



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 05:33 AM EDT

PDB ID : 6BZ6 / pdb\_00006bz6  
Title : Thermus thermophilus 70S complex containing 16S G347U ram mutation and empty A site  
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.  
Deposited on : 2017-12-22  
Resolution : 3.18 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                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

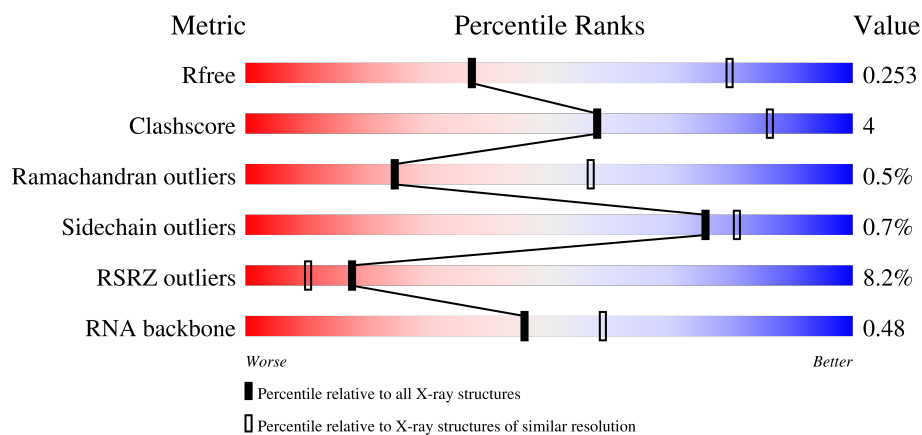
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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                      | 2001 (3.20-3.16)                                      |
| Clashscore            | 190562                      | 2119 (3.20-3.16)                                      |
| Ramachandran outliers | 187476                      | 2070 (3.20-3.16)                                      |
| Sidechain outliers    | 187428                      | 2069 (3.20-3.16)                                      |
| RSRZ outliers         | 180081                      | 2001 (3.20-3.16)                                      |
| RNA backbone          | 3983                        | 1138 (3.46-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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   | QA    | 1508   | <div> <div>9%</div> <div>65% 29% 5%</div> </div> |
| 1   | XA    | 1508   | <div> <div>6%</div> <div>67% 27% 5%</div> </div> |
| 2   | QB    | 256    | <div> <div>9%</div> <div>76% 15% 8%</div> </div> |
| 2   | XB    | 256    | <div> <div>6%</div> <div>80% 12% 8%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | QC    | 239    |                  |
| 3   | XC    | 239    |                  |
| 4   | QD    | 209    |                  |
| 4   | XD    | 209    |                  |
| 5   | QE    | 162    |                  |
| 5   | XE    | 162    |                  |
| 6   | QF    | 101    |                  |
| 6   | XF    | 101    |                  |
| 7   | QG    | 156    |                  |
| 7   | XG    | 156    |                  |
| 8   | QH    | 138    |                  |
| 8   | XH    | 138    |                  |
| 9   | QI    | 128    |                  |
| 9   | XI    | 128    |                  |
| 10  | QJ    | 105    |                  |
| 10  | XJ    | 105    |                  |
| 11  | QK    | 129    |                  |
| 11  | XK    | 129    |                  |
| 12  | QL    | 132    |                  |
| 12  | XL    | 132    |                  |
| 13  | QM    | 126    |                  |
| 13  | XM    | 126    |                  |
| 14  | QN    | 61     |                  |
| 14  | XN    | 61     |                  |
| 15  | QO    | 89     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | XO    | 89     |                  |
| 16  | QP    | 88     |                  |
| 16  | XP    | 88     |                  |
| 17  | QQ    | 105    |                  |
| 17  | XQ    | 105    |                  |
| 18  | QR    | 88     |                  |
| 18  | XR    | 88     |                  |
| 19  | QS    | 93     |                  |
| 19  | XS    | 93     |                  |
| 20  | QT    | 106    |                  |
| 20  | XT    | 106    |                  |
| 21  | QU    | 27     |                  |
| 21  | XU    | 27     |                  |
| 22  | QV    | 77     |                  |
| 22  | XV    | 77     |                  |
| 23  | QX    | 25     |                  |
| 23  | XX    | 25     |                  |
| 24  | RA    | 2915   |                  |
| 24  | YA    | 2915   |                  |
| 25  | RB    | 122    |                  |
| 25  | YB    | 122    |                  |
| 26  | RD    | 276    |                  |
| 26  | YD    | 276    |                  |
| 27  | RE    | 206    |                  |
| 27  | YE    | 206    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | RF    | 210    |                  |
| 28  | YF    | 210    |                  |
| 29  | RG    | 182    |                  |
| 29  | YG    | 182    |                  |
| 30  | RH    | 180    |                  |
| 30  | YH    | 180    |                  |
| 31  | RI    | 148    |                  |
| 31  | YI    | 148    |                  |
| 32  | RN    | 140    |                  |
| 32  | YN    | 140    |                  |
| 33  | RO    | 122    |                  |
| 33  | YO    | 122    |                  |
| 34  | RP    | 150    |                  |
| 34  | YP    | 150    |                  |
| 35  | RQ    | 141    |                  |
| 35  | YQ    | 141    |                  |
| 36  | RR    | 118    |                  |
| 36  | YR    | 118    |                  |
| 37  | RS    | 112    |                  |
| 37  | YS    | 112    |                  |
| 38  | RT    | 146    |                  |
| 38  | YT    | 146    |                  |
| 39  | RU    | 118    |                  |
| 39  | YU    | 118    |                  |
| 40  | RV    | 101    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | YV    | 101    |                  |
| 41  | RW    | 113    |                  |
| 41  | YW    | 113    |                  |
| 42  | RX    | 96     |                  |
| 42  | YX    | 96     |                  |
| 43  | RY    | 110    |                  |
| 43  | YY    | 110    |                  |
| 44  | RZ    | 206    |                  |
| 44  | YZ    | 206    |                  |
| 45  | R0    | 85     |                  |
| 45  | Y0    | 85     |                  |
| 46  | R1    | 98     |                  |
| 46  | Y1    | 98     |                  |
| 47  | R2    | 72     |                  |
| 47  | Y2    | 72     |                  |
| 48  | R3    | 60     |                  |
| 48  | Y3    | 60     |                  |
| 49  | R4    | 71     |                  |
| 49  | Y4    | 71     |                  |
| 50  | R5    | 60     |                  |
| 50  | Y5    | 60     |                  |
| 51  | R6    | 54     |                  |
| 51  | Y6    | 54     |                  |
| 52  | R7    | 49     |                  |
| 52  | Y7    | 49     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | R8    | 65     |                  |
| 53  | Y8    | 65     |                  |
| 54  | R9    | 37     |                  |
| 54  | Y9    | 37     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55  | MG   | RA    | 3003 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3012 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3013 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3030 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3031 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3044 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3049 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3050 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3053 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3061 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3087 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3094 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3212 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3407 | -         | -        | -       | X                |
| 55  | MG   | RA    | 3498 | -         | -        | -       | X                |
| 55  | MG   | Y8    | 101  | -         | -        | -       | X                |
| 55  | MG   | YA    | 3018 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3022 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3027 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3028 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3033 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3044 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3045 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3050 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3051 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3052 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3055 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3056 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3061 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3062 | -         | -        | -       | X                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 55  | MG   | YA    | 3063 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3065 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3088 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3114 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3118 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3134 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3137 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3140 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3184 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3186 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3209 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3234 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3280 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3291 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3534 | -         | -        | -       | X                |
| 55  | MG   | YA    | 3538 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 291753 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | QA    | 1498     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32202 | 14333 | 5970 | 10402 | 1497 |         |         |       |
| 1   | XA    | 1500     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32246 | 14353 | 5981 | 10413 | 1499 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference   |
|-------|---------|----------|--------|---------------------|-------------|
| QA    | 347     | U        | G      | engineered mutation | GB 55771382 |
| XA    | 347     | U        | G      | engineered mutation | GB 55771382 |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | QB    | 235      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1907  | 1217 | 342 | 343 | 5 |         |         |       |
| 2   | XB    | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1915  | 1223 | 343 | 344 | 5 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | QC    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1011 | 313 | 280 | 1 |         |         |       |
| 3   | XC    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1011 | 313 | 280 | 1 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | QD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | XD    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1703  | 1066 | 339 | 291 | 7 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | QE    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |
| 5   | XE    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1155  | 729 | 218 | 204 | 4 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | QF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |
| 6   | XF    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 843   | 531 | 155 | 154 | 3 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | QG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |
| 7   | XG    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1257  | 781 | 252 | 218 | 6 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | QH    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1108  | 700 | 214 | 192 | 2 |         |         |       |
| 8   | XH    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1108  | 700 | 214 | 192 | 2 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 9   | QI    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 1010  | 639 | 197 | 174 |         |         |       |
| 9   | XI    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 998   | 633 | 193 | 172 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | QJ    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 801   | 504 | 157 | 139 | 1 |         |         |       |
| 10  | XJ    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 777   | 487 | 153 | 136 | 1 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | QK    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 885   | 549 | 168 | 165 | 3 |         |         |       |
| 11  | XK    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 864   | 537 | 164 | 160 | 3 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | QL    | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 975   | 614 | 196 | 164 | 1 |         |         |       |
| 12  | XL    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 956   | 603 | 193 | 159 | 1 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | QM    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 591 | 197 | 165 | 2 |         |         |       |
| 13  | XM    | 119      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 946   | 585 | 195 | 164 | 2 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 14  | QN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 14  | XN    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | QO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 734   | 459 | 147 | 126 | 2 |         |         |       |
| 15  | XO    | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 729   | 457 | 146 | 124 | 2 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | QP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |
| 16  | XP    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 446 | 140 | 118 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | QQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |
| 17  | XQ    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 534 | 155 | 143 | 2 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|---------|-------|
| 18  | QR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |
| 18  | XR    | 70       | Total | C   | N   | O  | 0       | 0       | 0     |
|     |       |          | 574   | 367 | 112 | 95 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | QS    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 424 | 124 | 115 | 2 |         |         |       |
| 19  | XS    | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 674   | 430 | 126 | 116 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | QT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | XT    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 470 | 162 | 129 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 21  | QU    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |
| 21  | XU    | 25       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 217   | 134 | 52 | 31 |         |         |       |

- Molecule 22 is a RNA chain called tRNA fMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 22  | QV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1644  | 732 | 297 | 538 | 77 |         |         |       |
| 22  | XV    | 77       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1644  | 732 | 297 | 538 | 77 |         |         |       |

- Molecule 23 is a RNA chain called messenger RNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 23  | QX    | 12       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 259   | 116 | 48 | 83 | 12 |         |         |       |
| 23  | XX    | 11       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 239   | 107 | 46 | 75 | 11 |         |         |       |

- Molecule 24 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 24  | RA    | 2882     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62071 | 27627 | 11611 | 19952 | 2881 |         |         |       |
| 24  | YA    | 2883     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62091 | 27636 | 11613 | 19960 | 2882 |         |         |       |

- Molecule 25 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 25  | RB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |
| 25  | YB    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 26  | RD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |
| 26  | YD    | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | RE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |
| 27  | YE    | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 28  | RF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |
| 28  | YF    | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | RG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |
| 29  | YG    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | RH    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1336  | 848 | 251 | 236 | 1 |         |         |       |
| 30  | YH    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1336  | 848 | 251 | 236 | 1 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | RI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |
| 31  | YI    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | RN    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |
| 32  | YN    | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | RO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |
| 33  | YO    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | RP    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |
| 34  | YP    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 698 | 229 | 192 | 3 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | RQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 35  | YQ    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36  | RR    | 117      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36  | YR    | 117      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 960   | 599 | 202 | 159 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 37  | RS    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |
| 37  | YS    | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | RT    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |
| 38  | YT    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | RU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |
| 39  | YU    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | RV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |
| 40  | YV    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | RW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |
| 41  | YW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42  | RX    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |
| 42  | YX    | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

- Molecule 43 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | RY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 818   | 525 | 155 | 132 | 6 |         |         |       |
| 43  | YY    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 818   | 525 | 155 | 132 | 6 |         |         |       |

- Molecule 44 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | RZ    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1461  | 933 | 260 | 265 | 3 |         |         |       |
| 44  | YZ    | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1461  | 933 | 260 | 265 | 3 |         |         |       |

- Molecule 45 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45  | R0    | 81       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 643   | 398 | 137 | 107 | 1 |         |         |       |
| 45  | Y0    | 75       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 599   | 370 | 127 | 101 | 1 |         |         |       |

- Molecule 46 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | R1    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |
| 46  | Y1    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 729   | 457 | 145 | 126 | 1 |         |         |       |

- Molecule 47 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | R2    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |
| 47  | Y2    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |

- Molecule 48 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48  | R3    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |   |         |         |       |
| 48  | Y3    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |   |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 49  | R4    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 565   | 356 | 103 | 101 | 5 |         |         |       |
| 49  | Y4    | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 565   | 356 | 103 | 101 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | R5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 50  | Y5    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 51  | R6    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |
| 51  | Y6    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 52  | R7    | 47       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 409   | 251 | 102 | 54 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 52  | Y7    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

- Molecule 53 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 53  | R8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |
| 53  | Y8    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

- Molecule 54 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 54  | R9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 54  | Y9    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 55  | QA    | 80       | Total | Mg  | 0       | 0       |
|     |       |          | 80    | 80  |         |         |
| 55  | QC    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 55  | QF    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 55  | QH    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 55  | QT    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 55  | QV    | 6        | Total | Mg  | 0       | 0       |
|     |       |          | 6     | 6   |         |         |
| 55  | RA    | 521      | Total | Mg  | 0       | 0       |
|     |       |          | 521   | 521 |         |         |
| 55  | RB    | 11       | Total | Mg  | 0       | 0       |
|     |       |          | 11    | 11  |         |         |
| 55  | RD    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 55  | RE    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |

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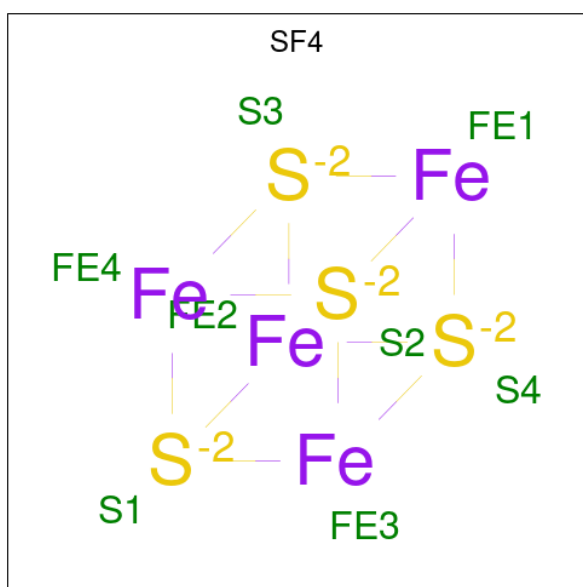
| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 55  | RN    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | RO    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | RP    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 55  | RQ    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 55  | RR    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | RT    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | R0    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | R8    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | XA    | 98       | Total<br>98  | Mg<br>98  | 0       | 0       |
| 55  | XE    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | XL    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | XM    | 2        | Total<br>2   | Mg<br>2   | 0       | 0       |
| 55  | XQ    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | XS    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | XV    | 8        | Total<br>8   | Mg<br>8   | 0       | 0       |
| 55  | XX    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 55  | YA    | 551      | Total<br>551 | Mg<br>551 | 0       | 0       |
| 55  | YB    | 12       | Total<br>12  | Mg<br>12  | 0       | 0       |
| 55  | YD    | 3        | Total<br>3   | Mg<br>3   | 0       | 0       |
| 55  | YE    | 4        | Total<br>4   | Mg<br>4   | 0       | 0       |
| 55  | YF    | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 55  | YO    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 55  | YP    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 55  | YQ    | 4        | Total<br>4 | Mg<br>4 | 0       | 0       |
| 55  | YU    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 55  | YX    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 55  | YY    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 55  | Y0    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |
| 55  | Y1    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 55  | Y5    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 55  | Y7    | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 55  | Y8    | 2        | Total<br>2 | Mg<br>2 | 0       | 0       |

- Molecule 56 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 56  | QD    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 56  | XD    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

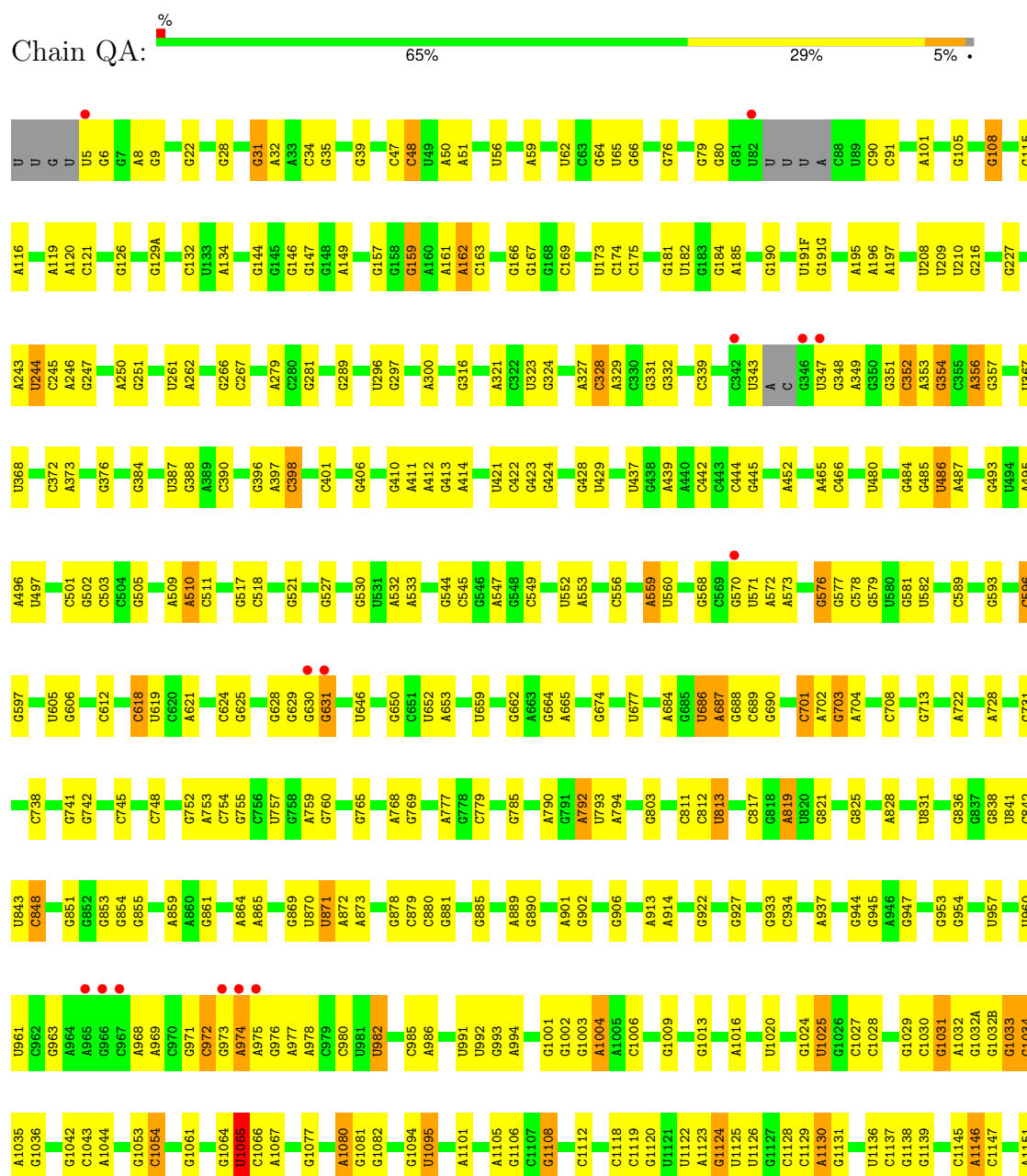
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 57  | QN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | RY    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | R4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | R5    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | R6    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | R9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | XN    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | YY    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | Y4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | Y5    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | Y6    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 57  | Y9    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

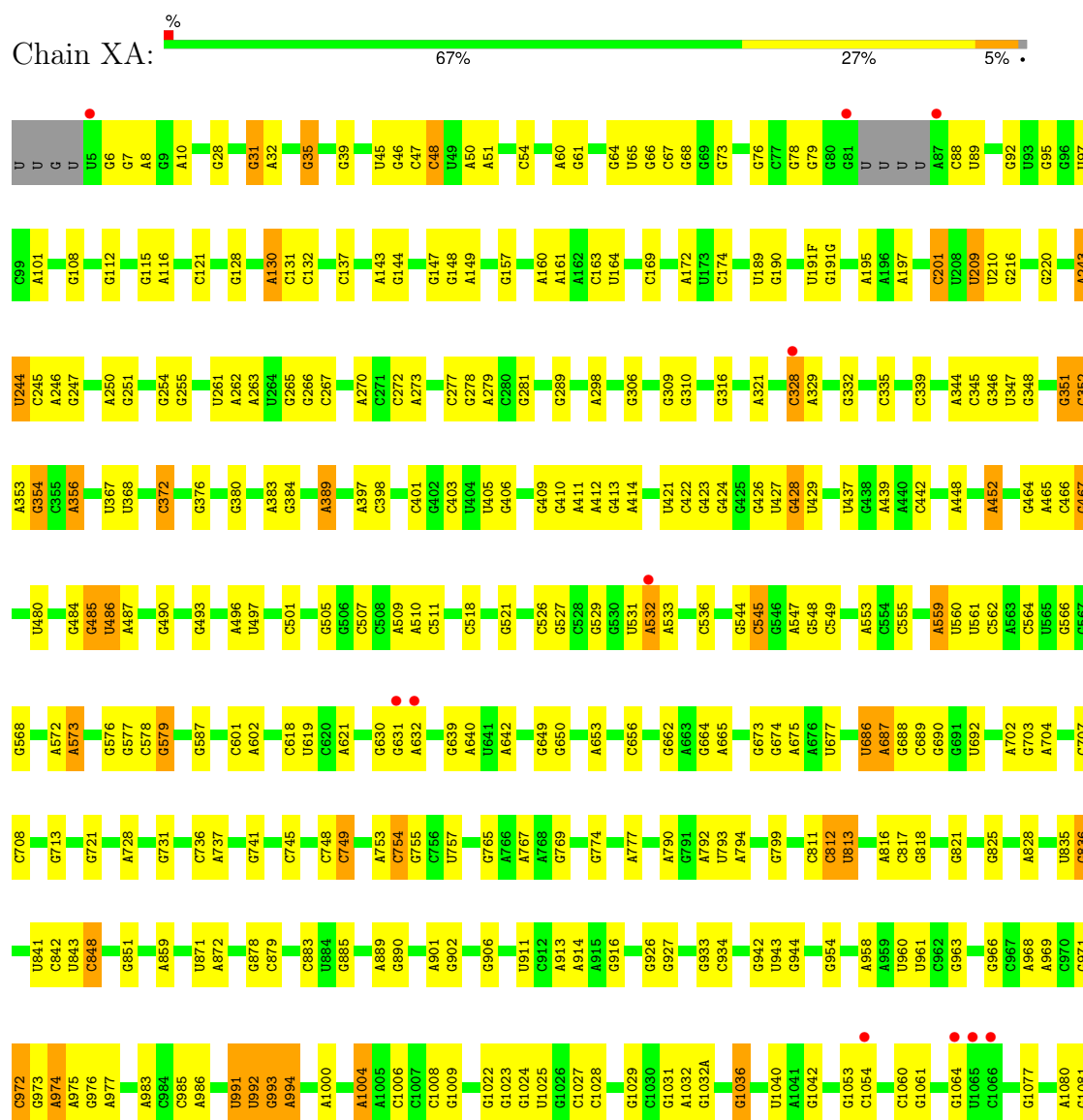
### 3 Residue-property plots

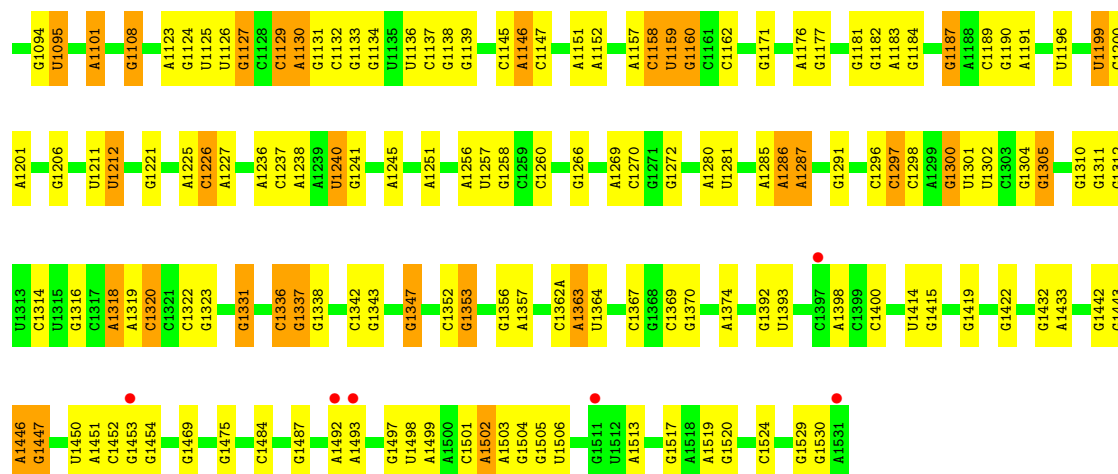
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 16S rRNA

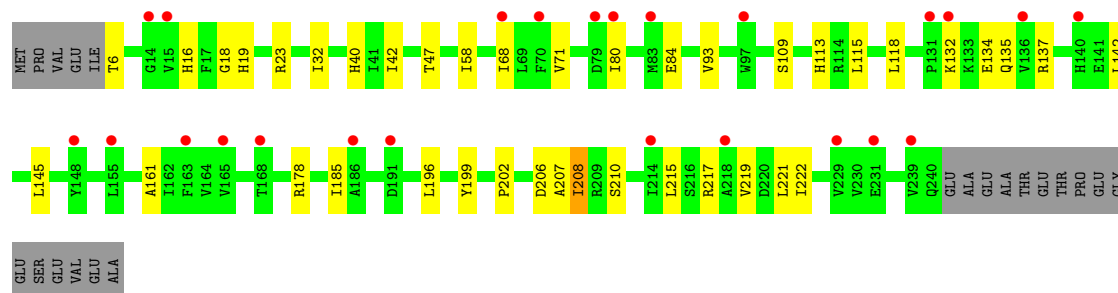
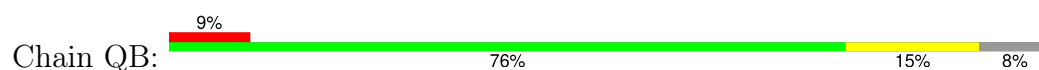


- Molecule 1: 16S rRNA

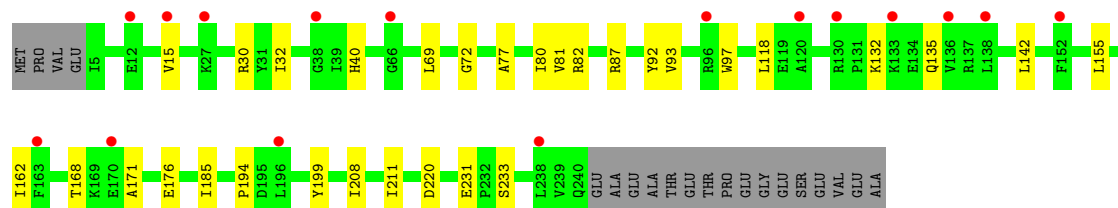
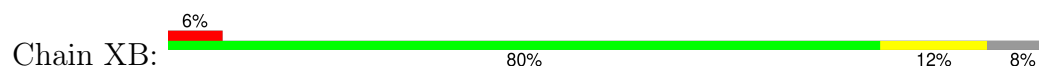




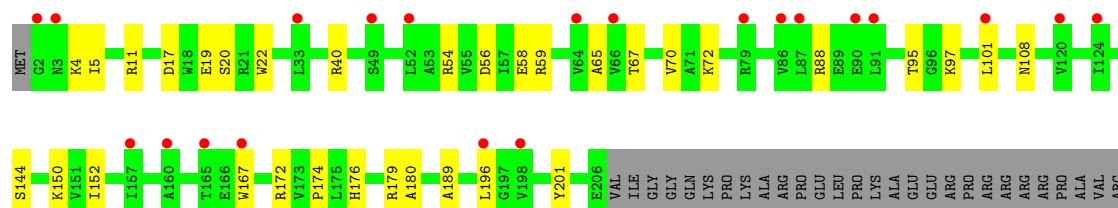
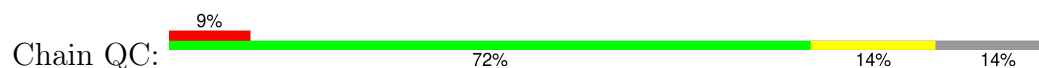
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2



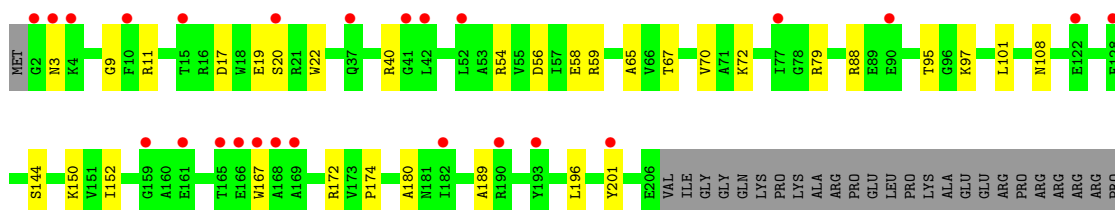
• Molecule 3: 30S ribosomal protein S3



VAL  
LYS  
LYS  
GLU  
GLU

• Molecule 3: 30S ribosomal protein S3

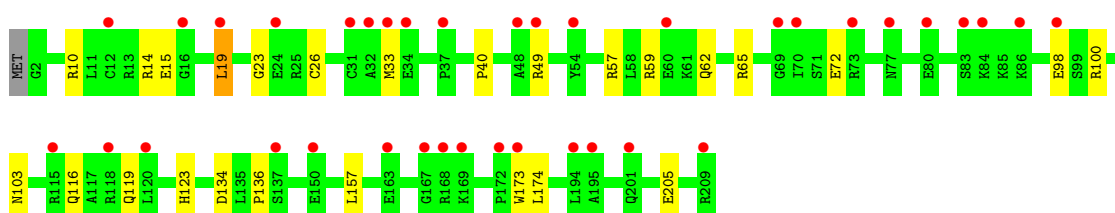
Chain XC: 



ALA  
VAL  
ARG  
VAL  
LYS  
LYS  
GLU  
GLU

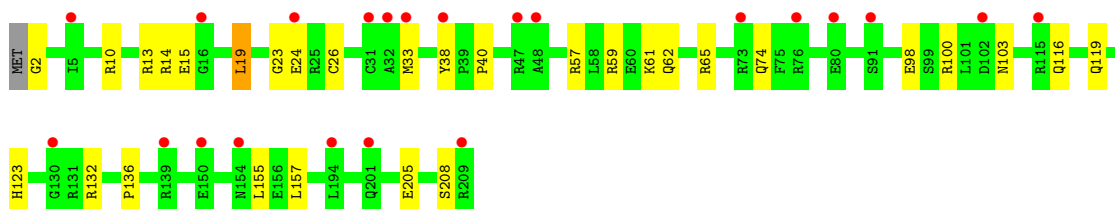
• Molecule 4: 30S ribosomal protein S4

Chain QD: 



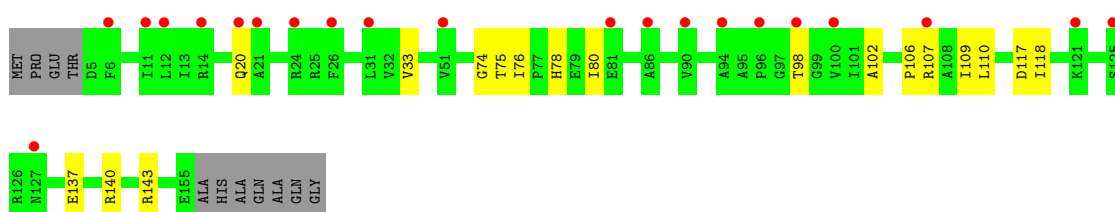
• Molecule 4: 30S ribosomal protein S4

Chain XD: 

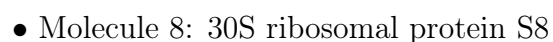


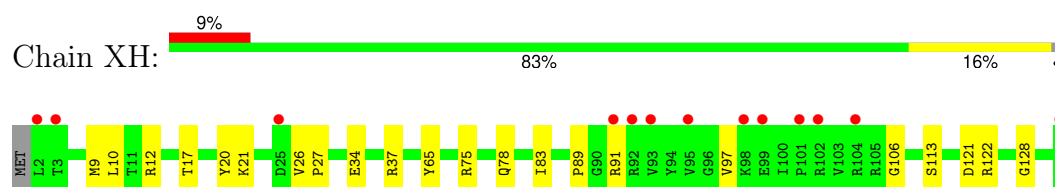
• Molecule 5: 30S ribosomal protein S5

Chain QE: 

