



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 18, 2022 – 05:38 PM EST

PDB ID : 7RQD  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with protein Y, A-site deacylated tRNA analog CACCA, P-site MTI-tripeptidyl-tRNA analog ACCA-ITM, and chloramphenicol at 2.50Å resolution  
Authors : Syroegin, E.A.; Flemmich, L.; Klepacki, D.; Vazquez-Laslop, N.; Micura, R.; Polikanov, Y.S.  
Deposited on : 2021-08-06  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.8.5 (274361), CSD as541be (2020)                                 |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.25   |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.25   |

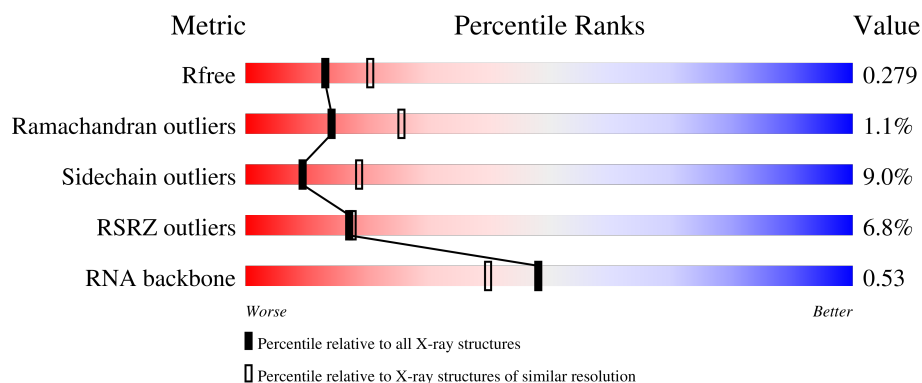
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 4661 (2.50-2.50)                                      |
| Ramachandran outliers | 138981                      | 5231 (2.50-2.50)                                      |
| Sidechain outliers    | 138945                      | 5233 (2.50-2.50)                                      |
| RSRZ outliers         | 127900                      | 4559 (2.50-2.50)                                      |
| RNA backbone          | 3102                        | 1008 (2.84-2.16)                                      |

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   | 1A    | 2915   | <div> <div>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div> |
| 1   | 2A    | 2915   | <div> <div>3%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>  |
| 2   | 1B    | 121    | <div> <div>91%</div> <div>8%</div> <div>.</div> </div>                 |
| 2   | 2B    | 121    | <div> <div>86%</div> <div>13%</div> <div>.</div> </div>                |
| 3   | 1D    | 276    | <div> <div>%</div> <div>95%</div> <div>5%</div> </div>                 |

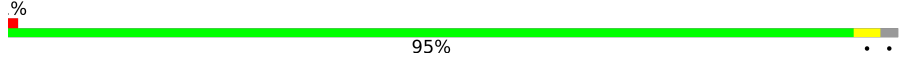
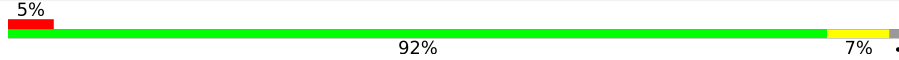
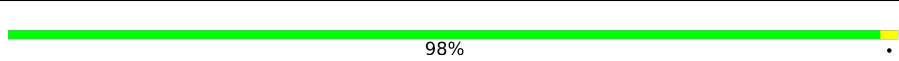

