/1118 | 0.76 | 0/1504 |
| 38 | BF | 0.64 | 0/835 | 0.75 | 0/1128 |
| 38 | DF | 0.55 | 0/835 | 0.73 | 0/1128 |
| 38 | FF | 0.54 | 0/835 | 0.73 | 0/1128 |
| 38 | HF | 0.58 | 0/835 | 0.72 | 0/1128 |
| 39 | BG | 0.48 | 0/1195 | 0.66 | 0/1602 |
| 39 | DG | 0.47 | 0/1195 | 0.66 | 0/1602 |
| 39 | FG | 0.51 | 0/1195 | 0.70 | 0/1602 |
| 39 | HG | 0.51 | 0/1195 | 0.73 | 0/1602 |
| 40 | BH | 0.48 | 0/989 | 0.63 | 0/1326 |
| 40 | DH | 0.50 | 0/989 | 0.65 | 0/1326 |
| 40 | FH | 0.50 | 0/989 | 0.72 | 0/1326 |
| 40 | HH | 0.45 | 0/989 | 0.66 | 0/1326 |
| 41 | BI | 0.52 | 0/1034 | 0.77 | 0/1375 |
| 41 | DI | 0.49 | 0/1034 | 0.72 | 1/1375 (0.1%) |
| 41 | FI | 0.52 | 0/1034 | 0.80 | 0/1375 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 41 | HI | 0.56 | 0/1034 | 0.76 | 1/1375 (0.1%) |
| 42 | BJ | 0.53 | 0/796 | 0.73 | 1/1077 (0.1%) |
| 42 | DJ | 0.55 | 0/796 | 0.75 | 0/1077 |
| 42 | FJ | 0.55 | 0/796 | 0.78 | 0/1077 |
| 42 | HJ | 0.54 | 0/796 | 0.77 | 0/1077 |
| 43 | BK | 0.59 | 0/893 | 0.81 | 0/1205 |
| 43 | DK | 0.51 | 0/893 | 0.80 | 1/1205 (0.1%) |
| 43 | FK | 0.52 | 0/893 | 0.72 | 0/1205 |
| 43 | HK | 0.71 | 0/893 | 0.92 | 2/1205 (0.2%) |
| 44 | BL | 0.55 | 0/969 | 0.78 | 0/1300 |
| 44 | DL | 0.54 | 0/969 | 0.79 | 0/1300 |
| 44 | FL | 0.51 | 0/969 | 0.75 | 1/1300 (0.1%) |
| 44 | HL | 0.50 | 0/969 | 0.78 | 0/1300 |
| 45 | BM | 0.48 | 0/892 | 0.72 | 0/1193 |
| 45 | DM | 0.48 | 0/892 | 0.70 | 0/1193 |
| 45 | FM | 0.46 | 0/892 | 0.72 | 0/1193 |
| 45 | HM | 0.60 | 0/892 | 0.83 | 0/1193 |
| 46 | BN | 0.53 | 0/785 | 0.73 | 0/1043 |
| 46 | DN | 0.53 | 0/785 | 0.68 | 0/1043 |
| 46 | FN | 0.59 | 0/785 | 0.80 | 0/1043 |
| 46 | HN | 0.48 | 0/785 | 0.67 | 0/1043 |
| 47 | BO | 0.46 | 0/722 | 0.65 | 0/964 |
| 47 | DO | 0.47 | 0/722 | 0.64 | 0/964 |
| 47 | FO | 0.44 | 0/722 | 0.63 | 0/964 |
| 47 | HO | 0.50 | 0/722 | 0.68 | 0/964 |
| 48 | BP | 0.51 | 0/659 | 0.74 | 0/884 |
| 48 | DP | 0.52 | 0/659 | 0.72 | 0/884 |
| 48 | FP | 0.48 | 0/659 | 0.70 | 0/884 |
| 48 | HP | 0.51 | 0/659 | 0.67 | 0/884 |
| 49 | BQ | 0.51 | 0/657 | 0.73 | 0/881 |
| 49 | DQ | 0.50 | 0/657 | 0.74 | 0/881 |
| 49 | FQ | 0.49 | 0/657 | 0.66 | 0/881 |
| 49 | HQ | 0.51 | 0/657 | 0.75 | 0/881 |
| 50 | BR | 0.53 | 0/462 | 0.67 | 0/621 |
| 50 | DR | 0.50 | 0/462 | 0.71 | 0/621 |
| 50 | FR | 0.48 | 0/462 | 0.63 | 0/621 |
| 50 | HR | 0.53 | 0/462 | 0.77 | 1/621 (0.2%) |
| 51 | BS | 0.47 | 0/652 | 0.78 | 0/877 |
| 51 | DS | 0.49 | 0/652 | 0.70 | 0/877 |
| 51 | FS | 0.48 | 0/652 | 0.72 | 0/877 |
| 51 | HS | 0.66 | 0/652 | 0.79 | 0/877 |
| 52 | BT | 0.50 | 0/671 | 0.65 | 0/888 |
| 52 | DT | 0.49 | 0/671 | 0.64 | 0/888 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 52 | FT | 0.48 | 0/671 | 0.68 | 0/888 |
| 52 | HT | 0.49 | 0/671 | 0.72 | 0/888 |
| 53 | BU | 0.67 | 0/430 | 0.75 | 0/570 |
| 53 | DU | 0.67 | 0/430 | 0.83 | 1/570 (0.2%) |
| 53 | FU | 0.69 | 0/430 | 0.83 | 0/570 |
| 53 | HU | 0.78 | 0/430 | 0.82 | 0/570 |
| 54 | BV | 0.48 | 0/5418 | 0.68 | 1/7329 (0.0%) |
| 54 | DV | 0.46 | 0/5418 | 0.66 | 1/7329 (0.0%) |
| 54 | FV | 0.57 | 0/5418 | 0.68 | 1/7329 (0.0%) |
| 54 | HV | 0.50 | 0/5418 | 0.70 | 1/7329 (0.0%) |
| 55 | BW | 2.44 | 1/11 (9.1%) | 1.38 | 0/13 |
| 55 | DW | 2.31 | 1/11 (9.1%) | 1.57 | 0/13 |
| 55 | FW | 2.44 | 1/11 (9.1%) | 2.53 | 1/13 (7.7%) |
| All | All | 0.68 | 73/635346 (0.0%) | 1.13 | 2493/946873 (0.3%) |

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 |
|-----|-------|---------------------|---------------------|
| 3 | CC | 0 | 1 |
| 3 | EC | 0 | 1 |
| 3 | GC | 0 | 1 |
| 4 | CD | 0 | 2 |
| 4 | ED | 0 | 1 |
| 4 | GD | 0 | 1 |
| 32 | A5 | 0 | 2 |
| 41 | FI | 0 | 1 |
| 44 | BL | 0 | 1 |
| 44 | DL | 0 | 1 |
| 44 | FL | 0 | 1 |
| 44 | HL | 0 | 1 |
| 54 | BV | 0 | 2 |
| 54 | DV | 0 | 2 |
| 54 | FV | 0 | 2 |
| 54 | HV | 0 | 3 |
| All | All | 0 | 23 |

The worst 5 of 73 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | EA | 984 | A | N9-C4 | -10.08 | 1.31 | 1.37 |
| 1 | EA | 528 | A | N9-C4 | -9.15 | 1.32 | 1.37 |
| 37 | BE | 94 | VAL | CB-CG2 | 9.12 | 1.72 | 1.52 |
| 13 | AM | 13 | HIS | CG-CD2 | 8.66 | 1.50 | 1.35 |
| 10 | EJ | 44 | TYR | CD1-CE1 | -7.92 | 1.27 | 1.39 |

The worst 5 of 2493 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | EA | 834 | G | N1-C6-O6 | 16.23 | 129.64 | 119.90 |
| 1 | EA | 984 | A | C2-N3-C4 | -15.83 | 102.68 | 110.60 |
| 1 | EA | 974 | G | C4-C5-N7 | 15.17 | 116.87 | 110.80 |
| 1 | AA | 2544 | G | N1-C6-O6 | 14.98 | 128.89 | 119.90 |
| 1 | AA | 2053 | G | N1-C6-O6 | 14.67 | 128.70 | 119.90 |

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 32 | A5 | 130 | PRO | Peptide |
| 32 | A5 | 134 | GLU | Peptide |
| 44 | BL | 23 | ALA | Peptide |
| 54 | BV | 218 | TRP | Peptide |
| 54 | BV | 304 | ASP | Peptide |

5.2 Too-close contacts [i](#)

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 | 61274 | 0 | 30818 | 1057 | 0 |
| 1 | CA | 61274 | 0 | 30819 | 919 | 0 |
| 1 | EA | 61274 | 0 | 30819 | 835 | 0 |
| 1 | GA | 61274 | 0 | 30819 | 917 | 3 |
| 2 | AB | 2529 | 0 | 1281 | 36 | 0 |
| 2 | CB | 2529 | 0 | 1281 | 34 | 0 |
| 2 | EB | 2529 | 0 | 1281 | 35 | 0 |
| 2 | GB | 2529 | 0 | 1281 | 37 | 0 |
| 3 | AC | 2082 | 0 | 2157 | 67 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | CC | 2082 | 0 | 2157 | 68 | 0 |
| 3 | EC | 2082 | 0 | 2157 | 65 | 0 |
| 3 | GC | 2082 | 0 | 2157 | 57 | 0 |
| 4 | AD | 1565 | 0 | 1616 | 78 | 0 |
| 4 | CD | 1565 | 0 | 1616 | 75 | 0 |
| 4 | ED | 1565 | 0 | 1616 | 72 | 0 |
| 4 | GD | 1565 | 0 | 1616 | 77 | 0 |
| 5 | AE | 1552 | 0 | 1619 | 63 | 0 |
| 5 | CE | 1552 | 0 | 1619 | 34 | 0 |
| 5 | EE | 1552 | 0 | 1619 | 42 | 0 |
| 5 | GE | 1552 | 0 | 1619 | 56 | 0 |
| 6 | AF | 1410 | 0 | 1447 | 133 | 0 |
| 6 | CF | 1410 | 0 | 1447 | 53 | 0 |
| 6 | EF | 1410 | 0 | 1447 | 60 | 0 |
| 6 | GF | 1410 | 0 | 1447 | 92 | 1 |
| 7 | AG | 1323 | 0 | 1374 | 65 | 0 |
| 7 | CG | 1323 | 0 | 1374 | 65 | 0 |
| 7 | EG | 1323 | 0 | 1374 | 48 | 0 |
| 7 | GG | 1323 | 0 | 1374 | 58 | 0 |
| 8 | AH | 384 | 0 | 405 | 12 | 0 |
| 8 | CH | 384 | 0 | 405 | 18 | 0 |
| 8 | EH | 384 | 0 | 405 | 15 | 0 |
| 8 | GH | 384 | 0 | 405 | 11 | 0 |
| 9 | AI | 1032 | 0 | 1088 | 70 | 0 |
| 9 | CI | 1032 | 0 | 1088 | 62 | 0 |
| 9 | EI | 1032 | 0 | 1088 | 48 | 0 |
| 9 | GI | 1032 | 0 | 1088 | 82 | 0 |
| 10 | AJ | 1129 | 0 | 1162 | 49 | 0 |
| 10 | CJ | 1129 | 0 | 1162 | 58 | 0 |
| 10 | EJ | 1129 | 0 | 1162 | 76 | 0 |
| 10 | GJ | 1129 | 0 | 1162 | 57 | 0 |
| 11 | AK | 938 | 0 | 1012 | 40 | 0 |
| 11 | CK | 938 | 0 | 1012 | 57 | 0 |
| 11 | EK | 938 | 0 | 1012 | 49 | 0 |
| 11 | GK | 938 | 0 | 1012 | 42 | 0 |
| 12 | AL | 1045 | 0 | 1117 | 51 | 0 |
| 12 | CL | 1045 | 0 | 1117 | 38 | 0 |
| 12 | EL | 1045 | 0 | 1117 | 35 | 0 |
| 12 | GL | 1045 | 0 | 1117 | 50 | 0 |
| 13 | AM | 1074 | 0 | 1157 | 29 | 0 |
| 13 | CM | 1074 | 0 | 1157 | 33 | 0 |
| 13 | EM | 1074 | 0 | 1157 | 29 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13 | GM | 1074 | 0 | 1157 | 24 | 0 |
| 14 | AN | 960 | 0 | 1000 | 35 | 0 |
| 14 | CN | 960 | 0 | 1000 | 44 | 0 |
| 14 | EN | 960 | 0 | 1000 | 33 | 0 |
| 14 | GN | 960 | 0 | 1000 | 36 | 0 |
| 15 | AO | 892 | 0 | 923 | 41 | 0 |
| 15 | CO | 892 | 0 | 923 | 32 | 0 |
| 15 | EO | 892 | 0 | 923 | 21 | 0 |
| 15 | GO | 892 | 0 | 923 | 29 | 0 |
| 16 | AP | 917 | 0 | 965 | 63 | 0 |
| 16 | CP | 917 | 0 | 965 | 58 | 0 |
| 16 | EP | 917 | 0 | 965 | 52 | 0 |
| 16 | GP | 917 | 0 | 965 | 49 | 0 |
| 17 | AQ | 947 | 0 | 1022 | 53 | 0 |
| 17 | CQ | 947 | 0 | 1022 | 56 | 0 |
| 17 | EQ | 947 | 0 | 1022 | 58 | 0 |
| 17 | GQ | 947 | 0 | 1022 | 56 | 0 |
| 18 | AR | 816 | 0 | 839 | 41 | 0 |
| 18 | CR | 816 | 0 | 839 | 49 | 0 |
| 18 | ER | 816 | 0 | 839 | 46 | 0 |
| 18 | GR | 816 | 0 | 839 | 34 | 0 |
| 19 | AS | 857 | 0 | 922 | 21 | 0 |
| 19 | CS | 857 | 0 | 922 | 27 | 0 |
| 19 | ES | 857 | 0 | 922 | 26 | 0 |
| 19 | GS | 857 | 0 | 922 | 30 | 0 |
| 20 | AT | 738 | 0 | 807 | 51 | 0 |
| 20 | CT | 738 | 0 | 807 | 54 | 0 |
| 20 | ET | 738 | 0 | 807 | 34 | 0 |
| 20 | GT | 738 | 0 | 807 | 47 | 0 |
| 21 | AU | 779 | 0 | 834 | 31 | 0 |
| 21 | CU | 779 | 0 | 834 | 19 | 0 |
| 21 | EU | 779 | 0 | 834 | 28 | 0 |
| 21 | GU | 779 | 0 | 834 | 27 | 1 |
| 22 | AV | 753 | 0 | 780 | 10 | 0 |
| 22 | CV | 753 | 0 | 780 | 16 | 0 |
| 22 | EV | 753 | 0 | 780 | 16 | 0 |
| 22 | GV | 753 | 0 | 780 | 25 | 0 |
| 23 | AW | 596 | 0 | 610 | 83 | 0 |
| 23 | CW | 596 | 0 | 610 | 78 | 0 |
| 23 | EW | 596 | 0 | 610 | 100 | 0 |
| 23 | GW | 596 | 0 | 610 | 85 | 0 |
| 24 | AX | 625 | 0 | 655 | 21 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24 | CX | 625 | 0 | 655 | 20 | 0 |
| 24 | EX | 625 | 0 | 655 | 26 | 0 |
| 24 | GX | 625 | 0 | 655 | 24 | 0 |
| 25 | AY | 509 | 0 | 543 | 12 | 0 |
| 25 | CY | 509 | 0 | 543 | 16 | 0 |
| 25 | EY | 509 | 0 | 543 | 17 | 0 |
| 25 | GY | 509 | 0 | 543 | 11 | 0 |
| 26 | AZ | 449 | 0 | 491 | 6 | 0 |
| 26 | CZ | 449 | 0 | 491 | 11 | 0 |
| 26 | EZ | 449 | 0 | 491 | 15 | 0 |
| 26 | GZ | 449 | 0 | 491 | 14 | 0 |
| 27 | A0 | 444 | 0 | 461 | 20 | 0 |
| 27 | C0 | 444 | 0 | 461 | 15 | 0 |
| 27 | E0 | 444 | 0 | 461 | 6 | 0 |
| 27 | G0 | 444 | 0 | 461 | 12 | 0 |
| 28 | A1 | 409 | 0 | 440 | 18 | 0 |
| 28 | C1 | 409 | 0 | 440 | 23 | 0 |
| 28 | E1 | 409 | 0 | 440 | 14 | 0 |
| 28 | G1 | 409 | 0 | 440 | 13 | 0 |
| 29 | A2 | 377 | 0 | 418 | 12 | 0 |
| 29 | C2 | 377 | 0 | 418 | 9 | 0 |
| 29 | E2 | 377 | 0 | 418 | 15 | 0 |
| 29 | G2 | 377 | 0 | 418 | 8 | 0 |
| 30 | A3 | 504 | 0 | 574 | 20 | 0 |
| 30 | C3 | 504 | 0 | 574 | 16 | 0 |
| 30 | E3 | 504 | 0 | 574 | 14 | 0 |
| 30 | G3 | 504 | 0 | 574 | 21 | 0 |
| 31 | A4 | 302 | 0 | 340 | 14 | 0 |
| 31 | C4 | 302 | 0 | 340 | 17 | 0 |
| 31 | E4 | 302 | 0 | 340 | 14 | 0 |
| 31 | G4 | 302 | 0 | 340 | 13 | 0 |
| 32 | A5 | 1117 | 0 | 1155 | 135 | 0 |
| 32 | E5 | 1092 | 0 | 1134 | 122 | 0 |
| 33 | BA | 32895 | 0 | 16553 | 571 | 0 |
| 33 | DA | 32895 | 0 | 16553 | 534 | 0 |
| 33 | FA | 32895 | 0 | 16553 | 435 | 3 |
| 33 | HA | 32895 | 0 | 16553 | 430 | 0 |
| 34 | BB | 1704 | 0 | 1732 | 67 | 0 |
| 34 | DB | 1704 | 0 | 1732 | 87 | 0 |
| 34 | FB | 1704 | 0 | 1732 | 79 | 0 |
| 34 | HB | 1704 | 0 | 1732 | 72 | 0 |
| 35 | BC | 1624 | 0 | 1696 | 52 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35 | DC | 1624 | 0 | 1696 | 40 | 0 |
| 35 | FC | 1624 | 0 | 1696 | 38 | 0 |
| 35 | HC | 1624 | 0 | 1696 | 50 | 0 |
| 36 | BD | 1643 | 0 | 1707 | 80 | 0 |
| 36 | DD | 1643 | 0 | 1707 | 83 | 0 |
| 36 | FD | 1643 | 0 | 1707 | 73 | 0 |
| 36 | HD | 1643 | 0 | 1707 | 72 | 0 |
| 37 | BE | 1105 | 0 | 1148 | 61 | 0 |
| 37 | DE | 1105 | 0 | 1148 | 33 | 0 |
| 37 | FE | 1105 | 0 | 1148 | 50 | 0 |
| 37 | HE | 1105 | 0 | 1148 | 37 | 0 |
| 38 | BF | 817 | 0 | 808 | 51 | 0 |
| 38 | DF | 817 | 0 | 808 | 28 | 0 |
| 38 | FF | 817 | 0 | 808 | 28 | 0 |
| 38 | HF | 817 | 0 | 808 | 25 | 0 |
| 39 | BG | 1181 | 0 | 1238 | 25 | 0 |
| 39 | DG | 1181 | 0 | 1238 | 31 | 0 |
| 39 | FG | 1181 | 0 | 1238 | 35 | 0 |
| 39 | HG | 1181 | 0 | 1238 | 38 | 0 |
| 40 | BH | 979 | 0 | 1031 | 50 | 0 |
| 40 | DH | 979 | 0 | 1031 | 28 | 0 |
| 40 | FH | 979 | 0 | 1031 | 34 | 0 |
| 40 | HH | 979 | 0 | 1031 | 28 | 0 |
| 41 | BI | 1022 | 0 | 1070 | 58 | 0 |
| 41 | DI | 1022 | 0 | 1070 | 53 | 0 |
| 41 | FI | 1022 | 0 | 1070 | 44 | 0 |
| 41 | HI | 1022 | 0 | 1070 | 59 | 0 |
| 42 | BJ | 786 | 0 | 828 | 26 | 0 |
| 42 | DJ | 786 | 0 | 828 | 34 | 0 |
| 42 | FJ | 786 | 0 | 828 | 43 | 0 |
| 42 | HJ | 786 | 0 | 828 | 34 | 0 |
| 43 | BK | 877 | 0 | 887 | 75 | 0 |
| 43 | DK | 877 | 0 | 887 | 45 | 0 |
| 43 | FK | 877 | 0 | 887 | 38 | 0 |
| 43 | HK | 877 | 0 | 887 | 75 | 0 |
| 44 | BL | 955 | 0 | 1016 | 55 | 0 |
| 44 | DL | 955 | 0 | 1016 | 52 | 0 |
| 44 | FL | 955 | 0 | 1016 | 51 | 0 |
| 44 | HL | 955 | 0 | 1016 | 39 | 0 |
| 45 | BM | 883 | 0 | 941 | 26 | 0 |
| 45 | DM | 883 | 0 | 941 | 25 | 0 |
| 45 | FM | 883 | 0 | 941 | 34 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 45 | HM | 883 | 0 | 941 | 53 | 0 |
| 46 | BN | 774 | 0 | 824 | 32 | 0 |
| 46 | DN | 774 | 0 | 824 | 21 | 0 |
| 46 | FN | 774 | 0 | 824 | 30 | 0 |
| 46 | HN | 774 | 0 | 824 | 29 | 0 |
| 47 | BO | 714 | 0 | 734 | 18 | 0 |
| 47 | DO | 714 | 0 | 734 | 13 | 0 |
| 47 | FO | 714 | 0 | 734 | 17 | 0 |
| 47 | HO | 714 | 0 | 734 | 21 | 0 |
| 48 | BP | 649 | 0 | 666 | 29 | 0 |
| 48 | DP | 649 | 0 | 666 | 25 | 0 |
| 48 | FP | 649 | 0 | 666 | 18 | 0 |
| 48 | HP | 649 | 0 | 666 | 19 | 0 |
| 49 | BQ | 648 | 0 | 691 | 19 | 0 |
| 49 | DQ | 648 | 0 | 691 | 21 | 0 |
| 49 | FQ | 648 | 0 | 691 | 16 | 0 |
| 49 | HQ | 648 | 0 | 691 | 21 | 0 |
| 50 | BR | 455 | 0 | 478 | 19 | 0 |
| 50 | DR | 455 | 0 | 478 | 16 | 0 |
| 50 | FR | 455 | 0 | 478 | 16 | 0 |
| 50 | HR | 455 | 0 | 478 | 15 | 0 |
| 51 | BS | 637 | 0 | 665 | 23 | 0 |
| 51 | DS | 637 | 0 | 665 | 17 | 0 |
| 51 | FS | 637 | 0 | 665 | 30 | 0 |
| 51 | HS | 637 | 0 | 665 | 21 | 0 |
| 52 | BT | 665 | 0 | 714 | 30 | 0 |
| 52 | DT | 665 | 0 | 714 | 26 | 0 |
| 52 | FT | 665 | 0 | 714 | 30 | 0 |
| 52 | HT | 665 | 0 | 714 | 19 | 0 |
| 53 | BU | 425 | 0 | 449 | 40 | 0 |
| 53 | DU | 425 | 0 | 449 | 28 | 0 |
| 53 | FU | 425 | 0 | 449 | 24 | 0 |
| 53 | HU | 425 | 0 | 449 | 36 | 0 |
| 54 | BV | 5319 | 0 | 5228 | 105 | 0 |
| 54 | DV | 5319 | 0 | 5228 | 113 | 0 |
| 54 | FV | 5319 | 0 | 5229 | 111 | 0 |
| 54 | HV | 5319 | 0 | 5227 | 145 | 0 |
| 55 | BW | 48 | 0 | 41 | 7 | 0 |
| 55 | DW | 48 | 0 | 41 | 8 | 0 |
| 55 | FW | 48 | 0 | 39 | 9 | 0 |
| 56 | A3 | 1 | 0 | 0 | 0 | 0 |
| 56 | AA | 130 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 56 | AB | 4 | 0 | 0 | 0 | 0 |
| 56 | AC | 3 | 0 | 0 | 0 | 0 |
| 56 | AD | 1 | 0 | 0 | 0 | 0 |
| 56 | AE | 1 | 0 | 0 | 0 | 0 |
| 56 | AT | 1 | 0 | 0 | 0 | 0 |
| 56 | BA | 40 | 0 | 0 | 0 | 0 |
| 56 | BE | 1 | 0 | 0 | 0 | 0 |
| 56 | BL | 1 | 0 | 0 | 0 | 0 |
| 56 | BU | 1 | 0 | 0 | 0 | 0 |
| 56 | BV | 1 | 0 | 0 | 0 | 0 |
| 56 | C4 | 1 | 0 | 0 | 0 | 0 |
| 56 | CA | 134 | 0 | 0 | 0 | 0 |
| 56 | CB | 4 | 0 | 0 | 0 | 0 |
| 56 | CD | 1 | 0 | 0 | 0 | 0 |
| 56 | CE | 1 | 0 | 0 | 0 | 0 |
| 56 | DA | 42 | 0 | 0 | 0 | 0 |
| 56 | DU | 1 | 0 | 0 | 0 | 0 |
| 56 | DV | 1 | 0 | 0 | 0 | 0 |
| 56 | EA | 133 | 0 | 0 | 0 | 0 |
| 56 | EB | 4 | 0 | 0 | 0 | 0 |
| 56 | EC | 1 | 0 | 0 | 0 | 0 |
| 56 | ED | 2 | 0 | 0 | 0 | 0 |
| 56 | EQ | 1 | 0 | 0 | 0 | 0 |
| 56 | FA | 41 | 0 | 0 | 0 | 0 |
| 56 | FE | 1 | 0 | 0 | 0 | 0 |
| 56 | FU | 1 | 0 | 0 | 0 | 0 |
| 56 | FV | 1 | 0 | 0 | 0 | 0 |
| 56 | GA | 134 | 0 | 0 | 0 | 0 |
| 56 | GB | 4 | 0 | 0 | 0 | 0 |
| 56 | GC | 1 | 0 | 0 | 0 | 0 |
| 56 | GL | 1 | 0 | 0 | 0 | 0 |
| 56 | GS | 1 | 0 | 0 | 0 | 0 |
| 56 | HA | 40 | 0 | 0 | 0 | 0 |
| 56 | HC | 1 | 0 | 0 | 0 | 0 |
| 56 | HE | 1 | 0 | 0 | 0 | 0 |
| 56 | HT | 1 | 0 | 0 | 0 | 0 |
| 56 | HV | 1 | 0 | 0 | 0 | 0 |
| 57 | A4 | 1 | 0 | 0 | 0 | 0 |
| 57 | C4 | 1 | 0 | 0 | 0 | 0 |
| 57 | E4 | 1 | 0 | 0 | 0 | 0 |
| 57 | G4 | 1 | 0 | 0 | 0 | 0 |
| 58 | BV | 32 | 0 | 14 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58 | DV | 32 | 0 | 14 | 1 | 0 |
| 58 | FV | 32 | 0 | 14 | 5 | 0 |
| 58 | HV | 32 | 0 | 14 | 1 | 0 |
| 59 | A0 | 1 | 0 | 0 | 0 | 0 |
| 59 | A3 | 1 | 0 | 0 | 0 | 0 |
| 59 | A4 | 2 | 0 | 0 | 0 | 0 |
| 59 | AA | 608 | 0 | 0 | 111 | 0 |
| 59 | AB | 19 | 0 | 0 | 1 | 0 |
| 59 | AC | 10 | 0 | 0 | 0 | 0 |
| 59 | AD | 3 | 0 | 0 | 0 | 0 |
| 59 | AE | 1 | 0 | 0 | 0 | 0 |
| 59 | AJ | 1 | 0 | 0 | 1 | 0 |
| 59 | AL | 7 | 0 | 0 | 1 | 0 |
| 59 | AN | 4 | 0 | 0 | 0 | 0 |
| 59 | AP | 1 | 0 | 0 | 0 | 0 |
| 59 | AQ | 1 | 0 | 0 | 0 | 0 |
| 59 | AS | 1 | 0 | 0 | 0 | 0 |
| 59 | AU | 1 | 0 | 0 | 0 | 0 |
| 59 | BA | 197 | 0 | 0 | 36 | 0 |
| 59 | BC | 1 | 0 | 0 | 0 | 0 |
| 59 | BD | 1 | 0 | 0 | 0 | 0 |
| 59 | BI | 1 | 0 | 0 | 0 | 0 |
| 59 | BK | 1 | 0 | 0 | 0 | 0 |
| 59 | BN | 3 | 0 | 0 | 0 | 0 |
| 59 | BT | 2 | 0 | 0 | 0 | 0 |
| 59 | BU | 1 | 0 | 0 | 0 | 0 |
| 59 | BV | 1 | 0 | 0 | 1 | 0 |
| 59 | C2 | 1 | 0 | 0 | 0 | 0 |
| 59 | C3 | 1 | 0 | 0 | 0 | 0 |
| 59 | C4 | 2 | 0 | 0 | 0 | 0 |
| 59 | CA | 604 | 0 | 0 | 104 | 0 |
| 59 | CB | 20 | 0 | 0 | 2 | 0 |
| 59 | CC | 11 | 0 | 0 | 4 | 0 |
| 59 | CD | 3 | 0 | 0 | 0 | 0 |
| 59 | CE | 1 | 0 | 0 | 0 | 0 |
| 59 | CF | 1 | 0 | 0 | 0 | 0 |
| 59 | CJ | 3 | 0 | 0 | 2 | 0 |
| 59 | CL | 6 | 0 | 0 | 1 | 0 |
| 59 | CN | 4 | 0 | 0 | 0 | 0 |
| 59 | CS | 1 | 0 | 0 | 0 | 0 |
| 59 | CT | 2 | 0 | 0 | 0 | 0 |
| 59 | DA | 193 | 0 | 0 | 32 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 59 | DC | 1 | 0 | 0 | 0 | 0 |
| 59 | DE | 2 | 0 | 0 | 0 | 0 |
| 59 | DG | 1 | 0 | 0 | 0 | 0 |
| 59 | DK | 1 | 0 | 0 | 0 | 0 |
| 59 | DL | 1 | 0 | 0 | 0 | 0 |
| 59 | DN | 6 | 0 | 0 | 0 | 0 |
| 59 | DQ | 1 | 0 | 0 | 0 | 0 |
| 59 | DT | 1 | 0 | 0 | 1 | 0 |
| 59 | DU | 1 | 0 | 0 | 0 | 0 |
| 59 | DV | 1 | 0 | 0 | 1 | 0 |
| 59 | E0 | 2 | 0 | 0 | 0 | 0 |
| 59 | E3 | 2 | 0 | 0 | 0 | 0 |
| 59 | E4 | 1 | 0 | 0 | 0 | 0 |
| 59 | EA | 617 | 0 | 0 | 88 | 0 |
| 59 | EB | 20 | 0 | 0 | 1 | 0 |
| 59 | EC | 8 | 0 | 0 | 0 | 0 |
| 59 | ED | 1 | 0 | 0 | 0 | 0 |
| 59 | EL | 4 | 0 | 0 | 0 | 0 |
| 59 | EN | 2 | 0 | 0 | 0 | 0 |
| 59 | ER | 1 | 0 | 0 | 0 | 0 |
| 59 | ET | 1 | 0 | 0 | 0 | 0 |
| 59 | EU | 1 | 0 | 0 | 0 | 0 |
| 59 | FA | 198 | 0 | 0 | 21 | 0 |
| 59 | FE | 1 | 0 | 0 | 0 | 0 |
| 59 | FK | 1 | 0 | 0 | 0 | 0 |
| 59 | FN | 3 | 0 | 0 | 0 | 0 |
| 59 | FQ | 1 | 0 | 0 | 0 | 0 |
| 59 | FT | 4 | 0 | 0 | 1 | 0 |
| 59 | FV | 1 | 0 | 0 | 1 | 0 |
| 59 | G2 | 2 | 0 | 0 | 0 | 0 |
| 59 | G3 | 1 | 0 | 0 | 0 | 0 |
| 59 | G4 | 1 | 0 | 0 | 0 | 0 |
| 59 | GA | 607 | 0 | 0 | 87 | 0 |
| 59 | GB | 19 | 0 | 0 | 1 | 0 |
| 59 | GC | 9 | 0 | 0 | 2 | 0 |
| 59 | GD | 4 | 0 | 0 | 0 | 0 |
| 59 | GE | 2 | 0 | 0 | 0 | 0 |
| 59 | GL | 4 | 0 | 0 | 1 | 0 |
| 59 | GN | 3 | 0 | 0 | 0 | 0 |
| 59 | GQ | 1 | 0 | 0 | 0 | 0 |
| 59 | GR | 2 | 0 | 0 | 0 | 0 |
| 59 | GS | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 59 | GT | 1 | 0 | 0 | 0 | 0 |
| 59 | GU | 2 | 0 | 0 | 0 | 0 |
| 59 | GV | 1 | 0 | 0 | 1 | 0 |
| 59 | HA | 197 | 0 | 0 | 33 | 0 |
| 59 | HD | 1 | 0 | 0 | 0 | 0 |
| 59 | HE | 3 | 0 | 0 | 0 | 0 |
| 59 | HN | 5 | 0 | 0 | 0 | 0 |
| 59 | HT | 1 | 0 | 0 | 0 | 0 |
| 59 | HU | 1 | 0 | 0 | 0 | 0 |
| 59 | HV | 1 | 0 | 0 | 1 | 0 |
| All | All | 590573 | 0 | 402393 | 12569 | 4 |