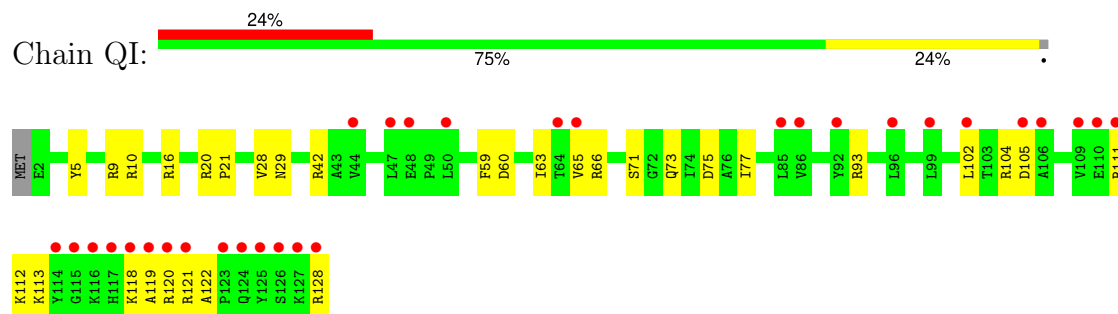


• Molecule 5: 30S ribosomal protein S5

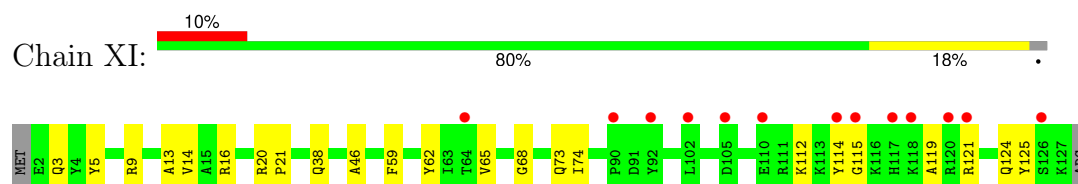




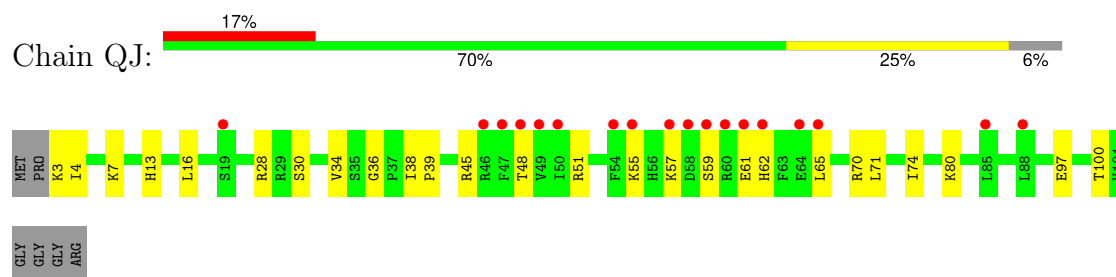
- Molecule 9: 30S ribosomal protein S9



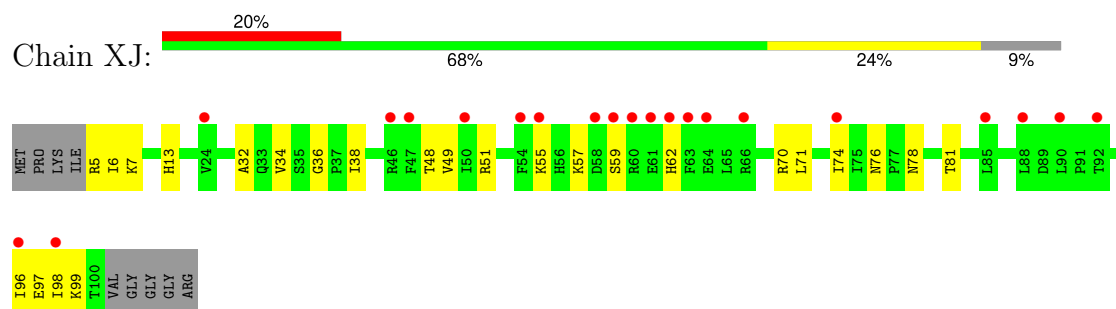
- Molecule 9: 30S ribosomal protein S9



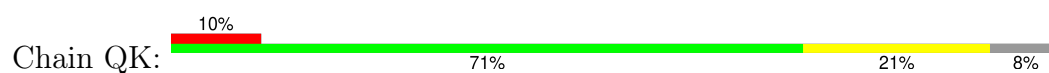
- Molecule 10: 30S ribosomal protein S10

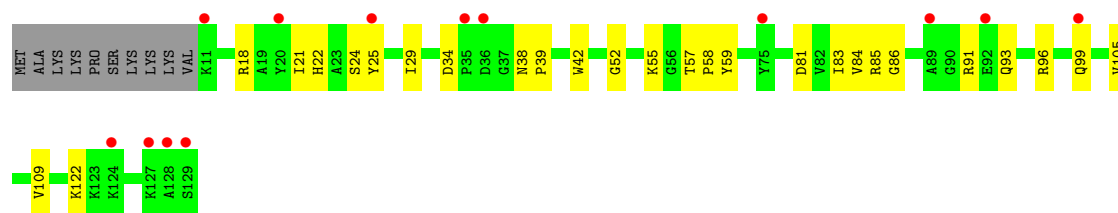


- Molecule 10: 30S ribosomal protein S10

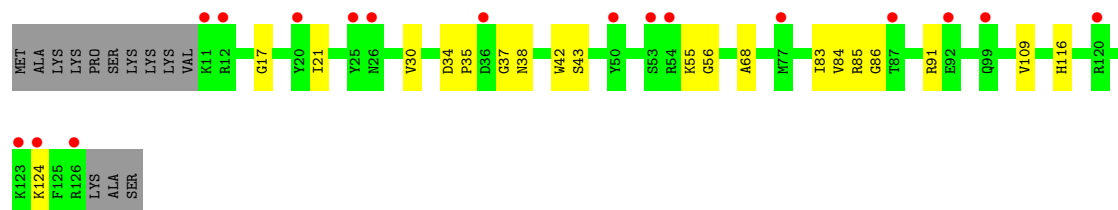
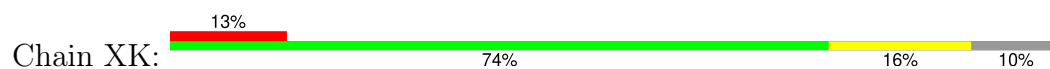


- Molecule 11: 30S ribosomal protein S11

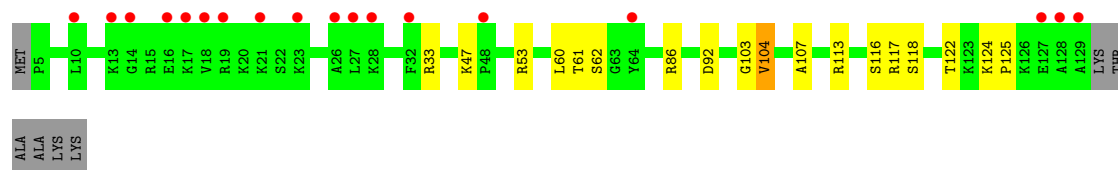
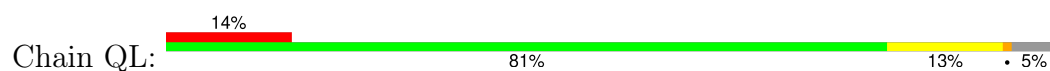




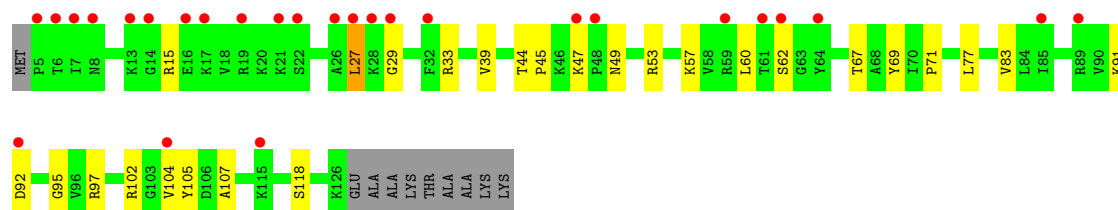
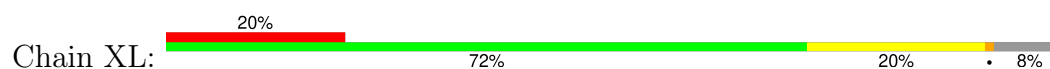
- Molecule 11: 30S ribosomal protein S11



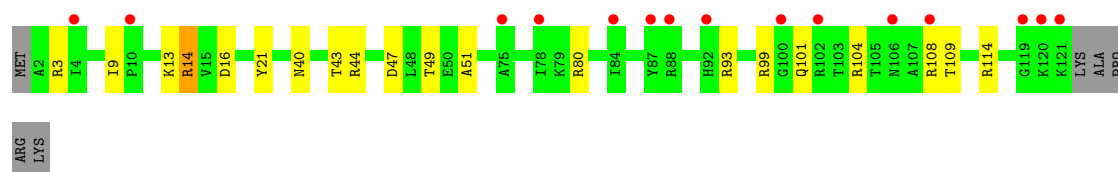
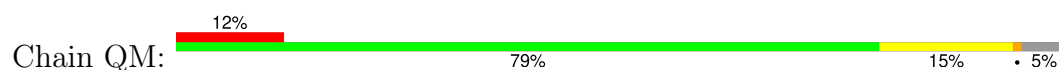
- Molecule 12: 30S ribosomal protein S12



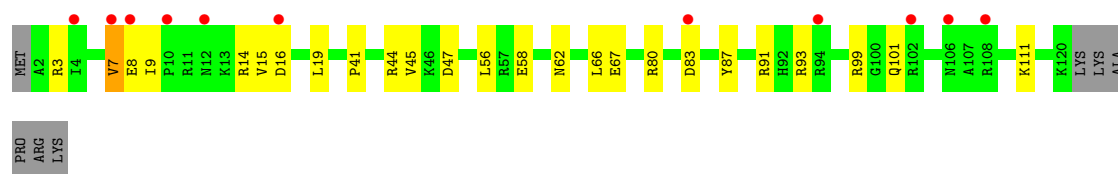
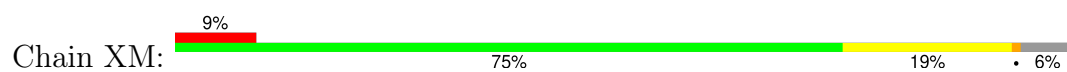
- Molecule 12: 30S ribosomal protein S12



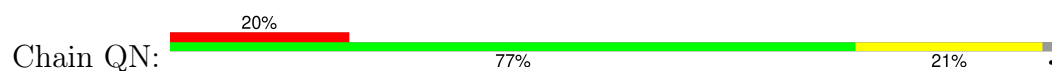
- Molecule 13: 30S ribosomal protein S13



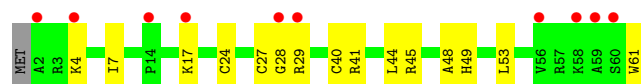
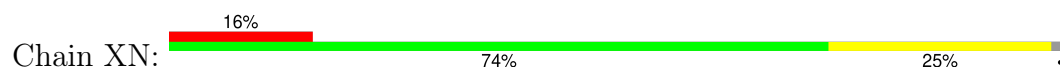
- Molecule 13: 30S ribosomal protein S13



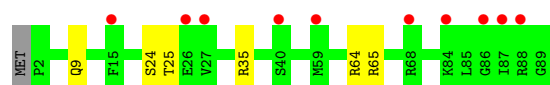
- Molecule 14: 30S ribosomal protein S14 type Z



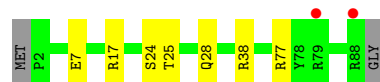
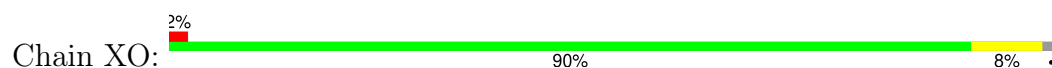
- Molecule 14: 30S ribosomal protein S14 type Z



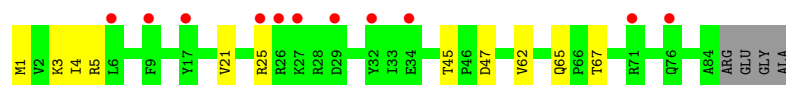
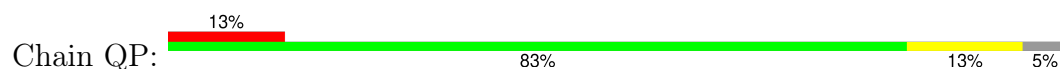
- Molecule 15: 30S ribosomal protein S15



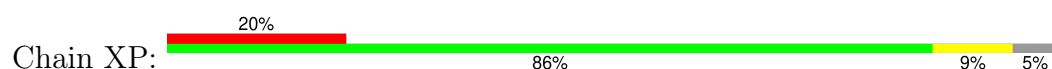
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

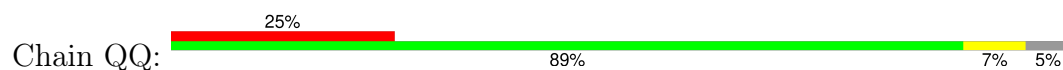


- Molecule 16: 30S ribosomal protein S16

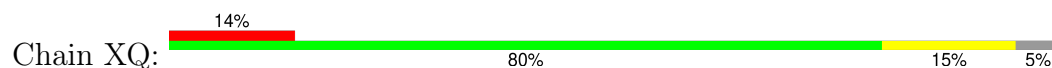




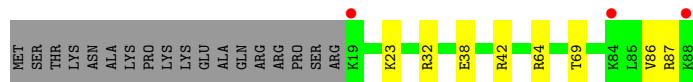
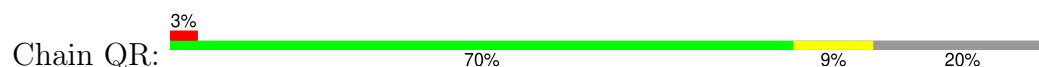
- Molecule 17: 30S ribosomal protein S17



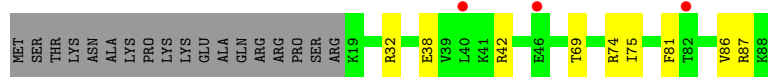
- Molecule 17: 30S ribosomal protein S17



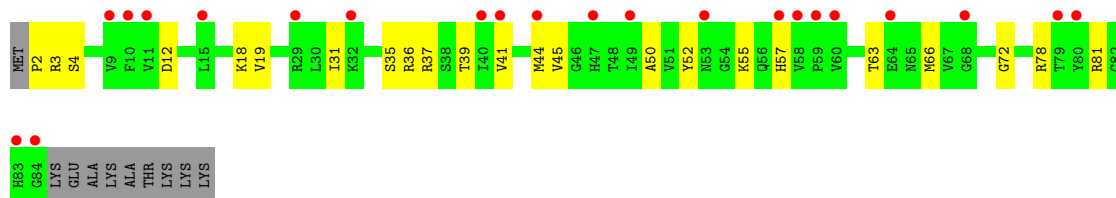
- Molecule 18: 30S ribosomal protein S18



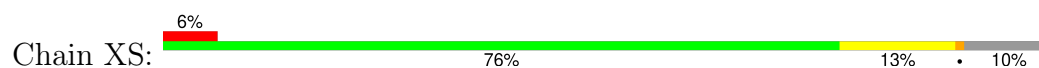
- Molecule 18: 30S ribosomal protein S18

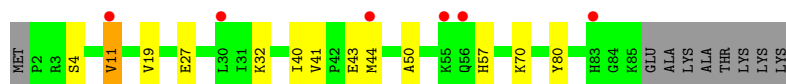


- Molecule 19: 30S ribosomal protein S19

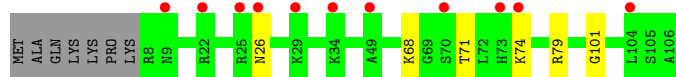
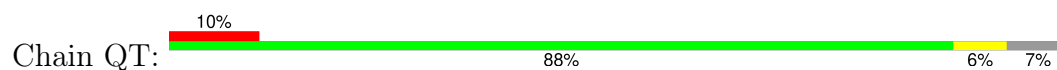


- Molecule 19: 30S ribosomal protein S19





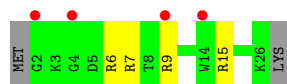
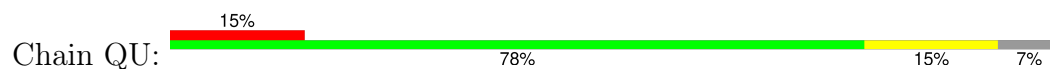
- Molecule 20: 30S ribosomal protein S20



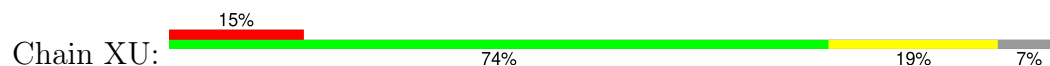
- Molecule 20: 30S ribosomal protein S20



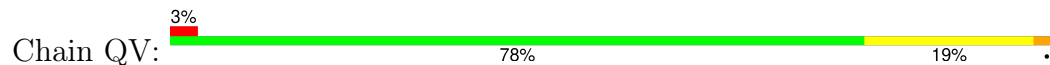
- Molecule 21: 30S ribosomal protein Thx



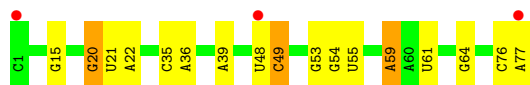
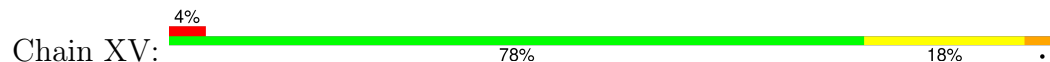
- Molecule 21: 30S ribosomal protein Thx



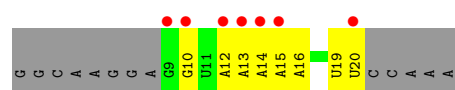
- Molecule 22: tRNA fMet



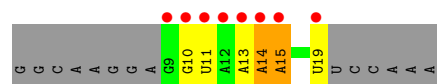
- Molecule 22: tRNA fMet



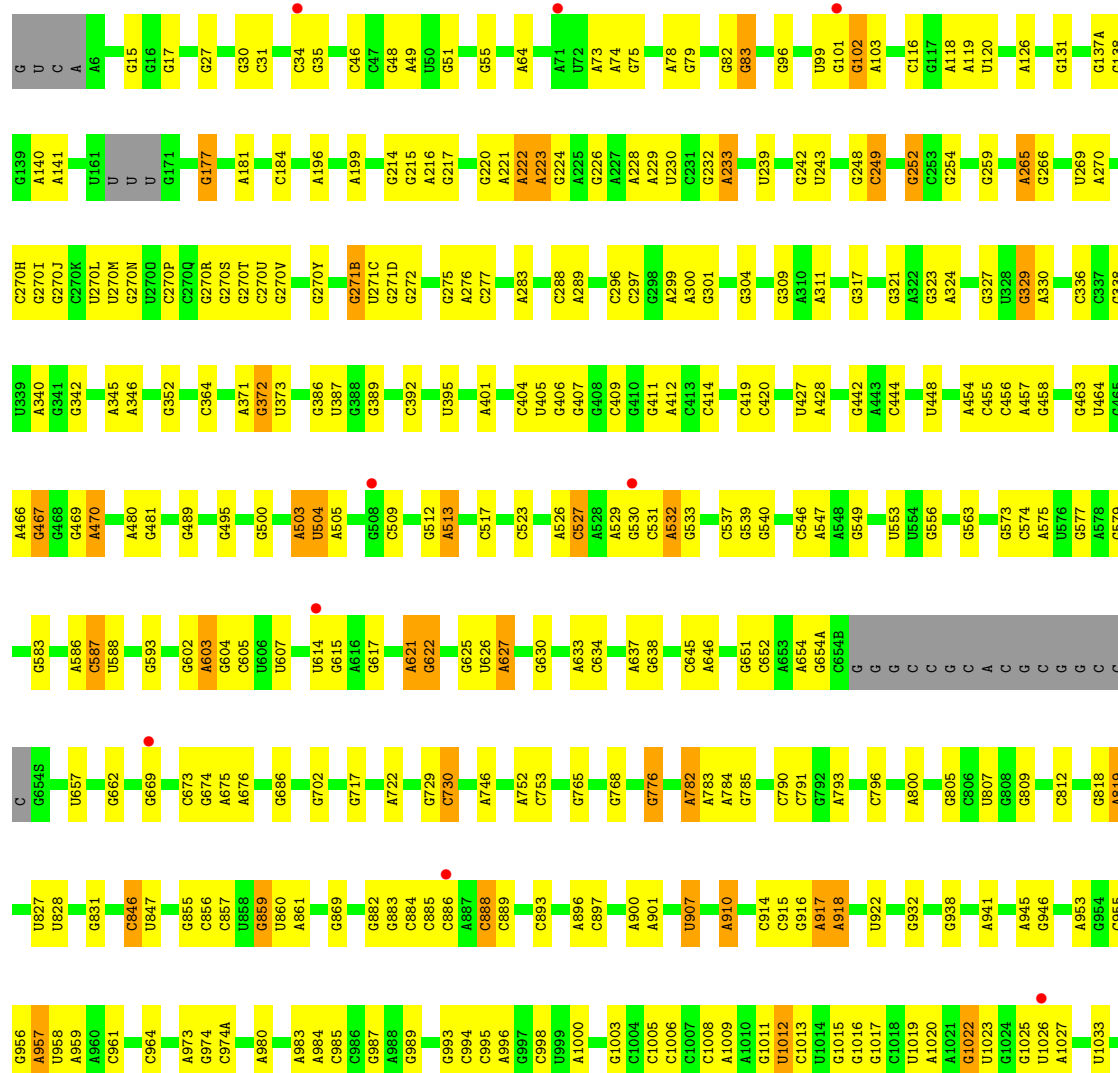
- Molecule 23: messenger RNA



Chain XX: 



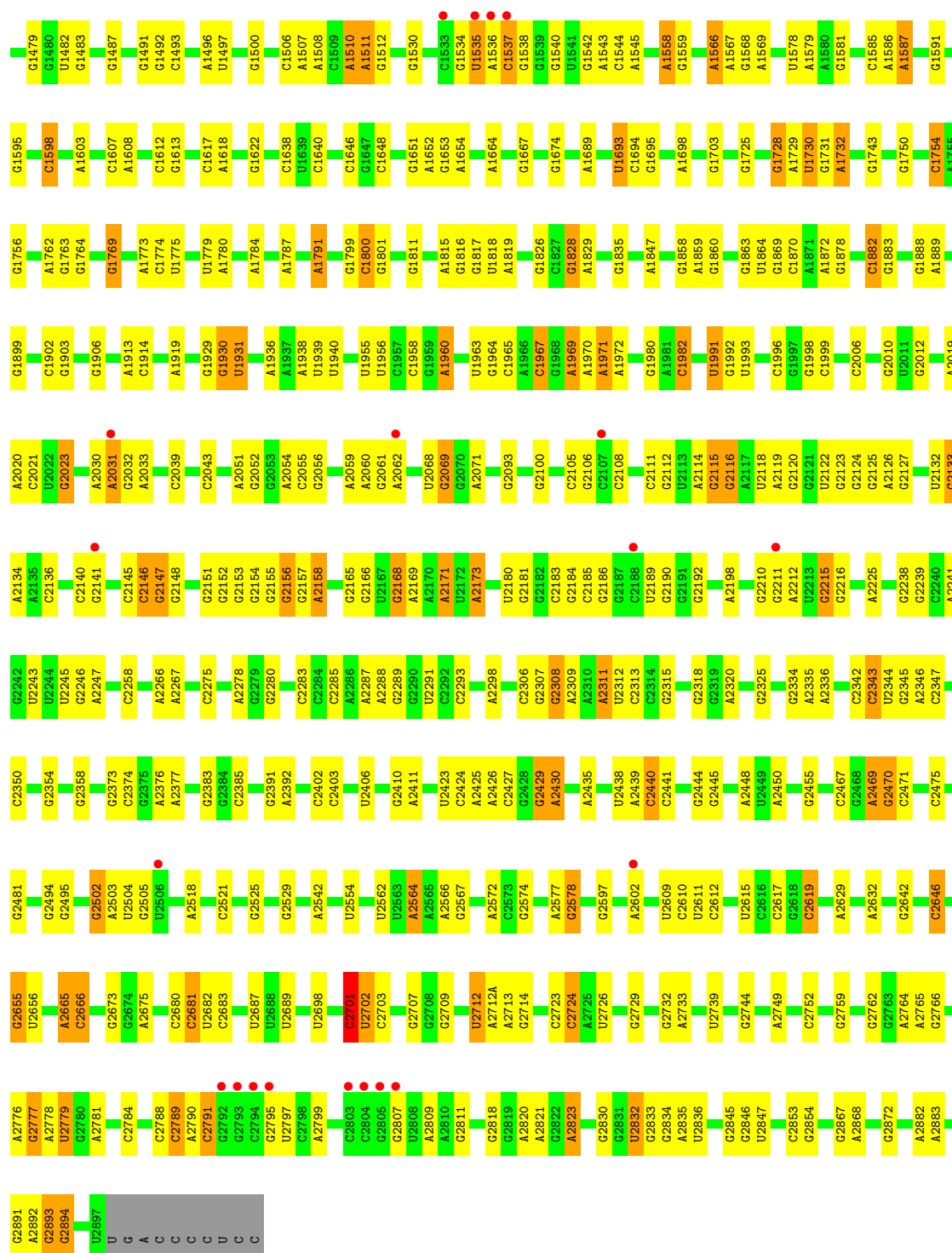
Chain RA: 



|       |       |       |       |       |       |       |       |        |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|-------|-------|
| G2744 | U2615 | G2318 | A2439 | G2093 | U1955 | G1811 | G1653 | U1535  | G1421 | G1271 | G1042 |
| G2751 | G2619 | G2319 | C2440 | G2210 | C1958 | G1816 | A1654 | A1536  | G1422 | A1272 | C1043 |
| C2752 | C2619 | A2320 | C2441 | G2211 | U1963 | G2112 | A1664 | C1537  | G1423 | G1136 | G1044 |
| C2753 | G2623 | G2325 | C2443 | U2213 | G1964 | U2113 | G1667 | U1541  | G1424 | G1137 | A1045 |
|       |       |       | C2444 | A2114 | U1819 | U1818 | A1668 | G1542  | G1425 | U1288 |       |
|       | A2629 | G2334 | G2445 | G2215 | C1967 | U1820 | U1668 | A1543  | G1426 | G1296 |       |
|       |       | A2335 |       | G2116 | G1968 | A1971 | G1674 | A1545  | A1427 | U1300 | A1050 |
|       | A2632 | A2336 |       | A2117 | A1969 | G1970 | C1675 |        | C1428 | U1410 |       |
|       |       |       |       | U2118 | A1971 | A1972 | A1689 |        | A1444 | A1301 | A1054 |
|       | U2636 | G2343 | G2470 | A2119 | A1972 |       | A1689 | C1547  | C1445 | G1309 | G1055 |
| U2637 | U2344 | U2344 |       | G2123 |       | G1828 | A1694 | A1558  |       | G1309 | G1059 |
| G2641 | G2345 | G2346 |       | G2124 | G1980 | A1829 | C1694 | A1449  | A1449 | U1312 | U1060 |
| G2642 | C2347 | C2347 |       | G2125 | A1981 | G1835 | A1698 | G1449A | A1555 | U1313 | U1061 |
|       |       |       |       | A2126 | C1982 |       | A1698 | G1465  |       | C1314 | G1062 |
| C2646 | C2350 | C2350 |       | G2127 | U1991 | A1847 | G1703 | C1565  | G1171 | G1173 | U1065 |
|       | U2244 | U2244 |       | C2128 | U1991 | A1848 | G1703 | A1566  | G1174 | A1174 | U1066 |
|       | G2246 | U2245 |       | G2131 | U1993 | G1849 | G1725 | A1567  | G1175 | U1175 | A1067 |
|       |       |       |       | U2132 | U1993 | G1850 | G1725 | A1569  | G1176 | G1176 | U1068 |
|       | G2250 | A2134 |       | G2133 | C1996 | A1854 | G1728 | U1578  | U1329 | C1178 | A1070 |
| A2503 | C2258 | A2135 |       | A2136 | C1999 | G1858 | U1730 | A1579  | U1329 | C1178 | A1070 |
| U2504 | G2265 | G2136 |       | C2136 | C1999 | A1859 | G1731 | A1580  | C1330 | G1179 | G1071 |
|       |       |       |       |       | C2006 | A1732 | A1732 |        | U1341 |       |       |
| U2506 | C2264 | G2141 |       | G2141 | C2006 | G1733 | G1733 |        | C1474 | U1341 | A1077 |
|       | A2273 | C2142 |       | C2142 | G2010 | A1864 | U1480 | A1583  | G1479 | A1349 | U1078 |
| U2519 | A2274 | G2143 |       | C2143 | U2011 | G1869 | G1480 | C1585  | U1482 | U1352 | C1079 |
| C2520 | C2275 | U2144 |       | U2144 | G2012 | C1870 | G1743 | A1586  | G1483 | U1359 | U1082 |
|       |       | C2145 |       | C2145 |       | G1878 | G1750 | U1590  | G1484 | A1395 | U1083 |
|       | A2278 | G2146 |       | C2146 | A2019 | C1882 | G1754 | G1591  | G1485 | G1195 | A1084 |
| G2529 | G2279 | G2147 |       | G2147 | A2020 | G1883 | A1755 | C1592  | G1486 | G1203 | A1085 |
| A2542 | G2280 | G2148 |       | G2148 |       | G1888 | G1756 | G1594  | G1487 | U1204 | A1086 |
| G2543 |       |       |       |       | G2023 | G1889 |       | G1595  | A1490 | U1205 | A1088 |
|       | C2283 |       |       | G2156 | A2031 | A1889 | A1762 | C1598  | G1491 | G1206 | G1091 |
|       | C2284 | G2157 |       | G2157 | G2032 | G1900 | G1763 | C1607  | G1492 | A1210 | G1092 |
|       | C2285 | A2158 |       | G2158 | A2033 | G1905 | G1764 | A1608  | C1493 | U1211 | G1093 |
|       | A2286 |       |       |       | G2052 | G1906 |       | A1609  | U1497 | A1214 | U1094 |
| A2560 | A2287 | C2161 |       | C2161 | C2039 | A1901 | G1769 | A1609  |       |       | A1095 |
| A2561 | A2288 | G2182 |       | G2182 |       | C1902 |       | A1610  |       |       | A1096 |
| U2562 |       | C2163 |       | C2163 | C2043 | G1905 | A1773 | C1617  | C1504 | A1220 | A1103 |
| A2566 | U2291 | C2164 |       | C2164 | C2043 | C1906 | U1774 | C1617  | C1505 | A1220 | A1103 |
| G2567 | C2402 | G2185 |       | G2185 | G2052 | G1905 | U1775 |        | A1507 | G1236 | C1104 |
| C2568 | C2403 | G2166 |       | G2166 |       | G1906 | G1776 | G1622  | A1508 | A1237 | U1105 |
| G2569 |       |       |       |       |       |       |       |        | C1509 | U1394 |       |
|       | U2406 |       |       | A2189 | C2055 | A1913 | U1779 | C1636  | C1509 | A1395 | G1110 |
|       |       |       |       | A2170 | G2056 | C1914 | A1780 | A1637  | A1510 | A1395 | A1111 |
|       |       |       |       |       |       |       | A1780 | A1637  | A1511 | A1408 | G1112 |
|       | C2424 |       |       | A2173 | A2059 | G1929 | C1781 | A1638  | A1511 | C1407 |       |
|       | A2425 |       |       |       | G2061 | G1930 | C1782 | U1639  | U1514 | A1253 | G1122 |
|       | A2426 |       |       |       | G2061 | G1930 | C1782 | U1639  | U1514 | A1254 | G1123 |
|       | C2427 |       |       |       | G2061 | A1936 | A1783 | C1640  | C1515 | U1255 | C1124 |
|       | G2307 | G2184 |       | G2184 | A2062 | A1937 | A1784 |        | C1515 | A1412 | G1125 |
|       | G2308 |       |       |       | C2063 | A1938 |       | G1645  | G1525 | G1413 |       |
|       | A2309 |       |       | C2188 |       | U1939 | A1791 | C1646  | G1530 | A1265 | A1126 |
|       | A2310 |       |       | U2189 |       | U1939 |       | C1647  | G1530 | A1265 |       |
|       | A2311 |       |       | G2190 |       | G1799 | G1799 | C1648  | G1530 | A1265 | A1129 |
|       | U2312 |       |       | G2191 |       | A1952 | C1800 | C1648  | G1530 | A1265 |       |
|       |       |       |       | G2191 |       |       | C1801 |        | C1533 | A1419 | C1134 |
|       | G2315 |       |       | G2192 |       |       | C1801 |        | C1534 | A1419 |       |

Chain YA:  %





• Molecule 25: 5S rRNA

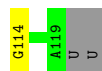
Chain RB: 66% 31% 3%





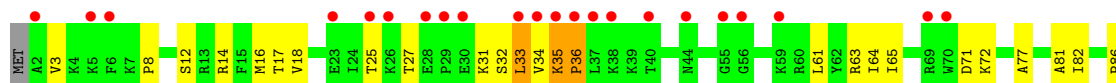
- Molecule 25: 5S rRNA

Chain YB: 2% 68% 28% ..



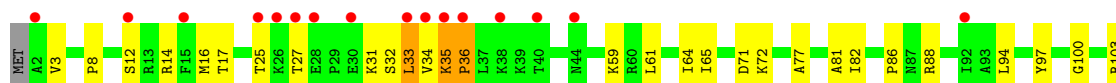
- Molecule 26: 50S ribosomal protein L2

Chain RD: 13% 76% 21% ..