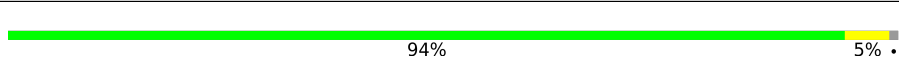
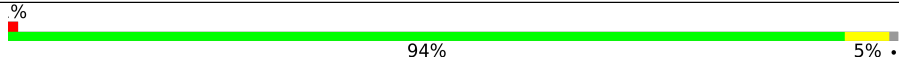
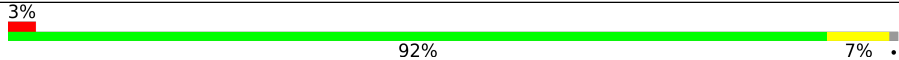
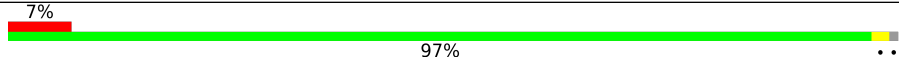
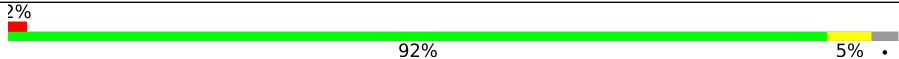
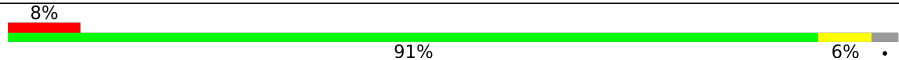
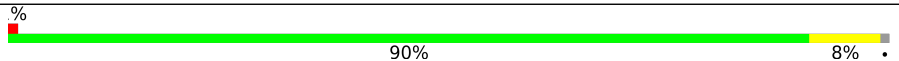
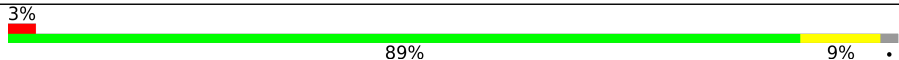
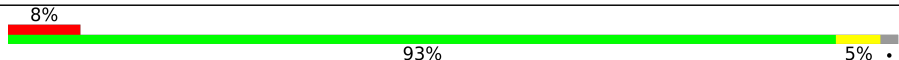
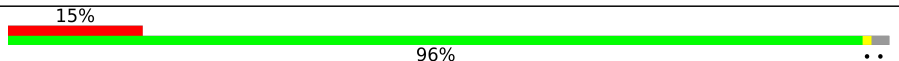
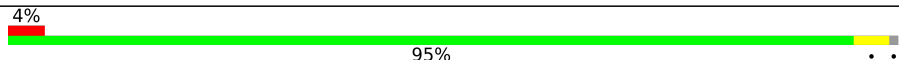
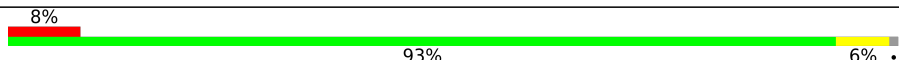
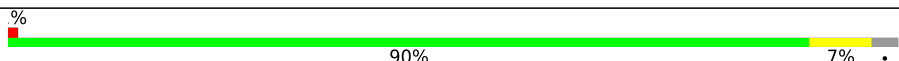
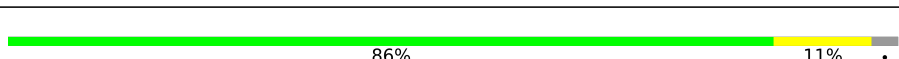
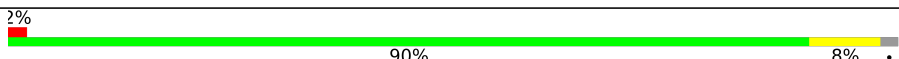
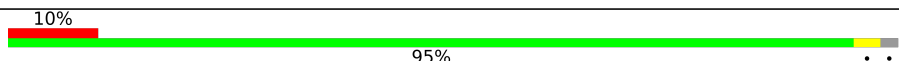
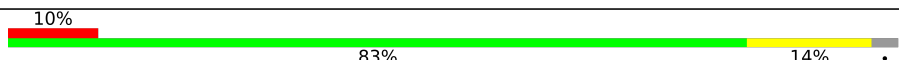
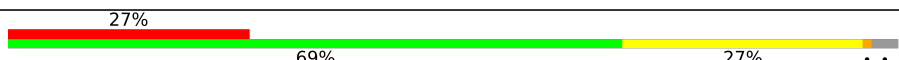
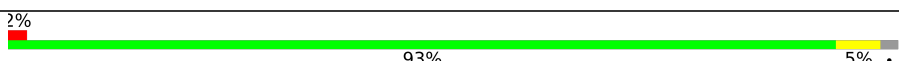
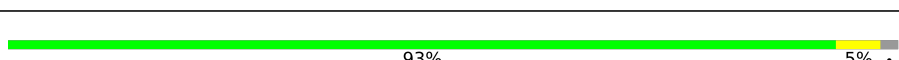
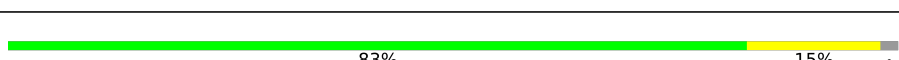
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | 2D    | 276    |                  |
| 4   | 1E    | 206    |                  |
| 4   | 2E    | 206    |                  |
| 5   | 1F    | 210    |                  |
| 5   | 2F    | 210    |                  |
| 6   | 1G    | 182    |                  |
| 6   | 2G    | 182    |                  |
| 7   | 1H    | 180    |                  |
| 7   | 2H    | 180    |                  |
| 8   | 1I    | 148    |                  |
| 8   | 2I    | 148    |                  |
| 9   | 1N    | 140    |                  |
| 9   | 2N    | 140    |                  |
| 10  | 1O    | 122    |                  |
| 10  | 2O    | 122    |                  |
| 11  | 1P    | 150    |                  |
| 11  | 2P    | 150    |                  |
| 12  | 1Q    | 141    |                  |
| 12  | 2Q    | 141    |                  |
| 13  | 1R    | 118    |                  |
| 13  | 2R    | 118    |                  |
| 14  | 1S    | 112    |                  |
| 14  | 2S    | 112    |                  |
| 15  | 1T    | 146    |                  |
| 15  | 2T    | 146    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 16  | 1U    | 118    |    |
| 16  | 2U    | 118    |    |
| 17  | 1V    | 101    |    |
| 17  | 2V    | 101    |    |
| 18  | 1W    | 113    |    |
| 18  | 2W    | 113    |    |
| 19  | 1X    | 96     |    |
| 19  | 2X    | 96     |    |
| 20  | 1Y    | 110    |    |
| 20  | 2Y    | 110    |    |
| 21  | 1Z    | 206    |    |
| 21  | 2Z    | 206    |   |
| 22  | 10    | 85     |  |
| 22  | 20    | 85     |  |
| 23  | 11    | 98     |  |
| 23  | 21    | 98     |  |
| 24  | 12    | 72     |  |
| 24  | 22    | 72     |  |
| 25  | 13    | 60     |  |
| 25  | 23    | 60     |  |
| 26  | 14    | 71     |  |
| 26  | 24    | 71     |  |
| 27  | 15    | 60     |  |
| 27  | 25    | 60     |  |
| 28  | 16    | 54     |  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 28  | 26    | 54     | <div> <div>4%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>                 |
| 29  | 17    | 49     | <div> <div>4%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>                  |
| 29  | 27    | 49     | <div> <div>4%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>                 |
| 30  | 18    | 65     | <div> <div>2%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>                  |
| 30  | 28    | 65     | <div> <div>12%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>                |
| 31  | 19    | 37     | <div> <div>97%</div> <div>.</div> </div>  |
| 31  | 29    | 37     | <div> <div>8%</div> <div>95%</div> <div>5%</div> </div>                               |
| 32  | 1a    | 1521   | <div> <div>3%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>                 |
| 32  | 2a    | 1521   | <div> <div>5%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>                |
| 33  | 1b    | 256    | <div> <div>11%</div> <div>77%</div> <div>12%</div> <div>.</div> <div>10%</div> </div> |
| 33  | 2b    | 256    | <div> <div>18%</div> <div>78%</div> <div>11%</div> <div>.</div> <div>10%</div> </div> |
| 34  | 1c    | 239    | <div> <div>17%</div> <div>83%</div> <div>.</div> <div>14%</div> </div>                |
| 34  | 2c    | 239    | <div> <div>28%</div> <div>74%</div> <div>11%</div> <div>14%</div> </div>              |
| 35  | 1d    | 209    | <div> <div>12%</div> <div>89%</div> <div>10%</div> </div>                             |
| 35  | 2d    | 209    | <div> <div>14%</div> <div>91%</div> <div>9%</div> </div>                              |
| 36  | 1e    | 162    | <div> <div>7%</div> <div>85%</div> <div>7%</div> <div>9%</div> </div>                 |
| 36  | 2e    | 162    | <div> <div>10%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>                |
| 37  | 1f    | 101    | <div> <div>2%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>                 |
| 37  | 2f    | 101    | <div> <div>%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>                   |
| 38  | 1g    | 156    | <div> <div>5%</div> <div>92%</div> <div>8%</div> <div>.</div> </div>                  |
| 38  | 2g    | 156    | <div> <div>22%</div> <div>90%</div> <div>9%</div> <div>..</div> </div>                |
| 39  | 1h    | 138    | <div> <div>7%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>                  |
| 39  | 2h    | 138    | <div> <div>8%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>                  |
| 40  | 1i    | 128    | <div> <div>33%</div> <div>87%</div> <div>12%</div> <div>..</div> </div>               |
| 40  | 2i    | 128    | <div> <div>66%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>                |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 41  | 1j    | 105    | <div> <div>19%</div> <div>81%</div> <div>11%</div> <div>8%</div> </div>           |
| 41  | 2j    | 105    | <div> <div>44%</div> <div>82%</div> <div>10%</div> <div>9%</div> </div>           |
| 42  | 1k    | 129    | <div> <div>%</div> <div>84%</div> <div>5%</div> <div>12%</div> </div>             |
| 42  | 2k    | 129    | <div> <div>15%</div> <div>80%</div> <div>9%</div> <div>12%</div> </div>           |
| 43  | 1l    | 132    | <div> <div>7%</div> <div>86%</div> <div>7%</div> <div>8%</div> </div>             |
| 43  | 2l    | 132    | <div> <div>5%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>             |
| 44  | 1m    | 126    | <div> <div>10%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>            |
| 44  | 2m    | 126    | <div> <div>17%</div> <div>75%</div> <div>15%</div> <div>10%</div> </div>          |
| 45  | 1n    | 61     | <div> <div>26%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>            |
| 45  | 2n    | 61     | <div> <div>67%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>            |
| 46  | 1o    | 89     | <div> <div>3%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>              |
| 46  | 2o    | 89     | <div> <div>3%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>              |
| 47  | 1p    | 88     | <div> <div>18%</div> <div>80%</div> <div>14%</div> <div>7%</div> </div>           |
| 47  | 2p    | 88     | <div> <div>8%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>             |
| 48  | 1q    | 105    | <div> <div>6%</div> <div>87%</div> <div>8%</div> <div>6%</div> </div>             |
| 48  | 2q    | 105    | <div> <div>11%</div> <div>90%</div> <div>.</div> <div>6%</div> </div>             |
| 49  | 1r    | 88     | <div> <div>2%</div> <div>67%</div> <div>10%</div> <div>23%</div> </div>           |
| 49  | 2r    | 88     | <div> <div>5%</div> <div>70%</div> <div>7%</div> <div>23%</div> </div>            |
| 50  | 1s    | 93     | <div> <div>2%</div> <div>84%</div> <div>5%</div> <div>11%</div> </div>            |
| 50  | 2s    | 93     | <div> <div>20%</div> <div>84%</div> <div>5%</div> <div>11%</div> </div>           |
| 51  | 1t    | 106    | <div> <div>11%</div> <div>82%</div> <div>8%</div> <div>9%</div> </div>            |
| 51  | 2t    | 106    | <div> <div>7%</div> <div>88%</div> <div>.</div> <div>.</div> <div>8%</div> </div> |
| 52  | 1u    | 27     | <div> <div>30%</div> <div>81%</div> <div>.</div> <div>15%</div> </div>            |
| 52  | 2u    | 27     | <div> <div>37%</div> <div>85%</div> <div>.</div> <div>15%</div> </div>            |
| 53  | 1y    | 113    | <div> <div>4%</div> <div>81%</div> <div>.</div> <div>14%</div> </div>             |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | 2y    | 113    |                  |
| 54  | 1w    | 5      |                  |
| 54  | 2w    | 5      |                  |
| 55  | 1x    | 4      |                  |
| 55  | 2x    | 4      |                  |
| 56  | 1v    | 3      |                  |
| 56  | 2v    | 3      |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57  | MG   | 1A    | 3002 | -         | -        | -       | X                |
| 57  | MG   | 1A    | 3212 | -         | -        | -       | X                |
| 57  | MG   | 1A    | 3772 | -         | -        | -       | X                |
| 57  | MG   | 1A    | 3898 | -         | -        | -       | X                |

## 2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 297630 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | 1A    | 2872     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61869 | 27540 | 11574 | 19884 | 2871 |         |         |       |
| 1   | 2A    | 2867     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 61758 | 27491 | 11552 | 19850 | 2865 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | 1B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2572  | 1145 | 476 | 832 | 119 |         |         |       |
| 2   | 2B    | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | 1D    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2131  | 1346 | 422 | 360 | 3 |         |         |       |
| 3   | 2D    | 275      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2136  | 1349 | 423 | 361 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | 1E    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |
| 4   | 2E    | 204      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1559  | 985 | 298 | 270 | 6 |         |         |       |