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 13.

The worst 5 of 12569 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:A5:117:LEU:CD2 | 32:A5:120:ALA:HA | 1.56 | 1.35 |
| 32:A5:24:SER:CB | 32:A5:116:GLU:HG2 | 1.59 | 1.32 |
| 32:A5:24:SER:O | 32:A5:116:GLU:HB3 | 1.37 | 1.24 |
| 32:E5:117:LEU:CD2 | 32:E5:120:ALA:HA | 1.70 | 1.20 |
| 32:E5:24:SER:CB | 32:E5:116:GLU:HG2 | 1.75 | 1.16 |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 33:FA:1029:U:O3' | 1:GA:1508:A:N6[1_565] | 2.13 | 0.07 |
| 33:FA:1029:U:OP2 | 1:GA:1509:A:N6[1_565] | 2.16 | 0.04 |
| 33:FA:1029:U:O2' | 1:GA:1508:A:N6[1_565] | 2.16 | 0.04 |
| 6:GF:20:ASN:ND2 | 21:GU:52:ASN:OD1[2_556] | 2.18 | 0.02 |

5.3 Torsion angles

5.3.1 Protein backbone

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 | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3 | AC | 269/273 (98%) | 220 (82%) | 34 (13%) | 15 (6%) | 2 | 6 |
| 3 | CC | 269/273 (98%) | 218 (81%) | 35 (13%) | 16 (6%) | 2 | 6 |
| 3 | EC | 269/273 (98%) | 219 (81%) | 36 (13%) | 14 (5%) | 2 | 8 |
| 3 | GC | 269/273 (98%) | 225 (84%) | 30 (11%) | 14 (5%) | 2 | 8 |
| 4 | AD | 207/209 (99%) | 161 (78%) | 33 (16%) | 13 (6%) | 1 | 4 |
| 4 | CD | 207/209 (99%) | 160 (77%) | 33 (16%) | 14 (7%) | 1 | 4 |
| 4 | ED | 207/209 (99%) | 155 (75%) | 34 (16%) | 18 (9%) | 1 | 2 |
| 4 | GD | 207/209 (99%) | 158 (76%) | 34 (16%) | 15 (7%) | 1 | 3 |
| 5 | AE | 199/201 (99%) | 163 (82%) | 24 (12%) | 12 (6%) | 2 | 5 |
| 5 | CE | 199/201 (99%) | 161 (81%) | 26 (13%) | 12 (6%) | 2 | 5 |
| 5 | EE | 199/201 (99%) | 162 (81%) | 25 (13%) | 12 (6%) | 2 | 5 |
| 5 | GE | 199/201 (99%) | 162 (81%) | 25 (13%) | 12 (6%) | 2 | 5 |
| 6 | AF | 175/179 (98%) | 128 (73%) | 41 (23%) | 6 (3%) | 4 | 18 |
| 6 | CF | 175/179 (98%) | 132 (75%) | 37 (21%) | 6 (3%) | 4 | 18 |
| 6 | EF | 175/179 (98%) | 139 (79%) | 29 (17%) | 7 (4%) | 3 | 14 |
| 6 | GF | 175/179 (98%) | 132 (75%) | 40 (23%) | 3 (2%) | 11 | 36 |
| 7 | AG | 174/177 (98%) | 124 (71%) | 33 (19%) | 17 (10%) | 1 | 1 |
| 7 | CG | 174/177 (98%) | 123 (71%) | 37 (21%) | 14 (8%) | 1 | 2 |
| 7 | EG | 174/177 (98%) | 120 (69%) | 43 (25%) | 11 (6%) | 1 | 4 |
| 7 | GG | 174/177 (98%) | 118 (68%) | 41 (24%) | 15 (9%) | 1 | 2 |
| 8 | AH | 48/50 (96%) | 24 (50%) | 19 (40%) | 5 (10%) | 0 | 1 |
| 8 | CH | 48/50 (96%) | 23 (48%) | 19 (40%) | 6 (12%) | 0 | 1 |
| 8 | EH | 48/50 (96%) | 24 (50%) | 19 (40%) | 5 (10%) | 0 | 1 |
| 8 | GH | 48/50 (96%) | 24 (50%) | 21 (44%) | 3 (6%) | 1 | 4 |
| 9 | AI | 139/142 (98%) | 87 (63%) | 45 (32%) | 7 (5%) | 2 | 8 |
| 9 | CI | 139/142 (98%) | 92 (66%) | 37 (27%) | 10 (7%) | 1 | 3 |
| 9 | EI | 139/142 (98%) | 90 (65%) | 42 (30%) | 7 (5%) | 2 | 8 |
| 9 | GI | 139/142 (98%) | 89 (64%) | 38 (27%) | 12 (9%) | 1 | 2 |
| 10 | AJ | 140/142 (99%) | 114 (81%) | 18 (13%) | 8 (6%) | 2 | 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 10 | CJ | 140/142 (99%) | 113 (81%) | 19 (14%) | 8 (6%) | 2 | 6 |
| 10 | EJ | 140/142 (99%) | 113 (81%) | 19 (14%) | 8 (6%) | 2 | 6 |
| 10 | GJ | 140/142 (99%) | 114 (81%) | 17 (12%) | 9 (6%) | 1 | 4 |
| 11 | AK | 120/123 (98%) | 93 (78%) | 17 (14%) | 10 (8%) | 1 | 2 |
| 11 | CK | 120/123 (98%) | 91 (76%) | 21 (18%) | 8 (7%) | 1 | 4 |
| 11 | EK | 120/123 (98%) | 92 (77%) | 17 (14%) | 11 (9%) | 1 | 2 |
| 11 | GK | 120/123 (98%) | 92 (77%) | 19 (16%) | 9 (8%) | 1 | 3 |
| 12 | AL | 141/144 (98%) | 107 (76%) | 26 (18%) | 8 (6%) | 2 | 6 |
| 12 | CL | 141/144 (98%) | 107 (76%) | 27 (19%) | 7 (5%) | 2 | 8 |
| 12 | EL | 141/144 (98%) | 108 (77%) | 26 (18%) | 7 (5%) | 2 | 8 |
| 12 | GL | 141/144 (98%) | 109 (77%) | 25 (18%) | 7 (5%) | 2 | 8 |
| 13 | AM | 134/136 (98%) | 105 (78%) | 22 (16%) | 7 (5%) | 2 | 8 |
| 13 | CM | 134/136 (98%) | 111 (83%) | 16 (12%) | 7 (5%) | 2 | 8 |
| 13 | EM | 134/136 (98%) | 110 (82%) | 18 (13%) | 6 (4%) | 3 | 11 |
| 13 | GM | 134/136 (98%) | 112 (84%) | 16 (12%) | 6 (4%) | 3 | 11 |
| 14 | AN | 118/127 (93%) | 101 (86%) | 15 (13%) | 2 (2%) | 11 | 36 |
| 14 | CN | 118/127 (93%) | 98 (83%) | 17 (14%) | 3 (2%) | 6 | 25 |
| 14 | EN | 118/127 (93%) | 101 (86%) | 14 (12%) | 3 (2%) | 6 | 25 |
| 14 | GN | 118/127 (93%) | 98 (83%) | 19 (16%) | 1 (1%) | 22 | 57 |
| 15 | AO | 114/117 (97%) | 99 (87%) | 14 (12%) | 1 (1%) | 20 | 54 |
| 15 | CO | 114/117 (97%) | 96 (84%) | 17 (15%) | 1 (1%) | 20 | 54 |
| 15 | EO | 114/117 (97%) | 96 (84%) | 18 (16%) | 0 | 100 | 100 |
| 15 | GO | 114/117 (97%) | 97 (85%) | 13 (11%) | 4 (4%) | 4 | 17 |
| 16 | AP | 112/115 (97%) | 83 (74%) | 22 (20%) | 7 (6%) | 1 | 4 |
| 16 | CP | 112/115 (97%) | 81 (72%) | 22 (20%) | 9 (8%) | 1 | 2 |
| 16 | EP | 112/115 (97%) | 83 (74%) | 22 (20%) | 7 (6%) | 1 | 4 |
| 16 | GP | 112/115 (97%) | 79 (70%) | 21 (19%) | 12 (11%) | 0 | 1 |
| 17 | AQ | 115/118 (98%) | 101 (88%) | 9 (8%) | 5 (4%) | 3 | 12 |
| 17 | CQ | 115/118 (98%) | 102 (89%) | 9 (8%) | 4 (4%) | 4 | 17 |
| 17 | EQ | 115/118 (98%) | 102 (89%) | 8 (7%) | 5 (4%) | 3 | 12 |
| 17 | GQ | 115/118 (98%) | 103 (90%) | 7 (6%) | 5 (4%) | 3 | 12 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|----------|----------|----------|-------------|----|
| 18 | AR | 101/103 (98%) | 83 (82%) | 15 (15%) | 3 (3%) | 5 | 20 |
| 18 | CR | 101/103 (98%) | 83 (82%) | 15 (15%) | 3 (3%) | 5 | 20 |
| 18 | ER | 101/103 (98%) | 83 (82%) | 15 (15%) | 3 (3%) | 5 | 20 |
| 18 | GR | 101/103 (98%) | 84 (83%) | 13 (13%) | 4 (4%) | 3 | 14 |
| 19 | AS | 108/110 (98%) | 93 (86%) | 10 (9%) | 5 (5%) | 3 | 11 |
| 19 | CS | 108/110 (98%) | 96 (89%) | 8 (7%) | 4 (4%) | 4 | 16 |
| 19 | ES | 108/110 (98%) | 91 (84%) | 12 (11%) | 5 (5%) | 3 | 11 |
| 19 | GS | 108/110 (98%) | 92 (85%) | 11 (10%) | 5 (5%) | 3 | 11 |
| 20 | AT | 91/100 (91%) | 59 (65%) | 24 (26%) | 8 (9%) | 1 | 2 |
| 20 | CT | 91/100 (91%) | 60 (66%) | 23 (25%) | 8 (9%) | 1 | 2 |
| 20 | ET | 91/100 (91%) | 59 (65%) | 25 (28%) | 7 (8%) | 1 | 3 |
| 20 | GT | 91/100 (91%) | 60 (66%) | 22 (24%) | 9 (10%) | 1 | 1 |
| 21 | AU | 100/104 (96%) | 73 (73%) | 18 (18%) | 9 (9%) | 1 | 2 |
| 21 | CU | 100/104 (96%) | 74 (74%) | 16 (16%) | 10 (10%) | 1 | 1 |
| 21 | EU | 100/104 (96%) | 74 (74%) | 13 (13%) | 13 (13%) | 0 | 1 |
| 21 | GU | 100/104 (96%) | 73 (73%) | 18 (18%) | 9 (9%) | 1 | 2 |
| 22 | AV | 92/94 (98%) | 82 (89%) | 9 (10%) | 1 (1%) | 17 | 48 |
| 22 | CV | 92/94 (98%) | 79 (86%) | 12 (13%) | 1 (1%) | 17 | 48 |
| 22 | EV | 92/94 (98%) | 82 (89%) | 9 (10%) | 1 (1%) | 17 | 48 |
| 22 | GV | 92/94 (98%) | 83 (90%) | 8 (9%) | 1 (1%) | 17 | 48 |
| 23 | AW | 77/85 (91%) | 41 (53%) | 19 (25%) | 17 (22%) | 0 | 0 |
| 23 | CW | 77/85 (91%) | 42 (54%) | 21 (27%) | 14 (18%) | 0 | 0 |
| 23 | EW | 77/85 (91%) | 42 (54%) | 19 (25%) | 16 (21%) | 0 | 0 |
| 23 | GW | 77/85 (91%) | 42 (54%) | 21 (27%) | 14 (18%) | 0 | 0 |
| 24 | AX | 75/78 (96%) | 65 (87%) | 7 (9%) | 3 (4%) | 3 | 14 |
| 24 | CX | 75/78 (96%) | 64 (85%) | 8 (11%) | 3 (4%) | 3 | 14 |
| 24 | EX | 75/78 (96%) | 64 (85%) | 9 (12%) | 2 (3%) | 6 | 23 |
| 24 | GX | 75/78 (96%) | 65 (87%) | 9 (12%) | 1 (1%) | 14 | 43 |
| 25 | AY | 61/63 (97%) | 40 (66%) | 19 (31%) | 2 (3%) | 4 | 18 |
| 25 | CY | 61/63 (97%) | 43 (70%) | 17 (28%) | 1 (2%) | 11 | 37 |
| 25 | EY | 61/63 (97%) | 38 (62%) | 19 (31%) | 4 (7%) | 1 | 4 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 25 | GY | 61/63 (97%) | 42 (69%) | 17 (28%) | 2 (3%) | 4 | 18 |
| 26 | AZ | 56/59 (95%) | 49 (88%) | 5 (9%) | 2 (4%) | 4 | 17 |
| 26 | CZ | 56/59 (95%) | 49 (88%) | 5 (9%) | 2 (4%) | 4 | 17 |
| 26 | EZ | 56/59 (95%) | 48 (86%) | 6 (11%) | 2 (4%) | 4 | 17 |
| 26 | GZ | 56/59 (95%) | 49 (88%) | 5 (9%) | 2 (4%) | 4 | 17 |
| 27 | A0 | 54/57 (95%) | 45 (83%) | 6 (11%) | 3 (6%) | 2 | 6 |
| 27 | C0 | 54/57 (95%) | 45 (83%) | 6 (11%) | 3 (6%) | 2 | 6 |
| 27 | E0 | 54/57 (95%) | 45 (83%) | 6 (11%) | 3 (6%) | 2 | 6 |
| 27 | G0 | 54/57 (95%) | 45 (83%) | 6 (11%) | 3 (6%) | 2 | 6 |
| 28 | A1 | 48/55 (87%) | 40 (83%) | 5 (10%) | 3 (6%) | 1 | 4 |
| 28 | C1 | 48/55 (87%) | 40 (83%) | 6 (12%) | 2 (4%) | 3 | 12 |
| 28 | E1 | 48/55 (87%) | 42 (88%) | 5 (10%) | 1 (2%) | 8 | 30 |
| 28 | G1 | 48/55 (87%) | 41 (85%) | 5 (10%) | 2 (4%) | 3 | 12 |
| 29 | A2 | 44/46 (96%) | 39 (89%) | 4 (9%) | 1 (2%) | 7 | 27 |
| 29 | C2 | 44/46 (96%) | 39 (89%) | 4 (9%) | 1 (2%) | 7 | 27 |
| 29 | E2 | 44/46 (96%) | 39 (89%) | 4 (9%) | 1 (2%) | 7 | 27 |
| 29 | G2 | 44/46 (96%) | 39 (89%) | 4 (9%) | 1 (2%) | 7 | 27 |
| 30 | A3 | 62/65 (95%) | 56 (90%) | 4 (6%) | 2 (3%) | 5 | 19 |
| 30 | C3 | 62/65 (95%) | 56 (90%) | 4 (6%) | 2 (3%) | 5 | 19 |
| 30 | E3 | 62/65 (95%) | 55 (89%) | 5 (8%) | 2 (3%) | 5 | 19 |
| 30 | G3 | 62/65 (95%) | 56 (90%) | 4 (6%) | 2 (3%) | 5 | 19 |
| 31 | A4 | 36/38 (95%) | 31 (86%) | 2 (6%) | 3 (8%) | 1 | 2 |
| 31 | C4 | 36/38 (95%) | 31 (86%) | 3 (8%) | 2 (6%) | 2 | 6 |
| 31 | E4 | 36/38 (95%) | 31 (86%) | 2 (6%) | 3 (8%) | 1 | 2 |
| 31 | G4 | 36/38 (95%) | 30 (83%) | 4 (11%) | 2 (6%) | 2 | 6 |
| 32 | A5 | 146/165 (88%) | 80 (55%) | 44 (30%) | 22 (15%) | 0 | 0 |
| 32 | E5 | 142/165 (86%) | 80 (56%) | 39 (28%) | 23 (16%) | 0 | 0 |
| 34 | BB | 216/241 (90%) | 147 (68%) | 57 (26%) | 12 (6%) | 2 | 6 |
| 34 | DB | 216/241 (90%) | 145 (67%) | 59 (27%) | 12 (6%) | 2 | 6 |
| 34 | FB | 216/241 (90%) | 146 (68%) | 60 (28%) | 10 (5%) | 3 | 11 |
| 34 | HB | 216/241 (90%) | 149 (69%) | 55 (26%) | 12 (6%) | 2 | 6 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 35 | BC | 204/233 (88%) | 180 (88%) | 16 (8%) | 8 (4%) | 3 | 14 |
| 35 | DC | 204/233 (88%) | 177 (87%) | 23 (11%) | 4 (2%) | 9 | 31 |
| 35 | FC | 204/233 (88%) | 181 (89%) | 17 (8%) | 6 (3%) | 5 | 21 |
| 35 | HC | 204/233 (88%) | 183 (90%) | 16 (8%) | 5 (2%) | 6 | 25 |
| 36 | BD | 203/206 (98%) | 157 (77%) | 34 (17%) | 12 (6%) | 2 | 6 |
| 36 | DD | 203/206 (98%) | 157 (77%) | 30 (15%) | 16 (8%) | 1 | 2 |
| 36 | FD | 203/206 (98%) | 155 (76%) | 34 (17%) | 14 (7%) | 1 | 3 |
| 36 | HD | 203/206 (98%) | 159 (78%) | 35 (17%) | 9 (4%) | 3 | 11 |
| 37 | BE | 148/167 (89%) | 124 (84%) | 19 (13%) | 5 (3%) | 4 | 18 |
| 37 | DE | 148/167 (89%) | 125 (84%) | 18 (12%) | 5 (3%) | 4 | 18 |
| 37 | FE | 148/167 (89%) | 122 (82%) | 22 (15%) | 4 (3%) | 6 | 23 |
| 37 | HE | 148/167 (89%) | 122 (82%) | 22 (15%) | 4 (3%) | 6 | 23 |
| 38 | BF | 98/135 (73%) | 73 (74%) | 20 (20%) | 5 (5%) | 2 | 8 |
| 38 | DF | 98/135 (73%) | 71 (72%) | 20 (20%) | 7 (7%) | 1 | 3 |
| 38 | FF | 98/135 (73%) | 72 (74%) | 16 (16%) | 10 (10%) | 1 | 1 |
| 38 | HF | 98/135 (73%) | 75 (76%) | 18 (18%) | 5 (5%) | 2 | 8 |
| 39 | BG | 149/179 (83%) | 126 (85%) | 23 (15%) | 0 | 100 | 100 |
| 39 | DG | 149/179 (83%) | 123 (83%) | 25 (17%) | 1 (1%) | 25 | 60 |
| 39 | FG | 149/179 (83%) | 126 (85%) | 23 (15%) | 0 | 100 | 100 |
| 39 | HG | 149/179 (83%) | 122 (82%) | 25 (17%) | 2 (1%) | 14 | 43 |
| 40 | BH | 127/130 (98%) | 108 (85%) | 18 (14%) | 1 (1%) | 22 | 57 |
| 40 | DH | 127/130 (98%) | 110 (87%) | 15 (12%) | 2 (2%) | 11 | 37 |
| 40 | FH | 127/130 (98%) | 113 (89%) | 12 (9%) | 2 (2%) | 11 | 37 |
| 40 | HH | 127/130 (98%) | 111 (87%) | 16 (13%) | 0 | 100 | 100 |
| 41 | BI | 125/130 (96%) | 96 (77%) | 21 (17%) | 8 (6%) | 1 | 4 |
| 41 | DI | 125/130 (96%) | 99 (79%) | 19 (15%) | 7 (6%) | 2 | 6 |
| 41 | FI | 125/130 (96%) | 97 (78%) | 22 (18%) | 6 (5%) | 2 | 10 |
| 41 | HI | 125/130 (96%) | 98 (78%) | 21 (17%) | 6 (5%) | 2 | 10 |
| 42 | BJ | 96/103 (93%) | 73 (76%) | 16 (17%) | 7 (7%) | 1 | 3 |
| 42 | DJ | 96/103 (93%) | 72 (75%) | 18 (19%) | 6 (6%) | 1 | 4 |
| 42 | FJ | 96/103 (93%) | 73 (76%) | 17 (18%) | 6 (6%) | 1 | 4 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|----------|----------|----------|-------------|-----|
| 42 | HJ | 96/103 (93%) | 73 (76%) | 19 (20%) | 4 (4%) | 3 | 12 |
| 43 | BK | 115/129 (89%) | 92 (80%) | 17 (15%) | 6 (5%) | 2 | 8 |
| 43 | DK | 115/129 (89%) | 90 (78%) | 23 (20%) | 2 (2%) | 11 | 36 |
| 43 | FK | 115/129 (89%) | 92 (80%) | 20 (17%) | 3 (3%) | 6 | 24 |
| 43 | HK | 115/129 (89%) | 87 (76%) | 24 (21%) | 4 (4%) | 4 | 17 |
| 44 | BL | 121/124 (98%) | 95 (78%) | 17 (14%) | 9 (7%) | 1 | 3 |
| 44 | DL | 121/124 (98%) | 95 (78%) | 18 (15%) | 8 (7%) | 1 | 4 |
| 44 | FL | 121/124 (98%) | 96 (79%) | 17 (14%) | 8 (7%) | 1 | 4 |
| 44 | HL | 121/124 (98%) | 97 (80%) | 15 (12%) | 9 (7%) | 1 | 3 |
| 45 | BM | 112/118 (95%) | 98 (88%) | 8 (7%) | 6 (5%) | 2 | 7 |
| 45 | DM | 112/118 (95%) | 99 (88%) | 7 (6%) | 6 (5%) | 2 | 7 |
| 45 | FM | 112/118 (95%) | 98 (88%) | 9 (8%) | 5 (4%) | 3 | 11 |
| 45 | HM | 112/118 (95%) | 91 (81%) | 14 (12%) | 7 (6%) | 1 | 4 |
| 46 | BN | 92/101 (91%) | 71 (77%) | 18 (20%) | 3 (3%) | 4 | 18 |
| 46 | DN | 92/101 (91%) | 71 (77%) | 19 (21%) | 2 (2%) | 8 | 29 |
| 46 | FN | 92/101 (91%) | 69 (75%) | 20 (22%) | 3 (3%) | 4 | 18 |
| 46 | HN | 92/101 (91%) | 70 (76%) | 20 (22%) | 2 (2%) | 8 | 29 |
| 47 | BO | 86/89 (97%) | 72 (84%) | 12 (14%) | 2 (2%) | 7 | 27 |
| 47 | DO | 86/89 (97%) | 73 (85%) | 11 (13%) | 2 (2%) | 7 | 27 |
| 47 | FO | 86/89 (97%) | 72 (84%) | 12 (14%) | 2 (2%) | 7 | 27 |
| 47 | HO | 86/89 (97%) | 70 (81%) | 14 (16%) | 2 (2%) | 7 | 27 |
| 48 | BP | 80/82 (98%) | 60 (75%) | 16 (20%) | 4 (5%) | 2 | 8 |
| 48 | DP | 80/82 (98%) | 62 (78%) | 16 (20%) | 2 (2%) | 6 | 25 |
| 48 | FP | 80/82 (98%) | 65 (81%) | 13 (16%) | 2 (2%) | 6 | 25 |
| 48 | HP | 80/82 (98%) | 61 (76%) | 15 (19%) | 4 (5%) | 2 | 8 |
| 49 | BQ | 78/84 (93%) | 54 (69%) | 19 (24%) | 5 (6%) | 1 | 4 |
| 49 | DQ | 78/84 (93%) | 56 (72%) | 16 (20%) | 6 (8%) | 1 | 3 |
| 49 | FQ | 78/84 (93%) | 57 (73%) | 18 (23%) | 3 (4%) | 4 | 15 |
| 49 | HQ | 78/84 (93%) | 57 (73%) | 16 (20%) | 5 (6%) | 1 | 4 |
| 50 | BR | 53/75 (71%) | 41 (77%) | 12 (23%) | 0 | 100 | 100 |
| 50 | DR | 53/75 (71%) | 43 (81%) | 10 (19%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-----------|-------------|-----|
| 50 | FR | 53/75 (71%) | 40 (76%) | 13 (24%) | 0 | 100 | 100 |
| 50 | HR | 53/75 (71%) | 43 (81%) | 10 (19%) | 0 | 100 | 100 |
| 51 | BS | 77/92 (84%) | 69 (90%) | 7 (9%) | 1 (1%) | 14 | 43 |
| 51 | DS | 77/92 (84%) | 70 (91%) | 6 (8%) | 1 (1%) | 14 | 43 |
| 51 | FS | 77/92 (84%) | 67 (87%) | 6 (8%) | 4 (5%) | 2 | 8 |
| 51 | HS | 77/92 (84%) | 68 (88%) | 9 (12%) | 0 | 100 | 100 |
| 52 | BT | 83/87 (95%) | 66 (80%) | 15 (18%) | 2 (2%) | 7 | 27 |
| 52 | DT | 83/87 (95%) | 69 (83%) | 11 (13%) | 3 (4%) | 4 | 17 |
| 52 | FT | 83/87 (95%) | 66 (80%) | 15 (18%) | 2 (2%) | 7 | 27 |
| 52 | HT | 83/87 (95%) | 68 (82%) | 14 (17%) | 1 (1%) | 15 | 46 |
| 53 | BU | 49/71 (69%) | 25 (51%) | 20 (41%) | 4 (8%) | 1 | 2 |
| 53 | DU | 49/71 (69%) | 27 (55%) | 20 (41%) | 2 (4%) | 3 | 13 |
| 53 | FU | 49/71 (69%) | 28 (57%) | 19 (39%) | 2 (4%) | 3 | 13 |
| 53 | HU | 49/71 (69%) | 24 (49%) | 22 (45%) | 3 (6%) | 2 | 5 |
| 54 | BV | 685/704 (97%) | 559 (82%) | 90 (13%) | 36 (5%) | 2 | 7 |
| 54 | DV | 685/704 (97%) | 558 (82%) | 92 (13%) | 35 (5%) | 2 | 8 |
| 54 | FV | 685/704 (97%) | 556 (81%) | 91 (13%) | 38 (6%) | 2 | 7 |
| 54 | HV | 685/704 (97%) | 556 (81%) | 91 (13%) | 38 (6%) | 2 | 7 |
| 55 | BW | 2/6 (33%) | 0 | 0 | 2 (100%) | 0 | 0 |
| 55 | DW | 2/6 (33%) | 1 (50%) | 1 (50%) | 0 | 100 | 100 |
| 55 | FW | 2/6 (33%) | 2 (100%) | 0 | 0 | 100 | 100 |
| All | All | 25122/26708 (94%) | 19751 (79%) | 4073 (16%) | 1298 (5%) | 2 | 8 |