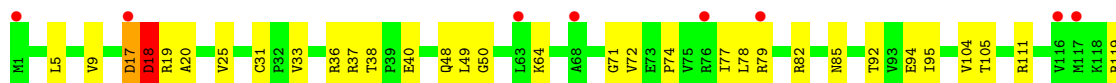
- Molecule 26: 50S ribosomal protein L2

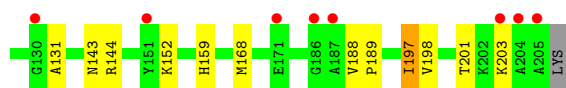
Chain YD: 8% 78% 19% ..



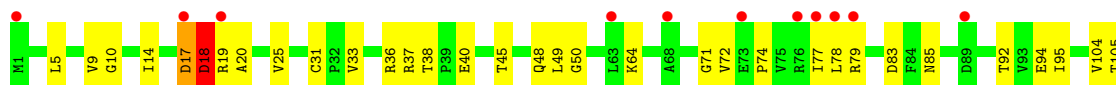
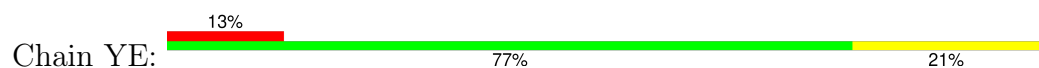
- Molecule 27: 50S ribosomal protein L3

Chain RE: 8% 78% 20% .

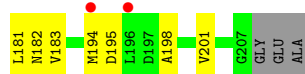
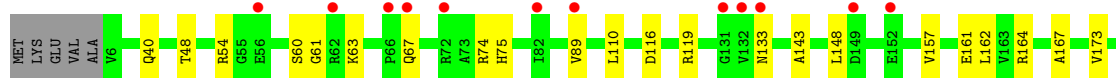
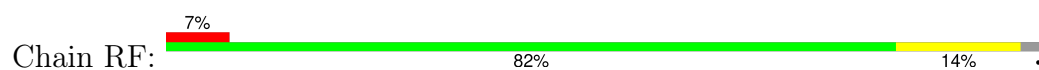




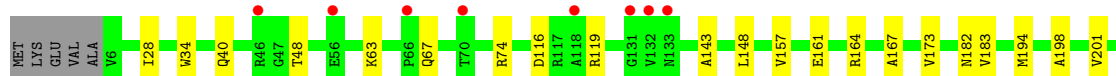
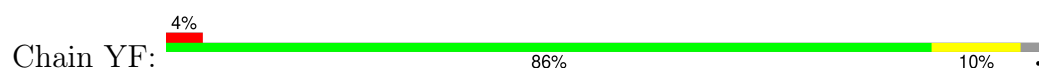
- Molecule 27: 50S ribosomal protein L3



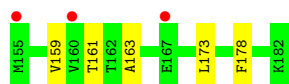
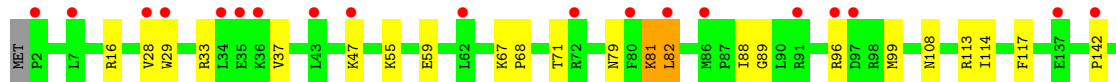
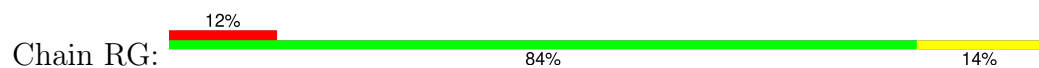
- Molecule 28: 50S ribosomal protein L4



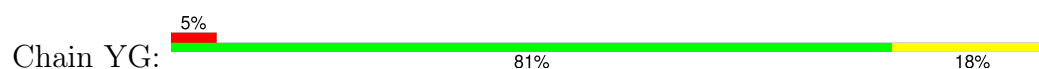
- Molecule 28: 50S ribosomal protein L4

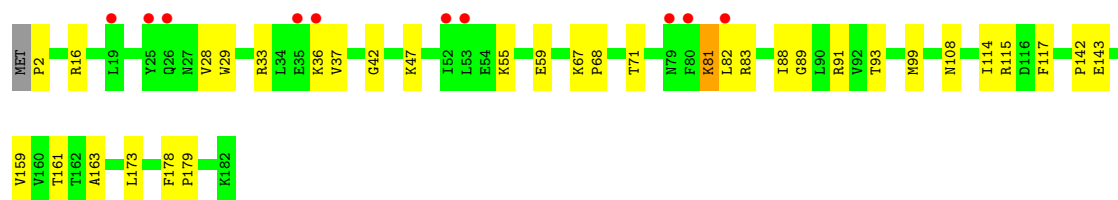


- Molecule 29: 50S ribosomal protein L5

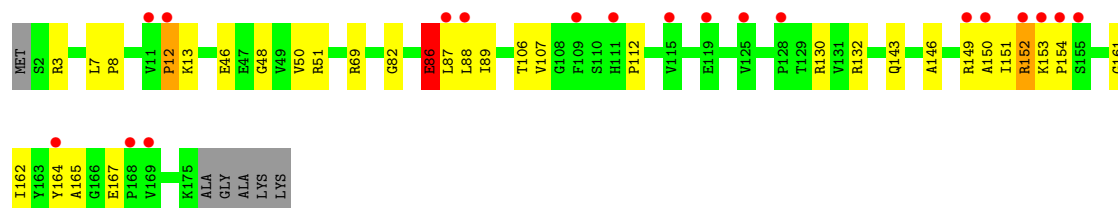
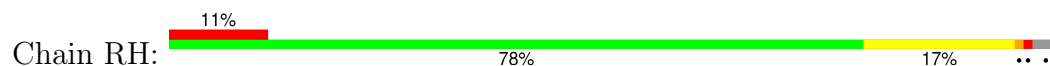


- Molecule 29: 50S ribosomal protein L5

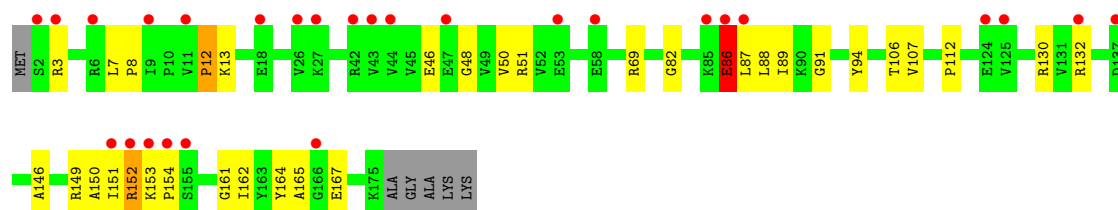
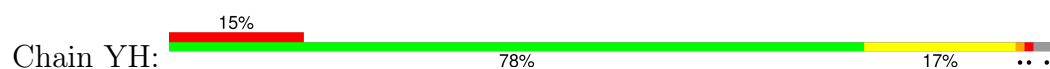




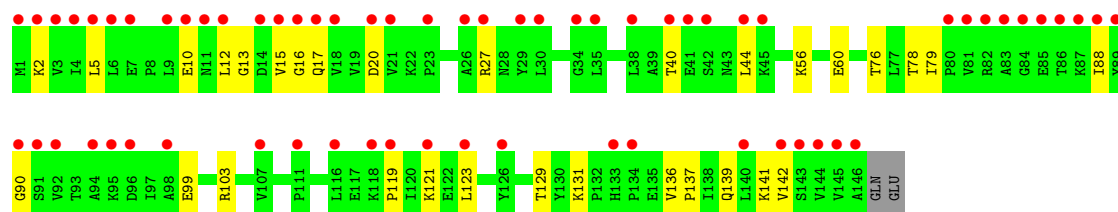
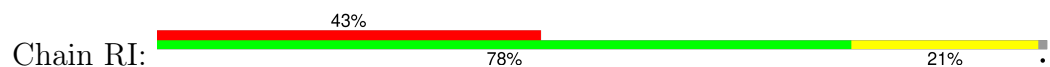
- Molecule 30: 50S ribosomal protein L6



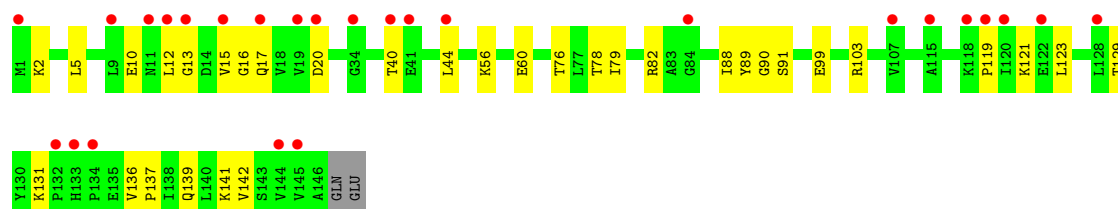
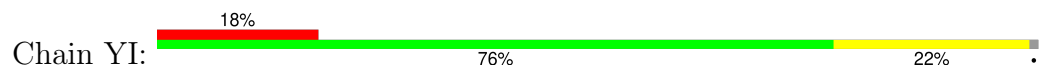
- Molecule 30: 50S ribosomal protein L6



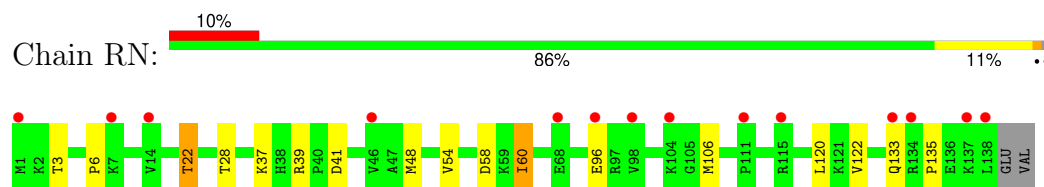
- Molecule 31: 50S ribosomal protein L9



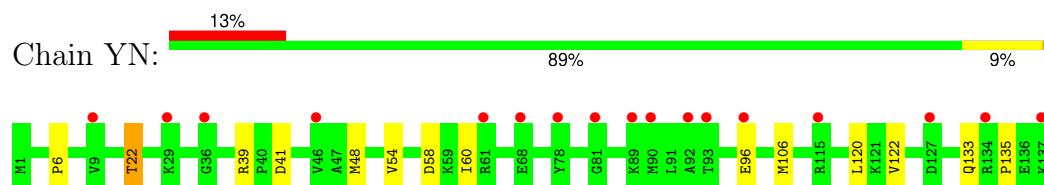
- Molecule 31: 50S ribosomal protein L9



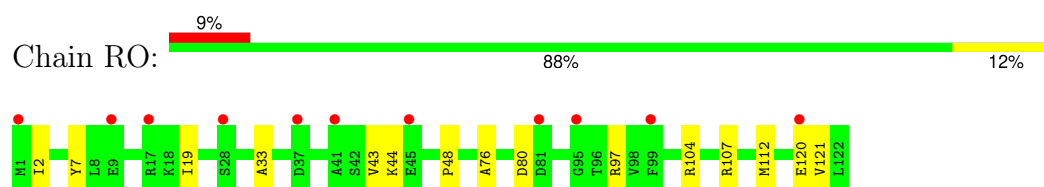
- Molecule 32: 50S ribosomal protein L13



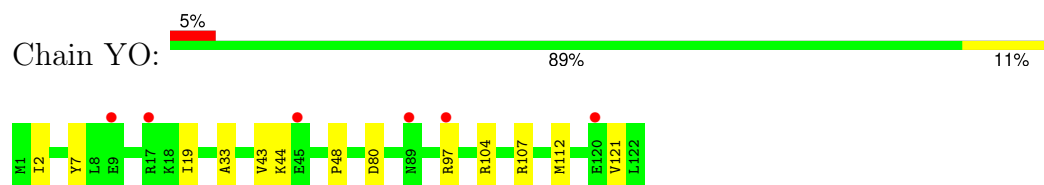
- Molecule 32: 50S ribosomal protein L13



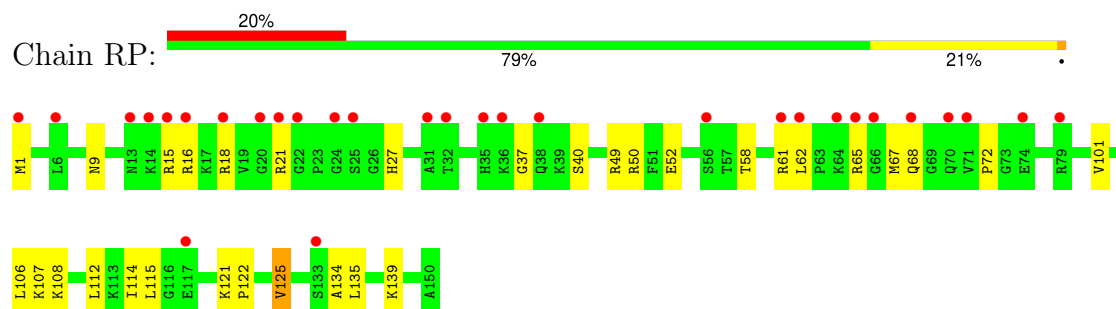
- Molecule 33: 50S ribosomal protein L14



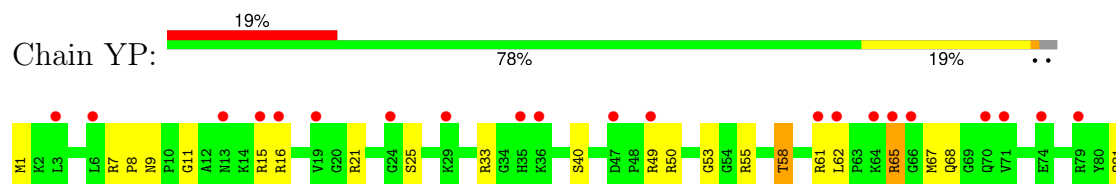
- Molecule 33: 50S ribosomal protein L14



- Molecule 34: 50S ribosomal protein L15

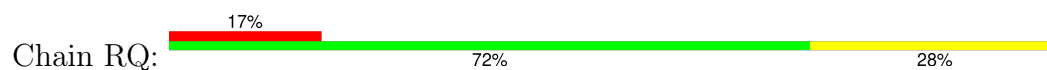


- Molecule 34: 50S ribosomal protein L15

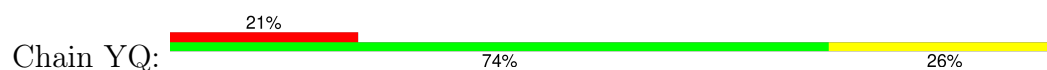




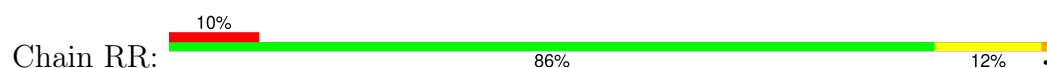
- Molecule 35: 50S ribosomal protein L16



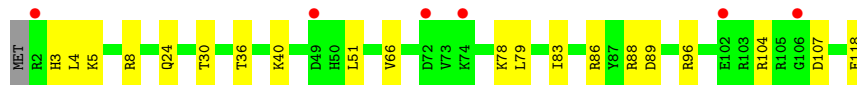
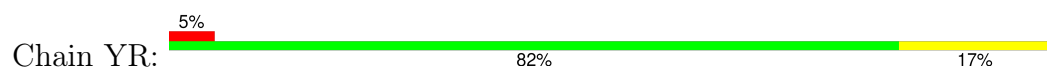
- Molecule 35: 50S ribosomal protein L16



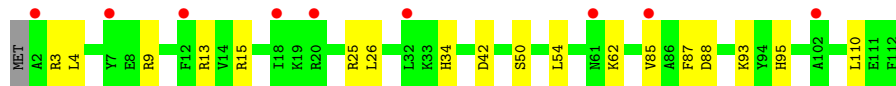
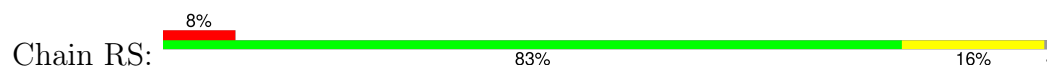
- Molecule 36: 50S ribosomal protein L17



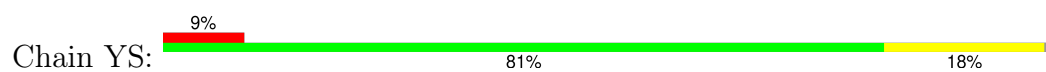
- Molecule 36: 50S ribosomal protein L17



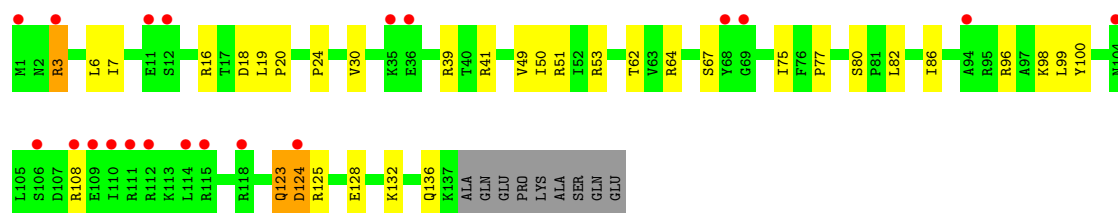
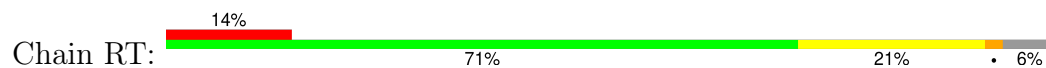
- Molecule 37: 50S ribosomal protein L18



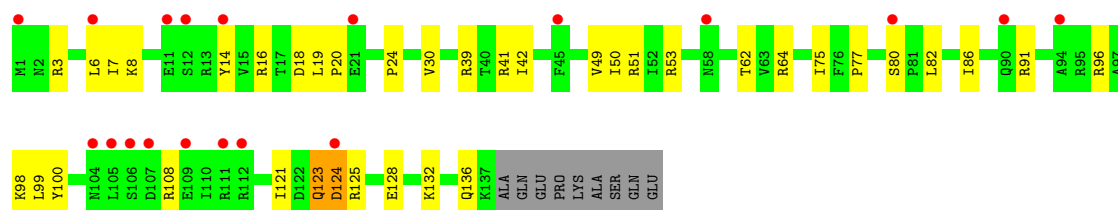
- Molecule 37: 50S ribosomal protein L18



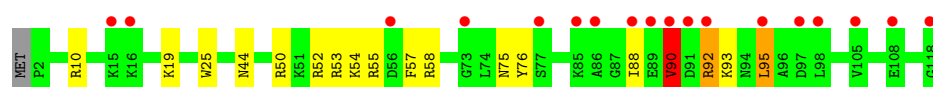
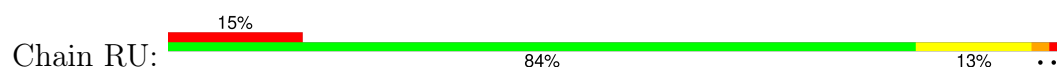
- Molecule 38: 50S ribosomal protein L19



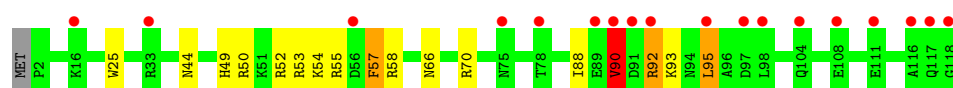
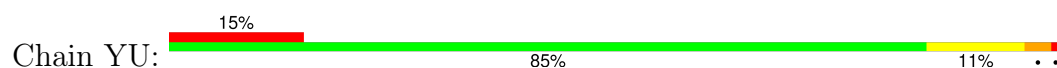
- Molecule 38: 50S ribosomal protein L19



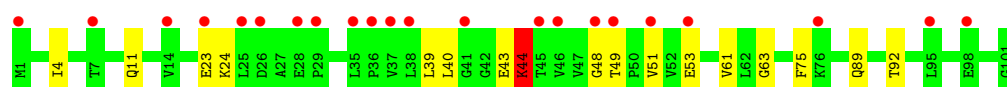
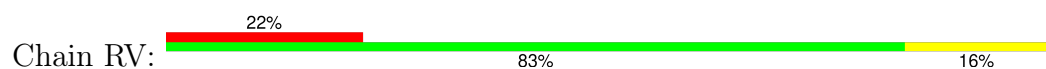
- Molecule 39: 50S ribosomal protein L20



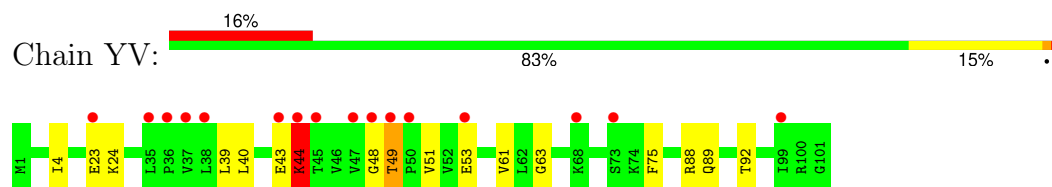
- Molecule 39: 50S ribosomal protein L20



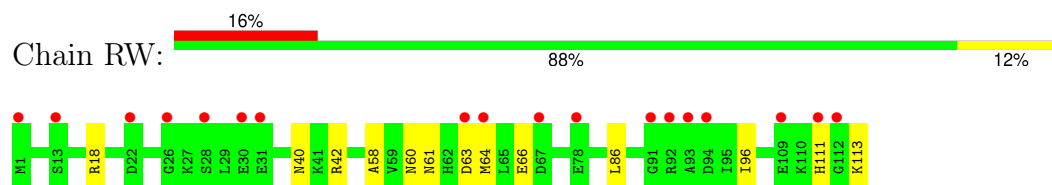
- Molecule 40: 50S ribosomal protein L21



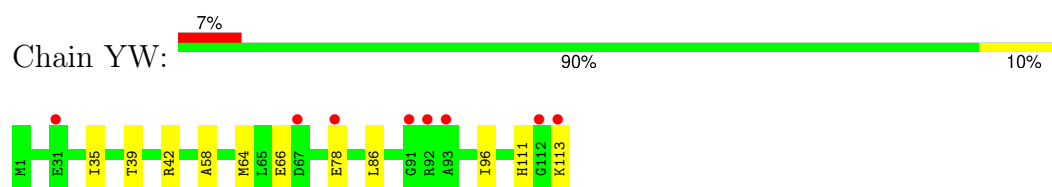
- Molecule 40: 50S ribosomal protein L21



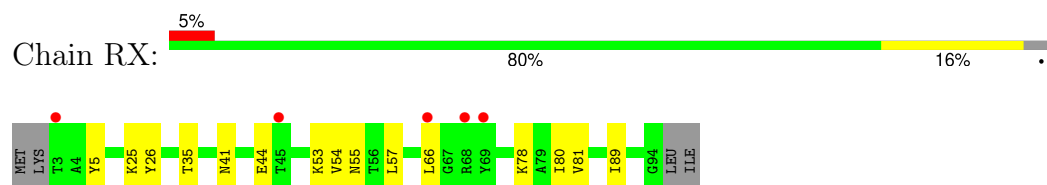
- Molecule 41: 50S ribosomal protein L22



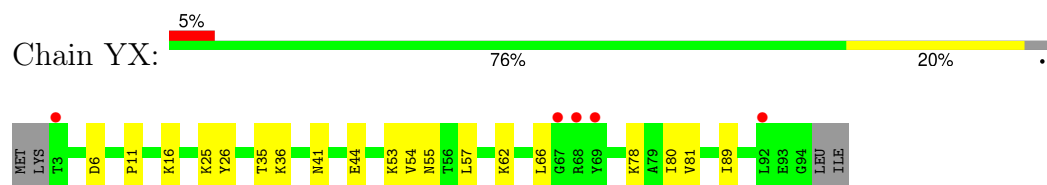
- Molecule 41: 50S ribosomal protein L22



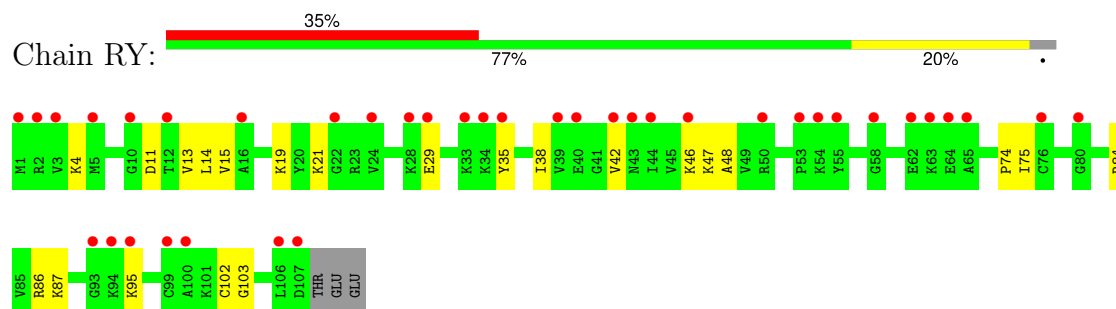
- Molecule 42: 50S ribosomal protein L23



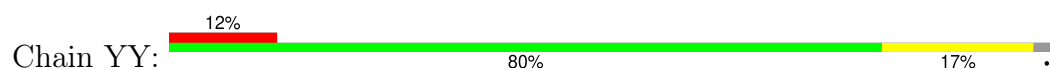
- Molecule 42: 50S ribosomal protein L23



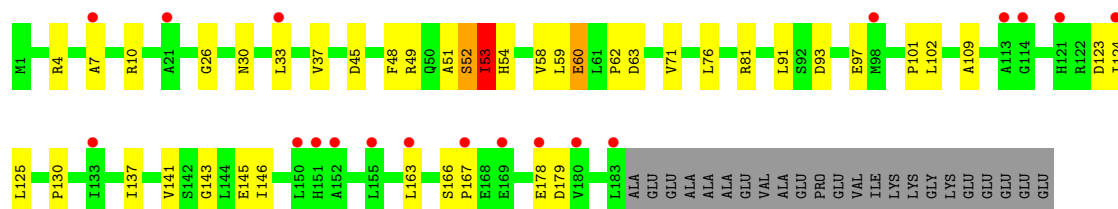
- Molecule 43: 50S ribosomal protein L24



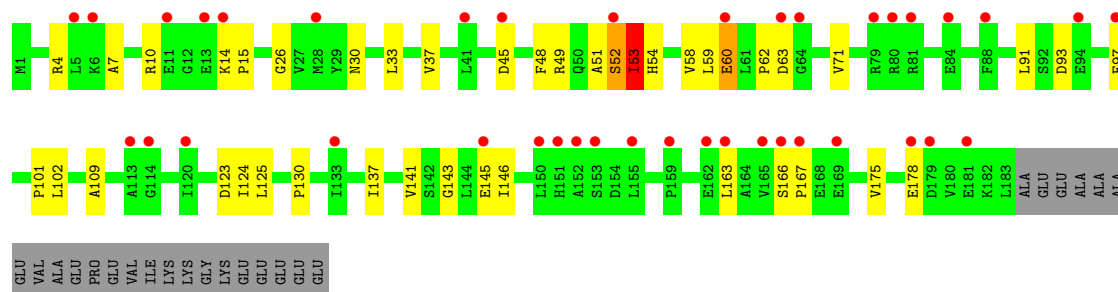
- Molecule 43: 50S ribosomal protein L24



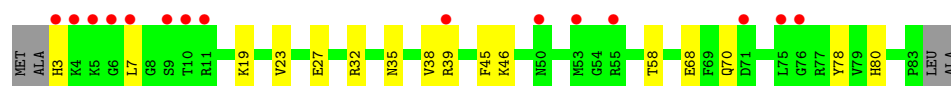
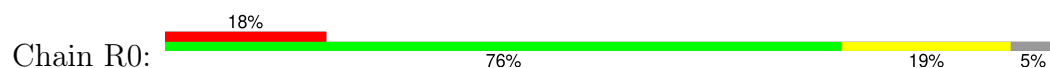
- Molecule 44: 50S ribosomal protein L25



- Molecule 44: 50S ribosomal protein L25



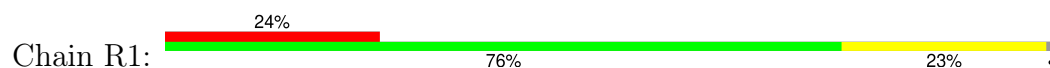
- Molecule 45: 50S ribosomal protein L27

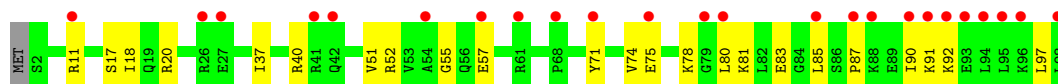


- Molecule 45: 50S ribosomal protein L27

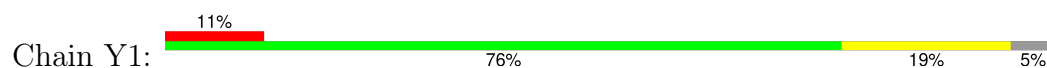


- Molecule 46: 50S ribosomal protein L28

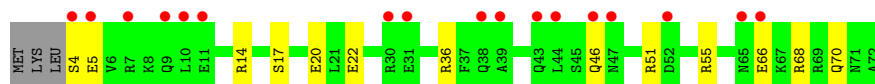
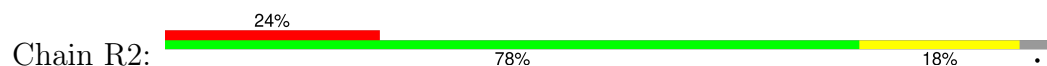




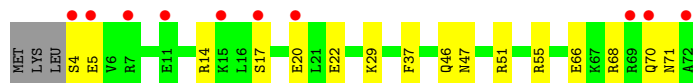
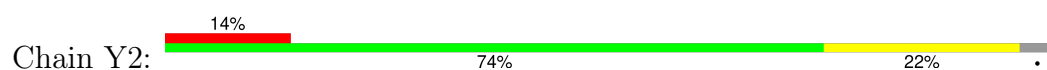
- Molecule 46: 50S ribosomal protein L28



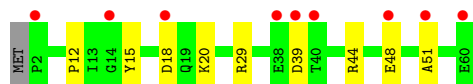
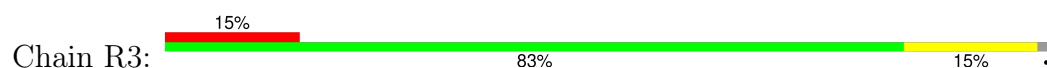
- Molecule 47: 50S ribosomal protein L29



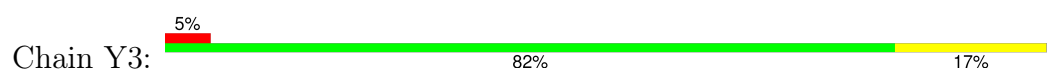
- Molecule 47: 50S ribosomal protein L29



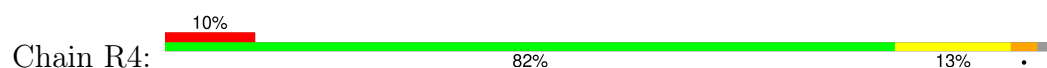
- Molecule 48: 50S ribosomal protein L30



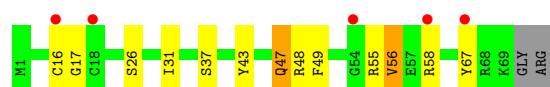
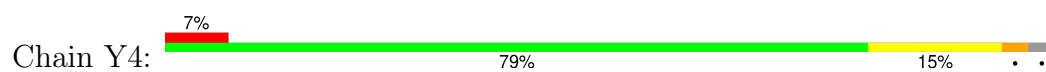
- Molecule 48: 50S ribosomal protein L30



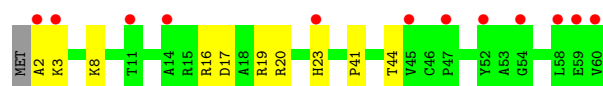
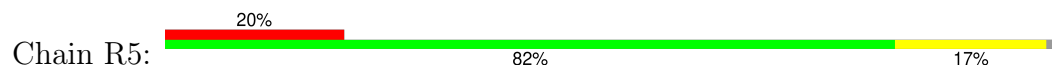
- Molecule 49: 50S ribosomal protein L31



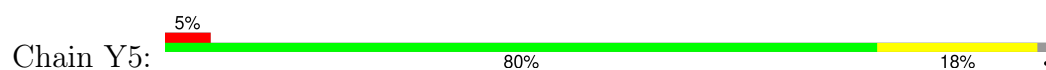
- Molecule 49: 50S ribosomal protein L31



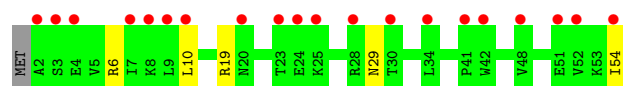
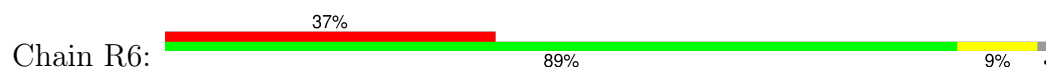
- Molecule 50: 50S ribosomal protein L32



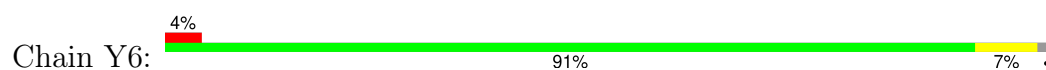
- Molecule 50: 50S ribosomal protein L32