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



| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | 1F    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1584  | 1009 | 298 | 275 | 2 |         |         |       |
| 5   | 2F    | 203      | Total | C    | N   | O   | S | 0       | 0       | 1     |
|     |       |          | 1580  | 1007 | 297 | 274 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | 1G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 916 | 253 | 253 | 4 |         |         |       |
| 6   | 2G    | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1424  | 912 | 259 | 249 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | 1H    | 174      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1330  | 845 | 248 | 236 | 1 |         |         |       |
| 7   | 2H    | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1324  | 842 | 247 | 234 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | 1I    | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1094  | 699 | 191 | 203 | 1 |         |         |       |
| 8   | 2I    | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1076  | 687 | 186 | 202 | 1 |         |         |       |

- Molecule 9 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | 1N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1121  | 722 | 208 | 187 | 4 |         |         |       |
| 9   | 2N    | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1117  | 719 | 207 | 187 | 4 |         |         |       |

- Molecule 10 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | 1O    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | 2O    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

- Molecule 11 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | 1P    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |
| 11  | 2P    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1135  | 706 | 230 | 196 | 3 |         |         |       |

- Molecule 12 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | 1Q    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |
| 12  | 2Q    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

- Molecule 13 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | 1R    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |
| 13  | 2R    | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

- Molecule 14 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14  | 1S    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 877   | 553 | 175 | 149 |         |         |       |
| 14  | 2S    | 110      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 870   | 549 | 173 | 148 |         |         |       |

- Molecule 15 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | 1T    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1091  | 680 | 225 | 185 | 1 |         |         |       |
| 15  | 2T    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1083  | 675 | 224 | 183 | 1 |         |         |       |

- Molecule 16 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | 1U    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |
| 16  | 2U    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 959   | 608 | 201 | 149 | 1 |         |         |       |

- Molecule 17 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | 1V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 775   | 498 | 141 | 135 | 1 |         |         |       |
| 17  | 2V    | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 771   | 495 | 140 | 135 | 1 |         |         |       |

- Molecule 18 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | 1W    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |
| 18  | 2W    | 112      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 886   | 557 | 174 | 153 | 2 |         |         |       |

- Molecule 19 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | 1X    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |
| 19  | 2X    | 95       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 750   | 488 | 135 | 126 | 1 |         |         |       |

- Molecule 20 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | 1Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 520 | 153 | 131 | 6 |         |         |       |
| 20  | 2Y    | 107      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 810   | 519 | 153 | 132 | 6 |         |         |       |

- Molecule 21 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 21  | 1Z    | 203      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1587  | 1011 | 282 | 292 | 2 |         |         |       |
| 21  | 2Z    | 201      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1557  | 995  | 274 | 286 | 2 |         |         |       |

- Molecule 22 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | 10    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 653   | 404 | 139 | 109 | 1 |         |         |       |
| 22  | 20    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 650   | 401 | 139 | 109 | 1 |         |         |       |

- Molecule 23 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | 11    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 754   | 475 | 148 | 130 | 1 |         |         |       |
| 23  | 21    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 759   | 478 | 149 | 131 | 1 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | 12    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 588   | 365 | 118 | 103 | 2 |         |         |       |
| 24  | 22    | 70       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 592   | 368 | 119 | 103 | 2 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 25  | 13    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |
| 25  | 23    | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 464   | 296 | 90 | 78 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 14    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 546   | 346 | 96 | 99 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26  | 24    | 69       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 536   | 342 | 98 | 91 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | 15    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |
| 27  | 25    | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 455   | 285 | 89 | 76 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | 16    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 453   | 281 | 91 | 77 | 4 |         |         |       |
| 28  | 26    | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 449   | 279 | 91 | 75 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29  | 17    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |
| 29  | 27    | 48       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 418   | 257 | 104 | 55 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30  | 18    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |
| 30  | 28    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | 19    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |
| 31  | 29    | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 32  | 1a    | 1500     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32246 | 14358 | 5975 | 10413 | 1500 |         |         |       |
| 32  | 2a    | 1504     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32331 | 14396 | 5990 | 10441 | 1504 |         |         |       |

- Molecule 33 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 33  | 1b    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1842  | 1175 | 330 | 332 | 5 |         |         |       |
| 33  | 2b    | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1825  | 1167 | 326 | 327 | 5 |         |         |       |

- Molecule 34 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | 1c    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1558  | 979 | 305 | 273 | 1 |         |         |       |
| 34  | 2c    | 206      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1542  | 968 | 300 | 273 | 1 |         |         |       |

- Molecule 35 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 35  | 1d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1665  | 1043 | 329 | 286 | 7 |         |         |       |
| 35  | 2d    | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1668  | 1047 | 330 | 284 | 7 |         |         |       |

- Molecule 36 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36  | 1e    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1133  | 716 | 214 | 199 | 4 |         |         |       |
| 36  | 2e    | 148      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1133  | 716 | 214 | 199 | 4 |         |         |       |

- Molecule 37 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | 1f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 814   | 516 | 144 | 151 | 3 |         |         |       |
| 37  | 2f    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 146 | 151 | 3 |         |         |       |

- Molecule 38 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | 1g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 769 | 244 | 216 | 6 |         |         |       |
| 38  | 2g    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1229  | 766 | 241 | 216 | 6 |         |         |       |

- Molecule 39 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | 1h    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1098  | 694 | 210 | 192 | 2 |         |         |       |
| 39  | 2h    | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1088  | 689 | 206 | 191 | 2 |         |         |       |

- Molecule 40 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 40  | 1i    | 127      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 986   | 625 | 193 | 168 |         |         |       |
| 40  | 2i    | 126      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 966   | 613 | 186 | 167 |         |         |       |

- Molecule 41 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 41  | 1j    | 97       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 719   | 446 | 142 | 131 |         |         |       |
| 41  | 2j    | 96       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 710   | 442 | 137 | 131 |         |         |       |

- Molecule 42 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | 1k    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 834   | 520 | 156 | 155 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | 2k    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 833   | 519 | 156 | 155 | 3 |         |         |       |

- Molecule 43 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43  | 1l    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 586 | 185 | 159 | 2 |         |         |       |
| 43  | 2l    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 932   | 586 | 185 | 159 | 2 |         |         |       |

- Molecule 44 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44  | 1m    | 116      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 914   | 564 | 189 | 159 | 2 |         |         |       |
| 44  | 2m    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 895   | 550 | 186 | 157 | 2 |         |         |       |

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 45  | 1n    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |
| 45  | 2n    | 60       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 492   | 312 | 104 | 72 | 4 |         |         |       |

- Molecule 46 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 46  | 1o    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 728   | 456 | 144 | 126 | 2 |         |         |       |
| 46  | 2o    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 728   | 456 | 144 | 126 | 2 |         |         |       |

- Molecule 47 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 47  | 1p    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 681   | 433 | 134 | 113 | 1 |         |         |       |
| 47  | 2p    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 677   | 430 | 133 | 113 | 1 |         |         |       |



- Molecule 48 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 48  | 1q    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |
| 48  | 2q    | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 823   | 528 | 151 | 142 | 2 |         |         |       |

- Molecule 49 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|--|---------|---------|-------|
| 49  | 1r    | 68       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |  |         |         |       |
| 49  | 2r    | 68       | Total | C   | N   | O  |  | 0       | 0       | 0     |
|     |       |          | 555   | 355 | 108 | 92 |  |         |         |       |

- Molecule 50 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 50  | 1s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 415 | 120 | 111 | 2 |         |         |       |
| 50  | 2s    | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 645   | 410 | 118 | 115 | 2 |         |         |       |

- Molecule 51 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 51  | 1t    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 732   | 449 | 157 | 124 | 2 |         |         |       |
| 51  | 2t    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 733   | 451 | 154 | 126 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 52  | 1u    | 23       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |  |         |         |       |
| 52  | 2u    | 23       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 199   | 122 | 48 | 29 |  |         |         |       |

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 53  | 1y    | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 764   | 478 | 144 | 139 | 3 |         |         |       |
| 53  | 2y    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 749   | 468 | 141 | 137 | 3 |         |         |       |

- Molecule 54 is a RNA chain called A-site Deacylated tRNA Analog.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 54  | 1w    | 4        | Total | C  | N  | O  | P | 0       | 0       | 1     |
|     |       |          | 63    | 28 | 11 | 21 | 3 |         |         |       |
| 54  | 2w    | 4        | Total | C  | N  | O  | P | 0       | 0       | 1     |
|     |       |          | 63    | 28 | 11 | 21 | 3 |         |         |       |

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA Analog RNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 55  | 1x    | 4        | Total | C  | N  | O  | P | 0       | 0       | 1     |
|     |       |          | 63    | 28 | 12 | 20 | 3 |         |         |       |
| 55  | 2x    | 4        | Total | C  | N  | O  | P | 0       | 0       | 1     |
|     |       |          | 63    | 28 | 12 | 20 | 3 |         |         |       |

- Molecule 56 is a protein called P-site Peptidyl-tRNA Analog Peptide.

| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---|---------|---------|-------|
| 56  | 1v    | 3        | Total | C  | N | O | S | 0       | 0       | 0     |
|     |       |          | 23    | 15 | 3 | 4 | 1 |         |         |       |
| 56  | 2v    | 3        | Total | C  | N | O | S | 0       | 0       | 0     |
|     |       |          | 23    | 15 | 3 | 4 | 1 |         |         |       |

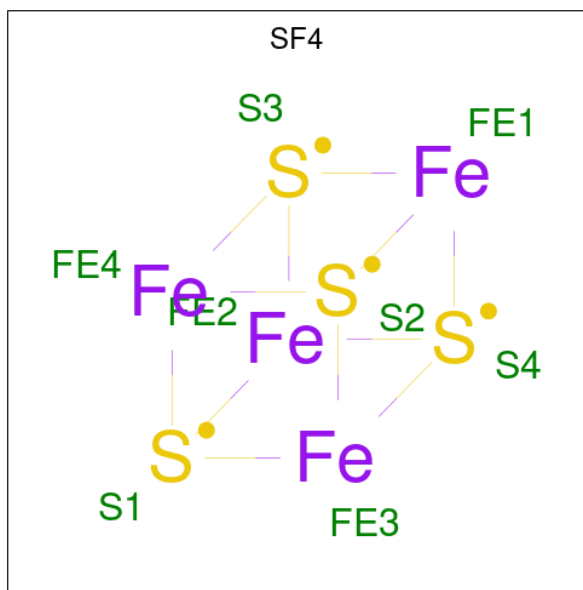
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |      | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 57  | 1A    | 1176     | Total | Mg   | 0       | 0       |
|     |       |          | 1176  | 1176 |         |         |
| 57  | 1a    | 306      | Total | Mg   | 0       | 0       |
|     |       |          | 306   | 306  |         |         |
| 57  | 2A    | 804      | Total | Mg   | 0       | 0       |
|     |       |          | 804   | 804  |         |         |
| 57  | 2a    | 200      | Total | Mg   | 0       | 0       |
|     |       |          | 200   | 200  |         |         |

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

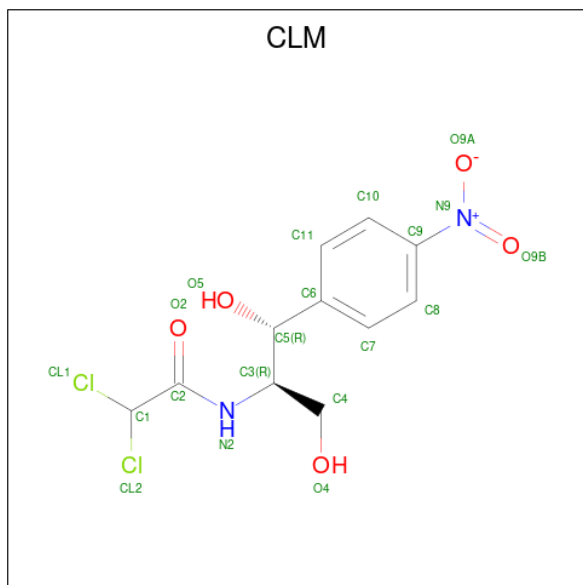
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58  | 1Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 14    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 15    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 16    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 19    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 1n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 2Y    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 24    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 25    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 26    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 29    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 58  | 2n    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



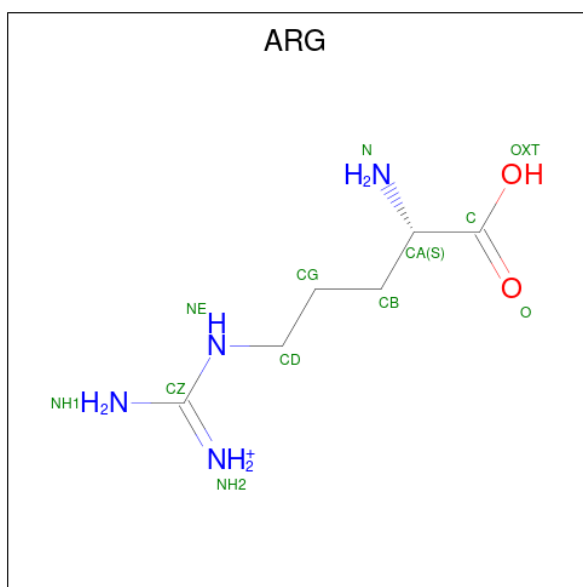
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 59  | 1d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 59  | 2d    | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 60 is CHLORAMPHENICOL (three-letter code: CLM) (formula:  $C_{11}H_{12}Cl_2N_2O_5$ ).



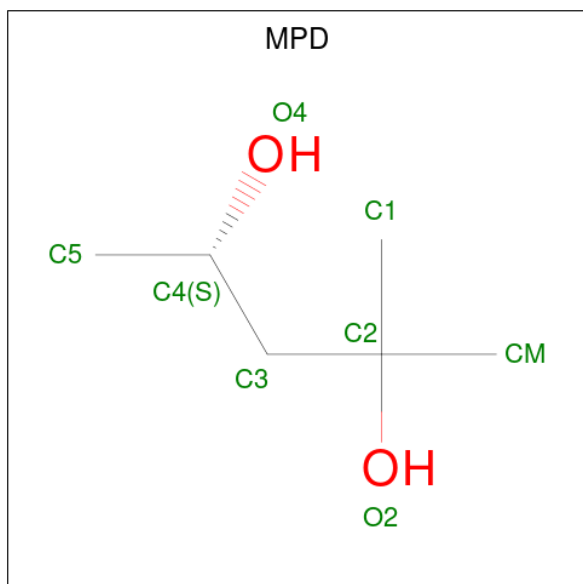
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 60  | 1z    | 1        | Total | C  | Cl | N | O       |         |
|     |       |          | 20    | 11 | 2  | 2 | 5       | 0       |
| 60  | 2z    | 1        | Total | C  | Cl | N | O       |         |
|     |       |          | 20    | 11 | 2  | 2 | 5       | 0       |

- Molecule 61 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 61  | 1z    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 6 | 4 | 2 |         |         |
| 61  | 1z    | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 6 | 4 | 2 |         |         |

- Molecule 62 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 62  | 1z    | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 62  | 1z    | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 62  | 1z    | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 62  | 1z    | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 62  | 2z    | 1        | Total C O<br>8 6 2 | 0       | 0       |
| 62  | 2z    | 1        | Total C O<br>8 6 2 | 0       | 0       |

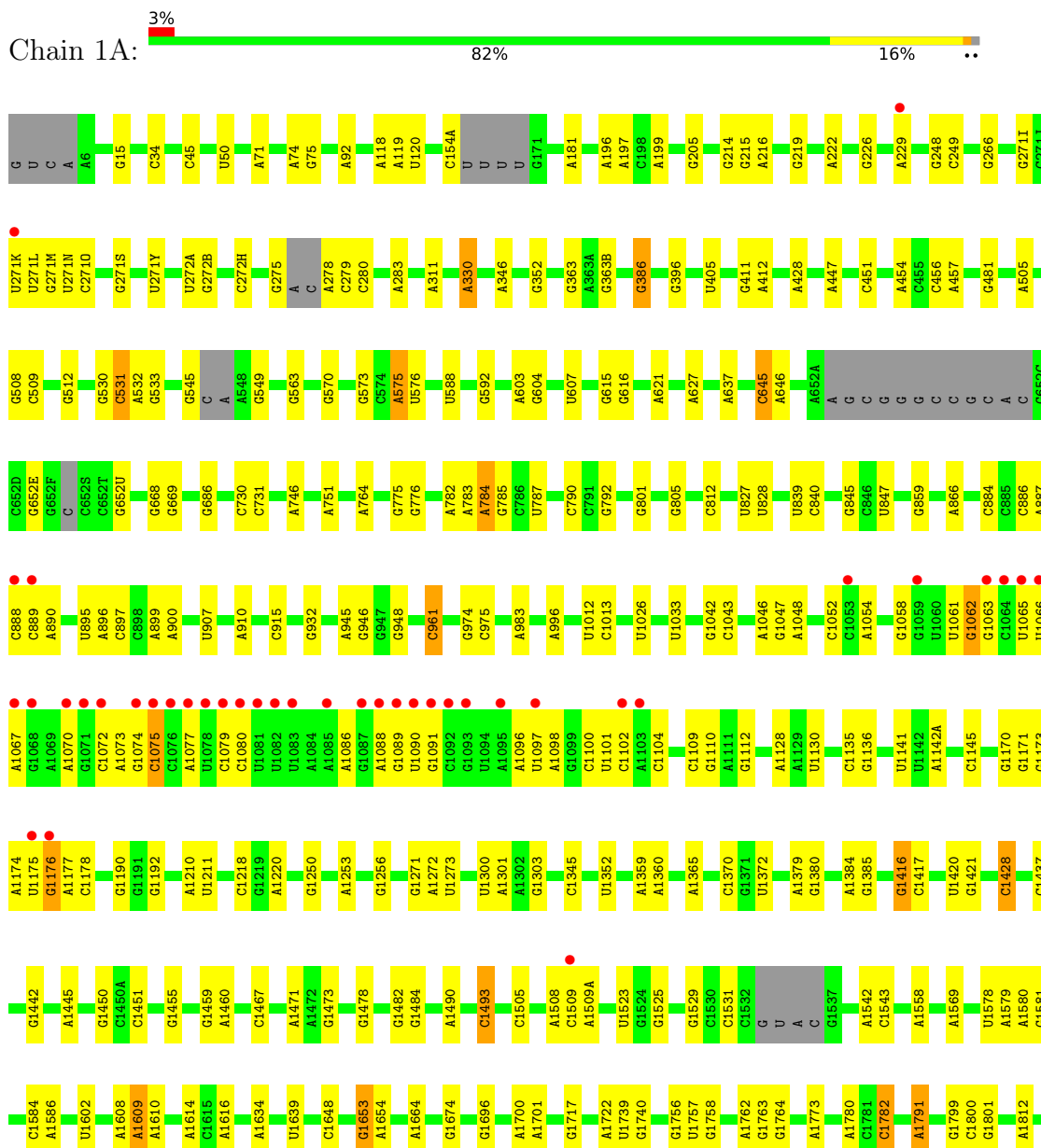
- Molecule 63 is water.