5 of 1298 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 70 | LYS |
| 3 | AC | 104 | LEU |
| 3 | AC | 121 | ALA |
| 3 | AC | 140 | VAL |
| 3 | AC | 256 | THR |

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 | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | AC | 216/218 (99%) | 203 (94%) | 13 (6%) | 22 | 54 |
| 3 | CC | 216/218 (99%) | 201 (93%) | 15 (7%) | 18 | 46 |
| 3 | EC | 216/218 (99%) | 200 (93%) | 16 (7%) | 16 | 42 |
| 3 | GC | 216/218 (99%) | 198 (92%) | 18 (8%) | 13 | 36 |
| 4 | AD | 164/164 (100%) | 153 (93%) | 11 (7%) | 19 | 48 |
| 4 | CD | 164/164 (100%) | 156 (95%) | 8 (5%) | 29 | 63 |
| 4 | ED | 164/164 (100%) | 155 (94%) | 9 (6%) | 25 | 58 |
| 4 | GD | 164/164 (100%) | 156 (95%) | 8 (5%) | 29 | 63 |
| 5 | AE | 165/165 (100%) | 154 (93%) | 11 (7%) | 19 | 48 |
| 5 | CE | 165/165 (100%) | 158 (96%) | 7 (4%) | 34 | 69 |
| 5 | EE | 165/165 (100%) | 153 (93%) | 12 (7%) | 16 | 43 |
| 5 | GE | 165/165 (100%) | 160 (97%) | 5 (3%) | 46 | 80 |
| 6 | AF | 148/150 (99%) | 140 (95%) | 8 (5%) | 26 | 59 |
| 6 | CF | 148/150 (99%) | 139 (94%) | 9 (6%) | 22 | 53 |
| 6 | EF | 148/150 (99%) | 138 (93%) | 10 (7%) | 18 | 47 |
| 6 | GF | 148/150 (99%) | 144 (97%) | 4 (3%) | 50 | 82 |
| 7 | AG | 137/138 (99%) | 126 (92%) | 11 (8%) | 14 | 38 |
| 7 | CG | 137/138 (99%) | 126 (92%) | 11 (8%) | 14 | 38 |
| 7 | EG | 137/138 (99%) | 125 (91%) | 12 (9%) | 12 | 34 |
| 7 | GG | 137/138 (99%) | 130 (95%) | 7 (5%) | 28 | 62 |
| 8 | AH | 40/40 (100%) | 38 (95%) | 2 (5%) | 28 | 62 |
| 8 | CH | 40/40 (100%) | 39 (98%) | 1 (2%) | 53 | 83 |
| 8 | EH | 40/40 (100%) | 36 (90%) | 4 (10%) | 9 | 27 |
| 8 | GH | 40/40 (100%) | 36 (90%) | 4 (10%) | 9 | 27 |
| 9 | AI | 109/110 (99%) | 105 (96%) | 4 (4%) | 39 | 74 |
| 9 | CI | 109/110 (99%) | 108 (99%) | 1 (1%) | 82 | 95 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 9 | EI | 109/110 (99%) | 108 (99%) | 1 (1%) | 82 | 95 |
| 9 | GI | 109/110 (99%) | 108 (99%) | 1 (1%) | 82 | 95 |
| 10 | AJ | 116/116 (100%) | 97 (84%) | 19 (16%) | 2 | 8 |
| 10 | CJ | 116/116 (100%) | 102 (88%) | 14 (12%) | 6 | 17 |
| 10 | EJ | 116/116 (100%) | 96 (83%) | 20 (17%) | 2 | 7 |
| 10 | GJ | 116/116 (100%) | 103 (89%) | 13 (11%) | 7 | 21 |
| 11 | AK | 103/104 (99%) | 93 (90%) | 10 (10%) | 9 | 29 |
| 11 | CK | 103/104 (99%) | 94 (91%) | 9 (9%) | 12 | 34 |
| 11 | EK | 103/104 (99%) | 95 (92%) | 8 (8%) | 15 | 39 |
| 11 | GK | 103/104 (99%) | 96 (93%) | 7 (7%) | 18 | 47 |
| 12 | AL | 102/103 (99%) | 96 (94%) | 6 (6%) | 23 | 55 |
| 12 | CL | 102/103 (99%) | 96 (94%) | 6 (6%) | 23 | 55 |
| 12 | EL | 102/103 (99%) | 97 (95%) | 5 (5%) | 29 | 63 |
| 12 | GL | 102/103 (99%) | 94 (92%) | 8 (8%) | 15 | 39 |
| 13 | AM | 109/109 (100%) | 94 (86%) | 15 (14%) | 4 | 12 |
| 13 | CM | 109/109 (100%) | 96 (88%) | 13 (12%) | 6 | 18 |
| 13 | EM | 109/109 (100%) | 100 (92%) | 9 (8%) | 13 | 36 |
| 13 | GM | 109/109 (100%) | 102 (94%) | 7 (6%) | 20 | 50 |
| 14 | AN | 100/103 (97%) | 94 (94%) | 6 (6%) | 22 | 54 |
| 14 | CN | 100/103 (97%) | 93 (93%) | 7 (7%) | 18 | 45 |
| 14 | EN | 100/103 (97%) | 98 (98%) | 2 (2%) | 60 | 87 |
| 14 | GN | 100/103 (97%) | 96 (96%) | 4 (4%) | 36 | 71 |
| 15 | AO | 86/87 (99%) | 81 (94%) | 5 (6%) | 23 | 56 |
| 15 | CO | 86/87 (99%) | 80 (93%) | 6 (7%) | 18 | 45 |
| 15 | EO | 86/87 (99%) | 79 (92%) | 7 (8%) | 14 | 38 |
| 15 | GO | 86/87 (99%) | 83 (96%) | 3 (4%) | 41 | 75 |
| 16 | AP | 99/100 (99%) | 85 (86%) | 14 (14%) | 4 | 12 |
| 16 | CP | 99/100 (99%) | 88 (89%) | 11 (11%) | 7 | 21 |
| 16 | EP | 99/100 (99%) | 91 (92%) | 8 (8%) | 14 | 38 |
| 16 | GP | 99/100 (99%) | 88 (89%) | 11 (11%) | 7 | 21 |
| 17 | AQ | 89/90 (99%) | 83 (93%) | 6 (7%) | 19 | 48 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------|-----------|----------|-------------|----|
| 17 | CQ | 89/90 (99%) | 82 (92%) | 7 (8%) | 14 | 39 |
| 17 | EQ | 89/90 (99%) | 80 (90%) | 9 (10%) | 9 | 27 |
| 17 | GQ | 89/90 (99%) | 86 (97%) | 3 (3%) | 42 | 76 |
| 18 | AR | 84/84 (100%) | 79 (94%) | 5 (6%) | 22 | 54 |
| 18 | CR | 84/84 (100%) | 78 (93%) | 6 (7%) | 17 | 44 |
| 18 | ER | 84/84 (100%) | 77 (92%) | 7 (8%) | 13 | 36 |
| 18 | GR | 84/84 (100%) | 80 (95%) | 4 (5%) | 30 | 64 |
| 19 | AS | 93/93 (100%) | 85 (91%) | 8 (9%) | 12 | 35 |
| 19 | CS | 93/93 (100%) | 86 (92%) | 7 (8%) | 16 | 42 |
| 19 | ES | 93/93 (100%) | 84 (90%) | 9 (10%) | 9 | 29 |
| 19 | GS | 93/93 (100%) | 86 (92%) | 7 (8%) | 16 | 42 |
| 20 | AT | 80/84 (95%) | 71 (89%) | 9 (11%) | 7 | 21 |
| 20 | CT | 80/84 (95%) | 77 (96%) | 3 (4%) | 38 | 73 |
| 20 | ET | 80/84 (95%) | 73 (91%) | 7 (9%) | 12 | 34 |
| 20 | GT | 80/84 (95%) | 76 (95%) | 4 (5%) | 28 | 62 |
| 21 | AU | 83/85 (98%) | 79 (95%) | 4 (5%) | 30 | 64 |
| 21 | CU | 83/85 (98%) | 80 (96%) | 3 (4%) | 40 | 75 |
| 21 | EU | 83/85 (98%) | 76 (92%) | 7 (8%) | 13 | 36 |
| 21 | GU | 83/85 (98%) | 80 (96%) | 3 (4%) | 40 | 75 |
| 22 | AV | 78/78 (100%) | 73 (94%) | 5 (6%) | 20 | 50 |
| 22 | CV | 78/78 (100%) | 75 (96%) | 3 (4%) | 38 | 73 |
| 22 | EV | 78/78 (100%) | 76 (97%) | 2 (3%) | 51 | 83 |
| 22 | GV | 78/78 (100%) | 75 (96%) | 3 (4%) | 38 | 73 |
| 23 | AW | 59/63 (94%) | 49 (83%) | 10 (17%) | 2 | 7 |
| 23 | CW | 59/63 (94%) | 51 (86%) | 8 (14%) | 4 | 12 |
| 23 | EW | 59/63 (94%) | 52 (88%) | 7 (12%) | 6 | 18 |
| 23 | GW | 59/63 (94%) | 53 (90%) | 6 (10%) | 8 | 26 |
| 24 | AX | 67/68 (98%) | 61 (91%) | 6 (9%) | 11 | 33 |
| 24 | CX | 67/68 (98%) | 60 (90%) | 7 (10%) | 8 | 25 |
| 24 | EX | 67/68 (98%) | 60 (90%) | 7 (10%) | 8 | 25 |
| 24 | GX | 67/68 (98%) | 61 (91%) | 6 (9%) | 11 | 33 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 25 | AY | 55/55 (100%) | 49 (89%) | 6 (11%) | 7 | 22 |
| 25 | CY | 55/55 (100%) | 53 (96%) | 2 (4%) | 40 | 75 |
| 25 | EY | 55/55 (100%) | 49 (89%) | 6 (11%) | 7 | 22 |
| 25 | GY | 55/55 (100%) | 51 (93%) | 4 (7%) | 16 | 43 |
| 26 | AZ | 48/49 (98%) | 44 (92%) | 4 (8%) | 13 | 36 |
| 26 | CZ | 48/49 (98%) | 43 (90%) | 5 (10%) | 8 | 25 |
| 26 | EZ | 48/49 (98%) | 44 (92%) | 4 (8%) | 13 | 36 |
| 26 | GZ | 48/49 (98%) | 43 (90%) | 5 (10%) | 8 | 25 |
| 27 | A0 | 47/48 (98%) | 47 (100%) | 0 | 100 | 100 |
| 27 | C0 | 47/48 (98%) | 45 (96%) | 2 (4%) | 33 | 68 |
| 27 | E0 | 47/48 (98%) | 45 (96%) | 2 (4%) | 33 | 68 |
| 27 | G0 | 47/48 (98%) | 47 (100%) | 0 | 100 | 100 |
| 28 | A1 | 45/49 (92%) | 42 (93%) | 3 (7%) | 19 | 48 |
| 28 | C1 | 45/49 (92%) | 41 (91%) | 4 (9%) | 11 | 33 |
| 28 | E1 | 45/49 (92%) | 43 (96%) | 2 (4%) | 33 | 67 |
| 28 | G1 | 45/49 (92%) | 44 (98%) | 1 (2%) | 57 | 86 |
| 29 | A2 | 38/38 (100%) | 37 (97%) | 1 (3%) | 51 | 83 |
| 29 | C2 | 38/38 (100%) | 35 (92%) | 3 (8%) | 14 | 39 |
| 29 | E2 | 38/38 (100%) | 33 (87%) | 5 (13%) | 5 | 14 |
| 29 | G2 | 38/38 (100%) | 34 (90%) | 4 (10%) | 8 | 24 |
| 30 | A3 | 51/52 (98%) | 49 (96%) | 2 (4%) | 37 | 72 |
| 30 | C3 | 51/52 (98%) | 50 (98%) | 1 (2%) | 60 | 87 |
| 30 | E3 | 51/52 (98%) | 47 (92%) | 4 (8%) | 15 | 39 |
| 30 | G3 | 51/52 (98%) | 47 (92%) | 4 (8%) | 15 | 39 |
| 31 | A4 | 34/34 (100%) | 32 (94%) | 2 (6%) | 23 | 55 |
| 31 | C4 | 34/34 (100%) | 32 (94%) | 2 (6%) | 23 | 55 |
| 31 | E4 | 34/34 (100%) | 32 (94%) | 2 (6%) | 23 | 55 |
| 31 | G4 | 34/34 (100%) | 31 (91%) | 3 (9%) | 12 | 34 |
| 32 | A5 | 112/123 (91%) | 95 (85%) | 17 (15%) | 3 | 10 |
| 32 | E5 | 110/123 (89%) | 96 (87%) | 14 (13%) | 5 | 15 |
| 34 | BB | 180/199 (90%) | 171 (95%) | 9 (5%) | 28 | 62 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 34 | DB | 180/199 (90%) | 171 (95%) | 9 (5%) | 28 | 62 |
| 34 | FB | 180/199 (90%) | 172 (96%) | 8 (4%) | 33 | 67 |
| 34 | HB | 180/199 (90%) | 170 (94%) | 10 (6%) | 25 | 57 |
| 35 | BC | 170/190 (90%) | 167 (98%) | 3 (2%) | 64 | 89 |
| 35 | DC | 170/190 (90%) | 166 (98%) | 4 (2%) | 54 | 84 |
| 35 | FC | 170/190 (90%) | 158 (93%) | 12 (7%) | 17 | 44 |
| 35 | HC | 170/190 (90%) | 164 (96%) | 6 (4%) | 41 | 75 |
| 36 | BD | 172/173 (99%) | 163 (95%) | 9 (5%) | 27 | 61 |
| 36 | DD | 172/173 (99%) | 162 (94%) | 10 (6%) | 23 | 56 |
| 36 | FD | 172/173 (99%) | 162 (94%) | 10 (6%) | 23 | 56 |
| 36 | HD | 172/173 (99%) | 163 (95%) | 9 (5%) | 27 | 61 |
| 37 | BE | 113/126 (90%) | 107 (95%) | 6 (5%) | 26 | 60 |
| 37 | DE | 113/126 (90%) | 110 (97%) | 3 (3%) | 50 | 82 |
| 37 | FE | 113/126 (90%) | 104 (92%) | 9 (8%) | 14 | 38 |
| 37 | HE | 113/126 (90%) | 106 (94%) | 7 (6%) | 21 | 52 |
| 38 | BF | 87/116 (75%) | 83 (95%) | 4 (5%) | 31 | 65 |
| 38 | DF | 87/116 (75%) | 85 (98%) | 2 (2%) | 56 | 85 |
| 38 | FF | 87/116 (75%) | 84 (97%) | 3 (3%) | 42 | 76 |
| 38 | HF | 87/116 (75%) | 85 (98%) | 2 (2%) | 56 | 85 |
| 39 | BG | 124/147 (84%) | 122 (98%) | 2 (2%) | 68 | 90 |
| 39 | DG | 124/147 (84%) | 121 (98%) | 3 (2%) | 54 | 84 |
| 39 | FG | 124/147 (84%) | 120 (97%) | 4 (3%) | 44 | 78 |
| 39 | HG | 124/147 (84%) | 123 (99%) | 1 (1%) | 85 | 96 |
| 40 | BH | 104/105 (99%) | 98 (94%) | 6 (6%) | 23 | 56 |
| 40 | DH | 104/105 (99%) | 97 (93%) | 7 (7%) | 19 | 48 |
| 40 | FH | 104/105 (99%) | 97 (93%) | 7 (7%) | 19 | 48 |
| 40 | HH | 104/105 (99%) | 98 (94%) | 6 (6%) | 23 | 56 |
| 41 | BI | 105/107 (98%) | 96 (91%) | 9 (9%) | 12 | 35 |
| 41 | DI | 105/107 (98%) | 102 (97%) | 3 (3%) | 48 | 81 |
| 41 | FI | 105/107 (98%) | 98 (93%) | 7 (7%) | 19 | 48 |
| 41 | HI | 105/107 (98%) | 99 (94%) | 6 (6%) | 24 | 56 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 42 | BJ | 86/90 (96%) | 85 (99%) | 1 (1%) | 75 | 93 |
| 42 | DJ | 86/90 (96%) | 80 (93%) | 6 (7%) | 18 | 45 |
| 42 | FJ | 86/90 (96%) | 84 (98%) | 2 (2%) | 56 | 85 |
| 42 | HJ | 86/90 (96%) | 83 (96%) | 3 (4%) | 41 | 75 |
| 43 | BK | 90/99 (91%) | 87 (97%) | 3 (3%) | 43 | 77 |
| 43 | DK | 90/99 (91%) | 88 (98%) | 2 (2%) | 57 | 86 |
| 43 | FK | 90/99 (91%) | 85 (94%) | 5 (6%) | 25 | 57 |
| 43 | HK | 90/99 (91%) | 82 (91%) | 8 (9%) | 11 | 33 |
| 44 | BL | 103/104 (99%) | 100 (97%) | 3 (3%) | 48 | 81 |
| 44 | DL | 103/104 (99%) | 101 (98%) | 2 (2%) | 62 | 88 |
| 44 | FL | 103/104 (99%) | 97 (94%) | 6 (6%) | 23 | 56 |
| 44 | HL | 103/104 (99%) | 94 (91%) | 9 (9%) | 12 | 34 |
| 45 | BM | 92/96 (96%) | 89 (97%) | 3 (3%) | 43 | 77 |
| 45 | DM | 92/96 (96%) | 92 (100%) | 0 | 100 | 100 |
| 45 | FM | 92/96 (96%) | 92 (100%) | 0 | 100 | 100 |
| 45 | HM | 92/96 (96%) | 92 (100%) | 0 | 100 | 100 |
| 46 | BN | 79/84 (94%) | 79 (100%) | 0 | 100 | 100 |
| 46 | DN | 79/84 (94%) | 78 (99%) | 1 (1%) | 73 | 93 |
| 46 | FN | 79/84 (94%) | 75 (95%) | 4 (5%) | 28 | 62 |
| 46 | HN | 79/84 (94%) | 77 (98%) | 2 (2%) | 53 | 83 |
| 47 | BO | 76/77 (99%) | 72 (95%) | 4 (5%) | 26 | 60 |
| 47 | DO | 76/77 (99%) | 74 (97%) | 2 (3%) | 51 | 83 |
| 47 | FO | 76/77 (99%) | 74 (97%) | 2 (3%) | 51 | 83 |
| 47 | HO | 76/77 (99%) | 74 (97%) | 2 (3%) | 51 | 83 |
| 48 | BP | 65/65 (100%) | 63 (97%) | 2 (3%) | 45 | 79 |
| 48 | DP | 65/65 (100%) | 60 (92%) | 5 (8%) | 15 | 40 |
| 48 | FP | 65/65 (100%) | 64 (98%) | 1 (2%) | 70 | 91 |
| 48 | HP | 65/65 (100%) | 63 (97%) | 2 (3%) | 45 | 79 |
| 49 | BQ | 74/78 (95%) | 70 (95%) | 4 (5%) | 26 | 59 |
| 49 | DQ | 74/78 (95%) | 72 (97%) | 2 (3%) | 50 | 82 |
| 49 | FQ | 74/78 (95%) | 73 (99%) | 1 (1%) | 71 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|-------------|-----|
| 49 | HQ | 74/78 (95%) | 69 (93%) | 5 (7%) | 18 | 47 |
| 50 | BR | 48/65 (74%) | 48 (100%) | 0 | 100 | 100 |
| 50 | DR | 48/65 (74%) | 48 (100%) | 0 | 100 | 100 |
| 50 | FR | 48/65 (74%) | 46 (96%) | 2 (4%) | 34 | 69 |
| 50 | HR | 48/65 (74%) | 48 (100%) | 0 | 100 | 100 |
| 51 | BS | 70/79 (89%) | 69 (99%) | 1 (1%) | 71 | 91 |
| 51 | DS | 70/79 (89%) | 67 (96%) | 3 (4%) | 33 | 68 |
| 51 | FS | 70/79 (89%) | 64 (91%) | 6 (9%) | 12 | 35 |
| 51 | HS | 70/79 (89%) | 67 (96%) | 3 (4%) | 33 | 68 |
| 52 | BT | 65/66 (98%) | 60 (92%) | 5 (8%) | 15 | 40 |
| 52 | DT | 65/66 (98%) | 58 (89%) | 7 (11%) | 7 | 23 |
| 52 | FT | 65/66 (98%) | 60 (92%) | 5 (8%) | 15 | 40 |
| 52 | HT | 65/66 (98%) | 60 (92%) | 5 (8%) | 15 | 40 |
| 53 | BU | 44/61 (72%) | 42 (96%) | 2 (4%) | 32 | 66 |
| 53 | DU | 44/61 (72%) | 41 (93%) | 3 (7%) | 18 | 47 |
| 53 | FU | 44/61 (72%) | 41 (93%) | 3 (7%) | 18 | 47 |
| 53 | HU | 44/61 (72%) | 42 (96%) | 2 (4%) | 32 | 66 |
| 54 | BV | 557/578 (96%) | 503 (90%) | 54 (10%) | 9 | 29 |
| 54 | DV | 557/578 (96%) | 508 (91%) | 49 (9%) | 12 | 34 |
| 54 | FV | 557/578 (96%) | 508 (91%) | 49 (9%) | 12 | 34 |
| 54 | HV | 557/578 (96%) | 507 (91%) | 50 (9%) | 11 | 33 |
| 55 | BW | 2/2 (100%) | 1 (50%) | 1 (50%) | 0 | 0 |
| 55 | DW | 2/2 (100%) | 1 (50%) | 1 (50%) | 0 | 0 |
| 55 | FW | 2/2 (100%) | 2 (100%) | 0 | 100 | 100 |
| All | All | 20824/21780 (96%) | 19507 (94%) | 1317 (6%) | 21 | 51 |