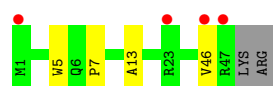
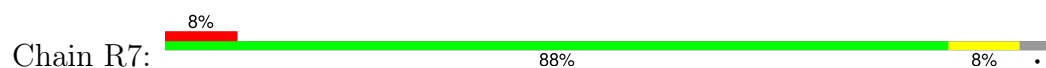
- Molecule 51: 50S ribosomal protein L33



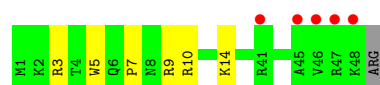
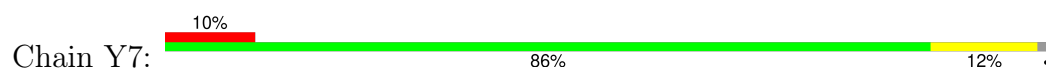
- Molecule 51: 50S ribosomal protein L33



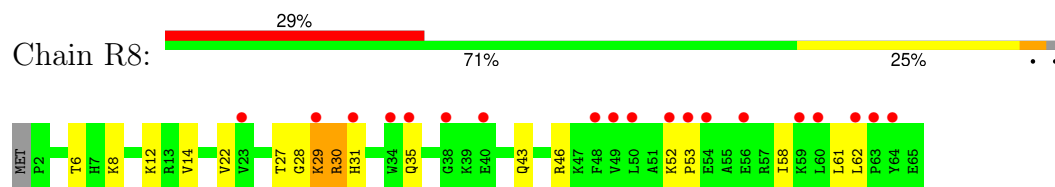
- Molecule 52: 50S ribosomal protein L34



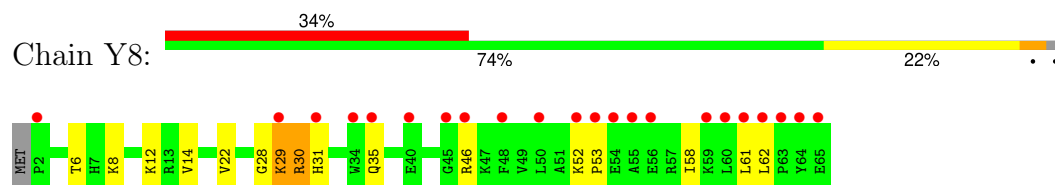
- Molecule 52: 50S ribosomal protein L34



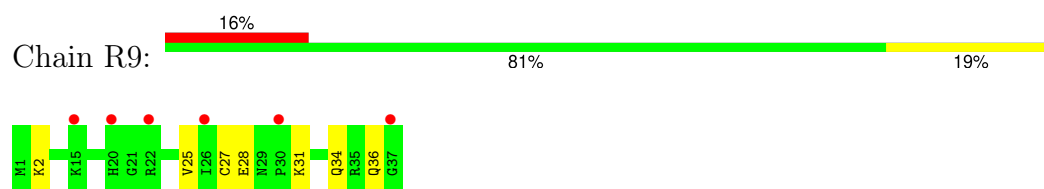
## ● Molecule 53: 50S ribosomal protein L35



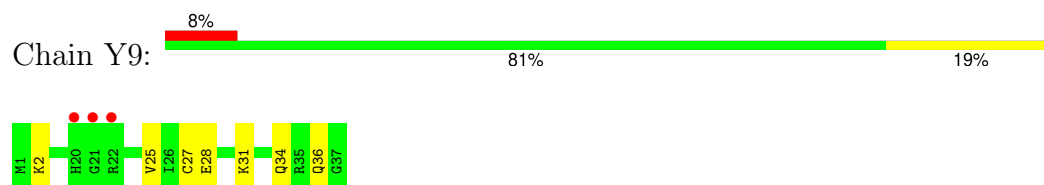
## ● Molecule 53: 50S ribosomal protein L35



## ● Molecule 54: 50S ribosomal protein L36



## ● Molecule 54: 50S ribosomal protein L36



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.65Å 447.95Å 618.80Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 124.48 – 3.18<br>124.48 – 3.18                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (124.48-3.18)<br>99.3 (124.48-3.18)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.30                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.31 (at 3.19Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.12                                                 | Depositor        |
| R, $R_{free}$                                                           | 0.232 , 0.251<br>0.233 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 44661 reflections (4.63%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 76.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.198                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 88.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 291753                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 104.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: ZN, SF4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$     |
| 1   | QA    | 0.39         | 0/36046       | 0.43        | 10/56257 (0.0%) |
| 1   | XA    | 0.45         | 0/36097       | 0.44        | 6/56339 (0.0%)  |
| 2   | QB    | 0.30         | 1/1942 (0.1%) | 0.66        | 2/2619 (0.1%)   |
| 2   | XB    | 0.36         | 0/1950        | 0.65        | 0/2630          |
| 3   | QC    | 0.30         | 0/1629        | 0.57        | 0/2195          |
| 3   | XC    | 0.30         | 0/1629        | 0.57        | 0/2195          |
| 4   | QD    | 0.37         | 0/1733        | 0.61        | 0/2318          |
| 4   | XD    | 0.37         | 0/1733        | 0.61        | 0/2318          |
| 5   | QE    | 0.33         | 0/1171        | 0.60        | 0/1576          |
| 5   | XE    | 0.33         | 0/1171        | 0.60        | 0/1576          |
| 6   | QF    | 0.32         | 0/856         | 0.49        | 0/1154          |
| 6   | XF    | 0.32         | 0/856         | 0.50        | 0/1154          |
| 7   | QG    | 0.29         | 0/1276        | 0.49        | 0/1709          |
| 7   | XG    | 0.29         | 0/1276        | 0.49        | 0/1709          |
| 8   | QH    | 0.35         | 0/1128        | 0.55        | 0/1517          |
| 8   | XH    | 0.35         | 0/1128        | 0.55        | 0/1517          |
| 9   | QI    | 0.32         | 0/1029        | 0.68        | 0/1379          |
| 9   | XI    | 0.37         | 0/1017        | 0.64        | 0/1365          |
| 10  | QJ    | 0.30         | 0/814         | 0.62        | 0/1095          |
| 10  | XJ    | 0.35         | 0/790         | 0.59        | 0/1063          |
| 11  | QK    | 0.33         | 0/900         | 0.52        | 0/1213          |
| 11  | XK    | 0.41         | 0/879         | 0.60        | 2/1187 (0.2%)   |
| 12  | QL    | 0.40         | 0/991         | 0.68        | 0/1327          |
| 12  | XL    | 0.48         | 0/972         | 0.74        | 2/1301 (0.2%)   |
| 13  | QM    | 0.32         | 0/965         | 0.76        | 2/1292 (0.2%)   |
| 13  | XM    | 0.35         | 0/956         | 0.76        | 1/1281 (0.1%)   |
| 14  | QN    | 0.38         | 0/501         | 0.73        | 0/664           |
| 14  | XN    | 0.38         | 0/501         | 0.73        | 0/664           |
| 15  | QO    | 0.30         | 0/745         | 0.52        | 0/992           |
| 15  | XO    | 0.35         | 0/740         | 0.52        | 0/987           |
| 16  | QP    | 0.39         | 0/721         | 0.61        | 0/970           |
| 16  | XP    | 0.39         | 0/721         | 0.61        | 0/970           |

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 17  | QQ    | 0.36         | 0/847   | 0.53        | 0/1131           |
| 17  | XQ    | 0.36         | 0/847   | 0.52        | 0/1131           |
| 18  | QR    | 0.36         | 0/579   | 0.58        | 0/768            |
| 18  | XR    | 0.36         | 0/579   | 0.58        | 0/768            |
| 19  | QS    | 0.31         | 0/680   | 0.84        | 0/915            |
| 19  | XS    | 0.38         | 0/689   | 0.83        | 1/926 (0.1%)     |
| 20  | QT    | 0.34         | 0/765   | 0.69        | 0/1007           |
| 20  | XT    | 0.34         | 0/765   | 0.69        | 0/1007           |
| 21  | QU    | 0.36         | 0/221   | 0.58        | 0/288            |
| 21  | XU    | 0.36         | 0/221   | 0.58        | 0/288            |
| 22  | QV    | 0.42         | 0/1836  | 0.41        | 0/2859           |
| 22  | XV    | 0.42         | 0/1836  | 0.41        | 0/2859           |
| 23  | QX    | 0.30         | 0/290   | 0.46        | 0/450            |
| 23  | XX    | 0.33         | 0/268   | 0.38        | 0/416            |
| 24  | RA    | 0.52         | 0/69521 | 0.45        | 7/108529 (0.0%)  |
| 24  | YA    | 0.60         | 0/69543 | 0.47        | 13/108563 (0.0%) |
| 25  | RB    | 0.42         | 0/2878  | 0.42        | 0/4490           |
| 25  | YB    | 0.42         | 0/2878  | 0.42        | 0/4490           |
| 26  | RD    | 0.58         | 0/2165  | 0.78        | 5/2919 (0.2%)    |
| 26  | YD    | 0.58         | 0/2165  | 0.77        | 5/2919 (0.2%)    |
| 27  | RE    | 0.51         | 0/1601  | 0.84        | 3/2160 (0.1%)    |
| 27  | YE    | 0.51         | 0/1601  | 0.84        | 3/2160 (0.1%)    |
| 28  | RF    | 0.50         | 0/1620  | 0.62        | 0/2194           |
| 28  | YF    | 0.50         | 0/1620  | 0.62        | 0/2194           |
| 29  | RG    | 0.38         | 0/1499  | 0.71        | 0/2016           |
| 29  | YG    | 0.38         | 0/1499  | 0.71        | 0/2016           |
| 30  | RH    | 0.36         | 0/1362  | 0.76        | 2/1841 (0.1%)    |
| 30  | YH    | 0.36         | 0/1362  | 0.76        | 2/1841 (0.1%)    |
| 31  | RI    | 0.34         | 0/1151  | 0.78        | 2/1558 (0.1%)    |
| 31  | YI    | 0.34         | 0/1151  | 0.78        | 2/1558 (0.1%)    |
| 32  | RN    | 0.46         | 0/1131  | 0.66        | 0/1525           |
| 32  | YN    | 0.46         | 0/1131  | 0.66        | 0/1525           |
| 33  | RO    | 0.50         | 0/943   | 0.59        | 0/1269           |
| 33  | YO    | 0.50         | 0/943   | 0.59        | 0/1269           |
| 34  | RP    | 0.47         | 0/1162  | 0.87        | 1/1544 (0.1%)    |
| 34  | YP    | 0.53         | 0/1139  | 0.92        | 2/1514 (0.1%)    |
| 35  | RQ    | 0.46         | 0/1143  | 0.75        | 0/1527           |
| 35  | YQ    | 0.46         | 0/1143  | 0.75        | 0/1527           |
| 36  | RR    | 0.51         | 0/974   | 0.72        | 0/1302           |
| 36  | YR    | 0.52         | 0/974   | 0.72        | 0/1302           |
| 37  | RS    | 0.36         | 0/892   | 0.78        | 0/1187           |
| 37  | YS    | 0.36         | 0/892   | 0.78        | 0/1187           |
| 38  | RT    | 0.45         | 0/1155  | 0.78        | 2/1542 (0.1%)    |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| 38  | YT    | 0.45         | 0/1155          | 0.78        | 0/1542           |
| 39  | RU    | 0.49         | 0/982           | 0.69        | 4/1306 (0.3%)    |
| 39  | YU    | 0.49         | 0/982           | 0.69        | 4/1306 (0.3%)    |
| 40  | RV    | 0.41         | 0/790           | 0.71        | 1/1057 (0.1%)    |
| 40  | YV    | 0.41         | 0/790           | 0.71        | 1/1057 (0.1%)    |
| 41  | RW    | 0.51         | 0/911           | 0.66        | 0/1220           |
| 41  | YW    | 0.51         | 0/911           | 0.66        | 0/1220           |
| 42  | RX    | 0.50         | 0/739           | 0.59        | 0/993            |
| 42  | YX    | 0.50         | 0/739           | 0.59        | 0/993            |
| 43  | RY    | 0.43         | 0/831           | 0.56        | 0/1108           |
| 43  | YY    | 0.43         | 0/831           | 0.56        | 0/1108           |
| 44  | RZ    | 0.36         | 0/1493          | 0.84        | 4/2026 (0.2%)    |
| 44  | YZ    | 0.36         | 0/1493          | 0.84        | 4/2026 (0.2%)    |
| 45  | R0    | 0.44         | 0/652           | 0.55        | 0/867            |
| 45  | Y0    | 0.54         | 0/607           | 0.60        | 0/809            |
| 46  | R1    | 0.49         | 0/770           | 0.78        | 1/1022 (0.1%)    |
| 46  | Y1    | 0.53         | 0/736           | 0.75        | 1/978 (0.1%)     |
| 47  | R2    | 0.36         | 0/583           | 0.60        | 0/771            |
| 47  | Y2    | 0.36         | 0/583           | 0.60        | 0/771            |
| 48  | R3    | 0.42         | 0/474           | 0.65        | 0/635            |
| 48  | Y3    | 0.42         | 0/474           | 0.65        | 0/635            |
| 49  | R4    | 0.31         | 0/578           | 0.85        | 0/776            |
| 49  | Y4    | 0.31         | 0/578           | 0.85        | 0/776            |
| 50  | R5    | 0.48         | 0/473           | 0.59        | 0/639            |
| 50  | Y5    | 0.47         | 0/473           | 0.59        | 0/639            |
| 51  | R6    | 0.26         | 0/460           | 0.50        | 0/613            |
| 51  | Y6    | 0.26         | 0/460           | 0.49        | 0/613            |
| 52  | R7    | 0.53         | 0/417           | 0.63        | 0/550            |
| 52  | Y7    | 0.61         | 0/426           | 0.63        | 0/561            |
| 53  | R8    | 0.58         | 0/525           | 0.92        | 0/691            |
| 53  | Y8    | 0.58         | 0/525           | 0.92        | 0/691            |
| 54  | R9    | 0.35         | 0/310           | 0.45        | 0/407            |
| 54  | Y9    | 0.35         | 0/310           | 0.45        | 0/407            |
| All | All   | 0.49         | 1/315585 (0.0%) | 0.52        | 95/471827 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4   | QD    | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4   | XD    | 0                   | 2                   |
| 12  | QL    | 0                   | 2                   |
| 12  | XL    | 0                   | 2                   |
| 19  | QS    | 0                   | 1                   |
| 26  | RD    | 0                   | 4                   |
| 26  | YD    | 0                   | 4                   |
| 27  | RE    | 0                   | 4                   |
| 27  | YE    | 0                   | 4                   |
| 29  | RG    | 0                   | 1                   |
| 29  | YG    | 0                   | 1                   |
| 30  | RH    | 0                   | 2                   |
| 30  | YH    | 0                   | 2                   |
| 31  | RI    | 0                   | 2                   |
| 31  | YI    | 0                   | 2                   |
| 32  | RN    | 0                   | 1                   |
| 32  | YN    | 0                   | 1                   |
| 34  | RP    | 0                   | 1                   |
| 34  | YP    | 0                   | 3                   |
| 35  | RQ    | 0                   | 1                   |
| 35  | YQ    | 0                   | 1                   |
| 39  | RU    | 0                   | 1                   |
| 39  | YU    | 0                   | 1                   |
| 40  | RV    | 0                   | 2                   |
| 40  | YV    | 0                   | 2                   |
| 44  | RZ    | 0                   | 4                   |
| 44  | YZ    | 0                   | 4                   |
| 47  | R2    | 0                   | 1                   |
| 47  | Y2    | 0                   | 1                   |
| 49  | R4    | 0                   | 2                   |
| 49  | Y4    | 0                   | 2                   |
| 53  | R8    | 0                   | 4                   |
| 53  | Y8    | 0                   | 4                   |
| All | All   | 0                   | 71                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | QB    | 23  | ARG  | CA-CB | 5.28 | 1.60        | 1.53     |

The worst 5 of 95 bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 46  | R1    | 75   | GLU  | N-CA-C      | -8.99 | 103.42      | 114.75   |
| 46  | Y1    | 75   | GLU  | N-CA-C      | -8.66 | 103.84      | 114.75   |
| 11  | XK    | 56   | GLY  | CA-C-N      | 7.39  | 130.67      | 120.39   |
| 11  | XK    | 56   | GLY  | C-N-CA      | 7.39  | 130.67      | 120.39   |
| 24  | YA    | 1130 | U    | C2'-C3'-O3' | 6.94  | 119.91      | 109.50   |

There are no chirality outliers.

5 of 71 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 4   | QD    | 19  | LEU  | Peptide |
| 4   | QD    | 33  | MET  | Peptide |
| 12  | QL    | 104 | VAL  | Peptide |
| 12  | QL    | 47  | LYS  | Peptide |
| 19  | QS    | 41  | VAL  | 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   | QA    | 32202 | 0        | 16255    | 210     | 0            |
| 1   | XA    | 32246 | 0        | 16277    | 184     | 0            |
| 2   | QB    | 1907  | 0        | 1958     | 20      | 0            |
| 2   | XB    | 1915  | 0        | 1969     | 17      | 0            |
| 3   | QC    | 1605  | 0        | 1668     | 22      | 0            |
| 3   | XC    | 1605  | 0        | 1668     | 20      | 2            |
| 4   | QD    | 1703  | 0        | 1766     | 17      | 0            |
| 4   | XD    | 1703  | 0        | 1767     | 22      | 0            |
| 5   | QE    | 1155  | 0        | 1213     | 11      | 0            |
| 5   | XE    | 1155  | 0        | 1213     | 8       | 0            |
| 6   | QF    | 843   | 0        | 857      | 10      | 0            |
| 6   | XF    | 843   | 0        | 857      | 8       | 0            |
| 7   | QG    | 1257  | 0        | 1296     | 11      | 0            |
| 7   | XG    | 1257  | 0        | 1296     | 10      | 0            |
| 8   | QH    | 1108  | 0        | 1164     | 17      | 0            |
| 8   | XH    | 1108  | 0        | 1165     | 15      | 0            |
| 9   | QI    | 1010  | 0        | 1037     | 26      | 0            |
| 9   | XI    | 998   | 0        | 1024     | 16      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | QJ    | 801   | 0        | 849      | 18      | 0            |
| 10  | XJ    | 777   | 0        | 816      | 19      | 0            |
| 11  | QK    | 885   | 0        | 904      | 20      | 2            |
| 11  | XK    | 864   | 0        | 881      | 14      | 0            |
| 12  | QL    | 975   | 0        | 1062     | 12      | 0            |
| 12  | XL    | 956   | 0        | 1046     | 16      | 0            |
| 13  | QM    | 955   | 0        | 1021     | 15      | 0            |
| 13  | XM    | 946   | 0        | 1008     | 17      | 0            |
| 14  | QN    | 492   | 0        | 529      | 7       | 0            |
| 14  | XN    | 492   | 0        | 529      | 9       | 0            |
| 15  | QO    | 734   | 0        | 771      | 5       | 0            |
| 15  | XO    | 729   | 0        | 768      | 4       | 0            |
| 16  | QP    | 705   | 0        | 725      | 7       | 0            |
| 16  | XP    | 705   | 0        | 725      | 4       | 0            |
| 17  | QQ    | 834   | 0        | 904      | 6       | 0            |
| 17  | XQ    | 834   | 0        | 904      | 15      | 0            |
| 18  | QR    | 574   | 0        | 644      | 6       | 0            |
| 18  | XR    | 574   | 0        | 644      | 7       | 0            |
| 19  | QS    | 665   | 0        | 686      | 16      | 0            |
| 19  | XS    | 674   | 0        | 699      | 10      | 0            |
| 20  | QT    | 763   | 0        | 860      | 6       | 0            |
| 20  | XT    | 763   | 0        | 861      | 5       | 0            |
| 21  | QU    | 217   | 0        | 234      | 4       | 0            |
| 21  | XU    | 217   | 0        | 234      | 5       | 0            |
| 22  | QV    | 1644  | 0        | 836      | 4       | 0            |
| 22  | XV    | 1644  | 0        | 836      | 4       | 0            |
| 23  | QX    | 259   | 0        | 129      | 2       | 0            |
| 23  | XX    | 239   | 0        | 119      | 1       | 0            |
| 24  | RA    | 62071 | 0        | 31285    | 282     | 0            |
| 24  | YA    | 62091 | 0        | 31293    | 278     | 0            |
| 25  | RB    | 2573  | 0        | 1306     | 14      | 0            |
| 25  | YB    | 2573  | 0        | 1306     | 12      | 0            |
| 26  | RD    | 2115  | 0        | 2195     | 41      | 0            |
| 26  | YD    | 2115  | 0        | 2195     | 39      | 0            |
| 27  | RE    | 1568  | 0        | 1634     | 26      | 0            |
| 27  | YE    | 1568  | 0        | 1634     | 27      | 0            |
| 28  | RF    | 1585  | 0        | 1632     | 20      | 0            |
| 28  | YF    | 1585  | 0        | 1632     | 14      | 0            |
| 29  | RG    | 1474  | 0        | 1535     | 18      | 0            |
| 29  | YG    | 1474  | 0        | 1535     | 22      | 0            |
| 30  | RH    | 1336  | 0        | 1418     | 19      | 0            |
| 30  | YH    | 1336  | 0        | 1418     | 20      | 1            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | RI    | 1136  | 0        | 1223     | 17      | 0            |
| 31  | YI    | 1136  | 0        | 1223     | 19      | 0            |
| 32  | RN    | 1104  | 0        | 1180     | 11      | 0            |
| 32  | YN    | 1104  | 0        | 1180     | 7       | 0            |
| 33  | RO    | 933   | 0        | 996      | 12      | 0            |
| 33  | YO    | 933   | 0        | 996      | 11      | 0            |
| 34  | RP    | 1145  | 0        | 1227     | 22      | 0            |
| 34  | YP    | 1122  | 0        | 1206     | 22      | 0            |
| 35  | RQ    | 1122  | 0        | 1179     | 27      | 0            |
| 35  | YQ    | 1122  | 0        | 1179     | 24      | 0            |
| 36  | RR    | 960   | 0        | 1021     | 9       | 0            |
| 36  | YR    | 960   | 0        | 1021     | 13      | 0            |
| 37  | RS    | 882   | 0        | 943      | 11      | 0            |
| 37  | YS    | 882   | 0        | 943      | 14      | 0            |
| 38  | RT    | 1141  | 0        | 1202     | 22      | 0            |
| 38  | YT    | 1141  | 0        | 1202     | 23      | 0            |
| 39  | RU    | 964   | 0        | 1022     | 21      | 0            |
| 39  | YU    | 964   | 0        | 1021     | 19      | 0            |
| 40  | RV    | 779   | 0        | 852      | 11      | 0            |
| 40  | YV    | 779   | 0        | 852      | 10      | 3            |
| 41  | RW    | 900   | 0        | 964      | 7       | 2            |
| 41  | YW    | 900   | 0        | 964      | 6       | 0            |
| 42  | RX    | 725   | 0        | 778      | 10      | 0            |
| 42  | YX    | 725   | 0        | 778      | 14      | 0            |
| 43  | RY    | 818   | 0        | 909      | 14      | 4            |
| 43  | YY    | 818   | 0        | 909      | 11      | 3            |
| 44  | RZ    | 1461  | 0        | 1493     | 22      | 0            |
| 44  | YZ    | 1461  | 0        | 1493     | 21      | 0            |
| 45  | R0    | 643   | 0        | 667      | 11      | 0            |
| 45  | Y0    | 599   | 0        | 617      | 12      | 0            |
| 46  | R1    | 763   | 0        | 848      | 15      | 0            |
| 46  | Y1    | 729   | 0        | 802      | 9       | 0            |
| 47  | R2    | 581   | 0        | 629      | 6       | 0            |
| 47  | Y2    | 581   | 0        | 629      | 8       | 4            |
| 48  | R3    | 469   | 0        | 518      | 8       | 0            |
| 48  | Y3    | 469   | 0        | 518      | 7       | 0            |
| 49  | R4    | 565   | 0        | 557      | 7       | 0            |
| 49  | Y4    | 565   | 0        | 557      | 9       | 0            |
| 50  | R5    | 459   | 0        | 476      | 9       | 0            |
| 50  | Y5    | 459   | 0        | 479      | 8       | 3            |
| 51  | R6    | 453   | 0        | 473      | 4       | 0            |
| 51  | Y6    | 453   | 0        | 473      | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 52  | R7    | 409   | 0        | 454      | 2       | 0            |
| 52  | Y7    | 418   | 0        | 467      | 5       | 0            |
| 53  | R8    | 517   | 0        | 582      | 14      | 0            |
| 53  | Y8    | 517   | 0        | 582      | 9       | 0            |
| 54  | R9    | 307   | 0        | 335      | 4       | 0            |
| 54  | Y9    | 307   | 0        | 335      | 4       | 0            |
| 55  | QA    | 80    | 0        | 0        | 0       | 0            |
| 55  | QC    | 1     | 0        | 0        | 0       | 0            |
| 55  | QF    | 1     | 0        | 0        | 0       | 0            |
| 55  | QH    | 1     | 0        | 0        | 0       | 0            |
| 55  | QT    | 1     | 0        | 0        | 0       | 0            |
| 55  | QV    | 6     | 0        | 0        | 0       | 0            |
| 55  | R0    | 2     | 0        | 0        | 0       | 0            |
| 55  | R8    | 1     | 0        | 0        | 0       | 0            |
| 55  | RA    | 521   | 0        | 0        | 0       | 0            |
| 55  | RB    | 11    | 0        | 0        | 0       | 0            |
| 55  | RD    | 1     | 0        | 0        | 0       | 0            |
| 55  | RE    | 4     | 0        | 0        | 0       | 0            |
| 55  | RN    | 1     | 0        | 0        | 0       | 0            |
| 55  | RO    | 1     | 0        | 0        | 0       | 0            |
| 55  | RP    | 3     | 0        | 0        | 0       | 0            |
| 55  | RQ    | 3     | 0        | 0        | 0       | 0            |
| 55  | RR    | 2     | 0        | 0        | 0       | 0            |
| 55  | RT    | 1     | 0        | 0        | 0       | 0            |
| 55  | XA    | 98    | 0        | 0        | 0       | 0            |
| 55  | XE    | 1     | 0        | 0        | 0       | 0            |
| 55  | XL    | 2     | 0        | 0        | 0       | 0            |
| 55  | XM    | 2     | 0        | 0        | 0       | 0            |
| 55  | XQ    | 1     | 0        | 0        | 0       | 0            |
| 55  | XS    | 1     | 0        | 0        | 0       | 0            |
| 55  | XV    | 8     | 0        | 0        | 0       | 0            |
| 55  | XX    | 1     | 0        | 0        | 0       | 0            |
| 55  | Y0    | 2     | 0        | 0        | 0       | 0            |
| 55  | Y1    | 1     | 0        | 0        | 0       | 0            |
| 55  | Y5    | 1     | 0        | 0        | 0       | 0            |
| 55  | Y7    | 1     | 0        | 0        | 0       | 0            |
| 55  | Y8    | 2     | 0        | 0        | 0       | 0            |
| 55  | YA    | 551   | 0        | 0        | 0       | 0            |
| 55  | YB    | 12    | 0        | 0        | 0       | 0            |
| 55  | YD    | 3     | 0        | 0        | 0       | 0            |
| 55  | YE    | 4     | 0        | 0        | 0       | 0            |
| 55  | YF    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 55  | YO    | 1      | 0        | 0        | 0       | 0            |
| 55  | YP    | 2      | 0        | 0        | 0       | 0            |
| 55  | YQ    | 4      | 0        | 0        | 0       | 0            |
| 55  | YU    | 1      | 0        | 0        | 0       | 0            |
| 55  | YX    | 2      | 0        | 0        | 0       | 0            |
| 55  | YY    | 1      | 0        | 0        | 0       | 0            |
| 56  | QD    | 8      | 0        | 0        | 0       | 0            |
| 56  | XD    | 8      | 0        | 0        | 0       | 0            |
| 57  | QN    | 1      | 0        | 0        | 0       | 0            |
| 57  | R4    | 1      | 0        | 0        | 0       | 0            |
| 57  | R5    | 1      | 0        | 0        | 0       | 0            |
| 57  | R6    | 1      | 0        | 0        | 0       | 0            |
| 57  | R9    | 1      | 0        | 0        | 0       | 0            |
| 57  | RY    | 1      | 0        | 0        | 0       | 0            |
| 57  | XN    | 1      | 0        | 0        | 0       | 0            |
| 57  | Y4    | 1      | 0        | 0        | 0       | 0            |
| 57  | Y5    | 1      | 0        | 0        | 0       | 0            |
| 57  | Y6    | 1      | 0        | 0        | 0       | 0            |
| 57  | Y9    | 1      | 0        | 0        | 0       | 0            |
| 57  | YY    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 291753 | 0        | 197646   | 1875    | 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 4.