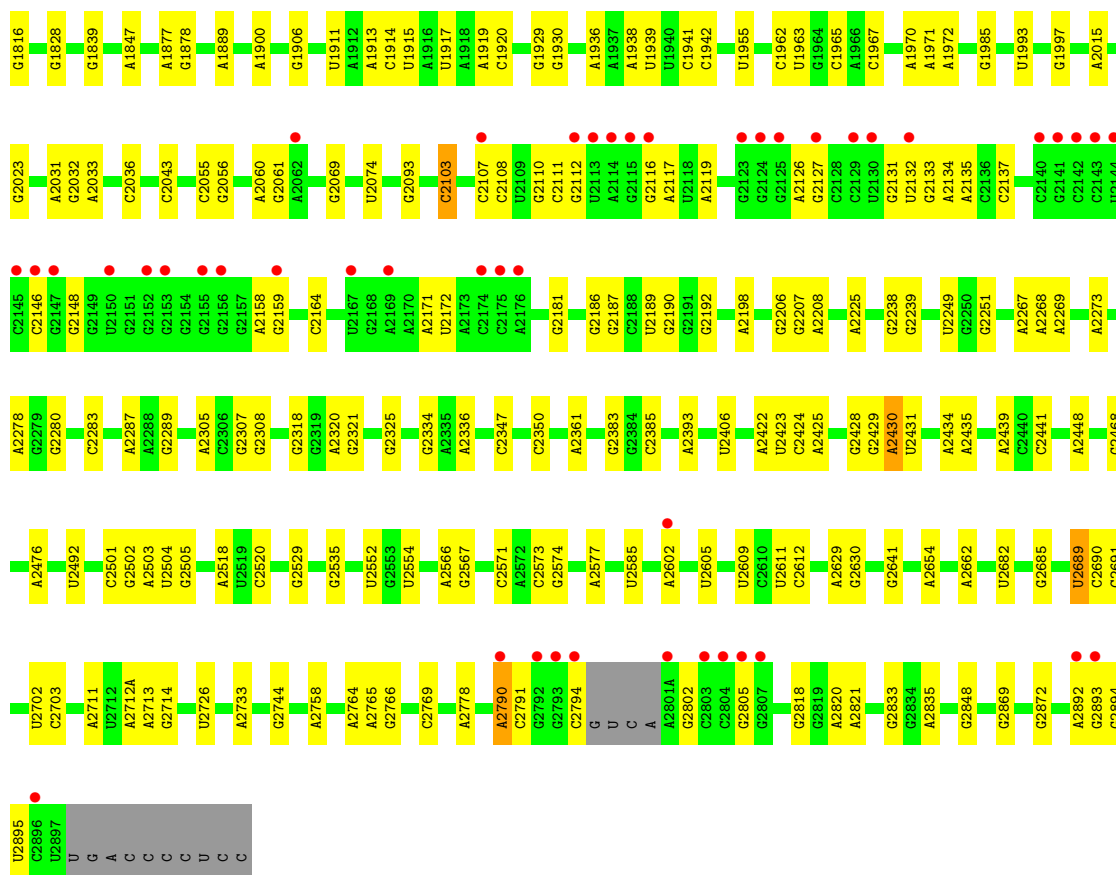
| Mol | Chain | Residues | Atoms                | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 63  | 1A    | 4956     | Total O<br>4956 4956 | 0       | 0       |
| 63  | 1a    | 454      | Total O<br>454 454   | 0       | 0       |
| 63  | 2A    | 2532     | Total O<br>2532 2532 | 0       | 0       |
| 63  | 2a    | 316      | Total O<br>316 316   | 0       | 0       |

### 3 Residue-property plots [i](#)

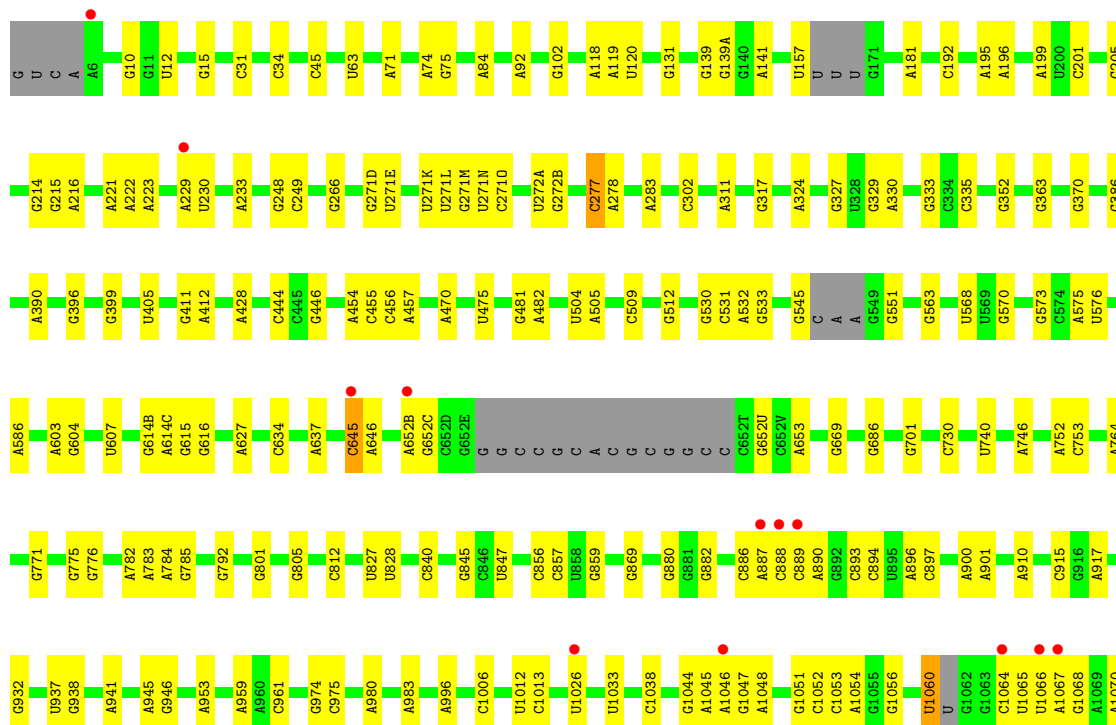
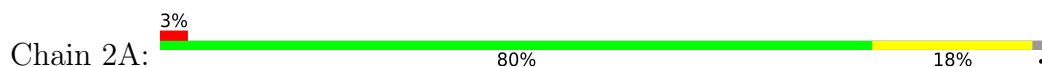
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S Ribosomal RNA