5 of 1317 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49 | DQ | 48 | ASP |
| 10 | EJ | 95 | ARG |
| 40 | HH | 94 | LYS |
| 54 | DV | 77 | LYS |
| 3 | EC | 176 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | EG | 115 | GLN |
| 34 | FB | 57 | ASN |
| 51 | HS | 52 | HIS |
| 9 | EI | 33 | ASN |
| 22 | EV | 80 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1 | AA | 2850/2904 (98%) | 472 (16%) | 0 |
| 1 | CA | 2850/2904 (98%) | 470 (16%) | 0 |
| 1 | EA | 2850/2904 (98%) | 471 (16%) | 0 |
| 1 | GA | 2850/2904 (98%) | 471 (16%) | 0 |
| 2 | AB | 117/120 (97%) | 17 (14%) | 0 |
| 2 | CB | 117/120 (97%) | 18 (15%) | 0 |
| 2 | EB | 117/120 (97%) | 17 (14%) | 0 |
| 2 | GB | 117/120 (97%) | 19 (16%) | 0 |
| 33 | BA | 1532/1542 (99%) | 272 (17%) | 0 |
| 33 | DA | 1532/1542 (99%) | 269 (17%) | 0 |
| 33 | FA | 1532/1542 (99%) | 265 (17%) | 0 |
| 33 | HA | 1532/1542 (99%) | 273 (17%) | 0 |
| All | All | 17996/18264 (98%) | 3034 (16%) | 0 |

5 of 3034 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 10 | A |
| 1 | AA | 12 | U |
| 1 | AA | 15 | G |
| 1 | AA | 34 | U |
| 1 | AA | 35 | G |

There are no RNA pucker outliers to report.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 55 | KBE | BW | 1 | 55 | 8,8,9 | 1.03 | 1 (12%) | 7,8,10 | 1.00 | 1 (14%) |
| 55 | DPP | BW | 2 | 55 | 4,5,6 | 1.11 | 0 | 1,5,7 | 1.50 | 0 |
| 55 | UAL | BW | 5 | 55 | 8,8,9 | 3.48 | 5 (62%) | 4,9,11 | 4.60 | 1 (25%) |
| 55 | 5OH | BW | 6 | 55 | 8,12,13 | 1.51 | 1 (12%) | 5,16,18 | 1.42 | 1 (20%) |
| 55 | KBE | DW | 1 | 55 | 8,8,9 | 1.05 | 1 (12%) | 7,8,10 | 1.05 | 1 (14%) |
| 55 | DPP | DW | 2 | 55 | 4,5,6 | 0.86 | 0 | 1,5,7 | 1.50 | 0 |
| 55 | UAL | DW | 5 | 55 | 8,8,9 | 3.21 | 5 (62%) | 4,9,11 | 4.40 | 1 (25%) |
| 55 | 5OH | DW | 6 | 55 | 8,12,13 | 1.57 | 2 (25%) | 5,16,18 | 1.50 | 1 (20%) |
| 55 | KBE | FW | 1 | 55 | 8,8,9 | 1.09 | 1 (12%) | 7,8,10 | 1.84 | 1 (14%) |
| 55 | DPP | FW | 2 | 55 | 4,5,6 | 1.35 | 1 (25%) | 1,5,7 | 1.42 | 0 |
| 55 | UAL | FW | 5 | 55 | 8,8,9 | 3.10 | 5 (62%) | 4,9,11 | 2.76 | 1 (25%) |
| 55 | 5OH | FW | 6 | 55 | 8,12,13 | 1.79 | 2 (25%) | 5,16,18 | 1.75 | 2 (40%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 55 | KBE | BW | 1 | 55 | - | 0/7/7/8 | 0/0/0/0 |
| 55 | DPP | BW | 2 | 55 | - | 0/2/4/6 | 0/0/0/0 |
| 55 | UAL | BW | 5 | 55 | - | 0/3/7/9 | 0/0/0/0 |
| 55 | 5OH | BW | 6 | 55 | - | 0/2/18/20 | 0/1/1/1 |
| 55 | KBE | DW | 1 | 55 | - | 0/7/7/8 | 0/0/0/0 |
| 55 | DPP | DW | 2 | 55 | - | 0/2/4/6 | 0/0/0/0 |
| 55 | UAL | DW | 5 | 55 | - | 0/3/7/9 | 0/0/0/0 |
| 55 | 5OH | DW | 6 | 55 | - | 0/2/18/20 | 0/1/1/1 |
| 55 | KBE | FW | 1 | 55 | - | 0/7/7/8 | 0/0/0/0 |
| 55 | DPP | FW | 2 | 55 | - | 0/2/4/6 | 0/0/0/0 |
| 55 | UAL | FW | 5 | 55 | - | 0/3/7/9 | 0/0/0/0 |
| 55 | 5OH | FW | 6 | 55 | - | 0/2/18/20 | 0/1/1/1 |

The worst 5 of 24 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 55 | FW | 6 | 5OH | CR-CB | -2.66 | 1.48 | 1.53 |
| 55 | DW | 6 | 5OH | CR-CB | -2.59 | 1.48 | 1.53 |
| 55 | FW | 1 | KBE | CB-N | -2.51 | 1.40 | 1.47 |
| 55 | DW | 1 | KBE | CB-N | -2.47 | 1.40 | 1.47 |
| 55 | BW | 1 | KBE | CB-N | -2.41 | 1.40 | 1.47 |

The worst 5 of 10 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 55 | BW | 5 | UAL | O-C-CA | -8.91 | 114.08 | 125.47 |
| 55 | DW | 5 | UAL | O-C-CA | -8.52 | 114.58 | 125.47 |
| 55 | FW | 5 | UAL | O-C-CA | -4.98 | 119.11 | 125.47 |
| 55 | DW | 6 | 5OH | O-C-CA | -2.56 | 119.17 | 125.15 |
| 55 | FW | 6 | 5OH | O-C-CA | -2.18 | 120.07 | 125.15 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 55 | BW | 1 | KBE | 2 | 0 |
| 55 | BW | 5 | UAL | 1 | 0 |
| 55 | BW | 6 | 5OH | 1 | 0 |
| 55 | DW | 1 | KBE | 1 | 0 |
| 55 | DW | 2 | DPP | 1 | 0 |
| 55 | DW | 5 | UAL | 2 | 0 |
| 55 | DW | 6 | 5OH | 3 | 0 |
| 55 | FW | 1 | KBE | 1 | 0 |
| 55 | FW | 2 | DPP | 1 | 0 |
| 55 | FW | 6 | 5OH | 3 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 748 ligands modelled in this entry, 744 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 58 | GCP | BV | 801 | 56 | 25,34,34 | 2.84 | 9 (36%) | 28,54,54 | 1.42 | 3 (10%) |
| 58 | GCP | DV | 801 | 56 | 25,34,34 | 2.80 | 8 (32%) | 28,54,54 | 1.25 | 3 (10%) |
| 58 | GCP | FV | 801 | 56 | 25,34,34 | 2.57 | 8 (32%) | 28,54,54 | 1.22 | 2 (7%) |
| 58 | GCP | HV | 801 | 56 | 25,34,34 | 2.70 | 9 (36%) | 28,54,54 | 1.38 | 3 (10%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 58 | GCP | BV | 801 | 56 | - | 0/18/38/38 | 0/3/3/3 |
| 58 | GCP | DV | 801 | 56 | - | 0/18/38/38 | 0/3/3/3 |
| 58 | GCP | FV | 801 | 56 | - | 0/18/38/38 | 0/3/3/3 |
| 58 | GCP | HV | 801 | 56 | - | 0/18/38/38 | 0/3/3/3 |

The worst 5 of 34 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 58 | FV | 801 | GCP | C4-N9 | -10.32 | 1.34 | 1.47 |
| 58 | BV | 801 | GCP | C5-C6 | -7.95 | 1.38 | 1.53 |
| 58 | BV | 801 | GCP | C4-N9 | -7.94 | 1.37 | 1.47 |
| 58 | DV | 801 | GCP | C5-C6 | -7.77 | 1.39 | 1.53 |
| 58 | DV | 801 | GCP | C4-N9 | -7.77 | 1.37 | 1.47 |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 58 | HV | 801 | GCP | PA-O3A-PB | -4.41 | 118.16 | 132.39 |
| 58 | BV | 801 | GCP | C4'-O4'-C1' | -4.17 | 100.17 | 109.47 |
| 58 | BV | 801 | GCP | PA-O3A-PB | -3.79 | 120.17 | 132.39 |
| 58 | FV | 801 | GCP | PA-O3A-PB | -3.68 | 120.54 | 132.39 |
| 58 | DV | 801 | GCP | C4'-O4'-C1' | -3.59 | 101.47 | 109.47 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 58 | BV | 801 | GCP | 2 | 0 |
| 58 | DV | 801 | GCP | 1 | 0 |
| 58 | FV | 801 | GCP | 5 | 0 |
| 58 | HV | 801 | GCP | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 2854/2904 (98%) | -0.24 | 60 (2%) 64 60 | 4, 28, 65, 87 | 0 |
| 1 | CA | 2854/2904 (98%) | -0.26 | 58 (2%) 65 62 | 3, 25, 63, 88 | 0 |
| 1 | EA | 2854/2904 (98%) | -0.25 | 45 (1%) 72 70 | 1, 14, 60, 92 | 0 |
| 1 | GA | 2854/2904 (98%) | -0.22 | 65 (2%) 61 57 | 5, 29, 68, 89 | 0 |
| 2 | AB | 118/120 (98%) | -0.49 | 0 100 100 | 18, 48, 62, 72 | 0 |
| 2 | CB | 118/120 (98%) | -0.61 | 0 100 100 | 18, 41, 54, 72 | 0 |
| 2 | EB | 118/120 (98%) | -0.52 | 0 100 100 | 3, 25, 45, 56 | 0 |
| 2 | GB | 118/120 (98%) | -0.52 | 1 (0%) 86 85 | 23, 44, 61, 78 | 0 |
| 3 | AC | 271/273 (99%) | -0.14 | 1 (0%) 92 92 | 5, 26, 40, 60 | 0 |
| 3 | CC | 271/273 (99%) | -0.23 | 0 100 100 | 2, 18, 34, 44 | 0 |
| 3 | EC | 271/273 (99%) | -0.30 | 0 100 100 | 1, 15, 32, 57 | 0 |
| 3 | GC | 271/273 (99%) | -0.28 | 0 100 100 | 3, 17, 30, 42 | 0 |
| 4 | AD | 209/209 (100%) | -0.09 | 2 (0%) 82 81 | 6, 27, 47, 60 | 0 |
| 4 | CD | 209/209 (100%) | -0.02 | 5 (2%) 59 55 | 3, 31, 52, 61 | 0 |
| 4 | ED | 209/209 (100%) | -0.18 | 2 (0%) 82 81 | 1, 20, 43, 56 | 0 |
| 4 | GD | 209/209 (100%) | 0.08 | 5 (2%) 59 55 | 4, 36, 54, 62 | 0 |
| 5 | AE | 201/201 (100%) | 0.17 | 6 (2%) 51 44 | 7, 33, 55, 63 | 0 |
| 5 | CE | 201/201 (100%) | 0.13 | 7 (3%) 44 38 | 4, 33, 54, 60 | 0 |
| 5 | EE | 201/201 (100%) | -0.05 | 2 (0%) 82 81 | 2, 19, 45, 69 | 0 |
| 5 | GE | 201/201 (100%) | 0.25 | 8 (3%) 39 34 | 7, 41, 56, 67 | 0 |
| 6 | AF | 177/179 (98%) | 2.43 | 93 (52%) 0 0 | 45, 61, 71, 79 | 0 |
| 6 | CF | 177/179 (98%) | 0.66 | 18 (10%) 7 5 | 32, 49, 63, 67 | 0 |
| 6 | EF | 177/179 (98%) | 0.55 | 15 (8%) 11 8 | 19, 42, 61, 68 | 0 |
| 6 | GF | 177/179 (98%) | 2.01 | 75 (42%) 0 0 | 36, 61, 72, 76 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 7 | AG | 176/177 (99%) | 0.41 | 16 (9%) 10 7 | 20, 42, 60, 69 | 0 |
| 7 | CG | 176/177 (99%) | 0.61 | 24 (13%) 3 2 | 23, 46, 61, 69 | 0 |
| 7 | EG | 176/177 (99%) | 0.11 | 8 (4%) 34 29 | 19, 37, 55, 63 | 0 |
| 7 | GG | 176/177 (99%) | 0.60 | 23 (13%) 4 2 | 32, 48, 63, 68 | 0 |
| 8 | AH | 50/50 (100%) | 1.28 | 10 (20%) 1 1 | 28, 51, 67, 77 | 0 |
| 8 | CH | 50/50 (100%) | 1.48 | 17 (34%) 0 0 | 39, 56, 68, 74 | 0 |
| 8 | EH | 50/50 (100%) | 1.31 | 14 (28%) 1 0 | 24, 49, 69, 79 | 0 |
| 8 | GH | 50/50 (100%) | 1.16 | 15 (30%) 1 0 | 26, 46, 64, 69 | 0 |
| 9 | AI | 141/142 (99%) | 2.13 | 58 (41%) 0 0 | 44, 64, 75, 82 | 0 |
| 9 | CI | 141/142 (99%) | 2.46 | 73 (51%) 0 0 | 49, 63, 73, 76 | 0 |
| 9 | EI | 141/142 (99%) | 2.84 | 81 (57%) 0 0 | 48, 65, 77, 82 | 0 |
| 9 | GI | 141/142 (99%) | 3.94 | 109 (77%) 0 0 | 49, 68, 77, 81 | 0 |
| 10 | AJ | 142/142 (100%) | -0.10 | 2 (1%) 75 74 | 12, 29, 41, 60 | 0 |
| 10 | CJ | 142/142 (100%) | -0.03 | 2 (1%) 75 74 | 13, 29, 42, 58 | 0 |
| 10 | EJ | 142/142 (100%) | -0.19 | 1 (0%) 87 86 | 3, 13, 30, 47 | 0 |
| 10 | GJ | 142/142 (100%) | 0.05 | 5 (3%) 44 38 | 15, 32, 47, 61 | 0 |
| 11 | AK | 122/123 (99%) | -0.20 | 1 (0%) 86 85 | 5, 19, 34, 54 | 0 |
| 11 | CK | 122/123 (99%) | -0.14 | 2 (1%) 72 70 | 9, 22, 39, 56 | 0 |
| 11 | EK | 122/123 (99%) | -0.07 | 2 (1%) 72 70 | 4, 18, 37, 49 | 0 |
| 11 | GK | 122/123 (99%) | 0.19 | 2 (1%) 72 70 | 13, 27, 42, 59 | 0 |
| 12 | AL | 143/144 (99%) | 0.21 | 7 (4%) 30 26 | 10, 30, 48, 58 | 0 |
| 12 | CL | 143/144 (99%) | 0.04 | 2 (1%) 75 74 | 3, 29, 47, 62 | 0 |
| 12 | EL | 143/144 (99%) | 0.09 | 3 (2%) 64 60 | 1, 18, 39, 54 | 0 |
| 12 | GL | 143/144 (99%) | 0.48 | 14 (9%) 8 6 | 10, 35, 53, 67 | 0 |
| 13 | AM | 136/136 (100%) | -0.07 | 2 (1%) 74 72 | 8, 19, 37, 55 | 0 |
| 13 | CM | 136/136 (100%) | -0.08 | 1 (0%) 87 86 | 8, 21, 38, 56 | 0 |
| 13 | EM | 136/136 (100%) | -0.21 | 2 (1%) 74 72 | 1, 11, 29, 60 | 0 |
| 13 | GM | 136/136 (100%) | 0.18 | 4 (2%) 52 46 | 11, 28, 45, 58 | 0 |
| 14 | AN | 120/127 (94%) | 0.08 | 2 (1%) 70 68 | 14, 29, 41, 62 | 0 |
| 14 | CN | 120/127 (94%) | 0.00 | 1 (0%) 86 85 | 18, 31, 43, 62 | 0 |
| 14 | EN | 120/127 (94%) | -0.10 | 1 (0%) 86 85 | 6, 19, 32, 61 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 14 | GN | 120/127 (94%) | -0.00 | 1 (0%) 86 85 | 19, 31, 43, 72 | 0 |
| 15 | AO | 116/117 (99%) | 0.60 | 11 (9%) 9 6 | 28, 47, 56, 62 | 0 |
| 15 | CO | 116/117 (99%) | 0.40 | 8 (6%) 18 13 | 28, 42, 55, 61 | 0 |
| 15 | EO | 116/117 (99%) | 0.09 | 3 (2%) 56 51 | 16, 30, 43, 55 | 0 |
| 15 | GO | 116/117 (99%) | 0.49 | 9 (7%) 14 10 | 28, 40, 58, 63 | 0 |
| 16 | AP | 114/115 (99%) | 0.08 | 1 (0%) 84 83 | 13, 31, 47, 62 | 0 |
| 16 | CP | 114/115 (99%) | 0.06 | 4 (3%) 44 38 | 17, 35, 49, 62 | 0 |
| 16 | EP | 114/115 (99%) | -0.21 | 2 (1%) 69 66 | 6, 24, 43, 66 | 0 |
| 16 | GP | 114/115 (99%) | 0.21 | 4 (3%) 44 38 | 14, 35, 50, 59 | 0 |
| 17 | AQ | 117/118 (99%) | 0.01 | 1 (0%) 84 83 | 10, 26, 43, 56 | 0 |
| 17 | CQ | 117/118 (99%) | -0.05 | 3 (2%) 56 51 | 6, 24, 39, 60 | 0 |
| 17 | EQ | 117/118 (99%) | -0.18 | 0 100 100 | 2, 9, 25, 46 | 0 |
| 17 | GQ | 117/118 (99%) | 0.15 | 4 (3%) 46 39 | 19, 29, 42, 56 | 0 |
| 18 | AR | 103/103 (100%) | 0.17 | 4 (3%) 40 35 | 10, 37, 52, 60 | 0 |
| 18 | CR | 103/103 (100%) | 0.06 | 2 (1%) 67 64 | 9, 34, 49, 63 | 0 |
| 18 | ER | 103/103 (100%) | -0.19 | 1 (0%) 82 81 | 2, 21, 41, 52 | 0 |
| 18 | GR | 103/103 (100%) | 0.46 | 6 (5%) 24 19 | 13, 40, 53, 63 | 0 |
| 19 | AS | 110/110 (100%) | 0.15 | 4 (3%) 43 37 | 13, 28, 45, 62 | 0 |
| 19 | CS | 110/110 (100%) | 0.11 | 2 (1%) 69 66 | 7, 27, 45, 65 | 0 |
| 19 | ES | 110/110 (100%) | -0.10 | 0 100 100 | 2, 12, 36, 49 | 0 |
| 19 | GS | 110/110 (100%) | 0.40 | 8 (7%) 16 11 | 12, 31, 50, 69 | 0 |
| 20 | AT | 93/100 (93%) | 0.59 | 10 (10%) 6 4 | 18, 37, 58, 63 | 0 |
| 20 | CT | 93/100 (93%) | 0.36 | 9 (9%) 8 6 | 14, 37, 57, 67 | 0 |
| 20 | ET | 93/100 (93%) | 0.36 | 8 (8%) 11 8 | 6, 24, 53, 61 | 0 |
| 20 | GT | 93/100 (93%) | 0.65 | 17 (18%) 1 1 | 19, 36, 57, 62 | 0 |
| 21 | AU | 102/104 (98%) | 0.73 | 14 (13%) 3 2 | 24, 40, 56, 64 | 0 |
| 21 | CU | 102/104 (98%) | 0.76 | 15 (14%) 3 2 | 24, 41, 61, 73 | 0 |
| 21 | EU | 102/104 (98%) | 0.34 | 5 (4%) 30 26 | 13, 28, 51, 65 | 0 |
| 21 | GU | 102/104 (98%) | 1.24 | 23 (22%) 1 0 | 32, 46, 63, 75 | 0 |
| 22 | AV | 94/94 (100%) | -0.12 | 2 (2%) 64 60 | 23, 38, 48, 57 | 0 |
| 22 | CV | 94/94 (100%) | 0.00 | 1 (1%) 80 79 | 25, 39, 52, 67 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|--------------|--------|--------------|-----------------------|-------|
| 22 | EV | 94/94 (100%) | -0.34 | 0 100 100 | 9, 22, 40, 45 | 0 |
| 22 | GV | 94/94 (100%) | 0.20 | 3 (3%) 48 42 | 29, 42, 55, 60 | 0 |
| 23 | AW | 79/85 (92%) | 0.54 | 9 (11%) 6 4 | 17, 35, 52, 61 | 0 |
| 23 | CW | 79/85 (92%) | 0.41 | 4 (5%) 29 24 | 15, 29, 51, 65 | 0 |
| 23 | EW | 79/85 (92%) | 0.38 | 4 (5%) 29 24 | 5, 17, 44, 50 | 0 |
| 23 | GW | 79/85 (92%) | 0.52 | 6 (7%) 15 10 | 15, 33, 55, 63 | 0 |
| 24 | AX | 77/78 (98%) | 0.34 | 2 (2%) 56 51 | 16, 31, 47, 57 | 0 |
| 24 | CX | 77/78 (98%) | 0.08 | 1 (1%) 77 76 | 8, 22, 46, 49 | 0 |
| 24 | EX | 77/78 (98%) | 0.01 | 0 100 100 | 4, 18, 40, 50 | 0 |
| 24 | GX | 77/78 (98%) | -0.01 | 1 (1%) 77 76 | 14, 25, 46, 56 | 0 |
| 25 | AY | 63/63 (100%) | 0.96 | 10 (15%) 2 1 | 30, 47, 61, 65 | 0 |
| 25 | CY | 63/63 (100%) | 0.63 | 6 (9%) 9 6 | 27, 44, 58, 67 | 0 |
| 25 | EY | 63/63 (100%) | 0.75 | 8 (12%) 4 3 | 13, 33, 51, 70 | 0 |
| 25 | GY | 63/63 (100%) | 1.11 | 9 (14%) 3 2 | 29, 45, 60, 68 | 0 |
| 26 | AZ | 58/59 (98%) | 0.37 | 2 (3%) 46 39 | 15, 31, 55, 71 | 0 |
| 26 | CZ | 58/59 (98%) | 0.25 | 3 (5%) 28 23 | 17, 30, 53, 65 | 0 |
| 26 | EZ | 58/59 (98%) | -0.14 | 1 (1%) 70 68 | 2, 10, 35, 59 | 0 |
| 26 | GZ | 58/59 (98%) | 0.27 | 3 (5%) 28 23 | 20, 32, 51, 53 | 0 |
| 27 | A0 | 56/57 (98%) | 0.37 | 2 (3%) 43 37 | 11, 33, 54, 62 | 0 |
| 27 | C0 | 56/57 (98%) | 0.18 | 1 (1%) 69 66 | 8, 35, 50, 60 | 0 |
| 27 | E0 | 56/57 (98%) | 0.11 | 1 (1%) 69 66 | 3, 25, 48, 56 | 0 |
| 27 | G0 | 56/57 (98%) | 0.31 | 3 (5%) 26 22 | 15, 35, 58, 67 | 0 |
| 28 | A1 | 50/55 (90%) | 1.09 | 9 (18%) 2 1 | 27, 38, 51, 61 | 0 |
| 28 | C1 | 50/55 (90%) | 0.79 | 5 (10%) 8 6 | 21, 35, 48, 59 | 0 |
| 28 | E1 | 50/55 (90%) | 0.44 | 4 (8%) 13 10 | 11, 26, 44, 47 | 0 |
| 28 | G1 | 50/55 (90%) | 1.24 | 15 (30%) 1 0 | 25, 38, 55, 61 | 0 |
| 29 | A2 | 46/46 (100%) | 0.07 | 1 (2%) 62 59 | 9, 22, 34, 55 | 0 |
| 29 | C2 | 46/46 (100%) | -0.04 | 2 (4%) 36 31 | 7, 14, 30, 54 | 0 |
| 29 | E2 | 46/46 (100%) | -0.22 | 1 (2%) 62 59 | 2, 7, 15, 53 | 0 |
| 29 | G2 | 46/46 (100%) | 0.05 | 2 (4%) 36 31 | 8, 17, 28, 51 | 0 |
| 30 | A3 | 64/65 (98%) | -0.00 | 0 100 100 | 12, 22, 37, 40 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 30 | C3 | 64/65 (98%) | -0.04 | 0 100 100 | 10, 18, 27, 35 | 0 |
| 30 | E3 | 64/65 (98%) | -0.13 | 0 100 100 | 2, 8, 14, 27 | 0 |
| 30 | G3 | 64/65 (98%) | 0.04 | 1 (1%) 72 70 | 13, 22, 37, 48 | 0 |
| 31 | A4 | 38/38 (100%) | 0.10 | 1 (2%) 56 51 | 13, 22, 36, 38 | 0 |
| 31 | C4 | 38/38 (100%) | 0.14 | 1 (2%) 56 51 | 14, 27, 39, 46 | 0 |
| 31 | E4 | 38/38 (100%) | -0.14 | 0 100 100 | 5, 16, 35, 38 | 0 |
| 31 | G4 | 38/38 (100%) | 0.34 | 1 (2%) 56 51 | 22, 33, 44, 49 | 0 |
| 32 | A5 | 148/165 (89%) | 2.99 | 83 (56%) 0 0 | 36, 54, 65, 74 | 0 |
| 32 | E5 | 144/165 (87%) | 3.51 | 102 (70%) 0 0 | 35, 61, 72, 82 | 0 |
| 33 | BA | 1533/1542 (99%) | -0.26 | 29 (1%) 67 64 | 11, 42, 70, 91 | 0 |
| 33 | DA | 1533/1542 (99%) | -0.27 | 25 (1%) 72 70 | 12, 43, 69, 85 | 0 |
| 33 | FA | 1533/1542 (99%) | -0.27 | 25 (1%) 72 70 | 8, 33, 61, 85 | 0 |
| 33 | HA | 1533/1542 (99%) | -0.13 | 51 (3%) 47 40 | 15, 41, 72, 90 | 0 |
| 34 | BB | 218/241 (90%) | 1.32 | 65 (29%) 1 0 | 41, 58, 69, 79 | 0 |
| 34 | DB | 218/241 (90%) | 1.46 | 67 (30%) 0 0 | 40, 57, 69, 79 | 0 |
| 34 | FB | 218/241 (90%) | 0.69 | 28 (12%) 4 3 | 26, 49, 63, 69 | 0 |
| 34 | HB | 218/241 (90%) | 1.11 | 45 (20%) 1 1 | 33, 51, 67, 73 | 0 |
| 35 | BC | 206/233 (88%) | 0.63 | 31 (15%) 3 2 | 30, 50, 60, 69 | 0 |
| 35 | DC | 206/233 (88%) | 0.41 | 18 (8%) 11 8 | 35, 50, 60, 67 | 0 |
| 35 | FC | 206/233 (88%) | -0.08 | 3 (1%) 74 72 | 13, 30, 46, 58 | 0 |
| 35 | HC | 206/233 (88%) | 0.32 | 11 (5%) 27 23 | 21, 40, 56, 66 | 0 |
| 36 | BD | 205/206 (99%) | 0.39 | 15 (7%) 16 11 | 23, 39, 57, 64 | 0 |
| 36 | DD | 205/206 (99%) | 0.89 | 33 (16%) 2 1 | 26, 47, 60, 65 | 0 |
| 36 | FD | 205/206 (99%) | 0.70 | 30 (14%) 3 2 | 27, 44, 60, 73 | 0 |
| 36 | HD | 205/206 (99%) | 0.59 | 23 (11%) 6 4 | 25, 47, 61, 79 | 0 |
| 37 | BE | 150/167 (89%) | 0.23 | 11 (7%) 16 11 | 17, 48, 63, 76 | 0 |
| 37 | DE | 150/167 (89%) | 0.16 | 7 (4%) 32 28 | 25, 45, 62, 71 | 0 |
| 37 | FE | 150/167 (89%) | -0.09 | 3 (2%) 65 62 | 18, 34, 50, 65 | 0 |
| 37 | HE | 150/167 (89%) | 0.06 | 4 (2%) 55 50 | 21, 37, 54, 67 | 0 |
| 38 | BF | 100/135 (74%) | 1.50 | 32 (32%) 0 0 | 50, 62, 70, 74 | 0 |
| 38 | DF | 100/135 (74%) | 0.61 | 15 (15%) 3 2 | 32, 49, 62, 69 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 38 | FF | 100/135 (74%) | 0.77 | 15 (15%) 3 2 | 32, 51, 63, 66 | 0 |
| 38 | HF | 100/135 (74%) | 0.54 | 9 (9%) 10 7 | 31, 51, 64, 71 | 0 |
| 39 | BG | 151/179 (84%) | 0.38 | 11 (7%) 16 11 | 28, 49, 60, 66 | 0 |
| 39 | DG | 151/179 (84%) | 0.34 | 8 (5%) 27 23 | 32, 46, 58, 63 | 0 |
| 39 | FG | 151/179 (84%) | 0.33 | 9 (5%) 23 17 | 23, 39, 55, 63 | 0 |
| 39 | HG | 151/179 (84%) | 0.79 | 21 (13%) 3 2 | 32, 48, 62, 68 | 0 |
| 40 | BH | 129/130 (99%) | 0.70 | 16 (12%) 4 3 | 40, 51, 62, 70 | 0 |
| 40 | DH | 129/130 (99%) | 0.58 | 14 (10%) 6 4 | 28, 47, 59, 73 | 0 |
| 40 | FH | 129/130 (99%) | -0.04 | 2 (1%) 72 70 | 20, 32, 47, 66 | 0 |
| 40 | HH | 129/130 (99%) | 0.27 | 5 (3%) 40 35 | 23, 35, 51, 69 | 0 |
| 41 | BI | 127/130 (97%) | 1.01 | 25 (19%) 1 1 | 24, 52, 65, 70 | 0 |
| 41 | DI | 127/130 (97%) | 0.97 | 18 (14%) 3 2 | 31, 52, 64, 74 | 0 |
| 41 | FI | 127/130 (97%) | 0.39 | 10 (7%) 13 10 | 14, 43, 60, 69 | 0 |
| 41 | HI | 127/130 (97%) | 1.29 | 34 (26%) 1 0 | 29, 55, 70, 75 | 0 |
| 42 | BJ | 98/103 (95%) | 1.83 | 39 (39%) 0 0 | 30, 55, 68, 72 | 0 |
| 42 | DJ | 98/103 (95%) | 1.73 | 36 (36%) 0 0 | 35, 57, 70, 74 | 0 |
| 42 | FJ | 98/103 (95%) | 0.54 | 12 (12%) 5 3 | 14, 32, 59, 65 | 0 |
| 42 | HJ | 98/103 (95%) | 1.27 | 27 (27%) 1 0 | 30, 51, 69, 78 | 0 |
| 43 | BK | 117/129 (90%) | 1.36 | 28 (23%) 1 0 | 33, 56, 66, 80 | 0 |
| 43 | DK | 117/129 (90%) | 0.16 | 9 (7%) 14 10 | 26, 41, 56, 60 | 0 |
| 43 | FK | 117/129 (90%) | 0.44 | 10 (8%) 11 8 | 18, 42, 59, 64 | 0 |
| 43 | HK | 117/129 (90%) | 1.41 | 32 (27%) 1 0 | 23, 50, 70, 74 | 0 |
| 44 | BL | 123/124 (99%) | -0.10 | 2 (1%) 72 70 | 15, 24, 43, 74 | 0 |
| 44 | DL | 123/124 (99%) | 0.02 | 5 (4%) 38 32 | 20, 34, 48, 61 | 0 |
| 44 | FL | 123/124 (99%) | -0.07 | 4 (3%) 47 40 | 9, 28, 44, 67 | 0 |
| 44 | HL | 123/124 (99%) | 0.19 | 7 (5%) 24 19 | 21, 37, 55, 63 | 0 |
| 45 | BM | 114/118 (96%) | 0.64 | 13 (11%) 6 4 | 28, 49, 64, 74 | 0 |
| 45 | DM | 114/118 (96%) | 0.45 | 6 (5%) 27 23 | 36, 50, 63, 67 | 0 |
| 45 | FM | 114/118 (96%) | 0.52 | 12 (10%) 7 5 | 19, 45, 63, 68 | 0 |
| 45 | HM | 114/118 (96%) | 2.55 | 60 (52%) 0 0 | 42, 63, 72, 75 | 0 |
| 46 | BN | 96/101 (95%) | 0.60 | 14 (14%) 3 2 | 32, 46, 60, 65 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|--------------|--------|--------------|-----------------------|-------|
| 46 | DN | 96/101 (95%) | 0.58 | 13 (13%) 3 2 | 30, 49, 62, 65 | 0 |
| 46 | FN | 96/101 (95%) | 0.00 | 2 (2%) 64 60 | 11, 24, 53, 60 | 0 |
| 46 | HN | 96/101 (95%) | 0.59 | 15 (15%) 2 1 | 27, 47, 64, 70 | 0 |
| 47 | BO | 88/89 (98%) | 0.59 | 8 (9%) 10 7 | 35, 50, 61, 64 | 0 |
| 47 | DO | 88/89 (98%) | 0.47 | 6 (6%) 18 13 | 31, 45, 56, 61 | 0 |
| 47 | FO | 88/89 (98%) | 0.36 | 2 (2%) 61 57 | 23, 37, 49, 56 | 0 |
| 47 | HO | 88/89 (98%) | 0.19 | 3 (3%) 46 39 | 22, 39, 53, 70 | 0 |
| 48 | BP | 82/82 (100%) | 0.65 | 9 (10%) 6 4 | 24, 35, 61, 68 | 0 |
| 48 | DP | 82/82 (100%) | 1.16 | 17 (20%) 1 1 | 28, 43, 62, 79 | 0 |
| 48 | FP | 82/82 (100%) | 0.24 | 5 (6%) 22 17 | 21, 34, 62, 77 | 0 |
| 48 | HP | 82/82 (100%) | 0.47 | 8 (9%) 8 6 | 22, 39, 62, 71 | 0 |
| 49 | BQ | 80/84 (95%) | 0.75 | 10 (12%) 4 3 | 30, 45, 55, 63 | 0 |
| 49 | DQ | 80/84 (95%) | 0.79 | 10 (12%) 4 3 | 29, 44, 57, 68 | 0 |
| 49 | FQ | 80/84 (95%) | 0.23 | 4 (5%) 30 25 | 22, 38, 54, 63 | 0 |
| 49 | HQ | 80/84 (95%) | 0.34 | 4 (5%) 30 25 | 27, 41, 51, 57 | 0 |
| 50 | BR | 55/75 (73%) | 1.75 | 20 (36%) 0 0 | 46, 55, 66, 69 | 0 |
| 50 | DR | 55/75 (73%) | 0.76 | 9 (16%) 2 1 | 35, 44, 60, 66 | 0 |
| 50 | FR | 55/75 (73%) | 0.43 | 6 (10%) 6 4 | 35, 44, 53, 61 | 0 |
| 50 | HR | 55/75 (73%) | 0.47 | 5 (9%) 10 7 | 26, 40, 55, 64 | 0 |
| 51 | BS | 79/92 (85%) | 0.32 | 5 (6%) 21 16 | 30, 44, 59, 64 | 0 |
| 51 | DS | 79/92 (85%) | 0.67 | 9 (11%) 6 4 | 36, 49, 63, 67 | 0 |
| 51 | FS | 79/92 (85%) | -0.20 | 2 (2%) 58 53 | 22, 32, 52, 63 | 0 |
| 51 | HS | 79/92 (85%) | 2.44 | 42 (53%) 0 0 | 43, 58, 70, 74 | 0 |
| 52 | BT | 85/87 (97%) | 0.53 | 5 (5%) 23 18 | 25, 40, 50, 59 | 0 |
| 52 | DT | 85/87 (97%) | 0.53 | 7 (8%) 12 9 | 30, 40, 55, 73 | 0 |
| 52 | FT | 85/87 (97%) | 0.22 | 5 (5%) 23 18 | 24, 36, 50, 63 | 0 |
| 52 | HT | 85/87 (97%) | 0.71 | 6 (7%) 17 12 | 23, 38, 53, 56 | 0 |
| 53 | BU | 51/71 (71%) | 3.68 | 34 (66%) 0 0 | 53, 62, 71, 82 | 0 |
| 53 | DU | 51/71 (71%) | 1.58 | 16 (31%) 0 0 | 40, 54, 69, 74 | 0 |
| 53 | FU | 51/71 (71%) | 1.37 | 19 (37%) 0 0 | 40, 53, 65, 69 | 0 |
| 53 | HU | 51/71 (71%) | 2.31 | 20 (39%) 0 0 | 40, 57, 67, 71 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|----------|
| 54 | BV | 689/704 (97%) | 0.39 | 65 (9%) 9 6 | 18, 46, 66, 76 | 0 |
| 54 | DV | 689/704 (97%) | 0.58 | 94 (13%) 3 2 | 27, 50, 68, 77 | 0 |
| 54 | FV | 689/704 (97%) | 2.68 | 366 (53%) 0 0 | 33, 66, 76, 82 | 0 |
| 54 | HV | 689/704 (97%) | 1.00 | 138 (20%) 1 1 | 32, 56, 70, 80 | 0 |
| 55 | BW | 2/6 (33%) | 4.02 | 1 (50%) 0 0 | 41, 41, 41, 43 | 2 (100%) |
| 55 | DW | 2/6 (33%) | 3.38 | 1 (50%) 0 0 | 40, 40, 40, 44 | 2 (100%) |
| 55 | FW | 2/6 (33%) | 2.97 | 2 (100%) 0 0 | 41, 41, 41, 42 | 2 (100%) |
| All | All | 43562/44972 (96%) | 0.24 | 3538 (8%) 13 9 | 1, 37, 66, 92 | 6 (0%) |