The worst 5 of 1875 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:RA:602:G:HO2'  | 24:RA:604:G:HO2'  | 1.26                     | 0.79              |
| 46:Y1:91:LYS:HE2  | 46:Y1:92:LYS:HE2  | 1.69                     | 0.74              |
| 1:QA:664:G:H22    | 1:QA:741:G:H1     | 1.36                     | 0.74              |
| 24:RA:2343:C:HO2' | 24:RA:2373:G:HO2' | 1.36                     | 0.73              |
| 1:XA:686:U:H1'    | 11:XK:42:TRP:HE1  | 1.54                     | 0.73              |

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) |
|-----------------|-------------------------|--------------------------|-------------------|
| 43:RY:21:LYS:NZ | 47:Y2:71:ASN:CB[3_555]  | 1.64                     | 0.56              |
| 43:RY:19:LYS:O  | 47:Y2:71:ASN:ND2[3_555] | 1.79                     | 0.41              |

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| Atom-1           | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 41:RW:63:ASP:OD1 | 43:YY:92:ASN:ND2[3_555] | 1.88                     | 0.32              |
| 40:YV:49:THR:O   | 50:Y5:59:GLU:OE2[4_445] | 1.90                     | 0.30              |
| 40:YV:49:THR:OG1 | 50:Y5:60:VAL:O[4_445]   | 1.91                     | 0.29              |

## 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   | QB    | 233/256 (91%) | 205 (88%) | 27 (12%) | 1 (0%)   | 30          | 60  |
| 2   | XB    | 234/256 (91%) | 210 (90%) | 24 (10%) | 0        | 100         | 100 |
| 3   | QC    | 203/239 (85%) | 188 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 3   | XC    | 203/239 (85%) | 188 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 4   | QD    | 206/209 (99%) | 193 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 4   | XD    | 206/209 (99%) | 193 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 5   | QE    | 149/162 (92%) | 142 (95%) | 6 (4%)   | 1 (1%)   | 18          | 50  |
| 5   | XE    | 149/162 (92%) | 142 (95%) | 6 (4%)   | 1 (1%)   | 18          | 50  |
| 6   | QF    | 99/101 (98%)  | 99 (100%) | 0        | 0        | 100         | 100 |
| 6   | XF    | 99/101 (98%)  | 99 (100%) | 0        | 0        | 100         | 100 |
| 7   | QG    | 153/156 (98%) | 150 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 7   | XG    | 153/156 (98%) | 150 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 8   | QH    | 135/138 (98%) | 132 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 8   | XH    | 135/138 (98%) | 132 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 9   | QI    | 125/128 (98%) | 114 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 9   | XI    | 124/128 (97%) | 114 (92%) | 10 (8%)  | 0        | 100         | 100 |
| 10  | QJ    | 97/105 (92%)  | 88 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 10  | XJ    | 94/105 (90%)  | 83 (88%)  | 11 (12%) | 0        | 100         | 100 |
| 11  | QK    | 117/129 (91%) | 109 (93%) | 8 (7%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 11  | XK    | 114/129 (88%) | 107 (94%) | 7 (6%)   | 0        | 100         | 100 |
| 12  | QL    | 123/132 (93%) | 104 (85%) | 19 (15%) | 0        | 100         | 100 |
| 12  | XL    | 120/132 (91%) | 105 (88%) | 14 (12%) | 1 (1%)   | 16          | 47  |
| 13  | QM    | 118/126 (94%) | 101 (86%) | 16 (14%) | 1 (1%)   | 16          | 47  |
| 13  | XM    | 117/126 (93%) | 100 (86%) | 17 (14%) | 0        | 100         | 100 |
| 14  | QN    | 58/61 (95%)   | 53 (91%)  | 4 (7%)   | 1 (2%)   | 7           | 32  |
| 14  | XN    | 58/61 (95%)   | 53 (91%)  | 4 (7%)   | 1 (2%)   | 7           | 32  |
| 15  | QO    | 86/89 (97%)   | 83 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 15  | XO    | 85/89 (96%)   | 85 (100%) | 0        | 0        | 100         | 100 |
| 16  | QP    | 82/88 (93%)   | 81 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 16  | XP    | 82/88 (93%)   | 81 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 17  | QQ    | 98/105 (93%)  | 97 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 17  | XQ    | 98/105 (93%)  | 97 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 18  | QR    | 68/88 (77%)   | 66 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 18  | XR    | 68/88 (77%)   | 66 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 19  | QS    | 81/93 (87%)   | 71 (88%)  | 10 (12%) | 0        | 100         | 100 |
| 19  | XS    | 82/93 (88%)   | 66 (80%)  | 15 (18%) | 1 (1%)   | 10          | 39  |
| 20  | QT    | 97/106 (92%)  | 90 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 20  | XT    | 97/106 (92%)  | 90 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 21  | QU    | 23/27 (85%)   | 21 (91%)  | 2 (9%)   | 0        | 100         | 100 |
| 21  | XU    | 23/27 (85%)   | 21 (91%)  | 2 (9%)   | 0        | 100         | 100 |
| 26  | RD    | 270/276 (98%) | 246 (91%) | 23 (8%)  | 1 (0%)   | 30          | 60  |
| 26  | YD    | 270/276 (98%) | 246 (91%) | 23 (8%)  | 1 (0%)   | 30          | 60  |
| 27  | RE    | 203/206 (98%) | 165 (81%) | 37 (18%) | 1 (0%)   | 24          | 57  |
| 27  | YE    | 203/206 (98%) | 165 (81%) | 37 (18%) | 1 (0%)   | 24          | 57  |
| 28  | RF    | 200/210 (95%) | 186 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 28  | YF    | 200/210 (95%) | 186 (93%) | 14 (7%)  | 0        | 100         | 100 |
| 29  | RG    | 179/182 (98%) | 152 (85%) | 26 (14%) | 1 (1%)   | 21          | 53  |
| 29  | YG    | 179/182 (98%) | 152 (85%) | 26 (14%) | 1 (1%)   | 21          | 53  |
| 30  | RH    | 172/180 (96%) | 149 (87%) | 19 (11%) | 4 (2%)   | 5           | 26  |
| 30  | YH    | 172/180 (96%) | 149 (87%) | 19 (11%) | 4 (2%)   | 5           | 26  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 31  | RI    | 144/148 (97%) | 126 (88%) | 16 (11%) | 2 (1%)   | 9           | 36  |
| 31  | YI    | 144/148 (97%) | 126 (88%) | 16 (11%) | 2 (1%)   | 9           | 36  |
| 32  | RN    | 136/140 (97%) | 124 (91%) | 11 (8%)  | 1 (1%)   | 18          | 50  |
| 32  | YN    | 136/140 (97%) | 124 (91%) | 11 (8%)  | 1 (1%)   | 18          | 50  |
| 33  | RO    | 120/122 (98%) | 115 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 33  | YO    | 120/122 (98%) | 115 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 34  | RP    | 148/150 (99%) | 122 (82%) | 25 (17%) | 1 (1%)   | 18          | 50  |
| 34  | YP    | 145/150 (97%) | 115 (79%) | 29 (20%) | 1 (1%)   | 18          | 50  |
| 35  | RQ    | 139/141 (99%) | 117 (84%) | 21 (15%) | 1 (1%)   | 18          | 50  |
| 35  | YQ    | 139/141 (99%) | 117 (84%) | 21 (15%) | 1 (1%)   | 18          | 50  |
| 36  | RR    | 115/118 (98%) | 107 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 36  | YR    | 115/118 (98%) | 107 (93%) | 7 (6%)   | 1 (1%)   | 14          | 45  |
| 37  | RS    | 109/112 (97%) | 91 (84%)  | 17 (16%) | 1 (1%)   | 14          | 45  |
| 37  | YS    | 109/112 (97%) | 91 (84%)  | 17 (16%) | 1 (1%)   | 14          | 45  |
| 38  | RT    | 135/146 (92%) | 120 (89%) | 13 (10%) | 2 (2%)   | 8           | 35  |
| 38  | YT    | 135/146 (92%) | 120 (89%) | 13 (10%) | 2 (2%)   | 8           | 35  |
| 39  | RU    | 115/118 (98%) | 107 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 39  | YU    | 115/118 (98%) | 107 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 40  | RV    | 99/101 (98%)  | 84 (85%)  | 14 (14%) | 1 (1%)   | 12          | 43  |
| 40  | YV    | 99/101 (98%)  | 84 (85%)  | 14 (14%) | 1 (1%)   | 12          | 43  |
| 41  | RW    | 111/113 (98%) | 105 (95%) | 5 (4%)   | 1 (1%)   | 14          | 45  |
| 41  | YW    | 111/113 (98%) | 105 (95%) | 5 (4%)   | 1 (1%)   | 14          | 45  |
| 42  | RX    | 90/96 (94%)   | 87 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 42  | YX    | 90/96 (94%)   | 86 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 43  | RY    | 105/110 (96%) | 98 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 43  | YY    | 105/110 (96%) | 98 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 44  | RZ    | 181/206 (88%) | 148 (82%) | 30 (17%) | 3 (2%)   | 7           | 32  |
| 44  | YZ    | 181/206 (88%) | 148 (82%) | 30 (17%) | 3 (2%)   | 7           | 32  |
| 45  | R0    | 79/85 (93%)   | 76 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 45  | Y0    | 73/85 (86%)   | 69 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 46  | R1    | 95/98 (97%)   | 84 (88%)  | 11 (12%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 46  | Y1    | 91/98 (93%)       | 80 (88%)    | 11 (12%)  | 0        | 100         | 100 |
| 47  | R2    | 67/72 (93%)       | 62 (92%)    | 4 (6%)    | 1 (2%)   | 8           | 35  |
| 47  | Y2    | 67/72 (93%)       | 62 (92%)    | 4 (6%)    | 1 (2%)   | 8           | 35  |
| 48  | R3    | 57/60 (95%)       | 56 (98%)    | 1 (2%)    | 0        | 100         | 100 |
| 48  | Y3    | 57/60 (95%)       | 56 (98%)    | 1 (2%)    | 0        | 100         | 100 |
| 49  | R4    | 67/71 (94%)       | 55 (82%)    | 11 (16%)  | 1 (2%)   | 8           | 35  |
| 49  | Y4    | 67/71 (94%)       | 55 (82%)    | 11 (16%)  | 1 (2%)   | 8           | 35  |
| 50  | R5    | 57/60 (95%)       | 55 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 50  | Y5    | 57/60 (95%)       | 55 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 51  | R6    | 51/54 (94%)       | 49 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 51  | Y6    | 51/54 (94%)       | 49 (96%)    | 2 (4%)    | 0        | 100         | 100 |
| 52  | R7    | 45/49 (92%)       | 45 (100%)   | 0         | 0        | 100         | 100 |
| 52  | Y7    | 46/49 (94%)       | 45 (98%)    | 1 (2%)    | 0        | 100         | 100 |
| 53  | R8    | 62/65 (95%)       | 49 (79%)    | 11 (18%)  | 2 (3%)   | 3           | 19  |
| 53  | Y8    | 62/65 (95%)       | 49 (79%)    | 11 (18%)  | 2 (3%)   | 3           | 19  |
| 54  | R9    | 35/37 (95%)       | 35 (100%)   | 0         | 0        | 100         | 100 |
| 54  | Y9    | 35/37 (95%)       | 35 (100%)   | 0         | 0        | 100         | 100 |
| All | All   | 11452/12128 (94%) | 10380 (91%) | 1015 (9%) | 57 (0%)  | 24          | 57  |

5 of 57 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | RE    | 18  | ASP  |
| 31  | RI    | 15  | VAL  |
| 38  | RT    | 124 | ASP  |
| 44  | RZ    | 53  | ILE  |
| 12  | XL    | 105 | TYR  |

### 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   | QB    | 203/220 (92%) | 202 (100%) | 1 (0%)   | 81          | 83  |
| 2   | XB    | 204/220 (93%) | 203 (100%) | 1 (0%)   | 81          | 83  |
| 3   | QC    | 159/188 (85%) | 159 (100%) | 0        | 100         | 100 |
| 3   | XC    | 159/188 (85%) | 159 (100%) | 0        | 100         | 100 |
| 4   | QD    | 180/181 (99%) | 179 (99%)  | 1 (1%)   | 78          | 82  |
| 4   | XD    | 180/181 (99%) | 179 (99%)  | 1 (1%)   | 78          | 82  |
| 5   | QE    | 116/123 (94%) | 116 (100%) | 0        | 100         | 100 |
| 5   | XE    | 116/123 (94%) | 116 (100%) | 0        | 100         | 100 |
| 6   | QF    | 90/90 (100%)  | 90 (100%)  | 0        | 100         | 100 |
| 6   | XF    | 90/90 (100%)  | 90 (100%)  | 0        | 100         | 100 |
| 7   | QG    | 126/127 (99%) | 126 (100%) | 0        | 100         | 100 |
| 7   | XG    | 126/127 (99%) | 126 (100%) | 0        | 100         | 100 |
| 8   | QH    | 118/119 (99%) | 118 (100%) | 0        | 100         | 100 |
| 8   | XH    | 118/119 (99%) | 118 (100%) | 0        | 100         | 100 |
| 9   | QI    | 98/99 (99%)   | 98 (100%)  | 0        | 100         | 100 |
| 9   | XI    | 97/99 (98%)   | 97 (100%)  | 0        | 100         | 100 |
| 10  | QJ    | 89/92 (97%)   | 89 (100%)  | 0        | 100         | 100 |
| 10  | XJ    | 86/92 (94%)   | 85 (99%)   | 1 (1%)   | 63          | 76  |
| 11  | QK    | 90/99 (91%)   | 89 (99%)   | 1 (1%)   | 65          | 77  |
| 11  | XK    | 88/99 (89%)   | 88 (100%)  | 0        | 100         | 100 |
| 12  | QL    | 104/109 (95%) | 103 (99%)  | 1 (1%)   | 68          | 78  |
| 12  | XL    | 103/109 (94%) | 102 (99%)  | 1 (1%)   | 68          | 78  |
| 13  | QM    | 96/101 (95%)  | 96 (100%)  | 0        | 100         | 100 |
| 13  | XM    | 95/101 (94%)  | 95 (100%)  | 0        | 100         | 100 |
| 14  | QN    | 49/50 (98%)   | 48 (98%)   | 1 (2%)   | 48          | 69  |
| 14  | XN    | 49/50 (98%)   | 48 (98%)   | 1 (2%)   | 48          | 69  |
| 15  | QO    | 79/80 (99%)   | 79 (100%)  | 0        | 100         | 100 |
| 15  | XO    | 79/80 (99%)   | 79 (100%)  | 0        | 100         | 100 |
| 16  | QP    | 72/74 (97%)   | 71 (99%)   | 1 (1%)   | 59          | 74  |
| 16  | XP    | 72/74 (97%)   | 71 (99%)   | 1 (1%)   | 59          | 74  |
| 17  | QQ    | 95/97 (98%)   | 95 (100%)  | 0        | 100         | 100 |
| 17  | XQ    | 95/97 (98%)   | 95 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 18  | QR    | 61/77 (79%)    | 61 (100%)  | 0        | 100         | 100 |
| 18  | XR    | 61/77 (79%)    | 61 (100%)  | 0        | 100         | 100 |
| 19  | QS    | 72/80 (90%)    | 71 (99%)   | 1 (1%)   | 59          | 74  |
| 19  | XS    | 73/80 (91%)    | 73 (100%)  | 0        | 100         | 100 |
| 20  | QT    | 76/82 (93%)    | 76 (100%)  | 0        | 100         | 100 |
| 20  | XT    | 76/82 (93%)    | 76 (100%)  | 0        | 100         | 100 |
| 21  | QU    | 20/22 (91%)    | 20 (100%)  | 0        | 100         | 100 |
| 21  | XU    | 20/22 (91%)    | 20 (100%)  | 0        | 100         | 100 |
| 26  | RD    | 214/218 (98%)  | 212 (99%)  | 2 (1%)   | 70          | 79  |
| 26  | YD    | 214/218 (98%)  | 212 (99%)  | 2 (1%)   | 70          | 79  |
| 27  | RE    | 165/166 (99%)  | 161 (98%)  | 4 (2%)   | 43          | 67  |
| 27  | YE    | 165/166 (99%)  | 161 (98%)  | 4 (2%)   | 43          | 67  |
| 28  | RF    | 161/166 (97%)  | 160 (99%)  | 1 (1%)   | 78          | 82  |
| 28  | YF    | 161/166 (97%)  | 160 (99%)  | 1 (1%)   | 78          | 82  |
| 29  | RG    | 155/156 (99%)  | 154 (99%)  | 1 (1%)   | 78          | 82  |
| 29  | YG    | 155/156 (99%)  | 154 (99%)  | 1 (1%)   | 78          | 82  |
| 30  | RH    | 145/148 (98%)  | 143 (99%)  | 2 (1%)   | 59          | 74  |
| 30  | YH    | 145/148 (98%)  | 143 (99%)  | 2 (1%)   | 59          | 74  |
| 31  | RI    | 122/124 (98%)  | 121 (99%)  | 1 (1%)   | 73          | 80  |
| 31  | YI    | 122/124 (98%)  | 121 (99%)  | 1 (1%)   | 73          | 80  |
| 32  | RN    | 117/119 (98%)  | 115 (98%)  | 2 (2%)   | 53          | 72  |
| 32  | YN    | 117/119 (98%)  | 115 (98%)  | 2 (2%)   | 53          | 72  |
| 33  | RO    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 33  | YO    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 34  | RP    | 116/116 (100%) | 115 (99%)  | 1 (1%)   | 70          | 79  |
| 34  | YP    | 114/116 (98%)  | 112 (98%)  | 2 (2%)   | 51          | 71  |
| 35  | RQ    | 111/111 (100%) | 109 (98%)  | 2 (2%)   | 51          | 71  |
| 35  | YQ    | 111/111 (100%) | 109 (98%)  | 2 (2%)   | 51          | 71  |
| 36  | RR    | 100/101 (99%)  | 99 (99%)   | 1 (1%)   | 68          | 78  |
| 36  | YR    | 100/101 (99%)  | 100 (100%) | 0        | 100         | 100 |
| 37  | RS    | 87/88 (99%)    | 87 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 37  | YS    | 87/88 (99%)   | 87 (100%) | 0        | 100         | 100 |
| 38  | RT    | 120/127 (94%) | 118 (98%) | 2 (2%)   | 53          | 72  |
| 38  | YT    | 120/127 (94%) | 118 (98%) | 2 (2%)   | 53          | 72  |
| 39  | RU    | 93/94 (99%)   | 91 (98%)  | 2 (2%)   | 45          | 68  |
| 39  | YU    | 93/94 (99%)   | 91 (98%)  | 2 (2%)   | 45          | 68  |
| 40  | RV    | 82/82 (100%)  | 82 (100%) | 0        | 100         | 100 |
| 40  | YV    | 82/82 (100%)  | 82 (100%) | 0        | 100         | 100 |
| 41  | RW    | 92/92 (100%)  | 92 (100%) | 0        | 100         | 100 |
| 41  | YW    | 92/92 (100%)  | 92 (100%) | 0        | 100         | 100 |
| 42  | RX    | 74/78 (95%)   | 73 (99%)  | 1 (1%)   | 59          | 74  |
| 42  | YX    | 74/78 (95%)   | 73 (99%)  | 1 (1%)   | 59          | 74  |
| 43  | RY    | 88/91 (97%)   | 88 (100%) | 0        | 100         | 100 |
| 43  | YY    | 88/91 (97%)   | 88 (100%) | 0        | 100         | 100 |
| 44  | RZ    | 162/179 (90%) | 161 (99%) | 1 (1%)   | 78          | 82  |
| 44  | YZ    | 162/179 (90%) | 161 (99%) | 1 (1%)   | 78          | 82  |
| 45  | R0    | 65/67 (97%)   | 65 (100%) | 0        | 100         | 100 |
| 45  | Y0    | 61/67 (91%)   | 61 (100%) | 0        | 100         | 100 |
| 46  | R1    | 82/83 (99%)   | 82 (100%) | 0        | 100         | 100 |
| 46  | Y1    | 78/83 (94%)   | 78 (100%) | 0        | 100         | 100 |
| 47  | R2    | 64/67 (96%)   | 64 (100%) | 0        | 100         | 100 |
| 47  | Y2    | 64/67 (96%)   | 64 (100%) | 0        | 100         | 100 |
| 48  | R3    | 51/52 (98%)   | 51 (100%) | 0        | 100         | 100 |
| 48  | Y3    | 51/52 (98%)   | 51 (100%) | 0        | 100         | 100 |
| 49  | R4    | 62/63 (98%)   | 61 (98%)  | 1 (2%)   | 55          | 72  |
| 49  | Y4    | 62/63 (98%)   | 61 (98%)  | 1 (2%)   | 55          | 72  |
| 50  | R5    | 51/52 (98%)   | 51 (100%) | 0        | 100         | 100 |
| 50  | Y5    | 51/52 (98%)   | 51 (100%) | 0        | 100         | 100 |
| 51  | R6    | 51/52 (98%)   | 51 (100%) | 0        | 100         | 100 |
| 51  | Y6    | 51/52 (98%)   | 51 (100%) | 0        | 100         | 100 |
| 52  | R7    | 40/42 (95%)   | 40 (100%) | 0        | 100         | 100 |
| 52  | Y7    | 41/42 (98%)   | 41 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 53  | R8    | 54/55 (98%)      | 53 (98%)   | 1 (2%)   | 50          | 70  |
| 53  | Y8    | 54/55 (98%)      | 53 (98%)   | 1 (2%)   | 50          | 70  |
| 54  | R9    | 34/34 (100%)     | 34 (100%)  | 0        | 100         | 100 |
| 54  | Y9    | 34/34 (100%)     | 34 (100%)  | 0        | 100         | 100 |
| All | All   | 9687/10066 (96%) | 9624 (99%) | 63 (1%)  | 76          | 81  |

5 of 63 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | RX    | 66  | LEU  |
| 38  | YT    | 30  | VAL  |
| 12  | XL    | 83  | VAL  |
| 35  | YQ    | 96  | VAL  |
| 42  | YX    | 66  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | XO    | 62  | GLN  |
| 35  | YQ    | 57  | HIS  |
| 19  | XS    | 47  | HIS  |
| 28  | YF    | 40  | GLN  |
| 36  | YR    | 71  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | QA    | 1496/1508 (99%) | 280 (18%)         | 35 (2%)         |
| 1   | XA    | 1498/1508 (99%) | 281 (18%)         | 31 (2%)         |
| 22  | QV    | 76/77 (98%)     | 14 (18%)          | 2 (2%)          |
| 22  | XV    | 76/77 (98%)     | 14 (18%)          | 2 (2%)          |
| 23  | QX    | 11/25 (44%)     | 5 (45%)           | 1 (9%)          |
| 23  | XX    | 10/25 (40%)     | 6 (60%)           | 0               |
| 24  | RA    | 2879/2915 (98%) | 580 (20%)         | 38 (1%)         |
| 24  | YA    | 2880/2915 (98%) | 574 (19%)         | 40 (1%)         |
| 25  | RB    | 119/122 (97%)   | 22 (18%)          | 2 (1%)          |
| 25  | YB    | 119/122 (97%)   | 22 (18%)          | 2 (1%)          |
| All | All   | 9164/9294 (98%) | 1798 (19%)        | 153 (1%)        |

5 of 1798 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | QA    | 6   | G    |
| 1   | QA    | 9   | G    |
| 1   | QA    | 22  | G    |
| 1   | QA    | 32  | A    |
| 1   | QA    | 39  | G    |

5 of 153 RNA pucker outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 24  | YA    | 271(B) | G    |
| 24  | YA    | 1992   | G    |
| 24  | YA    | 503    | A    |
| 24  | YA    | 1130   | U    |
| 24  | YA    | 2867   | 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 1358 ligands modelled in this entry, 1356 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 56  | SF4  | QD    | 301 | 4    | 0,12,12      | -    | -           | -           |      |             |
| 56  | SF4  | XD    | 301 | 4    | 0,12,12      | -    | -           | -           |      |             |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 56  | SF4  | QD    | 301 | 4    | -       | -        | 0/6/5/5 |
| 56  | SF4  | XD    | 301 | 4    | -       | -        | 0/6/5/5 |

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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   | QA    | 1498/1508 (99%) | 0.06   | 18 (1%) 76 57 | 69, 120, 217, 376     | 0     |
| 1   | XA    | 1500/1508 (99%) | -0.07  | 17 (1%) 78 60 | 52, 97, 195, 317      | 0     |
| 2   | QB    | 235/256 (91%)   | 0.92   | 24 (10%) 12 7 | 111, 178, 229, 291    | 0     |
| 2   | XB    | 236/256 (92%)   | 0.76   | 16 (6%) 23 13 | 86, 142, 206, 231     | 0     |
| 3   | QC    | 205/239 (85%)   | 0.85   | 21 (10%) 12 7 | 128, 179, 228, 264    | 0     |
| 3   | XC    | 205/239 (85%)   | 0.97   | 25 (12%) 8 5  | 78, 123, 180, 231     | 0     |
| 4   | QD    | 208/209 (99%)   | 1.34   | 37 (17%) 4 2  | 88, 132, 181, 220     | 0     |
| 4   | XD    | 208/209 (99%)   | 0.89   | 22 (10%) 11 6 | 69, 104, 143, 192     | 0     |
| 5   | QE    | 151/162 (93%)   | 1.10   | 21 (13%) 6 4  | 96, 137, 177, 195     | 0     |
| 5   | XE    | 151/162 (93%)   | 0.69   | 12 (7%) 18 11 | 67, 104, 149, 192     | 0     |
| 6   | QF    | 101/101 (100%)  | 0.62   | 6 (5%) 28 16  | 90, 135, 177, 215     | 0     |
| 6   | XF    | 101/101 (100%)  | 0.89   | 7 (6%) 23 13  | 75, 111, 163, 201     | 0     |
| 7   | QG    | 155/156 (99%)   | 0.80   | 12 (7%) 19 11 | 110, 145, 205, 236    | 0     |
| 7   | XG    | 155/156 (99%)   | 0.93   | 21 (13%) 7 5  | 85, 116, 162, 208     | 0     |
| 8   | QH    | 137/138 (99%)   | 1.02   | 20 (14%) 6 4  | 104, 141, 183, 222    | 0     |
| 8   | XH    | 137/138 (99%)   | 0.84   | 13 (9%) 14 8  | 78, 113, 150, 194     | 0     |
| 9   | QI    | 127/128 (99%)   | 1.53   | 31 (24%) 2 2  | 109, 159, 203, 254    | 0     |
| 9   | XI    | 126/128 (98%)   | 0.85   | 13 (10%) 12 7 | 66, 136, 176, 241     | 0     |
| 10  | QJ    | 99/105 (94%)    | 1.39   | 18 (18%) 3 2  | 128, 174, 236, 263    | 0     |
| 10  | XJ    | 96/105 (91%)    | 1.32   | 21 (21%) 2 2  | 98, 143, 196, 257     | 0     |
| 11  | QK    | 119/129 (92%)   | 1.00   | 13 (10%) 10 6 | 91, 122, 169, 230     | 0     |
| 11  | XK    | 116/129 (89%)   | 1.11   | 17 (14%) 6 4  | 60, 103, 157, 207     | 0     |
| 12  | QL    | 125/132 (94%)   | 1.11   | 18 (14%) 6 4  | 76, 106, 154, 233     | 0     |
| 12  | XL    | 122/132 (92%)   | 1.28   | 27 (22%) 2 2  | 48, 85, 137, 203      | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | QM    | 120/126 (95%)   | 0.86   | 15 (12%) 8 5  | 110, 155, 195, 248    | 0     |
| 13  | XM    | 119/126 (94%)   | 0.81   | 11 (9%) 14 8  | 81, 122, 172, 255     | 0     |
| 14  | QN    | 60/61 (98%)     | 1.26   | 12 (20%) 3 2  | 122, 164, 214, 227    | 0     |
| 14  | XN    | 60/61 (98%)     | 1.18   | 10 (16%) 4 2  | 87, 112, 152, 165     | 0     |
| 15  | QO    | 88/89 (98%)     | 1.01   | 10 (11%) 10 6 | 80, 129, 170, 209     | 0     |
| 15  | XO    | 87/89 (97%)     | 0.47   | 2 (2%) 61 40  | 56, 99, 147, 185      | 0     |
| 16  | QP    | 84/88 (95%)     | 1.00   | 11 (13%) 7 5  | 70, 112, 150, 190     | 0     |
| 16  | XP    | 84/88 (95%)     | 1.26   | 18 (21%) 2 2  | 85, 115, 160, 168     | 0     |
| 17  | QQ    | 100/105 (95%)   | 1.37   | 26 (26%) 1 1  | 82, 118, 158, 193     | 0     |
| 17  | XQ    | 100/105 (95%)   | 0.97   | 15 (15%) 5 3  | 74, 103, 153, 196     | 0     |
| 18  | QR    | 70/88 (79%)     | 0.58   | 3 (4%) 40 23  | 93, 131, 165, 199     | 0     |
| 18  | XR    | 70/88 (79%)     | 0.65   | 3 (4%) 40 23  | 57, 105, 148, 173     | 0     |
| 19  | QS    | 83/93 (89%)     | 1.31   | 22 (26%) 1 1  | 133, 168, 212, 243    | 0     |
| 19  | XS    | 84/93 (90%)     | 0.78   | 6 (7%) 22 13  | 83, 128, 172, 237     | 0     |
| 20  | QT    | 99/106 (93%)    | 1.02   | 11 (11%) 10 6 | 74, 112, 166, 226     | 0     |
| 20  | XT    | 99/106 (93%)    | 1.67   | 33 (33%) 1 1  | 83, 119, 185, 247     | 0     |
| 21  | QU    | 25/27 (92%)     | 1.34   | 4 (16%) 5 3   | 115, 151, 181, 206    | 0     |
| 21  | XU    | 25/27 (92%)     | 0.90   | 4 (16%) 5 3   | 98, 114, 170, 194     | 0     |
| 22  | QV    | 77/77 (100%)    | 0.40   | 2 (2%) 57 36  | 82, 119, 166, 238     | 0     |
| 22  | XV    | 77/77 (100%)    | 0.08   | 3 (3%) 43 25  | 58, 95, 144, 187      | 0     |
| 23  | QX    | 12/25 (48%)     | 1.84   | 7 (58%) 0 0   | 100, 204, 231, 274    | 0     |
| 23  | XX    | 11/25 (44%)     | 2.29   | 8 (72%) 0 0   | 61, 167, 243, 286     | 0     |
| 24  | RA    | 2882/2915 (98%) | -0.06  | 28 (0%) 79 62 | 43, 79, 228, 335      | 0     |
| 24  | YA    | 2883/2915 (98%) | -0.18  | 37 (1%) 75 55 | 33, 64, 225, 389      | 0     |
| 25  | RB    | 120/122 (98%)   | 0.19   | 1 (0%) 82 67  | 92, 139, 178, 207     | 0     |
| 25  | YB    | 120/122 (98%)   | -0.05  | 2 (1%) 69 49  | 67, 95, 127, 161      | 0     |
| 26  | RD    | 272/276 (98%)   | 0.91   | 35 (12%) 7 5  | 46, 72, 113, 261      | 0     |
| 26  | YD    | 272/276 (98%)   | 0.67   | 23 (8%) 16 10 | 25, 61, 105, 242      | 0     |
| 27  | RE    | 205/206 (99%)   | 0.68   | 16 (7%) 19 11 | 46, 81, 154, 244      | 0     |
| 27  | YE    | 205/206 (99%)   | 0.88   | 26 (12%) 8 5  | 30, 78, 157, 260      | 0     |
| 28  | RF    | 202/210 (96%)   | 0.73   | 14 (6%) 23 13 | 45, 92, 152, 218      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28  | YF    | 202/210 (96%)  | 0.55   | 9 (4%) 38 22  | 33, 72, 139, 233      | 0     |
| 29  | RG    | 181/182 (99%)  | 0.99   | 22 (12%) 8 5  | 112, 153, 203, 257    | 0     |
| 29  | YG    | 181/182 (99%)  | 0.65   | 10 (5%) 30 18 | 69, 101, 153, 235     | 0     |
| 30  | RH    | 174/180 (96%)  | 1.17   | 19 (10%) 10 6 | 107, 158, 215, 279    | 0     |
| 30  | YH    | 174/180 (96%)  | 0.97   | 27 (15%) 5 3  | 62, 91, 139, 255      | 0     |
| 31  | RI    | 146/148 (98%)  | 2.05   | 64 (43%) 0 1  | 95, 136, 197, 248     | 0     |
| 31  | YI    | 146/148 (98%)  | 1.19   | 26 (17%) 4 2  | 70, 131, 173, 241     | 0     |
| 32  | RN    | 138/140 (98%)  | 1.04   | 14 (10%) 12 7 | 55, 94, 148, 188      | 0     |
| 32  | YN    | 138/140 (98%)  | 0.93   | 18 (13%) 7 5  | 45, 77, 149, 171      | 0     |
| 33  | RO    | 122/122 (100%) | 0.85   | 11 (9%) 15 9  | 54, 84, 121, 159      | 0     |
| 33  | YO    | 122/122 (100%) | 0.59   | 6 (4%) 35 20  | 40, 66, 108, 127      | 0     |
| 34  | RP    | 150/150 (100%) | 1.20   | 30 (20%) 3 2  | 46, 106, 168, 224     | 0     |
| 34  | YP    | 147/150 (98%)  | 1.26   | 28 (19%) 3 2  | 39, 79, 128, 177      | 0     |
| 35  | RQ    | 141/141 (100%) | 1.10   | 24 (17%) 4 2  | 67, 103, 161, 220     | 0     |
| 35  | YQ    | 141/141 (100%) | 1.16   | 29 (20%) 2 2  | 40, 73, 143, 236      | 0     |
| 36  | RR    | 117/118 (99%)  | 0.81   | 12 (10%) 12 7 | 47, 75, 112, 192      | 0     |
| 36  | YR    | 117/118 (99%)  | 0.66   | 6 (5%) 33 20  | 41, 72, 110, 168      | 0     |
| 37  | RS    | 111/112 (99%)  | 0.75   | 9 (8%) 18 10  | 93, 133, 186, 216     | 0     |
| 37  | YS    | 111/112 (99%)  | 0.73   | 10 (9%) 15 9  | 68, 101, 153, 231     | 0     |
| 38  | RT    | 137/146 (93%)  | 1.02   | 20 (14%) 6 4  | 55, 92, 171, 242      | 0     |
| 38  | YT    | 137/146 (93%)  | 0.87   | 19 (13%) 6 4  | 49, 83, 165, 198      | 0     |
| 39  | RU    | 117/118 (99%)  | 1.08   | 18 (15%) 5 3  | 48, 89, 155, 203      | 0     |
| 39  | YU    | 117/118 (99%)  | 0.88   | 18 (15%) 5 3  | 38, 71, 139, 247      | 0     |
| 40  | RV    | 101/101 (100%) | 1.46   | 22 (21%) 2 2  | 58, 110, 165, 266     | 0     |
| 40  | YV    | 101/101 (100%) | 0.93   | 16 (15%) 5 3  | 28, 89, 151, 277      | 0     |
| 41  | RW    | 113/113 (100%) | 0.82   | 18 (15%) 5 3  | 42, 66, 119, 230      | 0     |
| 41  | YW    | 113/113 (100%) | 0.65   | 8 (7%) 22 13  | 46, 65, 122, 162      | 0     |
| 42  | RX    | 92/96 (95%)    | 0.74   | 5 (5%) 31 18  | 61, 88, 124, 149      | 0     |
| 42  | YX    | 92/96 (95%)    | 0.53   | 5 (5%) 31 18  | 42, 64, 106, 154      | 0     |
| 43  | RY    | 107/110 (97%)  | 1.86   | 38 (35%) 1 1  | 69, 106, 156, 185     | 0     |
| 43  | YY    | 107/110 (97%)  | 0.94   | 13 (12%) 8 5  | 60, 90, 138, 182      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | RZ    | 183/206 (88%)     | 1.05   | 19 (10%) 11 7   | 103, 148, 216, 251    | 0     |
| 44  | YZ    | 183/206 (88%)     | 1.19   | 39 (21%) 2 2    | 70, 108, 181, 229     | 0     |
| 45  | R0    | 81/85 (95%)       | 1.15   | 15 (18%) 3 2    | 71, 99, 133, 226      | 0     |
| 45  | Y0    | 75/85 (88%)       | 0.62   | 5 (6%) 24 14    | 46, 71, 97, 117       | 0     |
| 46  | R1    | 97/98 (98%)       | 1.37   | 24 (24%) 2 2    | 44, 87, 148, 231      | 0     |
| 46  | Y1    | 93/98 (94%)       | 0.89   | 11 (11%) 9 5    | 42, 69, 130, 176      | 0     |
| 47  | R2    | 69/72 (95%)       | 1.50   | 17 (24%) 2 2    | 77, 116, 184, 230     | 0     |
| 47  | Y2    | 69/72 (95%)       | 1.05   | 10 (14%) 6 4    | 50, 73, 145, 309      | 0     |
| 48  | R3    | 59/60 (98%)       | 1.14   | 9 (15%) 5 3     | 67, 97, 155, 189      | 0     |
| 48  | Y3    | 59/60 (98%)       | 0.57   | 3 (5%) 33 20    | 48, 73, 131, 173      | 0     |
| 49  | R4    | 69/71 (97%)       | 0.72   | 7 (10%) 12 7    | 124, 169, 239, 274    | 0     |
| 49  | Y4    | 69/71 (97%)       | 0.76   | 5 (7%) 21 12    | 87, 134, 226, 273     | 0     |
| 50  | R5    | 59/60 (98%)       | 1.18   | 12 (20%) 3 2    | 38, 85, 200, 218      | 0     |
| 50  | Y5    | 59/60 (98%)       | 0.68   | 3 (5%) 33 20    | 28, 73, 171, 221      | 0     |
| 51  | R6    | 53/54 (98%)       | 1.78   | 20 (37%) 1 1    | 109, 155, 205, 247    | 0     |
| 51  | Y6    | 53/54 (98%)       | 0.68   | 2 (3%) 44 26    | 104, 128, 178, 197    | 0     |
| 52  | R7    | 47/49 (95%)       | 0.58   | 4 (8%) 16 10    | 45, 61, 93, 177       | 0     |
| 52  | Y7    | 48/49 (97%)       | 0.50   | 5 (10%) 11 7    | 28, 52, 115, 150      | 0     |
| 53  | R8    | 64/65 (98%)       | 1.79   | 19 (29%) 1 1    | 54, 87, 143, 220      | 0     |
| 53  | Y8    | 64/65 (98%)       | 1.75   | 22 (34%) 1 1    | 39, 70, 125, 237      | 0     |
| 54  | R9    | 37/37 (100%)      | 1.30   | 6 (16%) 4 3     | 109, 132, 166, 193    | 0     |
| 54  | Y9    | 37/37 (100%)      | 1.13   | 3 (8%) 18 10    | 85, 102, 141, 153     | 0     |
| All | All   | 20828/21422 (97%) | 0.52   | 1702 (8%) 17 10 | 25, 99, 197, 389      | 0     |