• Molecule 1: 23S Ribosomal RNA





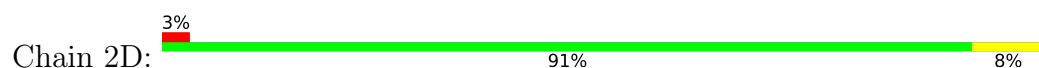




- Molecule 3: 50S ribosomal protein L2



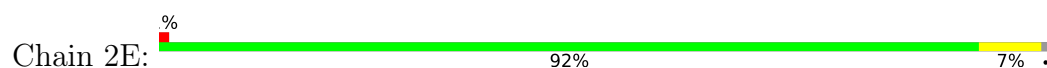
- Molecule 3: 50S ribosomal protein L2



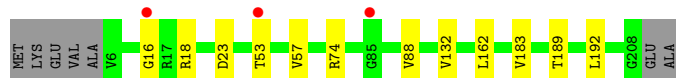
- Molecule 4: 50S ribosomal protein L3



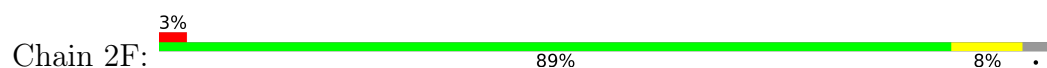
- Molecule 4: 50S ribosomal protein L3



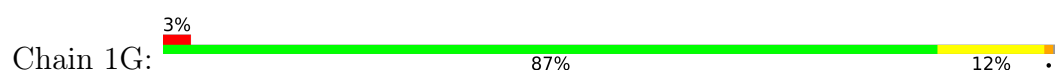
- Molecule 5: 50S ribosomal protein L4



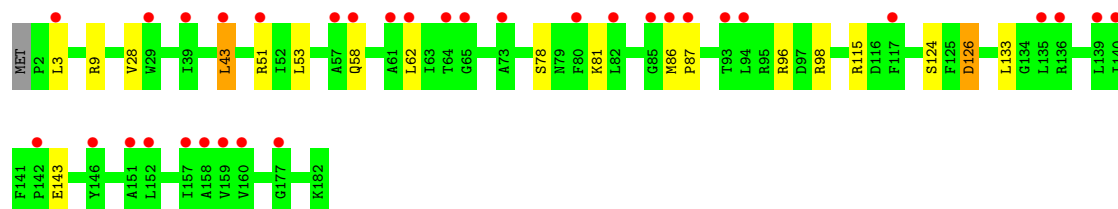
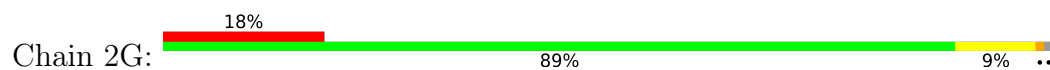
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



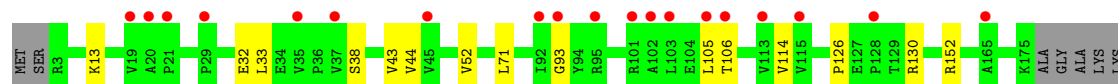
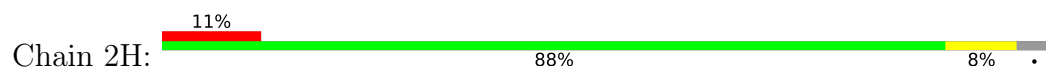
- Molecule 6: 50S ribosomal protein L5



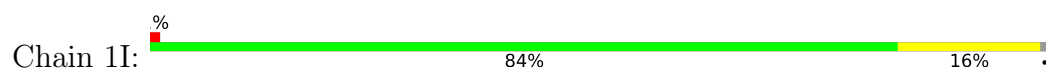
- Molecule 7: 50S ribosomal protein L6



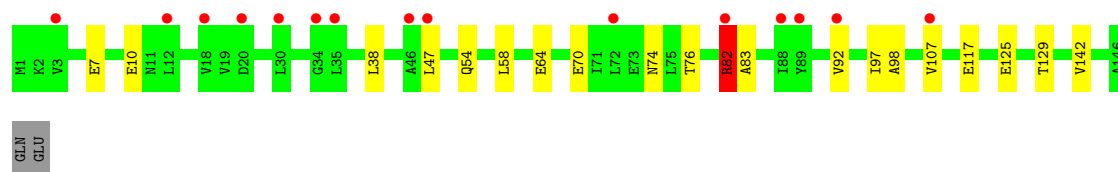
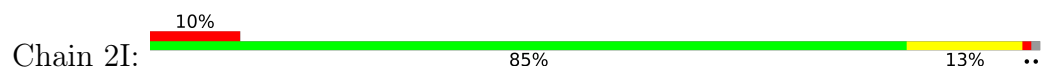
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



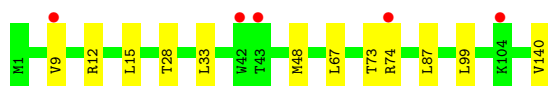
- Molecule 9: 50S ribosomal protein L13

Chain 1N:  91% 9%



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  4% 91% 9%



- Molecule 10: 50S ribosomal protein L14

Chain 1O:  95% 5%



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  96%



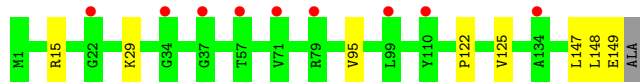
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  % 97% ..



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  6% 94% 5% .

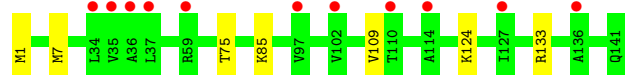


- Molecule 12: 50S ribosomal protein L16

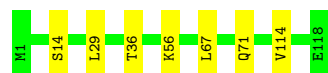
Chain 1Q:  97% .



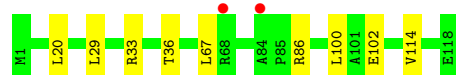
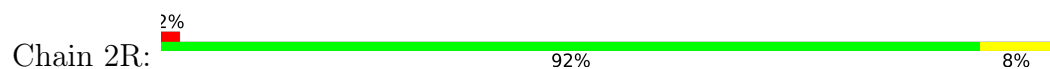
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



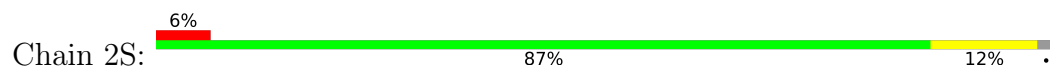
- Molecule 13: 50S ribosomal protein L17



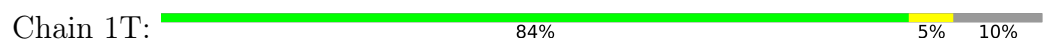
- Molecule 14: 50S ribosomal protein L18



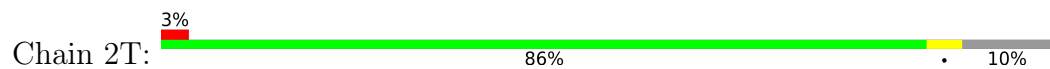
- Molecule 14: 50S ribosomal protein L18



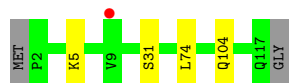
- Molecule 15: 50S ribosomal protein L19



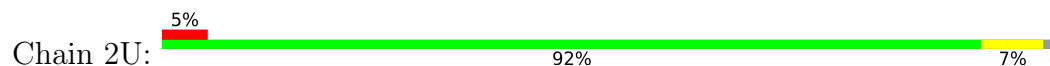
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



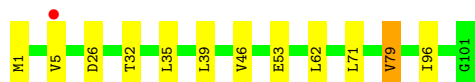
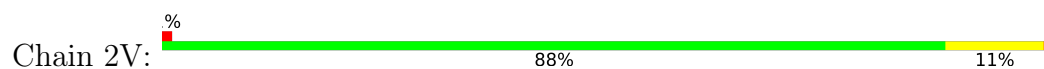
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



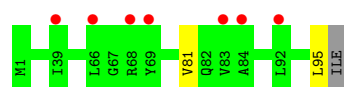
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



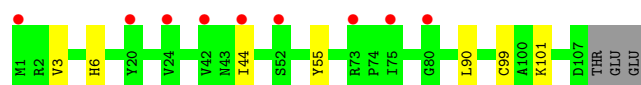
- Molecule 19: 50S ribosomal protein L23



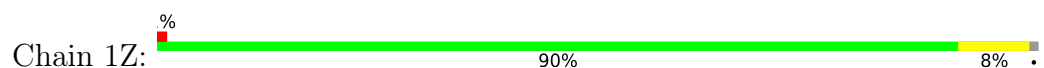
- Molecule 20: 50S ribosomal protein L24



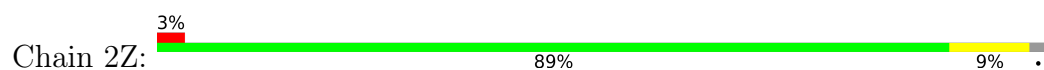
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



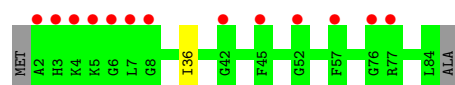
- Molecule 21: 50S ribosomal protein L25