The worst 5 of 3538 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 48 | DP | 81 | ALA | 20.0 |
| 32 | A5 | 112 | ALA | 16.9 |
| 9 | GI | 8 | VAL | 16.9 |
| 26 | AZ | 1 | ALA | 16.7 |
| 54 | FV | 588 | SER | 15.3 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 55 | 5OH | FW | 6 | 12/13 | 0.55 | 0.73 | - | 37,42,45,46 | 12 |
| 55 | DPP | BW | 2 | 6/7 | 0.85 | 0.56 | - | 34,36,39,40 | 6 |
| 55 | KBE | FW | 1 | 9/10 | 0.62 | 0.49 | - | 28,36,40,42 | 9 |
| 55 | 5OH | BW | 6 | 12/13 | 0.72 | 0.49 | - | 36,37,41,43 | 12 |
| 55 | KBE | DW | 1 | 9/10 | 0.68 | 0.37 | - | 32,33,40,41 | 9 |
| 55 | KBE | BW | 1 | 9/10 | 0.67 | 0.60 | - | 37,39,42,44 | 9 |
| 55 | 5OH | DW | 6 | 12/13 | 0.74 | 0.44 | - | 33,41,43,48 | 12 |
| 55 | UAL | FW | 5 | 9/10 | 0.67 | 0.57 | - | 35,37,39,41 | 9 |
| 55 | DPP | FW | 2 | 6/7 | 0.47 | 0.88 | - | 37,42,43,43 | 6 |
| 55 | UAL | DW | 5 | 9/10 | 0.78 | 0.44 | - | 35,39,42,46 | 9 |
| 55 | DPP | DW | 2 | 6/7 | 0.84 | 0.43 | - | 32,34,37,44 | 6 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 55 | UAL | BW | 5 | 9/10 | 0.69 | 0.62 | - | 32,40,42,42 | 9 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | AC | 303 | 1/1 | 0.94 | 1.01 | 30.19 | 34,34,34,34 | 0 |
| 56 | MG | EQ | 201 | 1/1 | 0.82 | 0.66 | 27.30 | 31,31,31,31 | 0 |
| 56 | MG | BA | 1606 | 1/1 | 0.97 | 0.53 | 25.25 | 39,39,39,39 | 0 |
| 56 | MG | EA | 3099 | 1/1 | 0.99 | 0.28 | 11.91 | 2,2,2,2 | 0 |
| 56 | MG | AA | 3098 | 1/1 | 0.98 | 0.23 | 10.88 | 5,5,5,5 | 0 |
| 56 | MG | GA | 3102 | 1/1 | 0.97 | 0.35 | 10.65 | 40,40,40,40 | 0 |
| 56 | MG | BA | 1614 | 1/1 | 0.82 | 0.38 | 10.44 | 26,26,26,26 | 0 |
| 56 | MG | FA | 1609 | 1/1 | 0.99 | 0.32 | 9.86 | 16,16,16,16 | 0 |
| 56 | MG | DA | 1628 | 1/1 | 0.96 | 0.33 | 9.14 | 37,37,37,37 | 0 |
| 56 | MG | HA | 1610 | 1/1 | 0.94 | 0.27 | 8.79 | 13,13,13,13 | 0 |
| 56 | MG | FA | 1623 | 1/1 | 0.99 | 0.21 | 8.49 | 7,7,7,7 | 0 |
| 56 | MG | AA | 3102 | 1/1 | 0.99 | 0.24 | 8.43 | 0,0,0,0 | 0 |
| 56 | MG | AA | 3028 | 1/1 | 0.99 | 0.28 | 7.53 | 2,2,2,2 | 0 |
| 56 | MG | GA | 3129 | 1/1 | 0.99 | 0.22 | 7.09 | 19,19,19,19 | 0 |
| 56 | MG | GA | 3063 | 1/1 | 0.99 | 0.27 | 7.02 | 3,3,3,3 | 0 |
| 56 | MG | GA | 3103 | 1/1 | 0.94 | 0.24 | 6.89 | 12,12,12,12 | 0 |
| 56 | MG | AC | 301 | 1/1 | 0.95 | 0.35 | 6.64 | 10,10,10,10 | 0 |
| 56 | MG | EA | 3042 | 1/1 | 0.99 | 0.19 | 6.09 | 2,2,2,2 | 0 |
| 56 | MG | HA | 1612 | 1/1 | 0.99 | 0.19 | 5.90 | 8,8,8,8 | 0 |
| 56 | MG | BA | 1612 | 1/1 | 0.96 | 0.22 | 5.75 | 5,5,5,5 | 0 |
| 56 | MG | AA | 3083 | 1/1 | 0.99 | 0.27 | 5.29 | 33,33,33,33 | 0 |
| 56 | MG | GA | 3014 | 1/1 | 0.98 | 0.28 | 5.18 | 8,8,8,8 | 0 |
| 56 | MG | BA | 1615 | 1/1 | 0.99 | 0.20 | 5.11 | 22,22,22,22 | 0 |
| 56 | MG | CA | 3077 | 1/1 | 0.90 | 0.27 | 5.05 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | HA | 1626 | 1/1 | 0.93 | 0.28 | 5.00 | 32,32,32,32 | 0 |
| 56 | MG | EA | 3049 | 1/1 | 0.99 | 0.23 | 4.81 | 8,8,8,8 | 0 |
| 56 | MG | CA | 3073 | 1/1 | 0.98 | 0.24 | 4.68 | 5,5,5,5 | 0 |
| 56 | MG | CA | 3079 | 1/1 | 0.99 | 0.22 | 4.64 | 12,12,12,12 | 0 |
| 56 | MG | CA | 3119 | 1/1 | 0.99 | 0.21 | 4.63 | 3,3,3,3 | 0 |
| 56 | MG | FA | 1621 | 1/1 | 0.98 | 0.18 | 4.53 | 10,10,10,10 | 0 |
| 56 | MG | EA | 3009 | 1/1 | 0.99 | 0.20 | 4.49 | 0,0,0,0 | 0 |
| 56 | MG | AA | 3107 | 1/1 | 0.99 | 0.19 | 4.46 | 18,18,18,18 | 0 |
| 56 | MG | GA | 3083 | 1/1 | 0.93 | 0.27 | 4.29 | 33,33,33,33 | 0 |
| 56 | MG | EA | 3078 | 1/1 | 0.98 | 0.18 | 4.18 | 3,3,3,3 | 0 |
| 56 | MG | AA | 3109 | 1/1 | 0.99 | 0.21 | 4.13 | 6,6,6,6 | 0 |
| 56 | MG | AA | 3009 | 1/1 | 0.99 | 0.22 | 4.01 | 12,12,12,12 | 0 |
| 56 | MG | EA | 3064 | 1/1 | 0.99 | 0.19 | 3.93 | 0,0,0,0 | 0 |
| 56 | MG | GA | 3060 | 1/1 | 0.94 | 0.28 | 3.70 | 23,23,23,23 | 0 |
| 56 | MG | GA | 3004 | 1/1 | 0.98 | 0.42 | 3.53 | 19,19,19,19 | 0 |
| 56 | MG | BA | 1622 | 1/1 | 0.98 | 0.21 | 3.43 | 32,32,32,32 | 0 |
| 56 | MG | DA | 1621 | 1/1 | 0.98 | 0.19 | 3.42 | 22,22,22,22 | 0 |
| 56 | MG | FA | 1627 | 1/1 | 0.84 | 0.26 | 3.35 | 23,23,23,23 | 0 |
| 56 | MG | EA | 3025 | 1/1 | 0.96 | 0.21 | 3.35 | 0,0,0,0 | 0 |
| 56 | MG | CA | 3040 | 1/1 | 0.99 | 0.19 | 3.32 | 12,12,12,12 | 0 |
| 56 | MG | GA | 3040 | 1/1 | 0.97 | 0.21 | 3.30 | 16,16,16,16 | 0 |
| 56 | MG | GA | 3078 | 1/1 | 0.97 | 0.24 | 3.22 | 40,40,40,40 | 0 |
| 56 | MG | DA | 1616 | 1/1 | 0.99 | 0.27 | 3.20 | 26,26,26,26 | 0 |
| 56 | MG | HA | 1632 | 1/1 | 0.99 | 0.21 | 3.16 | 25,25,25,25 | 0 |
| 56 | MG | GA | 3030 | 1/1 | 0.98 | 0.24 | 3.01 | 11,11,11,11 | 0 |
| 56 | MG | CA | 3028 | 1/1 | 0.98 | 0.21 | 2.84 | 7,7,7,7 | 0 |
| 56 | MG | EA | 3114 | 1/1 | 0.99 | 0.18 | 2.74 | 1,1,1,1 | 0 |
| 56 | MG | EA | 3131 | 1/1 | 0.99 | 0.20 | 2.62 | 5,5,5,5 | 0 |
| 56 | MG | GA | 3110 | 1/1 | 0.97 | 0.19 | 2.57 | 12,12,12,12 | 0 |
| 56 | MG | GA | 3114 | 1/1 | 0.98 | 0.17 | 2.47 | 10,10,10,10 | 0 |
| 56 | MG | CA | 3037 | 1/1 | 0.98 | 0.20 | 2.40 | 1,1,1,1 | 0 |
| 56 | MG | AA | 3017 | 1/1 | 1.00 | 0.20 | 2.34 | 1,1,1,1 | 0 |
| 56 | MG | GA | 3108 | 1/1 | 0.96 | 0.15 | 2.24 | 16,16,16,16 | 0 |
| 56 | MG | BA | 1619 | 1/1 | 0.99 | 0.18 | 2.22 | 28,28,28,28 | 0 |
| 56 | MG | EA | 3129 | 1/1 | 0.98 | 0.22 | 2.14 | 0,0,0,0 | 0 |
| 56 | MG | EA | 3118 | 1/1 | 0.99 | 0.19 | 2.12 | 1,1,1,1 | 0 |
| 56 | MG | DA | 1640 | 1/1 | 0.99 | 0.18 | 2.02 | 21,21,21,21 | 0 |
| 56 | MG | CA | 3123 | 1/1 | 0.98 | 0.17 | 1.99 | 8,8,8,8 | 0 |
| 56 | MG | EA | 3107 | 1/1 | 1.00 | 0.20 | 1.94 | 0,0,0,0 | 0 |
| 56 | MG | BA | 1616 | 1/1 | 0.98 | 0.22 | 1.93 | 35,35,35,35 | 0 |
| 56 | MG | FA | 1616 | 1/1 | 0.99 | 0.19 | 1.74 | 16,16,16,16 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | EA | 3024 | 1/1 | 0.97 | 0.19 | 1.74 | 0,0,0,0 | 0 |
| 56 | MG | AC | 302 | 1/1 | 0.97 | 0.23 | 1.69 | 19,19,19,19 | 0 |
| 56 | MG | AA | 3036 | 1/1 | 0.99 | 0.24 | 1.69 | 25,25,25,25 | 0 |
| 56 | MG | EA | 3102 | 1/1 | 0.97 | 0.21 | 1.68 | 0,0,0,0 | 0 |
| 56 | MG | CA | 3024 | 1/1 | 0.98 | 0.19 | 1.62 | 2,2,2,2 | 0 |
| 56 | MG | EA | 3002 | 1/1 | 1.00 | 0.17 | 1.58 | 4,4,4,4 | 0 |
| 56 | MG | EA | 3040 | 1/1 | 1.00 | 0.18 | 1.56 | 1,1,1,1 | 0 |
| 56 | MG | HA | 1606 | 1/1 | 0.99 | 0.16 | 1.53 | 17,17,17,17 | 0 |
| 56 | MG | CA | 3115 | 1/1 | 0.99 | 0.16 | 1.49 | 12,12,12,12 | 0 |
| 56 | MG | GA | 3066 | 1/1 | 0.98 | 0.17 | 1.47 | 4,4,4,4 | 0 |
| 56 | MG | HA | 1639 | 1/1 | 0.98 | 0.17 | 1.45 | 20,20,20,20 | 0 |
| 56 | MG | GA | 3013 | 1/1 | 0.99 | 0.21 | 1.41 | 1,1,1,1 | 0 |
| 56 | MG | FA | 1640 | 1/1 | 0.98 | 0.18 | 1.41 | 23,23,23,23 | 0 |
| 56 | MG | CA | 3066 | 1/1 | 0.99 | 0.17 | 1.40 | 2,2,2,2 | 0 |
| 56 | MG | AA | 3116 | 1/1 | 0.98 | 0.18 | 1.36 | 3,3,3,3 | 0 |
| 56 | MG | EA | 3103 | 1/1 | 0.98 | 0.21 | 1.33 | 10,10,10,10 | 0 |
| 56 | MG | AA | 3124 | 1/1 | 0.98 | 0.18 | 1.33 | 9,9,9,9 | 0 |
| 56 | MG | EA | 3053 | 1/1 | 0.98 | 0.18 | 1.33 | 1,1,1,1 | 0 |
| 56 | MG | AA | 3110 | 1/1 | 0.99 | 0.21 | 1.25 | 4,4,4,4 | 0 |
| 56 | MG | GA | 3027 | 1/1 | 0.99 | 0.17 | 1.24 | 6,6,6,6 | 0 |
| 56 | MG | AA | 3125 | 1/1 | 0.98 | 0.17 | 1.17 | 23,23,23,23 | 0 |
| 56 | MG | EA | 3014 | 1/1 | 0.98 | 0.19 | 1.13 | 0,0,0,0 | 0 |
| 56 | MG | GA | 3038 | 1/1 | 0.99 | 0.16 | 0.91 | 11,11,11,11 | 0 |
| 56 | MG | GA | 3009 | 1/1 | 0.98 | 0.17 | 0.85 | 20,20,20,20 | 0 |
| 56 | MG | BV | 802 | 1/1 | 1.00 | 0.17 | 0.81 | 27,27,27,27 | 0 |
| 56 | MG | CB | 1201 | 1/1 | 0.96 | 0.12 | 0.78 | 41,41,41,41 | 0 |
| 56 | MG | AA | 3106 | 1/1 | 0.99 | 0.18 | 0.76 | 9,9,9,9 | 0 |
| 56 | MG | EA | 3119 | 1/1 | 0.99 | 0.22 | 0.73 | 0,0,0,0 | 0 |
| 56 | MG | AA | 3105 | 1/1 | 0.98 | 0.19 | 0.72 | 12,12,12,12 | 0 |
| 56 | MG | GA | 3012 | 1/1 | 0.98 | 0.19 | 0.68 | 2,2,2,2 | 0 |
| 56 | MG | AA | 3103 | 1/1 | 0.99 | 0.17 | 0.68 | 10,10,10,10 | 0 |
| 56 | MG | EA | 3111 | 1/1 | 0.99 | 0.20 | 0.68 | 2,2,2,2 | 0 |
| 56 | MG | AA | 3101 | 1/1 | 0.99 | 0.17 | 0.66 | 7,7,7,7 | 0 |
| 56 | MG | GA | 3026 | 1/1 | 0.98 | 0.16 | 0.63 | 6,6,6,6 | 0 |
| 56 | MG | AA | 3024 | 1/1 | 0.97 | 0.18 | 0.58 | 20,20,20,20 | 0 |
| 56 | MG | EA | 3113 | 1/1 | 0.97 | 0.18 | 0.57 | 0,0,0,0 | 0 |
| 56 | MG | CA | 3100 | 1/1 | 0.99 | 0.17 | 0.56 | 1,1,1,1 | 0 |
| 56 | MG | GA | 3008 | 1/1 | 0.99 | 0.20 | 0.55 | 12,12,12,12 | 0 |
| 56 | MG | BA | 1609 | 1/1 | 0.84 | 0.11 | 0.54 | 38,38,38,38 | 0 |
| 56 | MG | CA | 3111 | 1/1 | 0.94 | 0.16 | 0.52 | 13,13,13,13 | 0 |
| 56 | MG | BA | 1626 | 1/1 | 0.98 | 0.16 | 0.49 | 36,36,36,36 | 0 |
| 56 | MG | GA | 3018 | 1/1 | 0.96 | 0.26 | 0.47 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | CA | 3103 | 1/1 | 0.98 | 0.17 | 0.44 | 0,0,0,0 | 0 |
| 56 | MG | FA | 1641 | 1/1 | 0.97 | 0.17 | 0.44 | 18,18,18,18 | 0 |
| 56 | MG | GA | 3023 | 1/1 | 0.95 | 0.17 | 0.43 | 7,7,7,7 | 0 |
| 56 | MG | FA | 1620 | 1/1 | 0.99 | 0.15 | 0.35 | 6,6,6,6 | 0 |
| 56 | MG | CA | 3129 | 1/1 | 0.99 | 0.17 | 0.35 | 9,9,9,9 | 0 |
| 56 | MG | DA | 1609 | 1/1 | 0.99 | 0.16 | 0.33 | 16,16,16,16 | 0 |
| 56 | MG | GA | 3065 | 1/1 | 0.98 | 0.15 | 0.28 | 3,3,3,3 | 0 |
| 56 | MG | GL | 201 | 1/1 | 0.98 | 0.19 | 0.27 | 7,7,7,7 | 0 |
| 56 | MG | AA | 3012 | 1/1 | 1.00 | 0.20 | 0.26 | 7,7,7,7 | 0 |
| 56 | MG | HA | 1627 | 1/1 | 0.99 | 0.14 | 0.23 | 24,24,24,24 | 0 |
| 56 | MG | BA | 1638 | 1/1 | 0.99 | 0.14 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | CA | 3032 | 1/1 | 0.99 | 0.18 | 0.15 | 3,3,3,3 | 0 |
| 56 | MG | ED | 302 | 1/1 | 0.99 | 0.17 | 0.15 | 2,2,2,2 | 0 |
| 56 | MG | AT | 201 | 1/1 | 0.93 | 0.17 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | AA | 3046 | 1/1 | 0.99 | 0.15 | 0.13 | 7,7,7,7 | 0 |
| 56 | MG | CA | 3130 | 1/1 | 1.00 | 0.17 | 0.06 | 1,1,1,1 | 0 |
| 56 | MG | AA | 3025 | 1/1 | 0.98 | 0.17 | 0.02 | 8,8,8,8 | 0 |
| 56 | MG | CA | 3134 | 1/1 | 0.98 | 0.18 | 0.01 | 23,23,23,23 | 0 |
| 56 | MG | EA | 3017 | 1/1 | 0.99 | 0.17 | 0.00 | 3,3,3,3 | 0 |
| 56 | MG | AA | 3023 | 1/1 | 1.00 | 0.17 | -0.06 | 3,3,3,3 | 0 |
| 56 | MG | EA | 3023 | 1/1 | 0.99 | 0.17 | -0.09 | 2,2,2,2 | 0 |
| 56 | MG | EA | 3035 | 1/1 | 0.99 | 0.17 | -0.16 | 0,0,0,0 | 0 |
| 56 | MG | CD | 301 | 1/1 | 0.99 | 0.17 | -0.19 | 3,3,3,3 | 0 |
| 56 | MG | AA | 3031 | 1/1 | 1.00 | 0.17 | -0.19 | 8,8,8,8 | 0 |
| 56 | MG | HA | 1619 | 1/1 | 0.94 | 0.16 | -0.20 | 34,34,34,34 | 0 |
| 56 | MG | EA | 3104 | 1/1 | 1.00 | 0.16 | -0.22 | 1,1,1,1 | 0 |
| 56 | MG | CA | 3023 | 1/1 | 0.99 | 0.17 | -0.23 | 5,5,5,5 | 0 |
| 56 | MG | AA | 3130 | 1/1 | 0.99 | 0.15 | -0.24 | 27,27,27,27 | 0 |
| 56 | MG | AA | 3072 | 1/1 | 0.99 | 0.16 | -0.28 | 7,7,7,7 | 0 |
| 56 | MG | DA | 1624 | 1/1 | 0.97 | 0.17 | -0.29 | 48,48,48,48 | 0 |
| 58 | GCP | DV | 801 | 32/32 | 0.96 | 0.14 | -0.32 | 20,38,49,52 | 0 |
| 56 | MG | CA | 3106 | 1/1 | 0.96 | 0.16 | -0.34 | 13,13,13,13 | 0 |
| 56 | MG | HA | 1616 | 1/1 | 0.99 | 0.16 | -0.37 | 33,33,33,33 | 0 |
| 56 | MG | EA | 3036 | 1/1 | 0.99 | 0.14 | -0.38 | 1,1,1,1 | 0 |
| 56 | MG | AA | 3119 | 1/1 | 1.00 | 0.15 | -0.42 | 13,13,13,13 | 0 |
| 56 | MG | GA | 3016 | 1/1 | 0.99 | 0.15 | -0.43 | 9,9,9,9 | 0 |
| 56 | MG | CA | 3132 | 1/1 | 0.98 | 0.17 | -0.43 | 2,2,2,2 | 0 |
| 58 | GCP | FV | 801 | 32/32 | 0.87 | 0.20 | -0.45 | 43,58,69,87 | 0 |
| 56 | MG | GA | 3022 | 1/1 | 0.98 | 0.16 | -0.45 | 16,16,16,16 | 0 |
| 56 | MG | BA | 1636 | 1/1 | 0.97 | 0.12 | -0.48 | 40,40,40,40 | 0 |
| 56 | MG | AA | 3049 | 1/1 | 0.99 | 0.15 | -0.52 | 3,3,3,3 | 0 |
| 58 | GCP | BV | 801 | 32/32 | 0.97 | 0.13 | -0.56 | 17,36,43,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | EA | 3022 | 1/1 | 0.98 | 0.15 | -0.57 | 0,0,0,0 | 0 |
| 56 | MG | EA | 3062 | 1/1 | 0.99 | 0.17 | -0.60 | 0,0,0,0 | 0 |
| 56 | MG | BA | 1634 | 1/1 | 0.97 | 0.14 | -0.63 | 14,14,14,14 | 0 |
| 56 | MG | EA | 3012 | 1/1 | 0.99 | 0.17 | -0.70 | 1,1,1,1 | 0 |
| 56 | MG | DA | 1642 | 1/1 | 0.96 | 0.16 | -0.71 | 29,29,29,29 | 0 |
| 56 | MG | CA | 3128 | 1/1 | 1.00 | 0.16 | -0.72 | 6,6,6,6 | 0 |
| 56 | MG | DA | 1634 | 1/1 | 0.99 | 0.13 | -0.74 | 33,33,33,33 | 0 |
| 56 | MG | CA | 3109 | 1/1 | 0.99 | 0.12 | -0.75 | 26,26,26,26 | 0 |
| 56 | MG | CA | 3015 | 1/1 | 0.96 | 0.16 | -0.78 | 14,14,14,14 | 0 |
| 56 | MG | BA | 1640 | 1/1 | 0.93 | 0.13 | -0.80 | 33,33,33,33 | 0 |
| 56 | MG | GA | 3006 | 1/1 | 0.97 | 0.12 | -0.83 | 25,25,25,25 | 0 |
| 56 | MG | EA | 3128 | 1/1 | 0.99 | 0.15 | -0.89 | 4,4,4,4 | 0 |
| 56 | MG | GA | 3005 | 1/1 | 0.99 | 0.13 | -0.89 | 15,15,15,15 | 0 |
| 56 | MG | GA | 3053 | 1/1 | 0.99 | 0.15 | -0.93 | 4,4,4,4 | 0 |
| 56 | MG | GA | 3105 | 1/1 | 0.99 | 0.15 | -0.96 | 3,3,3,3 | 0 |
| 56 | MG | EC | 301 | 1/1 | 0.99 | 0.14 | -0.98 | 1,1,1,1 | 0 |
| 56 | MG | GA | 3024 | 1/1 | 0.99 | 0.15 | -0.99 | 8,8,8,8 | 0 |
| 57 | ZN | C4 | 102 | 1/1 | 0.99 | 0.09 | -1.00 | 76,76,76,76 | 0 |
| 57 | ZN | A4 | 101 | 1/1 | 0.99 | 0.09 | -1.01 | 63,63,63,63 | 0 |
| 56 | MG | AA | 3011 | 1/1 | 0.93 | 0.17 | -1.08 | 18,18,18,18 | 0 |
| 56 | MG | FV | 802 | 1/1 | 0.97 | 0.12 | -1.10 | 48,48,48,48 | 0 |
| 56 | MG | EA | 3106 | 1/1 | 0.99 | 0.15 | -1.17 | 0,0,0,0 | 0 |
