



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:33 AM UTC

PDB ID : 4V8P / pdb\_00004v8p  
Title : T.thermophila 60S ribosomal subunit in complex with initiation factor 6.  
Authors : Klinge, S.; Voigts-Hoffmann, F.; Leibundgut, M.; Arpagaus, S.; Ban, N.  
Deposited on : 2011-09-14  
Resolution : 3.52 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

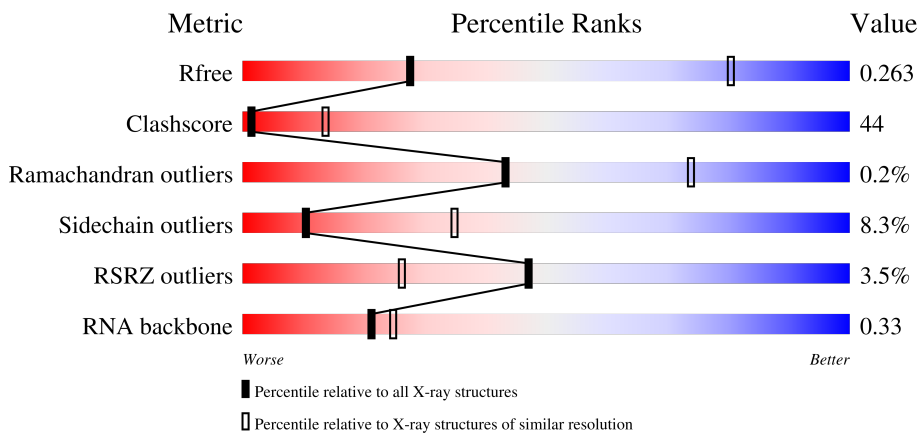
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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.



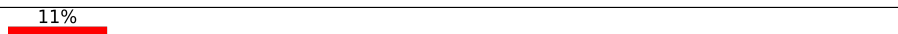
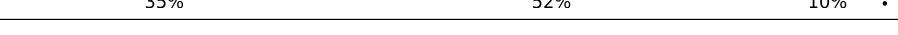
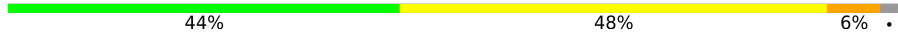
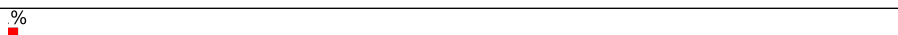
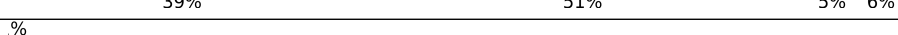
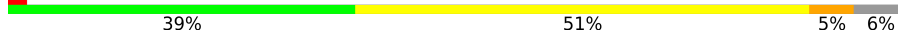
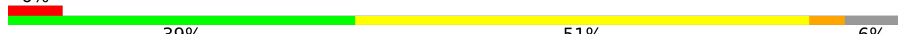
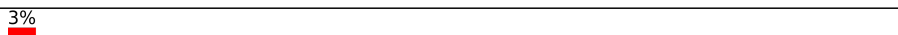
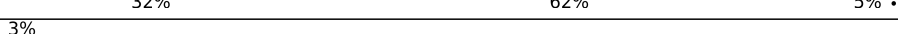
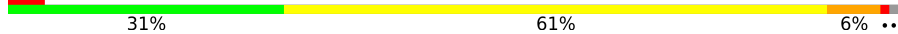
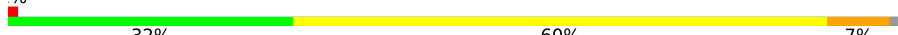
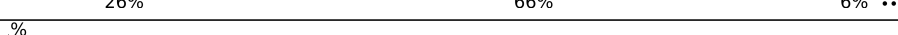
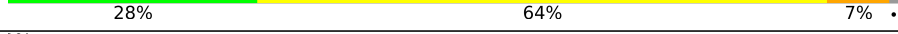
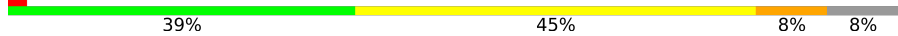
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1025 (3.56-3.48)                                      |
| Clashscore            | 190562                      | 1079 (3.56-3.48)                                      |
| Ramachandran outliers | 187476                      | 1052 (3.56-3.48)                                      |
| Sidechain outliers    | 187428                      | 1053 (3.56-3.48)                                      |
| RSRZ outliers         | 180081                      | 1024 (3.56-3.48)                                      |
| RNA backbone          | 3983                        | 1018 (4.00-3.04)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                       |
|-----|-------|--------|----------------------------------------------------------------------------------------|
| 1   | A1    | 3354   | <div> <div>3%</div> <div>18%</div> <div>46%</div> <div>29%</div> <div>7%</div> </div>  |
| 1   | D1    | 3354   | <div> <div>3%</div> <div>18%</div> <div>45%</div> <div>29%</div> <div>7%</div> </div>  |
| 1   | F1    | 3354   | <div> <div>4%</div> <div>18%</div> <div>45%</div> <div>29%</div> <div>7%</div> </div>  |
| 1   | H1    | 3354   | <div> <div>14%</div> <div>18%</div> <div>46%</div> <div>29%</div> <div>7%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | AA    | 94     |    |
| 2   | DA    | 94     |    |
| 2   | FA    | 94     |    |
| 2   | HA    | 94     |    |
| 3   | AB    | 52     |    |
| 3   | DB    | 52     |    |
| 3   | FB    | 52     |    |
| 3   | HB    | 52     |    |
| 4   | AC    | 109    |    |
| 4   | DC    | 109    |    |
| 4   | FC    | 109    |    |
| 4   | HC    | 109    |    |
| 5   | AE    | 191    |    |
| 5   | DE    | 191    |   |
| 5   | FE    | 191    |  |
| 5   | HE    | 191    |  |
| 6   | AF    | 126    |  |
| 6   | DF    | 126    |  |
| 6   | FF    | 126    |  |
| 6   | HF    | 126    |  |
| 7   | AG    | 104    |  |
| 7   | DG    | 104    |  |
| 7   | FG    | 104    |  |
| 7   | HG    | 104    |  |
| 8   | AH    | 113    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8   | DH    | 113    |                  |
| 8   | FH    | 113    |                  |
| 8   | HH    | 113    |                  |
| 9   | AJ    | 248    |                  |
| 9   | DJ    | 248    |                  |
| 9   | FJ    | 248    |                  |
| 9   | HJ    | 248    |                  |
| 10  | AK    | 129    |                  |
| 10  | DK    | 129    |                  |
| 10  | FK    | 129    |                  |
| 10  | HK    | 129    |                  |
| 11  | AL    | 123    |                  |
| 11  | DL    | 123    |                  |
| 11  | FL    | 123    |                  |
| 11  | HL    | 123    |                  |
| 12  | AM    | 118    |                  |
| 12  | DM    | 118    |                  |
| 12  | FM    | 118    |                  |
| 12  | HM    | 118    |                  |
| 13  | AN    | 144    |                  |
| 13  | DN    | 144    |                  |
| 13  | FN    | 144    |                  |
| 13  | HN    | 144    |                  |
| 14  | AO    | 134    |                  |
| 14  | DO    | 134    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14  | FO    | 134    |                  |
| 14  | HO    | 134    |                  |
| 15  | AP    | 89     |                  |
| 15  | DP    | 89     |                  |
| 15  | FP    | 89     |                  |
| 15  | HP    | 89     |                  |
| 16  | AQ    | 104    |                  |
| 16  | DQ    | 104    |                  |
| 16  | FQ    | 104    |                  |
| 16  | HQ    | 104    |                  |
| 17  | AT    | 66     |                  |
| 17  | DT    | 66     |                  |
| 17  | FT    | 66     |                  |
| 17  | HT    | 66     |                  |
| 18  | AU    | 206    |                  |
| 18  | DU    | 206    |                  |
| 18  | FU    | 206    |                  |
| 18  | HU    | 206    |                  |
| 19  | AX    | 189    |                  |
| 19  | DX    | 189    |                  |
| 19  | FX    | 189    |                  |
| 19  | HX    | 189    |                  |
| 20  | B2    | 154    |                  |
| 20  | C2    | 154    |                  |
| 20  | E2    | 154    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 20  | G2    | 154    |                  |
| 21  | B3    | 120    |                  |
| 21  | C3    | 120    |                  |
| 21  | E3    | 120    |                  |
| 21  | G3    | 120    |                  |
| 22  | BA    | 264    |                  |
| 22  | CA    | 264    |                  |
| 22  | EA    | 264    |                  |
| 22  | GA    | 264    |                  |
| 23  | BB    | 391    |                  |
| 23  | CB    | 391    |                  |
| 23  | EB    | 391    |                  |
| 23  | GB    | 391    |                  |
| 24  | BC    | 410    |                  |
| 24  | CC    | 410    |                  |
| 24  | EC    | 410    |                  |
| 24  | GC    | 410    |                  |
| 25  | BD    | 172    |                  |
| 25  | CD    | 172    |                  |
| 25  | ED    | 172    |                  |
| 25  | GD    | 172    |                  |
| 26  | BE    | 188    |                  |
| 26  | CE    | 188    |                  |
| 26  | EE    | 188    |                  |
| 26  | GE    | 188    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 27  | BF    | 255    |                  |
| 27  | CF    | 255    |                  |
| 27  | EF    | 255    |                  |
| 27  | GF    | 255    |                  |
| 28  | BG    | 123    |                  |
| 28  | CG    | 123    |                  |
| 28  | EG    | 123    |                  |
| 28  | GG    | 123    |                  |
| 29  | BH    | 215    |                  |
| 29  | CH    | 215    |                  |
| 29  | EH    | 215    |                  |
| 29  | GH    | 215    |                  |
| 30  | BI    | 198    |                  |
| 30  | CI    | 198    |                  |
| 30  | EI    | 198    |                  |
| 30  | GI    | 198    |                  |
| 31  | BJ    | 141    |                  |
| 31  | CJ    | 141    |                  |
| 31  | EJ    | 141    |                  |
| 31  | GJ    | 141    |                  |
| 32  | BK    | 149    |                  |
| 32  | CK    | 149    |                  |
| 32  | EK    | 149    |                  |
| 32  | GK    | 149    |                  |
| 33  | BL    | 204    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 33  | CL    | 204    |                  |
| 33  | EL    | 204    |                  |
| 33  | GL    | 204    |                  |
| 34  | BM    | 301    |                  |
| 34  | CM    | 301    |                  |
| 34  | EM    | 301    |                  |
| 34  | GM    | 301    |                  |
| 35  | BN    | 181    |                  |
| 35  | CN    | 181    |                  |
| 35  | EN    | 181    |                  |
| 35  | GN    | 181    |                  |
| 36  | BO    | 185    |                  |
| 36  | EO    | 185    |                  |
| 36  | GO    | 185    |                  |
| 37  | BP    | 157    |                  |
| 37  | CP    | 157    |                  |
| 37  | EP    | 157    |                  |
| 37  | GP    | 157    |                  |
| 38  | BQ    | 183    |                  |
| 38  | CQ    | 183    |                  |
| 38  | EQ    | 183    |                  |
| 38  | GQ    | 183    |                  |
| 39  | BR    | 150    |                  |
| 39  | CR    | 150    |                  |
| 39  | ER    | 150    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 39  | GR    | 150    |                  |
| 40  | BS    | 135    |                  |
| 40  | CS    | 135    |                  |
| 40  | ES    | 135    |                  |
| 40  | GS    | 135    |                  |
| 41  | BT    | 158    |                  |
| 41  | CT    | 158    |                  |
| 41  | ET    | 158    |                  |
| 41  | GT    | 158    |                  |
| 42  | BU    | 124    |                  |
| 42  | CU    | 124    |                  |
| 42  | EU    | 124    |                  |
| 42  | GU    | 124    |                  |
| 43  | BV    | 239    |                  |
| 43  | CV    | 239    |                  |
| 43  | EV    | 239    |                  |
| 43  | GV    | 239    |                  |
| 44  | BW    | 111    |                  |
| 44  | CW    | 111    |                  |
| 44  | EW    | 111    |                  |
| 44  | GW    | 111    |                  |
| 45  | BX    | 134    |                  |
| 45  | CX    | 134    |                  |
| 45  | EX    | 134    |                  |
| 45  | GX    | 134    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 46  | BY    | 103    |                  |
| 46  | CY    | 103    |                  |
| 46  | EY    | 103    |                  |
| 46  | GY    | 103    |                  |
| 47  | CO    | 185    |                  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 48  | MG   | H1    | 3551 | -         | -        | -       | X                |

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 511395 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 26S RRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | A1    | 3119     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 66769 | 29861 | 12195 | 21594 | 3119 |         |         |       |
| 1   | D1    | 3119     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 66769 | 29861 | 12195 | 21594 | 3119 |         |         |       |
| 1   | F1    | 3119     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 66769 | 29861 | 12195 | 21594 | 3119 |         |         |       |
| 1   | H1    | 3119     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 66769 | 29861 | 12195 | 21594 | 3119 |         |         |       |

- Molecule 2 is a protein called RIBOSOMAL PROTEIN L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | AA    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 721   | 440 | 158 | 116 | 7 |         |         |       |
| 2   | DA    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 721   | 440 | 158 | 116 | 7 |         |         |       |
| 2   | FA    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 721   | 440 | 158 | 116 | 7 |         |         |       |
| 2   | HA    | 91       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 721   | 440 | 158 | 116 | 7 |         |         |       |

- Molecule 3 is a protein called RPL39.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 3   | AB    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 97 | 70 | 1 |         |         |       |
| 3   | DB    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 97 | 70 | 1 |         |         |       |
| 3   | FB    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 97 | 70 | 1 |         |         |       |
| 3   | HB    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 97 | 70 | 1 |         |         |       |

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L36A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | AC    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 836   | 526 | 163 | 140 | 7 |         |         |       |
| 4   | DC    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 836   | 526 | 163 | 140 | 7 |         |         |       |
| 4   | FC    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 836   | 526 | 163 | 140 | 7 |         |         |       |
| 4   | HC    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 836   | 526 | 163 | 140 | 7 |         |         |       |

- Molecule 5 is a protein called RPL6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 190      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1525  | 966 | 286 | 272 | 1 |         |         |       |
| 5   | DE    | 190      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1525  | 966 | 286 | 272 | 1 |         |         |       |
| 5   | FE    | 190      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1525  | 966 | 286 | 272 | 1 |         |         |       |
| 5   | HE    | 190      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1525  | 966 | 286 | 272 | 1 |         |         |       |

- Molecule 6 is a protein called RPL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 659 | 192 | 169 | 1 |         |         |       |
| 6   | DF    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 659 | 192 | 169 | 1 |         |         |       |
| 6   | FF    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 659 | 192 | 169 | 1 |         |         |       |
| 6   | HF    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1021  | 659 | 192 | 169 | 1 |         |         |       |

- Molecule 7 is a protein called RPL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 455 | 129 | 138 | 5 |         |         |       |
| 7   | DG    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 455 | 129 | 138 | 5 |         |         |       |
| 7   | FG    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 455 | 129 | 138 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | HG    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 727   | 455 | 129 | 138 | 5 |         |         |       |

- Molecule 8 is a protein called RPL35A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 167 | 142 | 1 |         |         |       |
| 8   | DH    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 167 | 142 | 1 |         |         |       |
| 8   | FH    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 167 | 142 | 1 |         |         |       |
| 8   | HH    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 850   | 540 | 167 | 142 | 1 |         |         |       |

- Molecule 9 is a protein called TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 9   | AJ    | 226      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1716  | 1068 | 302 | 336 | 10 |         |         |       |
| 9   | DJ    | 226      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1716  | 1068 | 302 | 336 | 10 |         |         |       |
| 9   | FJ    | 226      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1716  | 1068 | 302 | 336 | 10 |         |         |       |
| 9   | HJ    | 226      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1716  | 1068 | 302 | 336 | 10 |         |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| AJ    | -2      | GLY      | -      | expression tag | UNP Q245F2 |
| AJ    | -1      | THR      | -      | expression tag | UNP Q245F2 |
| AJ    | 0       | SER      | -      | expression tag | UNP Q245F2 |
| DJ    | -2      | GLY      | -      | expression tag | UNP Q245F2 |
| DJ    | -1      | THR      | -      | expression tag | UNP Q245F2 |
| DJ    | 0       | SER      | -      | expression tag | UNP Q245F2 |
| FJ    | -2      | GLY      | -      | expression tag | UNP Q245F2 |
| FJ    | -1      | THR      | -      | expression tag | UNP Q245F2 |
| FJ    | 0       | SER      | -      | expression tag | UNP Q245F2 |
| HJ    | -2      | GLY      | -      | expression tag | UNP Q245F2 |
| HJ    | -1      | THR      | -      | expression tag | UNP Q245F2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| HJ    | 0       | SER      | -      | expression tag | UNP Q245F2 |

- Molecule 10 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | AK    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 415   | 257 | 83 | 69 | 6 |         |         |       |
| 10  | DK    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 415   | 257 | 83 | 69 | 6 |         |         |       |
| 10  | FK    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 415   | 257 | 83 | 69 | 6 |         |         |       |
| 10  | HK    | 52       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 415   | 257 | 83 | 69 | 6 |         |         |       |

- Molecule 11 is a protein called RPL34.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AL    | 108      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 529 | 170 | 147 | 6 |         |         |       |
| 11  | DL    | 108      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 529 | 170 | 147 | 6 |         |         |       |
| 11  | FL    | 108      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 529 | 170 | 147 | 6 |         |         |       |
| 11  | HL    | 108      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 852   | 529 | 170 | 147 | 6 |         |         |       |

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AM    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 819   | 530 | 137 | 151 | 1 |         |         |       |
| 12  | DM    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 819   | 530 | 137 | 151 | 1 |         |         |       |
| 12  | FM    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 819   | 530 | 137 | 151 | 1 |         |         |       |
| 12  | HM    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 819   | 530 | 137 | 151 | 1 |         |         |       |

- Molecule 13 is a protein called RPL27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AN    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1170  | 755 | 213 | 199 | 3 |         |         |       |
| 13  | DN    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1170  | 755 | 213 | 199 | 3 |         |         |       |
| 13  | FN    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1170  | 755 | 213 | 199 | 3 |         |         |       |
| 13  | HN    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1170  | 755 | 213 | 199 | 3 |         |         |       |

- Molecule 14 is a protein called RPL28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | AO    | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1034  | 650 | 204 | 179 | 1 |         |         |       |
| 14  | DO    | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1034  | 650 | 204 | 179 | 1 |         |         |       |
| 14  | FO    | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1034  | 650 | 204 | 179 | 1 |         |         |       |
| 14  | HO    | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1034  | 650 | 204 | 179 | 1 |         |         |       |

- Molecule 15 is a protein called RPL38.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 15  | AP    | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 551   | 367 | 93 | 90 | 1 |         |         |       |
| 15  | DP    | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 551   | 367 | 93 | 90 | 1 |         |         |       |
| 15  | FP    | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 551   | 367 | 93 | 90 | 1 |         |         |       |
| 15  | HP    | 66       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 551   | 367 | 93 | 90 | 1 |         |         |       |

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L36.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 16  | AQ    | 102      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 803   | 506 | 165 | 132 |         |         |       |
| 16  | DQ    | 102      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 803   | 506 | 165 | 132 |         |         |       |
| 16  | FQ    | 102      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 803   | 506 | 165 | 132 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 16  | HQ    | 102      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 803   | 506 | 165 | 132 |         |         |       |

- Molecule 17 is a protein called RPL29.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 17  | AT    | 65       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 533   | 324 | 117 | 92 |         |         |       |
| 17  | DT    | 65       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 533   | 324 | 117 | 92 |         |         |       |
| 17  | FT    | 65       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 533   | 324 | 117 | 92 |         |         |       |
| 17  | HT    | 65       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 533   | 324 | 117 | 92 |         |         |       |

- Molecule 18 is a protein called RPL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 18  | AU    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1015 | 328 | 279 | 2 |         |         |       |
| 18  | DU    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1015 | 328 | 279 | 2 |         |         |       |
| 18  | FU    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1015 | 328 | 279 | 2 |         |         |       |
| 18  | HU    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1624  | 1015 | 328 | 279 | 2 |         |         |       |

- Molecule 19 is a protein called RPL18A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AX    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1536  | 972 | 287 | 271 | 6 |         |         |       |
| 19  | DX    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1536  | 972 | 287 | 271 | 6 |         |         |       |
| 19  | FX    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1536  | 972 | 287 | 271 | 6 |         |         |       |
| 19  | HX    | 188      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1536  | 972 | 287 | 271 | 6 |         |         |       |

- Molecule 20 is a RNA chain called 5.8S RRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|---------|-------|
| 20  | B2    | 154      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3300  | 1475 | 602 | 1069 | 154 |         |         |       |
| 20  | C2    | 154      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3300  | 1475 | 602 | 1069 | 154 |         |         |       |
| 20  | E2    | 154      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3300  | 1475 | 602 | 1069 | 154 |         |         |       |
| 20  | G2    | 154      | Total | C    | N   | O    | P   | 0       | 0       | 0     |
|     |       |          | 3300  | 1475 | 602 | 1069 | 154 |         |         |       |

- Molecule 21 is a RNA chain called 5S RRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 21  | B3    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2566  | 1145 | 463 | 838 | 120 |         |         |       |
| 21  | C3    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2566  | 1145 | 463 | 838 | 120 |         |         |       |
| 21  | E3    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2566  | 1145 | 463 | 838 | 120 |         |         |       |
| 21  | G3    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2566  | 1145 | 463 | 838 | 120 |         |         |       |

- Molecule 22 is a protein called RPL8.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 22  | BA    | 257      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1977  | 1226 | 400 | 343 | 8 |         |         |       |
| 22  | CA    | 257      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1977  | 1226 | 400 | 343 | 8 |         |         |       |
| 22  | EA    | 257      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1977  | 1226 | 400 | 343 | 8 |         |         |       |
| 22  | GA    | 257      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1977  | 1226 | 400 | 343 | 8 |         |         |       |

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 23  | BB    | 386      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3080  | 1944 | 595 | 530 | 11 |         |         |       |
| 23  | CB    | 386      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3080  | 1944 | 595 | 530 | 11 |         |         |       |
| 23  | EB    | 386      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3080  | 1944 | 595 | 530 | 11 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 23  | GB    | 386      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3080  | 1944 | 595 | 530 | 11 |         |         |       |

- Molecule 24 is a protein called RPL4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24  | BC    | 409      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3172  | 1975 | 622 | 571 | 4 |         |         |       |
| 24  | CC    | 409      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3172  | 1975 | 622 | 571 | 4 |         |         |       |
| 24  | EC    | 409      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3172  | 1975 | 622 | 571 | 4 |         |         |       |
| 24  | GC    | 409      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3172  | 1975 | 622 | 571 | 4 |         |         |       |

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | BD    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1357  | 851 | 254 | 243 | 9 |         |         |       |
| 25  | CD    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1357  | 851 | 254 | 243 | 9 |         |         |       |
| 25  | ED    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1357  | 851 | 254 | 243 | 9 |         |         |       |
| 25  | GD    | 169      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1357  | 851 | 254 | 243 | 9 |         |         |       |

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | BE    | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1481  | 939 | 272 | 264 | 6 |         |         |       |
| 26  | CE    | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1481  | 939 | 272 | 264 | 6 |         |         |       |
| 26  | EE    | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1481  | 939 | 272 | 264 | 6 |         |         |       |
| 26  | GE    | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1481  | 939 | 272 | 264 | 6 |         |         |       |

- Molecule 27 is a protein called RPL7A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 27  | BF    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1860  | 1191 | 341 | 327 | 1 |         |         |       |
| 27  | CF    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1860  | 1191 | 341 | 327 | 1 |         |         |       |
| 27  | EF    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1860  | 1191 | 341 | 327 | 1 |         |         |       |
| 27  | GF    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1860  | 1191 | 341 | 327 | 1 |         |         |       |

- Molecule 28 is a protein called RPLP0.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 28  | BG    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 711   | 465 | 123 | 123 |         |         |       |
| 28  | CG    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 711   | 465 | 123 | 123 |         |         |       |
| 28  | EG    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 711   | 465 | 123 | 123 |         |         |       |
| 28  | GG    | 123      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 711   | 465 | 123 | 123 |         |         |       |

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 29  | BH    | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1620  | 1027 | 319 | 271 | 3 |         |         |       |
| 29  | CH    | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1620  | 1027 | 319 | 271 | 3 |         |         |       |
| 29  | EH    | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1620  | 1027 | 319 | 271 | 3 |         |         |       |
| 29  | GH    | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1620  | 1027 | 319 | 271 | 3 |         |         |       |

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN L13A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 30  | BI    | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1594  | 1019 | 308 | 263 | 4 |         |         |       |
| 30  | CI    | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1594  | 1019 | 308 | 263 | 4 |         |         |       |
| 30  | EI    | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1594  | 1019 | 308 | 263 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 30  | GI    | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1594  | 1019 | 308 | 263 | 4 |         |         |       |

- Molecule 31 is a protein called RPL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BJ    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 643 | 193 | 179 | 7 |         |         |       |
| 31  | CJ    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 643 | 193 | 179 | 7 |         |         |       |
| 31  | EJ    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 643 | 193 | 179 | 7 |         |         |       |
| 31  | GJ    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 643 | 193 | 179 | 7 |         |         |       |

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN L27A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BK    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1161  | 739 | 234 | 182 | 6 |         |         |       |
| 32  | CK    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1161  | 739 | 234 | 182 | 6 |         |         |       |
| 32  | EK    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1161  | 739 | 234 | 182 | 6 |         |         |       |
| 32  | GK    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1161  | 739 | 234 | 182 | 6 |         |         |       |

- Molecule 33 is a protein called RIBOSOMAL PROTEIN L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 33  | BL    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1691  | 1061 | 351 | 275 | 4 |         |         |       |
| 33  | CL    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1691  | 1061 | 351 | 275 | 4 |         |         |       |
| 33  | EL    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1691  | 1061 | 351 | 275 | 4 |         |         |       |
| 33  | GL    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1691  | 1061 | 351 | 275 | 4 |         |         |       |

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 34  | BM    | 298      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2409  | 1530 | 445 | 430 | 4 |         |         |       |
| 34  | CM    | 300      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2424  | 1541 | 447 | 432 | 4 |         |         |       |
| 34  | EM    | 300      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2424  | 1541 | 447 | 432 | 4 |         |         |       |
| 34  | GM    | 300      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2424  | 1541 | 447 | 432 | 4 |         |         |       |

- Molecule 35 is a protein called RPL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BN    | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 909 | 280 | 249 | 3 |         |         |       |
| 35  | CN    | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 909 | 280 | 249 | 3 |         |         |       |
| 35  | EN    | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 909 | 280 | 249 | 3 |         |         |       |
| 35  | GN    | 180      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1441  | 909 | 280 | 249 | 3 |         |         |       |

- Molecule 36 is a protein called RPL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | BO    | 184      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1491  | 924 | 311 | 251 | 5 |         |         |       |
| 36  | EO    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1192  | 745 | 249 | 193 | 5 |         |         |       |
| 36  | GO    | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1234  | 772 | 256 | 201 | 5 |         |         |       |

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BP    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1272  | 804 | 251 | 215 | 2 |         |         |       |
| 37  | CP    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1272  | 804 | 251 | 215 | 2 |         |         |       |
| 37  | EP    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1272  | 804 | 251 | 215 | 2 |         |         |       |
| 37  | GP    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1272  | 804 | 251 | 215 | 2 |         |         |       |

- Molecule 38 is a protein called RPL17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BQ    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1239  | 771 | 249 | 216 | 3 |         |         |       |
| 38  | CQ    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1239  | 771 | 249 | 216 | 3 |         |         |       |
| 38  | EQ    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1239  | 771 | 249 | 216 | 3 |         |         |       |
| 38  | GQ    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1239  | 771 | 249 | 216 | 3 |         |         |       |

- Molecule 39 is a protein called RPL23A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BR    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 613 | 176 | 173 | 3 |         |         |       |
| 39  | CR    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 613 | 176 | 173 | 3 |         |         |       |
| 39  | ER    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 613 | 176 | 173 | 3 |         |         |       |
| 39  | GR    | 121      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 965   | 613 | 176 | 173 | 3 |         |         |       |

- Molecule 40 is a protein called RPL26.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BS    | 126      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1013  | 638 | 200 | 173 | 2 |         |         |       |
| 40  | CS    | 126      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1013  | 638 | 200 | 173 | 2 |         |         |       |
| 40  | ES    | 126      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1013  | 638 | 200 | 173 | 2 |         |         |       |
| 40  | GS    | 126      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1013  | 638 | 200 | 173 | 2 |         |         |       |

- Molecule 41 is a protein called RPL24.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 41  | BT    | 61       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 510   | 331 | 100 | 76 | 3 |         |         |       |
| 41  | CT    | 61       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 510   | 331 | 100 | 76 | 3 |         |         |       |
| 41  | ET    | 61       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 510   | 331 | 100 | 76 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 41  | GT    | 61       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 510   | 331 | 100 | 76 | 3 |         |         |       |

- Molecule 42 is a protein called RPL35.

| Mol | Chain | Residues | Atoms |     |     |     |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 42  | BU    | 123      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 990   | 629 | 196 | 165 |  |         |         |       |
| 42  | CU    | 123      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 990   | 629 | 196 | 165 |  |         |         |       |
| 42  | EU    | 123      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 990   | 629 | 196 | 165 |  |         |         |       |
| 42  | GU    | 123      | Total | C   | N   | O   |  | 0       | 0       | 0     |
|     |       |          | 990   | 629 | 196 | 165 |  |         |         |       |

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 43  | BV    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1910  | 1221 | 362 | 323 | 4 |         |         |       |
| 43  | CV    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1910  | 1221 | 362 | 323 | 4 |         |         |       |
| 43  | EV    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1910  | 1221 | 362 | 323 | 4 |         |         |       |
| 43  | GV    | 234      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1910  | 1221 | 362 | 323 | 4 |         |         |       |

- Molecule 44 is a protein called 60S RIBOSOMAL PROTEIN L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | BW    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 901   | 563 | 171 | 164 | 3 |         |         |       |
| 44  | CW    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 901   | 563 | 171 | 164 | 3 |         |         |       |
| 44  | EW    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 901   | 563 | 171 | 164 | 3 |         |         |       |
| 44  | GW    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 901   | 563 | 171 | 164 | 3 |         |         |       |

- Molecule 45 is a protein called 60S RIBOSOMAL PROTEIN L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | BX    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1012  | 639 | 205 | 165 | 3 |         |         |       |
| 45  | CX    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1012  | 639 | 205 | 165 | 3 |         |         |       |
| 45  | EX    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1012  | 639 | 205 | 165 | 3 |         |         |       |
| 45  | GX    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1012  | 639 | 205 | 165 | 3 |         |         |       |

- Molecule 46 is a protein called RPL37A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | BY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 502 | 148 | 131 | 5 |         |         |       |
| 46  | CY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 502 | 148 | 131 | 5 |         |         |       |
| 46  | EY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 502 | 148 | 131 | 5 |         |         |       |
| 46  | GY    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 786   | 502 | 148 | 131 | 5 |         |         |       |

- Molecule 47 is a protein called RPL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | CO    | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1366  | 861 | 278 | 222 | 5 |         |         |       |

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 48  | A1    | 200      | Total | Mg  | 0       | 0       |
|     |       |          | 200   | 200 |         |         |
| 48  | AA    | 2        | Total | Mg  | 0       | 0       |
|     |       |          | 2     | 2   |         |         |
| 48  | AK    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 48  | B2    | 8        | Total | Mg  | 0       | 0       |
|     |       |          | 8     | 8   |         |         |
| 48  | B3    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 48  | BJ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 48  | BL    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | BN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | BP    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | BQ    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | BW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | C2    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 48  | C3    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 48  | CD    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | CJ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | CL    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | CN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | CQ    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | CW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | CY    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | D1    | 232      | Total<br>232 | Mg<br>232 | 0       | 0       |
| 48  | DA    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | DJ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | DK    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | DQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | E2    | 7        | Total<br>7   | Mg<br>7   | 0       | 0       |
| 48  | E3    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 48  | EJ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | EL    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | EN    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | EQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | EW    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | F1    | 184      | Total<br>184 | Mg<br>184 | 0       | 0       |
| 48  | FA    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | FK    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | FT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | G2    | 6        | Total<br>6   | Mg<br>6   | 0       | 0       |
| 48  | G3    | 5        | Total<br>5   | Mg<br>5   | 0       | 0       |
| 48  | GA    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | GJ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | GL    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | GN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | GO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | GP    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 48  | GQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | GW    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 48  | H1    | 155      | Total<br>155 | Mg<br>155 | 0       | 0       |
| 48  | HT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 49  | AA    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | AC    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | AK    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | AL    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | BY    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | CY    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | DA    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | DC    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | DK    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | DL    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | EY    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | FA    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | FC    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | FK    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | FL    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | GY    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | HA    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | HC    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | HK    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 49  | HL    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 50 is water.

| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 50  | A1    | 1134     | Total<br>1134 | O<br>1134 | 0       | 0       |
| 50  | AA    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 50  | AB    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 50  | AH    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 50  | AK    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 50  | AM    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 50  | AP    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | AT    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 50  | AU    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 50  | B2    | 54       | Total<br>54   | O<br>54   | 0       | 0       |
| 50  | B3    | 23       | Total<br>23   | O<br>23   | 0       | 0       |
| 50  | BA    | 12       | Total<br>12   | O<br>12   | 0       | 0       |
| 50  | BB    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 50  | BC    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 50  | BE    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 50  | BI    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 50  | BJ    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 50  | BK    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 50  | BL    | 8        | Total<br>8    | O<br>8    | 0       | 0       |
| 50  | BM    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | BN    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 50  | BO    | 2        | Total<br>2    | O<br>2    | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 50  | BP    | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 50  | BQ    | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 50  | BU    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 50  | BV    | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 50  | BW    | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 50  | BX    | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 50  | BY    | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 50  | C2    | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |
| 50  | C3    | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 50  | CA    | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 50  | CB    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 50  | CC    | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 50  | CD    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 50  | CE    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 50  | CI    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 50  | CJ    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 50  | CK    | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 50  | CL    | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |
| 50  | CM    | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 50  | CN    | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 50  | CO    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 50  | CP    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 50  | CQ    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 50  | CU    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 50  | CV    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 50  | CW    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 50  | CX    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 50  | CY    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 50  | D1    | 1341     | Total<br>1341 | O<br>1341 | 0       | 0       |
| 50  | DA    | 10       | Total<br>10   | O<br>10   | 0       | 0       |
| 50  | DB    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 50  | DE    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 50  | DJ    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | DK    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | DP    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 50  | DQ    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | DT    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 50  | DU    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 50  | DX    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | E2    | 44       | Total<br>44   | O<br>44   | 0       | 0       |
| 50  | E3    | 34       | Total<br>34   | O<br>34   | 0       | 0       |
| 50  | EA    | 4        | Total<br>4    | O<br>4    | 0       | 0       |

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| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 50  | EB    | 3        | Total<br>3    | O<br>3    | 0       | 0       |
| 50  | EC    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | EE    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | EJ    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 50  | EK    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 50  | EL    | 10       | Total<br>10   | O<br>10   | 0       | 0       |
| 50  | EM    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | EN    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 50  | EP    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 50  | EQ    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 50  | EV    | 6        | Total<br>6    | O<br>6    | 0       | 0       |
| 50  | EW    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 50  | EX    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 50  | EY    | 5        | Total<br>5    | O<br>5    | 0       | 0       |
| 50  | F1    | 1076     | Total<br>1076 | O<br>1076 | 0       | 0       |
| 50  | FA    | 7        | Total<br>7    | O<br>7    | 0       | 0       |
| 50  | FB    | 4        | Total<br>4    | O<br>4    | 0       | 0       |
| 50  | FE    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 50  | FH    | 1        | Total<br>1    | O<br>1    | 0       | 0       |
| 50  | FK    | 2        | Total<br>2    | O<br>2    | 0       | 0       |
| 50  | FL    | 3        | Total<br>3    | O<br>3    | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 50  | FP    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 50  | FT    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 50  | FU    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 50  | G2    | 34       | Total | O  | 0       | 0       |
|     |       |          | 34    | 34 |         |         |
| 50  | G3    | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 50  | GA    | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 50  | GB    | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 50  | GC    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 50  | GE    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 50  | GI    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 50  | GJ    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 50  | GK    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 50  | GL    | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 50  | GM    | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 50  | GN    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 50  | GO    | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 50  | GP    | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 50  | GQ    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 50  | GV    | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 50  | GW    | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 50  | GX    | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |

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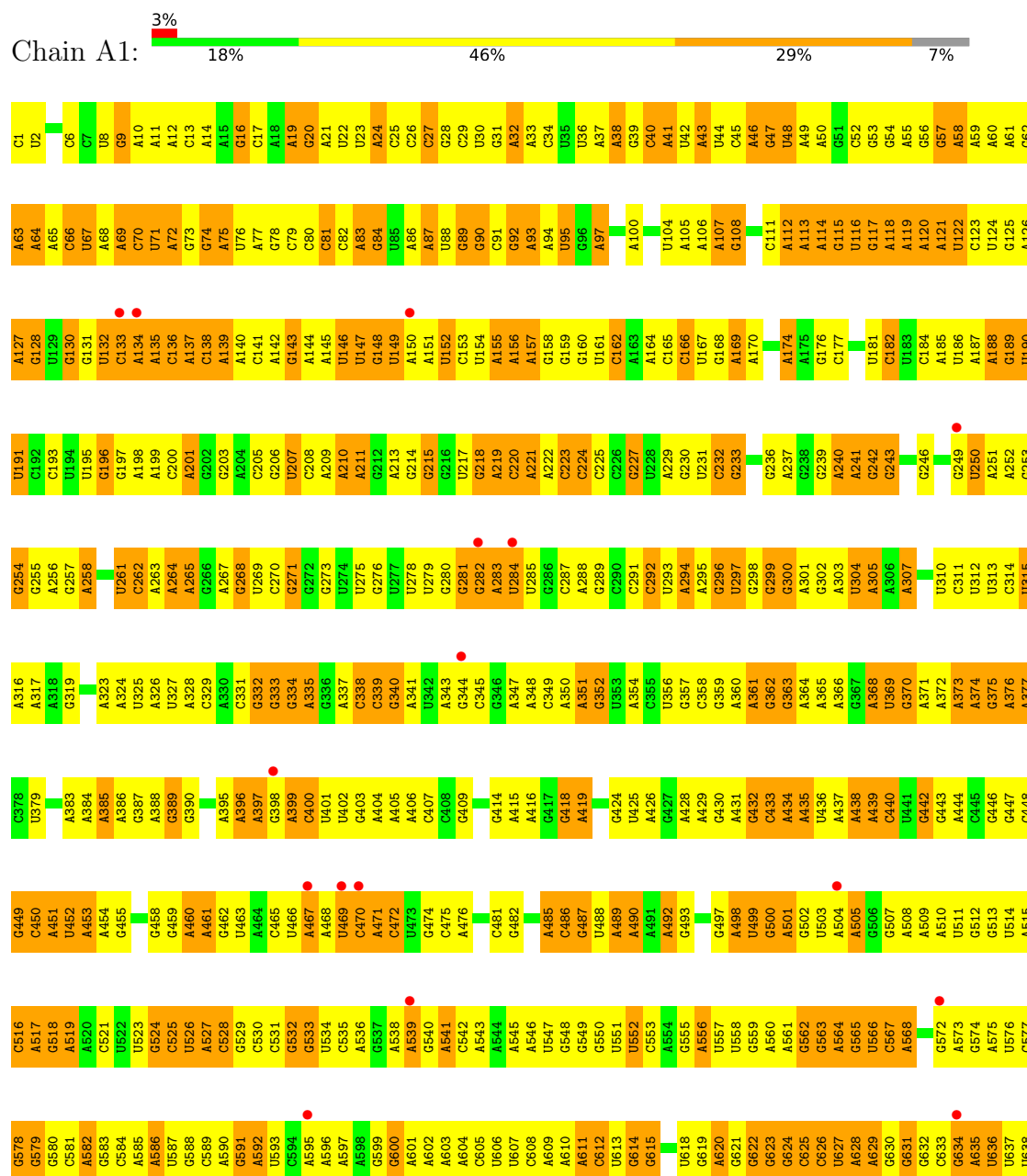
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 50  | GY    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 50  | H1    | 924      | Total<br>924 | O<br>924 | 0       | 0       |
| 50  | HA    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 50  | HB    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 50  | HJ    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 50  | HK    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 50  | HP    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 50  | HT    | 5        | Total<br>5   | O<br>5   | 0       | 0       |
| 50  | HU    | 2        | Total<br>2   | O<br>2   | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: 26S RRNA

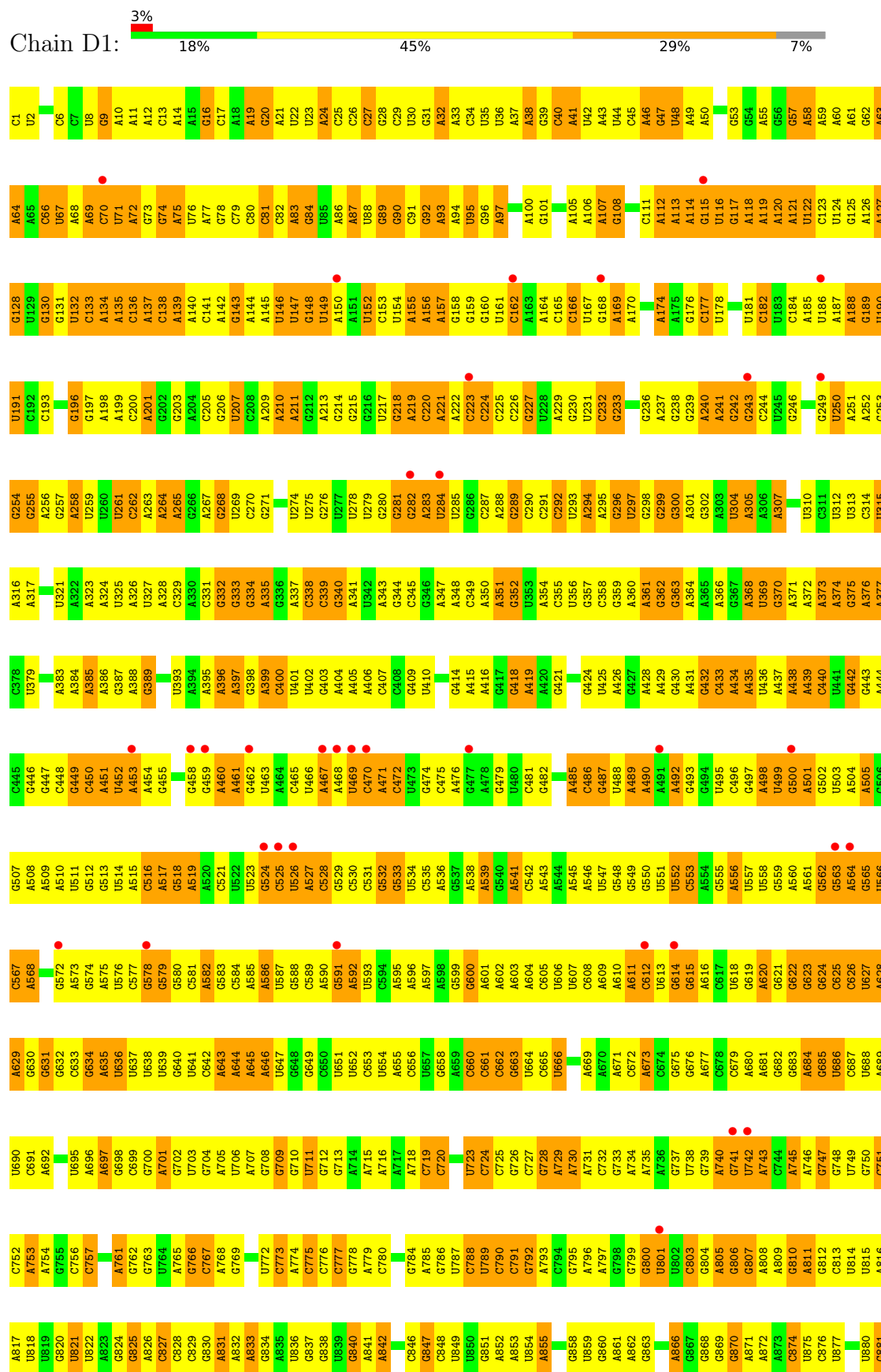


|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |    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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|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| U639 | U640 | U641 | U642 | U643 | U644 | U645 | U646 | U647 | U648 | U649 | U650 | U651 | U652 | U653 | U654 | U655 | U656 | U657 | U658 | U659 | U660 | U661 | U662 | U663 | U664 | U665 | U666 | U667 | U668 | U669 | U670 | U671 | U672 | U673 | U674 | U675 | U676 | U677 | U678 | U679 | U680 | U681 | U682 | U683 | U684 | U685 | U686 | U687 | U688 | U689 | U690 | U691 | U692 | U693 | U694 | U695 | U696 | U697 | U698 | U699 | U700 | U701 | U702 | U703 | U704 | U705 | U706 | U707 | U708 | U709 | U710 | U711 | U712 | U713 | U714 | U715 | U716 | U717 | U718 | U719 | U720 | U721 | U722 | U723 | U724 | U725 | U726 | U727 | U728 | U729 | U730 | U731 | U732 | U733 | U734 | U735 | U736 | U737 | U738 | U739 | U740 | U741 | U742 | U743 | U744 | U745 | U746 | U747 | U748 | U749 | U750 | U751 | U752 | U753 | U754 | U755 | U756 | U757 | U758 | U759 | U760 | U761 | U762 | U763 | U764 | U765 | U766 | U767 | U768 | U769 | U770 | U771 | U772 | U773 | U774 | U775 | U776 | U777 | U778 | U779 | U780 | U781 | U782 | U783 | U784 | U785 | U786 | U787 | U788 | U789 | U790 | U791 | U792 | U793 | U794 | U795 | U796 | U797 | U798 | U799 | U800 | U801 | U802 | U803 | U804 | U805 | U806 | U807 | U808 | U809 | U810 | U811 | U812 | U813 | U814 | U815 | U816 | U817 | U818 | U819 | U820 | U821 | U822 | U823 | U824 | U825 | U826 | U827 | U828 | U829 | U830 | U831 | U832 | U833 | U834 | U835 | U836 | U837 | U838 | U839 | U840 | U841 | U842 | U843 | U844 | U845 | U846 | U847 | U848 | U849 | U850 | U851 | U852 | U853 | U854 | U855 | U856 | U857 | U858 | U859 | U860 | U861 | U862 | U863 | U864 | U865 | U866 | U867 | U868 | U869 | U870 | U871 | U872 | U873 | U874 | U875 | U876 | U877 | U878 | U879 | U880 | U881 | U882 | U883 | U884 | U885 | U886 | U887 | U888 | U889 | U890 | U891 | U892 | U893 | U894 | U895 | U896 | U897 | U898 | U899 | U900 | U901 | U902 | U903 | U904 | U905 | U906 | U907 | U908 | U909 | U910 | U911 | U912 | U913 | U914 | U915 | U916 | U917 | U918 | U919 | U920 | U921 | U922 | U923 | U924 | U925 | U926 | U927 | U928 | U929 | U930 | U931 | U932 | U933 | U934 | U935 | U936 | U937 | U938 | U939 | U940 | U941 | U942 | U943 | U944 | U945 | U946 | U947 | U948 | U949 | U950 | U951 | U952 | U953 | U954 | U955 | U956 | U957 | U958 | U959 | U960 | U961 | U962 | U963 | U964 | U965 | U966 | U967 | U968 | U969 | U970 | U971 | U972 | U973 | U974 | U975 | U976 | U977 | U978 | U979 | U980 | U981 | U982 | U983 | U984 | U985 | U986 | U987 | U988 | U989 | U990 | U991 | U992 | U993 | U994 | U995 | U996 | U997 | U998 | U999 | U1000 | U1001 | U1002 | U1003 | U1004 | U1005 | U1006 | U1007 | U1008 | U1009 | U1010 | U1011 | U1012 | U1013 | U1014 | U1015 | U1016 | U1017 | U1018 | U1019 | U1020 | U1021 | U1022 | U1023 | U1024 | U1025 | U1026 | U1027 | U1028 | U1029 | U1030 | U1031 | U1032 | U1033 | U1034 | U1035 | U1036 | U1037 | U1038 | U1039 | U1040 | U1041 | U1042 | U1043 | U1044 | U1045 | U1046 | U1047 | U1048 | U1049 | U1050 | U1051 | U1052 | U1053 | U1054 | U1055 | U1056 | U1057 | U1058 | U1059 | U1060 | U1061 | U1062 | U1063 | U1064 | U1065 | U1066 | U1067 | U1068 | U1069 | U1070 | U1071 | U1072 | U1073 | U1074 | U1075 | U1076 | U1077 | U1078 | U1079 | U1080 | U1081 | U1082 | U1083 | U1084 | U1085 | U1086 | U1087 | U1088 | U1089 | U1090 | U1091 | U1092 | U1093 | U1094 | U1095 | U1096 | U1097 | U1098 | U1099 | U1100 | U1101 | U1102 | U1103 | U1104 | U1105 | U1106 | U1107 | U1108 | U1109 | U1110 | U1111 | U1112 | U1113 | U1114 | U1115 | U1116 | U1117 | U1118 | U1119 | U1120 | U1121 | U1122 | U1123 | U1124 | U1125 | U1126 | U1127 | U1128 | U1129 | U1130 | U1131 | U1132 | U1133 | U1134 | U1135 | U1136 | U1137 | U1138 | U1139 | U1140 | U1141 | U1142 | U1143 | U1144 | U1145 | U1146 | U1147 | U1148 | U1149 | U1150 | U1151 | U1152 | U1153 | U1154 | U1155 | U1156 | U1157 | U1158 | U1159 | U1160 | U1161 | U1162 | U1163 | U1164 | U1165 | U1166 | U1167 | U1168 | U1169 | U1170 | U1171 | U1172 | U1173 | U1174 | U1175 | U1176 | U1177 | U1178 | U1179 | U1180 | U1181 | U1182 | U1183 | U1184 | U1185 | U1186 | U1187 | U1188 | U1189 | U1190 | U1191 | U1192 | U1193 | U1194 | U1195 | U1196 | U1197 | U1198 | U1199 | U1200 | U1201 | U1202 | U1203 | U1204 | U1205 | U1206 | U1207 | U1208 | U1209 | U1210 | U1211 | U1212 | U1213 | U1214 | U1215 | U1216 | U1217 | U1218 | U1219 | U1220 | U1221 | U1222 | U1223 | U1224 | U1225 | U1226 | U1227 | U1228 | U1229 | U1230 | U1231 | U1232 | U1233 | U1234 | U1235 | U1236 | U1237 | U1238 | U1239 | U1240 | U1241 | U1242 | U1243 | U1244 | U1245 | U1246 | U1247 | U1248 | U1249 | U1250 | U1251 | U1252 | U1253 | U1254 | U1255 | U1256 | U1257 | U1258 | U1259 | U1260 | U1261 | U1262 | U1263 | U1264 | U1265 | U1266 | U1267 | U1268 | U1269 | U1270 | U1271 | U1272 | U1273 | U1274 | U1275 | U1276 | U1277 | U1278 | U1279 | U1280 | U1281 | U1282 | U1283 | U1284 | U1285 | U1286 | U1287 | U1288 | U1289 | U1290 | U1291 | U1292 | U1293 | U1294 | U1295 | U1296 | U1297 | U1298 | U1299 | U1300 | U1301 | U1302 | U1303 | U1304 | U1305 | U1306 | U1307 | U1308 | U1309 | U1310 | U1311 | U1312 | U1313 | U1314 | U1315 | U1316 | U1317 | U1318 | U1319 | U1320 | U1321 | U1322 | U1323 | U1324 | U1325 | U1326 | U1327 | U1328 | U1329 | U1330 | U1331 | U1332 | U1333 | U1334 | U1335 | U1336 | U1337 | U1338 | U1339 | U1340 | U1341 | U1342 | U1343 | U1344 | U1345 | U1346 | U1347 | U1348 | U1349 | U1350 | U1351 | U1352 | U1353 | U1354 | U1355 | U1356 | U1357 | U1358 | U1359 | U1360 | U1361 | U1362 | U1363 | U1364 | U1365 | U1366 | U1367 | U1368 | U1369 | U1370 | U1371 | U1372 | U1373 | U1374 | U1375 | U1376 | U1377 | U1378 | U1379 | U1380 | U1381 | U1382 | U1383 | U1384 | U1385 | U1386 | U1387 | U1388 | U1389 | U1390 | U1391 | U1392 | U1393 | U1394 | U1395 | U1396 | U1397 | U1398 | U1399 | U1400 | U1401 | U1402 | U1403 | U1404 | U1405 | U1406 | U1407 | U1408 | U1409 | U1410 | U1411 | U1412 | U1413 | U1414 | U1415 | U1416 | U1417 | U1418 | U1419 | U1420 | U1421 | U1422 | U1423 | U1424 | U1425 | U1426 | U1427 | U1428 | U1429 | U1430 | U1431 | U1432 | U1433 | 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U1559 | U1560 | U1561 | U1562 | U1563 | U1564 | U1565 | U1566 | U1567 | U1568 | U1569 | U1570 | U1571 | U1572 | U1573 | U1574 | U1575 | U1576 | U1577 | U1578 | U1579 | U1580 | U1581 | U1582 | U1583 | U1584 | U1585 | U1586 | U1587 | U1588 | U1589 | U1590 | U1591 | U1592 | U1593 | U1594 | U1595 | U1596 | U1597 | U1598 | U1599 | U1600 | U1601 | U1602 | U1603 | U1604 | U1605 | U1606 | U1607 | U1608 | U1609 | U1610 | U1611 | U1612 | U1613 | U1614 | U1615 | U1616 | U1617 | U1618 | U1619 | U1620 | U1621 | U1622 | U1623 | U1624 | U1625 | U1626 | U1627 | U1628 | U1629 | U1630 | U1631 | U1632 | U1633 | U1634 | U1635 | U1636 | U1637 | U1638 | U1639 | U1640 | U1641 | U1642 | U1643 | U1644 | U1645 | U1646 | U1647 | U1648 | U1649 | U1650 | U1651 | U1652 | U1653 | U1654 | U1655 | U1656 | U1657 | U1658 | U1659 | U1660 | U1661 | U1662 | U1663 | U1664 | U1665 | U1666 | U1667 | U1668 | U1669 | U1670 | U1671 | U1672 | U1673 | U1674 | U1675 | U1676 | U1677 | U1678 | U1679 | U1680 | U1681 | U1682 | U1683 | U1684 | U1685 | U1686 | U1687 | U1688 | U1689 | U1690 | U1691 | U1692 | U1693 | U1694 | U1695 | U1696 | U1697 | U1698 | U1699 | U1700 | U1701 | U1702 | U1703 | U1704 | U1705 | U1706 | U1707 | U1708 | U1709 | U1710 | U1711 | U1712 | U1713 | U1714 | U1715 | U1716 | U1717 | U1718 | U1719 | U1720 | U1721 | U1722 | U1723 | U1724 | U1725 | U1726 | U1727 | U1728 | U1729 | U1730 | U1731 | U1732 | U1733 | U1734 | U1735 | U1736 | U1737 | U1738 | U1739 | U1740 | U1741 | U1742 | U1743 | U1744 | U1745 | U1746 | U1747 | U1748 | U1749 | U1750 | U1751 | U1752 | U1753 | U1754 | U1755 | U1756 | U1757 | U1758 | U1759 | U1760 | U1761 | U1762 | U1763 | U1764 | U1765 | U1766 | U1767 | U1768 | U1769 | U1770 | U1771 | U1772 | U1773 | U1774 | U1775 | U1776 | U1777 | U1778 | U1779 | U1780 | U1781 | U1782 | U1783 | U1784 | U1785 | U1786 | U1787 | U1788 | U1789 | U1790 | U1791 | U1792 | U1793 | U1794 | U1795 | U1796 | U1797 | U1798 | U1799 | U1800 | U1801 | U1802 | U1803 | U1804 | U1805 | U1806 | U1807 | U1808 | 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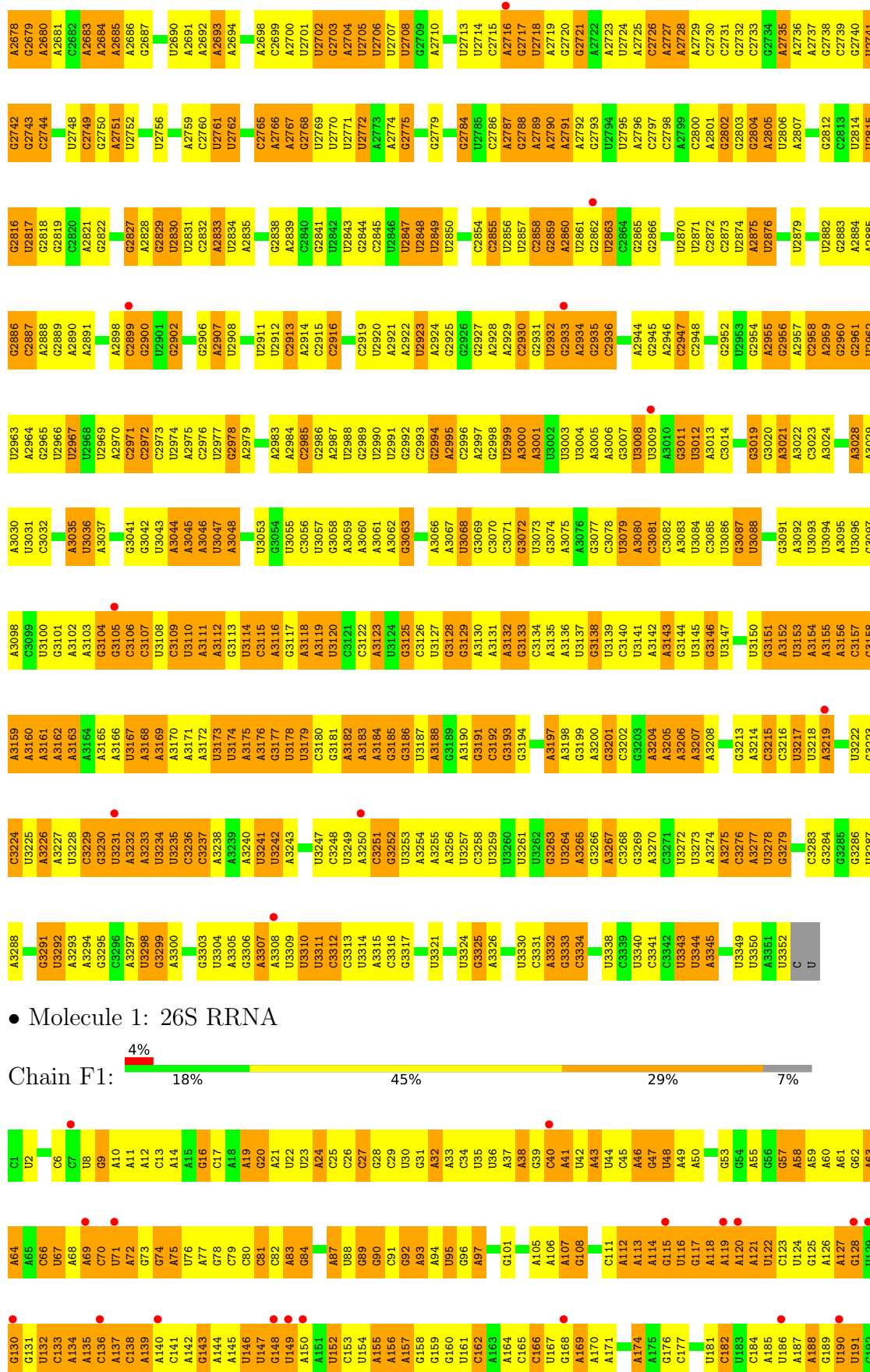
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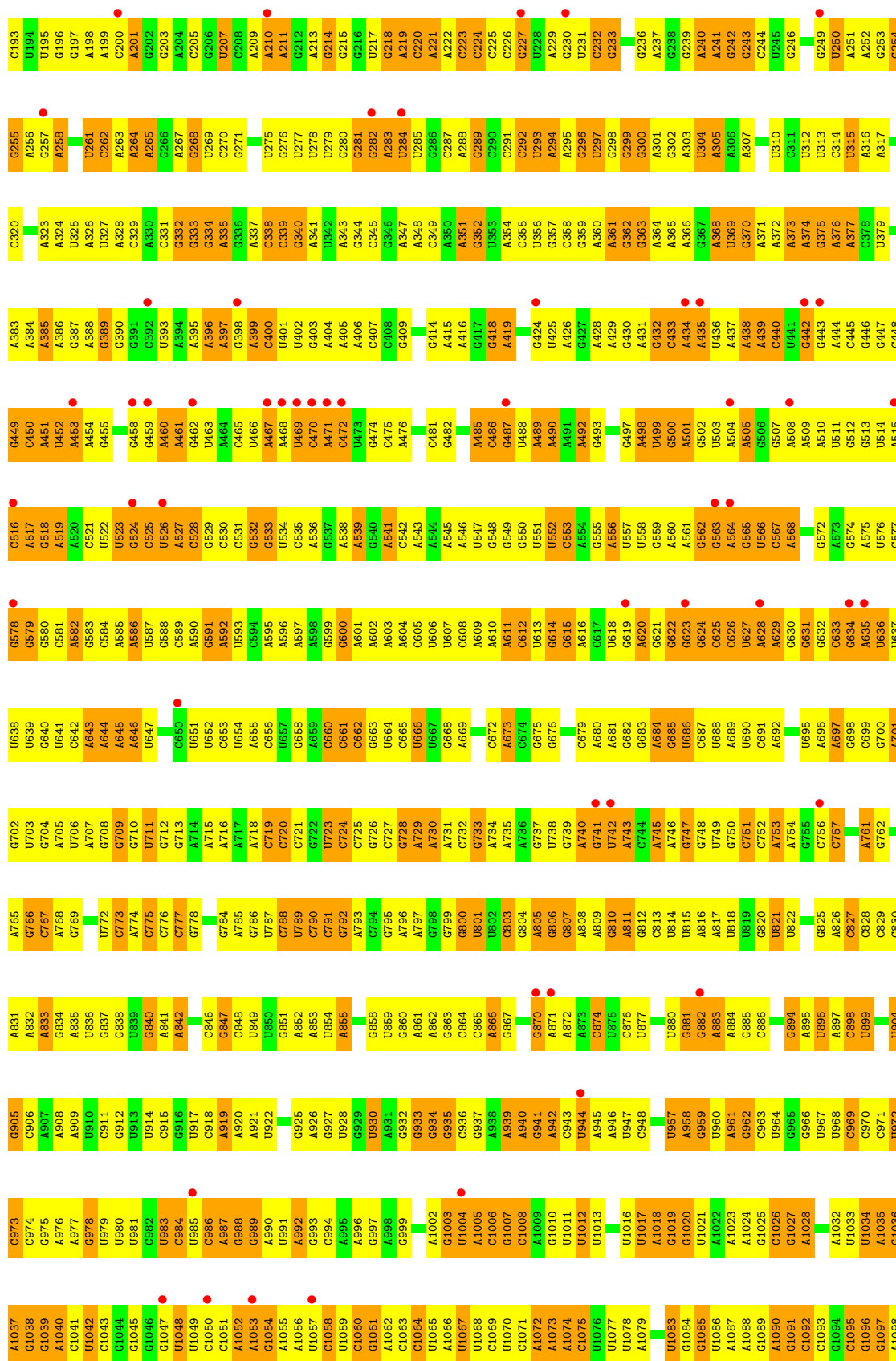
● Molecule 1: 26S RRNA