The worst 5 of 1702 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 31  | RI    | 16  | GLY  | 8.1  |
| 43  | RY    | 62  | GLU  | 8.0  |
| 12  | XL    | 28  | LYS  | 8.0  |
| 26  | RD    | 34  | VAL  | 7.9  |
| 26  | YD    | 34  | VAL  | 7.9  |

## 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3129 | 1/1   | 0.37 | 0.34 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3466 | 1/1   | 0.41 | 0.16 | 72,72,72,72                 | 0     |
| 55  | MG   | XA    | 1696 | 1/1   | 0.43 | 0.14 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3119 | 1/1   | 0.43 | 0.36 | 71,71,71,71                 | 0     |
| 55  | MG   | QA    | 1661 | 1/1   | 0.44 | 0.18 | 82,82,82,82                 | 0     |
| 55  | MG   | YA    | 3470 | 1/1   | 0.48 | 0.32 | 79,79,79,79                 | 0     |
| 55  | MG   | RA    | 3211 | 1/1   | 0.49 | 0.25 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3230 | 1/1   | 0.49 | 0.23 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3359 | 1/1   | 0.50 | 0.12 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3225 | 1/1   | 0.51 | 0.21 | 78,78,78,78                 | 0     |
| 55  | MG   | RA    | 3047 | 1/1   | 0.52 | 0.23 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3323 | 1/1   | 0.52 | 0.16 | 83,83,83,83                 | 0     |
| 55  | MG   | RA    | 3096 | 1/1   | 0.53 | 0.26 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3128 | 1/1   | 0.53 | 0.31 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3133 | 1/1   | 0.54 | 0.28 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3118 | 1/1   | 0.54 | 0.51 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3365 | 1/1   | 0.55 | 0.20 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3144 | 1/1   | 0.56 | 0.24 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3062 | 1/1   | 0.56 | 0.42 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3484 | 1/1   | 0.56 | 0.22 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3212 | 1/1   | 0.57 | 0.49 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3023 | 1/1   | 0.57 | 0.34 | 71,71,71,71                 | 0     |
| 55  | MG   | YB    | 212  | 1/1   | 0.57 | 0.11 | 82,82,82,82                 | 0     |
| 55  | MG   | RA    | 3428 | 1/1   | 0.58 | 0.10 | 105,105,105,105             | 0     |
| 55  | MG   | YA    | 3447 | 1/1   | 0.58 | 0.35 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3038 | 1/1   | 0.58 | 0.33 | 64,64,64,64                 | 0     |
| 55  | MG   | QA    | 1663 | 1/1   | 0.58 | 0.26 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3478 | 1/1   | 0.58 | 0.39 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3530 | 1/1   | 0.58 | 0.38 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3095 | 1/1   | 0.58 | 0.25 | 60,60,60,60                 | 0     |
| 55  | MG   | XA    | 1672 | 1/1   | 0.59 | 0.16 | 72,72,72,72                 | 0     |
| 55  | MG   | YQ    | 203  | 1/1   | 0.59 | 0.27 | 62,62,62,62                 | 0     |
| 57  | ZN   | R5    | 501  | 1/1   | 0.59 | 0.30 | 146,146,146,146             | 0     |
| 55  | MG   | YA    | 3209 | 1/1   | 0.60 | 0.58 | 63,63,63,63                 | 0     |
| 55  | MG   | XA    | 1601 | 1/1   | 0.60 | 0.27 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3509 | 1/1   | 0.60 | 0.24 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3538 | 1/1   | 0.60 | 0.55 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3261 | 1/1   | 0.60 | 0.37 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3516 | 1/1   | 0.60 | 0.27 | 78,78,78,78                 | 0     |
| 55  | MG   | YA    | 3001 | 1/1   | 0.60 | 0.38 | 71,71,71,71                 | 0     |
| 57  | ZN   | Y4    | 500  | 1/1   | 0.60 | 0.38 | 141,141,141,141             | 0     |
| 55  | MG   | RA    | 3410 | 1/1   | 0.61 | 0.18 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3414 | 1/1   | 0.61 | 0.27 | 77,77,77,77                 | 0     |
| 55  | MG   | YA    | 3193 | 1/1   | 0.61 | 0.19 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3201 | 1/1   | 0.61 | 0.20 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3304 | 1/1   | 0.61 | 0.21 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3065 | 1/1   | 0.61 | 0.25 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3199 | 1/1   | 0.62 | 0.19 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3508 | 1/1   | 0.62 | 0.15 | 81,81,81,81                 | 0     |
| 55  | MG   | RA    | 3092 | 1/1   | 0.62 | 0.26 | 61,61,61,61                 | 0     |
| 55  | MG   | XA    | 1655 | 1/1   | 0.62 | 0.31 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3506 | 1/1   | 0.63 | 0.23 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3197 | 1/1   | 0.63 | 0.22 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3317 | 1/1   | 0.63 | 0.15 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3404 | 1/1   | 0.63 | 0.29 | 77,77,77,77                 | 0     |
| 55  | MG   | YA    | 3024 | 1/1   | 0.63 | 0.36 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3074 | 1/1   | 0.64 | 0.31 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3275 | 1/1   | 0.64 | 0.17 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3521 | 1/1   | 0.64 | 0.21 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3050 | 1/1   | 0.64 | 0.55 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3319 | 1/1   | 0.64 | 0.21 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3097 | 1/1   | 0.64 | 0.26 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3451 | 1/1   | 0.64 | 0.18 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3022 | 1/1   | 0.64 | 0.34 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3002 | 1/1   | 0.64 | 0.21 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3331 | 1/1   | 0.65 | 0.27 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3237 | 1/1   | 0.65 | 0.21 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3039 | 1/1   | 0.65 | 0.39 | 62,62,62,62                 | 0     |
| 55  | MG   | XA    | 1646 | 1/1   | 0.65 | 0.22 | 77,77,77,77                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3307 | 1/1   | 0.65 | 0.26 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3138 | 1/1   | 0.65 | 0.38 | 72,72,72,72                 | 0     |
| 55  | MG   | XV    | 107  | 1/1   | 0.65 | 0.14 | 90,90,90,90                 | 0     |
| 55  | MG   | YA    | 3098 | 1/1   | 0.66 | 0.40 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3102 | 1/1   | 0.66 | 0.35 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3116 | 1/1   | 0.66 | 0.38 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3010 | 1/1   | 0.66 | 0.31 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3347 | 1/1   | 0.66 | 0.16 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3432 | 1/1   | 0.66 | 0.12 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3356 | 1/1   | 0.66 | 0.17 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3139 | 1/1   | 0.66 | 0.29 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3017 | 1/1   | 0.66 | 0.25 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3419 | 1/1   | 0.67 | 0.11 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3406 | 1/1   | 0.67 | 0.30 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3032 | 1/1   | 0.67 | 0.40 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3320 | 1/1   | 0.67 | 0.20 | 80,80,80,80                 | 0     |
| 55  | MG   | RA    | 3210 | 1/1   | 0.67 | 0.32 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3056 | 1/1   | 0.67 | 0.45 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3061 | 1/1   | 0.67 | 0.46 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3486 | 1/1   | 0.67 | 0.17 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3259 | 1/1   | 0.67 | 0.39 | 70,70,70,70                 | 0     |
| 55  | MG   | XA    | 1636 | 1/1   | 0.67 | 0.23 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3157 | 1/1   | 0.67 | 0.21 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3172 | 1/1   | 0.67 | 0.27 | 72,72,72,72                 | 0     |
| 55  | MG   | XA    | 1645 | 1/1   | 0.67 | 0.20 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3195 | 1/1   | 0.67 | 0.13 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3197 | 1/1   | 0.67 | 0.16 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3354 | 1/1   | 0.67 | 0.16 | 76,76,76,76                 | 0     |
| 55  | MG   | RD    | 301  | 1/1   | 0.68 | 0.20 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3088 | 1/1   | 0.68 | 0.39 | 72,72,72,72                 | 0     |
| 55  | MG   | QA    | 1656 | 1/1   | 0.68 | 0.16 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3012 | 1/1   | 0.68 | 0.30 | 73,73,73,73                 | 0     |
| 55  | MG   | XA    | 1638 | 1/1   | 0.68 | 0.33 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3476 | 1/1   | 0.68 | 0.21 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3031 | 1/1   | 0.68 | 0.46 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3025 | 1/1   | 0.68 | 0.33 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3150 | 1/1   | 0.68 | 0.24 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3488 | 1/1   | 0.68 | 0.21 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3353 | 1/1   | 0.68 | 0.28 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3184 | 1/1   | 0.68 | 0.42 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3187 | 1/1   | 0.68 | 0.19 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3201 | 1/1   | 0.68 | 0.14 | 72,72,72,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | Y1    | 101  | 1/1   | 0.68 | 0.12 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3420 | 1/1   | 0.68 | 0.13 | 72,72,72,72                 | 0     |
| 55  | MG   | XL    | 201  | 1/1   | 0.68 | 0.20 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3253 | 1/1   | 0.69 | 0.26 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3256 | 1/1   | 0.69 | 0.36 | 64,64,64,64                 | 0     |
| 55  | MG   | QV    | 101  | 1/1   | 0.69 | 0.30 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3022 | 1/1   | 0.69 | 0.44 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3085 | 1/1   | 0.69 | 0.23 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3295 | 1/1   | 0.69 | 0.35 | 78,78,78,78                 | 0     |
| 55  | MG   | YA    | 3143 | 1/1   | 0.69 | 0.19 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3308 | 1/1   | 0.69 | 0.18 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3310 | 1/1   | 0.69 | 0.26 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3200 | 1/1   | 0.69 | 0.20 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3120 | 1/1   | 0.69 | 0.32 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3544 | 1/1   | 0.69 | 0.12 | 64,64,64,64                 | 0     |
| 55  | MG   | YB    | 211  | 1/1   | 0.69 | 0.17 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3089 | 1/1   | 0.69 | 0.33 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3335 | 1/1   | 0.69 | 0.18 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3148 | 1/1   | 0.69 | 0.14 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3043 | 1/1   | 0.69 | 0.38 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3335 | 1/1   | 0.69 | 0.25 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3046 | 1/1   | 0.70 | 0.31 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3361 | 1/1   | 0.70 | 0.33 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3177 | 1/1   | 0.70 | 0.21 | 71,71,71,71                 | 0     |
| 55  | MG   | R0    | 102  | 1/1   | 0.70 | 0.19 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3290 | 1/1   | 0.70 | 0.14 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3373 | 1/1   | 0.70 | 0.14 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3314 | 1/1   | 0.70 | 0.31 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3377 | 1/1   | 0.70 | 0.13 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3194 | 1/1   | 0.70 | 0.16 | 61,61,61,61                 | 0     |
| 55  | MG   | RB    | 207  | 1/1   | 0.70 | 0.09 | 81,81,81,81                 | 0     |
| 55  | MG   | YA    | 3104 | 1/1   | 0.70 | 0.29 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3054 | 1/1   | 0.71 | 0.39 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3343 | 1/1   | 0.71 | 0.15 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3348 | 1/1   | 0.71 | 0.29 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3423 | 1/1   | 0.71 | 0.15 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3175 | 1/1   | 0.71 | 0.18 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3019 | 1/1   | 0.71 | 0.28 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3499 | 1/1   | 0.71 | 0.33 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3411 | 1/1   | 0.71 | 0.35 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3186 | 1/1   | 0.71 | 0.42 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3019 | 1/1   | 0.71 | 0.36 | 66,66,66,66                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | XA    | 1647 | 1/1   | 0.71 | 0.25 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3155 | 1/1   | 0.71 | 0.20 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3326 | 1/1   | 0.71 | 0.17 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3018 | 1/1   | 0.72 | 0.52 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3309 | 1/1   | 0.72 | 0.19 | 55,55,55,55                 | 0     |
| 55  | MG   | R0    | 101  | 1/1   | 0.72 | 0.40 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3020 | 1/1   | 0.72 | 0.24 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3217 | 1/1   | 0.72 | 0.31 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3170 | 1/1   | 0.72 | 0.20 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3323 | 1/1   | 0.72 | 0.29 | 78,78,78,78                 | 0     |
| 55  | MG   | RA    | 3239 | 1/1   | 0.72 | 0.35 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3429 | 1/1   | 0.72 | 0.29 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3036 | 1/1   | 0.72 | 0.27 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3258 | 1/1   | 0.72 | 0.27 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3462 | 1/1   | 0.72 | 0.15 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3472 | 1/1   | 0.72 | 0.17 | 77,77,77,77                 | 0     |
| 55  | MG   | YA    | 3189 | 1/1   | 0.72 | 0.21 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3193 | 1/1   | 0.72 | 0.30 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3132 | 1/1   | 0.72 | 0.14 | 82,82,82,82                 | 0     |
| 55  | MG   | XA    | 1667 | 1/1   | 0.72 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3074 | 1/1   | 0.72 | 0.21 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3461 | 1/1   | 0.72 | 0.18 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3498 | 1/1   | 0.72 | 0.61 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3092 | 1/1   | 0.72 | 0.39 | 67,67,67,67                 | 0     |
| 55  | MG   | XA    | 1684 | 1/1   | 0.72 | 0.13 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3081 | 1/1   | 0.72 | 0.34 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3100 | 1/1   | 0.72 | 0.36 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3235 | 1/1   | 0.72 | 0.23 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3518 | 1/1   | 0.72 | 0.20 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3236 | 1/1   | 0.72 | 0.18 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3039 | 1/1   | 0.72 | 0.27 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3030 | 1/1   | 0.72 | 0.60 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3114 | 1/1   | 0.72 | 0.44 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3510 | 1/1   | 0.72 | 0.26 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3418 | 1/1   | 0.72 | 0.08 | 70,70,70,70                 | 0     |
| 55  | MG   | YE    | 304  | 1/1   | 0.72 | 0.22 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3121 | 1/1   | 0.72 | 0.39 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3280 | 1/1   | 0.72 | 0.49 | 72,72,72,72                 | 0     |
| 55  | MG   | Y8    | 101  | 1/1   | 0.72 | 0.41 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3127 | 1/1   | 0.72 | 0.25 | 71,71,71,71                 | 0     |
| 55  | MG   | QA    | 1637 | 1/1   | 0.72 | 0.21 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3172 | 1/1   | 0.73 | 0.28 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3441 | 1/1   | 0.73 | 0.15 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3180 | 1/1   | 0.73 | 0.20 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3292 | 1/1   | 0.73 | 0.09 | 64,64,64,64                 | 0     |
| 55  | MG   | XA    | 1658 | 1/1   | 0.73 | 0.33 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3362 | 1/1   | 0.73 | 0.19 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3177 | 1/1   | 0.73 | 0.13 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3027 | 1/1   | 0.73 | 0.43 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3028 | 1/1   | 0.73 | 0.46 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3140 | 1/1   | 0.73 | 0.31 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3454 | 1/1   | 0.73 | 0.17 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3051 | 1/1   | 0.73 | 0.20 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3466 | 1/1   | 0.73 | 0.13 | 84,84,84,84                 | 0     |
| 55  | MG   | YA    | 3534 | 1/1   | 0.73 | 0.45 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3392 | 1/1   | 0.73 | 0.31 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3229 | 1/1   | 0.73 | 0.34 | 68,68,68,68                 | 0     |
| 55  | MG   | QA    | 1671 | 1/1   | 0.73 | 0.26 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3347 | 1/1   | 0.73 | 0.20 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3013 | 1/1   | 0.73 | 0.18 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3164 | 1/1   | 0.73 | 0.32 | 61,61,61,61                 | 0     |
| 55  | MG   | QA    | 1658 | 1/1   | 0.73 | 0.15 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3086 | 1/1   | 0.73 | 0.25 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3273 | 1/1   | 0.73 | 0.22 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3176 | 1/1   | 0.73 | 0.27 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3511 | 1/1   | 0.74 | 0.26 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3106 | 1/1   | 0.74 | 0.28 | 73,73,73,73                 | 0     |
| 55  | MG   | XA    | 1680 | 1/1   | 0.74 | 0.16 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3449 | 1/1   | 0.74 | 0.35 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3036 | 1/1   | 0.74 | 0.30 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3309 | 1/1   | 0.74 | 0.30 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3090 | 1/1   | 0.74 | 0.26 | 72,72,72,72                 | 0     |
| 55  | MG   | XM    | 202  | 1/1   | 0.74 | 0.11 | 88,88,88,88                 | 0     |
| 55  | MG   | RA    | 3321 | 1/1   | 0.74 | 0.33 | 79,79,79,79                 | 0     |
| 55  | MG   | YA    | 3048 | 1/1   | 0.74 | 0.27 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3051 | 1/1   | 0.74 | 0.47 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3044 | 1/1   | 0.74 | 0.45 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3243 | 1/1   | 0.74 | 0.32 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3529 | 1/1   | 0.74 | 0.21 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3415 | 1/1   | 0.74 | 0.32 | 80,80,80,80                 | 0     |
| 55  | MG   | YA    | 3148 | 1/1   | 0.74 | 0.25 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3334 | 1/1   | 0.74 | 0.21 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3252 | 1/1   | 0.74 | 0.27 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3013 | 1/1   | 0.74 | 0.42 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3232 | 1/1   | 0.74 | 0.14 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3080 | 1/1   | 0.74 | 0.24 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3166 | 1/1   | 0.74 | 0.15 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3259 | 1/1   | 0.74 | 0.31 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3246 | 1/1   | 0.74 | 0.29 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3156 | 1/1   | 0.74 | 0.23 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3059 | 1/1   | 0.74 | 0.10 | 77,77,77,77                 | 0     |
| 55  | MG   | XM    | 201  | 1/1   | 0.75 | 0.15 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3285 | 1/1   | 0.75 | 0.30 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3404 | 1/1   | 0.75 | 0.28 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3492 | 1/1   | 0.75 | 0.29 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3152 | 1/1   | 0.75 | 0.22 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3371 | 1/1   | 0.75 | 0.11 | 79,79,79,79                 | 0     |
| 55  | MG   | YA    | 3401 | 1/1   | 0.75 | 0.11 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3307 | 1/1   | 0.75 | 0.14 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3006 | 1/1   | 0.75 | 0.14 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3313 | 1/1   | 0.75 | 0.38 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3244 | 1/1   | 0.75 | 0.27 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3252 | 1/1   | 0.75 | 0.36 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3343 | 1/1   | 0.75 | 0.18 | 84,84,84,84                 | 0     |
| 55  | MG   | YA    | 3322 | 1/1   | 0.75 | 0.21 | 78,78,78,78                 | 0     |
| 55  | MG   | RA    | 3087 | 1/1   | 0.75 | 0.44 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3094 | 1/1   | 0.75 | 0.43 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3354 | 1/1   | 0.75 | 0.08 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3218 | 1/1   | 0.75 | 0.11 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3257 | 1/1   | 0.76 | 0.20 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3363 | 1/1   | 0.76 | 0.21 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3094 | 1/1   | 0.76 | 0.27 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3056 | 1/1   | 0.76 | 0.27 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3434 | 1/1   | 0.76 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3026 | 1/1   | 0.76 | 0.38 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3281 | 1/1   | 0.76 | 0.23 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3160 | 1/1   | 0.76 | 0.20 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3381 | 1/1   | 0.76 | 0.21 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3465 | 1/1   | 0.76 | 0.11 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3188 | 1/1   | 0.76 | 0.15 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3061 | 1/1   | 0.76 | 0.60 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3340 | 1/1   | 0.76 | 0.14 | 68,68,68,68                 | 0     |
| 55  | MG   | XV    | 103  | 1/1   | 0.76 | 0.18 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3484 | 1/1   | 0.76 | 0.15 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3044 | 1/1   | 0.76 | 0.66 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3481 | 1/1   | 0.76 | 0.28 | 80,80,80,80                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | XA    | 1617 | 1/1   | 0.76 | 0.18 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3215 | 1/1   | 0.76 | 0.23 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3137 | 1/1   | 0.76 | 0.46 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3138 | 1/1   | 0.76 | 0.36 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3329 | 1/1   | 0.76 | 0.23 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3003 | 1/1   | 0.76 | 0.42 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3489 | 1/1   | 0.76 | 0.30 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3179 | 1/1   | 0.76 | 0.17 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3063 | 1/1   | 0.76 | 0.50 | 67,67,67,67                 | 0     |
| 55  | MG   | YD    | 302  | 1/1   | 0.76 | 0.19 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3306 | 1/1   | 0.76 | 0.14 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3077 | 1/1   | 0.76 | 0.40 | 66,66,66,66                 | 0     |
| 55  | MG   | QA    | 1636 | 1/1   | 0.76 | 0.28 | 65,65,65,65                 | 0     |
| 55  | MG   | QA    | 1650 | 1/1   | 0.76 | 0.25 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3131 | 1/1   | 0.76 | 0.30 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3088 | 1/1   | 0.76 | 0.44 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3134 | 1/1   | 0.77 | 0.41 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3415 | 1/1   | 0.77 | 0.31 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3425 | 1/1   | 0.77 | 0.19 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3194 | 1/1   | 0.77 | 0.17 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3137 | 1/1   | 0.77 | 0.37 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3291 | 1/1   | 0.77 | 0.41 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3442 | 1/1   | 0.77 | 0.39 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3446 | 1/1   | 0.77 | 0.13 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3110 | 1/1   | 0.77 | 0.28 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3286 | 1/1   | 0.77 | 0.20 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3457 | 1/1   | 0.77 | 0.29 | 60,60,60,60                 | 0     |
| 55  | MG   | QV    | 106  | 1/1   | 0.77 | 0.18 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3053 | 1/1   | 0.77 | 0.55 | 70,70,70,70                 | 0     |
| 55  | MG   | XA    | 1640 | 1/1   | 0.77 | 0.15 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3214 | 1/1   | 0.77 | 0.32 | 69,69,69,69                 | 0     |
| 55  | MG   | XA    | 1641 | 1/1   | 0.77 | 0.28 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3503 | 1/1   | 0.77 | 0.27 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3227 | 1/1   | 0.77 | 0.19 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3045 | 1/1   | 0.77 | 0.45 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3430 | 1/1   | 0.77 | 0.17 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3234 | 1/1   | 0.77 | 0.45 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3181 | 1/1   | 0.77 | 0.37 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3173 | 1/1   | 0.77 | 0.37 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3103 | 1/1   | 0.77 | 0.35 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3055 | 1/1   | 0.77 | 0.22 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3407 | 1/1   | 0.77 | 0.46 | 72,72,72,72                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3018 | 1/1   | 0.77 | 0.40 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3353 | 1/1   | 0.77 | 0.36 | 68,68,68,68                 | 0     |
| 55  | MG   | QA    | 1673 | 1/1   | 0.77 | 0.40 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3358 | 1/1   | 0.77 | 0.22 | 74,74,74,74                 | 0     |
| 55  | MG   | QA    | 1603 | 1/1   | 0.77 | 0.27 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3121 | 1/1   | 0.77 | 0.11 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3393 | 1/1   | 0.77 | 0.24 | 83,83,83,83                 | 0     |
| 55  | MG   | YA    | 3065 | 1/1   | 0.77 | 0.57 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3268 | 1/1   | 0.77 | 0.16 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3159 | 1/1   | 0.77 | 0.18 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3414 | 1/1   | 0.78 | 0.16 | 67,67,67,67                 | 0     |
| 55  | MG   | RB    | 204  | 1/1   | 0.78 | 0.33 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3017 | 1/1   | 0.78 | 0.35 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3033 | 1/1   | 0.78 | 0.60 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3464 | 1/1   | 0.78 | 0.12 | 75,75,75,75                 | 0     |
| 55  | MG   | RP    | 201  | 1/1   | 0.78 | 0.22 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3042 | 1/1   | 0.78 | 0.36 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3325 | 1/1   | 0.78 | 0.18 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3119 | 1/1   | 0.78 | 0.17 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3169 | 1/1   | 0.78 | 0.20 | 59,59,59,59                 | 0     |
| 55  | MG   | QA    | 1667 | 1/1   | 0.78 | 0.29 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3050 | 1/1   | 0.78 | 0.47 | 67,67,67,67                 | 0     |
| 55  | MG   | XA    | 1630 | 1/1   | 0.78 | 0.26 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3052 | 1/1   | 0.78 | 0.54 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3007 | 1/1   | 0.78 | 0.15 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3055 | 1/1   | 0.78 | 0.41 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3320 | 1/1   | 0.78 | 0.23 | 72,72,72,72                 | 0     |
| 55  | MG   | QV    | 104  | 1/1   | 0.78 | 0.12 | 81,81,81,81                 | 0     |
| 55  | MG   | YA    | 3211 | 1/1   | 0.78 | 0.13 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3057 | 1/1   | 0.78 | 0.28 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3293 | 1/1   | 0.78 | 0.33 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3298 | 1/1   | 0.78 | 0.11 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3526 | 1/1   | 0.78 | 0.12 | 74,74,74,74                 | 0     |
| 55  | MG   | QT    | 201  | 1/1   | 0.78 | 0.31 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3025 | 1/1   | 0.78 | 0.30 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3067 | 1/1   | 0.78 | 0.38 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3149 | 1/1   | 0.78 | 0.25 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3069 | 1/1   | 0.78 | 0.33 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3155 | 1/1   | 0.78 | 0.38 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3240 | 1/1   | 0.78 | 0.40 | 79,79,79,79                 | 0     |
| 55  | MG   | YA    | 3161 | 1/1   | 0.78 | 0.24 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3076 | 1/1   | 0.78 | 0.30 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3014 | 1/1   | 0.78 | 0.30 | 61,61,61,61                 | 0     |
| 55  | MG   | Y0    | 102  | 1/1   | 0.78 | 0.27 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3079 | 1/1   | 0.78 | 0.24 | 68,68,68,68                 | 0     |
| 55  | MG   | Y7    | 101  | 1/1   | 0.78 | 0.21 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3317 | 1/1   | 0.78 | 0.17 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3158 | 1/1   | 0.78 | 0.11 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3198 | 1/1   | 0.78 | 0.24 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3070 | 1/1   | 0.79 | 0.37 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3231 | 1/1   | 0.79 | 0.33 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3459 | 1/1   | 0.79 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | QA    | 1675 | 1/1   | 0.79 | 0.12 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3248 | 1/1   | 0.79 | 0.18 | 74,74,74,74                 | 0     |
| 55  | MG   | XA    | 1679 | 1/1   | 0.79 | 0.20 | 79,79,79,79                 | 0     |
| 55  | MG   | RA    | 3518 | 1/1   | 0.79 | 0.39 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3521 | 1/1   | 0.79 | 0.25 | 91,91,91,91                 | 0     |
| 55  | MG   | RA    | 3319 | 1/1   | 0.79 | 0.21 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3457 | 1/1   | 0.79 | 0.26 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3458 | 1/1   | 0.79 | 0.13 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3496 | 1/1   | 0.79 | 0.07 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3499 | 1/1   | 0.79 | 0.12 | 83,83,83,83                 | 0     |
| 55  | MG   | QA    | 1642 | 1/1   | 0.79 | 0.21 | 67,67,67,67                 | 0     |
| 55  | MG   | XV    | 102  | 1/1   | 0.79 | 0.16 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3519 | 1/1   | 0.79 | 0.11 | 82,82,82,82                 | 0     |
| 55  | MG   | YA    | 3357 | 1/1   | 0.79 | 0.15 | 67,67,67,67                 | 0     |
| 55  | MG   | RP    | 202  | 1/1   | 0.79 | 0.13 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3105 | 1/1   | 0.79 | 0.34 | 62,62,62,62                 | 0     |
| 55  | MG   | QA    | 1612 | 1/1   | 0.79 | 0.28 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3403 | 1/1   | 0.79 | 0.25 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3124 | 1/1   | 0.79 | 0.27 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3261 | 1/1   | 0.79 | 0.15 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3549 | 1/1   | 0.79 | 0.34 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3166 | 1/1   | 0.79 | 0.12 | 71,71,71,71                 | 0     |
| 55  | MG   | XA    | 1631 | 1/1   | 0.79 | 0.12 | 71,71,71,71                 | 0     |
| 55  | MG   | YD    | 301  | 1/1   | 0.79 | 0.18 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3281 | 1/1   | 0.79 | 0.09 | 75,75,75,75                 | 0     |
| 55  | MG   | QA    | 1626 | 1/1   | 0.79 | 0.13 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3111 | 1/1   | 0.79 | 0.39 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3141 | 1/1   | 0.79 | 0.34 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3226 | 1/1   | 0.79 | 0.20 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3012 | 1/1   | 0.79 | 0.46 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3049 | 1/1   | 0.79 | 0.43 | 69,69,69,69                 | 0     |
| 57  | ZN   | RY    | 201  | 1/1   | 0.79 | 0.32 | 125,125,125,125             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | XA    | 1653 | 1/1   | 0.79 | 0.32 | 59,59,59,59                 | 0     |
| 55  | MG   | QV    | 105  | 1/1   | 0.79 | 0.27 | 74,74,74,74                 | 0     |
| 55  | MG   | XA    | 1610 | 1/1   | 0.80 | 0.34 | 73,73,73,73                 | 0     |
| 55  | MG   | QA    | 1670 | 1/1   | 0.80 | 0.09 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3008 | 1/1   | 0.80 | 0.17 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3409 | 1/1   | 0.80 | 0.14 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3507 | 1/1   | 0.80 | 0.15 | 78,78,78,78                 | 0     |
| 55  | MG   | YA    | 3255 | 1/1   | 0.80 | 0.16 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3514 | 1/1   | 0.80 | 0.15 | 81,81,81,81                 | 0     |
| 55  | MG   | YA    | 3171 | 1/1   | 0.80 | 0.29 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3046 | 1/1   | 0.80 | 0.58 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3274 | 1/1   | 0.80 | 0.34 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3430 | 1/1   | 0.80 | 0.26 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3164 | 1/1   | 0.80 | 0.32 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3433 | 1/1   | 0.80 | 0.16 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3114 | 1/1   | 0.80 | 0.17 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3140 | 1/1   | 0.80 | 0.47 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3072 | 1/1   | 0.80 | 0.31 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3443 | 1/1   | 0.80 | 0.32 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3181 | 1/1   | 0.80 | 0.38 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3183 | 1/1   | 0.80 | 0.19 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3105 | 1/1   | 0.80 | 0.28 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3032 | 1/1   | 0.80 | 0.37 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3171 | 1/1   | 0.80 | 0.25 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3460 | 1/1   | 0.80 | 0.27 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3108 | 1/1   | 0.80 | 0.12 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3200 | 1/1   | 0.80 | 0.25 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3191 | 1/1   | 0.80 | 0.21 | 54,54,54,54                 | 0     |
| 55  | MG   | YA    | 3374 | 1/1   | 0.80 | 0.23 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3475 | 1/1   | 0.80 | 0.21 | 79,79,79,79                 | 0     |
| 55  | MG   | YA    | 3387 | 1/1   | 0.80 | 0.16 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3303 | 1/1   | 0.80 | 0.29 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3417 | 1/1   | 0.81 | 0.11 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3473 | 1/1   | 0.81 | 0.15 | 81,81,81,81                 | 0     |
| 55  | MG   | YA    | 3073 | 1/1   | 0.81 | 0.27 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3364 | 1/1   | 0.81 | 0.21 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3477 | 1/1   | 0.81 | 0.18 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3221 | 1/1   | 0.81 | 0.12 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3216 | 1/1   | 0.81 | 0.33 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3469 | 1/1   | 0.81 | 0.14 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3495 | 1/1   | 0.81 | 0.23 | 81,81,81,81                 | 0     |
| 55  | MG   | YA    | 3388 | 1/1   | 0.81 | 0.39 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3024 | 1/1   | 0.81 | 0.57 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3506 | 1/1   | 0.81 | 0.14 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3303 | 1/1   | 0.81 | 0.17 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3403 | 1/1   | 0.81 | 0.18 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3043 | 1/1   | 0.81 | 0.39 | 67,67,67,67                 | 0     |