| 56 | MG | HA | 1638 | 1/1 | 0.98 | 0.09 | -1.22 | 26,26,26,26 | 0 |
| 56 | MG | AA | 3111 | 1/1 | 0.97 | 0.16 | -1.27 | 21,21,21,21 | 0 |
| 56 | MG | HV | 802 | 1/1 | 0.97 | 0.13 | -1.28 | 38,38,38,38 | 0 |
| 56 | MG | DV | 802 | 1/1 | 0.99 | 0.11 | -1.31 | 34,34,34,34 | 0 |
| 58 | GCP | HV | 801 | 32/32 | 0.97 | 0.11 | -1.37 | 24,48,54,56 | 0 |
| 56 | MG | FA | 1633 | 1/1 | 0.98 | 0.11 | -1.37 | 28,28,28,28 | 0 |
| 56 | MG | AA | 3128 | 1/1 | 1.00 | 0.14 | -1.38 | 2,2,2,2 | 0 |
| 56 | MG | HA | 1637 | 1/1 | 0.93 | 0.10 | -1.48 | 47,47,47,47 | 0 |
| 56 | MG | CA | 3113 | 1/1 | 0.99 | 0.11 | -1.49 | 14,14,14,14 | 0 |
| 56 | MG | BA | 1604 | 1/1 | 0.97 | 0.12 | -1.50 | 20,20,20,20 | 0 |
| 56 | MG | AA | 3088 | 1/1 | 0.97 | 0.13 | -1.52 | 14,14,14,14 | 0 |
| 57 | ZN | G4 | 101 | 1/1 | 0.99 | 0.09 | -1.52 | 69,69,69,69 | 0 |
| 56 | MG | AA | 3112 | 1/1 | 0.98 | 0.11 | -1.59 | 7,7,7,7 | 0 |
| 56 | MG | HA | 1628 | 1/1 | 0.99 | 0.14 | -1.66 | 30,30,30,30 | 0 |
| 56 | MG | A3 | 101 | 1/1 | 0.98 | 0.10 | -1.69 | 13,13,13,13 | 0 |
| 56 | MG | GA | 3132 | 1/1 | 0.99 | 0.14 | -1.75 | 7,7,7,7 | 0 |
| 56 | MG | GA | 3107 | 1/1 | 0.99 | 0.12 | -1.80 | 27,27,27,27 | 0 |
| 56 | MG | AA | 3090 | 1/1 | 0.94 | 0.10 | -1.81 | 23,23,23,23 | 0 |
| 56 | MG | AA | 3126 | 1/1 | 0.99 | 0.10 | -1.82 | 3,3,3,3 | 0 |
| 56 | MG | AA | 3027 | 1/1 | 0.99 | 0.15 | -1.90 | 8,8,8,8 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 56 | MG | EA | 3105 | 1/1 | 0.99 | 0.14 | -1.91 | 4,4,4,4 | 0 |
| 56 | MG | BA | 1627 | 1/1 | 0.98 | 0.08 | -1.94 | 25,25,25,25 | 0 |
| 57 | ZN | E4 | 101 | 1/1 | 0.99 | 0.09 | -2.02 | 54,54,54,54 | 0 |
| 56 | MG | FA | 1637 | 1/1 | 0.99 | 0.10 | -2.11 | 34,34,34,34 | 0 |
| 56 | MG | AA | 3076 | 1/1 | 0.98 | 0.09 | -2.14 | 21,21,21,21 | 0 |
| 56 | MG | GA | 3062 | 1/1 | 0.99 | 0.13 | -2.21 | 18,18,18,18 | 0 |
| 56 | MG | GA | 3130 | 1/1 | 0.99 | 0.09 | -2.26 | 9,9,9,9 | 0 |
| 56 | MG | FA | 1613 | 1/1 | 0.99 | 0.11 | -2.27 | 9,9,9,9 | 0 |
| 56 | MG | GA | 3112 | 1/1 | 0.99 | 0.10 | -2.29 | 15,15,15,15 | 0 |
| 56 | MG | GA | 3099 | 1/1 | 0.99 | 0.13 | -2.30 | 12,12,12,12 | 0 |
| 56 | MG | DA | 1641 | 1/1 | 0.94 | 0.12 | -2.37 | 30,30,30,30 | 0 |
| 56 | MG | CA | 3108 | 1/1 | 0.99 | 0.12 | -2.39 | 3,3,3,3 | 0 |
| 56 | MG | GA | 3090 | 1/1 | 0.99 | 0.08 | -2.44 | 26,26,26,26 | 0 |
| 56 | MG | CA | 3131 | 1/1 | 0.99 | 0.10 | -2.57 | 0,0,0,0 | 0 |
| 56 | MG | FA | 1617 | 1/1 | 0.97 | 0.12 | -2.70 | 9,9,9,9 | 0 |
| 56 | MG | CA | 3062 | 1/1 | 0.99 | 0.13 | -2.71 | 5,5,5,5 | 0 |
| 56 | MG | AA | 3003 | 1/1 | 0.99 | 0.10 | -2.81 | 26,26,26,26 | 0 |
| 56 | MG | EA | 3108 | 1/1 | 0.97 | 0.12 | -2.82 | 31,31,31,31 | 0 |
| 56 | MG | CA | 3071 | 1/1 | 0.99 | 0.14 | -2.90 | 2,2,2,2 | 0 |
| 56 | MG | AA | 3061 | 1/1 | 0.98 | 0.14 | -2.93 | 6,6,6,6 | 0 |
| 56 | MG | AA | 3104 | 1/1 | 0.99 | 0.13 | -2.94 | 12,12,12,12 | 0 |
| 56 | MG | HA | 1631 | 1/1 | 0.99 | 0.10 | -3.08 | 28,28,28,28 | 0 |
| 56 | MG | HA | 1622 | 1/1 | 0.99 | 0.10 | -3.09 | 36,36,36,36 | 0 |
| 56 | MG | EA | 3065 | 1/1 | 0.99 | 0.11 | -3.17 | 0,0,0,0 | 0 |
| 56 | MG | AA | 3040 | 1/1 | 0.99 | 0.12 | -3.32 | 24,24,24,24 | 0 |
| 56 | MG | AA | 3002 | 1/1 | 0.97 | 0.10 | -3.36 | 20,20,20,20 | 0 |
| 56 | MG | DA | 1610 | 1/1 | 0.95 | 0.04 | -3.39 | 48,48,48,48 | 0 |
| 56 | MG | AA | 3038 | 1/1 | 0.99 | 0.11 | -3.49 | 6,6,6,6 | 0 |
| 56 | MG | GA | 3021 | 1/1 | 1.00 | 0.12 | -3.61 | 9,9,9,9 | 0 |
| 56 | MG | BA | 1628 | 1/1 | 0.99 | 0.12 | -3.61 | 26,26,26,26 | 0 |
| 56 | MG | AA | 3095 | 1/1 | 0.99 | 0.10 | -3.64 | 9,9,9,9 | 0 |
| 56 | MG | DA | 1613 | 1/1 | 1.00 | 0.10 | -3.65 | 12,12,12,12 | 0 |
| 56 | MG | GA | 3128 | 1/1 | 0.99 | 0.09 | -3.72 | 20,20,20,20 | 0 |
| 56 | MG | CA | 3095 | 1/1 | 0.99 | 0.11 | -3.75 | 21,21,21,21 | 0 |
| 56 | MG | CA | 3065 | 1/1 | 0.99 | 0.11 | -3.76 | 1,1,1,1 | 0 |
| 56 | MG | CA | 3012 | 1/1 | 0.99 | 0.12 | -3.79 | 3,3,3,3 | 0 |
| 56 | MG | DA | 1607 | 1/1 | 0.98 | 0.13 | -3.81 | 16,16,16,16 | 0 |
| 56 | MG | FA | 1604 | 1/1 | 0.96 | 0.07 | -3.85 | 33,33,33,33 | 0 |
| 56 | MG | CA | 3104 | 1/1 | 0.99 | 0.14 | -3.88 | 4,4,4,4 | 0 |
| 56 | MG | EB | 1202 | 1/1 | 0.97 | 0.08 | -3.99 | 19,19,19,19 | 0 |
| 56 | MG | BA | 1603 | 1/1 | 0.98 | 0.06 | -4.08 | 21,21,21,21 | 0 |
| 56 | MG | DA | 1611 | 1/1 | 0.97 | 0.10 | -4.09 | 15,15,15,15 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 56 | MG | FA | 1629 | 1/1 | 0.98 | 0.10 | -4.19 | 16,16,16,16 | 0 |
| 56 | MG | GA | 3032 | 1/1 | 0.99 | 0.13 | -4.30 | 8,8,8,8 | 0 |
| 56 | MG | CA | 3022 | 1/1 | 0.99 | 0.12 | -4.45 | 0,0,0,0 | 0 |
| 56 | MG | FA | 1607 | 1/1 | 0.98 | 0.10 | -4.49 | 18,18,18,18 | 0 |
| 56 | MG | CA | 3036 | 1/1 | 0.99 | 0.08 | -4.55 | 19,19,19,19 | 0 |
| 56 | MG | DA | 1604 | 1/1 | 0.97 | 0.08 | -4.57 | 23,23,23,23 | 0 |
| 56 | MG | AA | 3053 | 1/1 | 0.99 | 0.10 | -4.68 | 6,6,6,6 | 0 |
| 56 | MG | DA | 1630 | 1/1 | 0.98 | 0.10 | -4.94 | 34,34,34,34 | 0 |
| 56 | MG | AA | 3082 | 1/1 | 0.98 | 0.03 | -5.27 | 29,29,29,29 | 0 |
| 56 | MG | BA | 1608 | 1/1 | 0.99 | 0.10 | -5.40 | 22,22,22,22 | 0 |
| 56 | MG | DA | 1638 | 1/1 | 0.98 | 0.04 | -5.41 | 40,40,40,40 | 0 |
| 56 | MG | BA | 1631 | 1/1 | 0.96 | 0.07 | -5.81 | 28,28,28,28 | 0 |
| 56 | MG | CA | 3053 | 1/1 | 1.00 | 0.12 | -6.81 | 5,5,5,5 | 0 |
| 56 | MG | EA | 3110 | 1/1 | 0.99 | 0.11 | -8.65 | 24,24,24,24 | 0 |
| 56 | MG | CA | 3025 | 1/1 | 0.99 | 0.10 | -9.36 | 7,7,7,7 | 0 |
| 56 | MG | CA | 3026 | 1/1 | 0.99 | 0.09 | -14.35 | 5,5,5,5 | 0 |
| 56 | MG | GA | 3085 | 1/1 | 1.00 | 0.15 | - | 16,16,16,16 | 0 |
| 56 | MG | DA | 1622 | 1/1 | 0.97 | 0.08 | - | 37,37,37,37 | 0 |
| 56 | MG | GA | 3116 | 1/1 | 0.99 | 0.14 | - | 3,3,3,3 | 0 |
| 56 | MG | FA | 1612 | 1/1 | 0.99 | 0.31 | - | 17,17,17,17 | 0 |
| 56 | MG | CA | 3114 | 1/1 | 0.92 | 0.56 | - | 25,25,25,25 | 0 |
| 56 | MG | AA | 3010 | 1/1 | 0.99 | 0.23 | - | 13,13,13,13 | 0 |
| 56 | MG | DA | 1620 | 1/1 | 0.98 | 0.08 | - | 22,22,22,22 | 0 |
| 56 | MG | EA | 3063 | 1/1 | 0.99 | 0.13 | - | 1,1,1,1 | 0 |
| 56 | MG | CA | 3002 | 1/1 | 0.99 | 0.14 | - | 17,17,17,17 | 0 |
| 56 | MG | AA | 3129 | 1/1 | 0.99 | 0.11 | - | 20,20,20,20 | 0 |
| 56 | MG | EA | 3100 | 1/1 | 0.99 | 0.14 | - | 0,0,0,0 | 0 |
| 56 | MG | EA | 3007 | 1/1 | 0.99 | 0.07 | - | 15,15,15,15 | 0 |
| 56 | MG | CA | 3049 | 1/1 | 0.99 | 0.18 | - | 9,9,9,9 | 0 |
| 56 | MG | CE | 301 | 1/1 | 0.94 | 0.25 | - | 16,16,16,16 | 0 |
| 56 | MG | EA | 3037 | 1/1 | 1.00 | 0.13 | - | 2,2,2,2 | 0 |
| 56 | MG | AA | 3117 | 1/1 | 0.99 | 0.25 | - | 7,7,7,7 | 0 |
| 56 | MG | FA | 1610 | 1/1 | 0.88 | 0.28 | - | 35,35,35,35 | 0 |
| 56 | MG | GA | 3097 | 1/1 | 0.99 | 0.17 | - | 26,26,26,26 | 0 |
| 56 | MG | CA | 3013 | 1/1 | 0.98 | 0.08 | - | 7,7,7,7 | 0 |
| 56 | MG | AA | 3075 | 1/1 | 0.98 | 0.09 | - | 15,15,15,15 | 0 |
| 56 | MG | BA | 1639 | 1/1 | 0.99 | 0.13 | - | 19,19,19,19 | 0 |
| 56 | MG | CA | 3101 | 1/1 | 0.99 | 0.15 | - | 10,10,10,10 | 0 |
| 56 | MG | EA | 3067 | 1/1 | 0.99 | 0.26 | - | 4,4,4,4 | 0 |
| 56 | MG | FA | 1614 | 1/1 | 1.00 | 0.13 | - | 5,5,5,5 | 0 |
| 56 | MG | GA | 3109 | 1/1 | 0.99 | 0.09 | - | 9,9,9,9 | 0 |
| 56 | MG | CA | 3133 | 1/1 | 0.99 | 0.12 | - | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3081 | 1/1 | 0.99 | 0.15 | - | 10,10,10,10 | 0 |
| 56 | MG | CA | 3019 | 1/1 | 0.98 | 0.10 | - | 22,22,22,22 | 0 |
| 56 | MG | GA | 3081 | 1/1 | 0.99 | 0.19 | - | 16,16,16,16 | 0 |
| 56 | MG | CA | 3059 | 1/1 | 0.99 | 0.17 | - | 3,3,3,3 | 0 |
| 56 | MG | AA | 3121 | 1/1 | 0.99 | 0.10 | - | 20,20,20,20 | 0 |
| 56 | MG | DA | 1614 | 1/1 | 0.95 | 0.12 | - | 44,44,44,44 | 0 |
| 56 | MG | AA | 3081 | 1/1 | 0.99 | 0.14 | - | 16,16,16,16 | 0 |
| 56 | MG | EA | 3044 | 1/1 | 0.96 | 0.13 | - | 11,11,11,11 | 0 |
| 56 | MG | CA | 3009 | 1/1 | 0.98 | 0.15 | - | 18,18,18,18 | 0 |
| 56 | MG | CA | 3124 | 1/1 | 0.99 | 0.15 | - | 0,0,0,0 | 0 |
| 56 | MG | CA | 3052 | 1/1 | 0.99 | 0.10 | - | 10,10,10,10 | 0 |
| 56 | MG | CA | 3014 | 1/1 | 0.99 | 0.12 | - | 9,9,9,9 | 0 |
| 56 | MG | CA | 3120 | 1/1 | 0.94 | 0.15 | - | 3,3,3,3 | 0 |
| 56 | MG | AA | 3113 | 1/1 | 1.00 | 0.11 | - | 8,8,8,8 | 0 |
| 56 | MG | BA | 1605 | 1/1 | 1.00 | 0.11 | - | 21,21,21,21 | 0 |
| 56 | MG | BA | 1637 | 1/1 | 0.92 | 0.29 | - | 29,29,29,29 | 0 |
| 56 | MG | GA | 3067 | 1/1 | 0.99 | 0.20 | - | 16,16,16,16 | 0 |
| 56 | MG | FA | 1631 | 1/1 | 0.99 | 0.06 | - | 21,21,21,21 | 0 |
| 56 | MG | EA | 3090 | 1/1 | 0.96 | 0.07 | - | 29,29,29,29 | 0 |
| 56 | MG | AA | 3051 | 1/1 | 0.99 | 0.08 | - | 4,4,4,4 | 0 |
| 56 | MG | GA | 3046 | 1/1 | 0.97 | 0.08 | - | 35,35,35,35 | 0 |
| 56 | MG | EA | 3058 | 1/1 | 0.98 | 0.13 | - | 6,6,6,6 | 0 |
| 56 | MG | AA | 3127 | 1/1 | 0.98 | 0.13 | - | 16,16,16,16 | 0 |
| 56 | MG | GA | 3061 | 1/1 | 0.95 | 0.20 | - | 10,10,10,10 | 0 |
| 56 | MG | AA | 3033 | 1/1 | 1.00 | 0.17 | - | 8,8,8,8 | 0 |
| 56 | MG | CA | 3043 | 1/1 | 0.99 | 0.11 | - | 5,5,5,5 | 0 |
| 56 | MG | AA | 3004 | 1/1 | 0.99 | 0.07 | - | 34,34,34,34 | 0 |
| 56 | MG | AA | 3034 | 1/1 | 0.99 | 0.11 | - | 14,14,14,14 | 0 |
| 56 | MG | EA | 3098 | 1/1 | 0.97 | 0.16 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3010 | 1/1 | 0.98 | 0.26 | - | 15,15,15,15 | 0 |
| 56 | MG | GA | 3121 | 1/1 | 0.99 | 0.14 | - | 4,4,4,4 | 0 |
| 56 | MG | BA | 1613 | 1/1 | 0.97 | 0.13 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 1617 | 1/1 | 0.99 | 0.13 | - | 45,45,45,45 | 0 |
| 56 | MG | FA | 1632 | 1/1 | 0.98 | 0.12 | - | 28,28,28,28 | 0 |
| 56 | MG | BA | 1629 | 1/1 | 0.97 | 0.15 | - | 41,41,41,41 | 0 |
| 56 | MG | GA | 3037 | 1/1 | 0.96 | 0.19 | - | 19,19,19,19 | 0 |
| 56 | MG | CA | 3102 | 1/1 | 0.99 | 0.07 | - | 32,32,32,32 | 0 |
| 56 | MG | EA | 3066 | 1/1 | 0.99 | 0.19 | - | 0,0,0,0 | 0 |
| 56 | MG | GA | 3091 | 1/1 | 0.97 | 0.14 | - | 11,11,11,11 | 0 |
| 56 | MG | AA | 3068 | 1/1 | 0.80 | 0.17 | - | 59,59,59,59 | 0 |
| 56 | MG | HA | 1611 | 1/1 | 0.98 | 0.23 | - | 20,20,20,20 | 0 |
| 56 | MG | EA | 3001 | 1/1 | 0.99 | 0.11 | - | 9,9,9,9 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 1631 | 1/1 | 0.97 | 0.17 | - | 25,25,25,25 | 0 |
| 56 | MG | AA | 3018 | 1/1 | 0.99 | 0.18 | - | 12,12,12,12 | 0 |
| 56 | MG | GA | 3075 | 1/1 | 0.96 | 0.15 | - | 7,7,7,7 | 0 |
| 56 | MG | CA | 3069 | 1/1 | 0.95 | 0.14 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 1632 | 1/1 | 0.98 | 0.15 | - | 28,28,28,28 | 0 |
| 56 | MG | CA | 3058 | 1/1 | 1.00 | 0.13 | - | 5,5,5,5 | 0 |
| 56 | MG | HE | 201 | 1/1 | 0.84 | 0.21 | - | 39,39,39,39 | 0 |
| 56 | MG | AA | 3091 | 1/1 | 0.98 | 0.14 | - | 16,16,16,16 | 0 |
| 56 | MG | BA | 1621 | 1/1 | 0.97 | 0.23 | - | 52,52,52,52 | 0 |
| 56 | MG | FA | 1639 | 1/1 | 0.97 | 0.26 | - | 25,25,25,25 | 0 |
| 56 | MG | EA | 3013 | 1/1 | 0.99 | 0.14 | - | 0,0,0,0 | 0 |
| 56 | MG | HA | 1604 | 1/1 | 0.96 | 0.17 | - | 27,27,27,27 | 0 |
| 56 | MG | EA | 3068 | 1/1 | 0.95 | 0.12 | - | 35,35,35,35 | 0 |
| 56 | MG | CA | 3082 | 1/1 | 0.99 | 0.12 | - | 15,15,15,15 | 0 |
| 56 | MG | DA | 1636 | 1/1 | 0.97 | 0.29 | - | 41,41,41,41 | 0 |
| 56 | MG | AA | 3043 | 1/1 | 1.00 | 0.13 | - | 21,21,21,21 | 0 |
| 56 | MG | EA | 3047 | 1/1 | 0.99 | 0.09 | - | 6,6,6,6 | 0 |
| 56 | MG | EA | 3121 | 1/1 | 0.98 | 0.24 | - | 1,1,1,1 | 0 |
| 56 | MG | GA | 3049 | 1/1 | 0.99 | 0.17 | - | 8,8,8,8 | 0 |
| 56 | MG | GA | 3118 | 1/1 | 0.97 | 0.29 | - | 9,9,9,9 | 0 |
| 56 | MG | GA | 3058 | 1/1 | 0.98 | 0.14 | - | 17,17,17,17 | 0 |
| 56 | MG | GA | 3113 | 1/1 | 0.96 | 0.10 | - | 26,26,26,26 | 0 |
| 56 | MG | CA | 3029 | 1/1 | 0.99 | 0.07 | - | 8,8,8,8 | 0 |
| 56 | MG | EA | 3095 | 1/1 | 0.99 | 0.17 | - | 5,5,5,5 | 0 |
| 56 | MG | GS | 201 | 1/1 | 0.94 | 0.48 | - | 33,33,33,33 | 0 |
| 56 | MG | GA | 3088 | 1/1 | 0.98 | 0.17 | - | 8,8,8,8 | 0 |
| 56 | MG | EA | 3130 | 1/1 | 0.89 | 0.21 | - | 29,29,29,29 | 0 |
| 56 | MG | CA | 3085 | 1/1 | 0.97 | 0.27 | - | 28,28,28,28 | 0 |
| 56 | MG | AA | 3115 | 1/1 | 0.80 | 0.14 | - | 32,32,32,32 | 0 |
| 56 | MG | EB | 1203 | 1/1 | 0.99 | 0.14 | - | 3,3,3,3 | 0 |
| 56 | MG | AA | 3062 | 1/1 | 0.99 | 0.18 | - | 2,2,2,2 | 0 |
| 56 | MG | AA | 3054 | 1/1 | 0.98 | 0.12 | - | 11,11,11,11 | 0 |
| 56 | MG | AA | 3066 | 1/1 | 1.00 | 0.17 | - | 6,6,6,6 | 0 |
| 56 | MG | CA | 3126 | 1/1 | 1.00 | 0.14 | - | 7,7,7,7 | 0 |
| 56 | MG | EA | 3027 | 1/1 | 0.99 | 0.20 | - | 0,0,0,0 | 0 |
| 56 | MG | AA | 3057 | 1/1 | 0.98 | 0.09 | - | 18,18,18,18 | 0 |
| 56 | MG | AA | 3039 | 1/1 | 0.99 | 0.18 | - | 5,5,5,5 | 0 |
| 56 | MG | FA | 1638 | 1/1 | 0.98 | 0.10 | - | 33,33,33,33 | 0 |
| 56 | MG | GA | 3056 | 1/1 | 1.00 | 0.12 | - | 4,4,4,4 | 0 |
| 56 | MG | AA | 3087 | 1/1 | 0.93 | 0.14 | - | 31,31,31,31 | 0 |
| 56 | MG | GA | 3011 | 1/1 | 0.98 | 0.10 | - | 46,46,46,46 | 0 |
| 56 | MG | HA | 1609 | 1/1 | 0.95 | 0.13 | - | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3031 | 1/1 | 0.99 | 0.14 | - | 11,11,11,11 | 0 |
| 56 | MG | GA | 3050 | 1/1 | 0.99 | 0.15 | - | 9,9,9,9 | 0 |