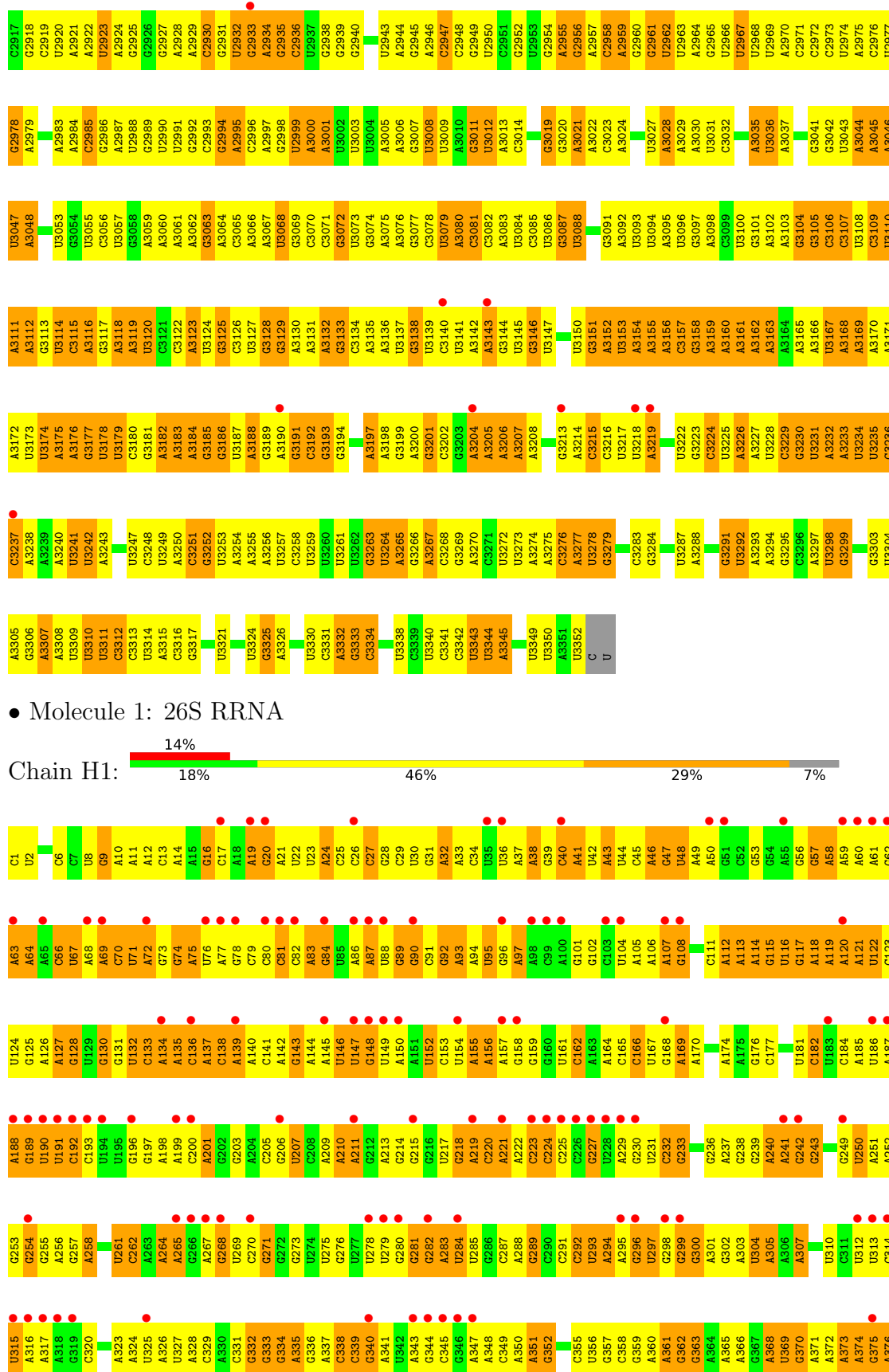






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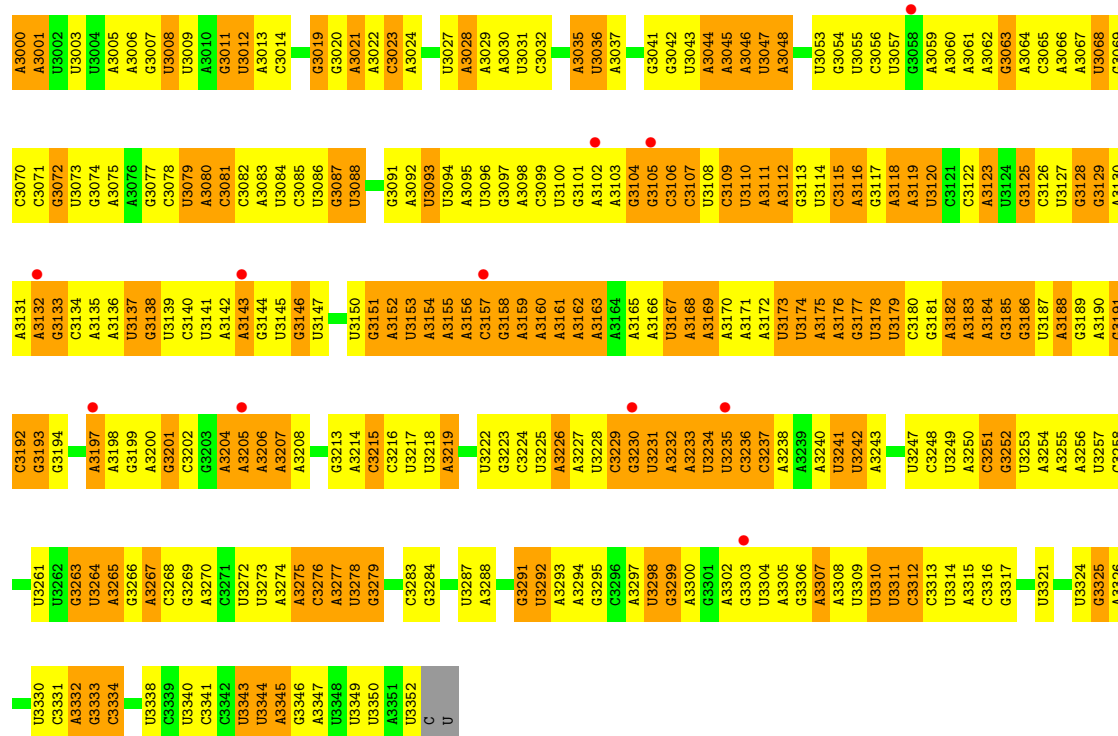




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|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
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| C2155 | G2156 | C2157 | C2158 | C2159 | A2162 | A2163 | C2164 | A2165 | U2168 | G2169 | A2170 | U2171 | G2172 | A2173 | U2178 | U2179 | G2180 | U2181 | G2182 | G2183 | U2184 | U2185 | U2186 | C2187 | U2188 | G2189 | C2190 | C2191 | A2192 | A2193 | G2194 | U2195 | G2196 | C2199 | U2200 | G2201 | A2202 | U2203 | U2204 | A2208 | A2209 | U2210 | G2211 | U2212 | A2214 | C2215 | A2216 | G2217 | A2218 | U2219 | U2220 | C2221 |       |       |       |       |       |       |
| C2222 | A2223 | A2227 | A2228 | A2238 | A2239 | C2240 | G2241 | G2242 | U2243 | G2244 | G2245 | G2246 | G2247 | G2248 | U2249 | A2250 | A2251 | G2252 | U2253 | A2254 | G2255 | G2256 | A2257 | U2258 | U2259 | U2260 | U2261 | G2262 | U2263 | U2264 | A2265 | G2266 | G2267 | G2268 | U2269 | A2270 | G2271 | C2272 | C2273 | C2274 | A2275 | A2276 | U2277 | G2278 | G2279 | C2280 | U2281 | C2282 | G2283 | U2284 | C2285 | A2286 | U2287 | C2288 | U2289 | C2290 | C2291 |       |
| U2292 | U2293 | A2294 | G2295 | A2298 | C2299 | C2300 | C2301 | G2302 | C2303 | A2304 | U2305 | G2306 | A2307 | A2308 | U2309 | G2310 | G2311 | U2312 | U2313 | U2314 | A2315 | A2316 | U2317 | G2318 | A2319 | U2320 | A2321 | U2322 | U2323 | A2324 | C2325 | C2326 | U2327 | U2328 | G2329 | G2330 | U2331 | C2332 | C2333 | C2334 | U2335 | U2339 | A2340 | U2342 | U2343 | U2344 | C2345 | U2346 | A2347 | G2348 | C2349 | G2350 | A2351 | C2352 | C2353 | C2354 |       |       |
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| U2418 | A2419 | U2420 | U2421 | C2422 | U2423 | U2424 | A2425 | C2426 | U2427 | U2428 | U2429 | U2430 | U2431 | U2432 | A2433 | U2434 | A2435 | U2436 | G2437 | A2438 | C2439 | A2440 | C     | U     | G     | U     | G     | G     | U     | A     | A     | C     | G     | C     | U     | A     | G     | U     | G     | A     | A     | G     | A     | U     | C     | G     | A     | U     | A     | U     | C     | C     | U     |       |       |       |       |       |
| G     | U     | A     | A     | A     | A     | A     | C     | C     | A     | U     | A     | C     | C     | C     | C     | C     | A     | U     | A     | U2498 | U2499 | C2500 | A2501 | U2502 | U2503 | U2504 | U2505 | U2506 | C2507 | U2508 | U2509 | A2510 | G2515 | U2516 | G2517 | A2518 | U2519 | G2520 | A2521 | A2522 | A2523 | A2524 | G2529 | U2530 | U2531 | G2532 | C2533 | A2534 | U2535 | A2536 | C2537 | U2538 | C2539 | G2540 | U2541 | U2542 | C2543 |       |



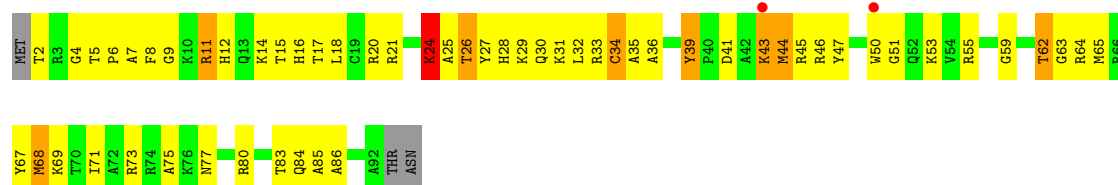
### • Molecule 2: RIBOSOMAL PROTEIN L37

Chain AA: 35% 53% 9%



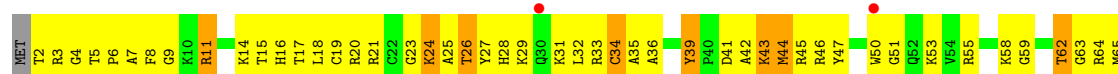
### • Molecule 2: RIBOSOMAL PROTEIN L37

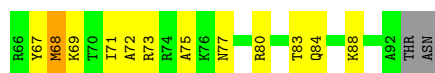
Chain DA: 2% 36% 51% 9%



### • Molecule 2: RIBOSOMAL PROTEIN L37

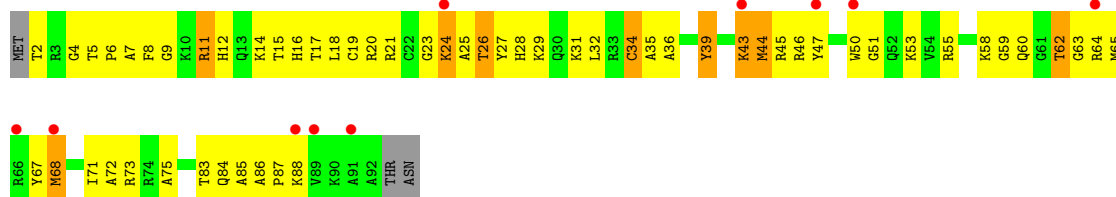
Chain FA: 2% 33% 54% 10%





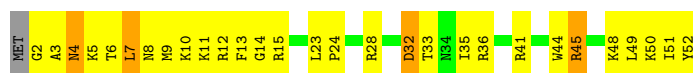
• Molecule 2: RIBOSOMAL PROTEIN L37

Chain HA: 11% 35% 52% 10%



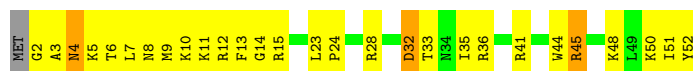
• Molecule 3: RPL39

Chain AB: 42% 48% 8%



• Molecule 3: RPL39

Chain DB: 44% 48% 6%



• Molecule 3: RPL39

Chain FB: 2% 42% 48% 8%



• Molecule 3: RPL39

Chain HB: 2% 40% 50% 8%



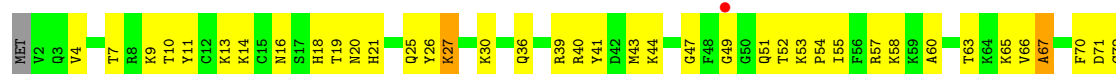
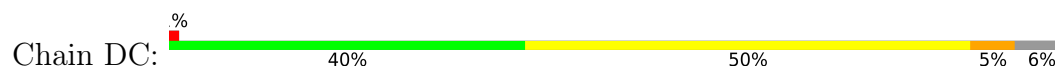
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A

Chain AC: % 39% 51% 5% 6%

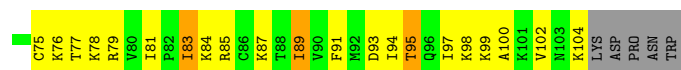
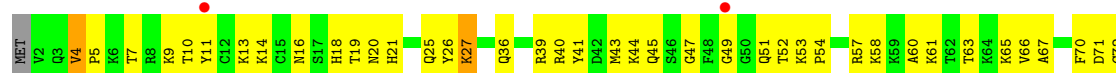




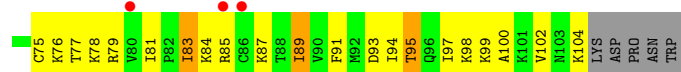
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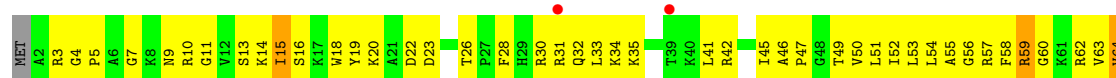
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A



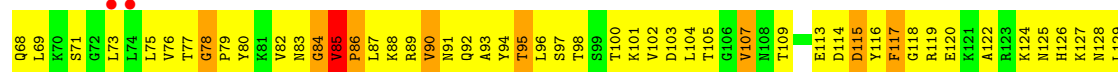
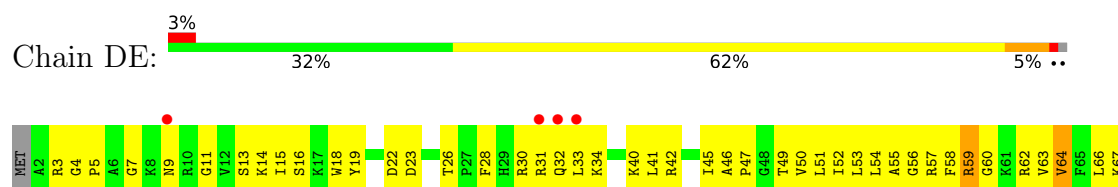
• Molecule 4: 60S RIBOSOMAL PROTEIN L36A



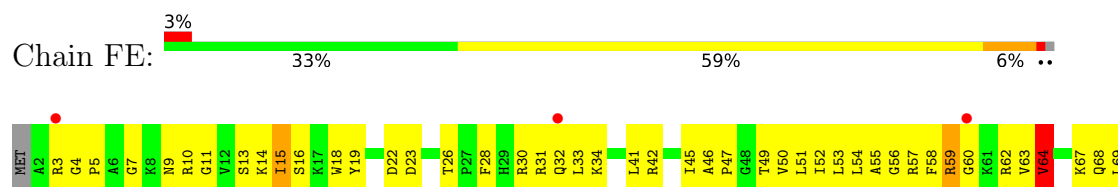
• Molecule 5: RPL6



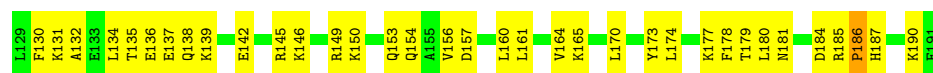
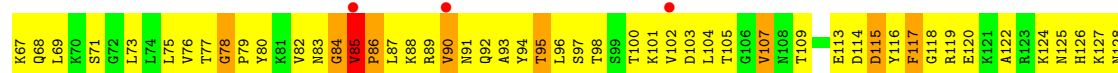
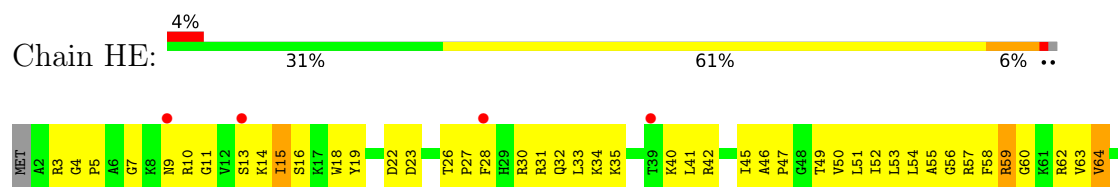
• Molecule 5: RPL6



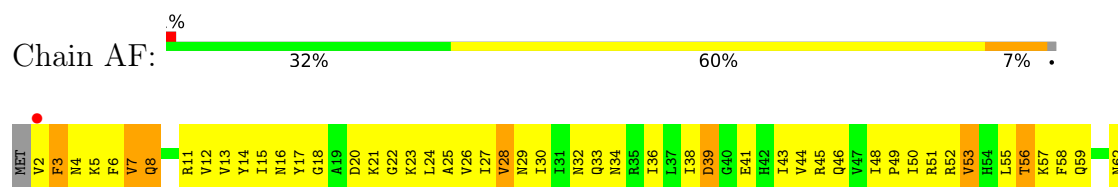
## • Molecule 5: RPL6



## • Molecule 5: RPL6



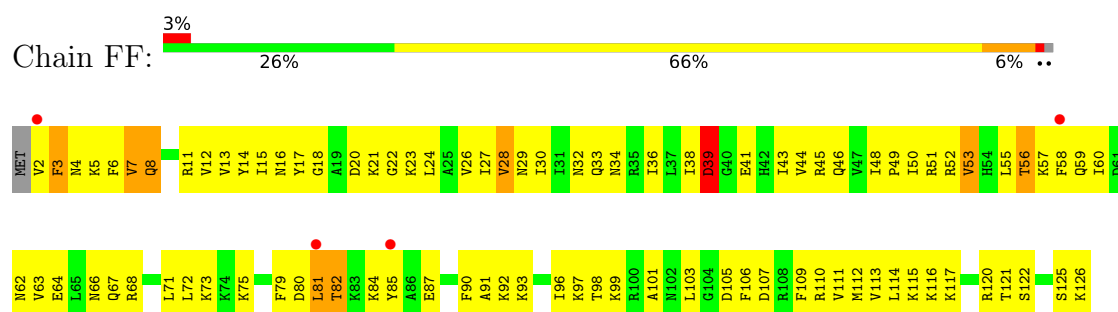
## • Molecule 6: RPL14



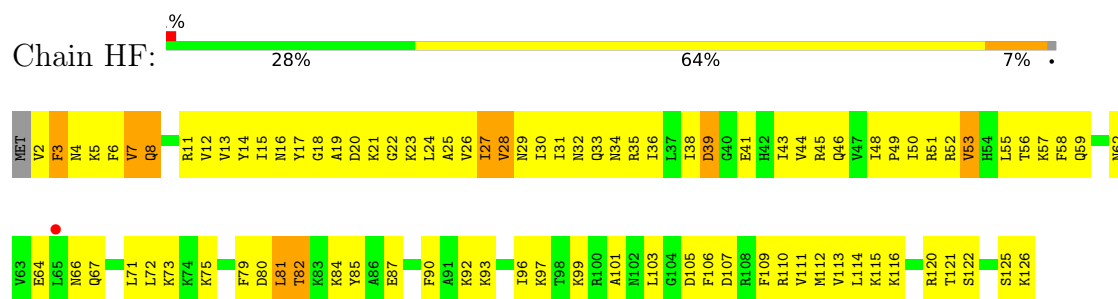
- Molecule 6: RPL14



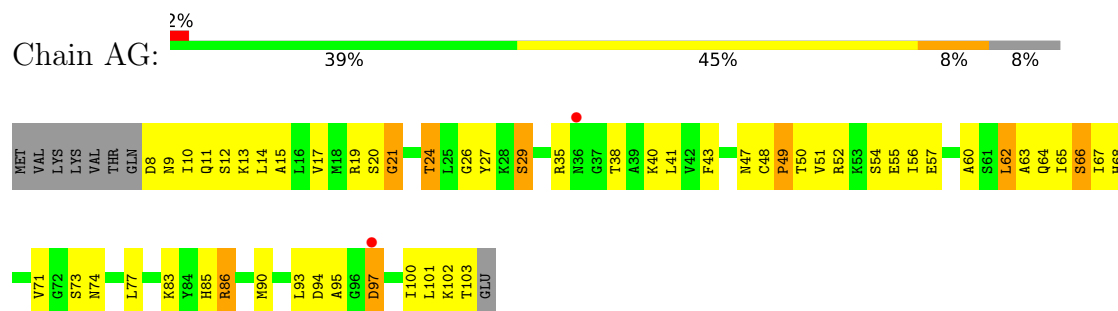
- Molecule 6: RPL14



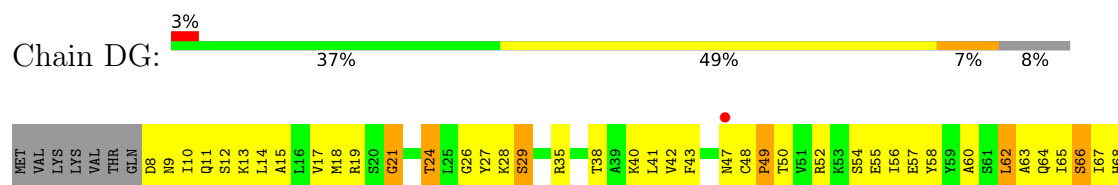
- Molecule 6: RPL14

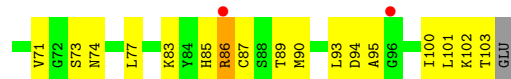


- Molecule 7: RPL30

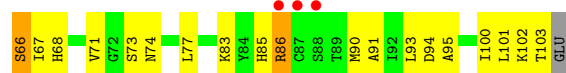
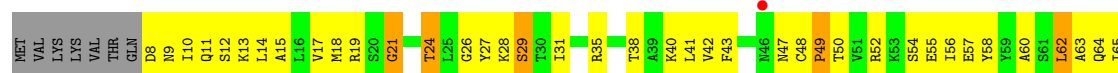


- Molecule 7: RPL30

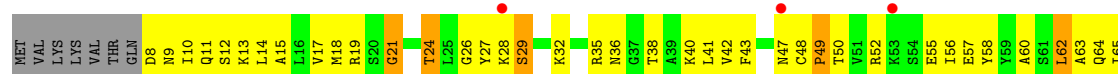




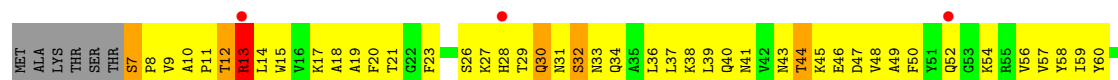
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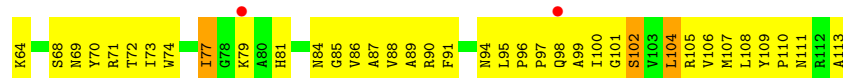
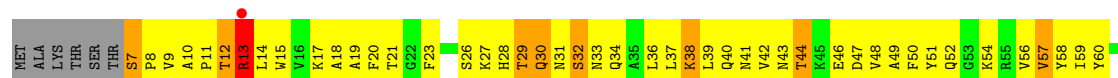
• Molecule 7: RPL30



• Molecule 8: RPL35A

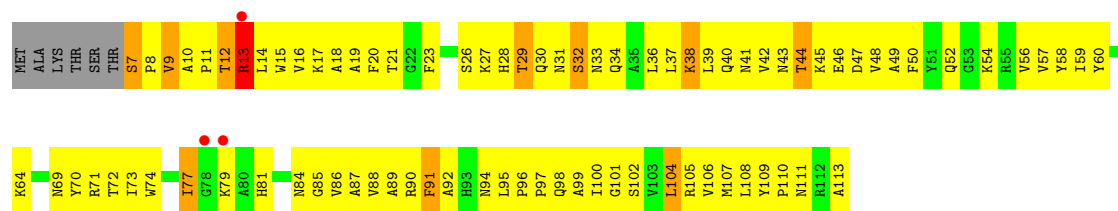


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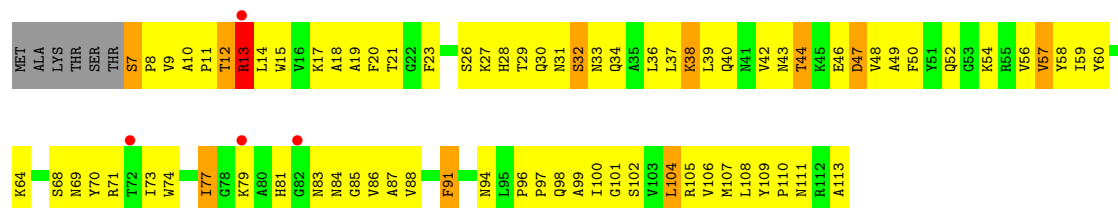


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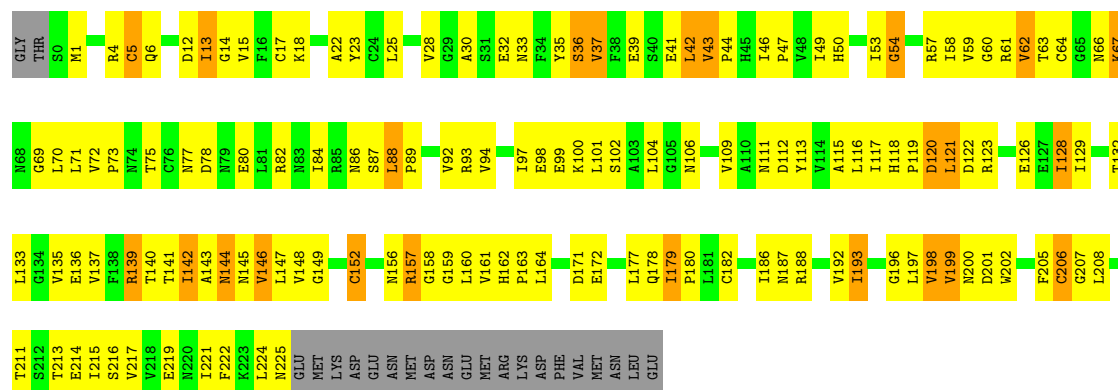




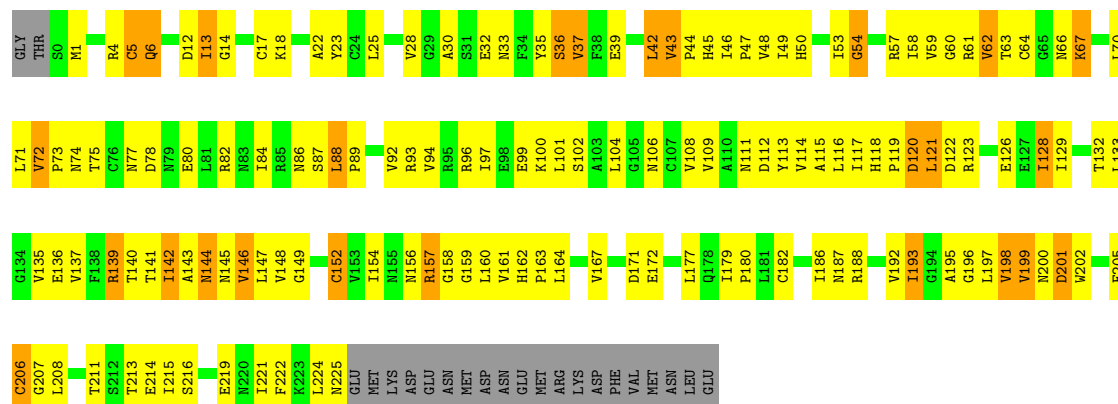
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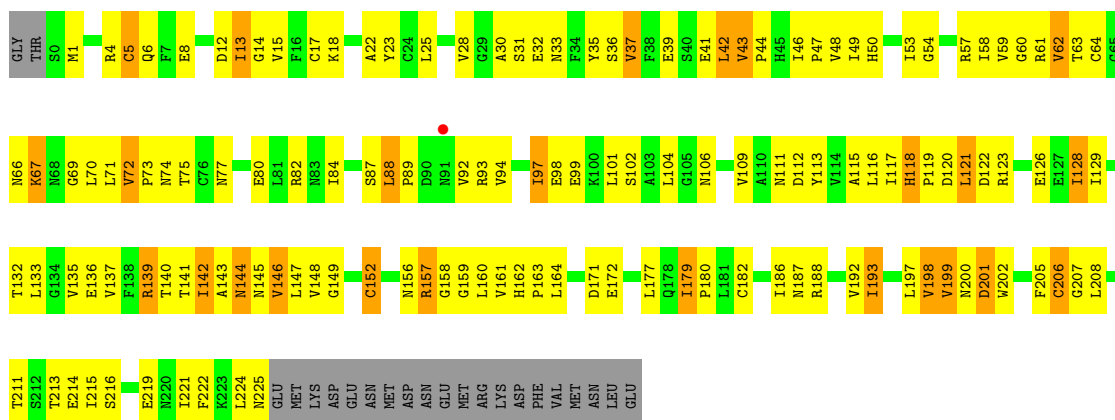
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN



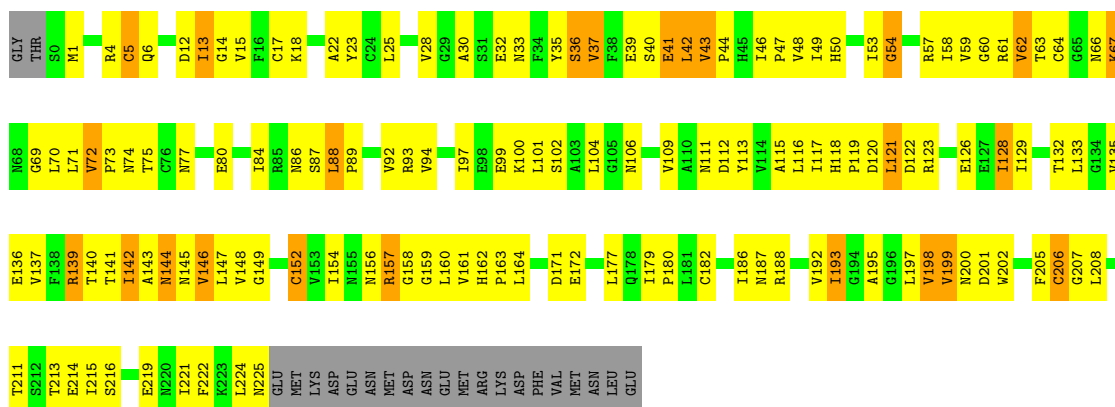
• Molecule 9: TRANSLATION INITIATION FACTOR EIF-6, PUTATIVE FAMILY PROTEIN



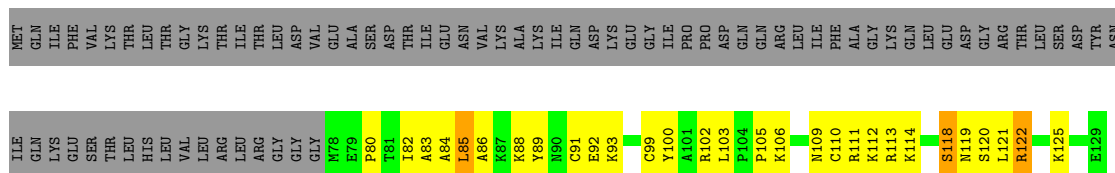
Chain FJ:  34% 47% 10% 9%



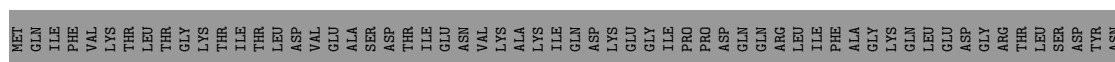
Chain HJ:  34% 48% 10% 9%



Chain AK:  18% 20% 60%

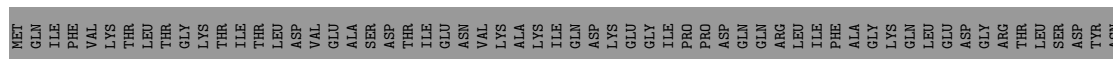


Chain DK: 

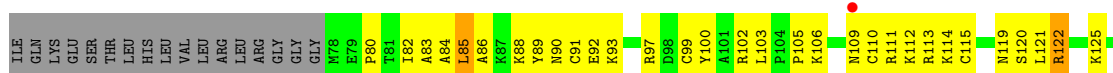




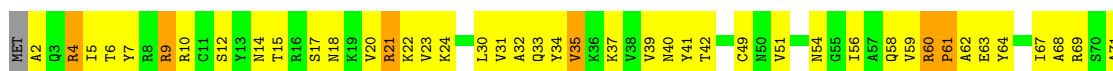
• Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



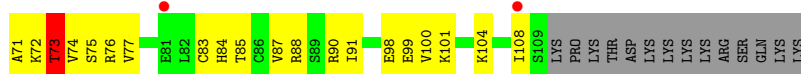
• Molecule 10: UBIQUITIN-60S RIBOSOMAL PROTEIN L40



• Molecule 11: RPL34

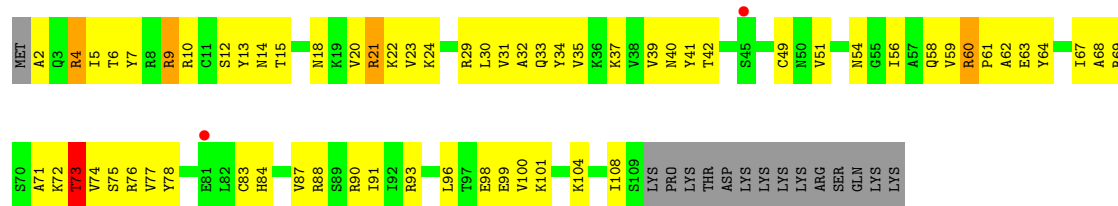


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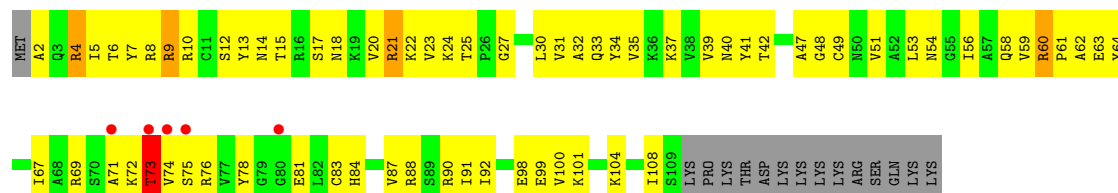


• Molecule 11: RPL34

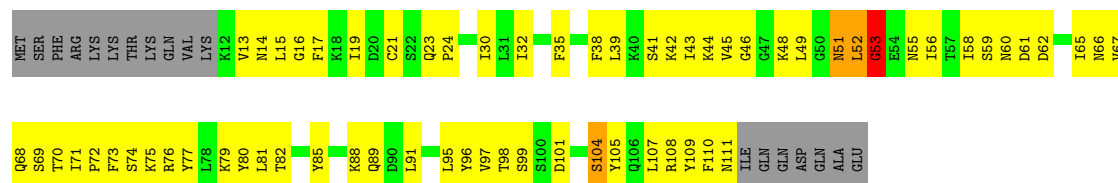




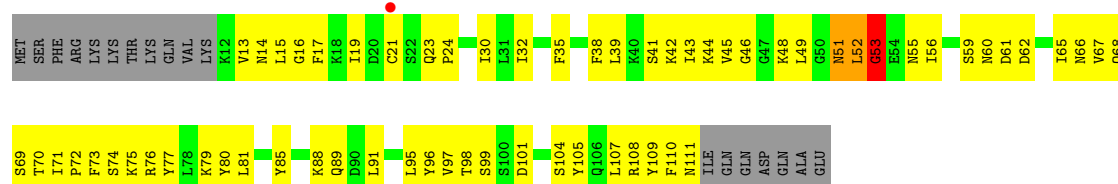
• Molecule 11: RPL34



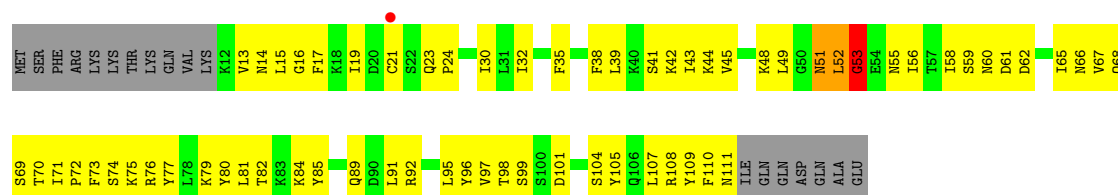
• Molecule 12: RIBOSOMAL PROTEIN L22



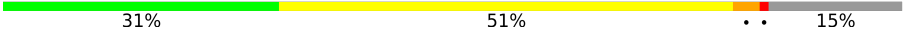
• Molecule 12: RIBOSOMAL PROTEIN L22

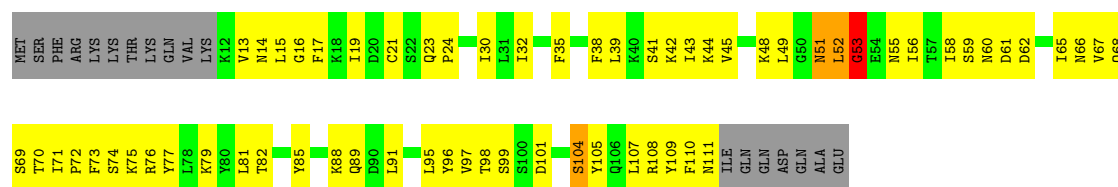


• Molecule 12: RIBOSOMAL PROTEIN L22



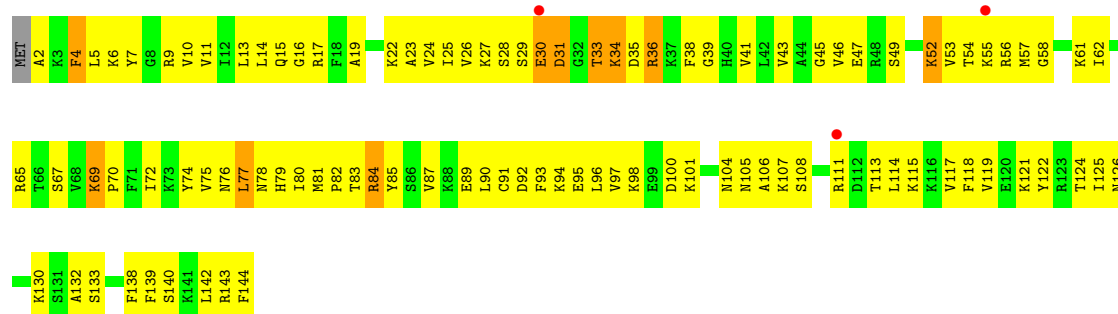
• Molecule 12: RIBOSOMAL PROTEIN L22

Chain HM: 



• Molecule 13: RPL27

Chain AN: 



• Molecule 13: RPL27

Chain DN: 

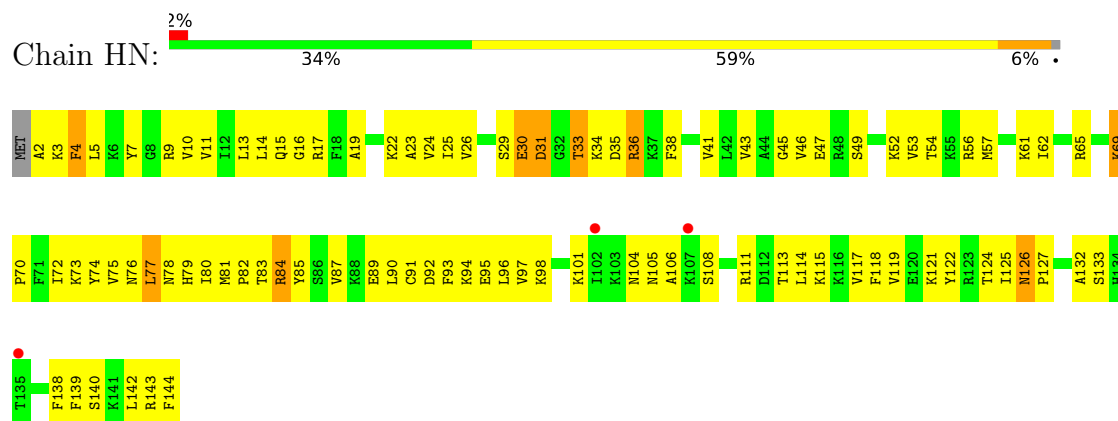


• Molecule 13: RPL27

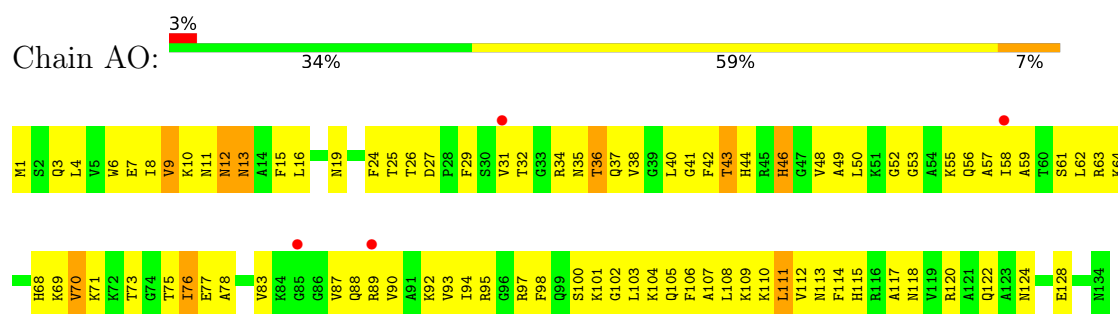
Chain FN: 



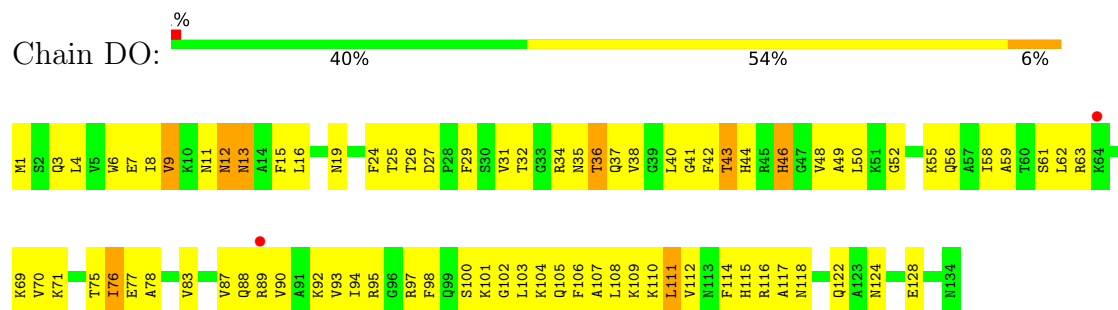
## ● Molecule 13: RPL27



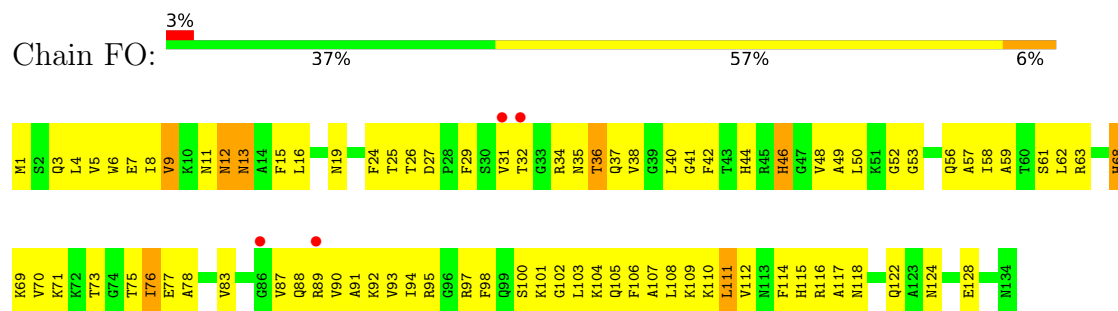
## ● Molecule 14: RPL28



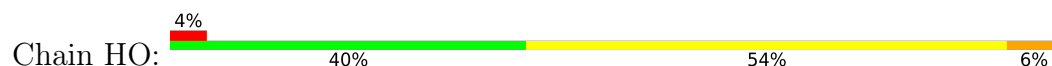
## ● Molecule 14: RPL28

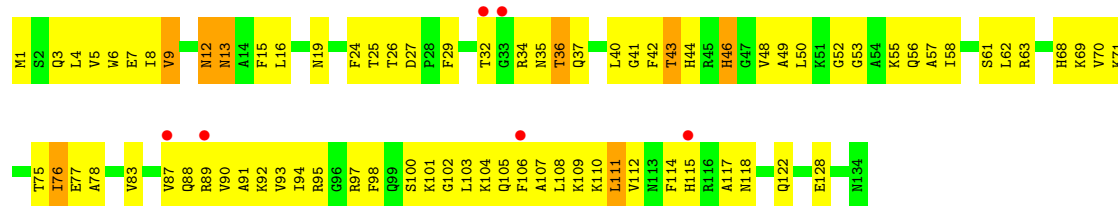


## ● Molecule 14: RPL28

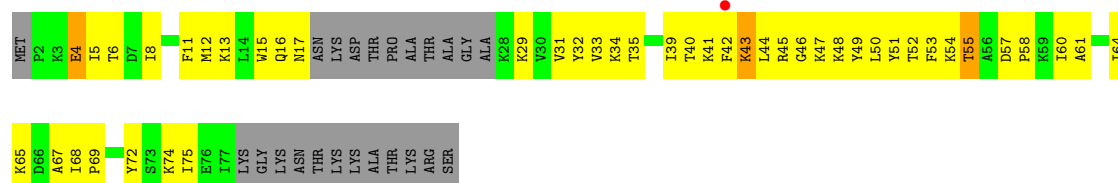


## ● Molecule 14: RPL28

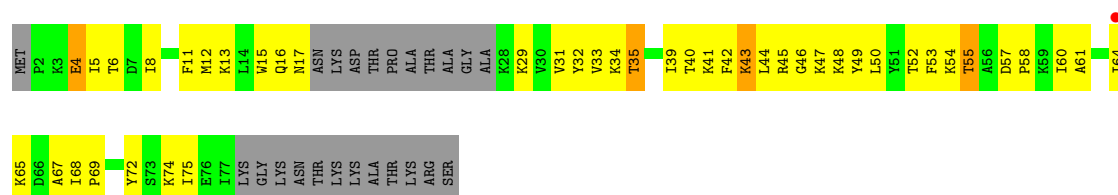




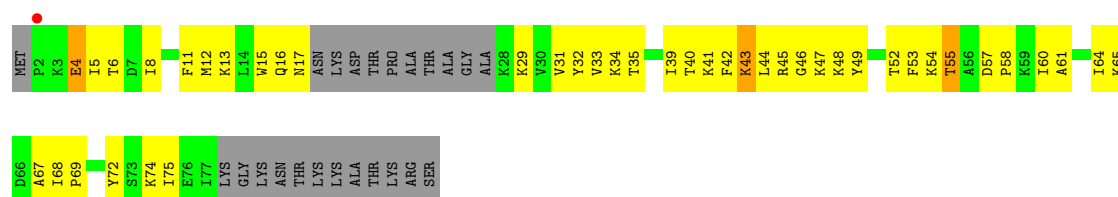
• Molecule 15: RPL38



• Molecule 15: RPL38



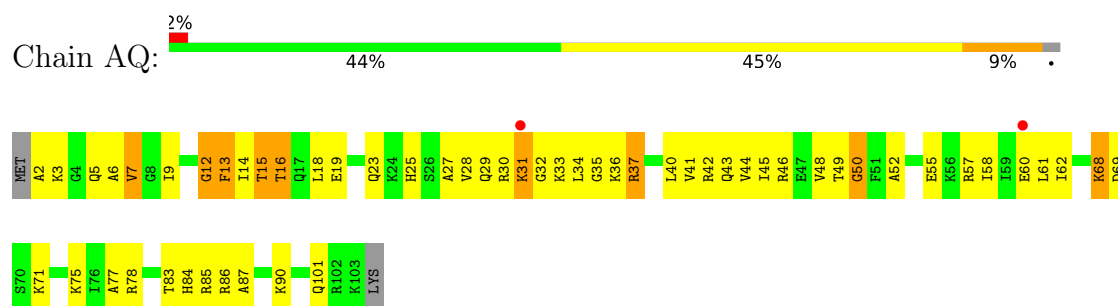
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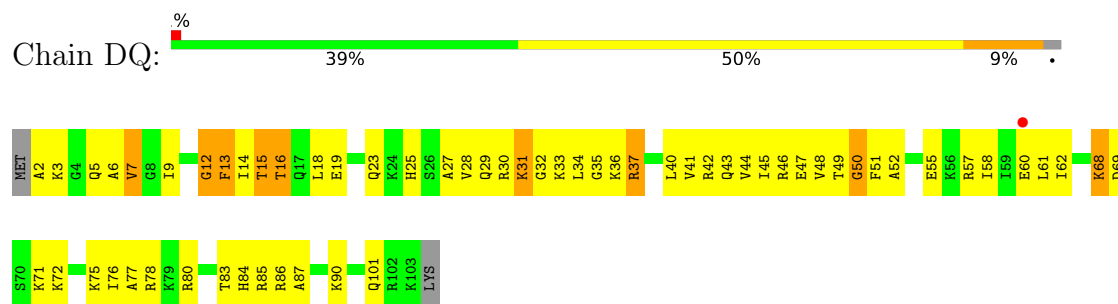
• Molecule 15: RPL38



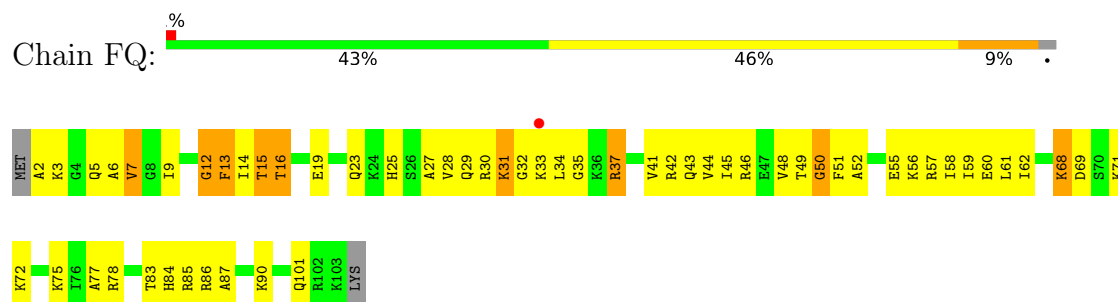
• Molecule 16: 60S RIBOSOMAL PROTEIN L36



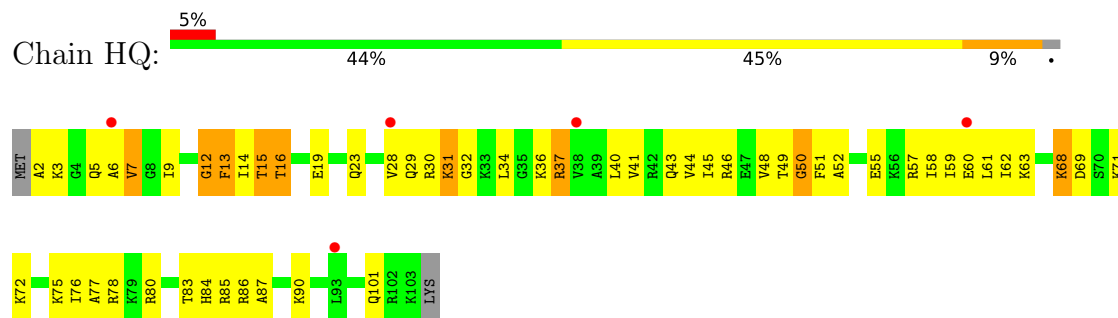
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



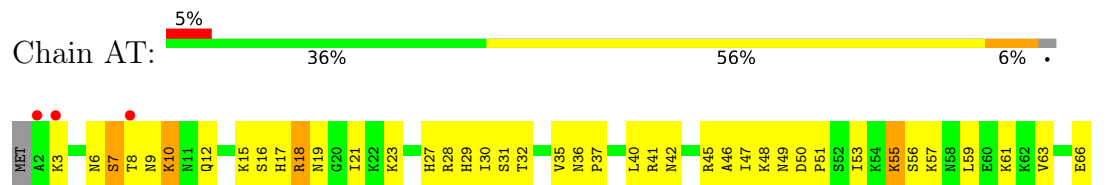
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



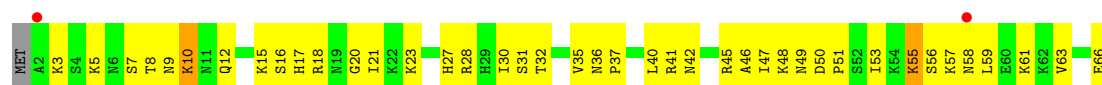
- Molecule 16: 60S RIBOSOMAL PROTEIN L36