| 55  | MG   | XA    | 1648 | 1/1   | 0.81 | 0.17 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3482 | 1/1   | 0.81 | 0.07 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3170 | 1/1   | 0.81 | 0.34 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3101 | 1/1   | 0.81 | 0.25 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3527 | 1/1   | 0.81 | 0.11 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3242 | 1/1   | 0.81 | 0.41 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3195 | 1/1   | 0.81 | 0.21 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3531 | 1/1   | 0.81 | 0.25 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3145 | 1/1   | 0.81 | 0.10 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3243 | 1/1   | 0.81 | 0.18 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3244 | 1/1   | 0.81 | 0.29 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3245 | 1/1   | 0.81 | 0.15 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3550 | 1/1   | 0.81 | 0.14 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3439 | 1/1   | 0.81 | 0.16 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3443 | 1/1   | 0.81 | 0.27 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3284 | 1/1   | 0.81 | 0.21 | 62,62,62,62                 | 0     |
| 55  | MG   | XA    | 1682 | 1/1   | 0.81 | 0.26 | 60,60,60,60                 | 0     |
| 55  | MG   | YE    | 301  | 1/1   | 0.81 | 0.36 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3161 | 1/1   | 0.81 | 0.13 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3337 | 1/1   | 0.81 | 0.25 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3339 | 1/1   | 0.81 | 0.19 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3456 | 1/1   | 0.81 | 0.07 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3116 | 1/1   | 0.81 | 0.14 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3030 | 1/1   | 0.81 | 0.51 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3260 | 1/1   | 0.81 | 0.63 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3250 | 1/1   | 0.81 | 0.28 | 80,80,80,80                 | 0     |
| 55  | MG   | RA    | 3322 | 1/1   | 0.81 | 0.17 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3147 | 1/1   | 0.82 | 0.29 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3458 | 1/1   | 0.82 | 0.26 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3083 | 1/1   | 0.82 | 0.29 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3391 | 1/1   | 0.82 | 0.26 | 81,81,81,81                 | 0     |
| 55  | MG   | XA    | 1651 | 1/1   | 0.82 | 0.11 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3031 | 1/1   | 0.82 | 0.33 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3033 | 1/1   | 0.82 | 0.26 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3242 | 1/1   | 0.82 | 0.15 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3512 | 1/1   | 0.82 | 0.18 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3515 | 1/1   | 0.82 | 0.14 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3349 | 1/1   | 0.82 | 0.27 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3399 | 1/1   | 0.82 | 0.23 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3040 | 1/1   | 0.82 | 0.32 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3356 | 1/1   | 0.82 | 0.35 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3485 | 1/1   | 0.82 | 0.23 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3247 | 1/1   | 0.82 | 0.40 | 82,82,82,82                 | 0     |
| 55  | MG   | RA    | 3251 | 1/1   | 0.82 | 0.39 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3220 | 1/1   | 0.82 | 0.13 | 70,70,70,70                 | 0     |
| 55  | MG   | RB    | 206  | 1/1   | 0.82 | 0.18 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3502 | 1/1   | 0.82 | 0.25 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3346 | 1/1   | 0.82 | 0.31 | 74,74,74,74                 | 0     |
| 55  | MG   | RB    | 211  | 1/1   | 0.82 | 0.08 | 84,84,84,84                 | 0     |
| 55  | MG   | YA    | 3385 | 1/1   | 0.82 | 0.30 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3117 | 1/1   | 0.82 | 0.26 | 64,64,64,64                 | 0     |
| 55  | MG   | RO    | 201  | 1/1   | 0.82 | 0.26 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3392 | 1/1   | 0.82 | 0.25 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3093 | 1/1   | 0.82 | 0.47 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3522 | 1/1   | 0.82 | 0.20 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3525 | 1/1   | 0.82 | 0.11 | 80,80,80,80                 | 0     |
| 55  | MG   | YA    | 3396 | 1/1   | 0.82 | 0.22 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3054 | 1/1   | 0.82 | 0.28 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3263 | 1/1   | 0.82 | 0.24 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3483 | 1/1   | 0.82 | 0.12 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3266 | 1/1   | 0.82 | 0.33 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3131 | 1/1   | 0.82 | 0.34 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3196 | 1/1   | 0.82 | 0.24 | 61,61,61,61                 | 0     |
| 55  | MG   | QA    | 1602 | 1/1   | 0.82 | 0.36 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3205 | 1/1   | 0.82 | 0.10 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3418 | 1/1   | 0.82 | 0.16 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3421 | 1/1   | 0.82 | 0.23 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3422 | 1/1   | 0.82 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3306 | 1/1   | 0.82 | 0.36 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3491 | 1/1   | 0.82 | 0.24 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3241 | 1/1   | 0.82 | 0.28 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3370 | 1/1   | 0.82 | 0.20 | 80,80,80,80                 | 0     |
| 55  | MG   | YA    | 3141 | 1/1   | 0.82 | 0.29 | 71,71,71,71                 | 0     |
| 55  | MG   | YQ    | 204  | 1/1   | 0.82 | 0.16 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3126 | 1/1   | 0.82 | 0.10 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3500 | 1/1   | 0.82 | 0.12 | 74,74,74,74                 | 0     |
| 55  | MG   | QA    | 1652 | 1/1   | 0.82 | 0.15 | 74,74,74,74                 | 0     |
| 55  | MG   | XA    | 1642 | 1/1   | 0.82 | 0.11 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3505 | 1/1   | 0.82 | 0.32 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3228 | 1/1   | 0.82 | 0.29 | 68,68,68,68                 | 0     |
| 57  | ZN   | R6    | 101  | 1/1   | 0.82 | 0.25 | 131,131,131,131             | 0     |
| 55  | MG   | RA    | 3449 | 1/1   | 0.82 | 0.11 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3472 | 1/1   | 0.83 | 0.17 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3450 | 1/1   | 0.83 | 0.20 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3341 | 1/1   | 0.83 | 0.08 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3359 | 1/1   | 0.83 | 0.07 | 74,74,74,74                 | 0     |
| 55  | MG   | QA    | 1635 | 1/1   | 0.83 | 0.17 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3123 | 1/1   | 0.83 | 0.11 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3006 | 1/1   | 0.83 | 0.26 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3265 | 1/1   | 0.83 | 0.43 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3379 | 1/1   | 0.83 | 0.21 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3064 | 1/1   | 0.83 | 0.46 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3351 | 1/1   | 0.83 | 0.23 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3352 | 1/1   | 0.83 | 0.14 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3501 | 1/1   | 0.83 | 0.15 | 54,54,54,54                 | 0     |
| 55  | MG   | YA    | 3068 | 1/1   | 0.83 | 0.31 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3408 | 1/1   | 0.83 | 0.18 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3202 | 1/1   | 0.83 | 0.24 | 77,77,77,77                 | 0     |
| 55  | MG   | RB    | 201  | 1/1   | 0.83 | 0.21 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3511 | 1/1   | 0.83 | 0.28 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3097 | 1/1   | 0.83 | 0.14 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3045 | 1/1   | 0.83 | 0.39 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3477 | 1/1   | 0.83 | 0.20 | 75,75,75,75                 | 0     |
| 55  | MG   | XA    | 1670 | 1/1   | 0.83 | 0.14 | 58,58,58,58                 | 0     |
| 55  | MG   | QA    | 1608 | 1/1   | 0.83 | 0.13 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3412 | 1/1   | 0.83 | 0.11 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3294 | 1/1   | 0.83 | 0.28 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3160 | 1/1   | 0.83 | 0.21 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3262 | 1/1   | 0.83 | 0.24 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3316 | 1/1   | 0.83 | 0.15 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3082 | 1/1   | 0.83 | 0.41 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3424 | 1/1   | 0.83 | 0.31 | 58,58,58,58                 | 0     |
| 55  | MG   | XA    | 1683 | 1/1   | 0.83 | 0.07 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3093 | 1/1   | 0.83 | 0.15 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3330 | 1/1   | 0.83 | 0.23 | 69,69,69,69                 | 0     |
| 55  | MG   | XA    | 1695 | 1/1   | 0.83 | 0.30 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3324 | 1/1   | 0.83 | 0.23 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3371 | 1/1   | 0.83 | 0.14 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3238 | 1/1   | 0.83 | 0.12 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3240 | 1/1   | 0.83 | 0.21 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3331 | 1/1   | 0.83 | 0.16 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YE    | 303  | 1/1   | 0.83 | 0.26 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3374 | 1/1   | 0.83 | 0.24 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3440 | 1/1   | 0.83 | 0.20 | 78,78,78,78                 | 0     |
| 55  | MG   | YA    | 3049 | 1/1   | 0.83 | 0.52 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3345 | 1/1   | 0.83 | 0.30 | 67,67,67,67                 | 0     |
| 55  | MG   | XS    | 101  | 1/1   | 0.83 | 0.07 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3154 | 1/1   | 0.83 | 0.25 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3251 | 1/1   | 0.83 | 0.23 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3444 | 1/1   | 0.83 | 0.09 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3446 | 1/1   | 0.83 | 0.17 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3355 | 1/1   | 0.83 | 0.16 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3042 | 1/1   | 0.83 | 0.32 | 62,62,62,62                 | 0     |
| 57  | ZN   | Y5    | 501  | 1/1   | 0.83 | 0.24 | 105,105,105,105             | 0     |
| 55  | MG   | YA    | 3368 | 1/1   | 0.84 | 0.29 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3058 | 1/1   | 0.84 | 0.34 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3373 | 1/1   | 0.84 | 0.40 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3035 | 1/1   | 0.84 | 0.49 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3293 | 1/1   | 0.84 | 0.18 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3384 | 1/1   | 0.84 | 0.25 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3496 | 1/1   | 0.84 | 0.42 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3488 | 1/1   | 0.84 | 0.23 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3270 | 1/1   | 0.84 | 0.18 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3219 | 1/1   | 0.84 | 0.34 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3497 | 1/1   | 0.84 | 0.34 | 72,72,72,72                 | 0     |
| 55  | MG   | XA    | 1603 | 1/1   | 0.84 | 0.34 | 61,61,61,61                 | 0     |
| 55  | MG   | XA    | 1604 | 1/1   | 0.84 | 0.08 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3447 | 1/1   | 0.84 | 0.26 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3130 | 1/1   | 0.84 | 0.35 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3349 | 1/1   | 0.84 | 0.12 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3047 | 1/1   | 0.84 | 0.38 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3167 | 1/1   | 0.84 | 0.22 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3080 | 1/1   | 0.84 | 0.24 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3099 | 1/1   | 0.84 | 0.23 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3405 | 1/1   | 0.84 | 0.27 | 79,79,79,79                 | 0     |
| 55  | MG   | RA    | 3278 | 1/1   | 0.84 | 0.41 | 73,73,73,73                 | 0     |
| 55  | MG   | XV    | 108  | 1/1   | 0.84 | 0.35 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3417 | 1/1   | 0.84 | 0.17 | 72,72,72,72                 | 0     |
| 55  | MG   | QA    | 1627 | 1/1   | 0.84 | 0.22 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3328 | 1/1   | 0.84 | 0.33 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3053 | 1/1   | 0.84 | 0.49 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3249 | 1/1   | 0.84 | 0.14 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3142 | 1/1   | 0.84 | 0.16 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3143 | 1/1   | 0.84 | 0.16 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3291 | 1/1   | 0.84 | 0.37 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3037 | 1/1   | 0.84 | 0.32 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3547 | 1/1   | 0.84 | 0.35 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3340 | 1/1   | 0.84 | 0.16 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3435 | 1/1   | 0.84 | 0.26 | 72,72,72,72                 | 0     |
| 55  | MG   | YB    | 202  | 1/1   | 0.84 | 0.12 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3341 | 1/1   | 0.84 | 0.15 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3328 | 1/1   | 0.84 | 0.17 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3329 | 1/1   | 0.84 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | RB    | 202  | 1/1   | 0.84 | 0.09 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3145 | 1/1   | 0.84 | 0.26 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3132 | 1/1   | 0.84 | 0.52 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3351 | 1/1   | 0.84 | 0.15 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3230 | 1/1   | 0.84 | 0.31 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3136 | 1/1   | 0.84 | 0.24 | 77,77,77,77                 | 0     |
| 55  | MG   | RA    | 3207 | 1/1   | 0.84 | 0.26 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3487 | 1/1   | 0.84 | 0.17 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3434 | 1/1   | 0.84 | 0.23 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3464 | 1/1   | 0.84 | 0.13 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3188 | 1/1   | 0.84 | 0.42 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3276 | 1/1   | 0.84 | 0.26 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3389 | 1/1   | 0.84 | 0.24 | 73,73,73,73                 | 0     |
| 57  | ZN   | YY    | 202  | 1/1   | 0.84 | 0.32 | 130,130,130,130             | 0     |
| 55  | MG   | YA    | 3144 | 1/1   | 0.84 | 0.17 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3367 | 1/1   | 0.84 | 0.28 | 65,65,65,65                 | 0     |
| 55  | MG   | XA    | 1613 | 1/1   | 0.85 | 0.26 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3289 | 1/1   | 0.85 | 0.19 | 55,55,55,55                 | 0     |
| 55  | MG   | XA    | 1625 | 1/1   | 0.85 | 0.16 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3365 | 1/1   | 0.85 | 0.27 | 75,75,75,75                 | 0     |
| 55  | MG   | XA    | 1629 | 1/1   | 0.85 | 0.23 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3125 | 1/1   | 0.85 | 0.26 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3284 | 1/1   | 0.85 | 0.51 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3174 | 1/1   | 0.85 | 0.13 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3016 | 1/1   | 0.85 | 0.35 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3178 | 1/1   | 0.85 | 0.16 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3003 | 1/1   | 0.85 | 0.27 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3301 | 1/1   | 0.85 | 0.26 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3386 | 1/1   | 0.85 | 0.30 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3133 | 1/1   | 0.85 | 0.32 | 71,71,71,71                 | 0     |
| 55  | MG   | QA    | 1677 | 1/1   | 0.85 | 0.21 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3389 | 1/1   | 0.85 | 0.27 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3210 | 1/1   | 0.85 | 0.38 | 68,68,68,68                 | 0     |
| 55  | MG   | QA    | 1678 | 1/1   | 0.85 | 0.16 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3183 | 1/1   | 0.85 | 0.32 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3398 | 1/1   | 0.85 | 0.29 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3015 | 1/1   | 0.85 | 0.28 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3311 | 1/1   | 0.85 | 0.28 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3516 | 1/1   | 0.85 | 0.17 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3184 | 1/1   | 0.85 | 0.14 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3255 | 1/1   | 0.85 | 0.26 | 61,61,61,61                 | 0     |
| 55  | MG   | QA    | 1625 | 1/1   | 0.85 | 0.09 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3057 | 1/1   | 0.85 | 0.41 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3523 | 1/1   | 0.85 | 0.19 | 79,79,79,79                 | 0     |
| 55  | MG   | RA    | 3411 | 1/1   | 0.85 | 0.17 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3075 | 1/1   | 0.85 | 0.33 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3023 | 1/1   | 0.85 | 0.45 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3416 | 1/1   | 0.85 | 0.29 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3413 | 1/1   | 0.85 | 0.25 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3076 | 1/1   | 0.85 | 0.36 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3420 | 1/1   | 0.85 | 0.30 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3325 | 1/1   | 0.85 | 0.10 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3314 | 1/1   | 0.85 | 0.31 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3227 | 1/1   | 0.85 | 0.36 | 66,66,66,66                 | 0     |
| 55  | MG   | XA    | 1663 | 1/1   | 0.85 | 0.23 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3332 | 1/1   | 0.85 | 0.20 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3077 | 1/1   | 0.85 | 0.22 | 67,67,67,67                 | 0     |
| 55  | MG   | YB    | 207  | 1/1   | 0.85 | 0.10 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3168 | 1/1   | 0.85 | 0.25 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3234 | 1/1   | 0.85 | 0.29 | 59,59,59,59                 | 0     |
| 55  | MG   | RE    | 304  | 1/1   | 0.85 | 0.26 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3436 | 1/1   | 0.85 | 0.35 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3421 | 1/1   | 0.85 | 0.19 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3236 | 1/1   | 0.85 | 0.38 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3366 | 1/1   | 0.85 | 0.25 | 58,58,58,58                 | 0     |
| 55  | MG   | YF    | 301  | 1/1   | 0.85 | 0.24 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3238 | 1/1   | 0.85 | 0.39 | 62,62,62,62                 | 0     |
| 55  | MG   | XA    | 1694 | 1/1   | 0.85 | 0.13 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3078 | 1/1   | 0.85 | 0.24 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3079 | 1/1   | 0.85 | 0.40 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3439 | 1/1   | 0.85 | 0.12 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3352 | 1/1   | 0.85 | 0.23 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3021 | 1/1   | 0.85 | 0.21 | 70,70,70,70                 | 0     |
| 57  | ZN   | R4    | 500  | 1/1   | 0.85 | 0.28 | 139,139,139,139             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3108 | 1/1   | 0.85 | 0.38 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3185 | 1/1   | 0.85 | 0.24 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3113 | 1/1   | 0.85 | 0.43 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3029 | 1/1   | 0.85 | 0.36 | 61,61,61,61                 | 0     |
| 55  | MG   | XQ    | 201  | 1/1   | 0.85 | 0.09 | 67,67,67,67                 | 0     |
| 55  | MG   | XA    | 1687 | 1/1   | 0.86 | 0.20 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3269 | 1/1   | 0.86 | 0.55 | 71,71,71,71                 | 0     |
| 55  | MG   | XA    | 1693 | 1/1   | 0.86 | 0.11 | 83,83,83,83                 | 0     |
| 55  | MG   | RA    | 3384 | 1/1   | 0.86 | 0.13 | 73,73,73,73                 | 0     |
| 55  | MG   | QA    | 1614 | 1/1   | 0.86 | 0.08 | 56,56,56,56                 | 0     |
| 55  | MG   | QA    | 1617 | 1/1   | 0.86 | 0.08 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3479 | 1/1   | 0.86 | 0.16 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3375 | 1/1   | 0.86 | 0.16 | 62,62,62,62                 | 0     |
| 55  | MG   | XA    | 1615 | 1/1   | 0.86 | 0.15 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3382 | 1/1   | 0.86 | 0.33 | 73,73,73,73                 | 0     |
| 55  | MG   | XA    | 1616 | 1/1   | 0.86 | 0.21 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3129 | 1/1   | 0.86 | 0.15 | 69,69,69,69                 | 0     |
| 55  | MG   | XA    | 1620 | 1/1   | 0.86 | 0.16 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3344 | 1/1   | 0.86 | 0.10 | 72,72,72,72                 | 0     |
| 55  | MG   | XA    | 1627 | 1/1   | 0.86 | 0.11 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3146 | 1/1   | 0.86 | 0.15 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3390 | 1/1   | 0.86 | 0.29 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3109 | 1/1   | 0.86 | 0.15 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3034 | 1/1   | 0.86 | 0.35 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3203 | 1/1   | 0.86 | 0.22 | 56,56,56,56                 | 0     |
| 55  | MG   | XA    | 1632 | 1/1   | 0.86 | 0.36 | 60,60,60,60                 | 0     |
| 55  | MG   | QA    | 1630 | 1/1   | 0.86 | 0.07 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3135 | 1/1   | 0.86 | 0.32 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3213 | 1/1   | 0.86 | 0.08 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3310 | 1/1   | 0.86 | 0.29 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3063 | 1/1   | 0.86 | 0.27 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3064 | 1/1   | 0.86 | 0.24 | 71,71,71,71                 | 0     |
| 55  | MG   | QA    | 1624 | 1/1   | 0.86 | 0.13 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3413 | 1/1   | 0.86 | 0.23 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3221 | 1/1   | 0.86 | 0.23 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3157 | 1/1   | 0.86 | 0.26 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3180 | 1/1   | 0.86 | 0.10 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3282 | 1/1   | 0.86 | 0.29 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3066 | 1/1   | 0.86 | 0.30 | 56,56,56,56                 | 0     |
| 55  | MG   | XA    | 1649 | 1/1   | 0.86 | 0.26 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3536 | 1/1   | 0.86 | 0.48 | 72,72,72,72                 | 0     |
| 55  | MG   | RB    | 205  | 1/1   | 0.86 | 0.10 | 79,79,79,79                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3539 | 1/1   | 0.86 | 0.53 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3475 | 1/1   | 0.86 | 0.13 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3078 | 1/1   | 0.86 | 0.32 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3247 | 1/1   | 0.86 | 0.18 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3367 | 1/1   | 0.86 | 0.12 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3288 | 1/1   | 0.86 | 0.08 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3163 | 1/1   | 0.86 | 0.20 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3084 | 1/1   | 0.86 | 0.32 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3165 | 1/1   | 0.86 | 0.18 | 78,78,78,78                 | 0     |
| 55  | MG   | QA    | 1609 | 1/1   | 0.86 | 0.09 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3344 | 1/1   | 0.86 | 0.27 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3029 | 1/1   | 0.86 | 0.31 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3168 | 1/1   | 0.86 | 0.32 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3103 | 1/1   | 0.86 | 0.22 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3248 | 1/1   | 0.86 | 0.24 | 63,63,63,63                 | 0     |
| 55  | MG   | YP    | 201  | 1/1   | 0.86 | 0.62 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3219 | 1/1   | 0.86 | 0.21 | 73,73,73,73                 | 0     |
| 55  | MG   | XA    | 1675 | 1/1   | 0.86 | 0.09 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3451 | 1/1   | 0.86 | 0.23 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3452 | 1/1   | 0.86 | 0.30 | 65,65,65,65                 | 0     |
| 55  | MG   | XA    | 1678 | 1/1   | 0.86 | 0.22 | 66,66,66,66                 | 0     |
| 55  | MG   | QA    | 1657 | 1/1   | 0.86 | 0.09 | 65,65,65,65                 | 0     |
| 55  | MG   | Y8    | 102  | 1/1   | 0.86 | 0.20 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3431 | 1/1   | 0.86 | 0.37 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3037 | 1/1   | 0.86 | 0.34 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3433 | 1/1   | 0.86 | 0.08 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3041 | 1/1   | 0.86 | 0.34 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3192 | 1/1   | 0.86 | 0.10 | 80,80,80,80                 | 0     |
| 55  | MG   | YA    | 3262 | 1/1   | 0.86 | 0.41 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3382 | 1/1   | 0.86 | 0.33 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3185 | 1/1   | 0.87 | 0.06 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3277 | 1/1   | 0.87 | 0.12 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3162 | 1/1   | 0.87 | 0.23 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3350 | 1/1   | 0.87 | 0.40 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3059 | 1/1   | 0.87 | 0.32 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3060 | 1/1   | 0.87 | 0.42 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3515 | 1/1   | 0.87 | 0.16 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3020 | 1/1   | 0.87 | 0.52 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3517 | 1/1   | 0.87 | 0.46 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3287 | 1/1   | 0.87 | 0.33 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3189 | 1/1   | 0.87 | 0.17 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3226 | 1/1   | 0.87 | 0.15 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | XA    | 1602 | 1/1   | 0.87 | 0.27 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3118 | 1/1   | 0.87 | 0.17 | 57,57,57,57                 | 0     |
| 55  | MG   | QA    | 1618 | 1/1   | 0.87 | 0.20 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3513 | 1/1   | 0.87 | 0.09 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3440 | 1/1   | 0.87 | 0.44 | 77,77,77,77                 | 0     |
| 55  | MG   | YA    | 3528 | 1/1   | 0.87 | 0.18 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3315 | 1/1   | 0.87 | 0.26 | 67,67,67,67                 | 0     |
| 55  | MG   | QA    | 1668 | 1/1   | 0.87 | 0.14 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3071 | 1/1   | 0.87 | 0.29 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3318 | 1/1   | 0.87 | 0.26 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3535 | 1/1   | 0.87 | 0.48 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3038 | 1/1   | 0.87 | 0.42 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3372 | 1/1   | 0.87 | 0.12 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3486 | 1/1   | 0.87 | 0.25 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3540 | 1/1   | 0.87 | 0.33 | 55,55,55,55                 | 0     |
| 55  | MG   | QA    | 1610 | 1/1   | 0.87 | 0.35 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3218 | 1/1   | 0.87 | 0.14 | 80,80,80,80                 | 0     |
| 55  | MG   | YA    | 3010 | 1/1   | 0.87 | 0.12 | 60,60,60,60                 | 0     |
| 55  | MG   | QA    | 1654 | 1/1   | 0.87 | 0.09 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3124 | 1/1   | 0.87 | 0.20 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3081 | 1/1   | 0.87 | 0.38 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3082 | 1/1   | 0.87 | 0.28 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3014 | 1/1   | 0.87 | 0.25 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3100 | 1/1   | 0.87 | 0.25 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3385 | 1/1   | 0.87 | 0.15 | 67,67,67,67                 | 0     |
| 55  | MG   | YD    | 303  | 1/1   | 0.87 | 0.38 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3388 | 1/1   | 0.87 | 0.14 | 81,81,81,81                 | 0     |
| 55  | MG   | YE    | 302  | 1/1   | 0.87 | 0.34 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3330 | 1/1   | 0.87 | 0.23 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3324 | 1/1   | 0.87 | 0.12 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3089 | 1/1   | 0.87 | 0.12 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3333 | 1/1   | 0.87 | 0.23 | 58,58,58,58                 | 0     |
| 55  | MG   | YP    | 202  | 1/1   | 0.87 | 0.18 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3222 | 1/1   | 0.87 | 0.24 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3091 | 1/1   | 0.87 | 0.53 | 72,72,72,72                 | 0     |
| 55  | MG   | YU    | 201  | 1/1   | 0.87 | 0.26 | 54,54,54,54                 | 0     |
| 55  | MG   | YA    | 3480 | 1/1   | 0.87 | 0.35 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3336 | 1/1   | 0.87 | 0.27 | 55,55,55,55                 | 0     |
| 55  | MG   | Y5    | 502  | 1/1   | 0.87 | 0.21 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3504 | 1/1   | 0.87 | 0.23 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3096 | 1/1   | 0.87 | 0.48 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3152 | 1/1   | 0.87 | 0.18 | 71,71,71,71                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3491 | 1/1   | 0.87 | 0.16 | 71,71,71,71                 | 0     |
| 55  | MG   | QA    | 1647 | 1/1   | 0.87 | 0.30 | 75,75,75,75                 | 0     |
| 55  | MG   | RR    | 202  | 1/1   | 0.87 | 0.20 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3159 | 1/1   | 0.87 | 0.30 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3026 | 1/1   | 0.87 | 0.25 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3500 | 1/1   | 0.87 | 0.13 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3346 | 1/1   | 0.87 | 0.38 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3102 | 1/1   | 0.88 | 0.26 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3493 | 1/1   | 0.88 | 0.17 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3128 | 1/1   | 0.88 | 0.35 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3402 | 1/1   | 0.88 | 0.19 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3191 | 1/1   | 0.88 | 0.10 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3085 | 1/1   | 0.88 | 0.31 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3507 | 1/1   | 0.88 | 0.10 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3173 | 1/1   | 0.88 | 0.18 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3212 | 1/1   | 0.88 | 0.10 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3104 | 1/1   | 0.88 | 0.32 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3312 | 1/1   | 0.88 | 0.29 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3399 | 1/1   | 0.88 | 0.14 | 77,77,77,77                 | 0     |
| 55  | MG   | XA    | 1634 | 1/1   | 0.88 | 0.18 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3004 | 1/1   | 0.88 | 0.17 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3364 | 1/1   | 0.88 | 0.30 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3066 | 1/1   | 0.88 | 0.38 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3318 | 1/1   | 0.88 | 0.36 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3008 | 1/1   | 0.88 | 0.11 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3409 | 1/1   | 0.88 | 0.22 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3295 | 1/1   | 0.88 | 0.30 | 69,69,69,69                 | 0     |
| 55  | MG   | QA    | 1634 | 1/1   | 0.88 | 0.10 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3459 | 1/1   | 0.88 | 0.16 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3524 | 1/1   | 0.88 | 0.19 | 81,81,81,81                 | 0     |
| 55  | MG   | YA    | 3229 | 1/1   | 0.88 | 0.20 | 70,70,70,70                 | 0     |
| 55  | MG   | XA    | 1643 | 1/1   | 0.88 | 0.17 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3461 | 1/1   | 0.88 | 0.17 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3419 | 1/1   | 0.88 | 0.23 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3299 | 1/1   | 0.88 | 0.16 | 65,65,65,65                 | 0     |
| 55  | MG   | QA    | 1629 | 1/1   | 0.88 | 0.07 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3107 | 1/1   | 0.88 | 0.28 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3158 | 1/1   | 0.88 | 0.27 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3416 | 1/1   | 0.88 | 0.20 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3470 | 1/1   | 0.88 | 0.11 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3471 | 1/1   | 0.88 | 0.26 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3241 | 1/1   | 0.88 | 0.09 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3162 | 1/1   | 0.88 | 0.28 | 69,69,69,69                 | 0     |
| 55  | MG   | RB    | 209  | 1/1   | 0.88 | 0.10 | 82,82,82,82                 | 0     |
| 55  | MG   | RA    | 3276 | 1/1   | 0.88 | 0.35 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3376 | 1/1   | 0.88 | 0.10 | 64,64,64,64                 | 0     |
| 55  | MG   | RE    | 303  | 1/1   | 0.88 | 0.08 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3551 | 1/1   | 0.88 | 0.27 | 72,72,72,72                 | 0     |
| 55  | MG   | XA    | 1671 | 1/1   | 0.88 | 0.28 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3134 | 1/1   | 0.88 | 0.26 | 72,72,72,72                 | 0     |
| 55  | MG   | YB    | 210  | 1/1   | 0.88 | 0.13 | 62,62,62,62                 | 0     |
| 55  | MG   | RN    | 201  | 1/1   | 0.88 | 0.33 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3380 | 1/1   | 0.88 | 0.27 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3422 | 1/1   | 0.88 | 0.21 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3279 | 1/1   | 0.88 | 0.23 | 66,66,66,66                 | 0     |
| 55  | MG   | XA    | 1681 | 1/1   | 0.88 | 0.33 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3425 | 1/1   | 0.88 | 0.25 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3312 | 1/1   | 0.88 | 0.20 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3178 | 1/1   | 0.88 | 0.14 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3383 | 1/1   | 0.88 | 0.16 | 76,76,76,76                 | 0     |
| 55  | MG   | YA    | 3101 | 1/1   | 0.88 | 0.43 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3264 | 1/1   | 0.88 | 0.44 | 66,66,66,66                 | 0     |
| 55  | MG   | XA    | 1685 | 1/1   | 0.88 | 0.09 | 70,70,70,70                 | 0     |
| 55  | MG   | QA    | 1632 | 1/1   | 0.88 | 0.28 | 59,59,59,59                 | 0     |
| 55  | MG   | XA    | 1689 | 1/1   | 0.88 | 0.24 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3270 | 1/1   | 0.88 | 0.31 | 66,66,66,66                 | 0     |
| 55  | MG   | YX    | 102  | 1/1   | 0.88 | 0.10 | 72,72,72,72                 | 0     |
| 55  | MG   | XA    | 1692 | 1/1   | 0.88 | 0.29 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3002 | 1/1   | 0.88 | 0.27 | 67,67,67,67                 | 0     |
| 55  | MG   | QV    | 103  | 1/1   | 0.88 | 0.15 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3370 | 1/1   | 0.88 | 0.12 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3494 | 1/1   | 0.88 | 0.17 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3231 | 1/1   | 0.88 | 0.33 | 67,67,67,67                 | 0     |
| 55  | MG   | XA    | 1697 | 1/1   | 0.88 | 0.12 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3004 | 1/1   | 0.88 | 0.28 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3483 | 1/1   | 0.88 | 0.22 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3256 | 1/1   | 0.88 | 0.28 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3288 | 1/1   | 0.88 | 0.31 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3396 | 1/1   | 0.88 | 0.17 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3502 | 1/1   | 0.88 | 0.32 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3345 | 1/1   | 0.89 | 0.18 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3239 | 1/1   | 0.89 | 0.20 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3400 | 1/1   | 0.89 | 0.08 | 60,60,60,60                 | 0     |
| 55  | MG   | RQ    | 201  | 1/1   | 0.89 | 0.41 | 75,75,75,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3402 | 1/1   | 0.89 | 0.29 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3316 | 1/1   | 0.89 | 0.24 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3504 | 1/1   | 0.89 | 0.27 | 67,67,67,67                 | 0     |