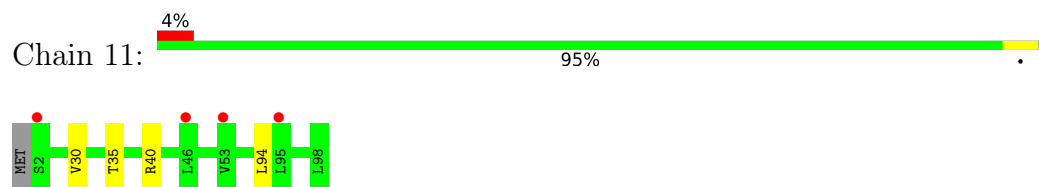
- Molecule 22: 50S ribosomal protein L27



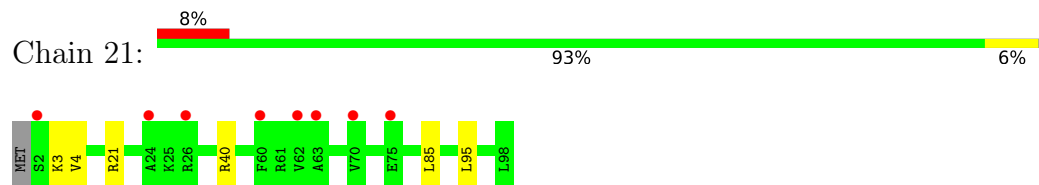
- Molecule 22: 50S ribosomal protein L27



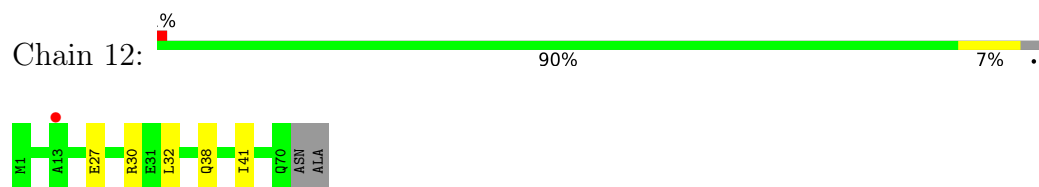
- Molecule 23: 50S ribosomal protein L28



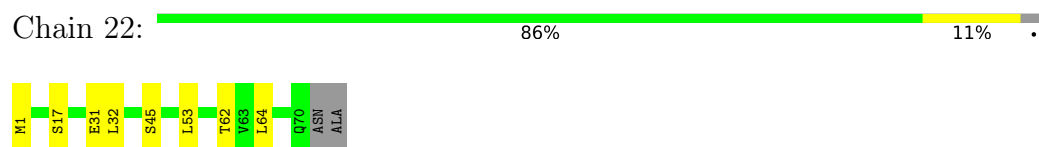
- Molecule 23: 50S ribosomal protein L28



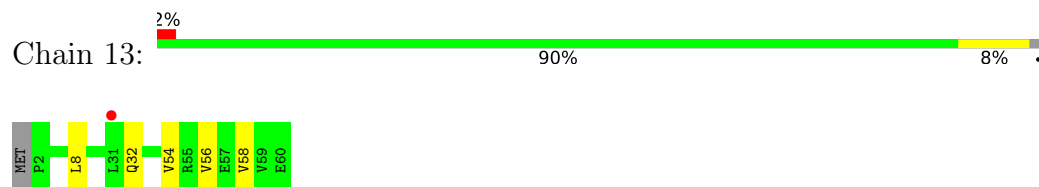
- Molecule 24: 50S ribosomal protein L29



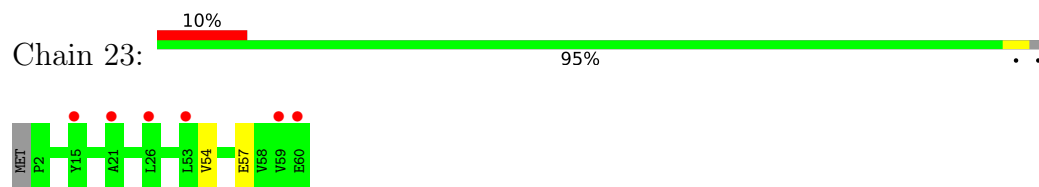
- Molecule 24: 50S ribosomal protein L29



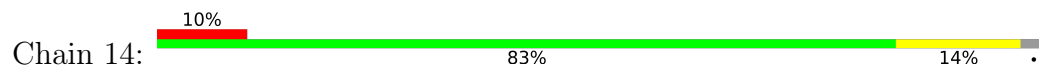
- Molecule 25: 50S ribosomal protein L30



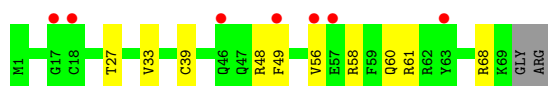
- Molecule 25: 50S ribosomal protein L30



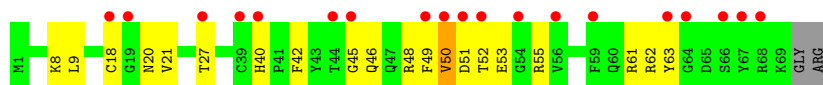
- Molecule 26: 50S ribosomal protein L31







- Molecule 26: 50S ribosomal protein L31



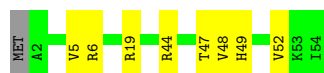
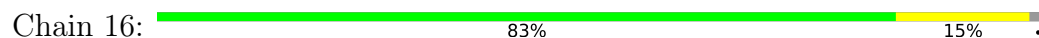
- Molecule 27: 50S ribosomal protein L32



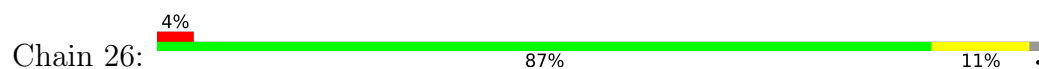
- Molecule 27: 50S ribosomal protein L32



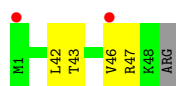
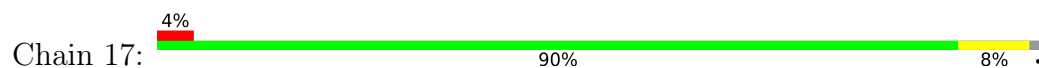
- Molecule 28: 50S ribosomal protein L33



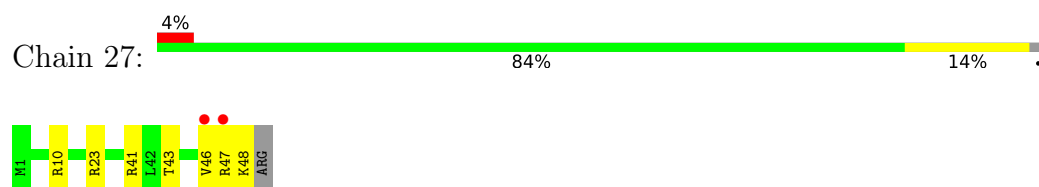
- Molecule 28: 50S ribosomal protein L33



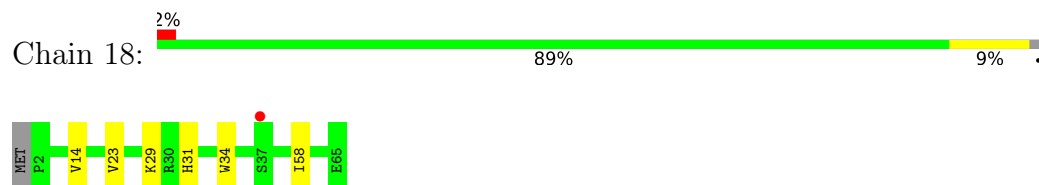
- Molecule 29: 50S ribosomal protein L34



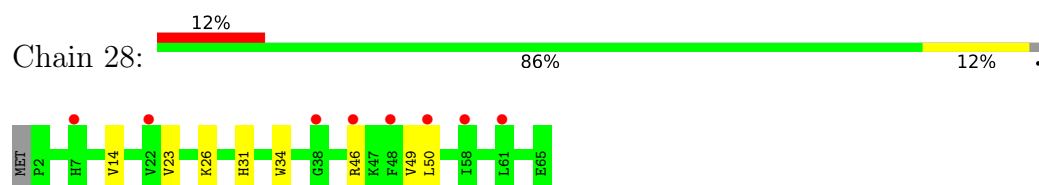
- Molecule 29: 50S ribosomal protein L34



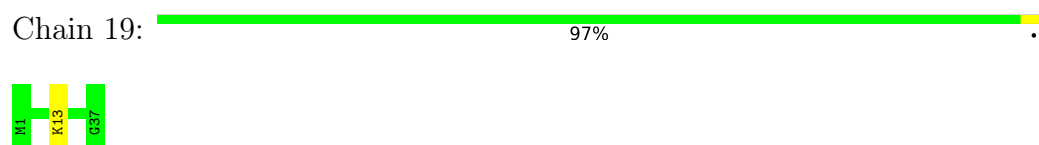
- Molecule 30: 50S ribosomal protein L35