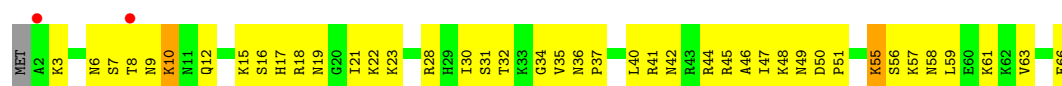
- Molecule 17: RPL29



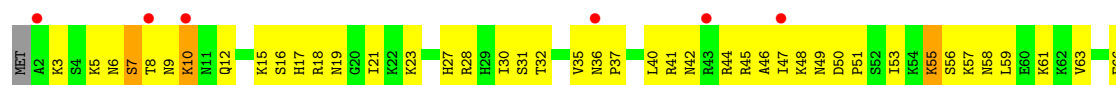
- Molecule 17: RPL29



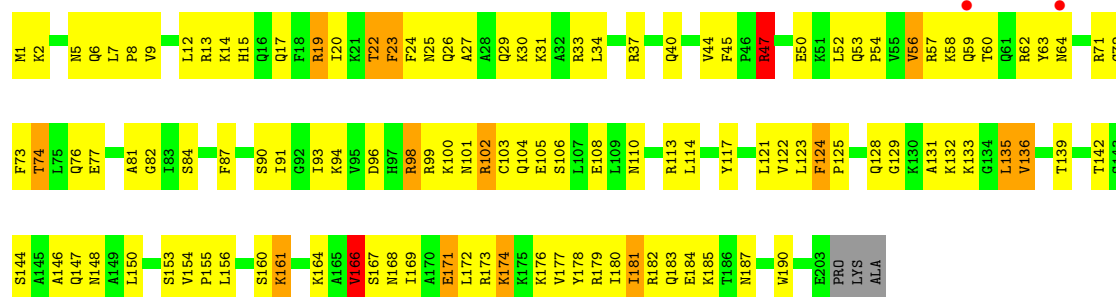
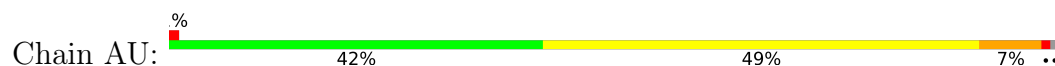
• Molecule 17: RPL29



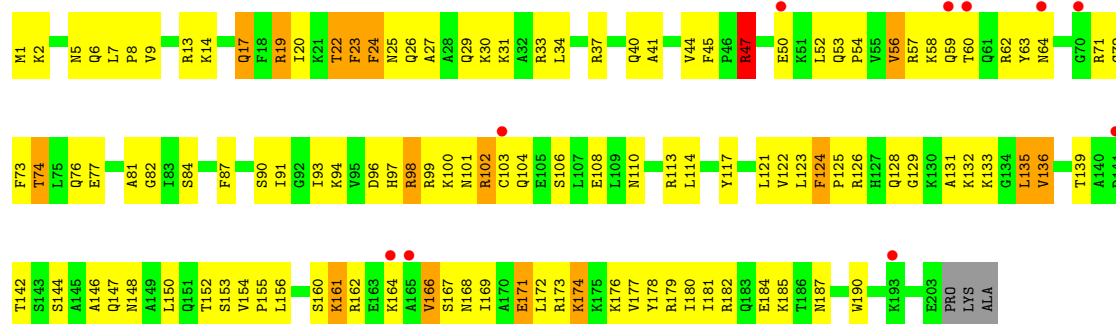
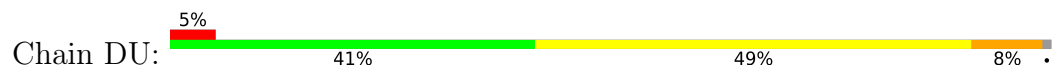
• Molecule 17: RPL29



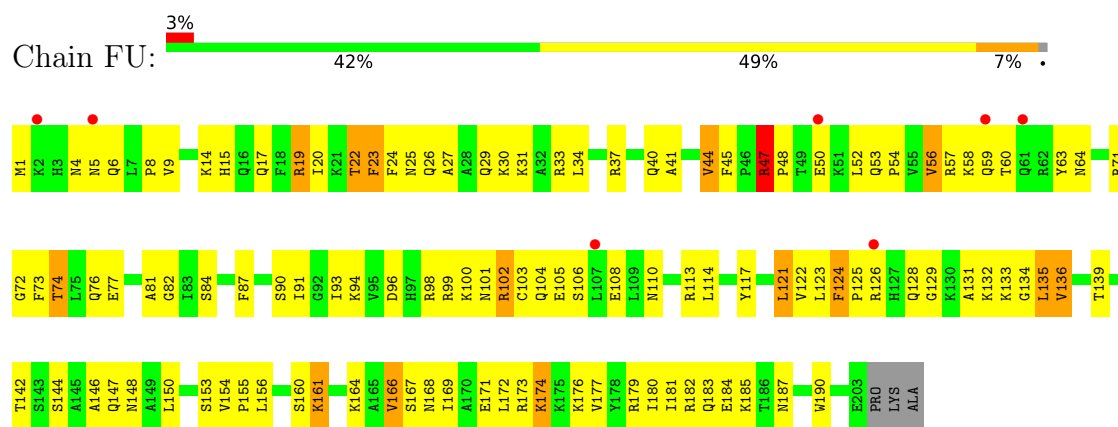
• Molecule 18: RPL13



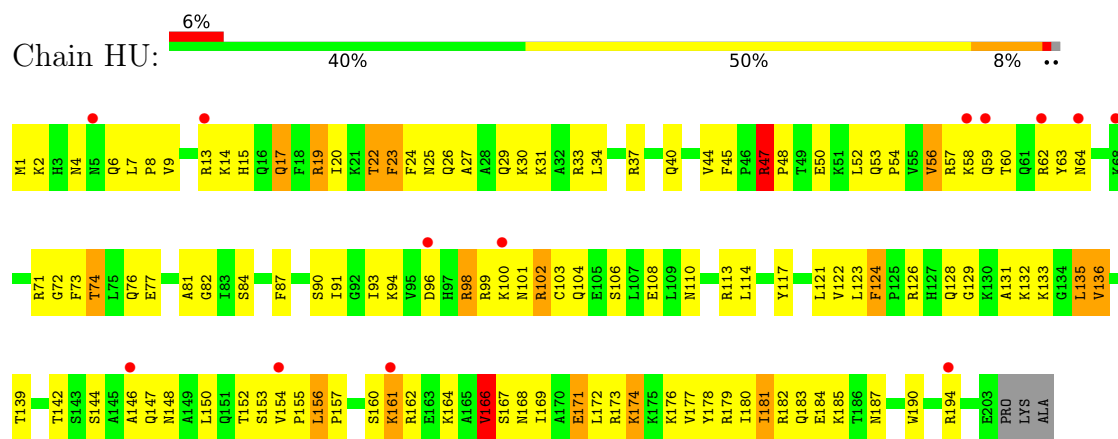
• Molecule 18: RPL13



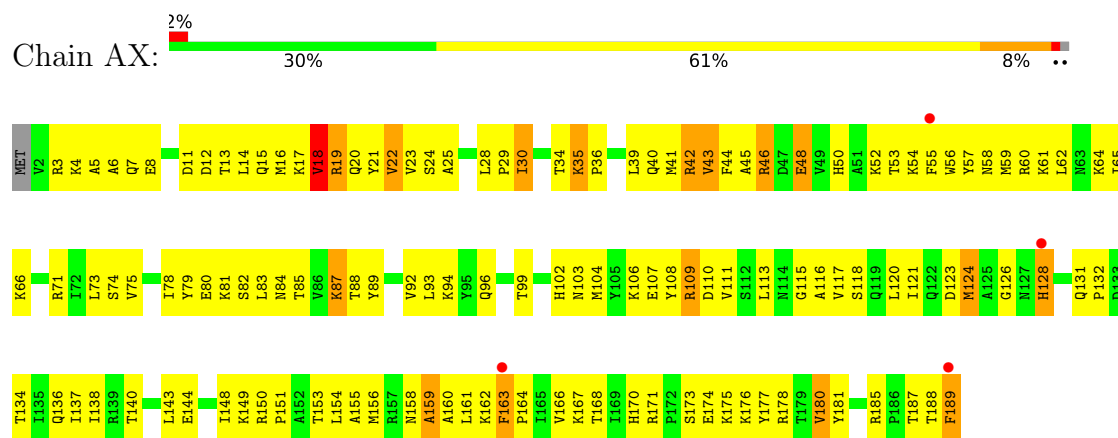
• Molecule 18: RPL13



## • Molecule 18: RPL13

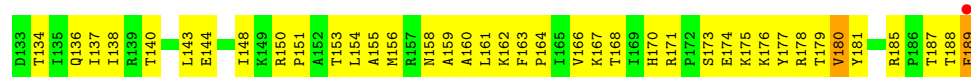


## • Molecule 19: RPL18A

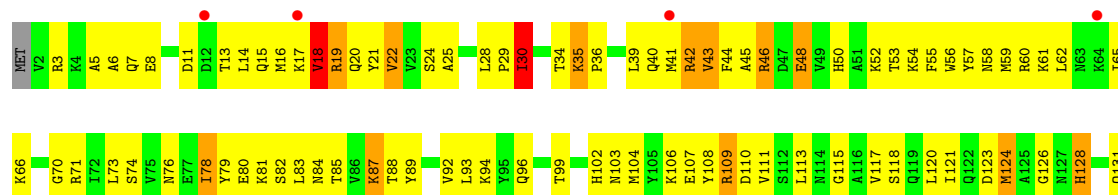


## • Molecule 19: RPL18A

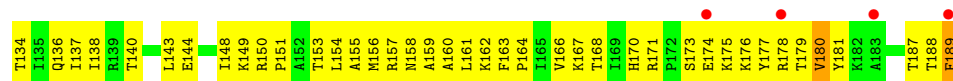
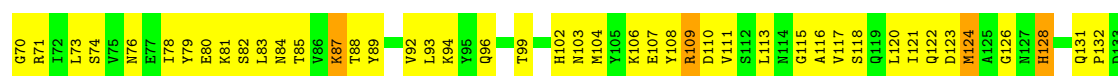
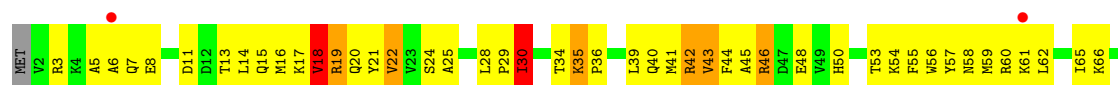




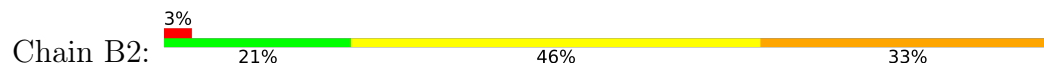
• Molecule 19: RPL18A



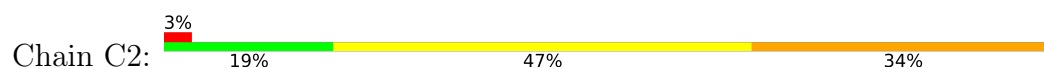
• Molecule 19: RPL18A



• Molecule 20: 5.8S RRNA

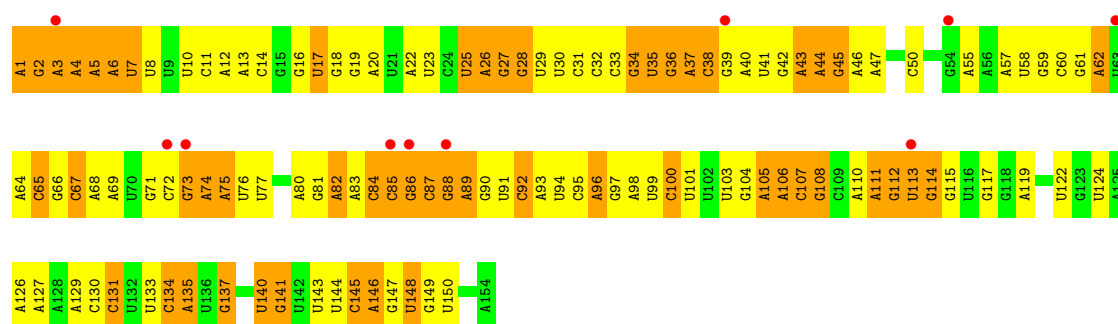
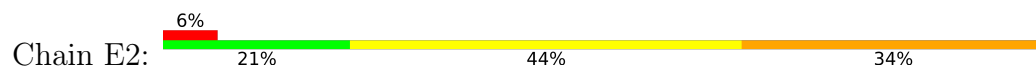


• Molecule 20: 5.8S RRNA

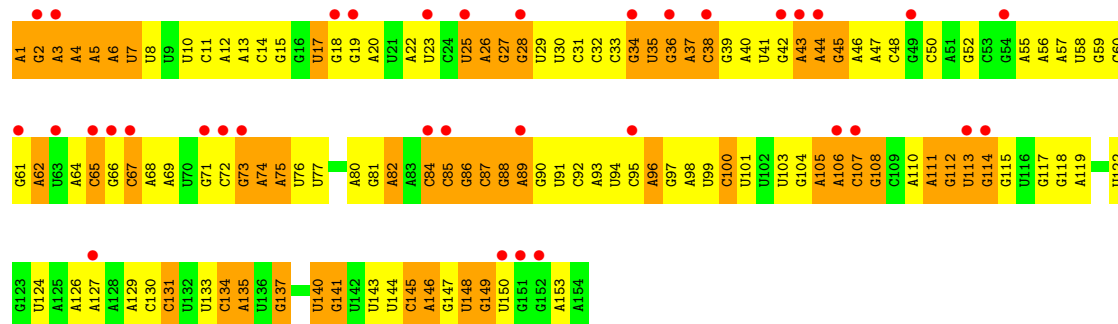
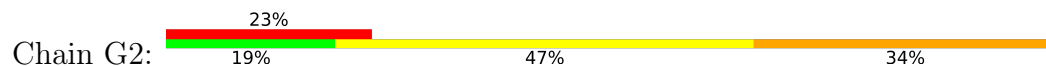




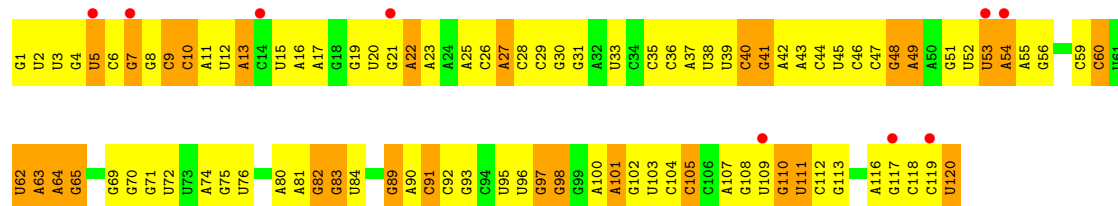
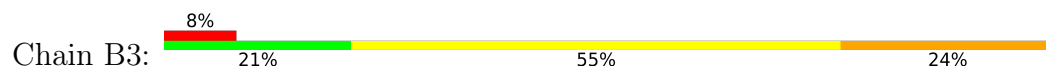
• Molecule 20: 5.8S rRNA



• Molecule 20: 5.8S rRNA

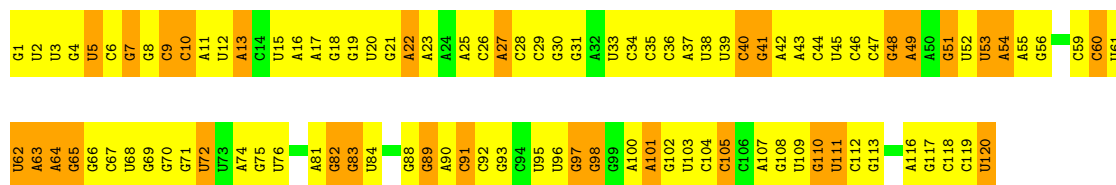


• Molecule 21: 5S rRNA



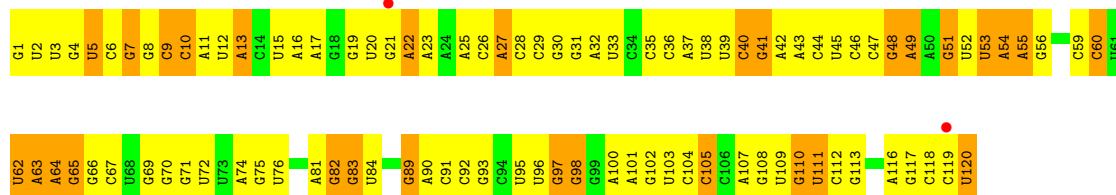
• Molecule 21: 5S rRNA

Chain C3: 16% 58% 26%



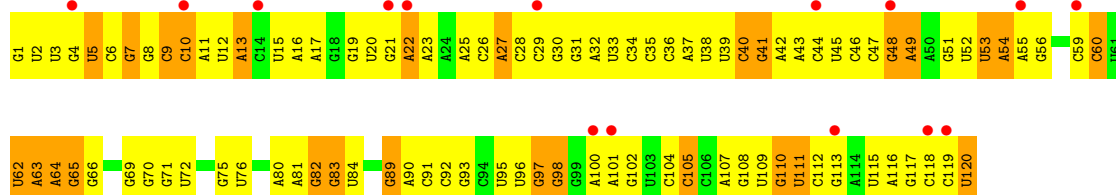
• Molecule 21: 5S RRNA

Chain E3: 2% 19% 57% 24%



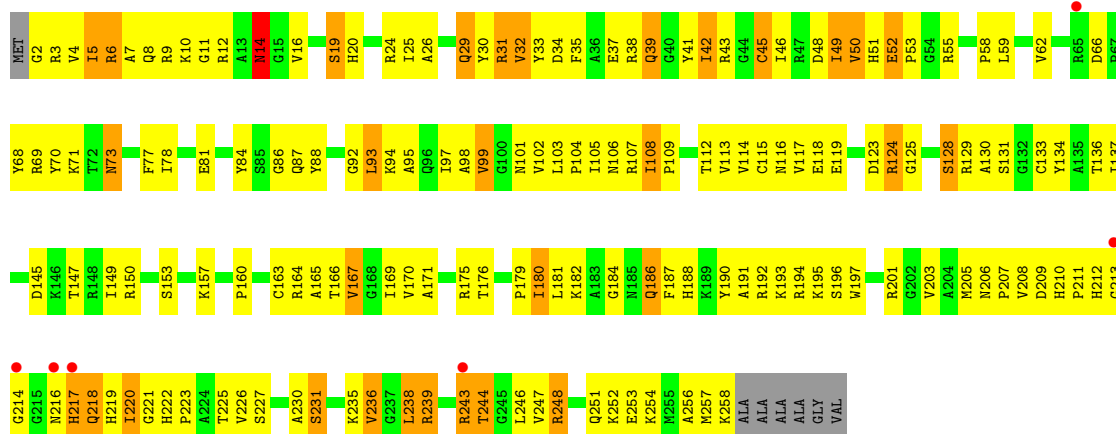
• Molecule 21: 5S RRNA

Chain G3: 12% 19% 58% 22%



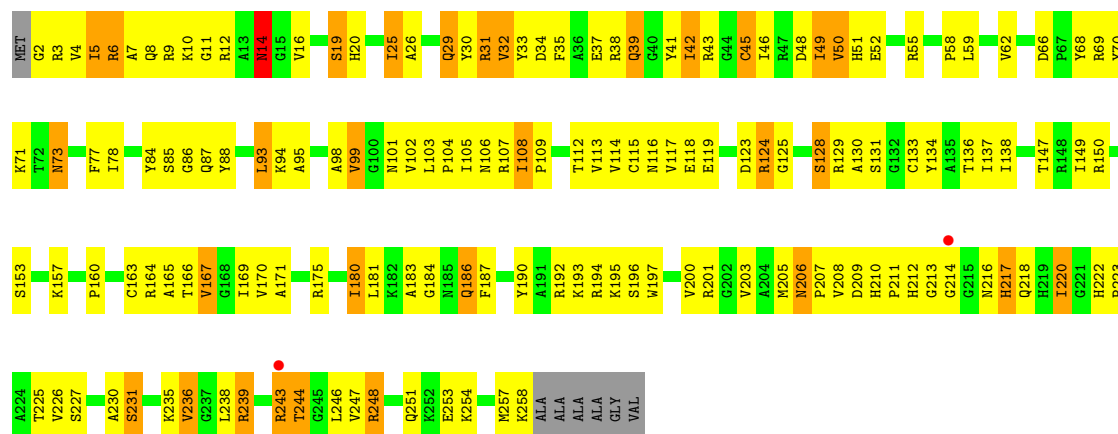
• Molecule 22: RPL8

Chain BA: 2% 35% 50% 12%

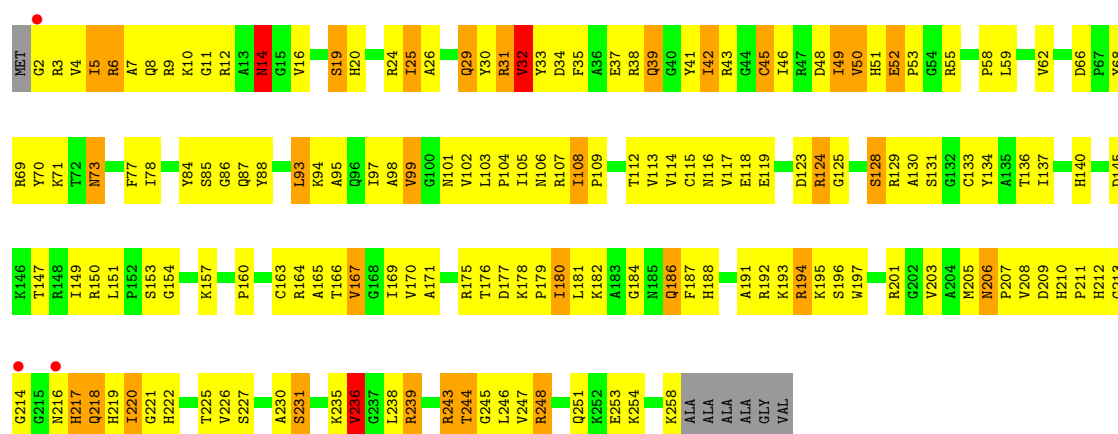


• Molecule 22: RPL8

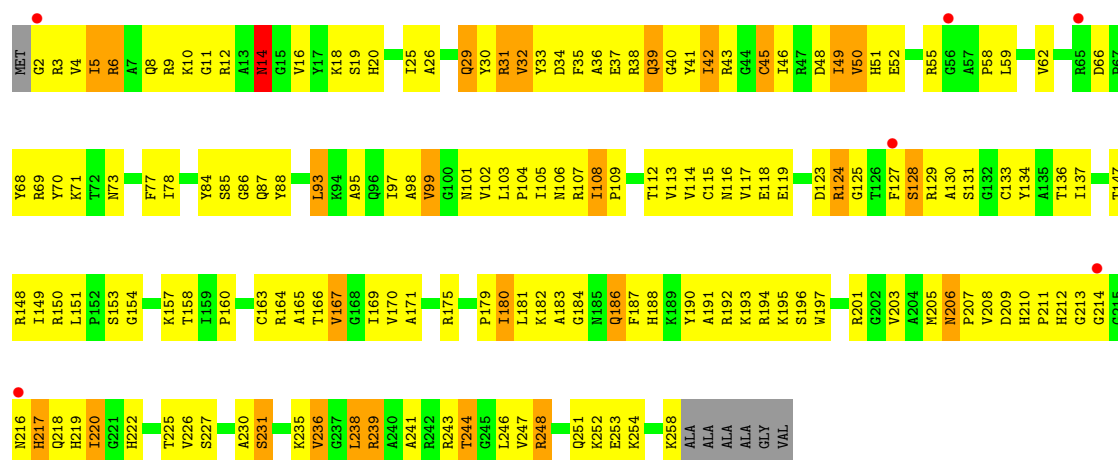
Chain CA: % 39% 47% 11%



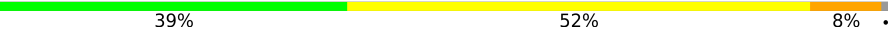
### • Molecule 22: RPL8

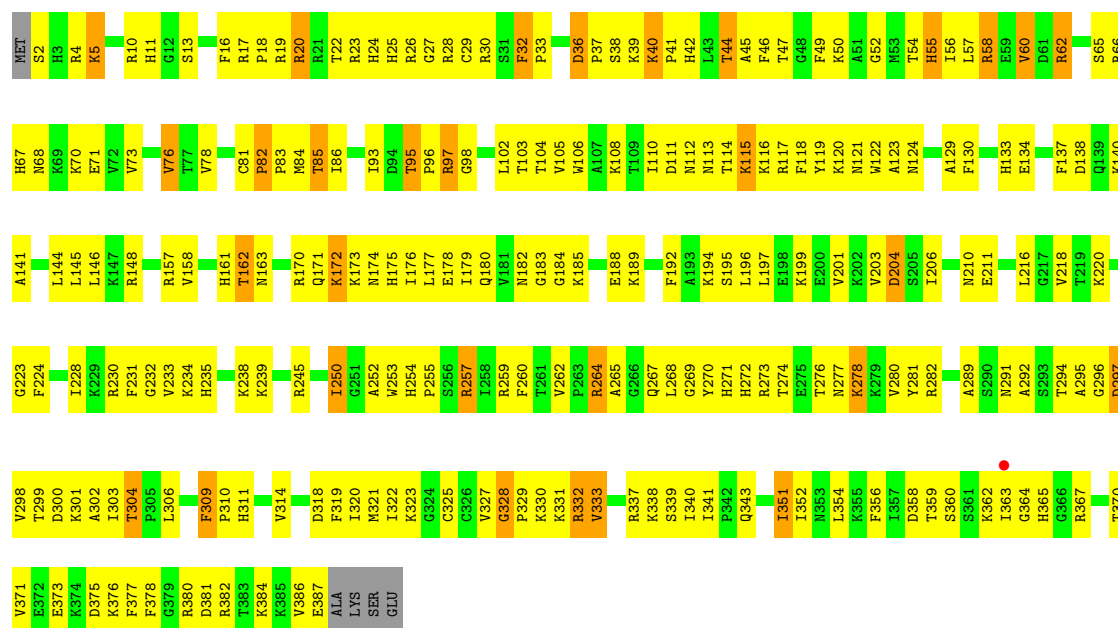


### • Molecule 22: RPL8



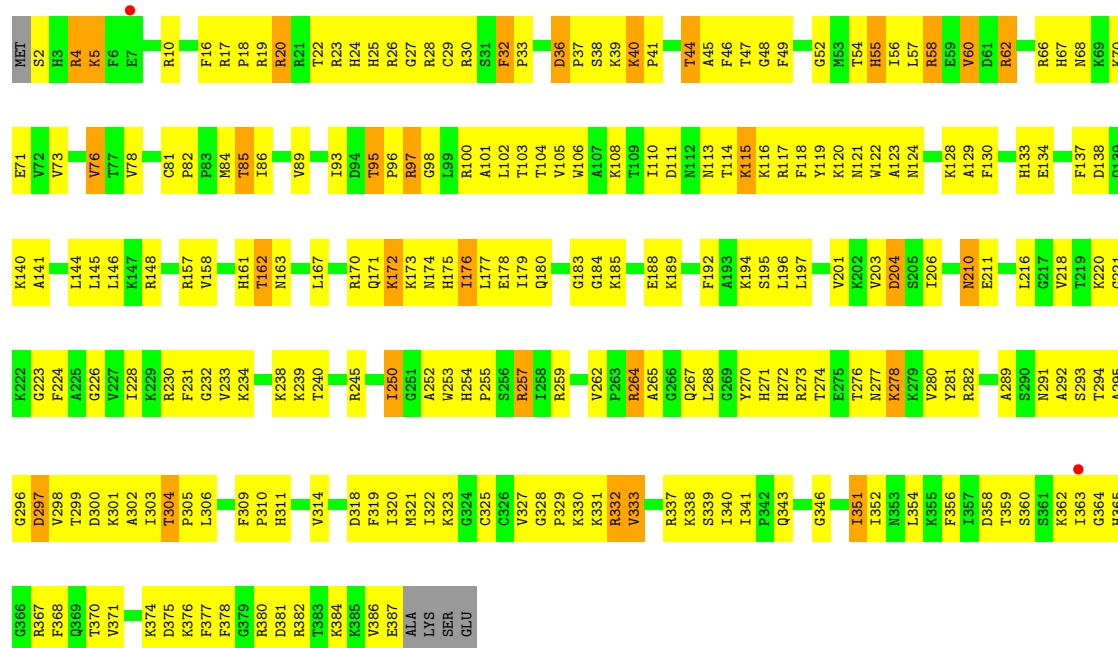
### • Molecule 23: RIBOSOMAL PROTEIN L3

Chain BB: 



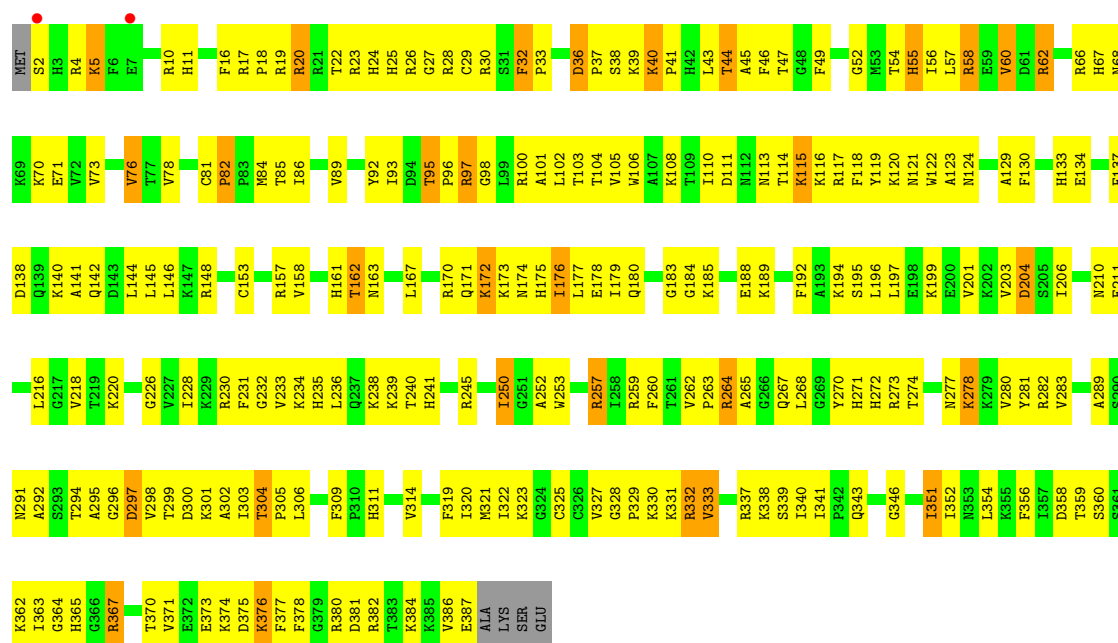
• Molecule 23: RIBOSOMAL PROTEIN L3

Chain CB: 

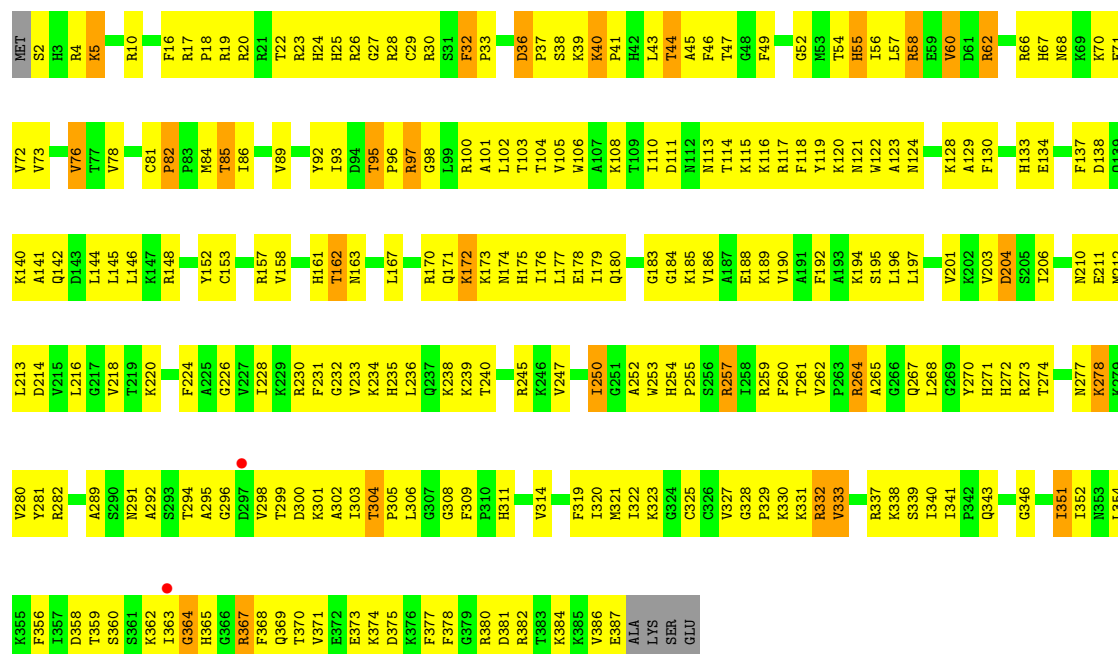


• Molecule 23: RIBOSOMAL PROTEIN L3

Chain EB: 



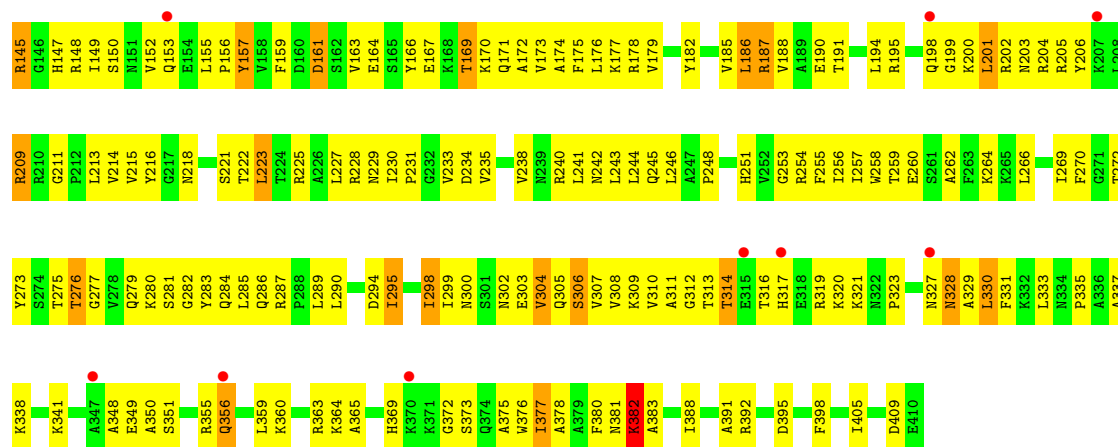
### • Molecule 23: RIBOSOMAL PROTEIN L3



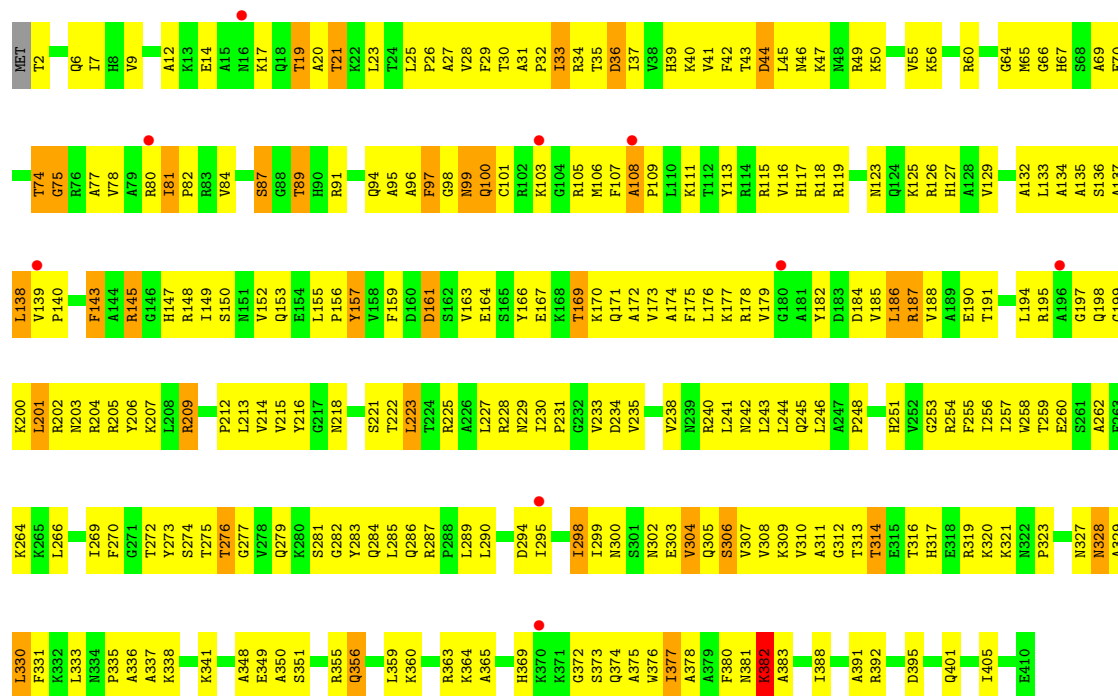
### • Molecule 24: RPL4



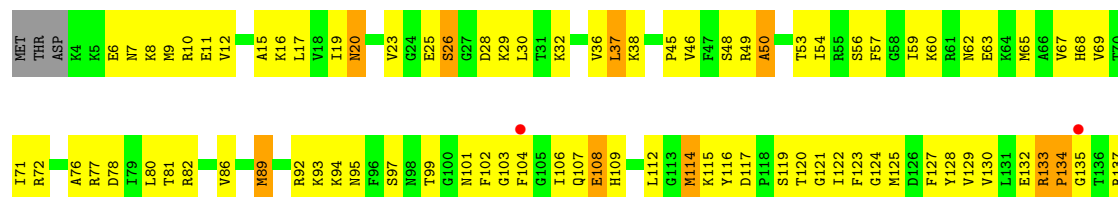




• Molecule 24: RPL4



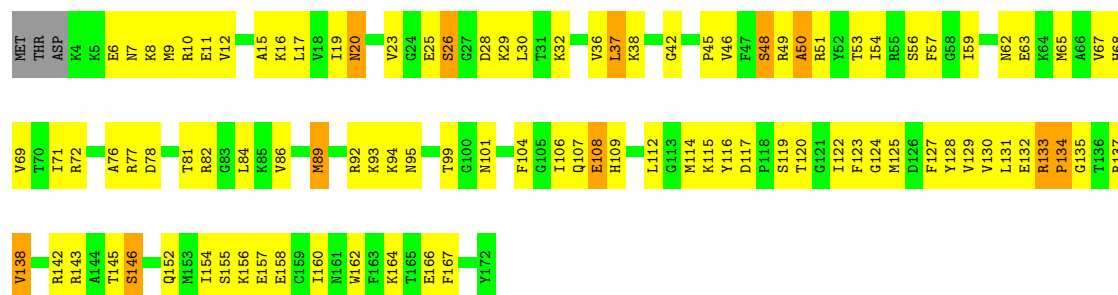
• Molecule 25: 60S RIBOSOMAL PROTEIN L11





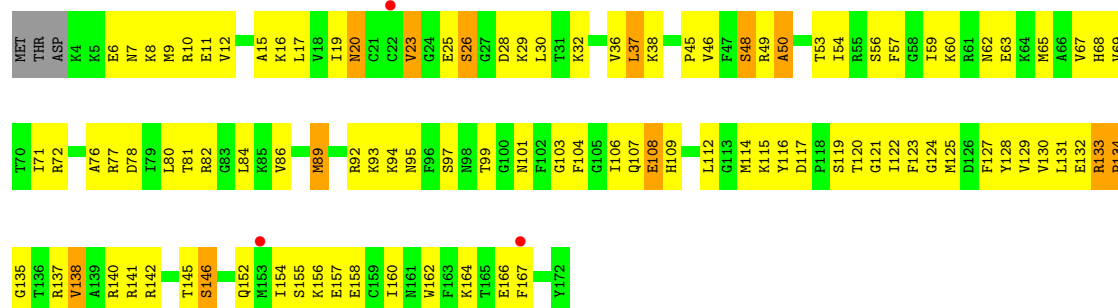
• Molecule 25: 60S RIBOSOMAL PROTEIN L11

Chain CD: 41% 51% 6%



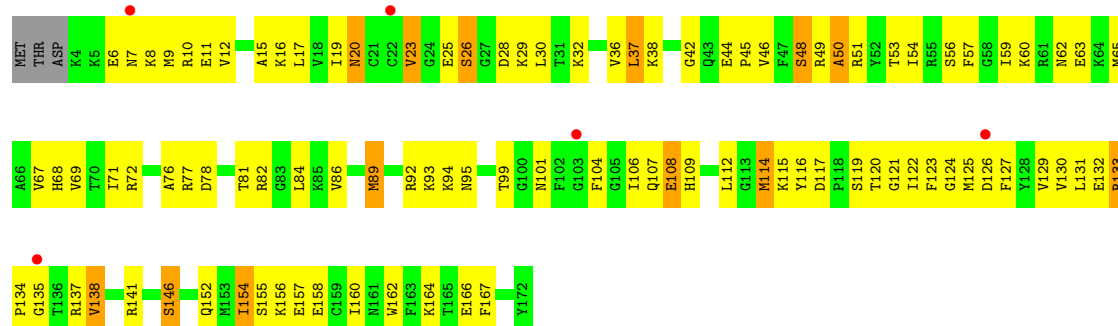
• Molecule 25: 60S RIBOSOMAL PROTEIN L11

Chain ED: 2% 39% 52% 7%



• Molecule 25: 60S RIBOSOMAL PROTEIN L11

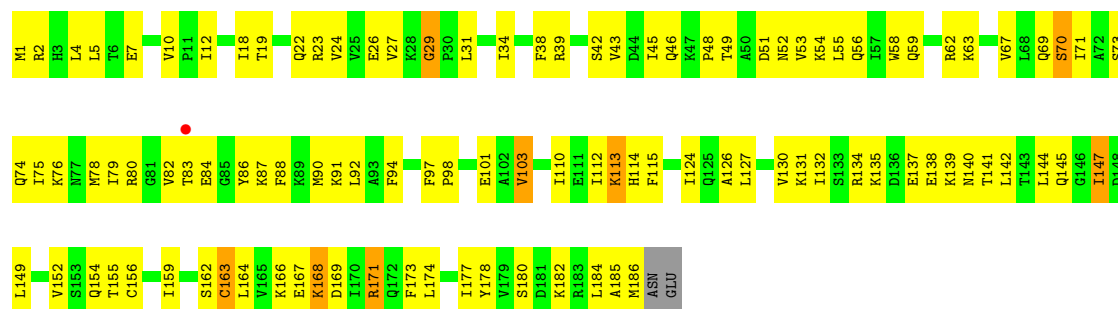
Chain GD: 3% 41% 50% 8%



• Molecule 26: 60S RIBOSOMAL PROTEIN L9

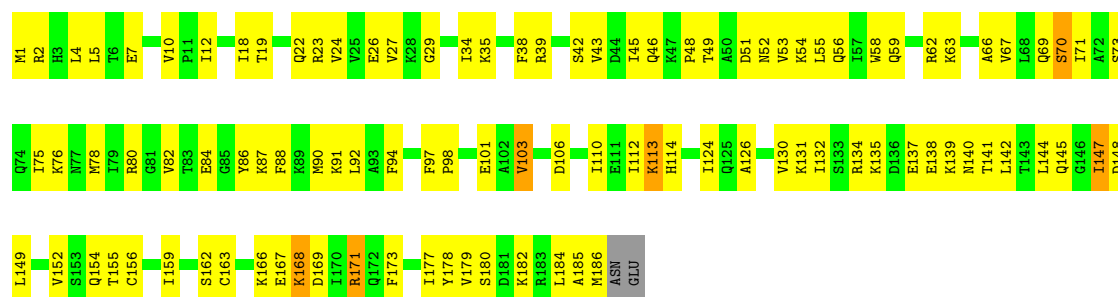
Chain BE: 43% 52%





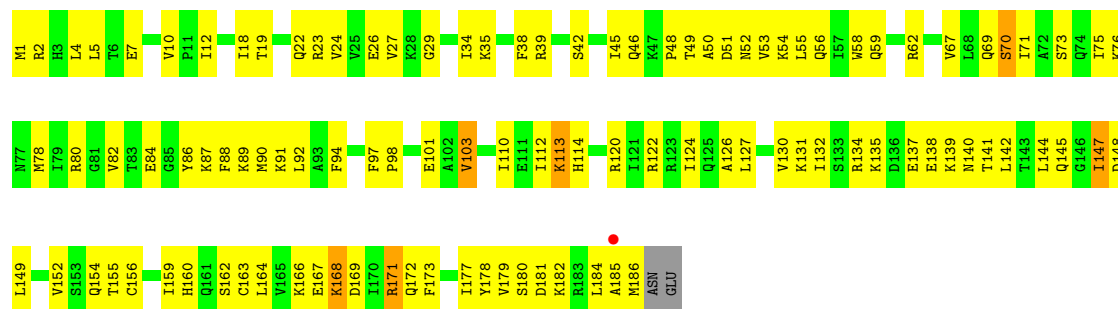
• Molecule 26: 60S RIBOSOMAL PROTEIN L9

Chain CE: 45% 51% ..



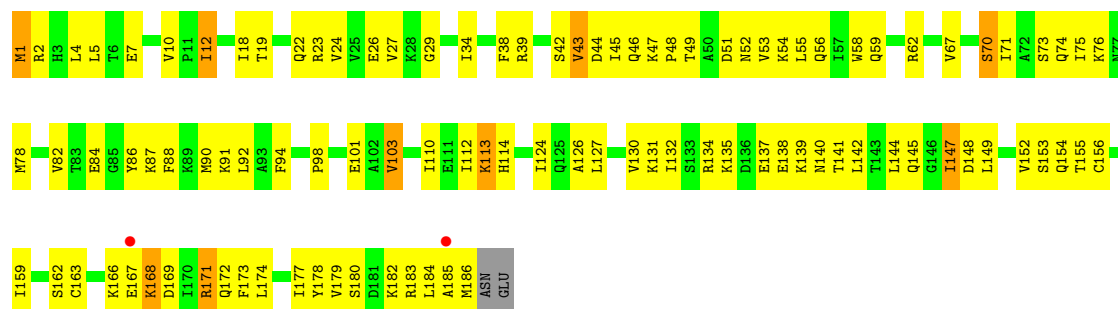
• Molecule 26: 60S RIBOSOMAL PROTEIN L9

Chain EE: 42% 54% ..

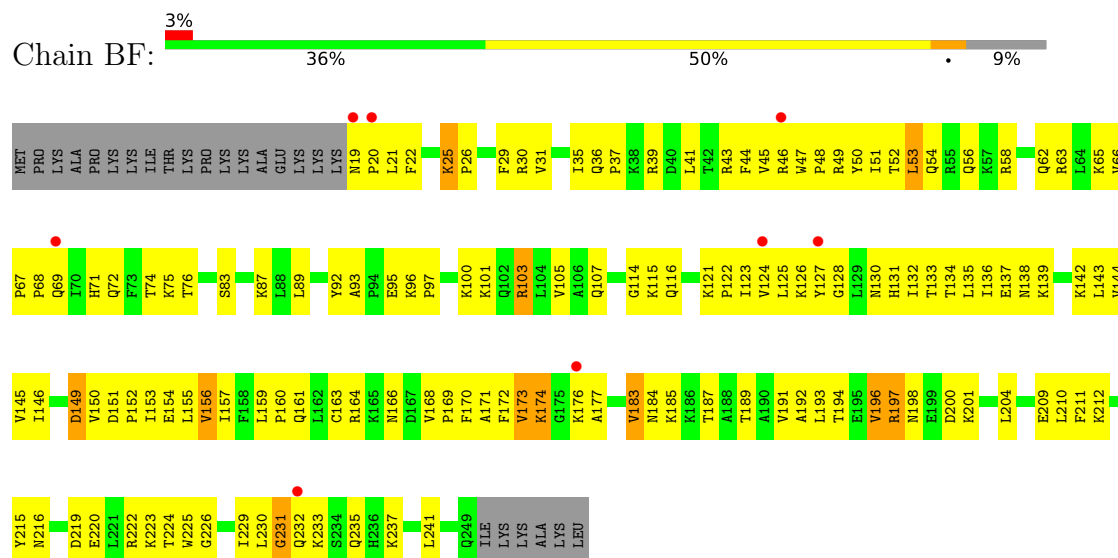


• Molecule 26: 60S RIBOSOMAL PROTEIN L9

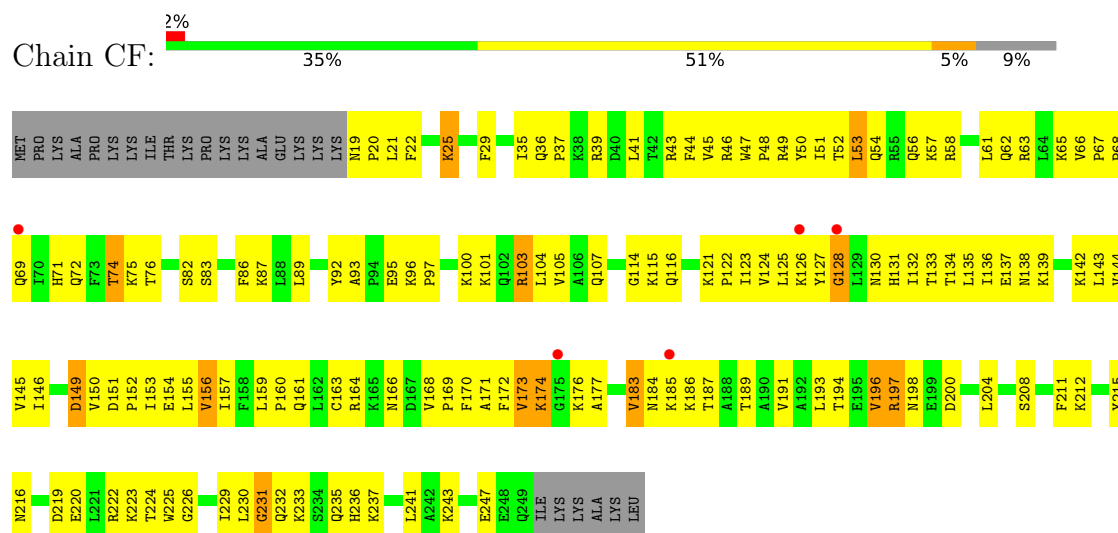
Chain GE: 44% 50% 5% .