| 55  | MG   | QA    | 1643 | 1/1   | 0.89 | 0.09 | 80,80,80,80                 | 0     |
| 55  | MG   | YA    | 3405 | 1/1   | 0.89 | 0.21 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3005 | 1/1   | 0.89 | 0.25 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3174 | 1/1   | 0.89 | 0.29 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3513 | 1/1   | 0.89 | 0.09 | 55,55,55,55                 | 0     |
| 55  | MG   | QA    | 1646 | 1/1   | 0.89 | 0.07 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3111 | 1/1   | 0.89 | 0.39 | 72,72,72,72                 | 0     |
| 55  | MG   | XA    | 1656 | 1/1   | 0.89 | 0.05 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3058 | 1/1   | 0.89 | 0.10 | 65,65,65,65                 | 0     |
| 55  | MG   | XA    | 1657 | 1/1   | 0.89 | 0.51 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3265 | 1/1   | 0.89 | 0.18 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3035 | 1/1   | 0.89 | 0.23 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3120 | 1/1   | 0.89 | 0.41 | 54,54,54,54                 | 0     |
| 55  | MG   | XA    | 1665 | 1/1   | 0.89 | 0.08 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3122 | 1/1   | 0.89 | 0.37 | 54,54,54,54                 | 0     |
| 55  | MG   | YA    | 3258 | 1/1   | 0.89 | 0.25 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3246 | 1/1   | 0.89 | 0.31 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3272 | 1/1   | 0.89 | 0.34 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3465 | 1/1   | 0.89 | 0.39 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3135 | 1/1   | 0.89 | 0.10 | 63,63,63,63                 | 0     |
| 55  | MG   | XA    | 1614 | 1/1   | 0.89 | 0.21 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3149 | 1/1   | 0.89 | 0.41 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3426 | 1/1   | 0.89 | 0.13 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3070 | 1/1   | 0.89 | 0.35 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3361 | 1/1   | 0.89 | 0.18 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3437 | 1/1   | 0.89 | 0.08 | 69,69,69,69                 | 0     |
| 55  | MG   | XA    | 1619 | 1/1   | 0.89 | 0.51 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3300 | 1/1   | 0.89 | 0.30 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3543 | 1/1   | 0.89 | 0.22 | 66,66,66,66                 | 0     |
| 55  | MG   | XA    | 1621 | 1/1   | 0.89 | 0.49 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3202 | 1/1   | 0.89 | 0.27 | 57,57,57,57                 | 0     |
| 55  | MG   | XA    | 1622 | 1/1   | 0.89 | 0.13 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3400 | 1/1   | 0.89 | 0.24 | 75,75,75,75                 | 0     |
| 55  | MG   | QA    | 1633 | 1/1   | 0.89 | 0.06 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3448 | 1/1   | 0.89 | 0.17 | 72,72,72,72                 | 0     |
| 55  | MG   | YB    | 203  | 1/1   | 0.89 | 0.08 | 61,61,61,61                 | 0     |
| 55  | MG   | YB    | 205  | 1/1   | 0.89 | 0.11 | 72,72,72,72                 | 0     |
| 55  | MG   | XA    | 1628 | 1/1   | 0.89 | 0.17 | 54,54,54,54                 | 0     |
| 55  | MG   | YA    | 3363 | 1/1   | 0.89 | 0.36 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3432 | 1/1   | 0.89 | 0.27 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3453 | 1/1   | 0.89 | 0.11 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3187 | 1/1   | 0.89 | 0.12 | 69,69,69,69                 | 0     |
| 55  | MG   | QA    | 1679 | 1/1   | 0.89 | 0.13 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3436 | 1/1   | 0.89 | 0.18 | 58,58,58,58                 | 0     |
| 55  | MG   | XA    | 1633 | 1/1   | 0.89 | 0.34 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3437 | 1/1   | 0.89 | 0.29 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3305 | 1/1   | 0.89 | 0.17 | 58,58,58,58                 | 0     |
| 55  | MG   | XE    | 201  | 1/1   | 0.89 | 0.06 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3223 | 1/1   | 0.89 | 0.11 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3156 | 1/1   | 0.89 | 0.22 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3471 | 1/1   | 0.89 | 0.09 | 80,80,80,80                 | 0     |
| 55  | MG   | YA    | 3378 | 1/1   | 0.89 | 0.20 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3067 | 1/1   | 0.89 | 0.34 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3474 | 1/1   | 0.89 | 0.10 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3380 | 1/1   | 0.89 | 0.22 | 58,58,58,58                 | 0     |
| 55  | MG   | XL    | 202  | 1/1   | 0.89 | 0.23 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3406 | 1/1   | 0.89 | 0.31 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3308 | 1/1   | 0.89 | 0.33 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3068 | 1/1   | 0.89 | 0.26 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3095 | 1/1   | 0.89 | 0.50 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3336 | 1/1   | 0.89 | 0.30 | 67,67,67,67                 | 0     |
| 55  | MG   | QA    | 1639 | 1/1   | 0.89 | 0.14 | 69,69,69,69                 | 0     |
| 55  | MG   | QA    | 1611 | 1/1   | 0.89 | 0.25 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3391 | 1/1   | 0.89 | 0.15 | 76,76,76,76                 | 0     |
| 55  | MG   | QA    | 1662 | 1/1   | 0.89 | 0.27 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3060 | 1/1   | 0.89 | 0.54 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3321 | 1/1   | 0.89 | 0.34 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3397 | 1/1   | 0.89 | 0.21 | 65,65,65,65                 | 0     |
| 57  | ZN   | Y6    | 101  | 1/1   | 0.89 | 0.28 | 133,133,133,133             | 0     |
| 55  | MG   | YA    | 3009 | 1/1   | 0.90 | 0.07 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3167 | 1/1   | 0.90 | 0.16 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3299 | 1/1   | 0.90 | 0.25 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3186 | 1/1   | 0.90 | 0.13 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3028 | 1/1   | 0.90 | 0.25 | 65,65,65,65                 | 0     |
| 55  | MG   | XA    | 1674 | 1/1   | 0.90 | 0.21 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3112 | 1/1   | 0.90 | 0.18 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3297 | 1/1   | 0.90 | 0.26 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3016 | 1/1   | 0.90 | 0.37 | 64,64,64,64                 | 0     |
| 55  | MG   | QA    | 1665 | 1/1   | 0.90 | 0.15 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3476 | 1/1   | 0.90 | 0.14 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3520 | 1/1   | 0.90 | 0.16 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3268 | 1/1   | 0.90 | 0.46 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3478 | 1/1   | 0.90 | 0.10 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3213 | 1/1   | 0.90 | 0.28 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3315 | 1/1   | 0.90 | 0.14 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3533 | 1/1   | 0.90 | 0.59 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3450 | 1/1   | 0.90 | 0.30 | 64,64,64,64                 | 0     |
| 55  | MG   | RB    | 203  | 1/1   | 0.90 | 0.11 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3214 | 1/1   | 0.90 | 0.10 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3126 | 1/1   | 0.90 | 0.20 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3073 | 1/1   | 0.90 | 0.35 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3305 | 1/1   | 0.90 | 0.40 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3541 | 1/1   | 0.90 | 0.22 | 66,66,66,66                 | 0     |
| 55  | MG   | XA    | 1691 | 1/1   | 0.90 | 0.13 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3130 | 1/1   | 0.90 | 0.24 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3545 | 1/1   | 0.90 | 0.20 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3334 | 1/1   | 0.90 | 0.17 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3441 | 1/1   | 0.90 | 0.35 | 76,76,76,76                 | 0     |
| 55  | MG   | RB    | 210  | 1/1   | 0.90 | 0.16 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3190 | 1/1   | 0.90 | 0.29 | 64,64,64,64                 | 0     |
| 55  | MG   | QA    | 1638 | 1/1   | 0.90 | 0.16 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3372 | 1/1   | 0.90 | 0.23 | 67,67,67,67                 | 0     |
| 55  | MG   | QA    | 1649 | 1/1   | 0.90 | 0.07 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3412 | 1/1   | 0.90 | 0.21 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3337 | 1/1   | 0.90 | 0.23 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3052 | 1/1   | 0.90 | 0.16 | 54,54,54,54                 | 0     |
| 55  | MG   | QA    | 1622 | 1/1   | 0.90 | 0.17 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3125 | 1/1   | 0.90 | 0.33 | 59,59,59,59                 | 0     |
| 55  | MG   | QA    | 1645 | 1/1   | 0.90 | 0.08 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3263 | 1/1   | 0.90 | 0.44 | 64,64,64,64                 | 0     |
| 55  | MG   | RQ    | 202  | 1/1   | 0.90 | 0.27 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3481 | 1/1   | 0.90 | 0.14 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3501 | 1/1   | 0.90 | 0.25 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3407 | 1/1   | 0.90 | 0.11 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3408 | 1/1   | 0.90 | 0.36 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3207 | 1/1   | 0.90 | 0.20 | 62,62,62,62                 | 0     |
| 55  | MG   | RT    | 201  | 1/1   | 0.90 | 0.08 | 73,73,73,73                 | 0     |
| 55  | MG   | YQ    | 201  | 1/1   | 0.90 | 0.14 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3005 | 1/1   | 0.90 | 0.47 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3492 | 1/1   | 0.90 | 0.12 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3274 | 1/1   | 0.90 | 0.10 | 71,71,71,71                 | 0     |
| 55  | MG   | QA    | 1653 | 1/1   | 0.90 | 0.08 | 74,74,74,74                 | 0     |
| 55  | MG   | YY    | 201  | 1/1   | 0.90 | 0.29 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | Y0    | 101  | 1/1   | 0.90 | 0.33 | 61,61,61,61                 | 0     |
| 55  | MG   | QA    | 1640 | 1/1   | 0.90 | 0.09 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3099 | 1/1   | 0.90 | 0.20 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3203 | 1/1   | 0.90 | 0.08 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3233 | 1/1   | 0.90 | 0.07 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3283 | 1/1   | 0.90 | 0.19 | 55,55,55,55                 | 0     |
| 55  | MG   | XA    | 1664 | 1/1   | 0.90 | 0.33 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3390 | 1/1   | 0.90 | 0.31 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3220 | 1/1   | 0.90 | 0.35 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3423 | 1/1   | 0.90 | 0.27 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3007 | 1/1   | 0.90 | 0.38 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3509 | 1/1   | 0.90 | 0.10 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3069 | 1/1   | 0.90 | 0.22 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3427 | 1/1   | 0.90 | 0.30 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3429 | 1/1   | 0.90 | 0.23 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3087 | 1/1   | 0.91 | 0.15 | 70,70,70,70                 | 0     |
| 55  | MG   | XA    | 1608 | 1/1   | 0.91 | 0.33 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3517 | 1/1   | 0.91 | 0.26 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3142 | 1/1   | 0.91 | 0.23 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3456 | 1/1   | 0.91 | 0.07 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3198 | 1/1   | 0.91 | 0.17 | 70,70,70,70                 | 0     |
| 55  | MG   | QA    | 1680 | 1/1   | 0.91 | 0.06 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3163 | 1/1   | 0.91 | 0.09 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3326 | 1/1   | 0.91 | 0.23 | 61,61,61,61                 | 0     |
| 55  | MG   | XA    | 1666 | 1/1   | 0.91 | 0.14 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3463 | 1/1   | 0.91 | 0.22 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3122 | 1/1   | 0.91 | 0.10 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3027 | 1/1   | 0.91 | 0.29 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3269 | 1/1   | 0.91 | 0.11 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3015 | 1/1   | 0.91 | 0.20 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3232 | 1/1   | 0.91 | 0.45 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3001 | 1/1   | 0.91 | 0.33 | 59,59,59,59                 | 0     |
| 55  | MG   | XA    | 1676 | 1/1   | 0.91 | 0.08 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3490 | 1/1   | 0.91 | 0.14 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3548 | 1/1   | 0.91 | 0.34 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3272 | 1/1   | 0.91 | 0.24 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3273 | 1/1   | 0.91 | 0.27 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3387 | 1/1   | 0.91 | 0.22 | 66,66,66,66                 | 0     |
| 55  | MG   | RB    | 208  | 1/1   | 0.91 | 0.24 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3190 | 1/1   | 0.91 | 0.17 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3107 | 1/1   | 0.91 | 0.23 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3302 | 1/1   | 0.91 | 0.27 | 76,76,76,76                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | YA    | 3110 | 1/1   | 0.91 | 0.23 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3235 | 1/1   | 0.91 | 0.40 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3327 | 1/1   | 0.91 | 0.18 | 72,72,72,72                 | 0     |
| 55  | MG   | RE    | 301  | 1/1   | 0.91 | 0.28 | 68,68,68,68                 | 0     |
| 55  | MG   | XA    | 1686 | 1/1   | 0.91 | 0.16 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3489 | 1/1   | 0.91 | 0.30 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3254 | 1/1   | 0.91 | 0.30 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3289 | 1/1   | 0.91 | 0.39 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3117 | 1/1   | 0.91 | 0.14 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3062 | 1/1   | 0.91 | 0.27 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3294 | 1/1   | 0.91 | 0.34 | 56,56,56,56                 | 0     |
| 55  | MG   | YO    | 201  | 1/1   | 0.91 | 0.29 | 67,67,67,67                 | 0     |
| 55  | MG   | XA    | 1635 | 1/1   | 0.91 | 0.26 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3298 | 1/1   | 0.91 | 0.26 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3460 | 1/1   | 0.91 | 0.09 | 58,58,58,58                 | 0     |
| 55  | MG   | YQ    | 202  | 1/1   | 0.91 | 0.26 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3300 | 1/1   | 0.91 | 0.28 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3398 | 1/1   | 0.91 | 0.15 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3362 | 1/1   | 0.91 | 0.19 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3280 | 1/1   | 0.91 | 0.30 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3304 | 1/1   | 0.91 | 0.21 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3204 | 1/1   | 0.91 | 0.19 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3401 | 1/1   | 0.91 | 0.08 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3257 | 1/1   | 0.91 | 0.09 | 84,84,84,84                 | 0     |
| 55  | MG   | QA    | 1641 | 1/1   | 0.91 | 0.22 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3153 | 1/1   | 0.91 | 0.22 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3260 | 1/1   | 0.91 | 0.18 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3313 | 1/1   | 0.91 | 0.27 | 73,73,73,73                 | 0     |
| 55  | MG   | R8    | 101  | 1/1   | 0.91 | 0.22 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3435 | 1/1   | 0.91 | 0.08 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3209 | 1/1   | 0.91 | 0.30 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3520 | 1/1   | 0.91 | 0.16 | 66,66,66,66                 | 0     |
| 55  | MG   | XV    | 101  | 1/1   | 0.91 | 0.29 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3224 | 1/1   | 0.91 | 0.40 | 57,57,57,57                 | 0     |
| 55  | MG   | RA    | 3438 | 1/1   | 0.91 | 0.10 | 81,81,81,81                 | 0     |
| 55  | MG   | XA    | 1605 | 1/1   | 0.91 | 0.18 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3182 | 1/1   | 0.92 | 0.11 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3040 | 1/1   | 0.92 | 0.52 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3278 | 1/1   | 0.92 | 0.42 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3532 | 1/1   | 0.92 | 0.19 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3279 | 1/1   | 0.92 | 0.27 | 70,70,70,70                 | 0     |
| 55  | MG   | QA    | 1672 | 1/1   | 0.92 | 0.22 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | XA    | 1673 | 1/1   | 0.92 | 0.21 | 63,63,63,63                 | 0     |
| 55  | MG   | QF    | 201  | 1/1   | 0.92 | 0.08 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3468 | 1/1   | 0.92 | 0.28 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3011 | 1/1   | 0.92 | 0.14 | 55,55,55,55                 | 0     |
| 55  | MG   | QH    | 201  | 1/1   | 0.92 | 0.15 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3283 | 1/1   | 0.92 | 0.20 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3542 | 1/1   | 0.92 | 0.12 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3480 | 1/1   | 0.92 | 0.08 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3179 | 1/1   | 0.92 | 0.20 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3139 | 1/1   | 0.92 | 0.12 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3292 | 1/1   | 0.92 | 0.29 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3223 | 1/1   | 0.92 | 0.20 | 55,55,55,55                 | 0     |
| 55  | MG   | QA    | 1666 | 1/1   | 0.92 | 0.22 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3090 | 1/1   | 0.92 | 0.13 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3296 | 1/1   | 0.92 | 0.28 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3011 | 1/1   | 0.92 | 0.20 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3136 | 1/1   | 0.92 | 0.18 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3086 | 1/1   | 0.92 | 0.27 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3485 | 1/1   | 0.92 | 0.20 | 64,64,64,64                 | 0     |
| 55  | MG   | YB    | 208  | 1/1   | 0.92 | 0.06 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3208 | 1/1   | 0.92 | 0.09 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3395 | 1/1   | 0.92 | 0.08 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3267 | 1/1   | 0.92 | 0.43 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3192 | 1/1   | 0.92 | 0.43 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3455 | 1/1   | 0.92 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | XA    | 1690 | 1/1   | 0.92 | 0.25 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3250 | 1/1   | 0.92 | 0.16 | 73,73,73,73                 | 0     |
| 55  | MG   | XA    | 1606 | 1/1   | 0.92 | 0.19 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3041 | 1/1   | 0.92 | 0.24 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3147 | 1/1   | 0.92 | 0.06 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3431 | 1/1   | 0.92 | 0.09 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3115 | 1/1   | 0.92 | 0.07 | 59,59,59,59                 | 0     |
| 55  | MG   | XA    | 1650 | 1/1   | 0.92 | 0.20 | 74,74,74,74                 | 0     |
| 55  | MG   | XA    | 1612 | 1/1   | 0.92 | 0.18 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3338 | 1/1   | 0.92 | 0.20 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3106 | 1/1   | 0.92 | 0.11 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3369 | 1/1   | 0.92 | 0.10 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3377 | 1/1   | 0.92 | 0.17 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3510 | 1/1   | 0.92 | 0.27 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3495 | 1/1   | 0.92 | 0.53 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3109 | 1/1   | 0.92 | 0.22 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3339 | 1/1   | 0.92 | 0.07 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | QA    | 1620 | 1/1   | 0.92 | 0.06 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3444 | 1/1   | 0.92 | 0.06 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3445 | 1/1   | 0.92 | 0.12 | 68,68,68,68                 | 0     |
| 55  | MG   | XA    | 1662 | 1/1   | 0.92 | 0.18 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3075 | 1/1   | 0.92 | 0.21 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3342 | 1/1   | 0.92 | 0.23 | 59,59,59,59                 | 0     |
| 56  | SF4  | QD    | 301  | 8/8   | 0.92 | 0.08 | 60,86,98,101                | 0     |
| 55  | MG   | RA    | 3296 | 1/1   | 0.92 | 0.30 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3327 | 1/1   | 0.92 | 0.20 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3271 | 1/1   | 0.92 | 0.37 | 68,68,68,68                 | 0     |
| 55  | MG   | QA    | 1651 | 1/1   | 0.92 | 0.07 | 66,66,66,66                 | 0     |
| 55  | MG   | QA    | 1605 | 1/1   | 0.92 | 0.38 | 60,60,60,60                 | 0     |
| 55  | MG   | XA    | 1668 | 1/1   | 0.92 | 0.20 | 70,70,70,70                 | 0     |
| 55  | MG   | QA    | 1616 | 1/1   | 0.92 | 0.06 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3395 | 1/1   | 0.92 | 0.05 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3153 | 1/1   | 0.93 | 0.08 | 62,62,62,62                 | 0     |
| 55  | MG   | YB    | 201  | 1/1   | 0.93 | 0.10 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3154 | 1/1   | 0.93 | 0.17 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3215 | 1/1   | 0.93 | 0.09 | 71,71,71,71                 | 0     |
| 55  | MG   | XA    | 1652 | 1/1   | 0.93 | 0.26 | 58,58,58,58                 | 0     |
| 55  | MG   | YA    | 3217 | 1/1   | 0.93 | 0.32 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3512 | 1/1   | 0.93 | 0.27 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3254 | 1/1   | 0.93 | 0.45 | 68,68,68,68                 | 0     |
| 55  | MG   | QA    | 1621 | 1/1   | 0.93 | 0.07 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3376 | 1/1   | 0.93 | 0.17 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3394 | 1/1   | 0.93 | 0.19 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3357 | 1/1   | 0.93 | 0.14 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3493 | 1/1   | 0.93 | 0.14 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3222 | 1/1   | 0.93 | 0.19 | 65,65,65,65                 | 0     |
| 55  | MG   | QV    | 102  | 1/1   | 0.93 | 0.10 | 71,71,71,71                 | 0     |
| 55  | MG   | YA    | 3383 | 1/1   | 0.93 | 0.23 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3206 | 1/1   | 0.93 | 0.08 | 66,66,66,66                 | 0     |
| 55  | MG   | QA    | 1619 | 1/1   | 0.93 | 0.06 | 60,60,60,60                 | 0     |
| 55  | MG   | QC    | 301  | 1/1   | 0.93 | 0.08 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3176 | 1/1   | 0.93 | 0.08 | 54,54,54,54                 | 0     |
| 55  | MG   | XA    | 1639 | 1/1   | 0.93 | 0.09 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3267 | 1/1   | 0.93 | 0.58 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3071 | 1/1   | 0.93 | 0.06 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3034 | 1/1   | 0.93 | 0.25 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3098 | 1/1   | 0.93 | 0.16 | 56,56,56,56                 | 0     |
| 55  | MG   | XA    | 1669 | 1/1   | 0.93 | 0.09 | 56,56,56,56                 | 0     |
| 55  | MG   | QA    | 1676 | 1/1   | 0.93 | 0.06 | 64,64,64,64                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | XA    | 1618 | 1/1   | 0.93 | 0.18 | 66,66,66,66                 | 0     |
| 55  | MG   | XA    | 1644 | 1/1   | 0.93 | 0.24 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3368 | 1/1   | 0.93 | 0.16 | 63,63,63,63                 | 0     |
| 55  | MG   | QA    | 1613 | 1/1   | 0.93 | 0.18 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3537 | 1/1   | 0.93 | 0.58 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3204 | 1/1   | 0.93 | 0.12 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3206 | 1/1   | 0.93 | 0.11 | 58,58,58,58                 | 0     |
| 55  | MG   | QA    | 1628 | 1/1   | 0.93 | 0.08 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3208 | 1/1   | 0.93 | 0.25 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3360 | 1/1   | 0.93 | 0.13 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3424 | 1/1   | 0.93 | 0.11 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3282 | 1/1   | 0.93 | 0.25 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3228 | 1/1   | 0.93 | 0.47 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3508 | 1/1   | 0.93 | 0.07 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3503 | 1/1   | 0.93 | 0.24 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3311 | 1/1   | 0.93 | 0.37 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3286 | 1/1   | 0.93 | 0.21 | 66,66,66,66                 | 0     |
| 55  | MG   | RR    | 201  | 1/1   | 0.94 | 0.15 | 68,68,68,68                 | 0     |
| 55  | MG   | RA    | 3199 | 1/1   | 0.94 | 0.10 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3113 | 1/1   | 0.94 | 0.14 | 60,60,60,60                 | 0     |
| 55  | MG   | RA    | 3468 | 1/1   | 0.94 | 0.12 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3072 | 1/1   | 0.94 | 0.34 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3438 | 1/1   | 0.94 | 0.10 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3084 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3386 | 1/1   | 0.94 | 0.20 | 64,64,64,64                 | 0     |
| 55  | MG   | XV    | 104  | 1/1   | 0.94 | 0.06 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3445 | 1/1   | 0.94 | 0.36 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3497 | 1/1   | 0.94 | 0.49 | 66,66,66,66                 | 0     |
| 55  | MG   | YB    | 204  | 1/1   | 0.94 | 0.06 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3205 | 1/1   | 0.94 | 0.22 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3297 | 1/1   | 0.94 | 0.32 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3348 | 1/1   | 0.94 | 0.30 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3473 | 1/1   | 0.94 | 0.12 | 69,69,69,69                 | 0     |
| 55  | MG   | QA    | 1623 | 1/1   | 0.94 | 0.21 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3427 | 1/1   | 0.94 | 0.12 | 73,73,73,73                 | 0     |
| 55  | MG   | QA    | 1674 | 1/1   | 0.94 | 0.18 | 73,73,73,73                 | 0     |
| 55  | MG   | XA    | 1609 | 1/1   | 0.94 | 0.06 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3009 | 1/1   | 0.94 | 0.39 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3169 | 1/1   | 0.94 | 0.22 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3455 | 1/1   | 0.94 | 0.07 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3479 | 1/1   | 0.94 | 0.10 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3453 | 1/1   | 0.94 | 0.09 | 58,58,58,58                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3237 | 1/1   | 0.94 | 0.23 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3277 | 1/1   | 0.94 | 0.21 | 57,57,57,57                 | 0     |
| 55  | MG   | RE    | 302  | 1/1   | 0.94 | 0.07 | 76,76,76,76                 | 0     |
| 55  | MG   | RA    | 3355 | 1/1   | 0.94 | 0.28 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3266 | 1/1   | 0.94 | 0.45 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3091 | 1/1   | 0.94 | 0.49 | 71,71,71,71                 | 0     |
| 55  | MG   | QA    | 1601 | 1/1   | 0.94 | 0.17 | 55,55,55,55                 | 0     |
| 55  | MG   | XA    | 1688 | 1/1   | 0.94 | 0.12 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3375 | 1/1   | 0.94 | 0.12 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3196 | 1/1   | 0.94 | 0.10 | 61,61,61,61                 | 0     |
| 55  | MG   | XA    | 1654 | 1/1   | 0.94 | 0.09 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3264 | 1/1   | 0.94 | 0.36 | 75,75,75,75                 | 0     |
| 55  | MG   | YA    | 3369 | 1/1   | 0.94 | 0.20 | 65,65,65,65                 | 0     |
| 55  | MG   | QA    | 1606 | 1/1   | 0.94 | 0.10 | 65,65,65,65                 | 0     |
| 55  | MG   | YA    | 3021 | 1/1   | 0.94 | 0.28 | 64,64,64,64                 | 0     |
| 55  | MG   | XA    | 1624 | 1/1   | 0.94 | 0.39 | 64,64,64,64                 | 0     |
| 55  | MG   | RA    | 3253 | 1/1   | 0.94 | 0.35 | 62,62,62,62                 | 0     |
| 55  | MG   | XA    | 1659 | 1/1   | 0.94 | 0.15 | 74,74,74,74                 | 0     |
| 55  | MG   | XA    | 1660 | 1/1   | 0.94 | 0.09 | 55,55,55,55                 | 0     |
| 55  | MG   | XA    | 1661 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 55  | MG   | XA    | 1626 | 1/1   | 0.94 | 0.10 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3482 | 1/1   | 0.94 | 0.15 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3083 | 1/1   | 0.94 | 0.18 | 60,60,60,60                 | 0     |
| 55  | MG   | RQ    | 203  | 1/1   | 0.94 | 0.10 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3151 | 1/1   | 0.94 | 0.26 | 64,64,64,64                 | 0     |
| 55  | MG   | YA    | 3381 | 1/1   | 0.94 | 0.29 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3487 | 1/1   | 0.94 | 0.07 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3378 | 1/1   | 0.95 | 0.12 | 72,72,72,72                 | 0     |
| 55  | MG   | RA    | 3151 | 1/1   | 0.95 | 0.42 | 70,70,70,70                 | 0     |
| 55  | MG   | QA    | 1669 | 1/1   | 0.95 | 0.08 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3146 | 1/1   | 0.95 | 0.29 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3175 | 1/1   | 0.95 | 0.12 | 65,65,65,65                 | 0     |
| 55  | MG   | QA    | 1607 | 1/1   | 0.95 | 0.06 | 67,67,67,67                 | 0     |
| 55  | MG   | RA    | 3271 | 1/1   | 0.95 | 0.33 | 74,74,74,74                 | 0     |
| 55  | MG   | YA    | 3249 | 1/1   | 0.95 | 0.07 | 66,66,66,66                 | 0     |
| 55  | MG   | XA    | 1677 | 1/1   | 0.95 | 0.27 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3224 | 1/1   | 0.95 | 0.11 | 62,62,62,62                 | 0     |
| 55  | MG   | XA    | 1637 | 1/1   | 0.95 | 0.07 | 71,71,71,71                 | 0     |
| 55  | MG   | RA    | 3301 | 1/1   | 0.95 | 0.25 | 54,54,54,54                 | 0     |
| 55  | MG   | RA    | 3448 | 1/1   | 0.95 | 0.07 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3332 | 1/1   | 0.95 | 0.22 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3333 | 1/1   | 0.95 | 0.11 | 55,55,55,55                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3360 | 1/1   | 0.95 | 0.06 | 59,59,59,59                 | 0     |
| 55  | MG   | YA    | 3338 | 1/1   | 0.95 | 0.48 | 71,71,71,71                 | 0     |
| 55  | MG   | XA    | 1623 | 1/1   | 0.95 | 0.26 | 63,63,63,63                 | 0     |
| 55  | MG   | YA    | 3454 | 1/1   | 0.95 | 0.08 | 61,61,61,61                 | 0     |
| 55  | MG   | QA    | 1655 | 1/1   | 0.95 | 0.14 | 70,70,70,70                 | 0     |
| 55  | MG   | RA    | 3165 | 1/1   | 0.95 | 0.12 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3428 | 1/1   | 0.95 | 0.39 | 68,68,68,68                 | 0     |
| 55  | MG   | YA    | 3490 | 1/1   | 0.95 | 0.19 | 75,75,75,75                 | 0     |
| 55  | MG   | RA    | 3150 | 1/1   | 0.95 | 0.25 | 58,58,58,58                 | 0     |
| 57  | ZN   | QN    | 101  | 1/1   | 0.95 | 0.09 | 108,108,108,108             | 0     |
| 55  | MG   | YB    | 206  | 1/1   | 0.95 | 0.24 | 58,58,58,58                 | 0     |
| 55  | MG   | XV    | 106  | 1/1   | 0.95 | 0.28 | 66,66,66,66                 | 0     |
| 55  | MG   | XA    | 1607 | 1/1   | 0.95 | 0.25 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3275 | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 55  | MG   | XX    | 101  | 1/1   | 0.95 | 0.08 | 73,73,73,73                 | 0     |
| 55  | MG   | RP    | 203  | 1/1   | 0.95 | 0.15 | 70,70,70,70                 | 0     |
| 55  | MG   | YA    | 3498 | 1/1   | 0.95 | 0.14 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3393 | 1/1   | 0.95 | 0.16 | 73,73,73,73                 | 0     |
| 55  | MG   | YA    | 3505 | 1/1   | 0.96 | 0.20 | 61,61,61,61                 | 0     |
| 55  | MG   | RA    | 3285 | 1/1   | 0.96 | 0.37 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3245 | 1/1   | 0.96 | 0.30 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3287 | 1/1   | 0.96 | 0.12 | 56,56,56,56                 | 0     |
| 55  | MG   | YA    | 3115 | 1/1   | 0.96 | 0.17 | 69,69,69,69                 | 0     |
| 55  | MG   | YA    | 3366 | 1/1   | 0.96 | 0.07 | 73,73,73,73                 | 0     |
| 55  | MG   | RA    | 3519 | 1/1   | 0.96 | 0.19 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3342 | 1/1   | 0.96 | 0.36 | 58,58,58,58                 | 0     |
| 55  | MG   | RA    | 3467 | 1/1   | 0.96 | 0.27 | 72,72,72,72                 | 0     |
| 55  | MG   | QA    | 1604 | 1/1   | 0.96 | 0.19 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3182 | 1/1   | 0.96 | 0.08 | 57,57,57,57                 | 0     |
| 55  | MG   | YA    | 3546 | 1/1   | 0.96 | 0.12 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3426 | 1/1   | 0.96 | 0.10 | 59,59,59,59                 | 0     |
| 55  | MG   | YX    | 101  | 1/1   | 0.96 | 0.10 | 62,62,62,62                 | 0     |
| 55  | MG   | XA    | 1698 | 1/1   | 0.96 | 0.04 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3112 | 1/1   | 0.96 | 0.08 | 62,62,62,62                 | 0     |
| 55  | MG   | RA    | 3350 | 1/1   | 0.96 | 0.29 | 67,67,67,67                 | 0     |
| 55  | MG   | QA    | 1631 | 1/1   | 0.96 | 0.08 | 66,66,66,66                 | 0     |
| 55  | MG   | YA    | 3123 | 1/1   | 0.96 | 0.19 | 67,67,67,67                 | 0     |
| 55  | MG   | YA    | 3302 | 1/1   | 0.96 | 0.30 | 59,59,59,59                 | 0     |
| 55  | MG   | RA    | 3379 | 1/1   | 0.96 | 0.18 | 72,72,72,72                 | 0     |
| 55  | MG   | YA    | 3462 | 1/1   | 0.96 | 0.32 | 61,61,61,61                 | 0     |
| 55  | MG   | YA    | 3233 | 1/1   | 0.96 | 0.21 | 62,62,62,62                 | 0     |
| 55  | MG   | QA    | 1648 | 1/1   | 0.96 | 0.06 | 61,61,61,61                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | MG   | RA    | 3474 | 1/1   | 0.96 | 0.33 | 74,74,74,74                 | 0     |
| 55  | MG   | RA    | 3048 | 1/1   | 0.96 | 0.21 | 64,64,64,64                 | 0     |
| 55  | MG   | YB    | 209  | 1/1   | 0.96 | 0.07 | 62,62,62,62                 | 0     |
| 55  | MG   | YA    | 3410 | 1/1   | 0.96 | 0.25 | 69,69,69,69                 | 0     |
| 55  | MG   | QA    | 1615 | 1/1   | 0.96 | 0.09 | 71,71,71,71                 | 0     |
| 57  | ZN   | R9    | 101  | 1/1   | 0.96 | 0.31 | 80,80,80,80                 | 0     |
| 55  | MG   | RA    | 3397 | 1/1   | 0.96 | 0.13 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3216 | 1/1   | 0.96 | 0.10 | 69,69,69,69                 | 0     |
| 55  | MG   | RA    | 3225 | 1/1   | 0.96 | 0.37 | 63,63,63,63                 | 0     |
| 55  | MG   | QA    | 1664 | 1/1   | 0.96 | 0.15 | 71,71,71,71                 | 0     |
| 56  | SF4  | XD    | 301  | 8/8   | 0.97 | 0.06 | 64,73,80,88                 | 0     |
| 55  | MG   | YA    | 3290 | 1/1   | 0.97 | 0.46 | 55,55,55,55                 | 0     |
| 55  | MG   | RA    | 3127 | 1/1   | 0.97 | 0.09 | 65,65,65,65                 | 0     |
| 55  | MG   | QA    | 1644 | 1/1   | 0.97 | 0.06 | 63,63,63,63                 | 0     |
| 55  | MG   | QA    | 1660 | 1/1   | 0.97 | 0.09 | 65,65,65,65                 | 0     |
| 55  | MG   | RA    | 3358 | 1/1   | 0.97 | 0.35 | 66,66,66,66                 | 0     |
| 55  | MG   | RA    | 3452 | 1/1   | 0.97 | 0.11 | 87,87,87,87                 | 0     |
| 55  | MG   | YA    | 3394 | 1/1   | 0.97 | 0.30 | 60,60,60,60                 | 0     |
| 55  | MG   | YA    | 3467 | 1/1   | 0.97 | 0.10 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3514 | 1/1   | 0.97 | 0.36 | 55,55,55,55                 | 0     |
| 55  | MG   | YA    | 3469 | 1/1   | 0.97 | 0.14 | 56,56,56,56                 | 0     |
| 57  | ZN   | XN    | 101  | 1/1   | 0.98 | 0.03 | 84,84,84,84                 | 0     |
| 55  | MG   | XA    | 1611 | 1/1   | 0.98 | 0.04 | 57,57,57,57                 | 0     |
| 55  | MG   | QA    | 1659 | 1/1   | 0.98 | 0.07 | 63,63,63,63                 | 0     |
| 55  | MG   | RA    | 3442 | 1/1   | 0.98 | 0.08 | 70,70,70,70                 | 0     |
| 55  | MG   | XV    | 105  | 1/1   | 0.98 | 0.10 | 62,62,62,62                 | 0     |
| 57  | ZN   | Y9    | 101  | 1/1   | 0.98 | 0.23 | 83,83,83,83                 | 0     |
| 55  | MG   | YA    | 3494 | 1/1   | 0.99 | 0.09 | 56,56,56,56                 | 0     |
| 55  | MG   | RA    | 3463 | 1/1   | 0.99 | 0.12 | 70,70,70,70                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.