| 56 | MG | EA | 3127 | 1/1 | 0.94 | 0.15 | - | 0,0,0,0 | 0 |
| 56 | MG | GB | 1203 | 1/1 | 0.97 | 0.13 | - | 16,16,16,16 | 0 |
| 56 | MG | DA | 1601 | 1/1 | 0.97 | 0.11 | - | 37,37,37,37 | 0 |
| 56 | MG | FA | 1625 | 1/1 | 0.99 | 0.09 | - | 18,18,18,18 | 0 |
| 56 | MG | EA | 3059 | 1/1 | 0.96 | 0.14 | - | 1,1,1,1 | 0 |
| 56 | MG | AA | 3120 | 1/1 | 0.99 | 0.18 | - | 6,6,6,6 | 0 |
| 56 | MG | EA | 3038 | 1/1 | 0.99 | 0.11 | - | 2,2,2,2 | 0 |
| 56 | MG | GA | 3079 | 1/1 | 0.99 | 0.12 | - | 18,18,18,18 | 0 |
| 56 | MG | AA | 3005 | 1/1 | 0.94 | 0.16 | - | 23,23,23,23 | 0 |
| 56 | MG | CA | 3067 | 1/1 | 0.99 | 0.11 | - | 4,4,4,4 | 0 |
| 56 | MG | EA | 3028 | 1/1 | 0.99 | 0.18 | - | 1,1,1,1 | 0 |
| 56 | MG | DA | 1602 | 1/1 | 0.91 | 0.34 | - | 31,31,31,31 | 0 |
| 56 | MG | AA | 3044 | 1/1 | 0.97 | 0.14 | - | 17,17,17,17 | 0 |
| 56 | MG | EA | 3080 | 1/1 | 0.97 | 0.20 | - | 3,3,3,3 | 0 |
| 56 | MG | CA | 3010 | 1/1 | 0.99 | 0.25 | - | 10,10,10,10 | 0 |
| 56 | MG | EA | 3008 | 1/1 | 0.99 | 0.18 | - | 1,1,1,1 | 0 |
| 56 | MG | EA | 3125 | 1/1 | 0.97 | 0.10 | - | 3,3,3,3 | 0 |
| 56 | MG | EA | 3054 | 1/1 | 0.99 | 0.13 | - | 5,5,5,5 | 0 |
| 56 | MG | AA | 3006 | 1/1 | 0.96 | 0.09 | - | 38,38,38,38 | 0 |
| 56 | MG | GA | 3015 | 1/1 | 0.99 | 0.11 | - | 18,18,18,18 | 0 |
| 56 | MG | EA | 3045 | 1/1 | 0.99 | 0.13 | - | 1,1,1,1 | 0 |
| 56 | MG | GA | 3084 | 1/1 | 0.98 | 0.30 | - | 25,25,25,25 | 0 |
| 56 | MG | EA | 3026 | 1/1 | 0.99 | 0.10 | - | 28,28,28,28 | 0 |
| 56 | MG | CA | 3092 | 1/1 | 0.88 | 0.17 | - | 30,30,30,30 | 0 |
| 56 | MG | HA | 1613 | 1/1 | 0.83 | 0.47 | - | 41,41,41,41 | 0 |
| 56 | MG | CA | 3050 | 1/1 | 0.99 | 0.11 | - | 12,12,12,12 | 0 |
| 56 | MG | EA | 3005 | 1/1 | 0.97 | 0.12 | - | 27,27,27,27 | 0 |
| 56 | MG | CA | 3055 | 1/1 | 0.98 | 0.13 | - | 20,20,20,20 | 0 |
| 56 | MG | CA | 3090 | 1/1 | 0.99 | 0.13 | - | 20,20,20,20 | 0 |
| 56 | MG | AA | 3035 | 1/1 | 0.99 | 0.20 | - | 3,3,3,3 | 0 |
| 56 | MG | CA | 3063 | 1/1 | 0.99 | 0.16 | - | 2,2,2,2 | 0 |
| 56 | MG | AA | 3074 | 1/1 | 0.98 | 0.17 | - | 9,9,9,9 | 0 |
| 56 | MG | DA | 1625 | 1/1 | 0.97 | 0.09 | - | 23,23,23,23 | 0 |
| 56 | MG | GA | 3126 | 1/1 | 0.98 | 0.09 | - | 18,18,18,18 | 0 |
| 56 | MG | CA | 3061 | 1/1 | 0.96 | 0.12 | - | 3,3,3,3 | 0 |
| 56 | MG | EA | 3091 | 1/1 | 1.00 | 0.14 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3061 | 1/1 | 0.99 | 0.22 | - | 0,0,0,0 | 0 |
| 56 | MG | FE | 201 | 1/1 | 0.88 | 0.50 | - | 52,52,52,52 | 0 |
| 56 | MG | HA | 1623 | 1/1 | 0.99 | 0.11 | - | 18,18,18,18 | 0 |
| 56 | MG | AA | 3073 | 1/1 | 0.99 | 0.16 | - | 8,8,8,8 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | GA | 3092 | 1/1 | 0.99 | 0.07 | - | 17,17,17,17 | 0 |
| 56 | MG | GA | 3051 | 1/1 | 0.99 | 0.19 | - | 4,4,4,4 | 0 |
| 56 | MG | GA | 3127 | 1/1 | 0.99 | 0.12 | - | 1,1,1,1 | 0 |
| 56 | MG | CA | 3046 | 1/1 | 0.99 | 0.16 | - | 17,17,17,17 | 0 |
| 56 | MG | BA | 1633 | 1/1 | 0.99 | 0.10 | - | 35,35,35,35 | 0 |
| 56 | MG | EA | 3101 | 1/1 | 0.99 | 0.13 | - | 26,26,26,26 | 0 |
| 56 | MG | EA | 3124 | 1/1 | 0.99 | 0.11 | - | 5,5,5,5 | 0 |
| 56 | MG | EA | 3039 | 1/1 | 0.99 | 0.19 | - | 0,0,0,0 | 0 |
| 56 | MG | GA | 3125 | 1/1 | 0.99 | 0.11 | - | 5,5,5,5 | 0 |
| 56 | MG | GA | 3036 | 1/1 | 0.98 | 0.14 | - | 35,35,35,35 | 0 |
| 56 | MG | CA | 3099 | 1/1 | 1.00 | 0.14 | - | 17,17,17,17 | 0 |
| 56 | MG | AA | 3045 | 1/1 | 0.99 | 0.13 | - | 18,18,18,18 | 0 |
| 56 | MG | BA | 1624 | 1/1 | 0.95 | 0.12 | - | 28,28,28,28 | 0 |
| 56 | MG | BA | 1607 | 1/1 | 0.99 | 0.26 | - | 8,8,8,8 | 0 |
| 56 | MG | DA | 1633 | 1/1 | 0.99 | 0.04 | - | 45,45,45,45 | 0 |
| 56 | MG | EA | 3088 | 1/1 | 0.96 | 0.16 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3057 | 1/1 | 0.92 | 0.11 | - | 22,22,22,22 | 0 |
| 56 | MG | AA | 3071 | 1/1 | 1.00 | 0.13 | - | 3,3,3,3 | 0 |
| 56 | MG | AA | 3069 | 1/1 | 0.96 | 0.17 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3093 | 1/1 | 0.96 | 0.49 | - | 28,28,28,28 | 0 |
| 56 | MG | FA | 1602 | 1/1 | 0.94 | 0.10 | - | 23,23,23,23 | 0 |
| 56 | MG | CA | 3039 | 1/1 | 0.99 | 0.21 | - | 6,6,6,6 | 0 |
| 56 | MG | EA | 3030 | 1/1 | 0.99 | 0.16 | - | 0,0,0,0 | 0 |
| 56 | MG | GA | 3039 | 1/1 | 1.00 | 0.17 | - | 15,15,15,15 | 0 |
| 56 | MG | HA | 1624 | 1/1 | 0.96 | 0.12 | - | 14,14,14,14 | 0 |
| 56 | MG | AA | 3070 | 1/1 | 1.00 | 0.13 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3085 | 1/1 | 0.99 | 0.19 | - | 4,4,4,4 | 0 |
| 56 | MG | CB | 1204 | 1/1 | 0.93 | 0.06 | - | 16,16,16,16 | 0 |
| 56 | MG | GA | 3070 | 1/1 | 0.99 | 0.23 | - | 13,13,13,13 | 0 |
| 56 | MG | AA | 3080 | 1/1 | 0.98 | 0.18 | - | 7,7,7,7 | 0 |
| 56 | MG | FA | 1603 | 1/1 | 0.98 | 0.11 | - | 30,30,30,30 | 0 |
| 56 | MG | GA | 3096 | 1/1 | 0.99 | 0.16 | - | 4,4,4,4 | 0 |
| 56 | MG | DA | 1612 | 1/1 | 0.98 | 0.19 | - | 11,11,11,11 | 0 |
| 56 | MG | AA | 3059 | 1/1 | 0.96 | 0.50 | - | 12,12,12,12 | 0 |
| 56 | MG | ED | 301 | 1/1 | 0.88 | 0.23 | - | 7,7,7,7 | 0 |
| 56 | MG | CA | 3088 | 1/1 | 0.99 | 0.11 | - | 28,28,28,28 | 0 |
| 56 | MG | EA | 3020 | 1/1 | 0.98 | 0.24 | - | 4,4,4,4 | 0 |
| 56 | MG | GA | 3115 | 1/1 | 0.99 | 0.23 | - | 23,23,23,23 | 0 |
| 56 | MG | CA | 3056 | 1/1 | 0.99 | 0.11 | - | 7,7,7,7 | 0 |
| 56 | MG | BA | 1632 | 1/1 | 0.99 | 0.10 | - | 40,40,40,40 | 0 |
| 56 | MG | DA | 1615 | 1/1 | 0.98 | 0.15 | - | 24,24,24,24 | 0 |
| 56 | MG | HA | 1621 | 1/1 | 0.97 | 0.28 | - | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | HA | 1617 | 1/1 | 0.83 | 0.16 | - | 62,62,62,62 | 0 |
| 56 | MG | HA | 1603 | 1/1 | 0.98 | 0.35 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 1626 | 1/1 | 0.97 | 0.08 | - | 24,24,24,24 | 0 |
| 56 | MG | EA | 3089 | 1/1 | 1.00 | 0.10 | - | 5,5,5,5 | 0 |
| 56 | MG | GA | 3120 | 1/1 | 0.98 | 0.21 | - | 5,5,5,5 | 0 |
| 56 | MG | AA | 3029 | 1/1 | 0.98 | 0.09 | - | 21,21,21,21 | 0 |
| 56 | MG | BU | 101 | 1/1 | 0.91 | 0.26 | - | 39,39,39,39 | 0 |
| 56 | MG | EA | 3034 | 1/1 | 0.98 | 0.21 | - | 0,0,0,0 | 0 |
| 56 | MG | CA | 3087 | 1/1 | 0.97 | 0.06 | - | 29,29,29,29 | 0 |
| 56 | MG | CA | 3084 | 1/1 | 0.99 | 0.21 | - | 4,4,4,4 | 0 |
| 56 | MG | EA | 3069 | 1/1 | 0.93 | 0.41 | - | 4,4,4,4 | 0 |
| 56 | MG | EA | 3055 | 1/1 | 0.97 | 0.43 | - | 14,14,14,14 | 0 |
| 56 | MG | EA | 3060 | 1/1 | 0.97 | 0.28 | - | 3,3,3,3 | 0 |
| 56 | MG | HA | 1640 | 1/1 | 0.99 | 0.10 | - | 15,15,15,15 | 0 |
| 56 | MG | HA | 1630 | 1/1 | 0.95 | 0.14 | - | 40,40,40,40 | 0 |
| 56 | MG | HA | 1634 | 1/1 | 0.95 | 0.13 | - | 24,24,24,24 | 0 |
| 56 | MG | HA | 1601 | 1/1 | 0.94 | 0.16 | - | 38,38,38,38 | 0 |
| 56 | MG | AE | 301 | 1/1 | 0.98 | 0.12 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3015 | 1/1 | 0.99 | 0.51 | - | 1,1,1,1 | 0 |
| 56 | MG | AA | 3123 | 1/1 | 0.99 | 0.17 | - | 14,14,14,14 | 0 |
| 56 | MG | BA | 1601 | 1/1 | 0.98 | 0.17 | - | 33,33,33,33 | 0 |
| 56 | MG | GA | 3095 | 1/1 | 0.98 | 0.18 | - | 2,2,2,2 | 0 |
| 56 | MG | AB | 1201 | 1/1 | 0.95 | 0.11 | - | 38,38,38,38 | 0 |
| 56 | MG | AA | 3008 | 1/1 | 0.99 | 0.12 | - | 15,15,15,15 | 0 |
| 56 | MG | AA | 3030 | 1/1 | 0.98 | 0.16 | - | 13,13,13,13 | 0 |
| 56 | MG | CA | 3105 | 1/1 | 0.98 | 0.17 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3072 | 1/1 | 0.97 | 0.15 | - | 13,13,13,13 | 0 |
| 56 | MG | GA | 3133 | 1/1 | 0.94 | 0.23 | - | 4,4,4,4 | 0 |
| 56 | MG | GA | 3077 | 1/1 | 0.96 | 0.10 | - | 33,33,33,33 | 0 |
| 56 | MG | AA | 3037 | 1/1 | 0.99 | 0.19 | - | 9,9,9,9 | 0 |
| 56 | MG | GA | 3052 | 1/1 | 0.99 | 0.18 | - | 8,8,8,8 | 0 |
| 56 | MG | EA | 3076 | 1/1 | 0.99 | 0.10 | - | 18,18,18,18 | 0 |
| 56 | MG | EA | 3056 | 1/1 | 0.97 | 0.08 | - | 2,2,2,2 | 0 |
| 56 | MG | CB | 1203 | 1/1 | 1.00 | 0.11 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3059 | 1/1 | 0.90 | 0.48 | - | 44,44,44,44 | 0 |
| 56 | MG | GB | 1202 | 1/1 | 0.96 | 0.16 | - | 36,36,36,36 | 0 |
| 56 | MG | EA | 3041 | 1/1 | 0.99 | 0.10 | - | 2,2,2,2 | 0 |
| 56 | MG | EA | 3083 | 1/1 | 0.98 | 0.14 | - | 1,1,1,1 | 0 |
| 56 | MG | GA | 3035 | 1/1 | 0.98 | 0.13 | - | 15,15,15,15 | 0 |
| 56 | MG | AA | 3052 | 1/1 | 0.99 | 0.12 | - | 2,2,2,2 | 0 |
| 56 | MG | AA | 3085 | 1/1 | 0.98 | 0.08 | - | 30,30,30,30 | 0 |
| 56 | MG | EA | 3116 | 1/1 | 0.99 | 0.15 | - | 0,0,0,0 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3078 | 1/1 | 0.99 | 0.10 | - | 25,25,25,25 | 0 |
| 56 | MG | AA | 3063 | 1/1 | 0.97 | 0.08 | - | 9,9,9,9 | 0 |
| 56 | MG | GA | 3025 | 1/1 | 0.98 | 0.17 | - | 18,18,18,18 | 0 |
| 56 | MG | DA | 1623 | 1/1 | 0.99 | 0.07 | - | 12,12,12,12 | 0 |
| 56 | MG | CA | 3035 | 1/1 | 0.99 | 0.16 | - | 3,3,3,3 | 0 |
| 56 | MG | BA | 1617 | 1/1 | 0.98 | 0.13 | - | 25,25,25,25 | 0 |
| 56 | MG | AA | 3079 | 1/1 | 1.00 | 0.16 | - | 11,11,11,11 | 0 |
| 56 | MG | GA | 3041 | 1/1 | 0.99 | 0.09 | - | 10,10,10,10 | 0 |
| 56 | MG | HA | 1602 | 1/1 | 0.98 | 0.36 | - | 48,48,48,48 | 0 |
| 56 | MG | GB | 1201 | 1/1 | 0.93 | 0.09 | - | 38,38,38,38 | 0 |
| 56 | MG | GA | 3134 | 1/1 | 0.99 | 0.05 | - | 16,16,16,16 | 0 |
| 56 | MG | GA | 3124 | 1/1 | 0.99 | 0.12 | - | 16,16,16,16 | 0 |
| 56 | MG | AA | 3118 | 1/1 | 0.99 | 0.11 | - | 11,11,11,11 | 0 |
| 56 | MG | GA | 3055 | 1/1 | 0.94 | 0.13 | - | 12,12,12,12 | 0 |
| 56 | MG | EA | 3051 | 1/1 | 1.00 | 0.15 | - | 0,0,0,0 | 0 |
| 56 | MG | CA | 3122 | 1/1 | 0.89 | 0.17 | - | 7,7,7,7 | 0 |
| 56 | MG | CA | 3038 | 1/1 | 0.99 | 0.18 | - | 7,7,7,7 | 0 |
| 56 | MG | CA | 3011 | 1/1 | 0.87 | 0.40 | - | 23,23,23,23 | 0 |
| 56 | MG | CA | 3001 | 1/1 | 0.99 | 0.15 | - | 10,10,10,10 | 0 |
| 56 | MG | EA | 3075 | 1/1 | 0.98 | 0.13 | - | 10,10,10,10 | 0 |
| 56 | MG | GC | 301 | 1/1 | 0.99 | 0.18 | - | 4,4,4,4 | 0 |
| 56 | MG | EA | 3010 | 1/1 | 0.93 | 0.16 | - | 11,11,11,11 | 0 |
| 56 | MG | AA | 3026 | 1/1 | 0.98 | 0.07 | - | 10,10,10,10 | 0 |
| 56 | MG | HT | 101 | 1/1 | 0.86 | 0.45 | - | 41,41,41,41 | 0 |
| 56 | MG | GA | 3123 | 1/1 | 0.99 | 0.20 | - | 11,11,11,11 | 0 |
| 56 | MG | AA | 3096 | 1/1 | 0.98 | 0.15 | - | 33,33,33,33 | 0 |
| 56 | MG | DA | 1635 | 1/1 | 0.99 | 0.08 | - | 38,38,38,38 | 0 |
| 56 | MG | EA | 3087 | 1/1 | 0.86 | 0.59 | - | 30,30,30,30 | 0 |
| 56 | MG | CA | 3097 | 1/1 | 0.94 | 0.67 | - | 22,22,22,22 | 0 |
| 56 | MG | AA | 3065 | 1/1 | 0.99 | 0.16 | - | 2,2,2,2 | 0 |
| 56 | MG | GA | 3033 | 1/1 | 0.98 | 0.24 | - | 12,12,12,12 | 0 |
| 56 | MG | CA | 3075 | 1/1 | 0.99 | 0.22 | - | 20,20,20,20 | 0 |
| 56 | MG | CA | 3048 | 1/1 | 0.99 | 0.09 | - | 13,13,13,13 | 0 |
| 56 | MG | EA | 3092 | 1/1 | 0.99 | 0.14 | - | 7,7,7,7 | 0 |
| 56 | MG | EA | 3123 | 1/1 | 0.99 | 0.29 | - | 2,2,2,2 | 0 |
| 56 | MG | DU | 101 | 1/1 | 0.96 | 0.28 | - | 36,36,36,36 | 0 |
| 56 | MG | CA | 3112 | 1/1 | 0.99 | 0.14 | - | 4,4,4,4 | 0 |
| 56 | MG | GA | 3111 | 1/1 | 0.97 | 0.17 | - | 11,11,11,11 | 0 |
| 56 | MG | FA | 1611 | 1/1 | 0.98 | 0.23 | - | 0,0,0,0 | 0 |
| 56 | MG | GA | 3047 | 1/1 | 0.98 | 0.18 | - | 27,27,27,27 | 0 |
| 56 | MG | AA | 3084 | 1/1 | 0.99 | 0.20 | - | 12,12,12,12 | 0 |
| 56 | MG | CA | 3044 | 1/1 | 0.92 | 0.13 | - | 22,22,22,22 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | HA | 1625 | 1/1 | 0.95 | 0.32 | - | 22,22,22,22 | 0 |
| 56 | MG | HA | 1607 | 1/1 | 0.99 | 0.20 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3109 | 1/1 | 0.88 | 0.17 | - | 8,8,8,8 | 0 |
| 56 | MG | AA | 3099 | 1/1 | 0.98 | 0.14 | - | 15,15,15,15 | 0 |
| 56 | MG | CA | 3005 | 1/1 | 0.96 | 0.17 | - | 31,31,31,31 | 0 |
| 56 | MG | CA | 3116 | 1/1 | 0.99 | 0.12 | - | 13,13,13,13 | 0 |
| 56 | MG | EA | 3032 | 1/1 | 0.99 | 0.16 | - | 0,0,0,0 | 0 |
| 56 | MG | CA | 3006 | 1/1 | 0.98 | 0.09 | - | 15,15,15,15 | 0 |
| 56 | MG | GA | 3003 | 1/1 | 0.99 | 0.12 | - | 15,15,15,15 | 0 |
| 56 | MG | CA | 3020 | 1/1 | 0.97 | 0.16 | - | 19,19,19,19 | 0 |
| 56 | MG | GA | 3104 | 1/1 | 0.98 | 0.20 | - | 6,6,6,6 | 0 |
| 56 | MG | CA | 3007 | 1/1 | 0.97 | 0.09 | - | 15,15,15,15 | 0 |
| 56 | MG | GB | 1204 | 1/1 | 0.98 | 0.07 | - | 21,21,21,21 | 0 |
| 56 | MG | GA | 3106 | 1/1 | 0.98 | 0.21 | - | 3,3,3,3 | 0 |
| 56 | MG | AB | 1204 | 1/1 | 0.98 | 0.07 | - | 8,8,8,8 | 0 |
| 56 | MG | BA | 1611 | 1/1 | 0.99 | 0.13 | - | 15,15,15,15 | 0 |
| 56 | MG | HA | 1605 | 1/1 | 0.99 | 0.11 | - | 39,39,39,39 | 0 |
| 56 | MG | EA | 3081 | 1/1 | 0.99 | 0.15 | - | 3,3,3,3 | 0 |
| 56 | MG | BA | 1623 | 1/1 | 0.97 | 0.10 | - | 24,24,24,24 | 0 |
| 56 | MG | AA | 3042 | 1/1 | 0.99 | 0.17 | - | 11,11,11,11 | 0 |
| 56 | MG | AA | 3092 | 1/1 | 0.97 | 0.05 | - | 31,31,31,31 | 0 |
| 56 | MG | FA | 1622 | 1/1 | 0.99 | 0.10 | - | 15,15,15,15 | 0 |
| 56 | MG | CA | 3047 | 1/1 | 0.99 | 0.10 | - | 31,31,31,31 | 0 |
| 56 | MG | GA | 3048 | 1/1 | 1.00 | 0.19 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3031 | 1/1 | 0.98 | 0.14 | - | 4,4,4,4 | 0 |
| 56 | MG | GA | 3074 | 1/1 | 0.99 | 0.14 | - | 2,2,2,2 | 0 |
| 56 | MG | DA | 1605 | 1/1 | 0.99 | 0.12 | - | 28,28,28,28 | 0 |
| 56 | MG | CA | 3076 | 1/1 | 0.98 | 0.08 | - | 25,25,25,25 | 0 |