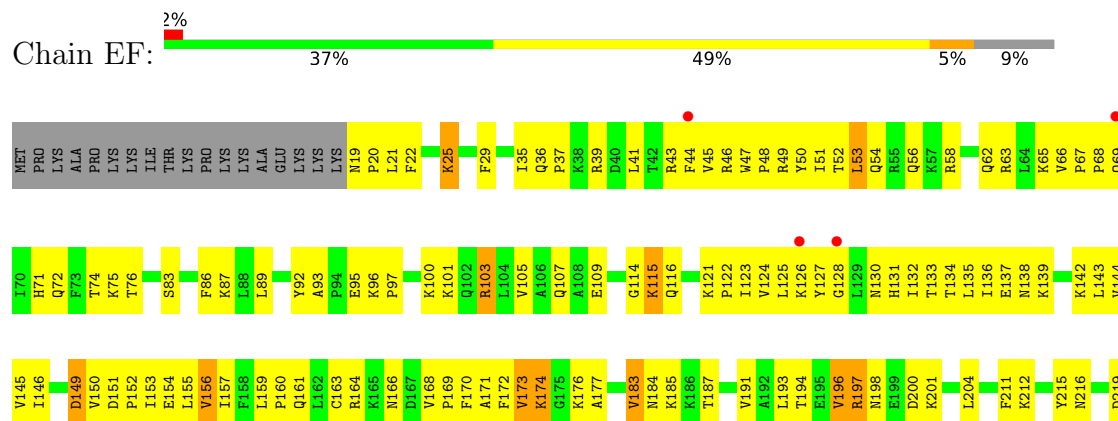
## • Molecule 27: RPL7A



## • Molecule 27: RPL7A



## • Molecule 27: RPL7A





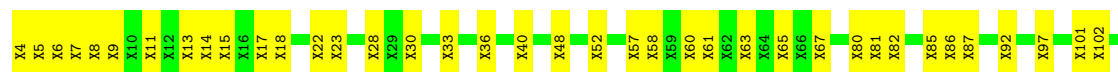
• Molecule 27: RPL7A



• Molecule 28: RPLP0



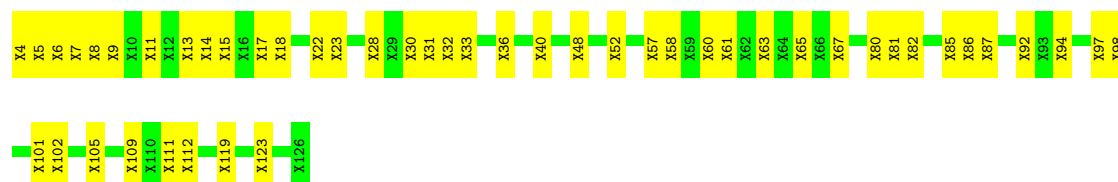
• Molecule 28: RPLP0



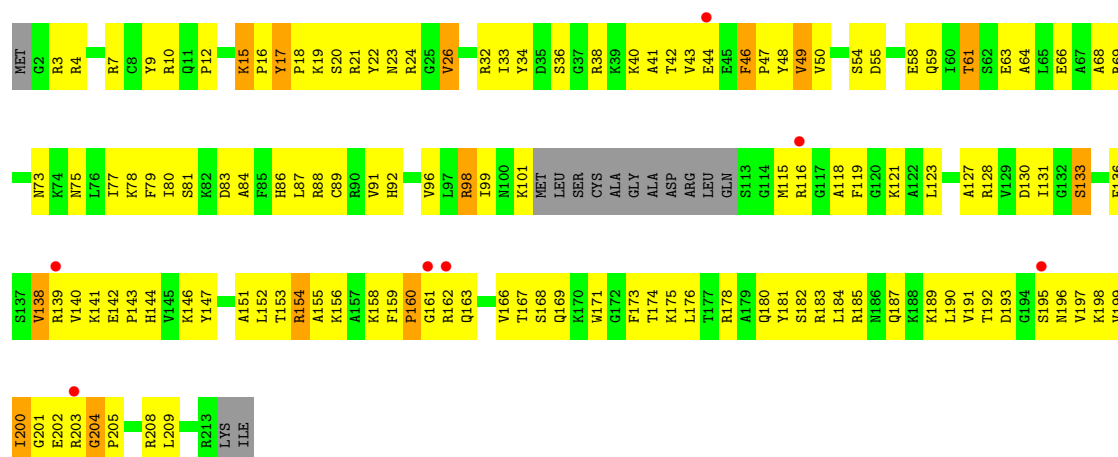
• Molecule 28: RPLP0



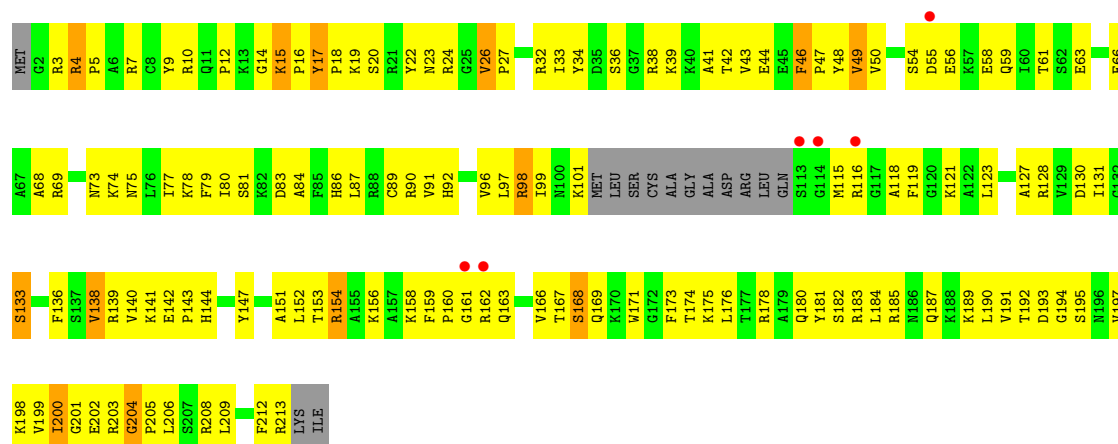
- Molecule 28: RPLP0

Chain GG:  61% 39%

- Molecule 29: 60S RIBOSOMAL PROTEIN L10

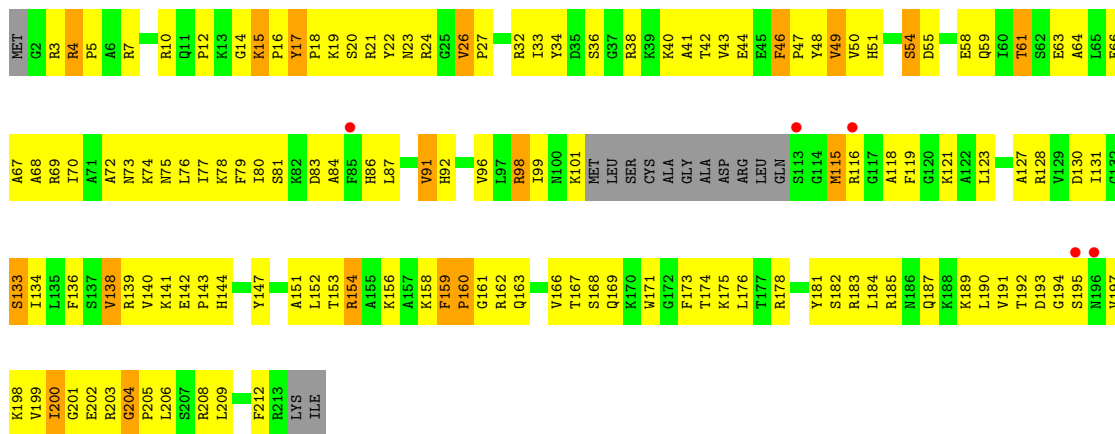
Chain BH:  3% 33% 54% 6% 7%

- Molecule 29: 60S RIBOSOMAL PROTEIN L10

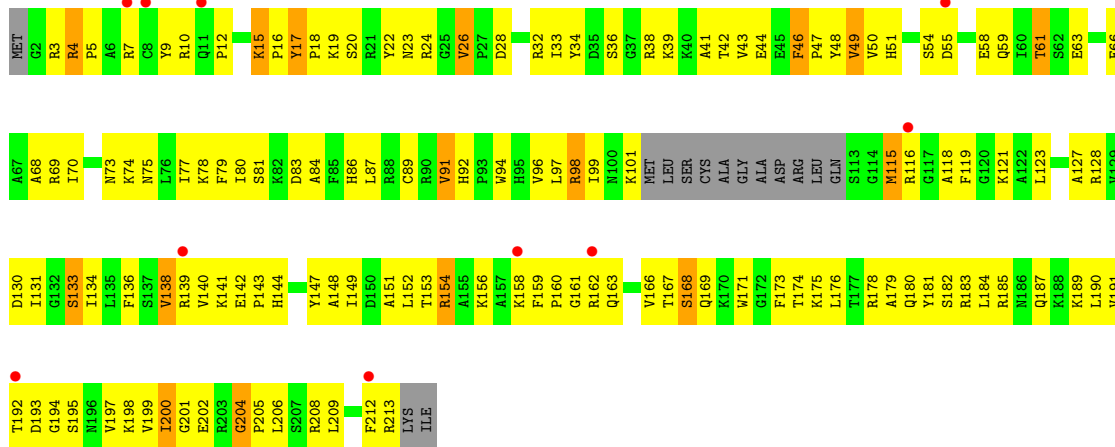
Chain CH:  3% 31% 56% 6% 7%

- Molecule 29: 60S RIBOSOMAL PROTEIN L10

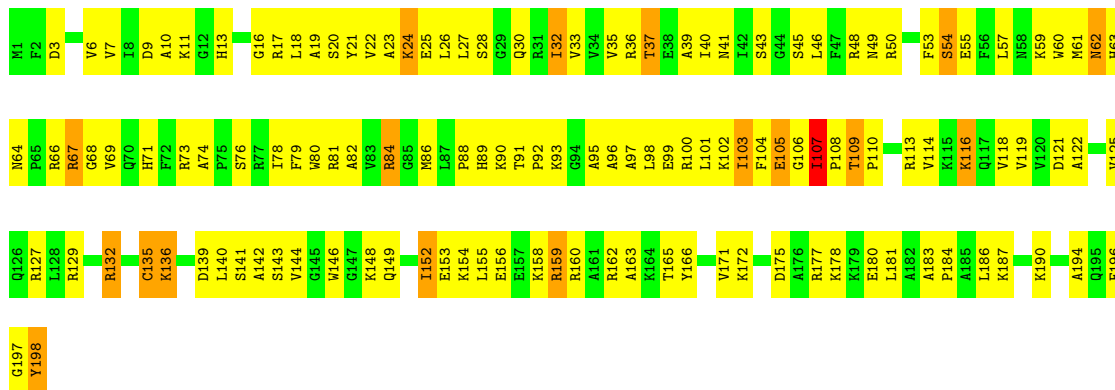
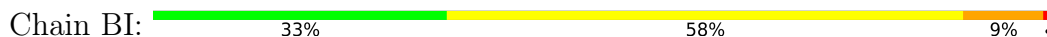
Chain EH:  2% 31% 54% 8% 7%



• Molecule 29: 60S RIBOSOMAL PROTEIN L10

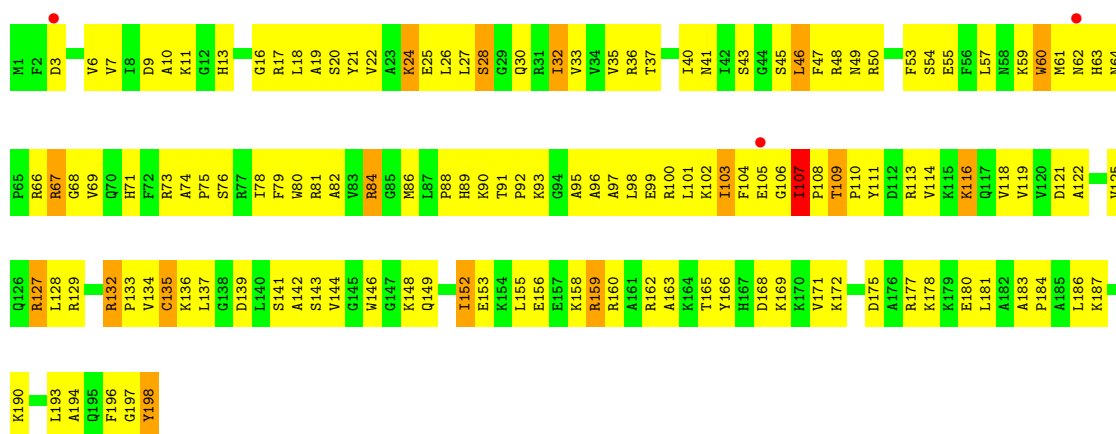


• Molecule 30: 60S RIBOSOMAL PROTEIN L13A

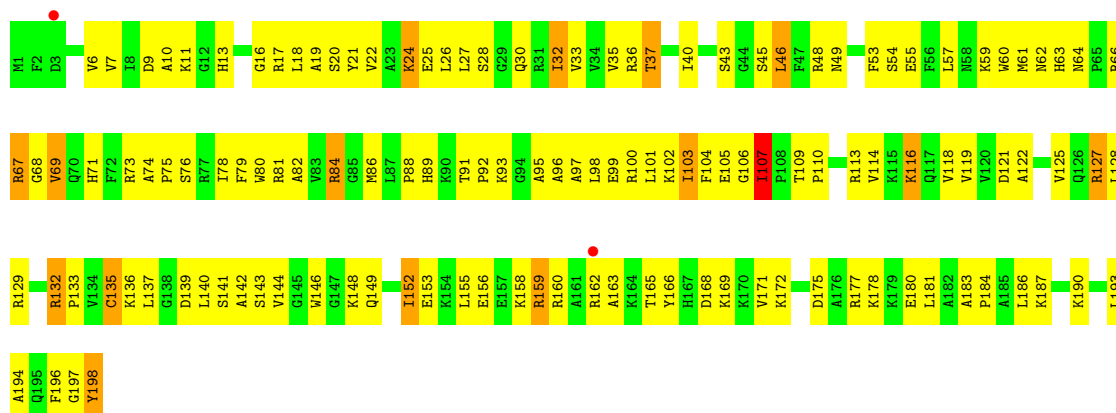


• Molecule 30: 60S RIBOSOMAL PROTEIN L13A

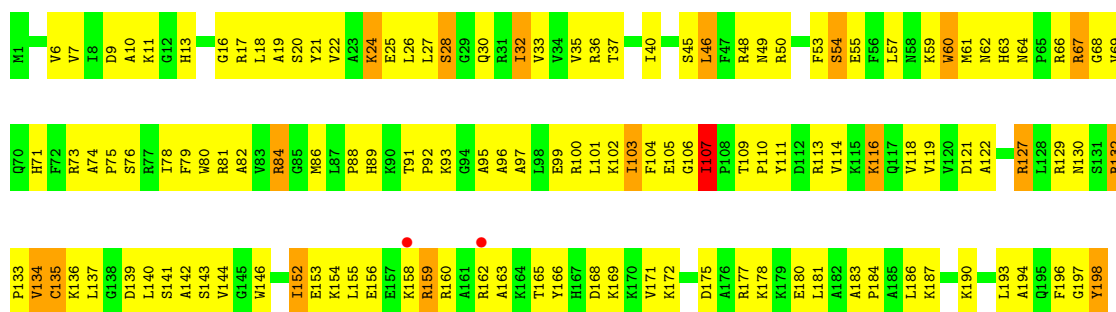




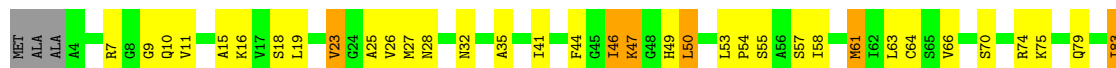
• Molecule 30: 60S RIBOSOMAL PROTEIN L13A



• Molecule 30: 60S RIBOSOMAL PROTEIN L13A



• Molecule 31: RPL23

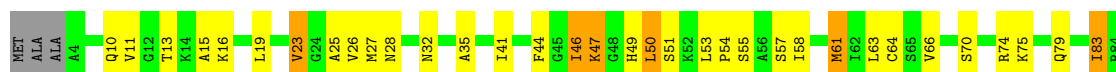




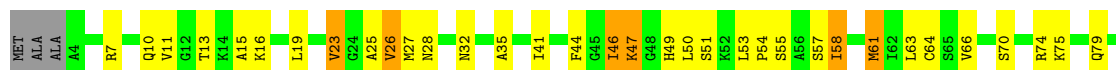
- Molecule 31: RPL23



- Molecule 31: RPL23



- Molecule 31: RPL23

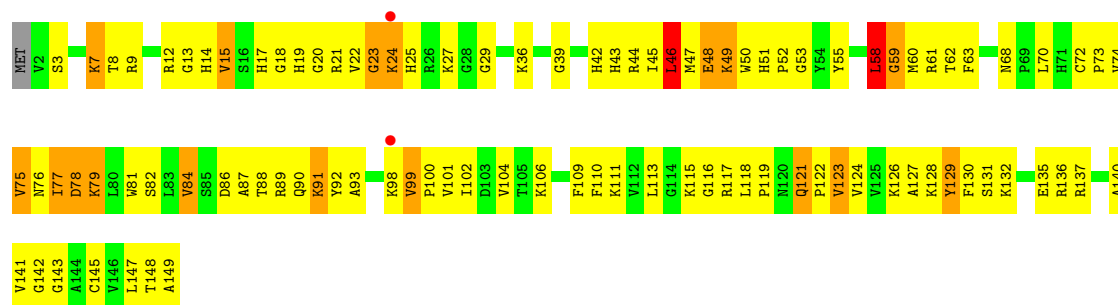


- Molecule 32: 60S RIBOSOMAL PROTEIN L27A

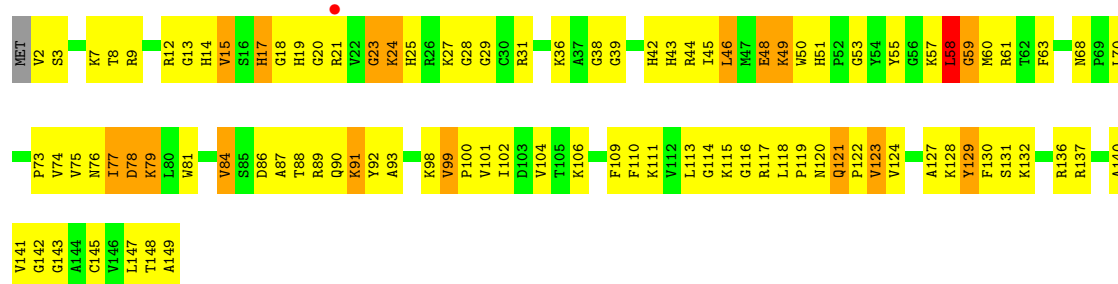


- Molecule 32: 60S RIBOSOMAL PROTEIN L27A

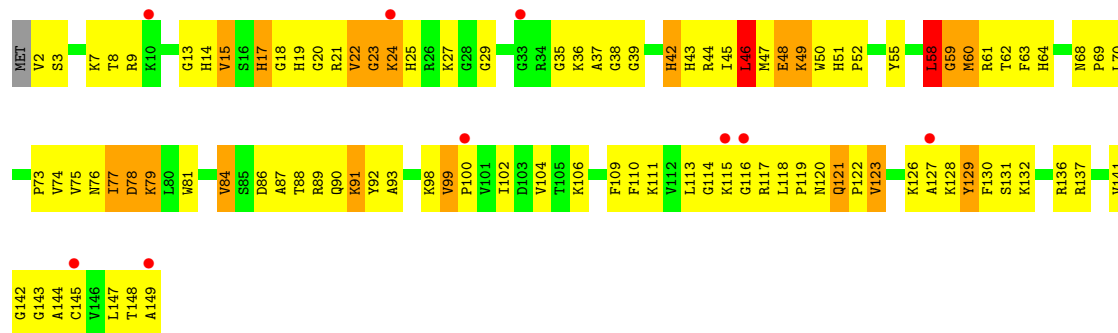




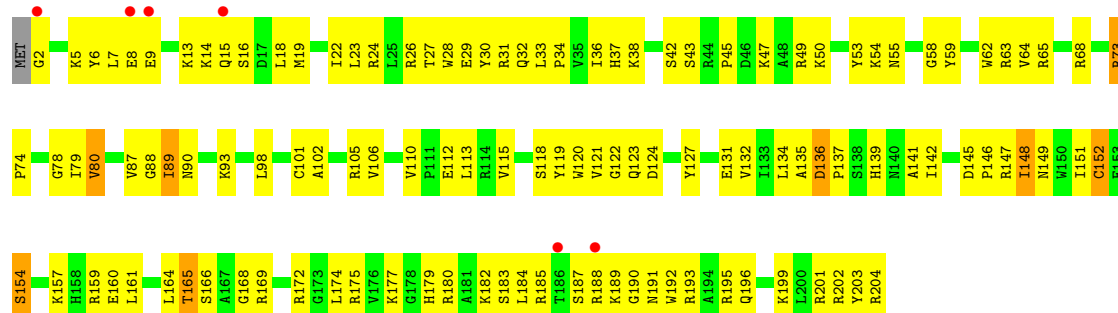
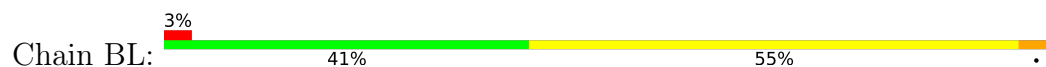
• Molecule 32: 60S RIBOSOMAL PROTEIN L27A



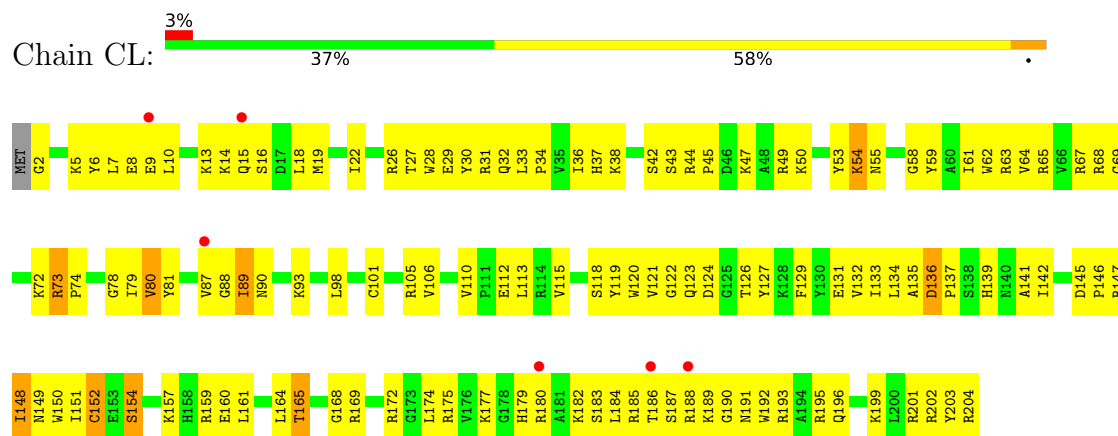
• Molecule 32: 60S RIBOSOMAL PROTEIN L27A



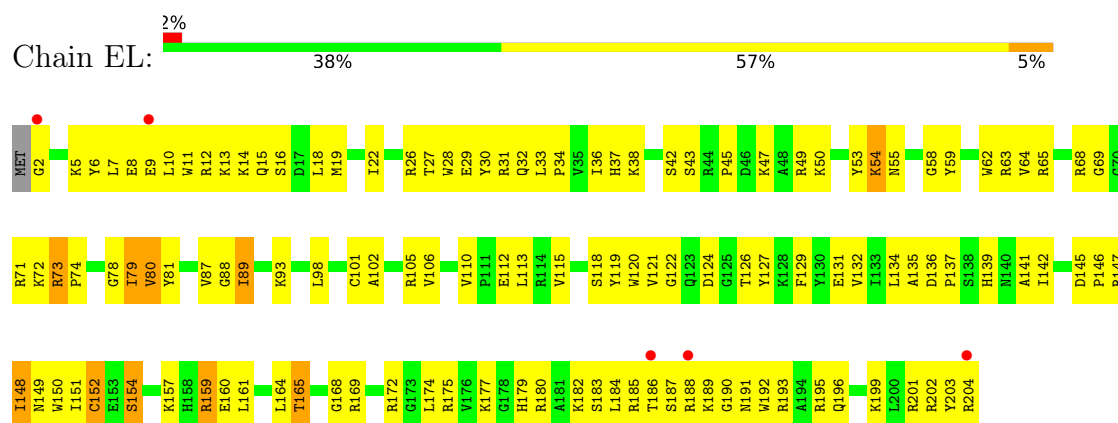
• Molecule 33: RIBOSOMAL PROTEIN L15



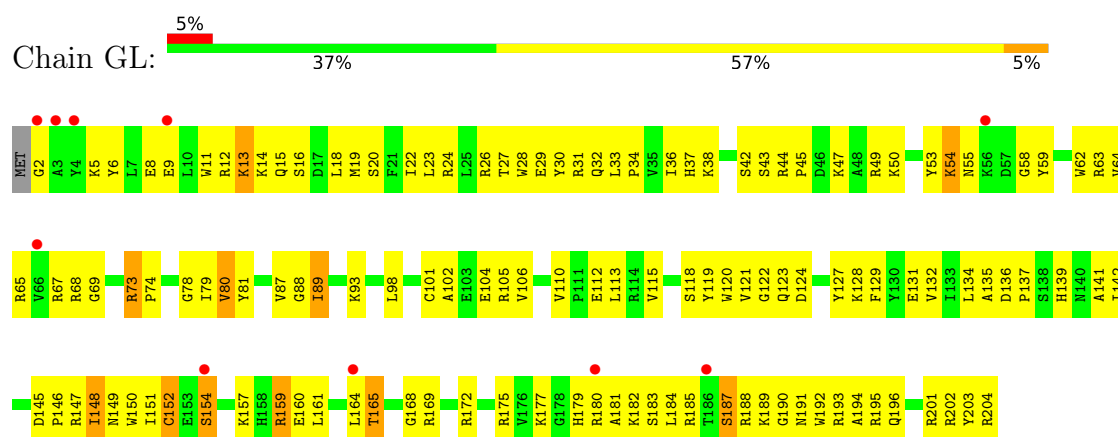
• Molecule 33: RIBOSOMAL PROTEIN L15



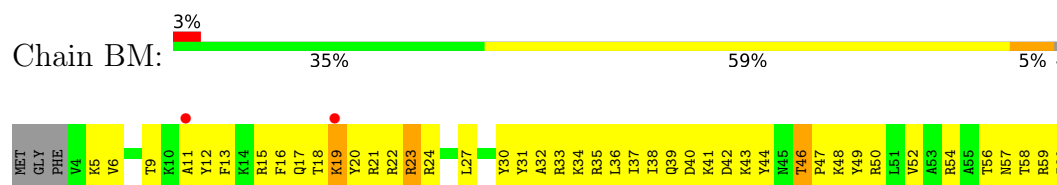
• Molecule 33: RIBOSOMAL PROTEIN L15

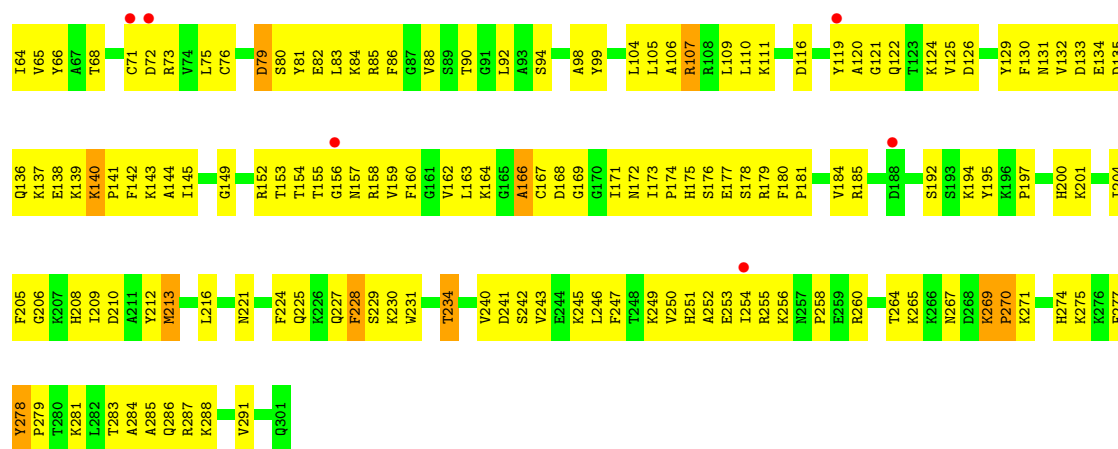


• Molecule 33: RIBOSOMAL PROTEIN L15

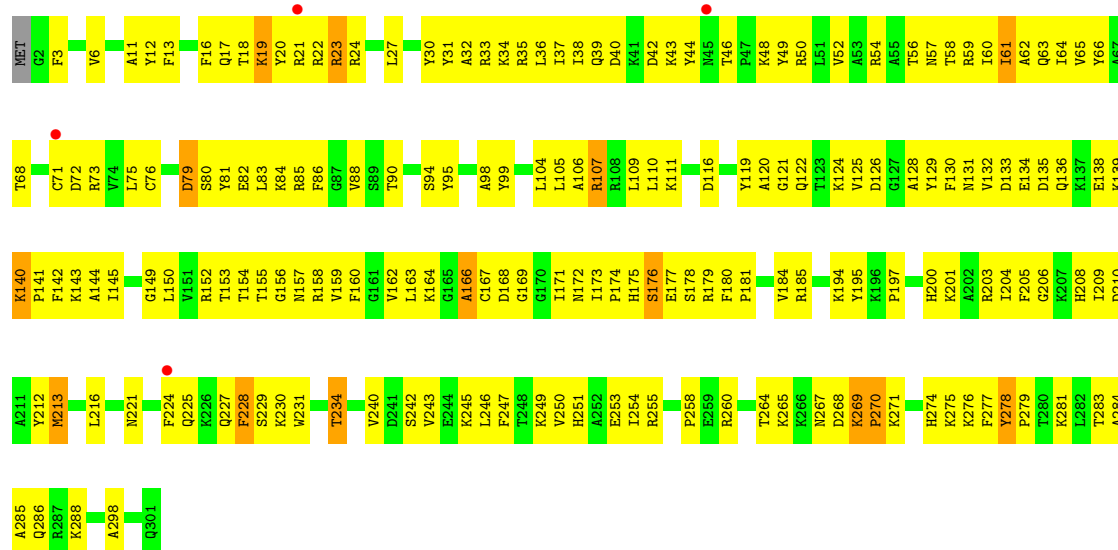


• Molecule 34: 60S RIBOSOMAL PROTEIN L5

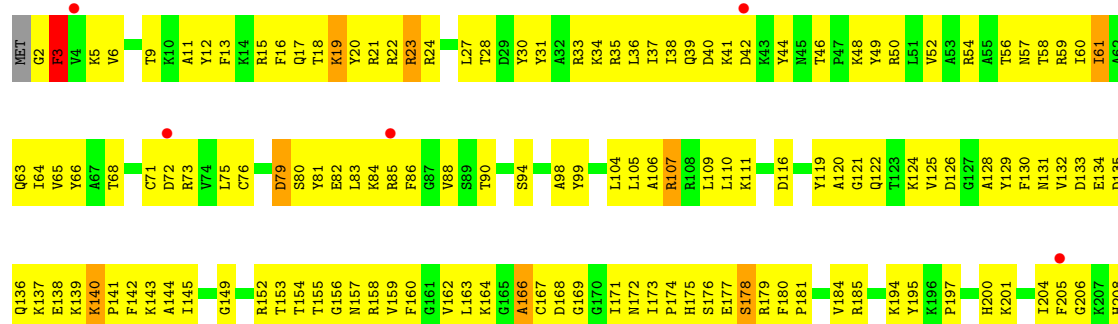


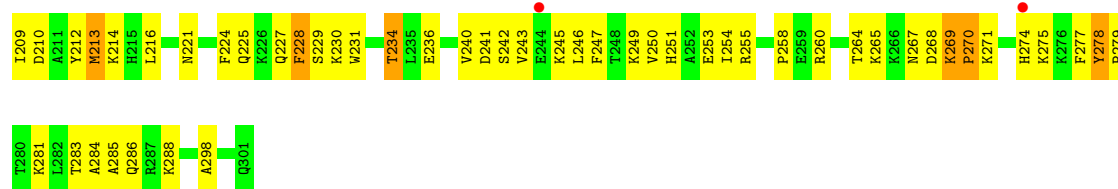


• Molecule 34: 60S RIBOSOMAL PROTEIN L5

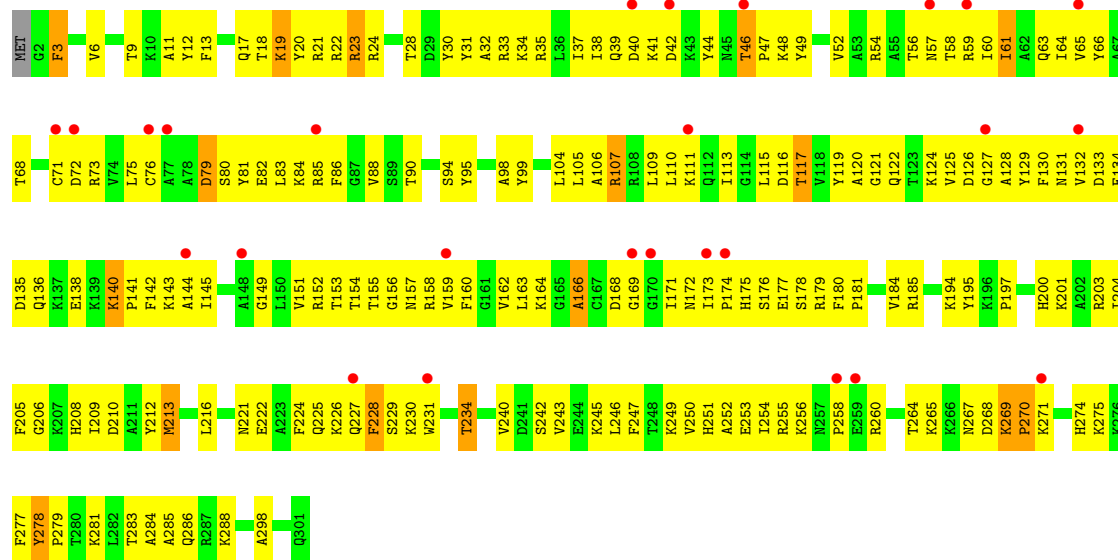


• Molecule 34: 60S RIBOSOMAL PROTEIN L5

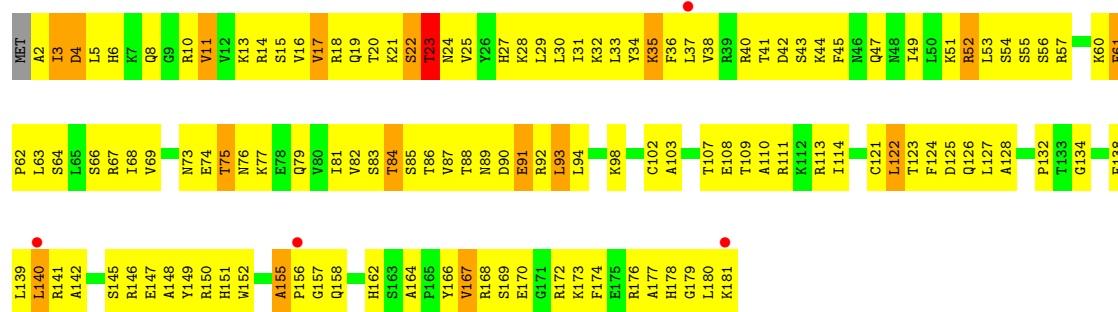




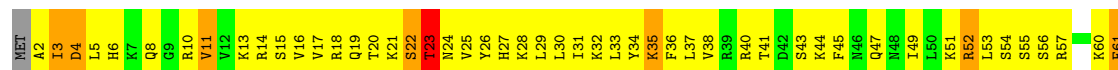
• Molecule 34: 60S RIBOSOMAL PROTEIN L5

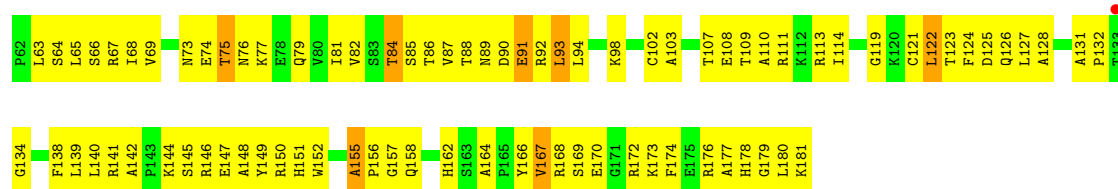


• Molecule 35: RPL18

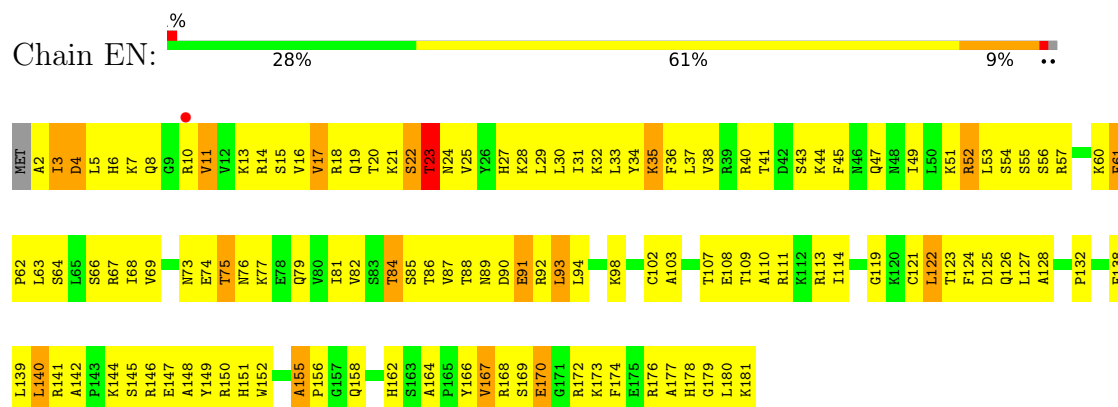


• Molecule 35: RPL18

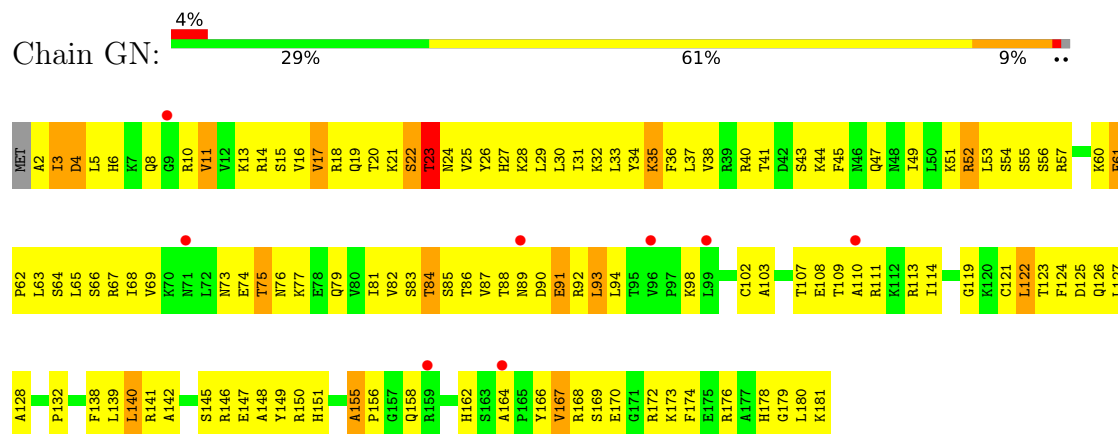




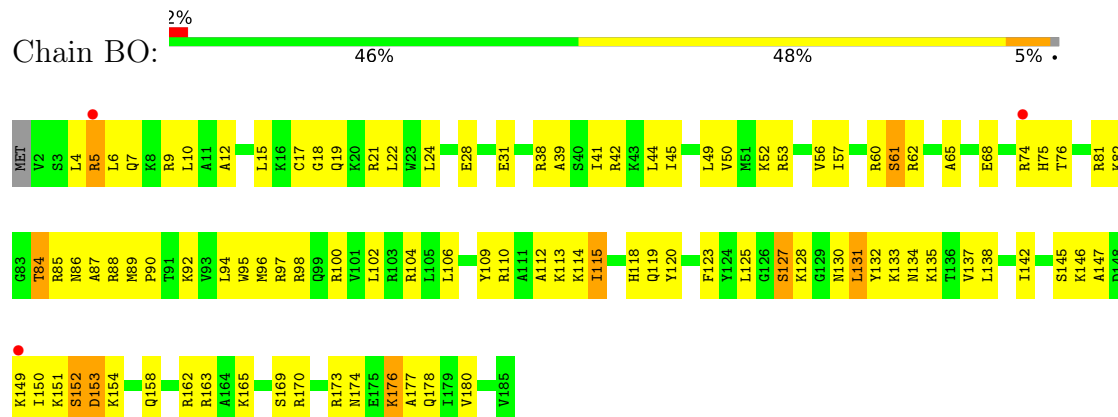
• Molecule 35: RPL18



• Molecule 35: RPL18

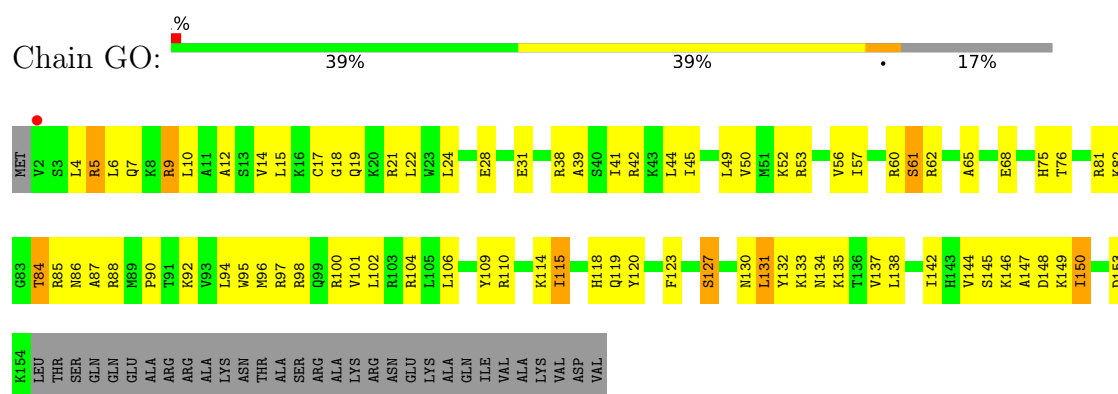


• Molecule 36: RPL19

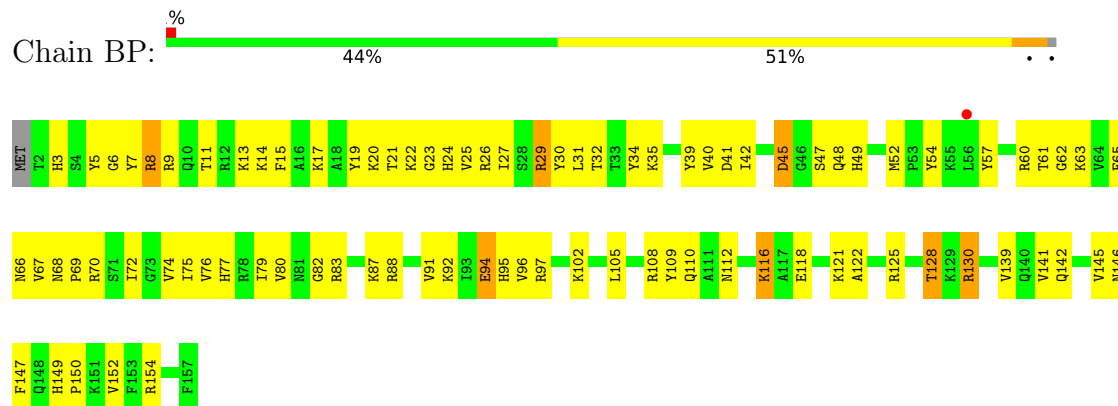


• Molecule 36: RPL19

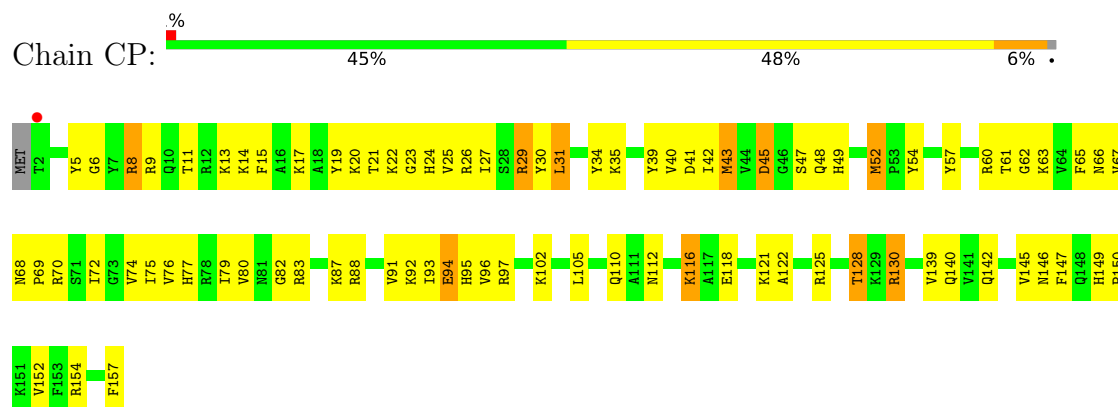
- Molecule 36: RPL19



● Molecule 37: 60S RIBOSOMAL PROTEIN L21



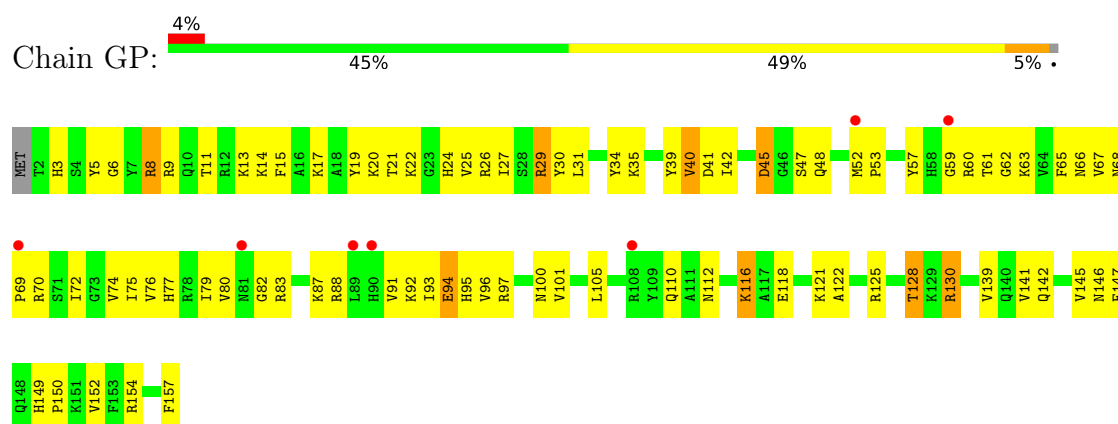
● Molecule 37: 60S RIBOSOMAL PROTEIN L21



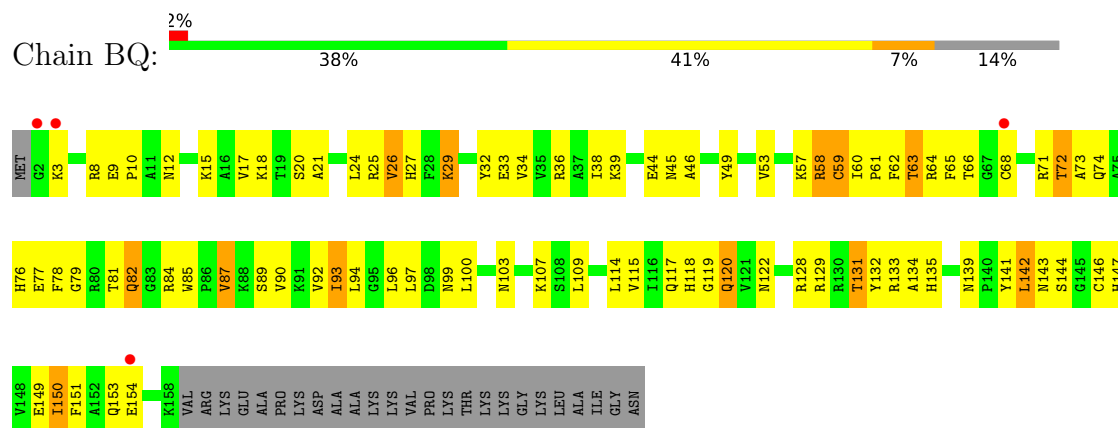
• Molecule 37: 60S RIBOSOMAL PROTEIN L21



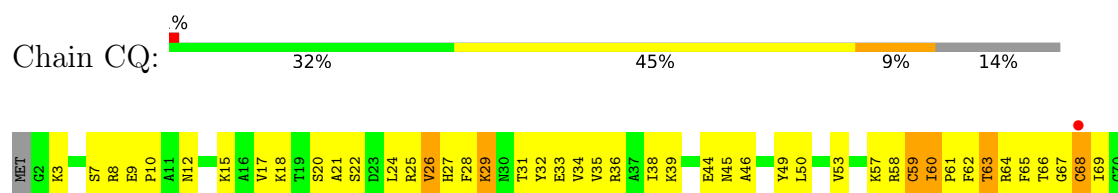
• Molecule 37: 60S RIBOSOMAL PROTEIN L21

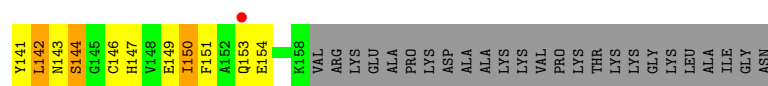


• Molecule 38: RPL17

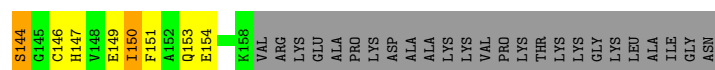
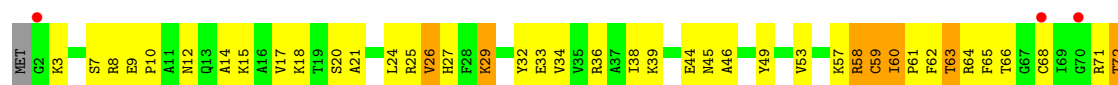


• Molecule 38: RPL17

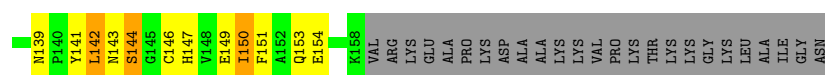




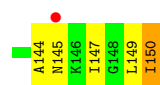
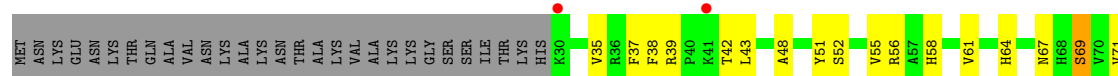
• Molecule 38: RPL17



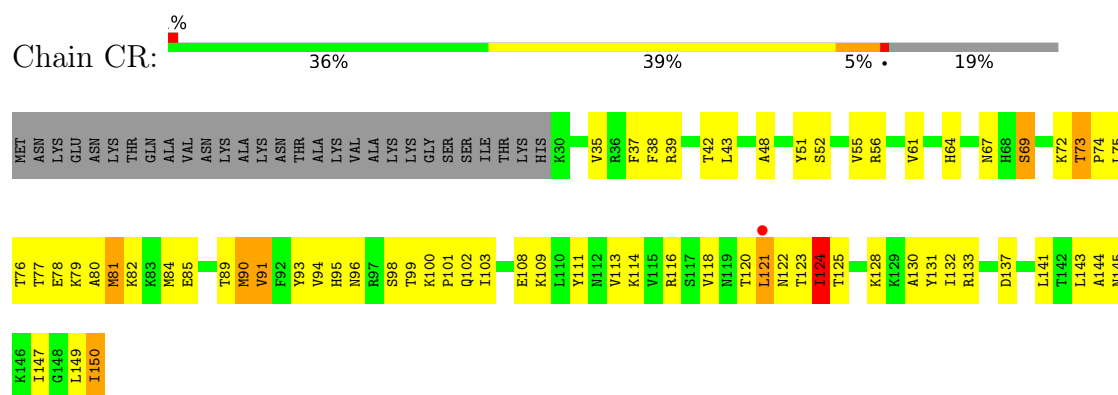
• Molecule 38: RPL17



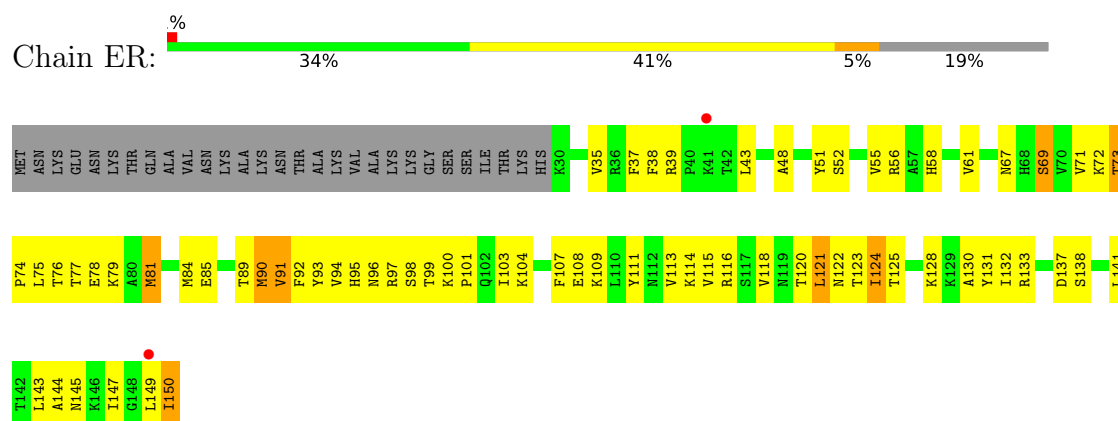
• Molecule 39: RPL23A



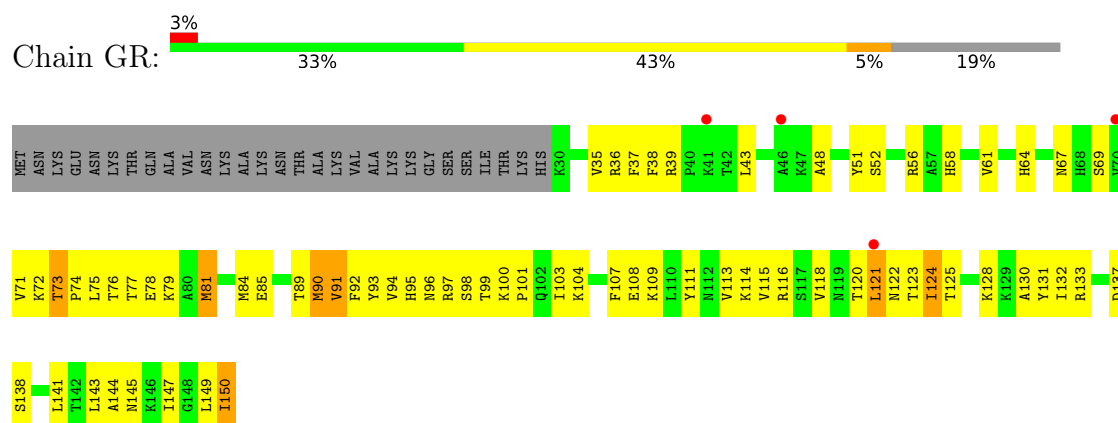
• Molecule 39: RPL23A



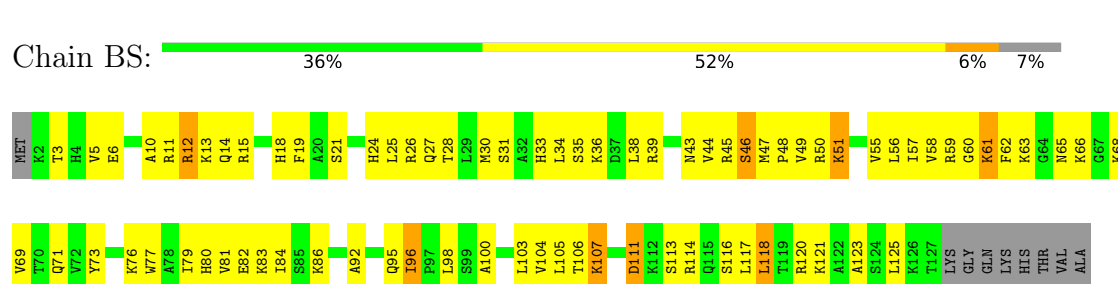
• Molecule 39: RPL23A



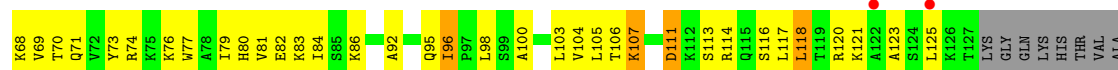
• Molecule 39: RPL23A



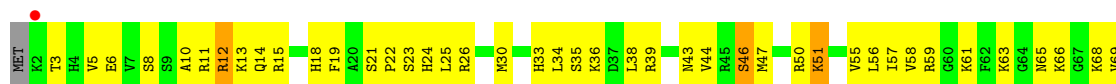
• Molecule 40: RPL26



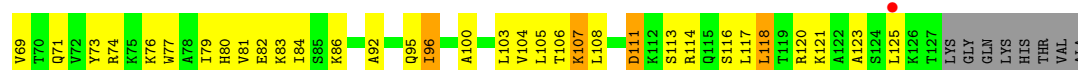
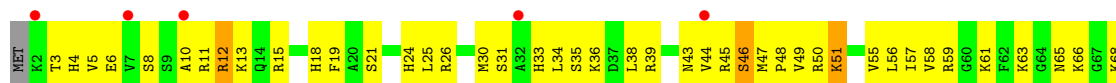
• Molecule 40: RPL26



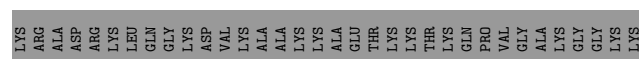
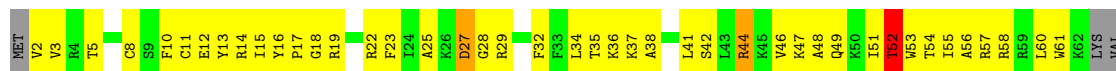
## • Molecule 40: RPL26



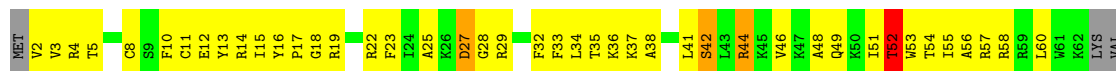
## • Molecule 40: RPL26



## • Molecule 41: RPL24



## • Molecule 41: RPL24



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| LYS | ALA | THR | ASP | ILE | ALA | GLN | LYS | LYS | LYS | LYS | ARG | ASN | VAL | VAL | THR | VAL | LYS | ALA | ARG | ALA | ALA | THR | ILE | VAL | GLY | ILE | THR | GLN | LEU | GLU | GLU | GLY | ILE | ASN | ARG | LYS | LYS | ASN | LEU | ASP | ALA | ALA | SER | HIS | LYS | LYS | ALA | ALA | GLU | ALA | GLU | LYS | VAL | ALA | VAL | VAL | ARG | GLU | LEU | LYS | GLN | LYS | LYS | LYS | ALA | ASN | ASP | ILE | LYS | VAL |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

• Molecule 41: RPL24

Chain ET:  11% 25% 61%

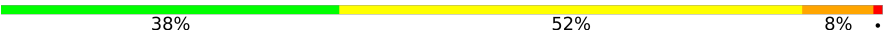
|     |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | V2 | V3 | R4 | T5 | C8 | S9 | F10 | C11 | E12 | Y13 | R14 | I15 | Y16 | P17 | G18 | R19 | R22 | F23 | I24 | A25 | K26 | D27 | G28 | R29 | F32 | F33 | L34 | T35 | K36 | K37 | A38 | L41 | S42 | L43 | R44 | K45 | V46 | K47 | A48 | Q49 | K50 | I51 | T52 | W53 | T54 | I55 | A56 | R57 | R58 | R59 | W61 | K62 | LYS | VAL |
|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

• Molecule 41: RPL24

Chain GT:  13% 23% 61%

|     |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | V2 | V3 | R4 | T5 | C8 | S9 | F10 | C11 | E12 | Y13 | R14 | I15 | Y16 | P17 | G18 | R19 | G20 | Q21 | F22 | I24 | A25 | K26 | D27 | G28 | R29 | F32 | F33 | L34 | T35 | K36 | K37 | A38 | L41 | S42 | L43 | R44 | K45 | V46 | K47 | A48 | Q49 | K50 | I51 | T52 | W53 | T54 | I55 | A56 | R57 | R58 | R59 | W61 | K62 | LYS |
|-----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

• Molecule 42: RPL35

Chain BU:  38% 52% 8%

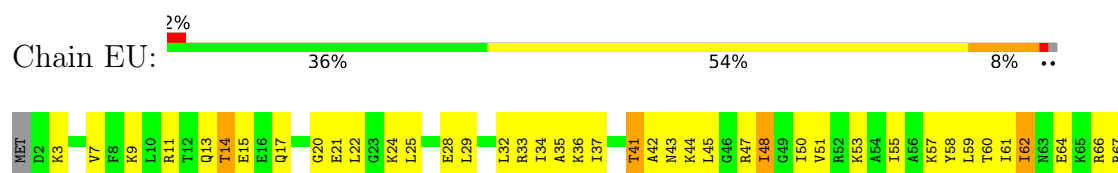
|     |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | D2 | K3 | R11 | T12 | Q13 | T14 | E15 | Q17 | G20 | E21 | L22 | G23 | K24 | L25 | E28 | L32 | R33 | T34 | A35 | K36 | I37 | T41 | A42 | M43 | K44 | T108 | G46 | R47 | I48 | V51 | R52 | K53 | A54 | I55 | Y58 | L59 | T60 | I61 | I62 | N63 | E64 | K65 | R66 | R67 | Q68 | A69 | D72 | Q73 | F74 | K75 |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

• Molecule 42: RPL35

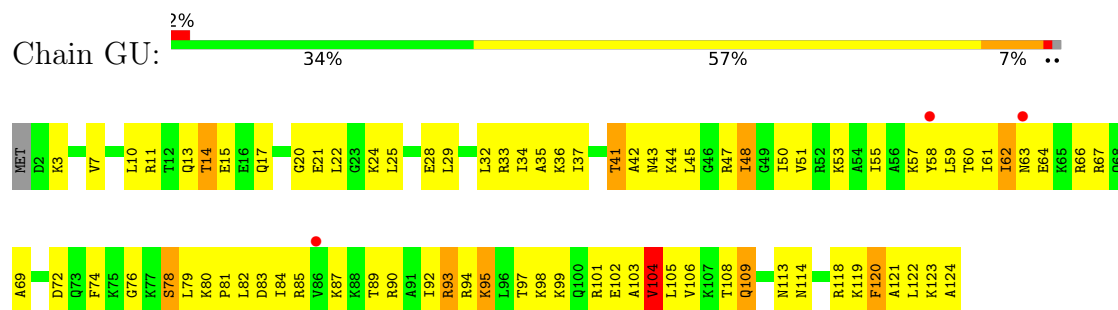
Chain CU:  36% 54% 8%

|     |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | D2 | K3 | V7 | R11 | T12 | Q13 | T14 | E15 | E16 | Q17 | G20 | E21 | L22 | G23 | K24 | L25 | E28 | L32 | R33 | T34 | A35 | K36 | I37 | T41 | A42 | M43 | K44 | L45 | G46 | R47 | I48 | V51 | R52 | K53 | A54 | I55 | A56 | K57 | Y58 | L59 | T60 | I61 | I62 | N63 | E64 | K65 | R66 | R67 | Q68 | A69 | D72 |
|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

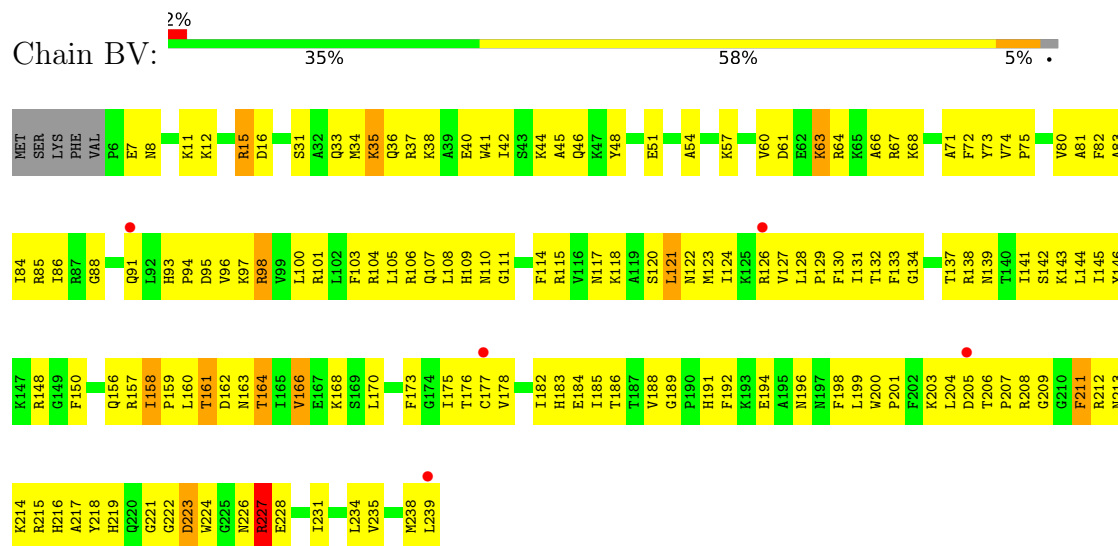
• Molecule 42: RPL35



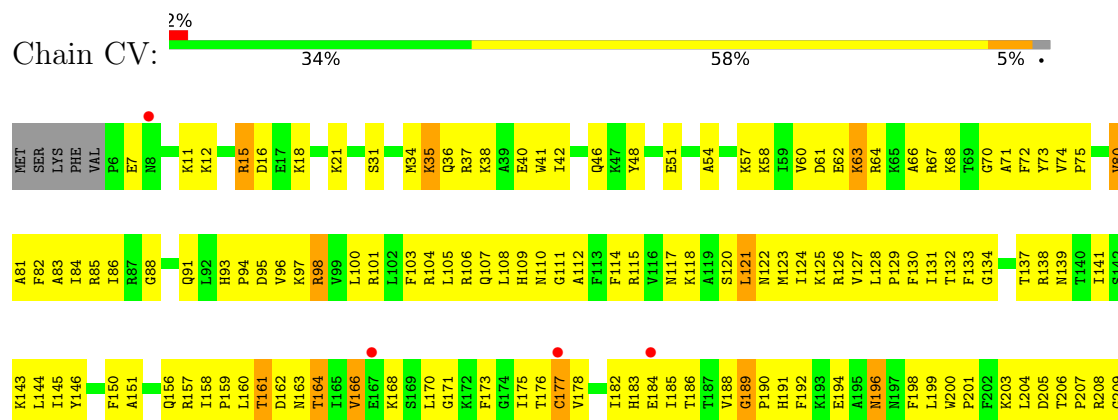
• Molecule 42: RPL35



• Molecule 43: 60S RIBOSOMAL PROTEIN L7



• Molecule 43: 60S RIBOSOMAL PROTEIN L7

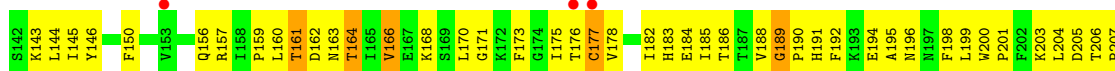
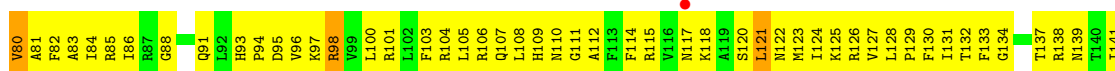
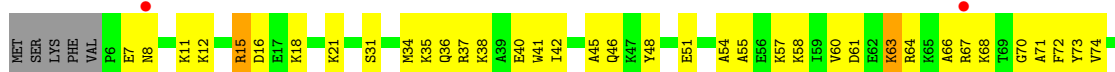




• Molecule 43: 60S RIBOSOMAL PROTEIN L7



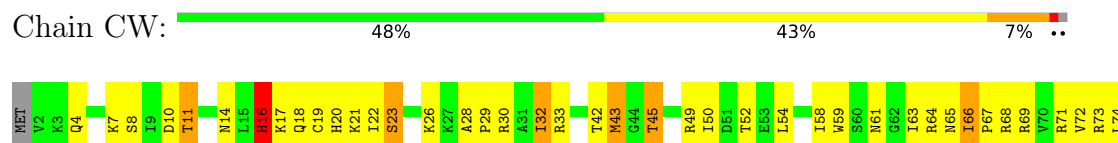
• Molecule 43: 60S RIBOSOMAL PROTEIN L7



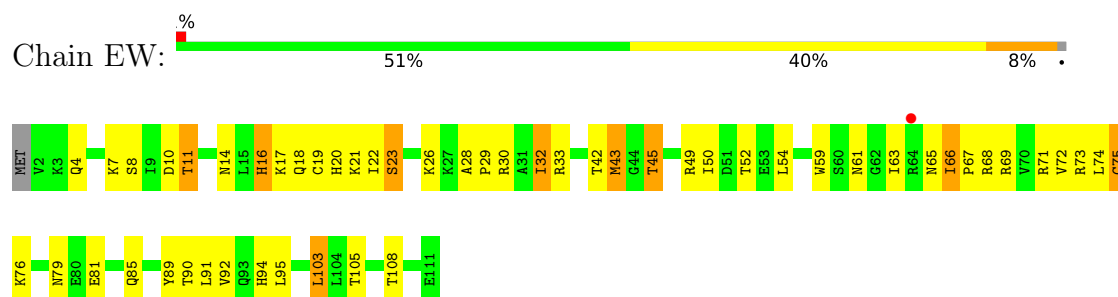
• Molecule 44: 60S RIBOSOMAL PROTEIN L31



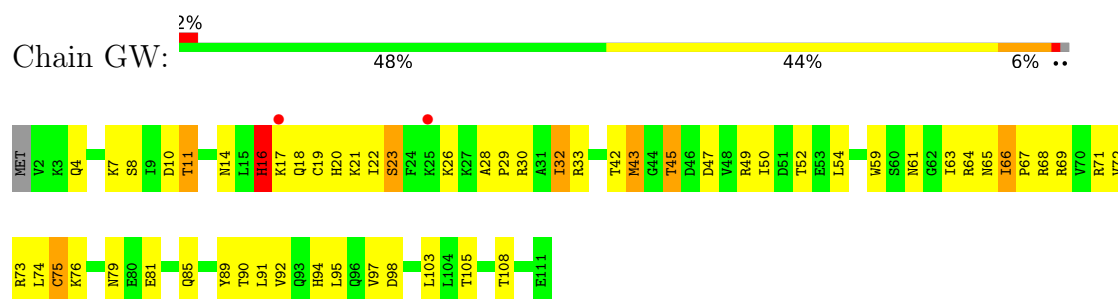
• Molecule 44: 60S RIBOSOMAL PROTEIN L31



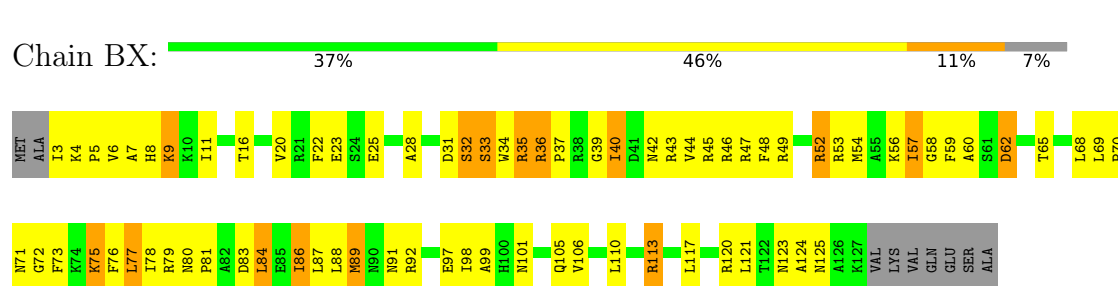
• Molecule 44: 60S RIBOSOMAL PROTEIN L31



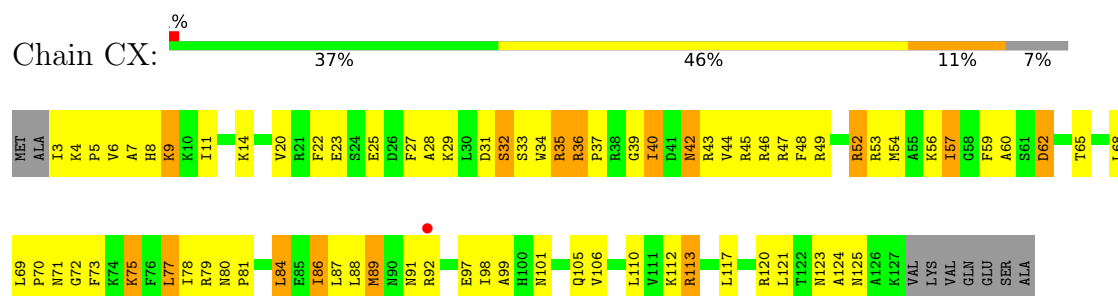
• Molecule 44: 60S RIBOSOMAL PROTEIN L31



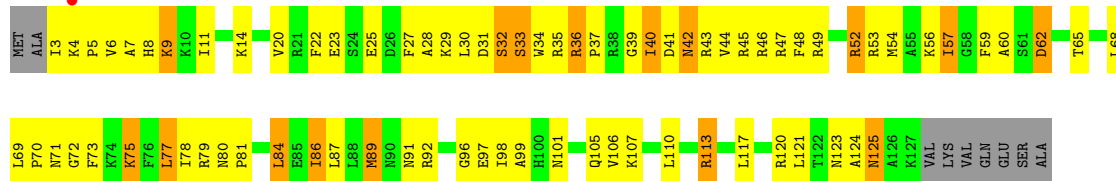
• Molecule 45: 60S RIBOSOMAL PROTEIN L32



• Molecule 45: 60S RIBOSOMAL PROTEIN L32



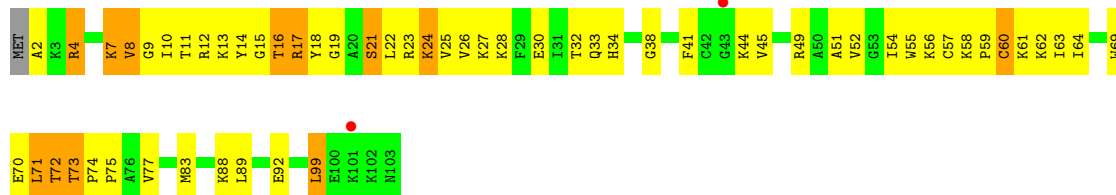
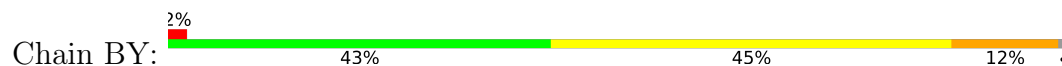
• Molecule 45: 60S RIBOSOMAL PROTEIN L32



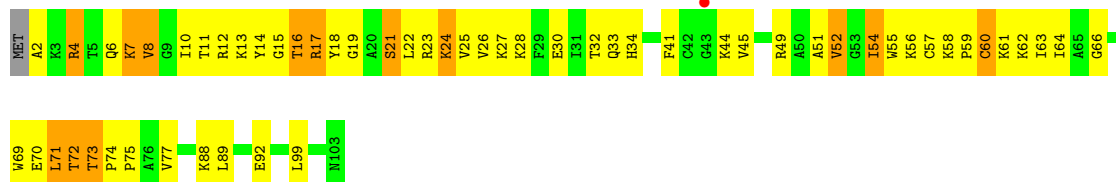
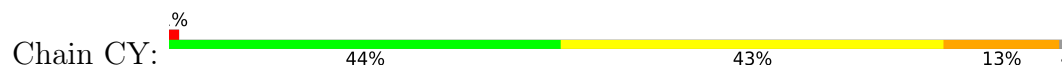
• Molecule 45: 60S RIBOSOMAL PROTEIN L32



• Molecule 46: RPL37A



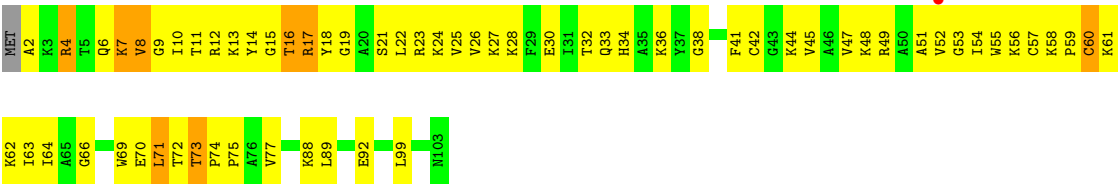
• Molecule 46: RPL37A



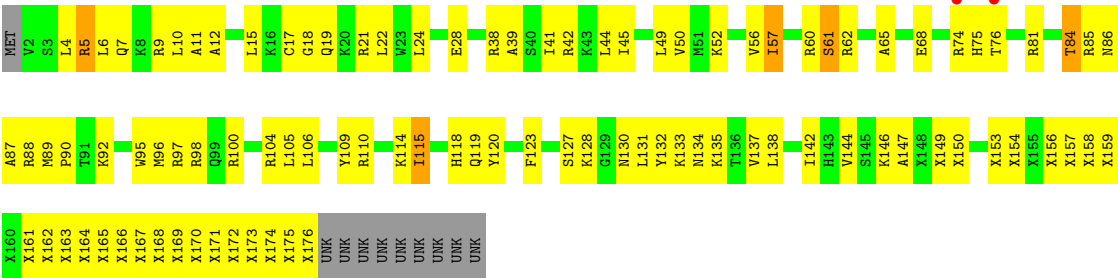
• Molecule 46: RPL37A



● Molecule 46: RPL37A



● Molecule 47: RPL19



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 320.19Å 289.25Å 535.04Å<br>90.00° 91.22° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 3.52<br>20.00 – 3.52                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.4 (20.00-3.52)<br>98.9 (20.00-3.52)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.13                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.87 (at 3.48Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (PHENIX.REFINE)                                      | Depositor        |
| R, $R_{free}$                                                           | 0.216 , 0.244<br>0.237 , 0.263                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10000 reflections (0.84%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 96.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.228                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 80.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | 0.028 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 511395                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 108.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, ZN

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   | A1    | 0.43         | 0/74792        | 0.48        | 0/116594        |
| 1   | D1    | 0.46         | 6/74792 (0.0%) | 0.48        | 0/116594        |
| 1   | F1    | 0.43         | 5/74792 (0.0%) | 0.48        | 3/116594 (0.0%) |
| 1   | H1    | 0.44         | 1/74792 (0.0%) | 0.49        | 0/116594        |
| 2   | AA    | 0.79         | 1/734 (0.1%)   | 1.15        | 4/972 (0.4%)    |
| 2   | DA    | 0.76         | 1/734 (0.1%)   | 1.15        | 4/972 (0.4%)    |
| 2   | FA    | 0.71         | 0/734          | 1.13        | 2/972 (0.2%)    |
| 2   | HA    | 0.72         | 0/734          | 1.11        | 2/972 (0.2%)    |
| 3   | AB    | 0.70         | 0/466          | 0.92        | 0/619           |
| 3   | DB    | 0.61         | 0/466          | 0.92        | 0/619           |
| 3   | FB    | 0.59         | 0/466          | 0.92        | 0/619           |
| 3   | HB    | 0.58         | 0/466          | 0.90        | 0/619           |
| 4   | AC    | 0.70         | 0/848          | 1.04        | 5/1123 (0.4%)   |
| 4   | DC    | 0.67         | 1/848 (0.1%)   | 1.03        | 5/1123 (0.4%)   |
| 4   | FC    | 0.65         | 0/848          | 1.04        | 5/1123 (0.4%)   |
| 4   | HC    | 0.70         | 0/848          | 1.03        | 3/1123 (0.3%)   |
| 5   | AE    | 0.59         | 0/1550         | 1.10        | 10/2077 (0.5%)  |
| 5   | DE    | 0.58         | 0/1550         | 1.11        | 9/2077 (0.4%)   |
| 5   | FE    | 0.59         | 0/1550         | 1.13        | 9/2077 (0.4%)   |
| 5   | HE    | 0.58         | 0/1550         | 1.13        | 10/2077 (0.5%)  |
| 6   | AF    | 0.67         | 0/1033         | 1.04        | 5/1380 (0.4%)   |
| 6   | DF    | 0.67         | 0/1033         | 1.04        | 6/1380 (0.4%)   |
| 6   | FF    | 0.69         | 0/1033         | 1.04        | 6/1380 (0.4%)   |
| 6   | HF    | 0.70         | 0/1033         | 1.06        | 6/1380 (0.4%)   |
| 7   | AG    | 0.70         | 0/736          | 1.12        | 3/990 (0.3%)    |
| 7   | DG    | 0.66         | 0/736          | 1.10        | 3/990 (0.3%)    |
| 7   | FG    | 0.65         | 0/736          | 1.12        | 3/990 (0.3%)    |
| 7   | HG    | 0.62         | 0/736          | 1.12        | 3/990 (0.3%)    |
| 8   | AH    | 0.82         | 3/870 (0.3%)   | 1.22        | 7/1175 (0.6%)   |
| 8   | DH    | 0.83         | 2/870 (0.2%)   | 1.23        | 9/1175 (0.8%)   |
| 8   | FH    | 0.84         | 3/870 (0.3%)   | 1.22        | 9/1175 (0.8%)   |
| 8   | HH    | 0.76         | 2/870 (0.2%)   | 1.21        | 7/1175 (0.6%)   |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 9   | AJ    | 0.68         | 0/1739  | 1.06        | 6/2368 (0.3%)  |
| 9   | DJ    | 0.65         | 0/1739  | 1.05        | 6/2368 (0.3%)  |
| 9   | FJ    | 0.70         | 0/1739  | 1.05        | 11/2368 (0.5%) |
| 9   | HJ    | 0.72         | 0/1739  | 1.05        | 7/2368 (0.3%)  |
| 10  | AK    | 0.60         | 0/421   | 1.06        | 0/558          |
| 10  | DK    | 0.61         | 0/421   | 1.07        | 0/558          |
| 10  | FK    | 0.60         | 0/421   | 1.05        | 0/558          |
| 10  | HK    | 0.62         | 0/421   | 1.07        | 0/558          |
| 11  | AL    | 0.80         | 0/861   | 1.10        | 5/1154 (0.4%)  |
| 11  | DL    | 0.72         | 0/861   | 1.08        | 4/1154 (0.3%)  |
| 11  | FL    | 0.66         | 0/861   | 1.06        | 4/1154 (0.3%)  |
| 11  | HL    | 0.61         | 0/861   | 1.06        | 4/1154 (0.3%)  |
| 12  | AM    | 0.55         | 0/832   | 0.97        | 2/1113 (0.2%)  |
| 12  | DM    | 0.52         | 0/832   | 0.99        | 1/1113 (0.1%)  |
| 12  | FM    | 0.50         | 0/832   | 0.99        | 1/1113 (0.1%)  |
| 12  | HM    | 0.50         | 0/832   | 0.98        | 2/1113 (0.2%)  |
| 13  | AN    | 0.55         | 0/1190  | 1.00        | 6/1582 (0.4%)  |
| 13  | DN    | 0.47         | 0/1190  | 0.98        | 5/1582 (0.3%)  |
| 13  | FN    | 0.46         | 0/1190  | 0.98        | 4/1582 (0.3%)  |
| 13  | HN    | 0.44         | 0/1190  | 0.97        | 4/1582 (0.3%)  |
| 14  | AO    | 0.62         | 0/1047  | 1.08        | 4/1400 (0.3%)  |
| 14  | DO    | 0.66         | 0/1047  | 1.09        | 4/1400 (0.3%)  |
| 14  | FO    | 0.62         | 0/1047  | 1.07        | 4/1400 (0.3%)  |
| 14  | HO    | 0.65         | 0/1047  | 1.08        | 3/1400 (0.2%)  |
| 15  | AP    | 0.55         | 0/561   | 0.98        | 2/745 (0.3%)   |
| 15  | DP    | 0.51         | 0/561   | 1.02        | 2/745 (0.3%)   |
| 15  | FP    | 0.52         | 0/561   | 1.00        | 2/745 (0.3%)   |
| 15  | HP    | 0.52         | 0/561   | 1.01        | 2/745 (0.3%)   |
| 16  | AQ    | 0.64         | 0/808   | 1.00        | 2/1068 (0.2%)  |
| 16  | DQ    | 0.66         | 0/808   | 0.98        | 3/1068 (0.3%)  |
| 16  | FQ    | 0.67         | 0/808   | 1.01        | 3/1068 (0.3%)  |
| 16  | HQ    | 0.65         | 0/808   | 0.99        | 2/1068 (0.2%)  |
| 17  | AT    | 0.63         | 0/539   | 1.06        | 0/711          |
| 17  | DT    | 0.62         | 0/539   | 1.04        | 0/711          |
| 17  | FT    | 0.63         | 0/539   | 1.04        | 0/711          |
| 17  | HT    | 0.65         | 0/539   | 1.08        | 0/711          |
| 18  | AU    | 0.71         | 0/1647  | 1.18        | 13/2201 (0.6%) |
| 18  | DU    | 0.70         | 0/1647  | 1.19        | 13/2201 (0.6%) |
| 18  | FU    | 0.70         | 0/1647  | 1.21        | 13/2201 (0.6%) |
| 18  | HU    | 0.75         | 0/1647  | 1.20        | 13/2201 (0.6%) |
| 19  | AX    | 0.62         | 0/1563  | 1.11        | 16/2104 (0.8%) |
| 19  | DX    | 0.67         | 0/1563  | 1.11        | 10/2104 (0.5%) |
| 19  | FX    | 0.66         | 0/1563  | 1.10        | 10/2104 (0.5%) |

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 19  | HX    | 0.66         | 0/1563        | 1.11        | 11/2104 (0.5%) |
| 20  | B2    | 0.40         | 0/3696        | 0.48        | 0/5761         |
| 20  | C2    | 0.42         | 0/3696        | 0.48        | 0/5761         |
| 20  | E2    | 0.37         | 0/3696        | 0.48        | 0/5761         |
| 20  | G2    | 0.46         | 0/3696        | 0.49        | 0/5761         |
| 21  | B3    | 0.38         | 0/2870        | 0.39        | 0/4473         |
| 21  | C3    | 0.36         | 0/2870        | 0.39        | 0/4473         |
| 21  | E3    | 0.33         | 0/2870        | 0.38        | 0/4473         |
| 21  | G3    | 0.35         | 0/2870        | 0.39        | 0/4473         |
| 22  | BA    | 0.79         | 0/2019        | 1.14        | 13/2712 (0.5%) |
| 22  | CA    | 0.76         | 0/2019        | 1.11        | 9/2712 (0.3%)  |
| 22  | EA    | 0.75         | 0/2019        | 1.13        | 14/2712 (0.5%) |
| 22  | GA    | 0.70         | 0/2019        | 1.11        | 10/2712 (0.4%) |
| 23  | BB    | 0.75         | 0/3144        | 1.11        | 21/4213 (0.5%) |
| 23  | CB    | 0.70         | 0/3144        | 1.09        | 17/4213 (0.4%) |
| 23  | EB    | 0.70         | 0/3144        | 1.10        | 23/4213 (0.5%) |
| 23  | GB    | 0.67         | 0/3144        | 1.10        | 17/4213 (0.4%) |
| 24  | BC    | 0.61         | 0/3222        | 1.03        | 11/4338 (0.3%) |
| 24  | CC    | 0.65         | 0/3222        | 1.02        | 9/4338 (0.2%)  |
| 24  | EC    | 0.62         | 0/3222        | 1.02        | 9/4338 (0.2%)  |
| 24  | GC    | 0.65         | 0/3222        | 1.02        | 6/4338 (0.1%)  |
| 25  | BD    | 0.60         | 0/1376        | 0.98        | 4/1833 (0.2%)  |
| 25  | CD    | 0.59         | 0/1376        | 0.98        | 5/1833 (0.3%)  |
| 25  | ED    | 0.58         | 0/1376        | 0.97        | 4/1833 (0.2%)  |
| 25  | GD    | 0.60         | 0/1376        | 0.99        | 5/1833 (0.3%)  |
| 26  | BE    | 0.60         | 0/1501        | 1.03        | 5/2015 (0.2%)  |
| 26  | CE    | 0.60         | 0/1501        | 1.03        | 4/2015 (0.2%)  |
| 26  | EE    | 0.61         | 0/1501        | 1.02        | 3/2015 (0.1%)  |
| 26  | GE    | 0.63         | 0/1501        | 1.05        | 5/2015 (0.2%)  |
| 27  | BF    | 0.63         | 0/1893        | 1.02        | 9/2548 (0.4%)  |
| 27  | CF    | 0.63         | 0/1893        | 1.03        | 10/2548 (0.4%) |
| 27  | EF    | 0.62         | 0/1893        | 1.02        | 9/2548 (0.4%)  |
| 27  | GF    | 0.61         | 0/1893        | 1.04        | 6/2548 (0.2%)  |
| 29  | BH    | 0.58         | 0/1652        | 1.12        | 12/2213 (0.5%) |
| 29  | CH    | 0.60         | 0/1652        | 1.10        | 10/2213 (0.5%) |
| 29  | EH    | 0.57         | 0/1652        | 1.11        | 15/2213 (0.7%) |
| 29  | GH    | 0.59         | 0/1652        | 1.11        | 11/2213 (0.5%) |
| 30  | BI    | 0.63         | 0/1624        | 1.03        | 7/2176 (0.3%)  |
| 30  | CI    | 0.63         | 1/1624 (0.1%) | 1.04        | 8/2176 (0.4%)  |
| 30  | EI    | 0.64         | 0/1624        | 1.05        | 7/2176 (0.3%)  |
| 30  | GI    | 0.93         | 5/1624 (0.3%) | 1.14        | 12/2176 (0.6%) |
| 31  | BJ    | 0.84         | 2/1038 (0.2%) | 1.11        | 6/1394 (0.4%)  |
| 31  | CJ    | 0.88         | 2/1038 (0.2%) | 1.12        | 7/1394 (0.5%)  |

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5        |
| 31  | EJ    | 0.83         | 1/1038 (0.1%) | 1.13        | 6/1394 (0.4%)  |
| 31  | GJ    | 0.90         | 3/1038 (0.3%) | 1.13        | 6/1394 (0.4%)  |
| 32  | BK    | 0.67         | 0/1189        | 1.22        | 6/1589 (0.4%)  |
| 32  | CK    | 0.69         | 0/1189        | 1.24        | 9/1589 (0.6%)  |
| 32  | EK    | 0.69         | 0/1189        | 1.24        | 7/1589 (0.4%)  |
| 32  | GK    | 0.74         | 0/1189        | 1.24        | 8/1589 (0.5%)  |
| 33  | BL    | 0.64         | 0/1727        | 1.12        | 5/2308 (0.2%)  |
| 33  | CL    | 0.64         | 0/1727        | 1.09        | 5/2308 (0.2%)  |
| 33  | EL    | 0.63         | 0/1727        | 1.14        | 6/2308 (0.3%)  |
| 33  | GL    | 0.68         | 0/1727        | 1.14        | 5/2308 (0.2%)  |
| 34  | BM    | 0.61         | 0/2453        | 1.05        | 10/3285 (0.3%) |
| 34  | CM    | 0.61         | 0/2469        | 1.06        | 11/3306 (0.3%) |
| 34  | EM    | 0.62         | 1/2469 (0.0%) | 1.06        | 11/3306 (0.3%) |
| 34  | GM    | 0.70         | 2/2469 (0.1%) | 1.08        | 14/3306 (0.4%) |
| 35  | BN    | 0.64         | 0/1464        | 1.20        | 7/1965 (0.4%)  |
| 35  | CN    | 0.66         | 0/1464        | 1.20        | 7/1965 (0.4%)  |
| 35  | EN    | 0.63         | 0/1464        | 1.19        | 7/1965 (0.4%)  |
| 35  | GN    | 0.67         | 0/1464        | 1.19        | 7/1965 (0.4%)  |
| 36  | BO    | 0.80         | 0/1507        | 1.00        | 5/2001 (0.2%)  |
| 36  | EO    | 0.58         | 0/1208        | 0.96        | 1/1604 (0.1%)  |
| 36  | GO    | 0.63         | 1/1250 (0.1%) | 0.99        | 2/1660 (0.1%)  |
| 37  | BP    | 0.62         | 0/1300        | 0.94        | 1/1743 (0.1%)  |
| 37  | CP    | 0.60         | 0/1300        | 0.93        | 2/1743 (0.1%)  |
| 37  | EP    | 0.59         | 0/1300        | 0.92        | 1/1743 (0.1%)  |
| 37  | GP    | 0.64         | 0/1300        | 0.93        | 2/1743 (0.1%)  |
| 38  | BQ    | 0.79         | 0/1259        | 1.13        | 3/1693 (0.2%)  |
| 38  | CQ    | 0.78         | 0/1259        | 1.12        | 4/1693 (0.2%)  |
| 38  | EQ    | 0.70         | 0/1259        | 1.15        | 5/1693 (0.3%)  |
| 38  | GQ    | 0.68         | 0/1259        | 1.15        | 2/1693 (0.1%)  |
| 39  | BR    | 0.69         | 0/981         | 1.01        | 3/1320 (0.2%)  |
| 39  | CR    | 0.61         | 0/981         | 1.02        | 4/1320 (0.3%)  |
| 39  | ER    | 0.57         | 0/981         | 1.00        | 2/1320 (0.2%)  |
| 39  | GR    | 0.60         | 0/981         | 1.01        | 2/1320 (0.2%)  |
| 40  | BS    | 0.53         | 0/1028        | 0.98        | 5/1372 (0.4%)  |
| 40  | CS    | 0.53         | 0/1028        | 0.97        | 5/1372 (0.4%)  |
| 40  | ES    | 0.52         | 0/1028        | 0.96        | 4/1372 (0.3%)  |
| 40  | GS    | 0.58         | 0/1028        | 0.98        | 5/1372 (0.4%)  |
| 41  | BT    | 0.66         | 0/521         | 1.01        | 4/693 (0.6%)   |
| 41  | CT    | 0.65         | 0/521         | 1.00        | 3/693 (0.4%)   |
| 41  | ET    | 0.63         | 0/521         | 1.00        | 3/693 (0.4%)   |
| 41  | GT    | 0.62         | 0/521         | 0.99        | 3/693 (0.4%)   |
| 42  | BU    | 0.57         | 0/995         | 0.96        | 4/1318 (0.3%)  |
| 42  | CU    | 0.56         | 0/995         | 0.96        | 2/1318 (0.2%)  |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 42  | EU    | 0.52         | 0/995            | 0.98        | 4/1318 (0.3%)     |
| 42  | GU    | 0.61         | 0/995            | 0.99        | 4/1318 (0.3%)     |
| 43  | BV    | 0.57         | 0/1950           | 1.00        | 8/2614 (0.3%)     |
| 43  | CV    | 0.63         | 0/1950           | 1.01        | 10/2614 (0.4%)    |
| 43  | EV    | 0.61         | 0/1950           | 1.01        | 10/2614 (0.4%)    |
| 43  | GV    | 0.61         | 0/1950           | 1.01        | 8/2614 (0.3%)     |
| 44  | BW    | 0.80         | 0/913            | 0.92        | 0/1222            |
| 44  | CW    | 0.71         | 0/913            | 0.93        | 2/1222 (0.2%)     |
| 44  | EW    | 0.62         | 0/913            | 0.92        | 1/1222 (0.1%)     |
| 44  | GW    | 0.61         | 0/913            | 0.91        | 1/1222 (0.1%)     |
| 45  | BX    | 0.59         | 0/1028           | 0.98        | 1/1371 (0.1%)     |
| 45  | CX    | 0.63         | 0/1028           | 0.98        | 2/1371 (0.1%)     |
| 45  | EX    | 0.57         | 0/1028           | 0.96        | 2/1371 (0.1%)     |
| 45  | GX    | 0.63         | 0/1028           | 1.01        | 2/1371 (0.1%)     |
| 46  | BY    | 0.79         | 0/799            | 1.19        | 5/1069 (0.5%)     |
| 46  | CY    | 0.74         | 1/799 (0.1%)     | 1.16        | 5/1069 (0.5%)     |
| 46  | EY    | 0.73         | 0/799            | 1.15        | 3/1069 (0.3%)     |
| 46  | GY    | 0.71         | 0/799            | 1.14        | 3/1069 (0.3%)     |
| 47  | CO    | 0.65         | 0/1208           | 0.94        | 1/1604 (0.1%)     |
| All | All   | 0.53         | 44/540737 (0.0%) | 0.75        | 951/795620 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | AA    | 0                   | 1                   |
| 2   | DA    | 0                   | 1                   |
| 2   | FA    | 0                   | 1                   |
| 2   | HA    | 0                   | 1                   |
| 8   | AH    | 0                   | 1                   |
| 12  | AM    | 0                   | 1                   |
| 12  | DM    | 0                   | 1                   |
| 12  | FM    | 0                   | 1                   |
| 12  | HM    | 0                   | 1                   |
| 16  | AQ    | 0                   | 1                   |
| 16  | DQ    | 0                   | 1                   |
| 16  | FQ    | 0                   | 1                   |
| 16  | HQ    | 0                   | 1                   |
| 18  | FU    | 0                   | 1                   |
| 27  | BF    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 27  | CF    | 0                   | 1                   |
| 27  | EF    | 0                   | 1                   |
| 27  | GF    | 0                   | 1                   |
| 32  | BK    | 0                   | 2                   |
| 32  | CK    | 0                   | 2                   |
| 32  | EK    | 0                   | 2                   |
| 32  | GK    | 0                   | 2                   |
| 38  | CQ    | 0                   | 1                   |
| 38  | GQ    | 0                   | 1                   |
| 42  | CU    | 0                   | 1                   |
| 45  | GX    | 0                   | 1                   |
| All | All   | 0                   | 30                  |

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

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 30  | GI    | 60   | TRP  | NE1-CE2 | -21.64 | 1.13        | 1.37     |
| 1   | F1    | 2239 | A    | O3'-P   | 20.53  | 1.92        | 1.61     |
| 34  | GM    | 117  | THR  | CA-CB   | -11.77 | 1.35        | 1.53     |
| 30  | GI    | 60   | TRP  | CG-CD2  | 11.01  | 1.63        | 1.43     |
| 30  | GI    | 60   | TRP  | CD2-CE2 | 9.77   | 1.57        | 1.41     |

The worst 5 of 951 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 33  | EL    | 73  | ARG  | CA-C-N | 14.37 | 133.91      | 119.82   |
| 33  | EL    | 73  | ARG  | C-N-CA | 14.37 | 133.91      | 119.82   |
| 33  | GL    | 73  | ARG  | CA-C-N | 13.63 | 133.18      | 119.82   |
| 33  | GL    | 73  | ARG  | C-N-CA | 13.63 | 133.18      | 119.82   |
| 33  | BL    | 73  | ARG  | CA-C-N | 12.90 | 132.47      | 119.82   |

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | AA    | 51  | GLY  | Peptide |
| 8   | AH    | 101 | GLY  | Peptide |
| 12  | AM    | 53  | GLY  | Peptide |
| 16  | AQ    | 12  | GLY  | Peptide |
| 27  | BF    | 174 | LYS  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A1    | 66769 | 0        | 33570    | 4651    | 2            |
| 1   | D1    | 66769 | 0        | 33568    | 4668    | 1            |
| 1   | F1    | 66769 | 0        | 33568    | 4673    | 3            |
| 1   | H1    | 66769 | 0        | 33570    | 4690    | 4            |
| 2   | AA    | 721   | 0        | 744      | 102     | 0            |
| 2   | DA    | 721   | 0        | 744      | 104     | 0            |
| 2   | FA    | 721   | 0        | 744      | 108     | 0            |
| 2   | HA    | 721   | 0        | 744      | 114     | 0            |
| 3   | AB    | 456   | 0        | 483      | 52      | 0            |
| 3   | DB    | 456   | 0        | 483      | 55      | 0            |
| 3   | FB    | 456   | 0        | 483      | 56      | 0            |
| 3   | HB    | 456   | 0        | 483      | 53      | 0            |
| 4   | AC    | 836   | 0        | 912      | 67      | 0            |
| 4   | DC    | 836   | 0        | 911      | 65      | 0            |
| 4   | FC    | 836   | 0        | 911      | 68      | 0            |
| 4   | HC    | 836   | 0        | 911      | 68      | 0            |
| 5   | AE    | 1525  | 0        | 1600     | 240     | 0            |
| 5   | DE    | 1525  | 0        | 1600     | 238     | 0            |
| 5   | FE    | 1525  | 0        | 1600     | 230     | 0            |
| 5   | HE    | 1525  | 0        | 1600     | 241     | 0            |
| 6   | AF    | 1021  | 0        | 1119     | 154     | 0            |
| 6   | DF    | 1021  | 0        | 1119     | 154     | 0            |
| 6   | FF    | 1021  | 0        | 1119     | 159     | 0            |
| 6   | HF    | 1021  | 0        | 1119     | 156     | 0            |
| 7   | AG    | 727   | 0        | 747      | 106     | 0            |
| 7   | DG    | 727   | 0        | 747      | 95      | 0            |
| 7   | FG    | 727   | 0        | 747      | 91      | 0            |
| 7   | HG    | 727   | 0        | 747      | 90      | 0            |
| 8   | AH    | 850   | 0        | 870      | 139     | 0            |
| 8   | DH    | 850   | 0        | 870      | 144     | 0            |
| 8   | FH    | 850   | 0        | 870      | 145     | 0            |
| 8   | HH    | 850   | 0        | 870      | 138     | 0            |
| 9   | AJ    | 1716  | 0        | 1712     | 168     | 0            |
| 9   | DJ    | 1716  | 0        | 1712     | 187     | 0            |
| 9   | FJ    | 1716  | 0        | 1712     | 182     | 0            |
| 9   | HJ    | 1716  | 0        | 1712     | 181     | 0            |
| 10  | AK    | 415   | 0        | 446      | 42      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | DK    | 415   | 0        | 446      | 40      | 0            |
| 10  | FK    | 415   | 0        | 446      | 36      | 0            |
| 10  | HK    | 415   | 0        | 446      | 36      | 0            |
| 11  | AL    | 852   | 0        | 906      | 93      | 0            |
| 11  | DL    | 852   | 0        | 906      | 97      | 0            |
| 11  | FL    | 852   | 0        | 906      | 91      | 0            |
| 11  | HL    | 852   | 0        | 906      | 92      | 0            |
| 12  | AM    | 819   | 0        | 855      | 77      | 0            |
| 12  | DM    | 819   | 0        | 855      | 74      | 0            |
| 12  | FM    | 819   | 0        | 855      | 78      | 0            |
| 12  | HM    | 819   | 0        | 855      | 75      | 0            |
| 13  | AN    | 1170  | 0        | 1259     | 162     | 0            |
| 13  | DN    | 1170  | 0        | 1259     | 140     | 0            |
| 13  | FN    | 1170  | 0        | 1259     | 161     | 0            |
| 13  | HN    | 1170  | 0        | 1259     | 139     | 0            |
| 14  | AO    | 1034  | 0        | 1101     | 146     | 0            |
| 14  | DO    | 1034  | 0        | 1101     | 133     | 0            |
| 14  | FO    | 1034  | 0        | 1101     | 135     | 0            |
| 14  | HO    | 1034  | 0        | 1101     | 124     | 0            |
| 15  | AP    | 551   | 0        | 614      | 53      | 0            |
| 15  | DP    | 551   | 0        | 614      | 57      | 2            |
| 15  | FP    | 551   | 0        | 614      | 50      | 0            |
| 15  | HP    | 551   | 0        | 614      | 58      | 0            |
| 16  | AQ    | 803   | 0        | 907      | 88      | 2            |
| 16  | DQ    | 803   | 0        | 907      | 100     | 0            |
| 16  | FQ    | 803   | 0        | 907      | 98      | 0            |
| 16  | HQ    | 803   | 0        | 907      | 83      | 0            |
| 17  | AT    | 533   | 0        | 578      | 67      | 0            |
| 17  | DT    | 533   | 0        | 578      | 56      | 0            |
| 17  | FT    | 533   | 0        | 578      | 58      | 0            |
| 17  | HT    | 533   | 0        | 578      | 62      | 0            |
| 18  | AU    | 1624  | 0        | 1733     | 212     | 0            |
| 18  | DU    | 1624  | 0        | 1733     | 221     | 0            |
| 18  | FU    | 1624  | 0        | 1733     | 214     | 0            |
| 18  | HU    | 1624  | 0        | 1733     | 242     | 0            |
| 19  | AX    | 1536  | 0        | 1613     | 224     | 0            |
| 19  | DX    | 1536  | 0        | 1613     | 224     | 0            |
| 19  | FX    | 1536  | 0        | 1613     | 229     | 0            |
| 19  | HX    | 1536  | 0        | 1613     | 219     | 0            |
| 20  | B2    | 3300  | 0        | 1657     | 220     | 1            |
| 20  | C2    | 3300  | 0        | 1657     | 224     | 0            |
| 20  | E2    | 3300  | 0        | 1657     | 229     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | G2    | 3300  | 0        | 1657     | 234     | 0            |
| 21  | B3    | 2566  | 0        | 1294     | 181     | 0            |
| 21  | C3    | 2566  | 0        | 1294     | 194     | 0            |
| 21  | E3    | 2566  | 0        | 1294     | 192     | 0            |
| 21  | G3    | 2566  | 0        | 1294     | 187     | 0            |
| 22  | BA    | 1977  | 0        | 2000     | 242     | 0            |
| 22  | CA    | 1977  | 0        | 2000     | 229     | 0            |
| 22  | EA    | 1977  | 0        | 2000     | 250     | 0            |
| 22  | GA    | 1977  | 0        | 2000     | 251     | 0            |
| 23  | BB    | 3080  | 0        | 3187     | 348     | 0            |
| 23  | CB    | 3080  | 0        | 3187     | 340     | 0            |
| 23  | EB    | 3080  | 0        | 3187     | 372     | 0            |
| 23  | GB    | 3080  | 0        | 3187     | 370     | 0            |
| 24  | BC    | 3172  | 0        | 3274     | 438     | 0            |
| 24  | CC    | 3172  | 0        | 3274     | 444     | 0            |
| 24  | EC    | 3172  | 0        | 3274     | 454     | 0            |
| 24  | GC    | 3172  | 0        | 3274     | 457     | 0            |
| 25  | BD    | 1357  | 0        | 1400     | 129     | 0            |
| 25  | CD    | 1357  | 0        | 1400     | 124     | 0            |
| 25  | ED    | 1357  | 0        | 1400     | 131     | 0            |
| 25  | GD    | 1357  | 0        | 1400     | 130     | 0            |
| 26  | BE    | 1481  | 0        | 1574     | 130     | 0            |
| 26  | CE    | 1481  | 0        | 1574     | 126     | 0            |
| 26  | EE    | 1481  | 0        | 1574     | 133     | 0            |
| 26  | GE    | 1481  | 0        | 1574     | 129     | 0            |
| 27  | BF    | 1860  | 0        | 1968     | 211     | 0            |
| 27  | CF    | 1860  | 0        | 1968     | 223     | 0            |
| 27  | EF    | 1860  | 0        | 1968     | 199     | 1            |
| 27  | GF    | 1860  | 0        | 1968     | 213     | 0            |
| 28  | BG    | 711   | 0        | 644      | 56      | 0            |
| 28  | CG    | 711   | 0        | 644      | 44      | 0            |
| 28  | EG    | 711   | 0        | 644      | 46      | 0            |
| 28  | GG    | 711   | 0        | 644      | 86      | 0            |
| 29  | BH    | 1620  | 0        | 1701     | 162     | 0            |
| 29  | CH    | 1620  | 0        | 1701     | 159     | 0            |
| 29  | EH    | 1620  | 0        | 1701     | 170     | 0            |
| 29  | GH    | 1620  | 0        | 1701     | 167     | 0            |
| 30  | BI    | 1594  | 0        | 1701     | 184     | 0            |
| 30  | CI    | 1594  | 0        | 1701     | 192     | 0            |
| 30  | EI    | 1594  | 0        | 1701     | 179     | 0            |
| 30  | GI    | 1594  | 0        | 1701     | 189     | 0            |
| 31  | BJ    | 1022  | 0        | 1078     | 68      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | CJ    | 1022  | 0        | 1079     | 69      | 0            |
| 31  | EJ    | 1022  | 0        | 1079     | 71      | 0            |
| 31  | GJ    | 1022  | 0        | 1078     | 74      | 0            |
| 32  | BK    | 1161  | 0        | 1227     | 193     | 0            |
| 32  | CK    | 1161  | 0        | 1227     | 186     | 0            |
| 32  | EK    | 1161  | 0        | 1227     | 185     | 0            |
| 32  | GK    | 1161  | 0        | 1227     | 202     | 0            |
| 33  | BL    | 1691  | 0        | 1762     | 189     | 0            |
| 33  | CL    | 1691  | 0        | 1762     | 195     | 0            |
| 33  | EL    | 1691  | 0        | 1762     | 202     | 0            |
| 33  | GL    | 1691  | 0        | 1762     | 206     | 0            |
| 34  | BM    | 2409  | 0        | 2497     | 331     | 0            |
| 34  | CM    | 2424  | 0        | 2509     | 320     | 1            |
| 34  | EM    | 2424  | 0        | 2509     | 319     | 4            |
| 34  | GM    | 2424  | 0        | 2509     | 293     | 2            |
| 35  | BN    | 1441  | 0        | 1534     | 223     | 0            |
| 35  | CN    | 1441  | 0        | 1534     | 236     | 0            |
| 35  | EN    | 1441  | 0        | 1534     | 229     | 0            |
| 35  | GN    | 1441  | 0        | 1534     | 241     | 0            |
| 36  | BO    | 1491  | 0        | 1618     | 109     | 0            |
| 36  | EO    | 1192  | 0        | 1296     | 88      | 0            |
| 36  | GO    | 1234  | 0        | 1323     | 90      | 0            |
| 37  | BP    | 1272  | 0        | 1310     | 133     | 0            |
| 37  | CP    | 1272  | 0        | 1310     | 127     | 0            |
| 37  | EP    | 1272  | 0        | 1310     | 137     | 0            |
| 37  | GP    | 1272  | 0        | 1310     | 123     | 0            |
| 38  | BQ    | 1239  | 0        | 1276     | 129     | 0            |
| 38  | CQ    | 1239  | 0        | 1276     | 138     | 0            |
| 38  | EQ    | 1239  | 0        | 1276     | 126     | 0            |
| 38  | GQ    | 1239  | 0        | 1276     | 136     | 0            |
| 39  | BR    | 965   | 0        | 1020     | 100     | 0            |
| 39  | CR    | 965   | 0        | 1020     | 87      | 0            |
| 39  | ER    | 965   | 0        | 1020     | 95      | 0            |
| 39  | GR    | 965   | 0        | 1020     | 99      | 0            |
| 40  | BS    | 1013  | 0        | 1101     | 95      | 0            |
| 40  | CS    | 1013  | 0        | 1101     | 101     | 1            |
| 40  | ES    | 1013  | 0        | 1101     | 98      | 0            |
| 40  | GS    | 1013  | 0        | 1101     | 96      | 0            |
| 41  | BT    | 510   | 0        | 546      | 51      | 0            |
| 41  | CT    | 510   | 0        | 546      | 51      | 0            |
| 41  | ET    | 510   | 0        | 546      | 59      | 0            |
| 41  | GT    | 510   | 0        | 546      | 52      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 42  | BU    | 990   | 0        | 1123     | 100     | 0            |
| 42  | CU    | 990   | 0        | 1123     | 107     | 0            |
| 42  | EU    | 990   | 0        | 1123     | 109     | 0            |
| 42  | GU    | 990   | 0        | 1123     | 120     | 0            |
| 43  | BV    | 1910  | 0        | 1983     | 211     | 0            |
| 43  | CV    | 1910  | 0        | 1983     | 209     | 0            |
| 43  | EV    | 1910  | 0        | 1983     | 224     | 0            |
| 43  | GV    | 1910  | 0        | 1983     | 209     | 0            |
| 44  | BW    | 901   | 0        | 937      | 68      | 0            |
| 44  | CW    | 901   | 0        | 937      | 69      | 0            |
| 44  | EW    | 901   | 0        | 937      | 70      | 0            |
| 44  | GW    | 901   | 0        | 937      | 72      | 0            |
| 45  | BX    | 1012  | 0        | 1079     | 115     | 0            |
| 45  | CX    | 1012  | 0        | 1079     | 116     | 0            |
| 45  | EX    | 1012  | 0        | 1079     | 122     | 0            |
| 45  | GX    | 1012  | 0        | 1079     | 128     | 0            |
| 46  | BY    | 786   | 0        | 851      | 87      | 0            |
| 46  | CY    | 786   | 0        | 849      | 92      | 0            |
| 46  | EY    | 786   | 0        | 851      | 111     | 0            |
| 46  | GY    | 786   | 0        | 851      | 99      | 0            |
| 47  | CO    | 1366  | 0        | 1470     | 143     | 0            |
| 48  | A1    | 200   | 0        | 0        | 0       | 0            |
| 48  | AA    | 2     | 0        | 0        | 0       | 0            |
| 48  | AK    | 1     | 0        | 0        | 0       | 0            |
| 48  | B2    | 8     | 0        | 0        | 0       | 0            |
| 48  | B3    | 3     | 0        | 0        | 0       | 0            |
| 48  | BJ    | 1     | 0        | 0        | 0       | 0            |
| 48  | BL    | 1     | 0        | 0        | 0       | 0            |
| 48  | BN    | 1     | 0        | 0        | 0       | 0            |
| 48  | BP    | 1     | 0        | 0        | 0       | 0            |
| 48  | BQ    | 2     | 0        | 0        | 0       | 0            |
| 48  | BW    | 1     | 0        | 0        | 0       | 0            |
| 48  | C2    | 6     | 0        | 0        | 0       | 0            |
| 48  | C3    | 7     | 0        | 0        | 0       | 0            |
| 48  | CD    | 1     | 0        | 0        | 0       | 0            |
| 48  | CJ    | 1     | 0        | 0        | 0       | 0            |
| 48  | CL    | 2     | 0        | 0        | 0       | 0            |
| 48  | CN    | 1     | 0        | 0        | 0       | 0            |
| 48  | CQ    | 2     | 0        | 0        | 0       | 0            |
| 48  | CW    | 1     | 0        | 0        | 0       | 0            |
| 48  | CY    | 1     | 0        | 0        | 0       | 0            |
| 48  | D1    | 232   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 48  | DA    | 2     | 0        | 0        | 0       | 0            |
| 48  | DJ    | 1     | 0        | 0        | 0       | 0            |
| 48  | DK    | 1     | 0        | 0        | 0       | 0            |
| 48  | DQ    | 1     | 0        | 0        | 0       | 0            |
| 48  | E2    | 7     | 0        | 0        | 0       | 0            |
| 48  | E3    | 6     | 0        | 0        | 0       | 0            |
| 48  | EJ    | 1     | 0        | 0        | 0       | 0            |
| 48  | EL    | 2     | 0        | 0        | 0       | 0            |
| 48  | EN    | 2     | 0        | 0        | 0       | 0            |
| 48  | EQ    | 1     | 0        | 0        | 0       | 0            |
| 48  | EW    | 2     | 0        | 0        | 0       | 0            |
| 48  | F1    | 184   | 0        | 0        | 0       | 0            |
| 48  | FA    | 2     | 0        | 0        | 0       | 0            |
| 48  | FK    | 1     | 0        | 0        | 0       | 0            |
| 48  | FT    | 1     | 0        | 0        | 0       | 0            |
| 48  | G2    | 6     | 0        | 0        | 0       | 0            |
| 48  | G3    | 5     | 0        | 0        | 0       | 0            |
| 48  | GA    | 1     | 0        | 0        | 0       | 0            |
| 48  | GJ    | 1     | 0        | 0        | 0       | 0            |
| 48  | GL    | 1     | 0        | 0        | 0       | 0            |
| 48  | GN    | 1     | 0        | 0        | 0       | 0            |
| 48  | GO    | 1     | 0        | 0        | 0       | 0            |
| 48  | GP    | 2     | 0        | 0        | 0       | 0            |
| 48  | GQ    | 1     | 0        | 0        | 0       | 0            |
| 48  | GW    | 1     | 0        | 0        | 0       | 0            |
| 48  | H1    | 155   | 0        | 0        | 0       | 0            |
| 48  | HT    | 1     | 0        | 0        | 0       | 0            |
| 49  | AA    | 1     | 0        | 0        | 0       | 0            |
| 49  | AC    | 1     | 0        | 0        | 0       | 0            |
| 49  | AK    | 1     | 0        | 0        | 0       | 0            |
| 49  | AL    | 1     | 0        | 0        | 0       | 0            |
| 49  | BY    | 1     | 0        | 0        | 0       | 0            |
| 49  | CY    | 1     | 0        | 0        | 0       | 0            |
| 49  | DA    | 1     | 0        | 0        | 0       | 0            |
| 49  | DC    | 1     | 0        | 0        | 0       | 0            |
| 49  | DK    | 1     | 0        | 0        | 0       | 0            |
| 49  | DL    | 1     | 0        | 0        | 0       | 0            |
| 49  | EY    | 1     | 0        | 0        | 0       | 0            |
| 49  | FA    | 1     | 0        | 0        | 0       | 0            |
| 49  | FC    | 1     | 0        | 0        | 0       | 0            |
| 49  | FK    | 1     | 0        | 0        | 0       | 0            |
| 49  | FL    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 49  | GY    | 1     | 0        | 0        | 0       | 0            |
| 49  | HA    | 1     | 0        | 0        | 0       | 0            |
| 49  | HC    | 1     | 0        | 0        | 0       | 0            |
| 49  | HK    | 1     | 0        | 0        | 0       | 0            |
| 49  | HL    | 1     | 0        | 0        | 0       | 0            |
| 50  | A1    | 1134  | 0        | 0        | 292     | 0            |
| 50  | AA    | 8     | 0        | 0        | 2       | 0            |
| 50  | AB    | 5     | 0        | 0        | 2       | 0            |
| 50  | AH    | 1     | 0        | 0        | 0       | 0            |
| 50  | AK    | 3     | 0        | 0        | 1       | 0            |
| 50  | AM    | 1     | 0        | 0        | 0       | 0            |
| 50  | AP    | 2     | 0        | 0        | 0       | 0            |
| 50  | AT    | 3     | 0        | 0        | 3       | 0            |
| 50  | AU    | 4     | 0        | 0        | 3       | 0            |
| 50  | B2    | 54    | 0        | 0        | 5       | 0            |
| 50  | B3    | 23    | 0        | 0        | 6       | 0            |
| 50  | BA    | 12    | 0        | 0        | 3       | 0            |
| 50  | BB    | 4     | 0        | 0        | 1       | 0            |
| 50  | BC    | 7     | 0        | 0        | 0       | 0            |
| 50  | BE    | 1     | 0        | 0        | 0       | 0            |
| 50  | BI    | 3     | 0        | 0        | 1       | 0            |
| 50  | BJ    | 5     | 0        | 0        | 1       | 0            |
| 50  | BK    | 3     | 0        | 0        | 1       | 0            |
| 50  | BL    | 8     | 0        | 0        | 0       | 0            |
| 50  | BM    | 2     | 0        | 0        | 1       | 0            |
| 50  | BN    | 5     | 0        | 0        | 0       | 0            |
| 50  | BO    | 2     | 0        | 0        | 2       | 0            |
| 50  | BP    | 5     | 0        | 0        | 2       | 0            |
| 50  | BQ    | 7     | 0        | 0        | 3       | 0            |
| 50  | BU    | 1     | 0        | 0        | 0       | 0            |
| 50  | BV    | 7     | 0        | 0        | 1       | 0            |
| 50  | BW    | 5     | 0        | 0        | 0       | 0            |
| 50  | BX    | 6     | 0        | 0        | 1       | 0            |
| 50  | BY    | 5     | 0        | 0        | 0       | 0            |
| 50  | C2    | 46    | 0        | 0        | 3       | 0            |
| 50  | C3    | 39    | 0        | 0        | 10      | 0            |
| 50  | CA    | 11    | 0        | 0        | 3       | 0            |
| 50  | CB    | 4     | 0        | 0        | 0       | 0            |
| 50  | CC    | 7     | 0        | 0        | 0       | 0            |
| 50  | CD    | 4     | 0        | 0        | 0       | 0            |
| 50  | CE    | 2     | 0        | 0        | 1       | 0            |
| 50  | CI    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 50  | CJ    | 4     | 0        | 0        | 3       | 0            |
| 50  | CK    | 3     | 0        | 0        | 1       | 0            |
| 50  | CL    | 12    | 0        | 0        | 2       | 0            |
| 50  | CM    | 6     | 0        | 0        | 1       | 0            |
| 50  | CN    | 7     | 0        | 0        | 5       | 0            |
| 50  | CO    | 2     | 0        | 0        | 1       | 0            |
| 50  | CP    | 6     | 0        | 0        | 1       | 0            |
| 50  | CQ    | 7     | 0        | 0        | 5       | 0            |
| 50  | CU    | 1     | 0        | 0        | 0       | 0            |
| 50  | CV    | 4     | 0        | 0        | 1       | 0            |
| 50  | CW    | 5     | 0        | 0        | 0       | 0            |
| 50  | CX    | 6     | 0        | 0        | 0       | 0            |
| 50  | CY    | 5     | 0        | 0        | 0       | 0            |
| 50  | D1    | 1341  | 0        | 0        | 313     | 0            |
| 50  | DA    | 10    | 0        | 0        | 1       | 0            |
| 50  | DB    | 4     | 0        | 0        | 2       | 0            |
| 50  | DE    | 1     | 0        | 0        | 0       | 0            |
| 50  | DJ    | 2     | 0        | 0        | 1       | 0            |
| 50  | DK    | 2     | 0        | 0        | 0       | 0            |
| 50  | DP    | 1     | 0        | 0        | 0       | 0            |
| 50  | DQ    | 2     | 0        | 0        | 2       | 0            |
| 50  | DT    | 4     | 0        | 0        | 3       | 0            |
| 50  | DU    | 3     | 0        | 0        | 0       | 0            |
| 50  | DX    | 2     | 0        | 0        | 0       | 0            |
| 50  | E2    | 44    | 0        | 0        | 8       | 0            |
| 50  | E3    | 34    | 0        | 0        | 4       | 0            |
| 50  | EA    | 4     | 0        | 0        | 4       | 0            |
| 50  | EB    | 3     | 0        | 0        | 0       | 0            |
| 50  | EC    | 2     | 0        | 0        | 0       | 0            |
| 50  | EE    | 2     | 0        | 0        | 0       | 0            |
| 50  | EJ    | 4     | 0        | 0        | 1       | 0            |
| 50  | EK    | 5     | 0        | 0        | 1       | 0            |
| 50  | EL    | 10    | 0        | 0        | 1       | 0            |
| 50  | EM    | 2     | 0        | 0        | 0       | 0            |
| 50  | EN    | 7     | 0        | 0        | 7       | 0            |
| 50  | EP    | 6     | 0        | 0        | 1       | 0            |
| 50  | EQ    | 4     | 0        | 0        | 4       | 0            |
| 50  | EV    | 6     | 0        | 0        | 1       | 0            |
| 50  | EW    | 7     | 0        | 0        | 0       | 0            |
| 50  | EX    | 5     | 0        | 0        | 2       | 0            |
| 50  | EY    | 5     | 0        | 0        | 0       | 0            |
| 50  | F1    | 1076  | 0        | 0        | 268     | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 50  | FA    | 7      | 0        | 0        | 2       | 0            |
| 50  | FB    | 4      | 0        | 0        | 1       | 0            |
| 50  | FE    | 1      | 0        | 0        | 0       | 0            |
| 50  | FH    | 1      | 0        | 0        | 0       | 0            |
| 50  | FK    | 2      | 0        | 0        | 0       | 0            |
| 50  | FL    | 3      | 0        | 0        | 1       | 0            |
| 50  | FP    | 2      | 0        | 0        | 0       | 0            |
| 50  | FT    | 4      | 0        | 0        | 4       | 0            |
| 50  | FU    | 4      | 0        | 0        | 0       | 0            |
| 50  | G2    | 34     | 0        | 0        | 2       | 0            |
| 50  | G3    | 26     | 0        | 0        | 9       | 0            |
| 50  | GA    | 6      | 0        | 0        | 6       | 0            |
| 50  | GB    | 3      | 0        | 0        | 0       | 0            |
| 50  | GC    | 2      | 0        | 0        | 0       | 0            |
| 50  | GE    | 2      | 0        | 0        | 0       | 0            |
| 50  | GI    | 1      | 0        | 0        | 0       | 0            |
| 50  | GJ    | 4      | 0        | 0        | 2       | 0            |
| 50  | GK    | 2      | 0        | 0        | 2       | 0            |
| 50  | GL    | 5      | 0        | 0        | 1       | 0            |
| 50  | GM    | 1      | 0        | 0        | 1       | 0            |
| 50  | GN    | 2      | 0        | 0        | 1       | 0            |
| 50  | GO    | 2      | 0        | 0        | 1       | 0            |
| 50  | GP    | 5      | 0        | 0        | 0       | 0            |
| 50  | GQ    | 4      | 0        | 0        | 2       | 0            |
| 50  | GV    | 3      | 0        | 0        | 0       | 0            |
| 50  | GW    | 4      | 0        | 0        | 0       | 0            |
| 50  | GX    | 5      | 0        | 0        | 1       | 0            |
| 50  | GY    | 1      | 0        | 0        | 0       | 0            |
| 50  | H1    | 924    | 0        | 0        | 218     | 0            |
| 50  | HA    | 4      | 0        | 0        | 1       | 0            |
| 50  | HB    | 4      | 0        | 0        | 2       | 0            |
| 50  | HJ    | 2      | 0        | 0        | 0       | 0            |
| 50  | HK    | 2      | 0        | 0        | 0       | 0            |
| 50  | HP    | 1      | 0        | 0        | 0       | 0            |
| 50  | HT    | 5      | 0        | 0        | 5       | 0            |
| 50  | HU    | 2      | 0        | 0        | 0       | 0            |
| All | All   | 511395 | 0        | 371708   | 38211   | 12           |

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 44.