| 56 | MG | CA | 3110 | 1/1 | 0.91 | 0.11 | - | 20,20,20,20 | 0 |
| 56 | MG | HC | 401 | 1/1 | 0.89 | 0.32 | - | 49,49,49,49 | 0 |
| 56 | MG | BL | 201 | 1/1 | 0.91 | 0.23 | - | 51,51,51,51 | 0 |
| 56 | MG | AA | 3094 | 1/1 | 0.99 | 0.06 | - | 20,20,20,20 | 0 |
| 56 | MG | EA | 3052 | 1/1 | 0.98 | 0.20 | - | 2,2,2,2 | 0 |
| 56 | MG | GA | 3086 | 1/1 | 0.99 | 0.04 | - | 26,26,26,26 | 0 |
| 56 | MG | GA | 3082 | 1/1 | 0.92 | 0.11 | - | 35,35,35,35 | 0 |
| 56 | MG | FA | 1628 | 1/1 | 0.97 | 0.18 | - | 19,19,19,19 | 0 |
| 56 | MG | CA | 3093 | 1/1 | 0.98 | 0.12 | - | 25,25,25,25 | 0 |
| 56 | MG | EA | 3016 | 1/1 | 0.95 | 0.12 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3117 | 1/1 | 0.99 | 0.07 | - | 22,22,22,22 | 0 |
| 56 | MG | CA | 3042 | 1/1 | 0.99 | 0.11 | - | 8,8,8,8 | 0 |
| 56 | MG | HA | 1618 | 1/1 | 0.98 | 0.08 | - | 19,19,19,19 | 0 |
| 56 | MG | EA | 3126 | 1/1 | 0.99 | 0.16 | - | 2,2,2,2 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | EA | 3031 | 1/1 | 0.98 | 0.23 | - | 2,2,2,2 | 0 |
| 56 | MG | EA | 3029 | 1/1 | 0.97 | 0.18 | - | 0,0,0,0 | 0 |
| 56 | MG | EA | 3086 | 1/1 | 0.98 | 0.07 | - | 34,34,34,34 | 0 |
| 56 | MG | AA | 3001 | 1/1 | 0.99 | 0.09 | - | 11,11,11,11 | 0 |
| 56 | MG | HA | 1633 | 1/1 | 0.94 | 0.19 | - | 52,52,52,52 | 0 |
| 56 | MG | AA | 3122 | 1/1 | 0.99 | 0.16 | - | 2,2,2,2 | 0 |
| 56 | MG | EA | 3122 | 1/1 | 0.98 | 0.19 | - | 0,0,0,0 | 0 |
| 56 | MG | EA | 3094 | 1/1 | 0.98 | 0.11 | - | 15,15,15,15 | 0 |
| 56 | MG | CA | 3118 | 1/1 | 0.89 | 0.33 | - | 29,29,29,29 | 0 |
| 56 | MG | EA | 3117 | 1/1 | 0.97 | 0.10 | - | 11,11,11,11 | 0 |
| 56 | MG | GA | 3076 | 1/1 | 0.98 | 0.14 | - | 23,23,23,23 | 0 |
| 56 | MG | CA | 3074 | 1/1 | 0.99 | 0.05 | - | 19,19,19,19 | 0 |
| 56 | MG | BA | 1625 | 1/1 | 0.98 | 0.20 | - | 21,21,21,21 | 0 |
| 56 | MG | EA | 3050 | 1/1 | 0.96 | 0.24 | - | 13,13,13,13 | 0 |
| 56 | MG | CA | 3033 | 1/1 | 0.99 | 0.18 | - | 9,9,9,9 | 0 |
| 56 | MG | CA | 3125 | 1/1 | 0.99 | 0.14 | - | 9,9,9,9 | 0 |
| 56 | MG | GA | 3044 | 1/1 | 0.98 | 0.20 | - | 23,23,23,23 | 0 |
| 56 | MG | GA | 3071 | 1/1 | 0.99 | 0.18 | - | 20,20,20,20 | 0 |
| 56 | MG | FA | 1634 | 1/1 | 0.99 | 0.07 | - | 19,19,19,19 | 0 |
| 56 | MG | CA | 3021 | 1/1 | 0.99 | 0.10 | - | 10,10,10,10 | 0 |
| 56 | MG | FA | 1619 | 1/1 | 0.99 | 0.10 | - | 25,25,25,25 | 0 |
| 56 | MG | GA | 3001 | 1/1 | 0.96 | 0.17 | - | 32,32,32,32 | 0 |
| 56 | MG | CA | 3096 | 1/1 | 0.99 | 0.21 | - | 10,10,10,10 | 0 |
| 56 | MG | CA | 3094 | 1/1 | 0.96 | 0.07 | - | 34,34,34,34 | 0 |
| 56 | MG | EA | 3133 | 1/1 | 0.82 | 0.13 | - | 32,32,32,32 | 0 |
| 56 | MG | CA | 3127 | 1/1 | 0.98 | 0.08 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3079 | 1/1 | 0.94 | 0.23 | - | 0,0,0,0 | 0 |
| 56 | MG | AA | 3041 | 1/1 | 0.99 | 0.18 | - | 2,2,2,2 | 0 |
| 56 | MG | FA | 1606 | 1/1 | 0.98 | 0.12 | - | 13,13,13,13 | 0 |
| 56 | MG | HA | 1635 | 1/1 | 0.99 | 0.15 | - | 17,17,17,17 | 0 |
| 56 | MG | CA | 3057 | 1/1 | 0.97 | 0.11 | - | 1,1,1,1 | 0 |
| 56 | MG | FA | 1605 | 1/1 | 0.98 | 0.15 | - | 36,36,36,36 | 0 |
| 56 | MG | EA | 3077 | 1/1 | 0.98 | 0.11 | - | 14,14,14,14 | 0 |
| 56 | MG | GA | 3087 | 1/1 | 0.94 | 0.19 | - | 19,19,19,19 | 0 |
| 56 | MG | AA | 3064 | 1/1 | 0.98 | 0.13 | - | 20,20,20,20 | 0 |
| 56 | MG | CA | 3018 | 1/1 | 0.99 | 0.10 | - | 26,26,26,26 | 0 |
| 56 | MG | EA | 3093 | 1/1 | 0.99 | 0.09 | - | 21,21,21,21 | 0 |
| 56 | MG | HA | 1608 | 1/1 | 0.95 | 0.14 | - | 14,14,14,14 | 0 |
| 56 | MG | AA | 3050 | 1/1 | 0.98 | 0.09 | - | 7,7,7,7 | 0 |
| 56 | MG | CA | 3089 | 1/1 | 0.99 | 0.15 | - | 2,2,2,2 | 0 |
| 56 | MG | AA | 3016 | 1/1 | 1.00 | 0.12 | - | 10,10,10,10 | 0 |
| 56 | MG | CA | 3068 | 1/1 | 0.98 | 0.13 | - | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3093 | 1/1 | 0.95 | 0.26 | - | 34,34,34,34 | 0 |
| 56 | MG | DA | 1606 | 1/1 | 0.96 | 0.11 | - | 26,26,26,26 | 0 |
| 56 | MG | AA | 3019 | 1/1 | 0.99 | 0.18 | - | 33,33,33,33 | 0 |
| 56 | MG | CA | 3083 | 1/1 | 0.96 | 0.12 | - | 22,22,22,22 | 0 |
| 56 | MG | AA | 3020 | 1/1 | 0.99 | 0.13 | - | 24,24,24,24 | 0 |
| 56 | MG | GA | 3034 | 1/1 | 0.99 | 0.19 | - | 16,16,16,16 | 0 |
| 56 | MG | EB | 1201 | 1/1 | 0.94 | 0.14 | - | 26,26,26,26 | 0 |
| 56 | MG | GA | 3069 | 1/1 | 0.82 | 0.07 | - | 63,63,63,63 | 0 |
| 56 | MG | C4 | 101 | 1/1 | 0.95 | 0.06 | - | 22,22,22,22 | 0 |
| 56 | MG | GA | 3131 | 1/1 | 0.94 | 0.13 | - | 41,41,41,41 | 0 |
| 56 | MG | EA | 3004 | 1/1 | 0.98 | 0.09 | - | 13,13,13,13 | 0 |
| 56 | MG | EA | 3074 | 1/1 | 0.99 | 0.18 | - | 4,4,4,4 | 0 |
| 56 | MG | BA | 1630 | 1/1 | 0.98 | 0.11 | - | 25,25,25,25 | 0 |
| 56 | MG | FU | 101 | 1/1 | 0.89 | 0.14 | - | 24,24,24,24 | 0 |
| 56 | MG | AA | 3067 | 1/1 | 0.99 | 0.09 | - | 29,29,29,29 | 0 |
| 56 | MG | GA | 3122 | 1/1 | 0.98 | 0.19 | - | 14,14,14,14 | 0 |
| 56 | MG | CA | 3117 | 1/1 | 0.99 | 0.07 | - | 7,7,7,7 | 0 |
| 56 | MG | FA | 1618 | 1/1 | 0.97 | 0.10 | - | 28,28,28,28 | 0 |
| 56 | MG | GA | 3101 | 1/1 | 0.99 | 0.10 | - | 15,15,15,15 | 0 |
| 56 | MG | GA | 3068 | 1/1 | 0.98 | 0.27 | - | 15,15,15,15 | 0 |
| 56 | MG | CA | 3008 | 1/1 | 0.98 | 0.17 | - | 15,15,15,15 | 0 |
| 56 | MG | GA | 3043 | 1/1 | 0.99 | 0.10 | - | 8,8,8,8 | 0 |
| 56 | MG | AA | 3077 | 1/1 | 0.96 | 0.06 | - | 36,36,36,36 | 0 |
| 56 | MG | AA | 3013 | 1/1 | 0.99 | 0.16 | - | 5,5,5,5 | 0 |
| 56 | MG | AA | 3007 | 1/1 | 0.94 | 0.18 | - | 44,44,44,44 | 0 |
| 56 | MG | FA | 1630 | 1/1 | 0.97 | 0.09 | - | 16,16,16,16 | 0 |
| 56 | MG | AA | 3047 | 1/1 | 0.99 | 0.10 | - | 30,30,30,30 | 0 |
| 56 | MG | BA | 1610 | 1/1 | 0.99 | 0.07 | - | 19,19,19,19 | 0 |
| 56 | MG | AA | 3089 | 1/1 | 0.97 | 0.06 | - | 26,26,26,26 | 0 |
| 56 | MG | DA | 1637 | 1/1 | 0.99 | 0.11 | - | 23,23,23,23 | 0 |
| 56 | MG | AA | 3015 | 1/1 | 0.94 | 0.15 | - | 22,22,22,22 | 0 |
| 56 | MG | DA | 1608 | 1/1 | 0.98 | 0.14 | - | 14,14,14,14 | 0 |
| 56 | MG | DA | 1639 | 1/1 | 0.96 | 0.10 | - | 40,40,40,40 | 0 |
| 56 | MG | AA | 3048 | 1/1 | 0.99 | 0.12 | - | 2,2,2,2 | 0 |
| 56 | MG | GA | 3100 | 1/1 | 0.97 | 0.22 | - | 19,19,19,19 | 0 |
| 56 | MG | CA | 3064 | 1/1 | 0.99 | 0.10 | - | 1,1,1,1 | 0 |
| 56 | MG | AA | 3058 | 1/1 | 0.99 | 0.19 | - | 9,9,9,9 | 0 |
| 56 | MG | CA | 3051 | 1/1 | 0.99 | 0.29 | - | 7,7,7,7 | 0 |
| 56 | MG | EA | 3082 | 1/1 | 0.96 | 0.07 | - | 13,13,13,13 | 0 |
| 56 | MG | AA | 3100 | 1/1 | 0.97 | 0.12 | - | 6,6,6,6 | 0 |
| 56 | MG | HA | 1629 | 1/1 | 0.97 | 0.10 | - | 17,17,17,17 | 0 |
| 56 | MG | AA | 3055 | 1/1 | 1.00 | 0.17 | - | 18,18,18,18 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3027 | 1/1 | 0.99 | 0.10 | - | 2,2,2,2 | 0 |
| 56 | MG | CA | 3107 | 1/1 | 1.00 | 0.20 | - | 6,6,6,6 | 0 |
| 56 | MG | BA | 1602 | 1/1 | 0.99 | 0.12 | - | 15,15,15,15 | 0 |
| 56 | MG | CA | 3034 | 1/1 | 0.99 | 0.19 | - | 18,18,18,18 | 0 |
| 56 | MG | CA | 3017 | 1/1 | 0.99 | 0.18 | - | 2,2,2,2 | 0 |
| 56 | MG | AA | 3086 | 1/1 | 0.97 | 0.07 | - | 35,35,35,35 | 0 |
| 56 | MG | FA | 1635 | 1/1 | 0.99 | 0.13 | - | 8,8,8,8 | 0 |
| 56 | MG | CA | 3016 | 1/1 | 0.96 | 0.21 | - | 8,8,8,8 | 0 |
| 56 | MG | EA | 3084 | 1/1 | 0.99 | 0.17 | - | 2,2,2,2 | 0 |
| 56 | MG | EA | 3072 | 1/1 | 0.99 | 0.15 | - | 8,8,8,8 | 0 |
| 56 | MG | FA | 1601 | 1/1 | 0.94 | 0.14 | - | 28,28,28,28 | 0 |
| 56 | MG | EA | 3011 | 1/1 | 0.96 | 0.86 | - | 17,17,17,17 | 0 |
| 56 | MG | FA | 1636 | 1/1 | 0.83 | 0.62 | - | 38,38,38,38 | 0 |
| 56 | MG | EA | 3021 | 1/1 | 0.99 | 0.12 | - | 5,5,5,5 | 0 |
| 56 | MG | EA | 3115 | 1/1 | 1.00 | 0.14 | - | 2,2,2,2 | 0 |
| 56 | MG | CA | 3086 | 1/1 | 0.99 | 0.19 | - | 20,20,20,20 | 0 |
| 56 | MG | EA | 3046 | 1/1 | 0.99 | 0.15 | - | 9,9,9,9 | 0 |
| 56 | MG | CA | 3054 | 1/1 | 0.99 | 0.17 | - | 6,6,6,6 | 0 |
| 56 | MG | EA | 3057 | 1/1 | 0.93 | 0.11 | - | 15,15,15,15 | 0 |
| 56 | MG | AA | 3032 | 1/1 | 1.00 | 0.16 | - | 14,14,14,14 | 0 |
| 56 | MG | FA | 1608 | 1/1 | 0.99 | 0.18 | - | 14,14,14,14 | 0 |
| 56 | MG | CA | 3003 | 1/1 | 0.98 | 0.13 | - | 12,12,12,12 | 0 |
| 56 | MG | EA | 3043 | 1/1 | 0.99 | 0.10 | - | 4,4,4,4 | 0 |
| 56 | MG | BA | 1635 | 1/1 | 0.97 | 0.23 | - | 29,29,29,29 | 0 |
| 56 | MG | AD | 301 | 1/1 | 0.97 | 0.14 | - | 6,6,6,6 | 0 |
| 56 | MG | EA | 3096 | 1/1 | 0.94 | 0.15 | - | 15,15,15,15 | 0 |
| 56 | MG | GA | 3045 | 1/1 | 0.98 | 0.17 | - | 7,7,7,7 | 0 |
| 56 | MG | CA | 3060 | 1/1 | 0.98 | 0.22 | - | 13,13,13,13 | 0 |
| 56 | MG | HA | 1620 | 1/1 | 0.99 | 0.08 | - | 14,14,14,14 | 0 |
| 56 | MG | AB | 1203 | 1/1 | 0.99 | 0.12 | - | 14,14,14,14 | 0 |
| 56 | MG | FA | 1624 | 1/1 | 0.99 | 0.18 | - | 18,18,18,18 | 0 |
| 56 | MG | GA | 3017 | 1/1 | 0.98 | 0.09 | - | 24,24,24,24 | 0 |
| 56 | MG | AA | 3078 | 1/1 | 0.82 | 0.24 | - | 29,29,29,29 | 0 |
| 56 | MG | DA | 1603 | 1/1 | 0.99 | 0.12 | - | 22,22,22,22 | 0 |
| 56 | MG | EA | 3070 | 1/1 | 1.00 | 0.14 | - | 3,3,3,3 | 0 |
| 56 | MG | CA | 3121 | 1/1 | 0.99 | 0.22 | - | 3,3,3,3 | 0 |
| 56 | MG | CA | 3091 | 1/1 | 0.91 | 0.21 | - | 40,40,40,40 | 0 |
| 56 | MG | GA | 3042 | 1/1 | 1.00 | 0.14 | - | 24,24,24,24 | 0 |
| 56 | MG | EB | 1204 | 1/1 | 0.98 | 0.06 | - | 12,12,12,12 | 0 |
| 56 | MG | GA | 3002 | 1/1 | 0.98 | 0.17 | - | 14,14,14,14 | 0 |
| 56 | MG | CA | 3041 | 1/1 | 0.99 | 0.13 | - | 13,13,13,13 | 0 |
| 56 | MG | EA | 3006 | 1/1 | 0.98 | 0.12 | - | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3021 | 1/1 | 0.99 | 0.11 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3132 | 1/1 | 0.99 | 0.23 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3098 | 1/1 | 0.98 | 0.15 | - | 25,25,25,25 | 0 |
| 56 | MG | EA | 3033 | 1/1 | 1.00 | 0.17 | - | 1,1,1,1 | 0 |
| 56 | MG | AB | 1202 | 1/1 | 0.95 | 0.24 | - | 44,44,44,44 | 0 |
| 56 | MG | GA | 3119 | 1/1 | 0.99 | 0.16 | - | 5,5,5,5 | 0 |
| 56 | MG | GA | 3073 | 1/1 | 0.91 | 0.47 | - | 20,20,20,20 | 0 |
| 56 | MG | BA | 1618 | 1/1 | 0.98 | 0.13 | - | 3,3,3,3 | 0 |
| 56 | MG | GA | 3054 | 1/1 | 0.99 | 0.14 | - | 1,1,1,1 | 0 |
| 56 | MG | AA | 3097 | 1/1 | 1.00 | 0.18 | - | 8,8,8,8 | 0 |
| 56 | MG | CA | 3030 | 1/1 | 0.98 | 0.21 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3019 | 1/1 | 0.98 | 0.08 | - | 13,13,13,13 | 0 |
| 56 | MG | CA | 3070 | 1/1 | 0.99 | 0.15 | - | 4,4,4,4 | 0 |
| 56 | MG | GA | 3029 | 1/1 | 0.97 | 0.20 | - | 5,5,5,5 | 0 |
| 56 | MG | HA | 1614 | 1/1 | 0.99 | 0.12 | - | 37,37,37,37 | 0 |
| 56 | MG | DA | 1618 | 1/1 | 0.97 | 0.09 | - | 33,33,33,33 | 0 |
| 56 | MG | AA | 3114 | 1/1 | 0.99 | 0.09 | - | 1,1,1,1 | 0 |
| 56 | MG | HA | 1615 | 1/1 | 0.98 | 0.27 | - | 38,38,38,38 | 0 |
| 56 | MG | CA | 3072 | 1/1 | 0.99 | 0.15 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3048 | 1/1 | 0.99 | 0.13 | - | 11,11,11,11 | 0 |
| 56 | MG | EA | 3097 | 1/1 | 1.00 | 0.19 | - | 2,2,2,2 | 0 |
| 56 | MG | EA | 3120 | 1/1 | 0.98 | 0.23 | - | 0,0,0,0 | 0 |
| 56 | MG | HA | 1636 | 1/1 | 0.98 | 0.05 | - | 21,21,21,21 | 0 |
| 56 | MG | BA | 1620 | 1/1 | 0.98 | 0.05 | - | 20,20,20,20 | 0 |
| 56 | MG | AA | 3060 | 1/1 | 0.98 | 0.46 | - | 25,25,25,25 | 0 |
| 56 | MG | BE | 201 | 1/1 | 0.88 | 0.14 | - | 43,43,43,43 | 0 |
| 56 | MG | EA | 3073 | 1/1 | 0.99 | 0.19 | - | 0,0,0,0 | 0 |
| 56 | MG | GA | 3019 | 1/1 | 0.99 | 0.10 | - | 5,5,5,5 | 0 |
| 56 | MG | AA | 3014 | 1/1 | 0.99 | 0.18 | - | 4,4,4,4 | 0 |
| 56 | MG | AA | 3108 | 1/1 | 0.99 | 0.16 | - | 21,21,21,21 | 0 |
| 56 | MG | AA | 3022 | 1/1 | 0.99 | 0.11 | - | 8,8,8,8 | 0 |
| 56 | MG | EA | 3018 | 1/1 | 1.00 | 0.14 | - | 8,8,8,8 | 0 |
| 56 | MG | GA | 3089 | 1/1 | 0.98 | 0.13 | - | 14,14,14,14 | 0 |
| 56 | MG | DA | 1619 | 1/1 | 0.99 | 0.12 | - | 33,33,33,33 | 0 |
| 56 | MG | GA | 3028 | 1/1 | 0.99 | 0.12 | - | 10,10,10,10 | 0 |
| 56 | MG | FA | 1626 | 1/1 | 0.99 | 0.16 | - | 15,15,15,15 | 0 |
| 56 | MG | GA | 3007 | 1/1 | 0.99 | 0.07 | - | 28,28,28,28 | 0 |
| 56 | MG | FA | 1615 | 1/1 | 0.98 | 0.18 | - | 16,16,16,16 | 0 |
| 56 | MG | CB | 1202 | 1/1 | 0.98 | 0.12 | - | 55,55,55,55 | 0 |
| 56 | MG | CA | 3098 | 1/1 | 0.99 | 0.21 | - | 10,10,10,10 | 0 |
| 56 | MG | EA | 3003 | 1/1 | 0.98 | 0.14 | - | 6,6,6,6 | 0 |
| 56 | MG | CA | 3080 | 1/1 | 0.99 | 0.16 | - | 8,8,8,8 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | AA | 3056 | 1/1 | 0.99 | 0.13 | - | 24,24,24,24 | 0 |
| 56 | MG | DA | 1629 | 1/1 | 0.93 | 0.47 | - | 54,54,54,54 | 0 |
| 56 | MG | CA | 3045 | 1/1 | 0.97 | 0.14 | - | 21,21,21,21 | 0 |
| 56 | MG | CA | 3004 | 1/1 | 0.99 | 0.08 | - | 6,6,6,6 | 0 |
| 56 | MG | GA | 3020 | 1/1 | 0.99 | 0.21 | - | 3,3,3,3 | 0 |
| 56 | MG | GA | 3080 | 1/1 | 0.99 | 0.26 | - | 5,5,5,5 | 0 |
| 56 | MG | GA | 3064 | 1/1 | 0.98 | 0.12 | - | 9,9,9,9 | 0 |
| 56 | MG | EA | 3112 | 1/1 | 1.00 | 0.15 | - | 5,5,5,5 | 0 |
| 56 | MG | DA | 1627 | 1/1 | 0.94 | 0.11 | - | 21,21,21,21 | 0 |
| 56 | MG | EA | 3071 | 1/1 | 0.97 | 0.13 | - | 2,2,2,2 | 0 |
| 56 | MG | GA | 3094 | 1/1 | 0.96 | 0.55 | - | 22,22,22,22 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.