The worst 5 of 38211 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) |
|-------------------|------------------|--------------------------|-------------------|
| 28:GG:8:UNK:CG    | 1:H1:1248:G:N2   | 1.82                     | 1.41              |
| 28:GG:8:UNK:HG3   | 1:H1:1248:G:N2   | 1.34                     | 1.40              |
| 1:F1:452:U:H5'    | 14:FO:56:GLN:NE2 | 1.41                     | 1.35              |
| 13:AN:130:LYS:HG2 | 1:H1:2664:C:OP1  | 1.22                     | 1.33              |
| 46:CY:28:LYS:NZ   | 1:F1:2252:C:OP1  | 1.60                     | 1.33              |

The worst 5 of 12 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) |
|-------------------|-------------------------|--------------------------|-------------------|
| 34:CM:276:LYS:NZ  | 1:D1:259:U:O3'[2_546]   | 1.54                     | 0.66              |
| 34:GM:117:THR:OG1 | 1:H1:192:C:C4'[2_445]   | 1.57                     | 0.63              |
| 34:EM:214:LYS:NZ  | 1:F1:171:A:O4'[2_456]   | 1.76                     | 0.44              |
| 20:B2:87:C:N4     | 40:CS:82:GLU:OE2[1_545] | 1.84                     | 0.36              |
| 1:A1:1840:U:O4    | 15:DP:74:LYS:N[1_545]   | 1.88                     | 0.32              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed      | Favoured | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|----------|---------|----------|-------------|-----|
| 2   | AA    | 89/94 (95%)   | 85 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 2   | DA    | 89/94 (95%)   | 85 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 2   | FA    | 89/94 (95%)   | 85 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 2   | HA    | 89/94 (95%)   | 85 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 3   | AB    | 49/52 (94%)   | 46 (94%) | 3 (6%)  | 0        | 100         | 100 |
| 3   | DB    | 49/52 (94%)   | 46 (94%) | 3 (6%)  | 0        | 100         | 100 |
| 3   | FB    | 49/52 (94%)   | 46 (94%) | 3 (6%)  | 0        | 100         | 100 |
| 3   | HB    | 49/52 (94%)   | 46 (94%) | 3 (6%)  | 0        | 100         | 100 |
| 4   | AC    | 101/109 (93%) | 99 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 4   | DC    | 101/109 (93%) | 99 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4   | FC    | 101/109 (93%) | 99 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 4   | HC    | 101/109 (93%) | 99 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 5   | AE    | 188/191 (98%) | 178 (95%) | 9 (5%)  | 1 (0%)   | 24          | 58  |
| 5   | DE    | 188/191 (98%) | 176 (94%) | 11 (6%) | 1 (0%)   | 24          | 58  |
| 5   | FE    | 188/191 (98%) | 178 (95%) | 9 (5%)  | 1 (0%)   | 24          | 58  |
| 5   | HE    | 188/191 (98%) | 177 (94%) | 10 (5%) | 1 (0%)   | 24          | 58  |
| 6   | AF    | 123/126 (98%) | 115 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 6   | DF    | 123/126 (98%) | 116 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 6   | FF    | 123/126 (98%) | 115 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 6   | HF    | 123/126 (98%) | 114 (93%) | 9 (7%)  | 0        | 100         | 100 |
| 7   | AG    | 94/104 (90%)  | 90 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 7   | DG    | 94/104 (90%)  | 90 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 7   | FG    | 94/104 (90%)  | 90 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 7   | HG    | 94/104 (90%)  | 90 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 8   | AH    | 105/113 (93%) | 100 (95%) | 5 (5%)  | 0        | 100         | 100 |
| 8   | DH    | 105/113 (93%) | 100 (95%) | 5 (5%)  | 0        | 100         | 100 |
| 8   | FH    | 105/113 (93%) | 100 (95%) | 4 (4%)  | 1 (1%)   | 12          | 45  |
| 8   | HH    | 105/113 (93%) | 100 (95%) | 5 (5%)  | 0        | 100         | 100 |
| 9   | AJ    | 224/248 (90%) | 211 (94%) | 11 (5%) | 2 (1%)   | 14          | 48  |
| 9   | DJ    | 224/248 (90%) | 211 (94%) | 11 (5%) | 2 (1%)   | 14          | 48  |
| 9   | FJ    | 224/248 (90%) | 212 (95%) | 10 (4%) | 2 (1%)   | 14          | 48  |
| 9   | HJ    | 224/248 (90%) | 213 (95%) | 9 (4%)  | 2 (1%)   | 14          | 48  |
| 10  | AK    | 50/129 (39%)  | 43 (86%)  | 7 (14%) | 0        | 100         | 100 |
| 10  | DK    | 50/129 (39%)  | 44 (88%)  | 6 (12%) | 0        | 100         | 100 |
| 10  | FK    | 50/129 (39%)  | 44 (88%)  | 6 (12%) | 0        | 100         | 100 |
| 10  | HK    | 50/129 (39%)  | 43 (86%)  | 7 (14%) | 0        | 100         | 100 |
| 11  | AL    | 106/123 (86%) | 98 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 11  | DL    | 106/123 (86%) | 98 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 11  | FL    | 106/123 (86%) | 98 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 11  | HL    | 106/123 (86%) | 98 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 12  | AM    | 98/118 (83%)  | 92 (94%)  | 5 (5%)  | 1 (1%)   | 12          | 45  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 12  | DM    | 98/118 (83%)  | 94 (96%)  | 3 (3%)   | 1 (1%)   | 12          | 45  |
| 12  | FM    | 98/118 (83%)  | 93 (95%)  | 4 (4%)   | 1 (1%)   | 12          | 45  |
| 12  | HM    | 98/118 (83%)  | 92 (94%)  | 5 (5%)   | 1 (1%)   | 12          | 45  |
| 13  | AN    | 141/144 (98%) | 133 (94%) | 7 (5%)   | 1 (1%)   | 18          | 52  |
| 13  | DN    | 141/144 (98%) | 133 (94%) | 7 (5%)   | 1 (1%)   | 18          | 52  |
| 13  | FN    | 141/144 (98%) | 133 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 13  | HN    | 141/144 (98%) | 133 (94%) | 7 (5%)   | 1 (1%)   | 18          | 52  |
| 14  | AO    | 132/134 (98%) | 125 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 14  | DO    | 132/134 (98%) | 125 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 14  | FO    | 132/134 (98%) | 125 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 14  | HO    | 132/134 (98%) | 125 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 15  | AP    | 62/89 (70%)   | 58 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 15  | DP    | 62/89 (70%)   | 58 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 15  | FP    | 62/89 (70%)   | 58 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 15  | HP    | 62/89 (70%)   | 58 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 16  | AQ    | 100/104 (96%) | 89 (89%)  | 9 (9%)   | 2 (2%)   | 6           | 32  |
| 16  | DQ    | 100/104 (96%) | 89 (89%)  | 9 (9%)   | 2 (2%)   | 6           | 32  |
| 16  | FQ    | 100/104 (96%) | 88 (88%)  | 10 (10%) | 2 (2%)   | 6           | 32  |
| 16  | HQ    | 100/104 (96%) | 89 (89%)  | 9 (9%)   | 2 (2%)   | 6           | 32  |
| 17  | AT    | 63/66 (96%)   | 59 (94%)  | 3 (5%)   | 1 (2%)   | 7           | 36  |
| 17  | DT    | 63/66 (96%)   | 60 (95%)  | 2 (3%)   | 1 (2%)   | 7           | 36  |
| 17  | FT    | 63/66 (96%)   | 60 (95%)  | 2 (3%)   | 1 (2%)   | 7           | 36  |
| 17  | HT    | 63/66 (96%)   | 60 (95%)  | 2 (3%)   | 1 (2%)   | 7           | 36  |
| 18  | AU    | 201/206 (98%) | 188 (94%) | 12 (6%)  | 1 (0%)   | 24          | 58  |
| 18  | DU    | 201/206 (98%) | 187 (93%) | 13 (6%)  | 1 (0%)   | 24          | 58  |
| 18  | FU    | 201/206 (98%) | 187 (93%) | 13 (6%)  | 1 (0%)   | 24          | 58  |
| 18  | HU    | 201/206 (98%) | 189 (94%) | 11 (6%)  | 1 (0%)   | 24          | 58  |
| 19  | AX    | 186/189 (98%) | 177 (95%) | 8 (4%)   | 1 (0%)   | 24          | 58  |
| 19  | DX    | 186/189 (98%) | 178 (96%) | 6 (3%)   | 2 (1%)   | 11          | 44  |
| 19  | FX    | 186/189 (98%) | 178 (96%) | 6 (3%)   | 2 (1%)   | 11          | 44  |
| 19  | HX    | 186/189 (98%) | 177 (95%) | 7 (4%)   | 2 (1%)   | 11          | 44  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 22  | BA    | 255/264 (97%) | 236 (92%) | 19 (8%) | 0        | 100         | 100 |
| 22  | CA    | 255/264 (97%) | 235 (92%) | 20 (8%) | 0        | 100         | 100 |
| 22  | EA    | 255/264 (97%) | 234 (92%) | 21 (8%) | 0        | 100         | 100 |
| 22  | GA    | 255/264 (97%) | 237 (93%) | 18 (7%) | 0        | 100         | 100 |
| 23  | BB    | 384/391 (98%) | 371 (97%) | 13 (3%) | 0        | 100         | 100 |
| 23  | CB    | 384/391 (98%) | 371 (97%) | 13 (3%) | 0        | 100         | 100 |
| 23  | EB    | 384/391 (98%) | 371 (97%) | 13 (3%) | 0        | 100         | 100 |
| 23  | GB    | 384/391 (98%) | 370 (96%) | 14 (4%) | 0        | 100         | 100 |
| 24  | BC    | 407/410 (99%) | 383 (94%) | 24 (6%) | 0        | 100         | 100 |
| 24  | CC    | 407/410 (99%) | 387 (95%) | 20 (5%) | 0        | 100         | 100 |
| 24  | EC    | 407/410 (99%) | 384 (94%) | 23 (6%) | 0        | 100         | 100 |
| 24  | GC    | 407/410 (99%) | 386 (95%) | 21 (5%) | 0        | 100         | 100 |
| 25  | BD    | 167/172 (97%) | 156 (93%) | 11 (7%) | 0        | 100         | 100 |
| 25  | CD    | 167/172 (97%) | 156 (93%) | 11 (7%) | 0        | 100         | 100 |
| 25  | ED    | 167/172 (97%) | 156 (93%) | 11 (7%) | 0        | 100         | 100 |
| 25  | GD    | 167/172 (97%) | 156 (93%) | 11 (7%) | 0        | 100         | 100 |
| 26  | BE    | 184/188 (98%) | 171 (93%) | 13 (7%) | 0        | 100         | 100 |
| 26  | CE    | 184/188 (98%) | 171 (93%) | 13 (7%) | 0        | 100         | 100 |
| 26  | EE    | 184/188 (98%) | 171 (93%) | 13 (7%) | 0        | 100         | 100 |
| 26  | GE    | 184/188 (98%) | 171 (93%) | 13 (7%) | 0        | 100         | 100 |
| 27  | BF    | 229/255 (90%) | 219 (96%) | 10 (4%) | 0        | 100         | 100 |
| 27  | CF    | 229/255 (90%) | 219 (96%) | 10 (4%) | 0        | 100         | 100 |
| 27  | EF    | 229/255 (90%) | 219 (96%) | 9 (4%)  | 1 (0%)   | 30          | 62  |
| 27  | GF    | 229/255 (90%) | 219 (96%) | 10 (4%) | 0        | 100         | 100 |
| 29  | BH    | 197/215 (92%) | 186 (94%) | 11 (6%) | 0        | 100         | 100 |
| 29  | CH    | 197/215 (92%) | 187 (95%) | 10 (5%) | 0        | 100         | 100 |
| 29  | EH    | 197/215 (92%) | 186 (94%) | 11 (6%) | 0        | 100         | 100 |
| 29  | GH    | 197/215 (92%) | 186 (94%) | 11 (6%) | 0        | 100         | 100 |
| 30  | BI    | 196/198 (99%) | 189 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 30  | CI    | 196/198 (99%) | 189 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 30  | EI    | 196/198 (99%) | 189 (96%) | 7 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 30  | GI    | 196/198 (99%) | 189 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 31  | BJ    | 136/141 (96%) | 132 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 31  | CJ    | 136/141 (96%) | 132 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 31  | EJ    | 136/141 (96%) | 131 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 31  | GJ    | 136/141 (96%) | 132 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 32  | BK    | 146/149 (98%) | 136 (93%) | 8 (6%)  | 2 (1%)   | 9           | 38  |
| 32  | CK    | 146/149 (98%) | 135 (92%) | 8 (6%)  | 3 (2%)   | 5           | 31  |
| 32  | EK    | 146/149 (98%) | 137 (94%) | 7 (5%)  | 2 (1%)   | 9           | 38  |
| 32  | GK    | 146/149 (98%) | 135 (92%) | 8 (6%)  | 3 (2%)   | 5           | 31  |
| 33  | BL    | 201/204 (98%) | 191 (95%) | 10 (5%) | 0        | 100         | 100 |
| 33  | CL    | 201/204 (98%) | 191 (95%) | 10 (5%) | 0        | 100         | 100 |
| 33  | EL    | 201/204 (98%) | 191 (95%) | 10 (5%) | 0        | 100         | 100 |
| 33  | GL    | 201/204 (98%) | 193 (96%) | 7 (4%)  | 1 (0%)   | 24          | 58  |
| 34  | BM    | 296/301 (98%) | 282 (95%) | 13 (4%) | 1 (0%)   | 36          | 66  |
| 34  | CM    | 298/301 (99%) | 282 (95%) | 15 (5%) | 1 (0%)   | 36          | 66  |
| 34  | EM    | 298/301 (99%) | 283 (95%) | 14 (5%) | 1 (0%)   | 36          | 66  |
| 34  | GM    | 298/301 (99%) | 285 (96%) | 12 (4%) | 1 (0%)   | 36          | 66  |
| 35  | BN    | 178/181 (98%) | 168 (94%) | 10 (6%) | 0        | 100         | 100 |
| 35  | CN    | 178/181 (98%) | 168 (94%) | 10 (6%) | 0        | 100         | 100 |
| 35  | EN    | 178/181 (98%) | 168 (94%) | 10 (6%) | 0        | 100         | 100 |
| 35  | GN    | 178/181 (98%) | 168 (94%) | 10 (6%) | 0        | 100         | 100 |
| 36  | BO    | 182/185 (98%) | 170 (93%) | 11 (6%) | 1 (0%)   | 24          | 58  |
| 36  | EO    | 144/185 (78%) | 137 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 36  | GO    | 151/185 (82%) | 143 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 37  | BP    | 154/157 (98%) | 148 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 37  | CP    | 154/157 (98%) | 147 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 37  | EP    | 154/157 (98%) | 148 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 37  | GP    | 154/157 (98%) | 147 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 38  | BQ    | 155/183 (85%) | 146 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 38  | CQ    | 155/183 (85%) | 147 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 38  | EQ    | 155/183 (85%) | 147 (95%) | 8 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 38  | GQ    | 155/183 (85%) | 147 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 39  | BR    | 119/150 (79%) | 115 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 39  | CR    | 119/150 (79%) | 116 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 39  | ER    | 119/150 (79%) | 115 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 39  | GR    | 119/150 (79%) | 114 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 40  | BS    | 124/135 (92%) | 119 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 40  | CS    | 124/135 (92%) | 119 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 40  | ES    | 124/135 (92%) | 119 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 40  | GS    | 124/135 (92%) | 118 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 41  | BT    | 59/158 (37%)  | 57 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 41  | CT    | 59/158 (37%)  | 56 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 41  | ET    | 59/158 (37%)  | 57 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 41  | GT    | 59/158 (37%)  | 57 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 42  | BU    | 121/124 (98%) | 112 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 42  | CU    | 121/124 (98%) | 111 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 42  | EU    | 121/124 (98%) | 113 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 42  | GU    | 121/124 (98%) | 112 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 43  | BV    | 232/239 (97%) | 216 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 43  | CV    | 232/239 (97%) | 216 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 43  | EV    | 232/239 (97%) | 216 (93%) | 15 (6%)  | 1 (0%)   | 30          | 62  |
| 43  | GV    | 232/239 (97%) | 216 (93%) | 15 (6%)  | 1 (0%)   | 30          | 62  |
| 44  | BW    | 108/111 (97%) | 102 (94%) | 6 (6%)   | 0        | 100         | 100 |
| 44  | CW    | 108/111 (97%) | 102 (94%) | 6 (6%)   | 0        | 100         | 100 |
| 44  | EW    | 108/111 (97%) | 101 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 44  | GW    | 108/111 (97%) | 102 (94%) | 6 (6%)   | 0        | 100         | 100 |
| 45  | BX    | 123/134 (92%) | 119 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 45  | CX    | 123/134 (92%) | 117 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 45  | EX    | 123/134 (92%) | 118 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 45  | GX    | 123/134 (92%) | 117 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 46  | BY    | 100/103 (97%) | 91 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 46  | CY    | 100/103 (97%) | 90 (90%)  | 10 (10%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 46  | EY    | 100/103 (97%)     | 90 (90%)    | 10 (10%)  | 0        | 100         | 100 |
| 46  | GY    | 100/103 (97%)     | 90 (90%)    | 10 (10%)  | 0        | 100         | 100 |
| 47  | CO    | 145/185 (78%)     | 138 (95%)   | 7 (5%)    | 0        | 100         | 100 |
| All | All   | 26160/28348 (92%) | 24720 (94%) | 1378 (5%) | 62 (0%)  | 43          | 74  |

5 of 62 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | AQ    | 7   | VAL  |
| 32  | BK    | 24  | LYS  |
| 32  | CK    | 24  | LYS  |
| 16  | DQ    | 7   | VAL  |
| 32  | EK    | 24  | LYS  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | AA    | 69/72 (96%)   | 58 (84%)  | 11 (16%) | 2           | 15 |
| 2   | DA    | 69/72 (96%)   | 57 (83%)  | 12 (17%) | 2           | 11 |
| 2   | FA    | 69/72 (96%)   | 57 (83%)  | 12 (17%) | 2           | 11 |
| 2   | HA    | 69/72 (96%)   | 57 (83%)  | 12 (17%) | 2           | 11 |
| 3   | AB    | 48/49 (98%)   | 42 (88%)  | 6 (12%)  | 4           | 22 |
| 3   | DB    | 48/49 (98%)   | 44 (92%)  | 4 (8%)   | 10          | 35 |
| 3   | FB    | 48/49 (98%)   | 44 (92%)  | 4 (8%)   | 10          | 35 |
| 3   | HB    | 48/49 (98%)   | 44 (92%)  | 4 (8%)   | 10          | 35 |
| 4   | AC    | 95/101 (94%)  | 91 (96%)  | 4 (4%)   | 26          | 52 |
| 4   | DC    | 95/101 (94%)  | 91 (96%)  | 4 (4%)   | 26          | 52 |
| 4   | FC    | 95/101 (94%)  | 91 (96%)  | 4 (4%)   | 26          | 52 |
| 4   | HC    | 95/101 (94%)  | 91 (96%)  | 4 (4%)   | 26          | 52 |
| 5   | AE    | 162/163 (99%) | 150 (93%) | 12 (7%)  | 13          | 38 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 5   | DE    | 162/163 (99%) | 152 (94%) | 10 (6%)  | 16          | 44 |
| 5   | FE    | 162/163 (99%) | 149 (92%) | 13 (8%)  | 11          | 36 |
| 5   | HE    | 162/163 (99%) | 150 (93%) | 12 (7%)  | 13          | 38 |
| 6   | AF    | 111/112 (99%) | 107 (96%) | 4 (4%)   | 31          | 57 |
| 6   | DF    | 111/112 (99%) | 107 (96%) | 4 (4%)   | 31          | 57 |
| 6   | FF    | 111/112 (99%) | 107 (96%) | 4 (4%)   | 31          | 57 |
| 6   | HF    | 111/112 (99%) | 107 (96%) | 4 (4%)   | 31          | 57 |
| 7   | AG    | 80/88 (91%)   | 75 (94%)  | 5 (6%)   | 16          | 43 |
| 7   | DG    | 80/88 (91%)   | 75 (94%)  | 5 (6%)   | 16          | 43 |
| 7   | FG    | 80/88 (91%)   | 75 (94%)  | 5 (6%)   | 16          | 43 |
| 7   | HG    | 80/88 (91%)   | 76 (95%)  | 4 (5%)   | 22          | 49 |
| 8   | AH    | 87/92 (95%)   | 79 (91%)  | 8 (9%)   | 8           | 32 |
| 8   | DH    | 87/92 (95%)   | 79 (91%)  | 8 (9%)   | 8           | 32 |
| 8   | FH    | 87/92 (95%)   | 79 (91%)  | 8 (9%)   | 8           | 32 |
| 8   | HH    | 87/92 (95%)   | 78 (90%)  | 9 (10%)  | 7           | 29 |
| 9   | AJ    | 195/216 (90%) | 173 (89%) | 22 (11%) | 5           | 26 |
| 9   | DJ    | 195/216 (90%) | 172 (88%) | 23 (12%) | 5           | 24 |
| 9   | FJ    | 195/216 (90%) | 173 (89%) | 22 (11%) | 5           | 26 |
| 9   | HJ    | 195/216 (90%) | 173 (89%) | 22 (11%) | 5           | 26 |
| 10  | AK    | 46/113 (41%)  | 41 (89%)  | 5 (11%)  | 6           | 27 |
| 10  | DK    | 46/113 (41%)  | 42 (91%)  | 4 (9%)   | 9           | 33 |
| 10  | FK    | 46/113 (41%)  | 40 (87%)  | 6 (13%)  | 4           | 21 |
| 10  | HK    | 46/113 (41%)  | 41 (89%)  | 5 (11%)  | 6           | 27 |
| 11  | AL    | 92/107 (86%)  | 85 (92%)  | 7 (8%)   | 12          | 38 |
| 11  | DL    | 92/107 (86%)  | 86 (94%)  | 6 (6%)   | 15          | 42 |
| 11  | FL    | 92/107 (86%)  | 86 (94%)  | 6 (6%)   | 15          | 42 |
| 11  | HL    | 92/107 (86%)  | 85 (92%)  | 7 (8%)   | 12          | 38 |
| 12  | AM    | 93/110 (84%)  | 92 (99%)  | 1 (1%)   | 65          | 75 |
| 12  | DM    | 93/110 (84%)  | 92 (99%)  | 1 (1%)   | 65          | 75 |
| 12  | FM    | 93/110 (84%)  | 92 (99%)  | 1 (1%)   | 65          | 75 |
| 12  | HM    | 93/110 (84%)  | 92 (99%)  | 1 (1%)   | 65          | 75 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 13  | AN    | 130/131 (99%)  | 120 (92%) | 10 (8%)  | 12          | 38 |
| 13  | DN    | 130/131 (99%)  | 122 (94%) | 8 (6%)   | 16          | 44 |
| 13  | FN    | 130/131 (99%)  | 122 (94%) | 8 (6%)   | 16          | 44 |
| 13  | HN    | 130/131 (99%)  | 121 (93%) | 9 (7%)   | 14          | 40 |
| 14  | AO    | 108/108 (100%) | 101 (94%) | 7 (6%)   | 15          | 42 |
| 14  | DO    | 108/108 (100%) | 102 (94%) | 6 (6%)   | 19          | 46 |
| 14  | FO    | 108/108 (100%) | 102 (94%) | 6 (6%)   | 19          | 46 |
| 14  | HO    | 108/108 (100%) | 102 (94%) | 6 (6%)   | 19          | 46 |
| 15  | AP    | 60/77 (78%)    | 54 (90%)  | 6 (10%)  | 7           | 29 |
| 15  | DP    | 60/77 (78%)    | 54 (90%)  | 6 (10%)  | 7           | 29 |
| 15  | FP    | 60/77 (78%)    | 54 (90%)  | 6 (10%)  | 7           | 29 |
| 15  | HP    | 60/77 (78%)    | 54 (90%)  | 6 (10%)  | 7           | 29 |
| 16  | AQ    | 81/83 (98%)    | 75 (93%)  | 6 (7%)   | 13          | 38 |
| 16  | DQ    | 81/83 (98%)    | 75 (93%)  | 6 (7%)   | 13          | 38 |
| 16  | FQ    | 81/83 (98%)    | 75 (93%)  | 6 (7%)   | 13          | 38 |
| 16  | HQ    | 81/83 (98%)    | 75 (93%)  | 6 (7%)   | 13          | 38 |
| 17  | AT    | 61/62 (98%)    | 57 (93%)  | 4 (7%)   | 15          | 42 |
| 17  | DT    | 61/62 (98%)    | 57 (93%)  | 4 (7%)   | 15          | 42 |
| 17  | FT    | 61/62 (98%)    | 57 (93%)  | 4 (7%)   | 15          | 42 |
| 17  | HT    | 61/62 (98%)    | 57 (93%)  | 4 (7%)   | 15          | 42 |
| 18  | AU    | 169/171 (99%)  | 158 (94%) | 11 (6%)  | 15          | 42 |
| 18  | DU    | 169/171 (99%)  | 159 (94%) | 10 (6%)  | 18          | 45 |
| 18  | FU    | 169/171 (99%)  | 159 (94%) | 10 (6%)  | 18          | 45 |
| 18  | HU    | 169/171 (99%)  | 158 (94%) | 11 (6%)  | 15          | 42 |
| 19  | AX    | 167/168 (99%)  | 151 (90%) | 16 (10%) | 8           | 31 |
| 19  | DX    | 167/168 (99%)  | 151 (90%) | 16 (10%) | 8           | 31 |
| 19  | FX    | 167/168 (99%)  | 149 (89%) | 18 (11%) | 6           | 27 |
| 19  | HX    | 167/168 (99%)  | 151 (90%) | 16 (10%) | 8           | 31 |
| 22  | BA    | 196/198 (99%)  | 163 (83%) | 33 (17%) | 2           | 13 |
| 22  | CA    | 196/198 (99%)  | 163 (83%) | 33 (17%) | 2           | 13 |
| 22  | EA    | 196/198 (99%)  | 162 (83%) | 34 (17%) | 2           | 12 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 22  | GA    | 196/198 (99%)  | 164 (84%) | 32 (16%) | 2           | 14 |
| 23  | BB    | 330/334 (99%)  | 302 (92%) | 28 (8%)  | 10          | 34 |
| 23  | CB    | 330/334 (99%)  | 300 (91%) | 30 (9%)  | 9           | 32 |
| 23  | EB    | 330/334 (99%)  | 304 (92%) | 26 (8%)  | 11          | 37 |
| 23  | GB    | 330/334 (99%)  | 302 (92%) | 28 (8%)  | 10          | 34 |
| 24  | BC    | 325/326 (100%) | 293 (90%) | 32 (10%) | 7           | 30 |
| 24  | CC    | 325/326 (100%) | 289 (89%) | 36 (11%) | 6           | 27 |
| 24  | EC    | 325/326 (100%) | 293 (90%) | 32 (10%) | 7           | 30 |
| 24  | GC    | 325/326 (100%) | 292 (90%) | 33 (10%) | 7           | 29 |
| 25  | BD    | 146/149 (98%)  | 133 (91%) | 13 (9%)  | 9           | 33 |
| 25  | CD    | 146/149 (98%)  | 133 (91%) | 13 (9%)  | 9           | 33 |
| 25  | ED    | 146/149 (98%)  | 133 (91%) | 13 (9%)  | 9           | 33 |
| 25  | GD    | 146/149 (98%)  | 133 (91%) | 13 (9%)  | 9           | 33 |
| 26  | BE    | 163/165 (99%)  | 157 (96%) | 6 (4%)   | 30          | 57 |
| 26  | CE    | 163/165 (99%)  | 157 (96%) | 6 (4%)   | 30          | 57 |
| 26  | EE    | 163/165 (99%)  | 157 (96%) | 6 (4%)   | 30          | 57 |
| 26  | GE    | 163/165 (99%)  | 156 (96%) | 7 (4%)   | 26          | 51 |
| 27  | BF    | 201/222 (90%)  | 193 (96%) | 8 (4%)   | 28          | 54 |
| 27  | CF    | 201/222 (90%)  | 193 (96%) | 8 (4%)   | 28          | 54 |
| 27  | EF    | 201/222 (90%)  | 193 (96%) | 8 (4%)   | 28          | 54 |
| 27  | GF    | 201/222 (90%)  | 193 (96%) | 8 (4%)   | 28          | 54 |
| 29  | BH    | 169/180 (94%)  | 155 (92%) | 14 (8%)  | 10          | 35 |
| 29  | CH    | 169/180 (94%)  | 155 (92%) | 14 (8%)  | 10          | 35 |
| 29  | EH    | 169/180 (94%)  | 155 (92%) | 14 (8%)  | 10          | 35 |
| 29  | GH    | 169/180 (94%)  | 155 (92%) | 14 (8%)  | 10          | 35 |
| 30  | BI    | 166/166 (100%) | 147 (89%) | 19 (11%) | 5           | 25 |
| 30  | CI    | 166/166 (100%) | 147 (89%) | 19 (11%) | 5           | 25 |
| 30  | EI    | 166/166 (100%) | 146 (88%) | 20 (12%) | 5           | 23 |
| 30  | GI    | 166/166 (100%) | 149 (90%) | 17 (10%) | 7           | 29 |
| 31  | BJ    | 107/108 (99%)  | 99 (92%)  | 8 (8%)   | 12          | 38 |
| 31  | CJ    | 107/108 (99%)  | 99 (92%)  | 8 (8%)   | 12          | 38 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 31  | EJ    | 107/108 (99%)  | 99 (92%)  | 8 (8%)   | 12          | 38 |
| 31  | GJ    | 107/108 (99%)  | 98 (92%)  | 9 (8%)   | 10          | 34 |
| 32  | BK    | 120/121 (99%)  | 105 (88%) | 15 (12%) | 4           | 22 |
| 32  | CK    | 120/121 (99%)  | 106 (88%) | 14 (12%) | 5           | 25 |
| 32  | EK    | 120/121 (99%)  | 107 (89%) | 13 (11%) | 6           | 27 |
| 32  | GK    | 120/121 (99%)  | 105 (88%) | 15 (12%) | 4           | 22 |
| 33  | BL    | 174/175 (99%)  | 165 (95%) | 9 (5%)   | 21          | 48 |
| 33  | CL    | 174/175 (99%)  | 164 (94%) | 10 (6%)  | 18          | 46 |
| 33  | EL    | 174/175 (99%)  | 164 (94%) | 10 (6%)  | 18          | 46 |
| 33  | GL    | 174/175 (99%)  | 165 (95%) | 9 (5%)   | 21          | 48 |
| 34  | BM    | 252/254 (99%)  | 241 (96%) | 11 (4%)  | 25          | 51 |
| 34  | CM    | 253/254 (100%) | 241 (95%) | 12 (5%)  | 23          | 50 |
| 34  | EM    | 253/254 (100%) | 241 (95%) | 12 (5%)  | 23          | 50 |
| 34  | GM    | 253/254 (100%) | 239 (94%) | 14 (6%)  | 19          | 46 |
| 35  | BN    | 159/160 (99%)  | 140 (88%) | 19 (12%) | 5           | 24 |
| 35  | CN    | 159/160 (99%)  | 142 (89%) | 17 (11%) | 6           | 28 |
| 35  | EN    | 159/160 (99%)  | 140 (88%) | 19 (12%) | 5           | 24 |
| 35  | GN    | 159/160 (99%)  | 140 (88%) | 19 (12%) | 5           | 24 |
| 36  | BO    | 158/159 (99%)  | 146 (92%) | 12 (8%)  | 12          | 38 |
| 36  | EO    | 126/159 (79%)  | 114 (90%) | 12 (10%) | 8           | 31 |
| 36  | GO    | 127/159 (80%)  | 115 (91%) | 12 (9%)  | 8           | 31 |
| 37  | BP    | 134/135 (99%)  | 125 (93%) | 9 (7%)   | 15          | 41 |
| 37  | CP    | 134/135 (99%)  | 123 (92%) | 11 (8%)  | 10          | 35 |
| 37  | EP    | 134/135 (99%)  | 125 (93%) | 9 (7%)   | 15          | 41 |
| 37  | GP    | 134/135 (99%)  | 124 (92%) | 10 (8%)  | 12          | 38 |
| 38  | BQ    | 128/148 (86%)  | 111 (87%) | 17 (13%) | 4           | 21 |
| 38  | CQ    | 128/148 (86%)  | 110 (86%) | 18 (14%) | 3           | 19 |
| 38  | EQ    | 128/148 (86%)  | 110 (86%) | 18 (14%) | 3           | 19 |
| 38  | GQ    | 128/148 (86%)  | 111 (87%) | 17 (13%) | 4           | 21 |
| 39  | BR    | 108/132 (82%)  | 100 (93%) | 8 (7%)   | 13          | 38 |
| 39  | CR    | 108/132 (82%)  | 100 (93%) | 8 (7%)   | 13          | 38 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 39  | ER    | 108/132 (82%) | 100 (93%) | 8 (7%)   | 13          | 38 |
| 39  | GR    | 108/132 (82%) | 101 (94%) | 7 (6%)   | 15          | 42 |
| 40  | BS    | 113/120 (94%) | 104 (92%) | 9 (8%)   | 11          | 36 |
| 40  | CS    | 113/120 (94%) | 104 (92%) | 9 (8%)   | 11          | 36 |
| 40  | ES    | 113/120 (94%) | 106 (94%) | 7 (6%)   | 16          | 44 |
| 40  | GS    | 113/120 (94%) | 105 (93%) | 8 (7%)   | 13          | 39 |
| 41  | BT    | 52/130 (40%)  | 48 (92%)  | 4 (8%)   | 12          | 38 |
| 41  | CT    | 52/130 (40%)  | 48 (92%)  | 4 (8%)   | 12          | 38 |
| 41  | ET    | 52/130 (40%)  | 48 (92%)  | 4 (8%)   | 12          | 38 |
| 41  | GT    | 52/130 (40%)  | 48 (92%)  | 4 (8%)   | 12          | 38 |
| 42  | BU    | 105/106 (99%) | 95 (90%)  | 10 (10%) | 8           | 31 |
| 42  | CU    | 105/106 (99%) | 95 (90%)  | 10 (10%) | 8           | 31 |
| 42  | EU    | 105/106 (99%) | 95 (90%)  | 10 (10%) | 8           | 31 |
| 42  | GU    | 105/106 (99%) | 95 (90%)  | 10 (10%) | 8           | 31 |
| 43  | BV    | 197/202 (98%) | 189 (96%) | 8 (4%)   | 27          | 53 |
| 43  | CV    | 197/202 (98%) | 189 (96%) | 8 (4%)   | 27          | 53 |
| 43  | EV    | 197/202 (98%) | 189 (96%) | 8 (4%)   | 27          | 53 |
| 43  | GV    | 197/202 (98%) | 189 (96%) | 8 (4%)   | 27          | 53 |
| 44  | BW    | 100/101 (99%) | 92 (92%)  | 8 (8%)   | 11          | 36 |
| 44  | CW    | 100/101 (99%) | 91 (91%)  | 9 (9%)   | 9           | 33 |
| 44  | EW    | 100/101 (99%) | 91 (91%)  | 9 (9%)   | 9           | 33 |
| 44  | GW    | 100/101 (99%) | 91 (91%)  | 9 (9%)   | 9           | 33 |
| 45  | BX    | 104/111 (94%) | 89 (86%)  | 15 (14%) | 3           | 18 |
| 45  | CX    | 104/111 (94%) | 89 (86%)  | 15 (14%) | 3           | 18 |
| 45  | EX    | 104/111 (94%) | 89 (86%)  | 15 (14%) | 3           | 18 |
| 45  | GX    | 104/111 (94%) | 89 (86%)  | 15 (14%) | 3           | 18 |
| 46  | BY    | 79/80 (99%)   | 70 (89%)  | 9 (11%)  | 5           | 25 |
| 46  | CY    | 79/80 (99%)   | 70 (89%)  | 9 (11%)  | 5           | 25 |
| 46  | EY    | 79/80 (99%)   | 71 (90%)  | 8 (10%)  | 7           | 29 |
| 46  | GY    | 79/80 (99%)   | 72 (91%)  | 7 (9%)   | 9           | 33 |
| 47  | CO    | 126/127 (99%) | 115 (91%) | 11 (9%)  | 9           | 33 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers  | Percentiles |
|-----|-------|-------------------|-------------|-----------|-------------|
| All | All   | 22468/23988 (94%) | 20597 (92%) | 1871 (8%) | 10 35       |

5 of 1871 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | DX    | 42  | ARG  |
| 8   | HH    | 38  | LYS  |
| 35  | EN    | 91  | GLU  |
| 5   | HE    | 90  | VAL  |
| 34  | GM    | 213 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 814 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | EI    | 13  | HIS  |
| 14  | FO    | 46  | HIS  |
| 18  | HU    | 137 | ASN  |
| 33  | EL    | 90  | ASN  |
| 29  | EH    | 144 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed          | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------------|-------------------|-----------------|
| 1   | A1    | 3114/3354 (92%)   | 1122 (36%)        | 209 (6%)        |
| 1   | D1    | 3114/3354 (92%)   | 1117 (35%)        | 215 (6%)        |
| 1   | F1    | 3114/3354 (92%)   | 1116 (35%)        | 211 (6%)        |
| 1   | H1    | 3114/3354 (92%)   | 1117 (35%)        | 210 (6%)        |
| 20  | B2    | 154/154 (100%)    | 58 (37%)          | 13 (8%)         |
| 20  | C2    | 154/154 (100%)    | 60 (38%)          | 13 (8%)         |
| 20  | E2    | 154/154 (100%)    | 60 (38%)          | 13 (8%)         |
| 20  | G2    | 154/154 (100%)    | 60 (38%)          | 13 (8%)         |
| 21  | B3    | 119/120 (99%)     | 38 (31%)          | 1 (0%)          |
| 21  | C3    | 119/120 (99%)     | 39 (32%)          | 1 (0%)          |
| 21  | E3    | 119/120 (99%)     | 38 (31%)          | 1 (0%)          |
| 21  | G3    | 119/120 (99%)     | 38 (31%)          | 1 (0%)          |
| All | All   | 13548/14512 (93%) | 4863 (35%)        | 901 (6%)        |

5 of 4863 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 9   | G    |
| 1   | A1    | 16  | G    |
| 1   | A1    | 17  | C    |
| 1   | A1    | 19  | A    |
| 1   | A1    | 20  | G    |

5 of 901 RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 20  | E2    | 112  | G    |
| 1   | H1    | 3205 | A    |
| 1   | F1    | 1617 | G    |
| 1   | H1    | 3162 | A    |
| 1   | H1    | 1617 | G    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 885 ligands modelled in this entry, 885 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | F1    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | F1    | 2239:A    | O3'    | 2240:C    | P      | 1.91         |

## 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, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----|-----|-----------------------|-------|
| 1   | A1    | 3119/3354 (92%) | 0.30   | 103 (3%)  | 49  | 27  | 42, 91, 187, 390      | 0     |
| 1   | D1    | 3119/3354 (92%) | 0.37   | 95 (3%)   | 52  | 29  | 40, 79, 164, 330      | 0     |
| 1   | F1    | 3119/3354 (92%) | 0.55   | 137 (4%)  | 39  | 21  | 51, 94, 176, 357      | 0     |
| 1   | H1    | 3119/3354 (92%) | 1.09   | 456 (14%) | 6   | 5   | 54, 121, 213, 367     | 0     |
| 2   | AA    | 91/94 (96%)     | 0.05   | 0         | 100 | 100 | 29, 65, 120, 243      | 0     |
| 2   | DA    | 91/94 (96%)     | 0.27   | 2 (2%)    | 62  | 35  | 34, 66, 123, 226      | 0     |
| 2   | FA    | 91/94 (96%)     | 0.16   | 2 (2%)    | 62  | 35  | 47, 83, 132, 204      | 0     |
| 2   | HA    | 91/94 (96%)     | 0.81   | 10 (10%)  | 10  | 7   | 74, 119, 186, 243     | 0     |
| 3   | AB    | 51/52 (98%)     | -0.11  | 0         | 100 | 100 | 44, 63, 110, 148      | 0     |
| 3   | DB    | 51/52 (98%)     | 0.02   | 0         | 100 | 100 | 49, 69, 111, 146      | 0     |
| 3   | FB    | 51/52 (98%)     | 0.10   | 1 (1%)    | 65  | 37  | 59, 86, 118, 167      | 0     |
| 3   | HB    | 51/52 (98%)     | 0.31   | 1 (1%)    | 65  | 37  | 90, 114, 144, 197     | 0     |
| 4   | AC    | 103/109 (94%)   | 0.20   | 1 (0%)    | 79  | 54  | 73, 117, 154, 228     | 0     |
| 4   | DC    | 103/109 (94%)   | 0.07   | 1 (0%)    | 79  | 54  | 46, 84, 135, 194      | 0     |
| 4   | FC    | 103/109 (94%)   | 0.21   | 2 (1%)    | 66  | 39  | 58, 96, 156, 192      | 0     |
| 4   | HC    | 103/109 (94%)   | 0.61   | 7 (6%)    | 23  | 14  | 81, 130, 176, 199     | 0     |
| 5   | AE    | 190/191 (99%)   | 0.21   | 2 (1%)    | 78  | 52  | 69, 122, 171, 214     | 0     |
| 5   | DE    | 190/191 (99%)   | 0.38   | 6 (3%)    | 50  | 28  | 74, 124, 169, 226     | 0     |
| 5   | FE    | 190/191 (99%)   | 0.40   | 5 (2%)    | 57  | 32  | 60, 123, 176, 227     | 0     |
| 5   | HE    | 190/191 (99%)   | 0.55   | 7 (3%)    | 45  | 25  | 76, 141, 194, 227     | 0     |
| 6   | AF    | 125/126 (99%)   | 0.12   | 1 (0%)    | 82  | 58  | 71, 111, 156, 213     | 0     |
| 6   | DF    | 125/126 (99%)   | 0.18   | 3 (2%)    | 59  | 34  | 70, 106, 157, 190     | 0     |
| 6   | FF    | 125/126 (99%)   | 0.22   | 4 (3%)    | 50  | 28  | 63, 109, 166, 245     | 0     |
| 6   | HF    | 125/126 (99%)   | 0.25   | 1 (0%)    | 82  | 58  | 74, 113, 163, 224     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 7   | AG    | 96/104 (92%)   | 0.28   | 2 (2%) 63 36 | 62, 103, 188, 218     | 0     |
| 7   | DG    | 96/104 (92%)   | 0.41   | 3 (3%) 51 29 | 57, 114, 179, 222     | 0     |
| 7   | FG    | 96/104 (92%)   | 0.33   | 4 (4%) 40 21 | 81, 112, 176, 199     | 0     |
| 7   | HG    | 96/104 (92%)   | 0.53   | 7 (7%) 21 13 | 94, 134, 183, 218     | 0     |
| 8   | AH    | 107/113 (94%)  | 0.23   | 7 (6%) 25 15 | 61, 91, 127, 159      | 0     |
| 8   | DH    | 107/113 (94%)  | 0.33   | 3 (2%) 55 31 | 54, 89, 127, 138      | 0     |
| 8   | FH    | 107/113 (94%)  | 0.45   | 3 (2%) 55 31 | 57, 89, 122, 164      | 0     |
| 8   | HH    | 107/113 (94%)  | 0.59   | 4 (3%) 45 25 | 68, 109, 141, 181     | 0     |
| 9   | AJ    | 226/248 (91%)  | -0.12  | 0 100 100    | 52, 90, 138, 190      | 0     |
| 9   | DJ    | 226/248 (91%)  | -0.06  | 0 100 100    | 51, 89, 136, 206      | 0     |
| 9   | FJ    | 226/248 (91%)  | -0.12  | 1 (0%) 88 70 | 38, 82, 130, 183      | 0     |
| 9   | HJ    | 226/248 (91%)  | -0.18  | 0 100 100    | 40, 78, 123, 155      | 0     |
| 10  | AK    | 52/129 (40%)   | -0.01  | 0 100 100    | 73, 101, 146, 182     | 0     |
| 10  | DK    | 52/129 (40%)   | 0.00   | 1 (1%) 66 39 | 53, 79, 134, 151      | 0     |
| 10  | FK    | 52/129 (40%)   | -0.16  | 0 100 100    | 56, 81, 139, 189      | 0     |
| 10  | HK    | 52/129 (40%)   | 0.15   | 1 (1%) 66 39 | 61, 77, 118, 158      | 0     |
| 11  | AL    | 108/123 (87%)  | 0.05   | 1 (0%) 81 56 | 38, 73, 130, 165      | 0     |
| 11  | DL    | 108/123 (87%)  | 0.14   | 2 (1%) 66 39 | 47, 85, 144, 217      | 0     |
| 11  | FL    | 108/123 (87%)  | 0.20   | 2 (1%) 66 39 | 66, 98, 135, 174      | 0     |
| 11  | HL    | 108/123 (87%)  | 0.52   | 5 (4%) 37 19 | 90, 117, 156, 183     | 0     |
| 12  | AM    | 100/118 (84%)  | 0.02   | 0 100 100    | 72, 121, 155, 185     | 0     |
| 12  | DM    | 100/118 (84%)  | 0.18   | 1 (1%) 79 54 | 73, 126, 179, 199     | 0     |
| 12  | FM    | 100/118 (84%)  | 0.17   | 1 (1%) 79 54 | 93, 144, 196, 208     | 0     |
| 12  | HM    | 100/118 (84%)  | 0.31   | 0 100 100    | 98, 151, 195, 214     | 0     |
| 13  | AN    | 143/144 (99%)  | 0.00   | 3 (2%) 63 36 | 59, 97, 163, 189      | 0     |
| 13  | DN    | 143/144 (99%)  | 0.14   | 3 (2%) 63 36 | 73, 121, 179, 214     | 0     |
| 13  | FN    | 143/144 (99%)  | 0.21   | 2 (1%) 73 46 | 72, 122, 175, 208     | 0     |
| 13  | HN    | 143/144 (99%)  | 0.40   | 3 (2%) 63 36 | 92, 148, 189, 217     | 0     |
| 14  | AO    | 134/134 (100%) | 0.21   | 4 (2%) 52 29 | 66, 116, 162, 202     | 0     |
| 14  | DO    | 134/134 (100%) | 0.25   | 2 (1%) 72 44 | 52, 99, 151, 209      | 0     |
| 14  | FO    | 134/134 (100%) | 0.39   | 4 (2%) 52 29 | 65, 118, 167, 219     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|-----|-----|-----------------------|-------|
| 14  | HO    | 134/134 (100%) | 0.52   | 6 (4%)   | 38  | 20  | 96, 143, 197, 227     | 0     |
| 15  | AP    | 66/89 (74%)    | 0.23   | 1 (1%)   | 72  | 44  | 55, 128, 209, 241     | 0     |
| 15  | DP    | 66/89 (74%)    | 0.29   | 1 (1%)   | 72  | 44  | 73, 116, 176, 245     | 0     |
| 15  | FP    | 66/89 (74%)    | 0.31   | 1 (1%)   | 72  | 44  | 99, 143, 202, 214     | 0     |
| 15  | HP    | 66/89 (74%)    | 0.61   | 0        | 100 | 100 | 99, 149, 219, 247     | 0     |
| 16  | AQ    | 102/104 (98%)  | 0.11   | 2 (1%)   | 65  | 37  | 72, 122, 172, 208     | 0     |
| 16  | DQ    | 102/104 (98%)  | 0.17   | 1 (0%)   | 79  | 54  | 63, 105, 151, 186     | 0     |
| 16  | FQ    | 102/104 (98%)  | 0.32   | 1 (0%)   | 79  | 54  | 72, 114, 166, 190     | 0     |
| 16  | HQ    | 102/104 (98%)  | 0.51   | 5 (4%)   | 35  | 19  | 110, 154, 195, 203    | 0     |
| 17  | AT    | 65/66 (98%)    | 0.41   | 3 (4%)   | 37  | 19  | 76, 121, 156, 193     | 0     |
| 17  | DT    | 65/66 (98%)    | 0.37   | 2 (3%)   | 51  | 29  | 51, 87, 122, 211      | 0     |
| 17  | FT    | 65/66 (98%)    | 0.58   | 2 (3%)   | 51  | 29  | 51, 107, 144, 201     | 0     |
| 17  | HT    | 65/66 (98%)    | 0.92   | 6 (9%)   | 14  | 9   | 69, 136, 171, 222     | 0     |
| 18  | AU    | 203/206 (98%)  | 0.23   | 2 (0%)   | 79  | 54  | 74, 122, 179, 233     | 0     |
| 18  | DU    | 203/206 (98%)  | 0.33   | 10 (4%)  | 35  | 19  | 48, 98, 158, 198      | 0     |
| 18  | FU    | 203/206 (98%)  | 0.48   | 7 (3%)   | 48  | 27  | 67, 116, 174, 203     | 0     |
| 18  | HU    | 203/206 (98%)  | 0.72   | 13 (6%)  | 25  | 15  | 102, 155, 206, 240    | 0     |
| 19  | AX    | 188/189 (99%)  | 0.04   | 4 (2%)   | 63  | 36  | 72, 105, 145, 201     | 0     |
| 19  | DX    | 188/189 (99%)  | 0.12   | 2 (1%)   | 78  | 52  | 54, 89, 128, 170      | 0     |
| 19  | FX    | 188/189 (99%)  | 0.26   | 5 (2%)   | 56  | 32  | 62, 98, 141, 179      | 0     |
| 19  | HX    | 188/189 (99%)  | 0.35   | 6 (3%)   | 50  | 28  | 74, 106, 135, 193     | 0     |
| 20  | B2    | 154/154 (100%) | 0.26   | 5 (3%)   | 50  | 28  | 61, 80, 118, 192      | 0     |
| 20  | C2    | 154/154 (100%) | 0.45   | 4 (2%)   | 57  | 32  | 54, 80, 120, 186      | 0     |
| 20  | E2    | 154/154 (100%) | 0.75   | 10 (6%)  | 25  | 15  | 74, 105, 142, 189     | 0     |
| 20  | G2    | 154/154 (100%) | 1.51   | 35 (22%) | 2   | 2   | 98, 146, 182, 210     | 0     |
| 21  | B3    | 120/120 (100%) | 1.01   | 9 (7%)   | 20  | 13  | 90, 150, 184, 217     | 0     |
| 21  | C3    | 120/120 (100%) | 0.36   | 0        | 100 | 100 | 64, 98, 116, 161      | 0     |
| 21  | E3    | 120/120 (100%) | 0.58   | 2 (1%)   | 69  | 41  | 72, 120, 147, 172     | 0     |
| 21  | G3    | 120/120 (100%) | 1.11   | 15 (12%) | 8   | 6   | 95, 138, 175, 235     | 0     |
| 22  | BA    | 257/264 (97%)  | 0.14   | 6 (2%)   | 61  | 35  | 30, 70, 134, 233      | 0     |
| 22  | CA    | 257/264 (97%)  | 0.01   | 2 (0%)   | 82  | 58  | 31, 75, 139, 238      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 22  | EA    | 257/264 (97%)  | 0.12   | 3 (1%) 76 50  | 40, 79, 136, 217      | 0     |
| 22  | GA    | 257/264 (97%)  | 0.44   | 6 (2%) 61 35  | 60, 106, 157, 242     | 0     |
| 23  | BB    | 386/391 (98%)  | -0.01  | 1 (0%) 90 75  | 33, 69, 120, 227      | 0     |
| 23  | CB    | 386/391 (98%)  | -0.09  | 2 (0%) 87 67  | 34, 75, 123, 222      | 0     |
| 23  | EB    | 386/391 (98%)  | -0.02  | 2 (0%) 87 67  | 38, 75, 123, 230      | 0     |
| 23  | GB    | 386/391 (98%)  | 0.04   | 2 (0%) 87 67  | 51, 82, 132, 217      | 0     |
| 24  | BC    | 409/410 (99%)  | 0.25   | 5 (1%) 76 50  | 37, 107, 173, 241     | 0     |
| 24  | CC    | 409/410 (99%)  | 0.18   | 2 (0%) 87 67  | 40, 91, 151, 206      | 0     |
| 24  | EC    | 409/410 (99%)  | 0.36   | 11 (2%) 56 32 | 54, 107, 162, 237     | 0     |
| 24  | GC    | 409/410 (99%)  | 0.67   | 9 (2%) 62 35  | 77, 143, 195, 252     | 0     |
| 25  | BD    | 169/172 (98%)  | 0.37   | 4 (2%) 59 34  | 116, 159, 200, 225    | 0     |
| 25  | CD    | 169/172 (98%)  | 0.12   | 0 100 100     | 70, 110, 151, 188     | 0     |
| 25  | ED    | 169/172 (98%)  | 0.25   | 3 (1%) 67 40  | 89, 133, 179, 209     | 0     |
| 25  | GD    | 169/172 (98%)  | 0.51   | 5 (2%) 52 29  | 96, 139, 182, 216     | 0     |
| 26  | BE    | 186/188 (98%)  | 0.23   | 1 (0%) 87 67  | 65, 109, 150, 194     | 0     |
| 26  | CE    | 186/188 (98%)  | 0.10   | 0 100 100     | 59, 94, 131, 171      | 0     |
| 26  | EE    | 186/188 (98%)  | 0.01   | 1 (0%) 87 67  | 60, 94, 139, 195      | 0     |
| 26  | GE    | 186/188 (98%)  | 0.14   | 2 (1%) 78 52  | 53, 91, 135, 220      | 0     |
| 27  | BF    | 231/255 (90%)  | 0.32   | 8 (3%) 47 26  | 70, 122, 176, 252     | 0     |
| 27  | CF    | 231/255 (90%)  | 0.20   | 5 (2%) 62 35  | 71, 115, 175, 233     | 0     |
| 27  | EF    | 231/255 (90%)  | 0.37   | 4 (1%) 69 41  | 76, 120, 187, 241     | 0     |
| 27  | GF    | 231/255 (90%)  | 0.52   | 4 (1%) 69 41  | 112, 166, 210, 233    | 0     |
| 28  | BG    | 0/123          | -      | -             | -                     | -     |
| 28  | CG    | 0/123          | -      | -             | -                     | -     |
| 28  | EG    | 0/123          | -      | -             | -                     | -     |
| 28  | GG    | 0/123          | -      | -             | -                     | -     |
| 29  | BH    | 201/215 (93%)  | 0.43   | 7 (3%) 47 26  | 79, 133, 181, 221     | 0     |
| 29  | CH    | 201/215 (93%)  | 0.14   | 6 (2%) 52 29  | 42, 93, 139, 153      | 0     |
| 29  | EH    | 201/215 (93%)  | 0.20   | 5 (2%) 58 33  | 50, 105, 158, 202     | 0     |
| 29  | GH    | 201/215 (93%)  | 0.37   | 10 (4%) 34 19 | 71, 118, 171, 203     | 0     |
| 30  | BI    | 198/198 (100%) | 0.02   | 0 100 100     | 51, 85, 152, 185      | 0     |
| 30  | CI    | 198/198 (100%) | -0.05  | 3 (1%) 72 44  | 48, 78, 149, 208      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------|-----|-----|-----------------------|-------|
| 30  | EI    | 198/198 (100%) | -0.07  | 2 (1%)  | 79  | 54  | 47, 79, 152, 174      | 0     |
| 30  | GI    | 198/198 (100%) | 0.02   | 2 (1%)  | 79  | 54  | 53, 91, 151, 195      | 0     |
| 31  | BJ    | 138/141 (97%)  | -0.06  | 0       | 100 | 100 | 42, 68, 112, 160      | 0     |
| 31  | CJ    | 138/141 (97%)  | -0.15  | 0       | 100 | 100 | 40, 65, 108, 150      | 0     |
| 31  | EJ    | 138/141 (97%)  | -0.24  | 1 (0%)  | 84  | 61  | 40, 65, 108, 202      | 0     |
| 31  | GJ    | 138/141 (97%)  | -0.17  | 0       | 100 | 100 | 30, 60, 98, 186       | 0     |
| 32  | BK    | 148/149 (99%)  | 0.37   | 7 (4%)  | 36  | 19  | 50, 105, 158, 221     | 0     |
| 32  | CK    | 148/149 (99%)  | 0.05   | 2 (1%)  | 73  | 46  | 36, 74, 124, 184      | 0     |
| 32  | EK    | 148/149 (99%)  | 0.29   | 1 (0%)  | 84  | 61  | 50, 95, 140, 228      | 0     |
| 32  | GK    | 148/149 (99%)  | 0.81   | 9 (6%)  | 27  | 16  | 78, 129, 181, 208     | 0     |
| 33  | BL    | 203/204 (99%)  | 0.21   | 6 (2%)  | 52  | 29  | 57, 83, 120, 153      | 0     |
| 33  | CL    | 203/204 (99%)  | 0.06   | 6 (2%)  | 52  | 29  | 37, 74, 106, 180      | 0     |
| 33  | EL    | 203/204 (99%)  | 0.27   | 5 (2%)  | 58  | 33  | 51, 89, 121, 160      | 0     |
| 33  | GL    | 203/204 (99%)  | 0.75   | 10 (4%) | 35  | 19  | 89, 133, 165, 205     | 0     |
| 34  | BM    | 298/301 (99%)  | 0.56   | 9 (3%)  | 52  | 29  | 87, 152, 201, 240     | 0     |
| 34  | CM    | 300/301 (99%)  | 0.26   | 4 (1%)  | 75  | 48  | 61, 110, 166, 208     | 0     |
| 34  | EM    | 300/301 (99%)  | 0.39   | 7 (2%)  | 61  | 35  | 76, 127, 183, 233     | 0     |
| 34  | GM    | 300/301 (99%)  | 0.85   | 26 (8%) | 16  | 10  | 98, 157, 204, 233     | 0     |
| 35  | BN    | 180/181 (99%)  | 0.29   | 4 (2%)  | 62  | 35  | 68, 110, 150, 224     | 0     |
| 35  | CN    | 180/181 (99%)  | 0.05   | 1 (0%)  | 85  | 64  | 47, 82, 125, 185      | 0     |
| 35  | EN    | 180/181 (99%)  | 0.29   | 1 (0%)  | 85  | 64  | 63, 101, 142, 187     | 0     |
| 35  | GN    | 180/181 (99%)  | 0.61   | 8 (4%)  | 39  | 21  | 94, 139, 188, 248     | 0     |
| 36  | BO    | 184/185 (99%)  | 0.03   | 3 (1%)  | 70  | 43  | 29, 78, 184, 207      | 0     |
| 36  | EO    | 146/185 (78%)  | 0.04   | 0       | 100 | 100 | 57, 95, 128, 194      | 0     |
| 36  | GO    | 153/185 (82%)  | 0.25   | 1 (0%)  | 84  | 61  | 67, 109, 153, 262     | 0     |
| 37  | BP    | 156/157 (99%)  | 0.35   | 1 (0%)  | 85  | 64  | 70, 116, 169, 203     | 0     |
| 37  | CP    | 156/157 (99%)  | -0.04  | 1 (0%)  | 85  | 64  | 42, 79, 136, 152      | 0     |
| 37  | EP    | 156/157 (99%)  | 0.24   | 0       | 100 | 100 | 56, 100, 148, 183     | 0     |
| 37  | GP    | 156/157 (99%)  | 0.62   | 7 (4%)  | 38  | 20  | 69, 122, 163, 222     | 0     |
| 38  | BQ    | 157/183 (85%)  | 0.04   | 4 (2%)  | 58  | 33  | 31, 68, 121, 173      | 0     |
| 38  | CQ    | 157/183 (85%)  | -0.06  | 2 (1%)  | 75  | 48  | 26, 70, 124, 158      | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------|-----|-----|-----------------------|-------|
| 38  | EQ    | 157/183 (85%) | 0.14   | 3 (1%)  | 66  | 39  | 48, 86, 141, 177      | 0     |
| 38  | GQ    | 157/183 (85%) | 0.33   | 6 (3%)  | 44  | 24  | 60, 106, 157, 200     | 0     |
| 39  | BR    | 121/150 (80%) | 0.13   | 3 (2%)  | 58  | 33  | 42, 78, 129, 185      | 0     |
| 39  | CR    | 121/150 (80%) | 0.08   | 1 (0%)  | 82  | 58  | 54, 88, 129, 172      | 0     |
| 39  | ER    | 121/150 (80%) | 0.20   | 2 (1%)  | 69  | 41  | 65, 112, 146, 172     | 0     |
| 39  | GR    | 121/150 (80%) | 0.48   | 4 (3%)  | 49  | 27  | 97, 138, 175, 191     | 0     |
| 40  | BS    | 126/135 (93%) | 0.05   | 0       | 100 | 100 | 62, 98, 133, 177      | 0     |
| 40  | CS    | 126/135 (93%) | 0.27   | 4 (3%)  | 50  | 28  | 46, 89, 127, 152      | 0     |
| 40  | ES    | 126/135 (93%) | 0.40   | 2 (1%)  | 70  | 43  | 74, 112, 151, 184     | 0     |
| 40  | GS    | 126/135 (93%) | 0.67   | 6 (4%)  | 35  | 19  | 101, 143, 186, 218    | 0     |
| 41  | BT    | 61/158 (38%)  | -0.08  | 0       | 100 | 100 | 39, 73, 127, 158      | 0     |
| 41  | CT    | 61/158 (38%)  | -0.09  | 0       | 100 | 100 | 37, 73, 105, 137      | 0     |
| 41  | ET    | 61/158 (38%)  | -0.11  | 0       | 100 | 100 | 45, 78, 113, 147      | 0     |
| 41  | GT    | 61/158 (38%)  | -0.07  | 2 (3%)  | 49  | 27  | 42, 76, 115, 138      | 0     |
| 42  | BU    | 123/124 (99%) | 0.13   | 0       | 100 | 100 | 59, 101, 139, 204     | 0     |
| 42  | CU    | 123/124 (99%) | 0.29   | 3 (2%)  | 59  | 34  | 49, 92, 143, 163      | 0     |
| 42  | EU    | 123/124 (99%) | 0.21   | 2 (1%)  | 70  | 43  | 79, 114, 157, 220     | 0     |
| 42  | GU    | 123/124 (99%) | 0.51   | 3 (2%)  | 59  | 34  | 113, 156, 193, 233    | 0     |
| 43  | BV    | 234/239 (97%) | 0.19   | 5 (2%)  | 63  | 36  | 61, 107, 160, 213     | 0     |
| 43  | CV    | 234/239 (97%) | 0.08   | 4 (1%)  | 69  | 41  | 47, 87, 145, 213      | 0     |
| 43  | EV    | 234/239 (97%) | 0.23   | 4 (1%)  | 69  | 41  | 53, 102, 159, 232     | 0     |
| 43  | GV    | 234/239 (97%) | 0.39   | 7 (2%)  | 52  | 29  | 75, 121, 173, 239     | 0     |
| 44  | BW    | 110/111 (99%) | -0.03  | 1 (0%)  | 81  | 56  | 36, 64, 155, 204      | 0     |
| 44  | CW    | 110/111 (99%) | -0.09  | 0       | 100 | 100 | 43, 76, 138, 178      | 0     |
| 44  | EW    | 110/111 (99%) | 0.08   | 1 (0%)  | 81  | 56  | 56, 88, 170, 227      | 0     |
| 44  | GW    | 110/111 (99%) | 0.08   | 2 (1%)  | 67  | 40  | 63, 102, 183, 216     | 0     |
| 45  | BX    | 125/134 (93%) | 0.15   | 0       | 100 | 100 | 53, 89, 128, 202      | 0     |
| 45  | CX    | 125/134 (93%) | 0.02   | 1 (0%)  | 82  | 58  | 40, 78, 116, 196      | 0     |
| 45  | EX    | 125/134 (93%) | 0.12   | 1 (0%)  | 82  | 58  | 49, 88, 129, 233      | 0     |
| 45  | GX    | 125/134 (93%) | 0.49   | 4 (3%)  | 50  | 28  | 73, 117, 162, 215     | 0     |
| 46  | BY    | 102/103 (99%) | 0.08   | 2 (1%)  | 65  | 37  | 40, 74, 164, 222      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2   |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------|----|----|-----------------------|-------|
| 46  | CY    | 102/103 (99%)     | -0.04  | 1 (0%)    | 79 | 54 | 41, 83, 173, 196      | 0     |
| 46  | EY    | 102/103 (99%)     | 0.09   | 1 (0%)    | 79 | 54 | 45, 84, 156, 193      | 0     |
| 46  | GY    | 102/103 (99%)     | 0.24   | 1 (0%)    | 79 | 54 | 53, 102, 189, 222     | 0     |
| 47  | CO    | 146/185 (78%)     | -0.06  | 2 (1%)    | 73 | 46 | 45, 79, 115, 148      | 0     |
| All | All   | 40083/43352 (92%) | 0.35   | 1403 (3%) | 47 | 26 | 26, 101, 177, 390     | 0     |

The worst 5 of 1403 RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 46  | EY    | 2    | ALA  | 6.1  |
| 33  | CL    | 9    | GLU  | 5.4  |
| 1   | A1    | 1308 | U    | 5.2  |
| 1   | F1    | 1109 | A    | 5.2  |
| 1   | F1    | 2278 | G    | 5.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 48  | MG   | H1    | 3536 | 1/1   | 0.14 | 0.29 | 168,168,168,168            | 0     |
| 48  | MG   | H1    | 3489 | 1/1   | 0.15 | 0.14 | 206,206,206,206            | 0     |
| 48  | MG   | F1    | 3411 | 1/1   | 0.15 | 0.27 | 142,142,142,142            | 0     |
| 48  | MG   | H1    | 3412 | 1/1   | 0.16 | 0.40 | 173,173,173,173            | 0     |
| 48  | MG   | E2    | 205  | 1/1   | 0.18 | 0.27 | 140,140,140,140            | 0     |
| 48  | MG   | G2    | 204  | 1/1   | 0.20 | 0.21 | 181,181,181,181            | 0     |
| 48  | MG   | H1    | 3547 | 1/1   | 0.23 | 0.15 | 175,175,175,175            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | E3    | 204  | 1/1   | 0.27 | 0.34 | 199,199,199,199             | 0     |
| 48  | MG   | A1    | 3568 | 1/1   | 0.31 | 0.14 | 173,173,173,173             | 0     |
| 48  | MG   | H1    | 3534 | 1/1   | 0.32 | 0.28 | 221,221,221,221             | 0     |
| 48  | MG   | EW    | 201  | 1/1   | 0.36 | 0.12 | 172,172,172,172             | 0     |
| 48  | MG   | C3    | 205  | 1/1   | 0.39 | 0.20 | 175,175,175,175             | 0     |
| 48  | MG   | D1    | 3463 | 1/1   | 0.39 | 0.23 | 176,176,176,176             | 0     |
| 48  | MG   | H1    | 3551 | 1/1   | 0.39 | 0.43 | 202,202,202,202             | 0     |
| 48  | MG   | G3    | 202  | 1/1   | 0.40 | 0.23 | 136,136,136,136             | 0     |
| 48  | MG   | D1    | 3446 | 1/1   | 0.43 | 0.24 | 176,176,176,176             | 0     |
| 48  | MG   | D1    | 3611 | 1/1   | 0.44 | 0.31 | 205,205,205,205             | 0     |
| 48  | MG   | F1    | 3566 | 1/1   | 0.44 | 0.35 | 146,146,146,146             | 0     |
| 48  | MG   | C3    | 207  | 1/1   | 0.45 | 0.22 | 160,160,160,160             | 0     |
| 48  | MG   | H1    | 3532 | 1/1   | 0.46 | 0.17 | 162,162,162,162             | 0     |
| 48  | MG   | F1    | 3422 | 1/1   | 0.47 | 0.19 | 149,149,149,149             | 0     |
| 48  | MG   | F1    | 3430 | 1/1   | 0.49 | 0.13 | 128,128,128,128             | 0     |
| 48  | MG   | A1    | 3593 | 1/1   | 0.50 | 0.17 | 158,158,158,158             | 0     |
| 48  | MG   | A1    | 3427 | 1/1   | 0.51 | 0.16 | 152,152,152,152             | 0     |
| 48  | MG   | B3    | 203  | 1/1   | 0.52 | 0.12 | 160,160,160,160             | 0     |
| 48  | MG   | D1    | 3528 | 1/1   | 0.53 | 0.15 | 123,123,123,123             | 0     |
| 48  | MG   | H1    | 3479 | 1/1   | 0.54 | 0.19 | 132,132,132,132             | 0     |
| 48  | MG   | A1    | 3585 | 1/1   | 0.55 | 0.16 | 152,152,152,152             | 0     |
| 48  | MG   | A1    | 3522 | 1/1   | 0.55 | 0.29 | 146,146,146,146             | 0     |
| 48  | MG   | D1    | 3592 | 1/1   | 0.56 | 0.27 | 159,159,159,159             | 0     |
| 48  | MG   | A1    | 3588 | 1/1   | 0.58 | 0.16 | 144,144,144,144             | 0     |
| 48  | MG   | F1    | 3575 | 1/1   | 0.58 | 0.14 | 130,130,130,130             | 0     |
| 48  | MG   | D1    | 3625 | 1/1   | 0.58 | 0.10 | 164,164,164,164             | 0     |
| 48  | MG   | E2    | 206  | 1/1   | 0.59 | 0.17 | 151,151,151,151             | 0     |
| 48  | MG   | A1    | 3573 | 1/1   | 0.59 | 0.28 | 186,186,186,186             | 0     |
| 48  | MG   | G3    | 205  | 1/1   | 0.60 | 0.16 | 171,171,171,171             | 0     |
| 48  | MG   | H1    | 3406 | 1/1   | 0.60 | 0.09 | 143,143,143,143             | 0     |
| 48  | MG   | B2    | 207  | 1/1   | 0.61 | 0.21 | 149,149,149,149             | 0     |
| 48  | MG   | G2    | 206  | 1/1   | 0.61 | 0.24 | 174,174,174,174             | 0     |
| 48  | MG   | H1    | 3531 | 1/1   | 0.61 | 0.15 | 157,157,157,157             | 0     |
| 48  | MG   | F1    | 3561 | 1/1   | 0.61 | 0.16 | 167,167,167,167             | 0     |
| 48  | MG   | D1    | 3608 | 1/1   | 0.62 | 0.12 | 115,115,115,115             | 0     |
| 48  | MG   | H1    | 3450 | 1/1   | 0.62 | 0.14 | 156,156,156,156             | 0     |
| 48  | MG   | D1    | 3548 | 1/1   | 0.62 | 0.16 | 183,183,183,183             | 0     |
| 48  | MG   | GN    | 201  | 1/1   | 0.62 | 0.19 | 212,212,212,212             | 0     |
| 48  | MG   | D1    | 3470 | 1/1   | 0.62 | 0.19 | 134,134,134,134             | 0     |
| 48  | MG   | H1    | 3529 | 1/1   | 0.63 | 0.26 | 214,214,214,214             | 0     |
| 48  | MG   | H1    | 3540 | 1/1   | 0.63 | 0.12 | 136,136,136,136             | 0     |
| 48  | MG   | F1    | 3560 | 1/1   | 0.64 | 0.15 | 169,169,169,169             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | F1    | 3421 | 1/1   | 0.64 | 0.16 | 174,174,174,174             | 0     |
| 48  | MG   | D1    | 3433 | 1/1   | 0.64 | 0.10 | 149,149,149,149             | 0     |
| 48  | MG   | H1    | 3414 | 1/1   | 0.64 | 0.14 | 169,169,169,169             | 0     |
| 48  | MG   | D1    | 3437 | 1/1   | 0.64 | 0.12 | 148,148,148,148             | 0     |
| 48  | MG   | F1    | 3509 | 1/1   | 0.65 | 0.10 | 144,144,144,144             | 0     |
| 48  | MG   | A1    | 3430 | 1/1   | 0.65 | 0.14 | 146,146,146,146             | 0     |
| 48  | MG   | A1    | 3587 | 1/1   | 0.65 | 0.24 | 182,182,182,182             | 0     |
| 48  | MG   | D1    | 3624 | 1/1   | 0.65 | 0.17 | 162,162,162,162             | 0     |
| 48  | MG   | A1    | 3527 | 1/1   | 0.66 | 0.13 | 119,119,119,119             | 0     |
| 48  | MG   | A1    | 3437 | 1/1   | 0.66 | 0.19 | 141,141,141,141             | 0     |
| 48  | MG   | A1    | 3451 | 1/1   | 0.66 | 0.11 | 146,146,146,146             | 0     |
| 48  | MG   | D1    | 3598 | 1/1   | 0.66 | 0.11 | 159,159,159,159             | 0     |
| 48  | MG   | A1    | 3435 | 1/1   | 0.66 | 0.24 | 151,151,151,151             | 0     |
| 48  | MG   | F1    | 3574 | 1/1   | 0.67 | 0.19 | 161,161,161,161             | 0     |
| 48  | MG   | F1    | 3539 | 1/1   | 0.67 | 0.23 | 187,187,187,187             | 0     |
| 48  | MG   | F1    | 3490 | 1/1   | 0.67 | 0.12 | 139,139,139,139             | 0     |
| 48  | MG   | F1    | 3565 | 1/1   | 0.68 | 0.16 | 168,168,168,168             | 0     |
| 48  | MG   | H1    | 3477 | 1/1   | 0.68 | 0.17 | 103,103,103,103             | 0     |
| 48  | MG   | H1    | 3511 | 1/1   | 0.69 | 0.12 | 140,140,140,140             | 0     |
| 48  | MG   | H1    | 3525 | 1/1   | 0.69 | 0.17 | 157,157,157,157             | 0     |
| 48  | MG   | D1    | 3550 | 1/1   | 0.69 | 0.16 | 136,136,136,136             | 0     |
| 48  | MG   | C2    | 206  | 1/1   | 0.69 | 0.14 | 123,123,123,123             | 0     |
| 48  | MG   | A1    | 3402 | 1/1   | 0.69 | 0.15 | 143,143,143,143             | 0     |
| 48  | MG   | A1    | 3515 | 1/1   | 0.70 | 0.17 | 111,111,111,111             | 0     |
| 48  | MG   | H1    | 3436 | 1/1   | 0.70 | 0.10 | 146,146,146,146             | 0     |
| 48  | MG   | F1    | 3415 | 1/1   | 0.70 | 0.12 | 118,118,118,118             | 0     |
| 48  | MG   | F1    | 3493 | 1/1   | 0.70 | 0.19 | 145,145,145,145             | 0     |
| 48  | MG   | F1    | 3483 | 1/1   | 0.71 | 0.15 | 129,129,129,129             | 0     |
| 48  | MG   | H1    | 3537 | 1/1   | 0.71 | 0.11 | 152,152,152,152             | 0     |
| 48  | MG   | F1    | 3537 | 1/1   | 0.71 | 0.14 | 136,136,136,136             | 0     |
| 48  | MG   | D1    | 3603 | 1/1   | 0.71 | 0.18 | 125,125,125,125             | 0     |
| 48  | MG   | H1    | 3550 | 1/1   | 0.71 | 0.10 | 152,152,152,152             | 0     |
| 48  | MG   | A1    | 3530 | 1/1   | 0.71 | 0.12 | 149,149,149,149             | 0     |
| 48  | MG   | E2    | 207  | 1/1   | 0.72 | 0.14 | 147,147,147,147             | 0     |
| 48  | MG   | A1    | 3586 | 1/1   | 0.72 | 0.11 | 177,177,177,177             | 0     |
| 48  | MG   | H1    | 3544 | 1/1   | 0.72 | 0.18 | 146,146,146,146             | 0     |
| 48  | MG   | H1    | 3418 | 1/1   | 0.72 | 0.11 | 141,141,141,141             | 0     |
| 48  | MG   | F1    | 3578 | 1/1   | 0.72 | 0.20 | 161,161,161,161             | 0     |
| 48  | MG   | H1    | 3410 | 1/1   | 0.72 | 0.13 | 192,192,192,192             | 0     |
| 48  | MG   | H1    | 3538 | 1/1   | 0.73 | 0.14 | 140,140,140,140             | 0     |
| 48  | MG   | D1    | 3583 | 1/1   | 0.73 | 0.09 | 139,139,139,139             | 0     |
| 48  | MG   | H1    | 3473 | 1/1   | 0.73 | 0.10 | 123,123,123,123             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | H1    | 3519 | 1/1   | 0.73 | 0.13 | 151,151,151,151             | 0     |
| 48  | MG   | A1    | 3420 | 1/1   | 0.73 | 0.15 | 155,155,155,155             | 0     |
| 48  | MG   | A1    | 3428 | 1/1   | 0.73 | 0.16 | 159,159,159,159             | 0     |
| 48  | MG   | D1    | 3426 | 1/1   | 0.74 | 0.13 | 143,143,143,143             | 0     |
| 48  | MG   | H1    | 3535 | 1/1   | 0.74 | 0.18 | 150,150,150,150             | 0     |
| 48  | MG   | A1    | 3449 | 1/1   | 0.74 | 0.14 | 115,115,115,115             | 0     |
| 48  | MG   | D1    | 3434 | 1/1   | 0.74 | 0.12 | 144,144,144,144             | 0     |
| 48  | MG   | A1    | 3416 | 1/1   | 0.74 | 0.11 | 140,140,140,140             | 0     |
| 48  | MG   | D1    | 3606 | 1/1   | 0.74 | 0.17 | 157,157,157,157             | 0     |
| 48  | MG   | H1    | 3543 | 1/1   | 0.74 | 0.06 | 183,183,183,183             | 0     |
| 48  | MG   | F1    | 3540 | 1/1   | 0.74 | 0.12 | 111,111,111,111             | 0     |
| 48  | MG   | F1    | 3545 | 1/1   | 0.74 | 0.09 | 137,137,137,137             | 0     |
| 48  | MG   | A1    | 3438 | 1/1   | 0.74 | 0.10 | 148,148,148,148             | 0     |
| 48  | MG   | D1    | 3609 | 1/1   | 0.74 | 0.18 | 120,120,120,120             | 0     |
| 48  | MG   | A1    | 3453 | 1/1   | 0.75 | 0.14 | 184,184,184,184             | 0     |
| 48  | MG   | H1    | 3481 | 1/1   | 0.75 | 0.16 | 134,134,134,134             | 0     |
| 48  | MG   | D1    | 3576 | 1/1   | 0.75 | 0.13 | 150,150,150,150             | 0     |
| 48  | MG   | F1    | 3576 | 1/1   | 0.75 | 0.12 | 142,142,142,142             | 0     |
| 48  | MG   | B3    | 201  | 1/1   | 0.76 | 0.10 | 129,129,129,129             | 0     |
| 48  | MG   | A1    | 3580 | 1/1   | 0.76 | 0.10 | 130,130,130,130             | 0     |
| 48  | MG   | D1    | 3597 | 1/1   | 0.76 | 0.13 | 158,158,158,158             | 0     |
| 48  | MG   | EN    | 202  | 1/1   | 0.76 | 0.38 | 238,238,238,238             | 0     |
| 48  | MG   | A1    | 3551 | 1/1   | 0.77 | 0.18 | 123,123,123,123             | 0     |
| 48  | MG   | D1    | 3401 | 1/1   | 0.77 | 0.15 | 109,109,109,109             | 0     |
| 48  | MG   | F1    | 3424 | 1/1   | 0.77 | 0.14 | 114,114,114,114             | 0     |
| 48  | MG   | D1    | 3421 | 1/1   | 0.77 | 0.10 | 126,126,126,126             | 0     |
| 48  | MG   | H1    | 3470 | 1/1   | 0.77 | 0.11 | 140,140,140,140             | 0     |
| 48  | MG   | H1    | 3401 | 1/1   | 0.77 | 0.09 | 146,146,146,146             | 0     |
| 48  | MG   | B2    | 208  | 1/1   | 0.77 | 0.14 | 138,138,138,138             | 0     |
| 48  | MG   | A1    | 3555 | 1/1   | 0.77 | 0.17 | 128,128,128,128             | 0     |
| 48  | MG   | D1    | 3588 | 1/1   | 0.77 | 0.12 | 156,156,156,156             | 0     |
| 48  | MG   | G3    | 204  | 1/1   | 0.78 | 0.23 | 143,143,143,143             | 0     |
| 48  | MG   | F1    | 3555 | 1/1   | 0.78 | 0.16 | 168,168,168,168             | 0     |
| 48  | MG   | D1    | 3593 | 1/1   | 0.78 | 0.15 | 180,180,180,180             | 0     |
| 48  | MG   | G2    | 205  | 1/1   | 0.78 | 0.10 | 146,146,146,146             | 0     |
| 48  | MG   | H1    | 3482 | 1/1   | 0.78 | 0.12 | 162,162,162,162             | 0     |
| 48  | MG   | A1    | 3556 | 1/1   | 0.78 | 0.15 | 124,124,124,124             | 0     |
| 48  | MG   | H1    | 3548 | 1/1   | 0.78 | 0.11 | 188,188,188,188             | 0     |
| 48  | MG   | H1    | 3549 | 1/1   | 0.78 | 0.19 | 124,124,124,124             | 0     |
| 48  | MG   | H1    | 3501 | 1/1   | 0.78 | 0.16 | 110,110,110,110             | 0     |
| 48  | MG   | A1    | 3472 | 1/1   | 0.78 | 0.15 | 149,149,149,149             | 0     |
| 48  | MG   | H1    | 3546 | 1/1   | 0.79 | 0.14 | 120,120,120,120             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | D1    | 3616 | 1/1   | 0.79 | 0.09 | 150,150,150,150             | 0     |
| 48  | MG   | D1    | 3599 | 1/1   | 0.79 | 0.11 | 126,126,126,126             | 0     |
| 48  | MG   | D1    | 3605 | 1/1   | 0.79 | 0.11 | 108,108,108,108             | 0     |
| 48  | MG   | D1    | 3626 | 1/1   | 0.79 | 0.11 | 137,137,137,137             | 0     |
| 48  | MG   | F1    | 3522 | 1/1   | 0.79 | 0.10 | 111,111,111,111             | 0     |
| 48  | MG   | HT    | 101  | 1/1   | 0.79 | 0.07 | 174,174,174,174             | 0     |
| 48  | MG   | F1    | 3414 | 1/1   | 0.80 | 0.11 | 123,123,123,123             | 0     |
| 48  | MG   | D1    | 3497 | 1/1   | 0.80 | 0.20 | 151,151,151,151             | 0     |
| 48  | MG   | D1    | 3514 | 1/1   | 0.80 | 0.08 | 128,128,128,128             | 0     |
| 48  | MG   | A1    | 3414 | 1/1   | 0.80 | 0.08 | 142,142,142,142             | 0     |
| 48  | MG   | A1    | 3576 | 1/1   | 0.80 | 0.19 | 122,122,122,122             | 0     |
| 48  | MG   | A1    | 3567 | 1/1   | 0.80 | 0.14 | 144,144,144,144             | 0     |
| 48  | MG   | D1    | 3445 | 1/1   | 0.80 | 0.14 | 126,126,126,126             | 0     |
| 48  | MG   | A1    | 3422 | 1/1   | 0.80 | 0.13 | 144,144,144,144             | 0     |
| 48  | MG   | F1    | 3572 | 1/1   | 0.80 | 0.18 | 155,155,155,155             | 0     |
| 48  | MG   | H1    | 3516 | 1/1   | 0.80 | 0.08 | 129,129,129,129             | 0     |
| 48  | MG   | E3    | 205  | 1/1   | 0.80 | 0.15 | 127,127,127,127             | 0     |
| 48  | MG   | D1    | 3448 | 1/1   | 0.80 | 0.10 | 125,125,125,125             | 0     |
| 48  | MG   | F1    | 3511 | 1/1   | 0.80 | 0.14 | 154,154,154,154             | 0     |
| 48  | MG   | D1    | 3422 | 1/1   | 0.80 | 0.10 | 150,150,150,150             | 0     |
| 48  | MG   | B2    | 201  | 1/1   | 0.80 | 0.12 | 119,119,119,119             | 0     |
| 48  | MG   | A1    | 3578 | 1/1   | 0.81 | 0.09 | 117,117,117,117             | 0     |
| 48  | MG   | A1    | 3595 | 1/1   | 0.81 | 0.26 | 151,151,151,151             | 0     |
| 48  | MG   | F1    | 3567 | 1/1   | 0.81 | 0.14 | 128,128,128,128             | 0     |
| 48  | MG   | F1    | 3570 | 1/1   | 0.81 | 0.14 | 113,113,113,113             | 0     |
| 48  | MG   | A1    | 3417 | 1/1   | 0.81 | 0.12 | 150,150,150,150             | 0     |
| 48  | MG   | H1    | 3541 | 1/1   | 0.81 | 0.12 | 154,154,154,154             | 0     |
| 48  | MG   | D1    | 3521 | 1/1   | 0.81 | 0.21 | 129,129,129,129             | 0     |
| 48  | MG   | H1    | 3411 | 1/1   | 0.81 | 0.09 | 120,120,120,120             | 0     |
| 48  | MG   | D1    | 3424 | 1/1   | 0.81 | 0.13 | 150,150,150,150             | 0     |
| 48  | MG   | D1    | 3596 | 1/1   | 0.81 | 0.13 | 165,165,165,165             | 0     |
| 48  | MG   | F1    | 3477 | 1/1   | 0.81 | 0.12 | 146,146,146,146             | 0     |
| 48  | MG   | D1    | 3540 | 1/1   | 0.81 | 0.12 | 139,139,139,139             | 0     |
| 48  | MG   | A1    | 3401 | 1/1   | 0.81 | 0.10 | 108,108,108,108             | 0     |
| 48  | MG   | A1    | 3589 | 1/1   | 0.81 | 0.11 | 113,113,113,113             | 0     |
| 48  | MG   | F1    | 3563 | 1/1   | 0.81 | 0.13 | 124,124,124,124             | 0     |
| 48  | MG   | F1    | 3580 | 1/1   | 0.82 | 0.11 | 147,147,147,147             | 0     |
| 48  | MG   | D1    | 3571 | 1/1   | 0.82 | 0.28 | 130,130,130,130             | 0     |
| 48  | MG   | A1    | 3592 | 1/1   | 0.82 | 0.08 | 134,134,134,134             | 0     |
| 48  | MG   | F1    | 3457 | 1/1   | 0.82 | 0.12 | 91,91,91,91                 | 0     |
| 48  | MG   | H1    | 3465 | 1/1   | 0.82 | 0.07 | 143,143,143,143             | 0     |
| 48  | MG   | H1    | 3553 | 1/1   | 0.82 | 0.13 | 146,146,146,146             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | GO    | 201  | 1/1   | 0.82 | 0.14 | 141,141,141,141             | 0     |
| 48  | MG   | H1    | 3457 | 1/1   | 0.83 | 0.11 | 147,147,147,147             | 0     |
| 48  | MG   | A1    | 3594 | 1/1   | 0.83 | 0.15 | 150,150,150,150             | 0     |
| 48  | MG   | F1    | 3569 | 1/1   | 0.83 | 0.14 | 130,130,130,130             | 0     |
| 48  | MG   | A1    | 3424 | 1/1   | 0.83 | 0.20 | 150,150,150,150             | 0     |
| 48  | MG   | A1    | 3596 | 1/1   | 0.83 | 0.09 | 163,163,163,163             | 0     |
| 48  | MG   | F1    | 3482 | 1/1   | 0.83 | 0.12 | 130,130,130,130             | 0     |
| 48  | MG   | D1    | 3565 | 1/1   | 0.83 | 0.12 | 114,114,114,114             | 0     |
| 48  | MG   | H1    | 3402 | 1/1   | 0.83 | 0.09 | 118,118,118,118             | 0     |
| 48  | MG   | F1    | 3419 | 1/1   | 0.83 | 0.07 | 124,124,124,124             | 0     |
| 48  | MG   | D1    | 3522 | 1/1   | 0.83 | 0.16 | 162,162,162,162             | 0     |
| 48  | MG   | F1    | 3496 | 1/1   | 0.83 | 0.14 | 122,122,122,122             | 0     |
| 48  | MG   | FK    | 201  | 1/1   | 0.83 | 0.21 | 168,168,168,168             | 0     |
| 48  | MG   | G2    | 201  | 1/1   | 0.83 | 0.09 | 141,141,141,141             | 0     |
| 48  | MG   | E3    | 206  | 1/1   | 0.83 | 0.12 | 132,132,132,132             | 0     |
| 48  | MG   | A1    | 3513 | 1/1   | 0.83 | 0.10 | 133,133,133,133             | 0     |
| 48  | MG   | H1    | 3443 | 1/1   | 0.83 | 0.11 | 157,157,157,157             | 0     |
| 48  | MG   | F1    | 3515 | 1/1   | 0.83 | 0.08 | 143,143,143,143             | 0     |
| 48  | MG   | F1    | 3564 | 1/1   | 0.84 | 0.11 | 143,143,143,143             | 0     |
| 48  | MG   | H1    | 3521 | 1/1   | 0.84 | 0.14 | 123,123,123,123             | 0     |
| 48  | MG   | C2    | 205  | 1/1   | 0.84 | 0.11 | 127,127,127,127             | 0     |
| 48  | MG   | D1    | 3547 | 1/1   | 0.84 | 0.10 | 109,109,109,109             | 0     |
| 48  | MG   | D1    | 3516 | 1/1   | 0.84 | 0.15 | 82,82,82,82                 | 0     |
| 48  | MG   | F1    | 3548 | 1/1   | 0.84 | 0.11 | 106,106,106,106             | 0     |
| 48  | MG   | H1    | 3533 | 1/1   | 0.84 | 0.15 | 153,153,153,153             | 0     |
| 48  | MG   | H1    | 3484 | 1/1   | 0.84 | 0.10 | 166,166,166,166             | 0     |
| 48  | MG   | D1    | 3601 | 1/1   | 0.84 | 0.11 | 124,124,124,124             | 0     |
| 48  | MG   | B2    | 202  | 1/1   | 0.84 | 0.09 | 103,103,103,103             | 0     |
| 48  | MG   | D1    | 3417 | 1/1   | 0.84 | 0.10 | 132,132,132,132             | 0     |
| 48  | MG   | BN    | 201  | 1/1   | 0.84 | 0.11 | 147,147,147,147             | 0     |
| 48  | MG   | F1    | 3448 | 1/1   | 0.85 | 0.07 | 126,126,126,126             | 0     |
| 48  | MG   | D1    | 3427 | 1/1   | 0.85 | 0.12 | 153,153,153,153             | 0     |
| 48  | MG   | A1    | 3444 | 1/1   | 0.85 | 0.10 | 126,126,126,126             | 0     |
| 48  | MG   | H1    | 3523 | 1/1   | 0.85 | 0.09 | 167,167,167,167             | 0     |
| 48  | MG   | CN    | 201  | 1/1   | 0.85 | 0.15 | 175,175,175,175             | 0     |
| 48  | MG   | AK    | 202  | 1/1   | 0.85 | 0.11 | 179,179,179,179             | 0     |
| 48  | MG   | H1    | 3415 | 1/1   | 0.85 | 0.08 | 133,133,133,133             | 0     |
| 48  | MG   | D1    | 3551 | 1/1   | 0.85 | 0.10 | 142,142,142,142             | 0     |
| 48  | MG   | H1    | 3420 | 1/1   | 0.85 | 0.12 | 113,113,113,113             | 0     |
| 48  | MG   | F1    | 3401 | 1/1   | 0.85 | 0.13 | 101,101,101,101             | 0     |
| 48  | MG   | A1    | 3441 | 1/1   | 0.85 | 0.12 | 127,127,127,127             | 0     |
| 48  | MG   | H1    | 3449 | 1/1   | 0.85 | 0.17 | 118,118,118,118             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | H1    | 3554 | 1/1   | 0.85 | 0.13 | 128,128,128,128             | 0     |
| 48  | MG   | F1    | 3444 | 1/1   | 0.85 | 0.09 | 155,155,155,155             | 0     |
| 48  | MG   | F1    | 3549 | 1/1   | 0.86 | 0.07 | 125,125,125,125             | 0     |
| 48  | MG   | H1    | 3404 | 1/1   | 0.86 | 0.07 | 132,132,132,132             | 0     |
| 48  | MG   | F1    | 3428 | 1/1   | 0.86 | 0.09 | 111,111,111,111             | 0     |
| 48  | MG   | H1    | 3409 | 1/1   | 0.86 | 0.15 | 193,193,193,193             | 0     |
| 48  | MG   | D1    | 3543 | 1/1   | 0.86 | 0.12 | 127,127,127,127             | 0     |
| 48  | MG   | H1    | 3539 | 1/1   | 0.86 | 0.10 | 128,128,128,128             | 0     |
| 48  | MG   | D1    | 3575 | 1/1   | 0.86 | 0.09 | 124,124,124,124             | 0     |
| 48  | MG   | F1    | 3503 | 1/1   | 0.86 | 0.12 | 129,129,129,129             | 0     |
| 48  | MG   | H1    | 3542 | 1/1   | 0.86 | 0.13 | 137,137,137,137             | 0     |
| 48  | MG   | D1    | 3475 | 1/1   | 0.86 | 0.15 | 120,120,120,120             | 0     |
| 48  | MG   | F1    | 3453 | 1/1   | 0.86 | 0.12 | 131,131,131,131             | 0     |
| 48  | MG   | DJ    | 301  | 1/1   | 0.86 | 0.07 | 150,150,150,150             | 0     |
| 48  | MG   | F1    | 3462 | 1/1   | 0.86 | 0.07 | 118,118,118,118             | 0     |
| 48  | MG   | F1    | 3466 | 1/1   | 0.86 | 0.09 | 140,140,140,140             | 0     |
| 48  | MG   | E2    | 201  | 1/1   | 0.86 | 0.08 | 156,156,156,156             | 0     |
| 48  | MG   | GA    | 301  | 1/1   | 0.86 | 0.07 | 142,142,142,142             | 0     |
| 48  | MG   | A1    | 3510 | 1/1   | 0.86 | 0.10 | 109,109,109,109             | 0     |
| 48  | MG   | D1    | 3586 | 1/1   | 0.86 | 0.09 | 109,109,109,109             | 0     |
| 48  | MG   | GP    | 202  | 1/1   | 0.86 | 0.08 | 137,137,137,137             | 0     |
| 48  | MG   | F1    | 3488 | 1/1   | 0.86 | 0.12 | 110,110,110,110             | 0     |
| 48  | MG   | A1    | 3547 | 1/1   | 0.87 | 0.16 | 81,81,81,81                 | 0     |
| 48  | MG   | D1    | 3604 | 1/1   | 0.87 | 0.09 | 141,141,141,141             | 0     |
| 48  | MG   | D1    | 3622 | 1/1   | 0.87 | 0.15 | 133,133,133,133             | 0     |
| 48  | MG   | A1    | 3574 | 1/1   | 0.87 | 0.08 | 119,119,119,119             | 0     |
| 48  | MG   | H1    | 3496 | 1/1   | 0.87 | 0.10 | 141,141,141,141             | 0     |
| 48  | MG   | F1    | 3473 | 1/1   | 0.87 | 0.09 | 156,156,156,156             | 0     |
| 48  | MG   | D1    | 3444 | 1/1   | 0.87 | 0.07 | 139,139,139,139             | 0     |
| 48  | MG   | A1    | 3485 | 1/1   | 0.87 | 0.12 | 137,137,137,137             | 0     |
| 48  | MG   | F1    | 3447 | 1/1   | 0.87 | 0.07 | 156,156,156,156             | 0     |
| 48  | MG   | F1    | 3529 | 1/1   | 0.87 | 0.21 | 140,140,140,140             | 0     |
| 48  | MG   | A1    | 3504 | 1/1   | 0.87 | 0.19 | 138,138,138,138             | 0     |
| 48  | MG   | F1    | 3538 | 1/1   | 0.87 | 0.22 | 113,113,113,113             | 0     |
| 48  | MG   | H1    | 3448 | 1/1   | 0.88 | 0.10 | 98,98,98,98                 | 0     |
| 48  | MG   | H1    | 3509 | 1/1   | 0.88 | 0.07 | 143,143,143,143             | 0     |
| 48  | MG   | D1    | 3439 | 1/1   | 0.88 | 0.10 | 146,146,146,146             | 0     |
| 48  | MG   | A1    | 3491 | 1/1   | 0.88 | 0.08 | 125,125,125,125             | 0     |
| 48  | MG   | D1    | 3482 | 1/1   | 0.88 | 0.08 | 106,106,106,106             | 0     |
| 48  | MG   | F1    | 3559 | 1/1   | 0.88 | 0.07 | 133,133,133,133             | 0     |
| 48  | MG   | H1    | 3469 | 1/1   | 0.88 | 0.11 | 119,119,119,119             | 0     |
| 48  | MG   | D1    | 3623 | 1/1   | 0.88 | 0.11 | 151,151,151,151             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | F1    | 3469 | 1/1   | 0.88 | 0.09 | 112,112,112,112             | 0     |
| 48  | MG   | F1    | 3562 | 1/1   | 0.88 | 0.09 | 140,140,140,140             | 0     |
| 48  | MG   | B2    | 206  | 1/1   | 0.88 | 0.13 | 139,139,139,139             | 0     |
| 48  | MG   | F1    | 3501 | 1/1   | 0.88 | 0.08 | 116,116,116,116             | 0     |
| 48  | MG   | F1    | 3475 | 1/1   | 0.88 | 0.13 | 93,93,93,93                 | 0     |
| 48  | MG   | H1    | 3552 | 1/1   | 0.88 | 0.10 | 131,131,131,131             | 0     |
| 48  | MG   | H1    | 3431 | 1/1   | 0.88 | 0.10 | 94,94,94,94                 | 0     |
| 48  | MG   | FT    | 101  | 1/1   | 0.88 | 0.07 | 124,124,124,124             | 0     |
| 48  | MG   | D1    | 3467 | 1/1   | 0.88 | 0.08 | 123,123,123,123             | 0     |
| 48  | MG   | A1    | 3581 | 1/1   | 0.89 | 0.10 | 126,126,126,126             | 0     |
| 48  | MG   | A1    | 3584 | 1/1   | 0.89 | 0.11 | 125,125,125,125             | 0     |
| 48  | MG   | H1    | 3472 | 1/1   | 0.89 | 0.11 | 104,104,104,104             | 0     |
| 48  | MG   | F1    | 3431 | 1/1   | 0.89 | 0.07 | 103,103,103,103             | 0     |
| 48  | MG   | A1    | 3423 | 1/1   | 0.89 | 0.08 | 115,115,115,115             | 0     |
| 48  | MG   | D1    | 3613 | 1/1   | 0.89 | 0.07 | 120,120,120,120             | 0     |
| 48  | MG   | A1    | 3554 | 1/1   | 0.89 | 0.12 | 76,76,76,76                 | 0     |
| 48  | MG   | D1    | 3617 | 1/1   | 0.89 | 0.17 | 113,113,113,113             | 0     |
| 48  | MG   | D1    | 3442 | 1/1   | 0.89 | 0.12 | 126,126,126,126             | 0     |
| 48  | MG   | H1    | 3486 | 1/1   | 0.89 | 0.09 | 105,105,105,105             | 0     |
| 48  | MG   | D1    | 3506 | 1/1   | 0.89 | 0.09 | 132,132,132,132             | 0     |
| 48  | MG   | A1    | 3412 | 1/1   | 0.89 | 0.14 | 117,117,117,117             | 0     |
| 48  | MG   | H1    | 3422 | 1/1   | 0.89 | 0.06 | 151,151,151,151             | 0     |
| 48  | MG   | F1    | 3527 | 1/1   | 0.89 | 0.17 | 105,105,105,105             | 0     |
| 48  | MG   | H1    | 3510 | 1/1   | 0.89 | 0.13 | 120,120,120,120             | 0     |
| 48  | MG   | C2    | 201  | 1/1   | 0.89 | 0.08 | 121,121,121,121             | 0     |
| 48  | MG   | D1    | 3517 | 1/1   | 0.89 | 0.13 | 127,127,127,127             | 0     |
| 48  | MG   | A1    | 3531 | 1/1   | 0.89 | 0.10 | 128,128,128,128             | 0     |
| 48  | MG   | F1    | 3571 | 1/1   | 0.89 | 0.09 | 132,132,132,132             | 0     |
| 48  | MG   | A1    | 3564 | 1/1   | 0.89 | 0.06 | 141,141,141,141             | 0     |
| 48  | MG   | H1    | 3524 | 1/1   | 0.89 | 0.13 | 139,139,139,139             | 0     |
| 48  | MG   | E2    | 202  | 1/1   | 0.89 | 0.11 | 89,89,89,89                 | 0     |
| 48  | MG   | A1    | 3408 | 1/1   | 0.89 | 0.09 | 122,122,122,122             | 0     |
| 48  | MG   | H1    | 3530 | 1/1   | 0.89 | 0.07 | 154,154,154,154             | 0     |
| 48  | MG   | F1    | 3464 | 1/1   | 0.90 | 0.11 | 120,120,120,120             | 0     |
| 48  | MG   | D1    | 3499 | 1/1   | 0.90 | 0.09 | 118,118,118,118             | 0     |
| 48  | MG   | H1    | 3468 | 1/1   | 0.90 | 0.09 | 121,121,121,121             | 0     |
| 48  | MG   | F1    | 3468 | 1/1   | 0.90 | 0.10 | 103,103,103,103             | 0     |
| 48  | MG   | A1    | 3507 | 1/1   | 0.90 | 0.08 | 129,129,129,129             | 0     |
| 48  | MG   | A1    | 3579 | 1/1   | 0.90 | 0.28 | 94,94,94,94                 | 0     |
| 48  | MG   | D1    | 3562 | 1/1   | 0.90 | 0.09 | 93,93,93,93                 | 0     |
| 48  | MG   | A1    | 3436 | 1/1   | 0.90 | 0.09 | 110,110,110,110             | 0     |
| 48  | MG   | H1    | 3408 | 1/1   | 0.90 | 0.09 | 111,111,111,111             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | F1    | 3542 | 1/1   | 0.90 | 0.09 | 107,107,107,107             | 0     |
| 48  | MG   | F1    | 3577 | 1/1   | 0.90 | 0.07 | 152,152,152,152             | 0     |
| 48  | MG   | A1    | 3403 | 1/1   | 0.90 | 0.08 | 96,96,96,96                 | 0     |
| 48  | MG   | D1    | 3412 | 1/1   | 0.90 | 0.12 | 95,95,95,95                 | 0     |
| 48  | MG   | D1    | 3416 | 1/1   | 0.90 | 0.11 | 110,110,110,110             | 0     |
| 48  | MG   | F1    | 3446 | 1/1   | 0.90 | 0.11 | 130,130,130,130             | 0     |
| 48  | MG   | A1    | 3583 | 1/1   | 0.90 | 0.15 | 112,112,112,112             | 0     |
| 48  | MG   | A1    | 3505 | 1/1   | 0.90 | 0.11 | 137,137,137,137             | 0     |
| 48  | MG   | F1    | 3498 | 1/1   | 0.90 | 0.06 | 141,141,141,141             | 0     |
| 48  | MG   | F1    | 3451 | 1/1   | 0.90 | 0.16 | 122,122,122,122             | 0     |
| 48  | MG   | H1    | 3433 | 1/1   | 0.90 | 0.08 | 132,132,132,132             | 0     |
| 48  | MG   | G3    | 201  | 1/1   | 0.90 | 0.08 | 119,119,119,119             | 0     |
| 48  | MG   | D1    | 3491 | 1/1   | 0.90 | 0.07 | 97,97,97,97                 | 0     |
| 48  | MG   | A1    | 3516 | 1/1   | 0.90 | 0.11 | 88,88,88,88                 | 0     |
| 48  | MG   | F1    | 3417 | 1/1   | 0.90 | 0.09 | 110,110,110,110             | 0     |
| 48  | MG   | F1    | 3463 | 1/1   | 0.90 | 0.09 | 100,100,100,100             | 0     |
| 48  | MG   | H1    | 3528 | 1/1   | 0.90 | 0.10 | 119,119,119,119             | 0     |
| 48  | MG   | D1    | 3525 | 1/1   | 0.91 | 0.09 | 113,113,113,113             | 0     |
| 48  | MG   | F1    | 3413 | 1/1   | 0.91 | 0.12 | 110,110,110,110             | 0     |
| 48  | MG   | D1    | 3574 | 1/1   | 0.91 | 0.13 | 80,80,80,80                 | 0     |
| 48  | MG   | A1    | 3470 | 1/1   | 0.91 | 0.08 | 164,164,164,164             | 0     |
| 48  | MG   | H1    | 3474 | 1/1   | 0.91 | 0.07 | 123,123,123,123             | 0     |
| 48  | MG   | A1    | 3575 | 1/1   | 0.91 | 0.08 | 143,143,143,143             | 0     |
| 48  | MG   | G2    | 202  | 1/1   | 0.91 | 0.11 | 122,122,122,122             | 0     |
| 48  | MG   | D1    | 3579 | 1/1   | 0.91 | 0.06 | 97,97,97,97                 | 0     |
| 48  | MG   | F1    | 3465 | 1/1   | 0.91 | 0.08 | 101,101,101,101             | 0     |
| 48  | MG   | H1    | 3416 | 1/1   | 0.91 | 0.21 | 113,113,113,113             | 0     |
| 48  | MG   | A1    | 3536 | 1/1   | 0.91 | 0.08 | 104,104,104,104             | 0     |
| 48  | MG   | H1    | 3487 | 1/1   | 0.91 | 0.09 | 122,122,122,122             | 0     |
| 48  | MG   | D1    | 3432 | 1/1   | 0.91 | 0.07 | 118,118,118,118             | 0     |
| 48  | MG   | H1    | 3490 | 1/1   | 0.91 | 0.10 | 122,122,122,122             | 0     |
| 48  | MG   | A1    | 3497 | 1/1   | 0.91 | 0.06 | 116,116,116,116             | 0     |
| 48  | MG   | A1    | 3565 | 1/1   | 0.91 | 0.08 | 132,132,132,132             | 0     |
| 48  | MG   | A1    | 3450 | 1/1   | 0.91 | 0.05 | 133,133,133,133             | 0     |
| 48  | MG   | F1    | 3476 | 1/1   | 0.91 | 0.07 | 99,99,99,99                 | 0     |
| 48  | MG   | D1    | 3555 | 1/1   | 0.91 | 0.09 | 119,119,119,119             | 0     |
| 48  | MG   | EN    | 201  | 1/1   | 0.91 | 0.09 | 111,111,111,111             | 0     |
| 48  | MG   | F1    | 3541 | 1/1   | 0.91 | 0.10 | 112,112,112,112             | 0     |
| 48  | MG   | GW    | 201  | 1/1   | 0.91 | 0.11 | 114,114,114,114             | 0     |
| 48  | MG   | D1    | 3557 | 1/1   | 0.91 | 0.07 | 116,116,116,116             | 0     |
| 48  | MG   | H1    | 3461 | 1/1   | 0.91 | 0.10 | 134,134,134,134             | 0     |
| 48  | MG   | A1    | 3553 | 1/1   | 0.91 | 0.07 | 108,108,108,108             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | H1    | 3555 | 1/1   | 0.91 | 0.08 | 123,123,123,123             | 0     |
| 48  | MG   | A1    | 3454 | 1/1   | 0.91 | 0.07 | 101,101,101,101             | 0     |
| 48  | MG   | D1    | 3425 | 1/1   | 0.92 | 0.18 | 123,123,123,123             | 0     |
| 48  | MG   | A1    | 3560 | 1/1   | 0.92 | 0.10 | 138,138,138,138             | 0     |
| 48  | MG   | A1    | 3490 | 1/1   | 0.92 | 0.10 | 105,105,105,105             | 0     |
| 48  | MG   | A1    | 3411 | 1/1   | 0.92 | 0.08 | 83,83,83,83                 | 0     |
| 48  | MG   | GP    | 201  | 1/1   | 0.92 | 0.11 | 109,109,109,109             | 0     |
| 48  | MG   | H1    | 3464 | 1/1   | 0.92 | 0.06 | 108,108,108,108             | 0     |
| 48  | MG   | CL    | 301  | 1/1   | 0.92 | 0.07 | 109,109,109,109             | 0     |
| 48  | MG   | A1    | 3528 | 1/1   | 0.92 | 0.13 | 120,120,120,120             | 0     |
| 48  | MG   | D1    | 3498 | 1/1   | 0.92 | 0.17 | 99,99,99,99                 | 0     |
| 48  | MG   | A1    | 3483 | 1/1   | 0.92 | 0.07 | 83,83,83,83                 | 0     |
| 48  | MG   | D1    | 3408 | 1/1   | 0.92 | 0.10 | 106,106,106,106             | 0     |
| 48  | MG   | H1    | 3405 | 1/1   | 0.92 | 0.07 | 101,101,101,101             | 0     |
| 48  | MG   | A1    | 3569 | 1/1   | 0.92 | 0.07 | 91,91,91,91                 | 0     |
| 48  | MG   | D1    | 3515 | 1/1   | 0.92 | 0.06 | 106,106,106,106             | 0     |
| 48  | MG   | H1    | 3478 | 1/1   | 0.92 | 0.06 | 114,114,114,114             | 0     |
| 48  | MG   | A1    | 3582 | 1/1   | 0.92 | 0.05 | 110,110,110,110             | 0     |
| 48  | MG   | F1    | 3579 | 1/1   | 0.92 | 0.12 | 166,166,166,166             | 0     |
| 48  | MG   | A1    | 3572 | 1/1   | 0.92 | 0.09 | 121,121,121,121             | 0     |
| 48  | MG   | F1    | 3583 | 1/1   | 0.92 | 0.07 | 104,104,104,104             | 0     |
| 48  | MG   | F1    | 3491 | 1/1   | 0.92 | 0.08 | 96,96,96,96                 | 0     |
| 48  | MG   | F1    | 3550 | 1/1   | 0.92 | 0.13 | 154,154,154,154             | 0     |
| 48  | MG   | H1    | 3545 | 1/1   | 0.92 | 0.10 | 156,156,156,156             | 0     |
| 48  | MG   | F1    | 3554 | 1/1   | 0.92 | 0.07 | 131,131,131,131             | 0     |
| 48  | MG   | BQ    | 201  | 1/1   | 0.92 | 0.09 | 122,122,122,122             | 0     |
| 48  | MG   | A1    | 3431 | 1/1   | 0.92 | 0.07 | 90,90,90,90                 | 0     |
| 48  | MG   | F1    | 3497 | 1/1   | 0.92 | 0.08 | 93,93,93,93                 | 0     |
| 48  | MG   | H1    | 3503 | 1/1   | 0.92 | 0.17 | 91,91,91,91                 | 0     |
| 48  | MG   | H1    | 3425 | 1/1   | 0.92 | 0.07 | 108,108,108,108             | 0     |
| 48  | MG   | A1    | 3487 | 1/1   | 0.92 | 0.11 | 121,121,121,121             | 0     |
| 48  | MG   | D1    | 3466 | 1/1   | 0.92 | 0.07 | 132,132,132,132             | 0     |
| 48  | MG   | H1    | 3512 | 1/1   | 0.92 | 0.09 | 121,121,121,121             | 0     |
| 48  | MG   | D1    | 3618 | 1/1   | 0.92 | 0.07 | 95,95,95,95                 | 0     |
| 48  | MG   | D1    | 3537 | 1/1   | 0.92 | 0.10 | 121,121,121,121             | 0     |
| 48  | MG   | D1    | 3451 | 1/1   | 0.93 | 0.08 | 115,115,115,115             | 0     |
| 48  | MG   | B3    | 202  | 1/1   | 0.93 | 0.07 | 113,113,113,113             | 0     |
| 48  | MG   | DK    | 201  | 1/1   | 0.93 | 0.07 | 101,101,101,101             | 0     |
| 48  | MG   | H1    | 3417 | 1/1   | 0.93 | 0.07 | 114,114,114,114             | 0     |
| 48  | MG   | A1    | 3500 | 1/1   | 0.93 | 0.13 | 89,89,89,89                 | 0     |
| 48  | MG   | D1    | 3595 | 1/1   | 0.93 | 0.10 | 94,94,94,94                 | 0     |
| 48  | MG   | F1    | 3532 | 1/1   | 0.93 | 0.11 | 87,87,87,87                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | H1    | 3423 | 1/1   | 0.93 | 0.09 | 98,98,98,98                 | 0     |
| 48  | MG   | A1    | 3590 | 1/1   | 0.93 | 0.11 | 142,142,142,142             | 0     |
| 48  | MG   | FA    | 101  | 1/1   | 0.93 | 0.06 | 97,97,97,97                 | 0     |
| 48  | MG   | D1    | 3541 | 1/1   | 0.93 | 0.15 | 114,114,114,114             | 0     |
| 48  | MG   | H1    | 3526 | 1/1   | 0.93 | 0.15 | 94,94,94,94                 | 0     |
| 48  | MG   | A1    | 3591 | 1/1   | 0.93 | 0.08 | 121,121,121,121             | 0     |
| 48  | MG   | A1    | 3503 | 1/1   | 0.93 | 0.07 | 95,95,95,95                 | 0     |
| 48  | MG   | D1    | 3600 | 1/1   | 0.93 | 0.08 | 123,123,123,123             | 0     |
| 48  | MG   | D1    | 3481 | 1/1   | 0.93 | 0.12 | 114,114,114,114             | 0     |
| 48  | MG   | A1    | 3562 | 1/1   | 0.93 | 0.07 | 91,91,91,91                 | 0     |
| 48  | MG   | H1    | 3454 | 1/1   | 0.93 | 0.07 | 111,111,111,111             | 0     |
| 48  | MG   | D1    | 3484 | 1/1   | 0.93 | 0.07 | 96,96,96,96                 | 0     |
| 48  | MG   | D1    | 3431 | 1/1   | 0.93 | 0.08 | 95,95,95,95                 | 0     |
| 48  | MG   | H1    | 3462 | 1/1   | 0.93 | 0.09 | 131,131,131,131             | 0     |
| 48  | MG   | EW    | 202  | 1/1   | 0.93 | 0.06 | 121,121,121,121             | 0     |
| 48  | MG   | A1    | 3563 | 1/1   | 0.93 | 0.07 | 100,100,100,100             | 0     |
| 48  | MG   | D1    | 3561 | 1/1   | 0.93 | 0.09 | 57,57,57,57                 | 0     |
| 48  | MG   | F1    | 3556 | 1/1   | 0.93 | 0.06 | 90,90,90,90                 | 0     |
| 48  | MG   | F1    | 3558 | 1/1   | 0.93 | 0.09 | 144,144,144,144             | 0     |
| 48  | MG   | A1    | 3415 | 1/1   | 0.93 | 0.09 | 120,120,120,120             | 0     |
| 48  | MG   | A1    | 3419 | 1/1   | 0.93 | 0.08 | 100,100,100,100             | 0     |
| 48  | MG   | A1    | 3455 | 1/1   | 0.93 | 0.07 | 111,111,111,111             | 0     |
| 48  | MG   | D1    | 3615 | 1/1   | 0.93 | 0.09 | 132,132,132,132             | 0     |
| 48  | MG   | A1    | 3468 | 1/1   | 0.93 | 0.11 | 109,109,109,109             | 0     |
| 48  | MG   | F1    | 3492 | 1/1   | 0.93 | 0.14 | 78,78,78,78                 | 0     |
| 48  | MG   | A1    | 3407 | 1/1   | 0.93 | 0.07 | 83,83,83,83                 | 0     |
| 48  | MG   | A1    | 3571 | 1/1   | 0.93 | 0.11 | 100,100,100,100             | 0     |
| 48  | MG   | D1    | 3619 | 1/1   | 0.93 | 0.07 | 101,101,101,101             | 0     |
| 48  | MG   | H1    | 3407 | 1/1   | 0.93 | 0.06 | 105,105,105,105             | 0     |
| 48  | MG   | A1    | 3496 | 1/1   | 0.93 | 0.10 | 137,137,137,137             | 0     |
| 48  | MG   | D1    | 3582 | 1/1   | 0.93 | 0.08 | 93,93,93,93                 | 0     |
| 48  | MG   | F1    | 3502 | 1/1   | 0.93 | 0.10 | 108,108,108,108             | 0     |
| 48  | MG   | A1    | 3443 | 1/1   | 0.93 | 0.07 | 90,90,90,90                 | 0     |
| 48  | MG   | A1    | 3499 | 1/1   | 0.93 | 0.06 | 117,117,117,117             | 0     |
| 48  | MG   | BP    | 200  | 1/1   | 0.94 | 0.06 | 123,123,123,123             | 0     |
| 48  | MG   | F1    | 3519 | 1/1   | 0.94 | 0.07 | 65,65,65,65                 | 0     |
| 48  | MG   | H1    | 3413 | 1/1   | 0.94 | 0.15 | 117,117,117,117             | 0     |
| 48  | MG   | A1    | 3512 | 1/1   | 0.94 | 0.07 | 90,90,90,90                 | 0     |
| 48  | MG   | D1    | 3419 | 1/1   | 0.94 | 0.07 | 92,92,92,92                 | 0     |
| 48  | MG   | A1    | 3493 | 1/1   | 0.94 | 0.09 | 113,113,113,113             | 0     |
| 48  | MG   | F1    | 3461 | 1/1   | 0.94 | 0.20 | 106,106,106,106             | 0     |
| 48  | MG   | H1    | 3505 | 1/1   | 0.94 | 0.06 | 95,95,95,95                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | D1    | 3511 | 1/1   | 0.94 | 0.09 | 118,118,118,118             | 0     |
| 48  | MG   | D1    | 3513 | 1/1   | 0.94 | 0.06 | 89,89,89,89                 | 0     |
| 48  | MG   | D1    | 3447 | 1/1   | 0.94 | 0.09 | 101,101,101,101             | 0     |
| 48  | MG   | A1    | 3467 | 1/1   | 0.94 | 0.07 | 106,106,106,106             | 0     |
| 48  | MG   | A1    | 3541 | 1/1   | 0.94 | 0.09 | 86,86,86,86                 | 0     |
| 48  | MG   | H1    | 3427 | 1/1   | 0.94 | 0.09 | 83,83,83,83                 | 0     |
| 48  | MG   | H1    | 3520 | 1/1   | 0.94 | 0.06 | 114,114,114,114             | 0     |
| 48  | MG   | A1    | 3544 | 1/1   | 0.94 | 0.14 | 135,135,135,135             | 0     |
| 48  | MG   | A1    | 3425 | 1/1   | 0.94 | 0.06 | 107,107,107,107             | 0     |
| 48  | MG   | H1    | 3434 | 1/1   | 0.94 | 0.08 | 93,93,93,93                 | 0     |
| 48  | MG   | A1    | 3548 | 1/1   | 0.94 | 0.07 | 124,124,124,124             | 0     |
| 48  | MG   | H1    | 3438 | 1/1   | 0.94 | 0.12 | 120,120,120,120             | 0     |
| 48  | MG   | F1    | 3407 | 1/1   | 0.94 | 0.07 | 111,111,111,111             | 0     |
| 48  | MG   | H1    | 3446 | 1/1   | 0.94 | 0.10 | 120,120,120,120             | 0     |
| 48  | MG   | A1    | 3519 | 1/1   | 0.94 | 0.05 | 113,113,113,113             | 0     |
| 48  | MG   | F1    | 3552 | 1/1   | 0.94 | 0.10 | 139,139,139,139             | 0     |
| 48  | MG   | D1    | 3527 | 1/1   | 0.94 | 0.12 | 106,106,106,106             | 0     |
| 48  | MG   | CQ    | 201  | 1/1   | 0.94 | 0.09 | 127,127,127,127             | 0     |
| 48  | MG   | H1    | 3455 | 1/1   | 0.94 | 0.06 | 113,113,113,113             | 0     |
| 48  | MG   | H1    | 3456 | 1/1   | 0.94 | 0.15 | 145,145,145,145             | 0     |
| 48  | MG   | D1    | 3585 | 1/1   | 0.94 | 0.06 | 108,108,108,108             | 0     |
| 48  | MG   | H1    | 3459 | 1/1   | 0.94 | 0.07 | 97,97,97,97                 | 0     |
| 48  | MG   | D1    | 3530 | 1/1   | 0.94 | 0.08 | 94,94,94,94                 | 0     |
| 48  | MG   | D1    | 3621 | 1/1   | 0.94 | 0.05 | 110,110,110,110             | 0     |
| 48  | MG   | D1    | 3532 | 1/1   | 0.94 | 0.06 | 119,119,119,119             | 0     |
| 48  | MG   | D1    | 3590 | 1/1   | 0.94 | 0.08 | 89,89,89,89                 | 0     |
| 48  | MG   | H1    | 3466 | 1/1   | 0.94 | 0.06 | 107,107,107,107             | 0     |
| 48  | MG   | H1    | 3467 | 1/1   | 0.94 | 0.07 | 95,95,95,95                 | 0     |
| 48  | MG   | CY    | 201  | 1/1   | 0.94 | 0.07 | 99,99,99,99                 | 0     |
| 48  | MG   | F1    | 3425 | 1/1   | 0.94 | 0.07 | 115,115,115,115             | 0     |
| 48  | MG   | A1    | 3461 | 1/1   | 0.94 | 0.06 | 67,67,67,67                 | 0     |
| 48  | MG   | H1    | 3471 | 1/1   | 0.94 | 0.09 | 124,124,124,124             | 0     |
| 48  | MG   | D1    | 3594 | 1/1   | 0.94 | 0.17 | 106,106,106,106             | 0     |
| 48  | MG   | H1    | 3403 | 1/1   | 0.94 | 0.07 | 111,111,111,111             | 0     |
| 48  | MG   | D1    | 3627 | 1/1   | 0.94 | 0.05 | 119,119,119,119             | 0     |
| 48  | MG   | F1    | 3433 | 1/1   | 0.94 | 0.15 | 95,95,95,95                 | 0     |
| 48  | MG   | F1    | 3568 | 1/1   | 0.94 | 0.07 | 98,98,98,98                 | 0     |
| 48  | MG   | A1    | 3509 | 1/1   | 0.94 | 0.05 | 128,128,128,128             | 0     |
| 48  | MG   | F1    | 3506 | 1/1   | 0.94 | 0.10 | 114,114,114,114             | 0     |
| 48  | MG   | A1    | 3492 | 1/1   | 0.94 | 0.09 | 127,127,127,127             | 0     |
| 48  | MG   | D1    | 3492 | 1/1   | 0.94 | 0.08 | 125,125,125,125             | 0     |
| 48  | MG   | CW    | 201  | 1/1   | 0.95 | 0.09 | 90,90,90,90                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | A1    | 3433 | 1/1   | 0.95 | 0.06 | 84,84,84,84                 | 0     |
| 48  | MG   | H1    | 3492 | 1/1   | 0.95 | 0.06 | 96,96,96,96                 | 0     |
| 48  | MG   | D1    | 3602 | 1/1   | 0.95 | 0.06 | 118,118,118,118             | 0     |
| 48  | MG   | A1    | 3566 | 1/1   | 0.95 | 0.08 | 75,75,75,75                 | 0     |
| 48  | MG   | F1    | 3530 | 1/1   | 0.95 | 0.07 | 107,107,107,107             | 0     |
| 48  | MG   | A1    | 3486 | 1/1   | 0.95 | 0.07 | 93,93,93,93                 | 0     |
| 48  | MG   | F1    | 3533 | 1/1   | 0.95 | 0.07 | 101,101,101,101             | 0     |
| 48  | MG   | F1    | 3534 | 1/1   | 0.95 | 0.06 | 79,79,79,79                 | 0     |
| 48  | MG   | D1    | 3518 | 1/1   | 0.95 | 0.08 | 92,92,92,92                 | 0     |
| 48  | MG   | D1    | 3573 | 1/1   | 0.95 | 0.07 | 126,126,126,126             | 0     |
| 48  | MG   | G2    | 203  | 1/1   | 0.95 | 0.05 | 112,112,112,112             | 0     |
| 48  | MG   | D1    | 3607 | 1/1   | 0.95 | 0.15 | 89,89,89,89                 | 0     |
| 48  | MG   | D1    | 3472 | 1/1   | 0.95 | 0.08 | 82,82,82,82                 | 0     |
| 48  | MG   | A1    | 3409 | 1/1   | 0.95 | 0.06 | 87,87,87,87                 | 0     |
| 48  | MG   | D1    | 3523 | 1/1   | 0.95 | 0.06 | 105,105,105,105             | 0     |
| 48  | MG   | F1    | 3471 | 1/1   | 0.95 | 0.09 | 90,90,90,90                 | 0     |
| 48  | MG   | H1    | 3451 | 1/1   | 0.95 | 0.06 | 78,78,78,78                 | 0     |
| 48  | MG   | F1    | 3472 | 1/1   | 0.95 | 0.05 | 111,111,111,111             | 0     |
| 48  | MG   | D1    | 3415 | 1/1   | 0.95 | 0.07 | 117,117,117,117             | 0     |
| 48  | MG   | D1    | 3614 | 1/1   | 0.95 | 0.06 | 129,129,129,129             | 0     |
| 48  | MG   | GL    | 301  | 1/1   | 0.95 | 0.06 | 113,113,113,113             | 0     |
| 48  | MG   | D1    | 3580 | 1/1   | 0.95 | 0.06 | 95,95,95,95                 | 0     |
| 48  | MG   | A1    | 3577 | 1/1   | 0.95 | 0.09 | 104,104,104,104             | 0     |
| 48  | MG   | C3    | 201  | 1/1   | 0.95 | 0.08 | 123,123,123,123             | 0     |
| 48  | MG   | D1    | 3485 | 1/1   | 0.95 | 0.06 | 120,120,120,120             | 0     |
| 48  | MG   | F1    | 3485 | 1/1   | 0.95 | 0.08 | 117,117,117,117             | 0     |
| 48  | MG   | F1    | 3418 | 1/1   | 0.95 | 0.10 | 126,126,126,126             | 0     |
| 48  | MG   | D1    | 3443 | 1/1   | 0.95 | 0.09 | 112,112,112,112             | 0     |
| 48  | MG   | D1    | 3620 | 1/1   | 0.95 | 0.10 | 106,106,106,106             | 0     |
| 48  | MG   | A1    | 3552 | 1/1   | 0.95 | 0.07 | 97,97,97,97                 | 0     |
| 48  | MG   | D1    | 3589 | 1/1   | 0.95 | 0.08 | 107,107,107,107             | 0     |
| 48  | MG   | F1    | 3494 | 1/1   | 0.95 | 0.08 | 97,97,97,97                 | 0     |
| 48  | MG   | D1    | 3494 | 1/1   | 0.95 | 0.07 | 78,78,78,78                 | 0     |
| 48  | MG   | D1    | 3496 | 1/1   | 0.95 | 0.07 | 78,78,78,78                 | 0     |
| 48  | MG   | C3    | 206  | 1/1   | 0.95 | 0.10 | 120,120,120,120             | 0     |
| 48  | MG   | A1    | 3518 | 1/1   | 0.95 | 0.06 | 109,109,109,109             | 0     |
| 48  | MG   | A1    | 3529 | 1/1   | 0.95 | 0.08 | 96,96,96,96                 | 0     |
| 48  | MG   | F1    | 3441 | 1/1   | 0.95 | 0.06 | 111,111,111,111             | 0     |
| 48  | MG   | H1    | 3480 | 1/1   | 0.95 | 0.10 | 81,81,81,81                 | 0     |
| 48  | MG   | D1    | 3549 | 1/1   | 0.95 | 0.07 | 99,99,99,99                 | 0     |
| 48  | MG   | F1    | 3508 | 1/1   | 0.95 | 0.06 | 127,127,127,127             | 0     |
| 48  | MG   | H1    | 3483 | 1/1   | 0.95 | 0.07 | 108,108,108,108             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | A1    | 3598 | 1/1   | 0.95 | 0.07 | 111,111,111,111             | 0     |
| 48  | MG   | H1    | 3485 | 1/1   | 0.95 | 0.06 | 104,104,104,104             | 0     |
| 48  | MG   | A1    | 3599 | 1/1   | 0.95 | 0.08 | 103,103,103,103             | 0     |
| 48  | MG   | D1    | 3452 | 1/1   | 0.95 | 0.10 | 106,106,106,106             | 0     |
| 48  | MG   | H1    | 3488 | 1/1   | 0.95 | 0.06 | 108,108,108,108             | 0     |
| 48  | MG   | D1    | 3542 | 1/1   | 0.96 | 0.04 | 71,71,71,71                 | 0     |
| 48  | MG   | F1    | 3581 | 1/1   | 0.96 | 0.07 | 144,144,144,144             | 0     |
| 48  | MG   | A1    | 3540 | 1/1   | 0.96 | 0.08 | 66,66,66,66                 | 0     |
| 48  | MG   | A1    | 3523 | 1/1   | 0.96 | 0.06 | 91,91,91,91                 | 0     |
| 48  | MG   | D1    | 3490 | 1/1   | 0.96 | 0.08 | 92,92,92,92                 | 0     |
| 48  | MG   | F1    | 3416 | 1/1   | 0.96 | 0.10 | 116,116,116,116             | 0     |
| 48  | MG   | D1    | 3436 | 1/1   | 0.96 | 0.05 | 78,78,78,78                 | 0     |
| 48  | MG   | A1    | 3557 | 1/1   | 0.96 | 0.08 | 104,104,104,104             | 0     |
| 48  | MG   | D1    | 3493 | 1/1   | 0.96 | 0.06 | 128,128,128,128             | 0     |
| 48  | MG   | F1    | 3420 | 1/1   | 0.96 | 0.07 | 88,88,88,88                 | 0     |
| 48  | MG   | A1    | 3558 | 1/1   | 0.96 | 0.06 | 91,91,91,91                 | 0     |
| 48  | MG   | F1    | 3512 | 1/1   | 0.96 | 0.05 | 94,94,94,94                 | 0     |
| 48  | MG   | F1    | 3513 | 1/1   | 0.96 | 0.07 | 79,79,79,79                 | 0     |
| 48  | MG   | D1    | 3610 | 1/1   | 0.96 | 0.06 | 66,66,66,66                 | 0     |
| 48  | MG   | F1    | 3516 | 1/1   | 0.96 | 0.05 | 121,121,121,121             | 0     |
| 48  | MG   | F1    | 3517 | 1/1   | 0.96 | 0.07 | 62,62,62,62                 | 0     |
| 48  | MG   | D1    | 3495 | 1/1   | 0.96 | 0.05 | 88,88,88,88                 | 0     |
| 48  | MG   | D1    | 3612 | 1/1   | 0.96 | 0.07 | 123,123,123,123             | 0     |
| 48  | MG   | F1    | 3526 | 1/1   | 0.96 | 0.06 | 72,72,72,72                 | 0     |
| 48  | MG   | D1    | 3440 | 1/1   | 0.96 | 0.05 | 99,99,99,99                 | 0     |
| 48  | MG   | A1    | 3542 | 1/1   | 0.96 | 0.07 | 96,96,96,96                 | 0     |
| 48  | MG   | D1    | 3563 | 1/1   | 0.96 | 0.07 | 93,93,93,93                 | 0     |
| 48  | MG   | GQ    | 201  | 1/1   | 0.96 | 0.08 | 102,102,102,102             | 0     |
| 48  | MG   | A1    | 3600 | 1/1   | 0.96 | 0.05 | 111,111,111,111             | 0     |
| 48  | MG   | F1    | 3437 | 1/1   | 0.96 | 0.09 | 100,100,100,100             | 0     |
| 48  | MG   | F1    | 3439 | 1/1   | 0.96 | 0.07 | 62,62,62,62                 | 0     |
| 48  | MG   | F1    | 3440 | 1/1   | 0.96 | 0.05 | 82,82,82,82                 | 0     |
| 48  | MG   | H1    | 3500 | 1/1   | 0.96 | 0.08 | 82,82,82,82                 | 0     |
| 48  | MG   | D1    | 3567 | 1/1   | 0.96 | 0.10 | 60,60,60,60                 | 0     |
| 48  | MG   | F1    | 3442 | 1/1   | 0.96 | 0.06 | 109,109,109,109             | 0     |
| 48  | MG   | D1    | 3414 | 1/1   | 0.96 | 0.08 | 96,96,96,96                 | 0     |
| 48  | MG   | D1    | 3572 | 1/1   | 0.96 | 0.10 | 69,69,69,69                 | 0     |
| 48  | MG   | C2    | 202  | 1/1   | 0.96 | 0.07 | 112,112,112,112             | 0     |
| 48  | MG   | F1    | 3543 | 1/1   | 0.96 | 0.08 | 71,71,71,71                 | 0     |
| 48  | MG   | F1    | 3544 | 1/1   | 0.96 | 0.07 | 97,97,97,97                 | 0     |
| 48  | MG   | H1    | 3513 | 1/1   | 0.96 | 0.06 | 87,87,87,87                 | 0     |
| 48  | MG   | D1    | 3510 | 1/1   | 0.96 | 0.06 | 81,81,81,81                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | H1    | 3517 | 1/1   | 0.96 | 0.07 | 79,79,79,79                 | 0     |
| 48  | MG   | A1    | 3484 | 1/1   | 0.96 | 0.07 | 108,108,108,108             | 0     |
| 48  | MG   | A1    | 3469 | 1/1   | 0.96 | 0.06 | 113,113,113,113             | 0     |
| 48  | MG   | D1    | 3418 | 1/1   | 0.96 | 0.04 | 114,114,114,114             | 0     |
| 48  | MG   | F1    | 3551 | 1/1   | 0.96 | 0.08 | 91,91,91,91                 | 0     |
| 48  | MG   | F1    | 3458 | 1/1   | 0.96 | 0.05 | 95,95,95,95                 | 0     |
| 48  | MG   | F1    | 3553 | 1/1   | 0.96 | 0.06 | 68,68,68,68                 | 0     |
| 48  | MG   | A1    | 3498 | 1/1   | 0.96 | 0.04 | 116,116,116,116             | 0     |
| 48  | MG   | D1    | 3581 | 1/1   | 0.96 | 0.06 | 68,68,68,68                 | 0     |
| 48  | MG   | C3    | 202  | 1/1   | 0.96 | 0.05 | 135,135,135,135             | 0     |
| 48  | MG   | D1    | 3628 | 1/1   | 0.96 | 0.05 | 107,107,107,107             | 0     |
| 48  | MG   | D1    | 3629 | 1/1   | 0.96 | 0.07 | 121,121,121,121             | 0     |
| 48  | MG   | H1    | 3426 | 1/1   | 0.96 | 0.07 | 105,105,105,105             | 0     |
| 48  | MG   | D1    | 3454 | 1/1   | 0.96 | 0.11 | 64,64,64,64                 | 0     |
| 48  | MG   | H1    | 3428 | 1/1   | 0.96 | 0.11 | 77,77,77,77                 | 0     |
| 48  | MG   | H1    | 3429 | 1/1   | 0.96 | 0.07 | 87,87,87,87                 | 0     |
| 48  | MG   | H1    | 3430 | 1/1   | 0.96 | 0.07 | 82,82,82,82                 | 0     |
| 48  | MG   | D1    | 3461 | 1/1   | 0.96 | 0.05 | 86,86,86,86                 | 0     |
| 48  | MG   | D1    | 3462 | 1/1   | 0.96 | 0.10 | 116,116,116,116             | 0     |
| 48  | MG   | C3    | 204  | 1/1   | 0.96 | 0.05 | 85,85,85,85                 | 0     |
| 48  | MG   | B2    | 204  | 1/1   | 0.96 | 0.06 | 85,85,85,85                 | 0     |
| 48  | MG   | A1    | 3479 | 1/1   | 0.96 | 0.09 | 120,120,120,120             | 0     |
| 48  | MG   | H1    | 3441 | 1/1   | 0.96 | 0.05 | 102,102,102,102             | 0     |
| 48  | MG   | D1    | 3468 | 1/1   | 0.96 | 0.05 | 75,75,75,75                 | 0     |
| 48  | MG   | E3    | 203  | 1/1   | 0.96 | 0.07 | 104,104,104,104             | 0     |
| 48  | MG   | H1    | 3447 | 1/1   | 0.96 | 0.06 | 110,110,110,110             | 0     |
| 48  | MG   | A1    | 3429 | 1/1   | 0.96 | 0.04 | 122,122,122,122             | 0     |
| 48  | MG   | F1    | 3479 | 1/1   | 0.96 | 0.15 | 81,81,81,81                 | 0     |
| 48  | MG   | CD    | 201  | 1/1   | 0.96 | 0.10 | 93,93,93,93                 | 0     |
| 48  | MG   | D1    | 3531 | 1/1   | 0.96 | 0.05 | 87,87,87,87                 | 0     |
| 48  | MG   | D1    | 3429 | 1/1   | 0.96 | 0.08 | 113,113,113,113             | 0     |
| 48  | MG   | D1    | 3534 | 1/1   | 0.96 | 0.09 | 98,98,98,98                 | 0     |
| 48  | MG   | D1    | 3476 | 1/1   | 0.96 | 0.06 | 43,43,43,43                 | 0     |
| 48  | MG   | D1    | 3538 | 1/1   | 0.96 | 0.07 | 119,119,119,119             | 0     |
| 48  | MG   | A1    | 3533 | 1/1   | 0.96 | 0.12 | 73,73,73,73                 | 0     |
| 48  | MG   | F1    | 3403 | 1/1   | 0.96 | 0.04 | 96,96,96,96                 | 0     |
| 48  | MG   | A1    | 3494 | 1/1   | 0.96 | 0.07 | 98,98,98,98                 | 0     |
| 49  | ZN   | AC    | 201  | 1/1   | 0.96 | 0.06 | 143,143,143,143             | 0     |
| 48  | MG   | A1    | 3480 | 1/1   | 0.97 | 0.09 | 120,120,120,120             | 0     |
| 48  | MG   | D1    | 3420 | 1/1   | 0.97 | 0.05 | 105,105,105,105             | 0     |
| 48  | MG   | D1    | 3504 | 1/1   | 0.97 | 0.10 | 98,98,98,98                 | 0     |
| 48  | MG   | A1    | 3481 | 1/1   | 0.97 | 0.07 | 88,88,88,88                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | EJ    | 201  | 1/1   | 0.97 | 0.06 | 69,69,69,69                 | 0     |
| 48  | MG   | F1    | 3547 | 1/1   | 0.97 | 0.04 | 112,112,112,112             | 0     |
| 48  | MG   | EL    | 301  | 1/1   | 0.97 | 0.03 | 119,119,119,119             | 0     |
| 48  | MG   | D1    | 3552 | 1/1   | 0.97 | 0.06 | 55,55,55,55                 | 0     |
| 48  | MG   | D1    | 3553 | 1/1   | 0.97 | 0.05 | 90,90,90,90                 | 0     |
| 48  | MG   | EQ    | 201  | 1/1   | 0.97 | 0.08 | 88,88,88,88                 | 0     |
| 48  | MG   | D1    | 3508 | 1/1   | 0.97 | 0.05 | 86,86,86,86                 | 0     |
| 48  | MG   | D1    | 3556 | 1/1   | 0.97 | 0.06 | 76,76,76,76                 | 0     |
| 48  | MG   | D1    | 3455 | 1/1   | 0.97 | 0.04 | 80,80,80,80                 | 0     |
| 48  | MG   | D1    | 3558 | 1/1   | 0.97 | 0.05 | 56,56,56,56                 | 0     |
| 48  | MG   | H1    | 3491 | 1/1   | 0.97 | 0.06 | 111,111,111,111             | 0     |
| 48  | MG   | F1    | 3405 | 1/1   | 0.97 | 0.05 | 79,79,79,79                 | 0     |
| 48  | MG   | F1    | 3557 | 1/1   | 0.97 | 0.05 | 84,84,84,84                 | 0     |
| 48  | MG   | H1    | 3499 | 1/1   | 0.97 | 0.06 | 75,75,75,75                 | 0     |
| 48  | MG   | D1    | 3560 | 1/1   | 0.97 | 0.06 | 64,64,64,64                 | 0     |
| 48  | MG   | D1    | 3456 | 1/1   | 0.97 | 0.06 | 70,70,70,70                 | 0     |
| 48  | MG   | D1    | 3512 | 1/1   | 0.97 | 0.05 | 101,101,101,101             | 0     |
| 48  | MG   | H1    | 3504 | 1/1   | 0.97 | 0.05 | 111,111,111,111             | 0     |
| 48  | MG   | F1    | 3489 | 1/1   | 0.97 | 0.04 | 85,85,85,85                 | 0     |
| 48  | MG   | H1    | 3508 | 1/1   | 0.97 | 0.07 | 80,80,80,80                 | 0     |
| 48  | MG   | D1    | 3458 | 1/1   | 0.97 | 0.05 | 51,51,51,51                 | 0     |
| 48  | MG   | D1    | 3564 | 1/1   | 0.97 | 0.12 | 92,92,92,92                 | 0     |
| 48  | MG   | A1    | 3549 | 1/1   | 0.97 | 0.06 | 54,54,54,54                 | 0     |
| 48  | MG   | A1    | 3550 | 1/1   | 0.97 | 0.05 | 69,69,69,69                 | 0     |
| 48  | MG   | H1    | 3424 | 1/1   | 0.97 | 0.03 | 96,96,96,96                 | 0     |
| 48  | MG   | A1    | 3521 | 1/1   | 0.97 | 0.06 | 105,105,105,105             | 0     |
| 48  | MG   | F1    | 3495 | 1/1   | 0.97 | 0.05 | 83,83,83,83                 | 0     |
| 48  | MG   | H1    | 3518 | 1/1   | 0.97 | 0.07 | 110,110,110,110             | 0     |
| 48  | MG   | A1    | 3459 | 1/1   | 0.97 | 0.07 | 90,90,90,90                 | 0     |
| 48  | MG   | A1    | 3404 | 1/1   | 0.97 | 0.04 | 94,94,94,94                 | 0     |
| 48  | MG   | A1    | 3501 | 1/1   | 0.97 | 0.08 | 102,102,102,102             | 0     |
| 48  | MG   | H1    | 3522 | 1/1   | 0.97 | 0.07 | 107,107,107,107             | 0     |
| 48  | MG   | F1    | 3500 | 1/1   | 0.97 | 0.08 | 105,105,105,105             | 0     |
| 48  | MG   | A1    | 3413 | 1/1   | 0.97 | 0.07 | 136,136,136,136             | 0     |
| 48  | MG   | F1    | 3573 | 1/1   | 0.97 | 0.07 | 84,84,84,84                 | 0     |
| 48  | MG   | A1    | 3439 | 1/1   | 0.97 | 0.04 | 106,106,106,106             | 0     |
| 48  | MG   | H1    | 3435 | 1/1   | 0.97 | 0.05 | 116,116,116,116             | 0     |
| 48  | MG   | A1    | 3445 | 1/1   | 0.97 | 0.08 | 88,88,88,88                 | 0     |
| 48  | MG   | F1    | 3504 | 1/1   | 0.97 | 0.06 | 84,84,84,84                 | 0     |
| 48  | MG   | A1    | 3488 | 1/1   | 0.97 | 0.05 | 91,91,91,91                 | 0     |
| 48  | MG   | A1    | 3559 | 1/1   | 0.97 | 0.04 | 89,89,89,89                 | 0     |
| 48  | MG   | A1    | 3532 | 1/1   | 0.97 | 0.05 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | A1    | 3447 | 1/1   | 0.97 | 0.08 | 58,58,58,58                 | 0     |
| 48  | MG   | F1    | 3434 | 1/1   | 0.97 | 0.04 | 83,83,83,83                 | 0     |
| 48  | MG   | D1    | 3584 | 1/1   | 0.97 | 0.06 | 101,101,101,101             | 0     |
| 48  | MG   | F1    | 3584 | 1/1   | 0.97 | 0.06 | 97,97,97,97                 | 0     |
| 48  | MG   | F1    | 3514 | 1/1   | 0.97 | 0.06 | 70,70,70,70                 | 0     |
| 48  | MG   | FA    | 102  | 1/1   | 0.97 | 0.06 | 84,84,84,84                 | 0     |
| 48  | MG   | F1    | 3438 | 1/1   | 0.97 | 0.05 | 58,58,58,58                 | 0     |
| 48  | MG   | D1    | 3406 | 1/1   | 0.97 | 0.06 | 67,67,67,67                 | 0     |
| 48  | MG   | D1    | 3441 | 1/1   | 0.97 | 0.07 | 75,75,75,75                 | 0     |
| 48  | MG   | D1    | 3535 | 1/1   | 0.97 | 0.06 | 86,86,86,86                 | 0     |
| 48  | MG   | A1    | 3535 | 1/1   | 0.97 | 0.05 | 99,99,99,99                 | 0     |
| 48  | MG   | D1    | 3631 | 1/1   | 0.97 | 0.05 | 78,78,78,78                 | 0     |
| 48  | MG   | F1    | 3445 | 1/1   | 0.97 | 0.08 | 78,78,78,78                 | 0     |
| 48  | MG   | D1    | 3632 | 1/1   | 0.97 | 0.04 | 83,83,83,83                 | 0     |
| 48  | MG   | A1    | 3471 | 1/1   | 0.97 | 0.04 | 88,88,88,88                 | 0     |
| 48  | MG   | F1    | 3531 | 1/1   | 0.97 | 0.04 | 95,95,95,95                 | 0     |
| 48  | MG   | D1    | 3591 | 1/1   | 0.97 | 0.05 | 55,55,55,55                 | 0     |
| 48  | MG   | DQ    | 201  | 1/1   | 0.97 | 0.05 | 118,118,118,118             | 0     |
| 48  | MG   | A1    | 3448 | 1/1   | 0.97 | 0.05 | 78,78,78,78                 | 0     |
| 48  | MG   | A1    | 3474 | 1/1   | 0.97 | 0.07 | 88,88,88,88                 | 0     |
| 48  | MG   | A1    | 3477 | 1/1   | 0.97 | 0.06 | 62,62,62,62                 | 0     |
| 48  | MG   | A1    | 3458 | 1/1   | 0.97 | 0.06 | 59,59,59,59                 | 0     |
| 48  | MG   | A1    | 3545 | 1/1   | 0.97 | 0.09 | 71,71,71,71                 | 0     |
| 48  | MG   | H1    | 3475 | 1/1   | 0.97 | 0.07 | 70,70,70,70                 | 0     |
| 49  | ZN   | HC    | 201  | 1/1   | 0.97 | 0.04 | 168,168,168,168             | 0     |
| 48  | MG   | D1    | 3505 | 1/1   | 0.98 | 0.04 | 84,84,84,84                 | 0     |
| 48  | MG   | D1    | 3453 | 1/1   | 0.98 | 0.05 | 54,54,54,54                 | 0     |
| 48  | MG   | H1    | 3463 | 1/1   | 0.98 | 0.05 | 78,78,78,78                 | 0     |
| 48  | MG   | D1    | 3507 | 1/1   | 0.98 | 0.07 | 75,75,75,75                 | 0     |
| 48  | MG   | A1    | 3482 | 1/1   | 0.98 | 0.05 | 62,62,62,62                 | 0     |
| 48  | MG   | F1    | 3582 | 1/1   | 0.98 | 0.06 | 77,77,77,77                 | 0     |
| 48  | MG   | AA    | 102  | 1/1   | 0.98 | 0.04 | 98,98,98,98                 | 0     |
| 48  | MG   | C3    | 203  | 1/1   | 0.98 | 0.06 | 69,69,69,69                 | 0     |
| 48  | MG   | A1    | 3506 | 1/1   | 0.98 | 0.08 | 77,77,77,77                 | 0     |
| 48  | MG   | D1    | 3460 | 1/1   | 0.98 | 0.05 | 85,85,85,85                 | 0     |
| 48  | MG   | D1    | 3568 | 1/1   | 0.98 | 0.07 | 105,105,105,105             | 0     |
| 48  | MG   | A1    | 3524 | 1/1   | 0.98 | 0.05 | 63,63,63,63                 | 0     |
| 48  | MG   | F1    | 3507 | 1/1   | 0.98 | 0.04 | 87,87,87,87                 | 0     |
| 48  | MG   | F1    | 3423 | 1/1   | 0.98 | 0.04 | 56,56,56,56                 | 0     |
| 48  | MG   | A1    | 3440 | 1/1   | 0.98 | 0.04 | 78,78,78,78                 | 0     |
| 48  | MG   | A1    | 3508 | 1/1   | 0.98 | 0.04 | 89,89,89,89                 | 0     |
| 48  | MG   | F1    | 3426 | 1/1   | 0.98 | 0.06 | 110,110,110,110             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | B2    | 205  | 1/1   | 0.98 | 0.04 | 81,81,81,81                 | 0     |
| 48  | MG   | F1    | 3429 | 1/1   | 0.98 | 0.07 | 73,73,73,73                 | 0     |
| 48  | MG   | D1    | 3428 | 1/1   | 0.98 | 0.03 | 106,106,106,106             | 0     |
| 48  | MG   | D1    | 3519 | 1/1   | 0.98 | 0.03 | 72,72,72,72                 | 0     |
| 48  | MG   | D1    | 3577 | 1/1   | 0.98 | 0.04 | 121,121,121,121             | 0     |
| 48  | MG   | F1    | 3518 | 1/1   | 0.98 | 0.08 | 77,77,77,77                 | 0     |
| 48  | MG   | GJ    | 201  | 1/1   | 0.98 | 0.06 | 69,69,69,69                 | 0     |
| 48  | MG   | D1    | 3578 | 1/1   | 0.98 | 0.03 | 88,88,88,88                 | 0     |
| 48  | MG   | F1    | 3520 | 1/1   | 0.98 | 0.06 | 85,85,85,85                 | 0     |
| 48  | MG   | F1    | 3436 | 1/1   | 0.98 | 0.04 | 70,70,70,70                 | 0     |
| 48  | MG   | F1    | 3524 | 1/1   | 0.98 | 0.06 | 56,56,56,56                 | 0     |
| 48  | MG   | F1    | 3525 | 1/1   | 0.98 | 0.04 | 73,73,73,73                 | 0     |
| 48  | MG   | CJ    | 201  | 1/1   | 0.98 | 0.04 | 64,64,64,64                 | 0     |
| 48  | MG   | D1    | 3469 | 1/1   | 0.98 | 0.05 | 64,64,64,64                 | 0     |
| 48  | MG   | A1    | 3446 | 1/1   | 0.98 | 0.04 | 64,64,64,64                 | 0     |
| 48  | MG   | D1    | 3524 | 1/1   | 0.98 | 0.04 | 69,69,69,69                 | 0     |
| 48  | MG   | D1    | 3471 | 1/1   | 0.98 | 0.09 | 40,40,40,40                 | 0     |
| 48  | MG   | A1    | 3434 | 1/1   | 0.98 | 0.06 | 74,74,74,74                 | 0     |
| 48  | MG   | H1    | 3502 | 1/1   | 0.98 | 0.05 | 82,82,82,82                 | 0     |
| 48  | MG   | DA    | 101  | 1/1   | 0.98 | 0.04 | 82,82,82,82                 | 0     |
| 48  | MG   | DA    | 102  | 1/1   | 0.98 | 0.06 | 115,115,115,115             | 0     |
| 48  | MG   | F1    | 3536 | 1/1   | 0.98 | 0.05 | 67,67,67,67                 | 0     |
| 48  | MG   | H1    | 3507 | 1/1   | 0.98 | 0.05 | 64,64,64,64                 | 0     |
| 48  | MG   | D1    | 3474 | 1/1   | 0.98 | 0.06 | 58,58,58,58                 | 0     |
| 48  | MG   | A1    | 3511 | 1/1   | 0.98 | 0.04 | 90,90,90,90                 | 0     |
| 48  | MG   | D1    | 3587 | 1/1   | 0.98 | 0.07 | 93,93,93,93                 | 0     |
| 48  | MG   | F1    | 3449 | 1/1   | 0.98 | 0.05 | 90,90,90,90                 | 0     |
| 48  | MG   | A1    | 3462 | 1/1   | 0.98 | 0.05 | 46,46,46,46                 | 0     |
| 48  | MG   | F1    | 3452 | 1/1   | 0.98 | 0.05 | 50,50,50,50                 | 0     |
| 48  | MG   | D1    | 3477 | 1/1   | 0.98 | 0.04 | 60,60,60,60                 | 0     |
| 48  | MG   | E2    | 203  | 1/1   | 0.98 | 0.05 | 77,77,77,77                 | 0     |
| 48  | MG   | D1    | 3478 | 1/1   | 0.98 | 0.04 | 81,81,81,81                 | 0     |
| 48  | MG   | D1    | 3435 | 1/1   | 0.98 | 0.04 | 108,108,108,108             | 0     |
| 48  | MG   | A1    | 3466 | 1/1   | 0.98 | 0.03 | 40,40,40,40                 | 0     |
| 48  | MG   | H1    | 3419 | 1/1   | 0.98 | 0.06 | 62,62,62,62                 | 0     |
| 48  | MG   | E3    | 201  | 1/1   | 0.98 | 0.05 | 90,90,90,90                 | 0     |
| 48  | MG   | H1    | 3421 | 1/1   | 0.98 | 0.06 | 97,97,97,97                 | 0     |
| 48  | MG   | E3    | 202  | 1/1   | 0.98 | 0.05 | 122,122,122,122             | 0     |
| 48  | MG   | D1    | 3483 | 1/1   | 0.98 | 0.05 | 88,88,88,88                 | 0     |
| 48  | MG   | A1    | 3534 | 1/1   | 0.98 | 0.05 | 62,62,62,62                 | 0     |
| 48  | MG   | H1    | 3527 | 1/1   | 0.98 | 0.04 | 99,99,99,99                 | 0     |
| 48  | MG   | D1    | 3403 | 1/1   | 0.98 | 0.05 | 89,89,89,89                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | D1    | 3487 | 1/1   | 0.98 | 0.04 | 65,65,65,65                 | 0     |
| 48  | MG   | BJ    | 201  | 1/1   | 0.98 | 0.06 | 66,66,66,66                 | 0     |
| 48  | MG   | D1    | 3545 | 1/1   | 0.98 | 0.06 | 88,88,88,88                 | 0     |
| 48  | MG   | EL    | 302  | 1/1   | 0.98 | 0.05 | 68,68,68,68                 | 0     |
| 48  | MG   | F1    | 3474 | 1/1   | 0.98 | 0.12 | 64,64,64,64                 | 0     |
| 48  | MG   | D1    | 3407 | 1/1   | 0.98 | 0.03 | 70,70,70,70                 | 0     |
| 48  | MG   | H1    | 3432 | 1/1   | 0.98 | 0.04 | 91,91,91,91                 | 0     |
| 48  | MG   | A1    | 3514 | 1/1   | 0.98 | 0.06 | 59,59,59,59                 | 0     |
| 48  | MG   | D1    | 3409 | 1/1   | 0.98 | 0.07 | 57,57,57,57                 | 0     |
| 48  | MG   | A1    | 3478 | 1/1   | 0.98 | 0.06 | 79,79,79,79                 | 0     |
| 48  | MG   | F1    | 3480 | 1/1   | 0.98 | 0.05 | 59,59,59,59                 | 0     |
| 48  | MG   | H1    | 3437 | 1/1   | 0.98 | 0.04 | 93,93,93,93                 | 0     |
| 48  | MG   | F1    | 3481 | 1/1   | 0.98 | 0.08 | 45,45,45,45                 | 0     |
| 48  | MG   | H1    | 3439 | 1/1   | 0.98 | 0.08 | 75,75,75,75                 | 0     |
| 48  | MG   | D1    | 3413 | 1/1   | 0.98 | 0.05 | 51,51,51,51                 | 0     |
| 48  | MG   | H1    | 3442 | 1/1   | 0.98 | 0.06 | 79,79,79,79                 | 0     |
| 48  | MG   | A1    | 3405 | 1/1   | 0.98 | 0.07 | 65,65,65,65                 | 0     |
| 48  | MG   | F1    | 3484 | 1/1   | 0.98 | 0.04 | 78,78,78,78                 | 0     |
| 48  | MG   | F1    | 3402 | 1/1   | 0.98 | 0.04 | 83,83,83,83                 | 0     |
| 48  | MG   | F1    | 3486 | 1/1   | 0.98 | 0.06 | 90,90,90,90                 | 0     |
| 48  | MG   | F1    | 3487 | 1/1   | 0.98 | 0.04 | 60,60,60,60                 | 0     |
| 48  | MG   | A1    | 3502 | 1/1   | 0.98 | 0.06 | 80,80,80,80                 | 0     |
| 48  | MG   | F1    | 3404 | 1/1   | 0.98 | 0.05 | 75,75,75,75                 | 0     |
| 48  | MG   | H1    | 3452 | 1/1   | 0.98 | 0.06 | 108,108,108,108             | 0     |
| 48  | MG   | A1    | 3597 | 1/1   | 0.98 | 0.05 | 133,133,133,133             | 0     |
| 48  | MG   | F1    | 3406 | 1/1   | 0.98 | 0.04 | 83,83,83,83                 | 0     |
| 48  | MG   | A1    | 3418 | 1/1   | 0.98 | 0.04 | 117,117,117,117             | 0     |
| 48  | MG   | F1    | 3408 | 1/1   | 0.98 | 0.09 | 82,82,82,82                 | 0     |
| 48  | MG   | A1    | 3457 | 1/1   | 0.98 | 0.11 | 94,94,94,94                 | 0     |
| 49  | ZN   | FA    | 103  | 1/1   | 0.98 | 0.05 | 80,80,80,80                 | 0     |
| 48  | MG   | H1    | 3460 | 1/1   | 0.98 | 0.06 | 69,69,69,69                 | 0     |
| 48  | MG   | D1    | 3536 | 1/1   | 0.99 | 0.04 | 73,73,73,73                 | 0     |
| 48  | MG   | F1    | 3412 | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |
| 48  | MG   | AA    | 103  | 1/1   | 0.99 | 0.03 | 56,56,56,56                 | 0     |
| 48  | MG   | D1    | 3430 | 1/1   | 0.99 | 0.02 | 59,59,59,59                 | 0     |
| 48  | MG   | D1    | 3539 | 1/1   | 0.99 | 0.04 | 57,57,57,57                 | 0     |
| 48  | MG   | A1    | 3442 | 1/1   | 0.99 | 0.03 | 52,52,52,52                 | 0     |
| 48  | MG   | D1    | 3480 | 1/1   | 0.99 | 0.04 | 32,32,32,32                 | 0     |
| 48  | MG   | A1    | 3473 | 1/1   | 0.99 | 0.03 | 55,55,55,55                 | 0     |
| 48  | MG   | A1    | 3463 | 1/1   | 0.99 | 0.06 | 59,59,59,59                 | 0     |
| 48  | MG   | D1    | 3544 | 1/1   | 0.99 | 0.04 | 50,50,50,50                 | 0     |
| 48  | MG   | B2    | 203  | 1/1   | 0.99 | 0.03 | 81,81,81,81                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | F1    | 3505 | 1/1   | 0.99 | 0.04 | 83,83,83,83                 | 0     |
| 48  | MG   | CL    | 302  | 1/1   | 0.99 | 0.06 | 68,68,68,68                 | 0     |
| 48  | MG   | A1    | 3517 | 1/1   | 0.99 | 0.05 | 74,74,74,74                 | 0     |
| 48  | MG   | D1    | 3486 | 1/1   | 0.99 | 0.08 | 47,47,47,47                 | 0     |
| 48  | MG   | H1    | 3476 | 1/1   | 0.99 | 0.03 | 52,52,52,52                 | 0     |
| 48  | MG   | A1    | 3475 | 1/1   | 0.99 | 0.04 | 80,80,80,80                 | 0     |
| 48  | MG   | F1    | 3510 | 1/1   | 0.99 | 0.04 | 95,95,95,95                 | 0     |
| 48  | MG   | D1    | 3488 | 1/1   | 0.99 | 0.03 | 97,97,97,97                 | 0     |
| 48  | MG   | G3    | 203  | 1/1   | 0.99 | 0.06 | 86,86,86,86                 | 0     |
| 48  | MG   | F1    | 3427 | 1/1   | 0.99 | 0.03 | 51,51,51,51                 | 0     |
| 48  | MG   | D1    | 3489 | 1/1   | 0.99 | 0.04 | 44,44,44,44                 | 0     |
| 48  | MG   | D1    | 3438 | 1/1   | 0.99 | 0.07 | 39,39,39,39                 | 0     |
| 48  | MG   | D1    | 3554 | 1/1   | 0.99 | 0.04 | 59,59,59,59                 | 0     |
| 48  | MG   | CQ    | 202  | 1/1   | 0.99 | 0.03 | 62,62,62,62                 | 0     |
| 48  | MG   | A1    | 3537 | 1/1   | 0.99 | 0.06 | 54,54,54,54                 | 0     |
| 48  | MG   | A1    | 3538 | 1/1   | 0.99 | 0.04 | 49,49,49,49                 | 0     |
| 48  | MG   | F1    | 3435 | 1/1   | 0.99 | 0.04 | 44,44,44,44                 | 0     |
| 48  | MG   | A1    | 3561 | 1/1   | 0.99 | 0.05 | 60,60,60,60                 | 0     |
| 48  | MG   | F1    | 3521 | 1/1   | 0.99 | 0.05 | 65,65,65,65                 | 0     |
| 48  | MG   | D1    | 3559 | 1/1   | 0.99 | 0.05 | 55,55,55,55                 | 0     |
| 48  | MG   | D1    | 3402 | 1/1   | 0.99 | 0.03 | 52,52,52,52                 | 0     |
| 48  | MG   | H1    | 3493 | 1/1   | 0.99 | 0.04 | 79,79,79,79                 | 0     |
| 48  | MG   | H1    | 3494 | 1/1   | 0.99 | 0.06 | 56,56,56,56                 | 0     |
| 48  | MG   | H1    | 3495 | 1/1   | 0.99 | 0.03 | 65,65,65,65                 | 0     |
| 48  | MG   | A1    | 3539 | 1/1   | 0.99 | 0.03 | 46,46,46,46                 | 0     |
| 48  | MG   | H1    | 3497 | 1/1   | 0.99 | 0.04 | 50,50,50,50                 | 0     |
| 48  | MG   | H1    | 3498 | 1/1   | 0.99 | 0.03 | 60,60,60,60                 | 0     |
| 48  | MG   | D1    | 3404 | 1/1   | 0.99 | 0.04 | 55,55,55,55                 | 0     |
| 48  | MG   | D1    | 3405 | 1/1   | 0.99 | 0.03 | 59,59,59,59                 | 0     |
| 48  | MG   | F1    | 3528 | 1/1   | 0.99 | 0.04 | 75,75,75,75                 | 0     |
| 48  | MG   | A1    | 3476 | 1/1   | 0.99 | 0.03 | 59,59,59,59                 | 0     |
| 48  | MG   | F1    | 3443 | 1/1   | 0.99 | 0.06 | 104,104,104,104             | 0     |
| 48  | MG   | D1    | 3500 | 1/1   | 0.99 | 0.08 | 44,44,44,44                 | 0     |
| 48  | MG   | D1    | 3630 | 1/1   | 0.99 | 0.05 | 71,71,71,71                 | 0     |
| 48  | MG   | H1    | 3506 | 1/1   | 0.99 | 0.05 | 75,75,75,75                 | 0     |
| 48  | MG   | D1    | 3566 | 1/1   | 0.99 | 0.03 | 80,80,80,80                 | 0     |
| 48  | MG   | D1    | 3501 | 1/1   | 0.99 | 0.04 | 51,51,51,51                 | 0     |
| 48  | MG   | F1    | 3535 | 1/1   | 0.99 | 0.07 | 58,58,58,58                 | 0     |
| 48  | MG   | D1    | 3502 | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 48  | MG   | D1    | 3569 | 1/1   | 0.99 | 0.03 | 48,48,48,48                 | 0     |
| 48  | MG   | D1    | 3570 | 1/1   | 0.99 | 0.09 | 54,54,54,54                 | 0     |
| 48  | MG   | D1    | 3503 | 1/1   | 0.99 | 0.04 | 82,82,82,82                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | H1    | 3514 | 1/1   | 0.99 | 0.04 | 66,66,66,66                 | 0     |
| 48  | MG   | H1    | 3515 | 1/1   | 0.99 | 0.07 | 73,73,73,73                 | 0     |
| 48  | MG   | A1    | 3520 | 1/1   | 0.99 | 0.04 | 70,70,70,70                 | 0     |
| 48  | MG   | F1    | 3454 | 1/1   | 0.99 | 0.03 | 56,56,56,56                 | 0     |
| 48  | MG   | F1    | 3455 | 1/1   | 0.99 | 0.06 | 65,65,65,65                 | 0     |
| 48  | MG   | F1    | 3456 | 1/1   | 0.99 | 0.04 | 62,62,62,62                 | 0     |
| 48  | MG   | D1    | 3449 | 1/1   | 0.99 | 0.03 | 68,68,68,68                 | 0     |
| 48  | MG   | A1    | 3464 | 1/1   | 0.99 | 0.04 | 64,64,64,64                 | 0     |
| 48  | MG   | F1    | 3546 | 1/1   | 0.99 | 0.04 | 59,59,59,59                 | 0     |
| 48  | MG   | F1    | 3459 | 1/1   | 0.99 | 0.06 | 79,79,79,79                 | 0     |
| 48  | MG   | BL    | 301  | 1/1   | 0.99 | 0.04 | 71,71,71,71                 | 0     |
| 48  | MG   | E2    | 204  | 1/1   | 0.99 | 0.03 | 75,75,75,75                 | 0     |
| 48  | MG   | D1    | 3411 | 1/1   | 0.99 | 0.04 | 44,44,44,44                 | 0     |
| 48  | MG   | A1    | 3543 | 1/1   | 0.99 | 0.10 | 96,96,96,96                 | 0     |
| 48  | MG   | A1    | 3465 | 1/1   | 0.99 | 0.04 | 54,54,54,54                 | 0     |
| 48  | MG   | A1    | 3456 | 1/1   | 0.99 | 0.04 | 49,49,49,49                 | 0     |
| 48  | MG   | D1    | 3457 | 1/1   | 0.99 | 0.05 | 34,34,34,34                 | 0     |
| 48  | MG   | BQ    | 202  | 1/1   | 0.99 | 0.03 | 53,53,53,53                 | 0     |
| 48  | MG   | F1    | 3470 | 1/1   | 0.99 | 0.04 | 49,49,49,49                 | 0     |
| 48  | MG   | D1    | 3459 | 1/1   | 0.99 | 0.04 | 63,63,63,63                 | 0     |
| 48  | MG   | BW    | 201  | 1/1   | 0.99 | 0.05 | 67,67,67,67                 | 0     |
| 48  | MG   | A1    | 3546 | 1/1   | 0.99 | 0.09 | 51,51,51,51                 | 0     |
| 48  | MG   | A1    | 3570 | 1/1   | 0.99 | 0.05 | 70,70,70,70                 | 0     |
| 48  | MG   | C2    | 203  | 1/1   | 0.99 | 0.03 | 63,63,63,63                 | 0     |
| 48  | MG   | D1    | 3520 | 1/1   | 0.99 | 0.03 | 93,93,93,93                 | 0     |
| 48  | MG   | H1    | 3440 | 1/1   | 0.99 | 0.03 | 73,73,73,73                 | 0     |
| 48  | MG   | D1    | 3464 | 1/1   | 0.99 | 0.04 | 44,44,44,44                 | 0     |
| 48  | MG   | F1    | 3478 | 1/1   | 0.99 | 0.05 | 73,73,73,73                 | 0     |
| 48  | MG   | D1    | 3465 | 1/1   | 0.99 | 0.05 | 65,65,65,65                 | 0     |
| 48  | MG   | H1    | 3444 | 1/1   | 0.99 | 0.04 | 65,65,65,65                 | 0     |
| 48  | MG   | H1    | 3445 | 1/1   | 0.99 | 0.04 | 68,68,68,68                 | 0     |
| 48  | MG   | C2    | 204  | 1/1   | 0.99 | 0.03 | 75,75,75,75                 | 0     |
| 48  | MG   | A1    | 3426 | 1/1   | 0.99 | 0.04 | 73,73,73,73                 | 0     |
| 48  | MG   | A1    | 3526 | 1/1   | 0.99 | 0.04 | 48,48,48,48                 | 0     |
| 48  | MG   | D1    | 3423 | 1/1   | 0.99 | 0.05 | 67,67,67,67                 | 0     |
| 48  | MG   | A1    | 3495 | 1/1   | 0.99 | 0.03 | 70,70,70,70                 | 0     |
| 48  | MG   | D1    | 3529 | 1/1   | 0.99 | 0.05 | 80,80,80,80                 | 0     |
| 48  | MG   | A1    | 3452 | 1/1   | 0.99 | 0.06 | 90,90,90,90                 | 0     |
| 48  | MG   | H1    | 3453 | 1/1   | 0.99 | 0.05 | 66,66,66,66                 | 0     |
| 48  | MG   | A1    | 3406 | 1/1   | 0.99 | 0.04 | 75,75,75,75                 | 0     |
| 48  | MG   | D1    | 3473 | 1/1   | 0.99 | 0.03 | 63,63,63,63                 | 0     |
| 48  | MG   | A1    | 3460 | 1/1   | 0.99 | 0.04 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 48  | MG   | A1    | 3421 | 1/1   | 0.99 | 0.03 | 71,71,71,71                 | 0     |
| 49  | ZN   | AA    | 101  | 1/1   | 0.99 | 0.05 | 64,64,64,64                 | 0     |
| 48  | MG   | H1    | 3458 | 1/1   | 0.99 | 0.04 | 90,90,90,90                 | 0     |
| 49  | ZN   | AK    | 201  | 1/1   | 0.99 | 0.03 | 89,89,89,89                 | 0     |
| 49  | ZN   | DL    | 201  | 1/1   | 0.99 | 0.04 | 86,86,86,86                 | 0     |
| 49  | ZN   | EY    | 201  | 1/1   | 0.99 | 0.02 | 77,77,77,77                 | 0     |
| 48  | MG   | F1    | 3409 | 1/1   | 0.99 | 0.04 | 60,60,60,60                 | 0     |
| 49  | ZN   | FC    | 201  | 1/1   | 0.99 | 0.03 | 108,108,108,108             | 0     |
| 49  | ZN   | FL    | 201  | 1/1   | 0.99 | 0.04 | 86,86,86,86                 | 0     |
| 49  | ZN   | GY    | 201  | 1/1   | 0.99 | 0.04 | 116,116,116,116             | 0     |
| 49  | ZN   | HA    | 101  | 1/1   | 0.99 | 0.05 | 112,112,112,112             | 0     |
| 48  | MG   | F1    | 3410 | 1/1   | 0.99 | 0.04 | 42,42,42,42                 | 0     |
| 49  | ZN   | HL    | 201  | 1/1   | 0.99 | 0.02 | 118,118,118,118             | 0     |
| 48  | MG   | F1    | 3460 | 1/1   | 1.00 | 0.02 | 36,36,36,36                 | 0     |
| 48  | MG   | F1    | 3523 | 1/1   | 1.00 | 0.04 | 55,55,55,55                 | 0     |
| 48  | MG   | D1    | 3410 | 1/1   | 1.00 | 0.01 | 39,39,39,39                 | 0     |
| 48  | MG   | A1    | 3525 | 1/1   | 1.00 | 0.03 | 51,51,51,51                 | 0     |
| 48  | MG   | A1    | 3489 | 1/1   | 1.00 | 0.02 | 33,33,33,33                 | 0     |
| 48  | MG   | F1    | 3450 | 1/1   | 1.00 | 0.02 | 59,59,59,59                 | 0     |
| 48  | MG   | A1    | 3410 | 1/1   | 1.00 | 0.04 | 62,62,62,62                 | 0     |
| 48  | MG   | D1    | 3479 | 1/1   | 1.00 | 0.02 | 50,50,50,50                 | 0     |
| 49  | ZN   | AL    | 201  | 1/1   | 1.00 | 0.01 | 70,70,70,70                 | 0     |
| 49  | ZN   | BY    | 201  | 1/1   | 1.00 | 0.02 | 59,59,59,59                 | 0     |
| 49  | ZN   | CY    | 202  | 1/1   | 1.00 | 0.02 | 70,70,70,70                 | 0     |
| 49  | ZN   | DA    | 103  | 1/1   | 1.00 | 0.05 | 69,69,69,69                 | 0     |
| 49  | ZN   | DC    | 201  | 1/1   | 1.00 | 0.05 | 89,89,89,89                 | 0     |
| 49  | ZN   | DK    | 202  | 1/1   | 1.00 | 0.02 | 68,68,68,68                 | 0     |
| 48  | MG   | F1    | 3467 | 1/1   | 1.00 | 0.04 | 57,57,57,57                 | 0     |
| 48  | MG   | D1    | 3533 | 1/1   | 1.00 | 0.02 | 41,41,41,41                 | 0     |
| 48  | MG   | F1    | 3499 | 1/1   | 1.00 | 0.02 | 57,57,57,57                 | 0     |
| 48  | MG   | A1    | 3432 | 1/1   | 1.00 | 0.03 | 45,45,45,45                 | 0     |
| 49  | ZN   | FK    | 202  | 1/1   | 1.00 | 0.04 | 74,74,74,74                 | 0     |
| 48  | MG   | D1    | 3509 | 1/1   | 1.00 | 0.03 | 41,41,41,41                 | 0     |
| 48  | MG   | D1    | 3546 | 1/1   | 1.00 | 0.03 | 49,49,49,49                 | 0     |
| 48  | MG   | F1    | 3432 | 1/1   | 1.00 | 0.02 | 68,68,68,68                 | 0     |
| 48  | MG   | D1    | 3526 | 1/1   | 1.00 | 0.03 | 54,54,54,54                 | 0     |
| 49  | ZN   | HK    | 201  | 1/1   | 1.00 | 0.03 | 70,70,70,70                 | 0     |
| 48  | MG   | D1    | 3450 | 1/1   | 1.00 | 0.02 | 49,49,49,49                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.