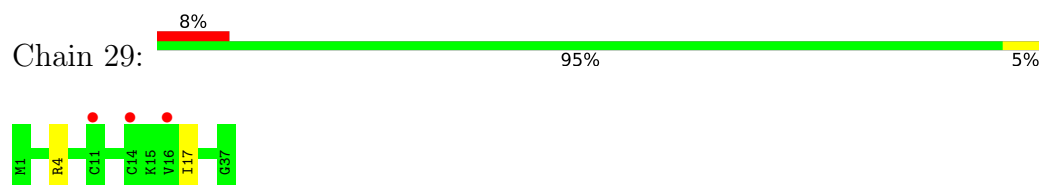
- Molecule 30: 50S ribosomal protein L35



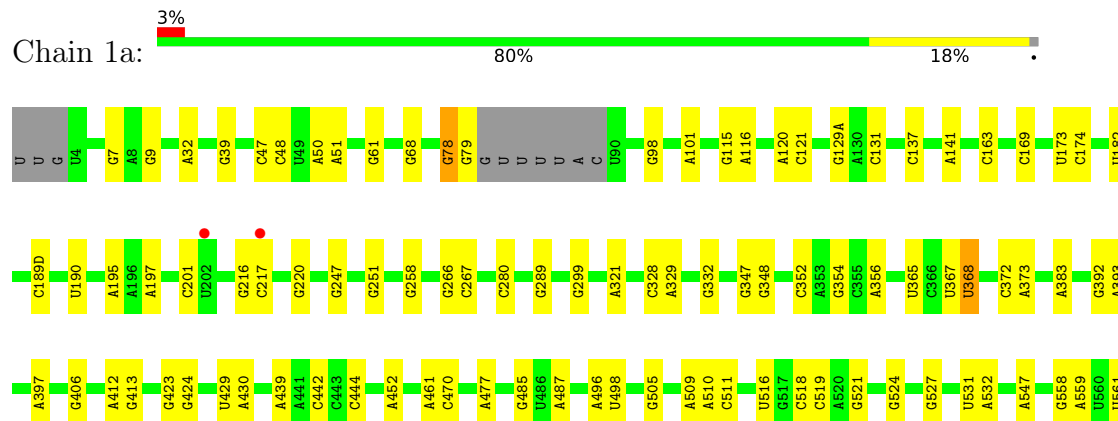
- Molecule 31: 50S ribosomal protein L36

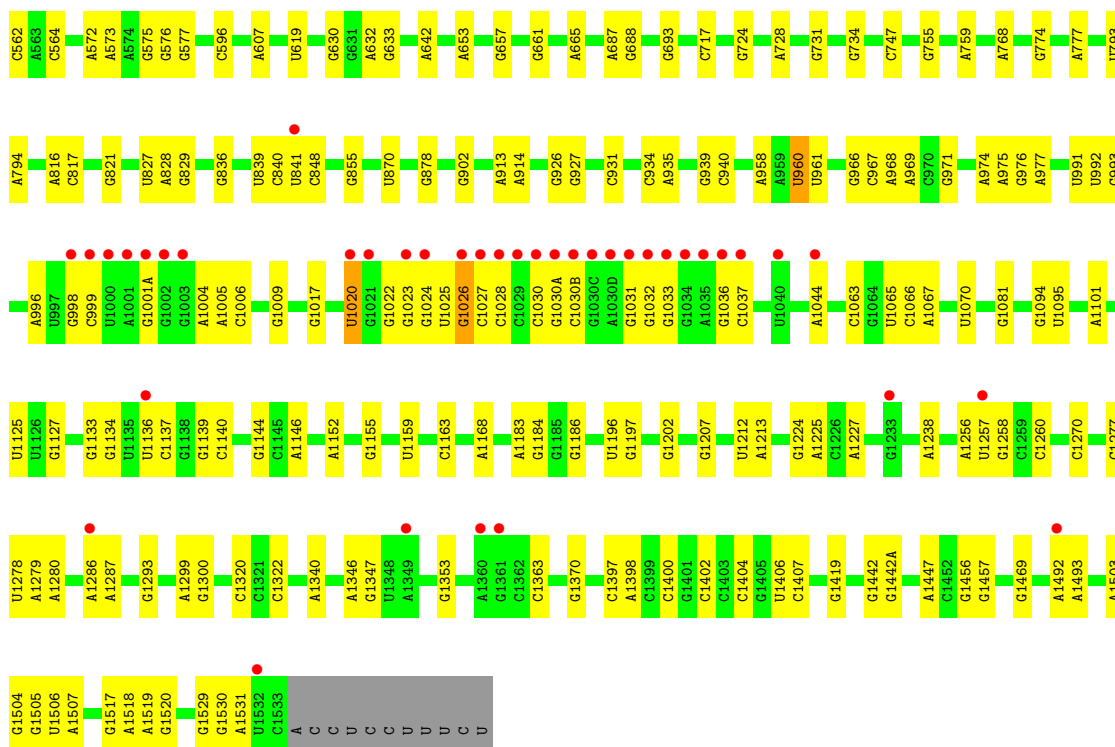


- Molecule 31: 50S ribosomal protein L36

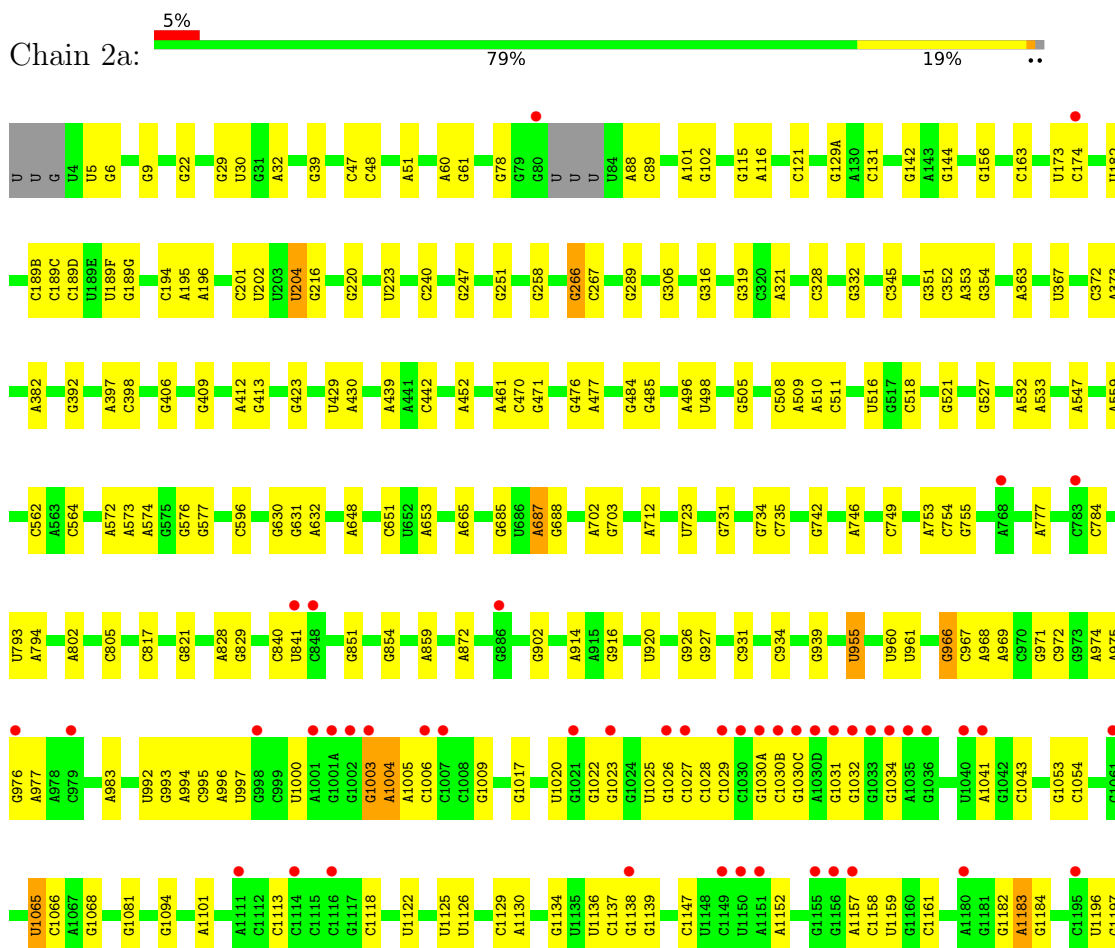


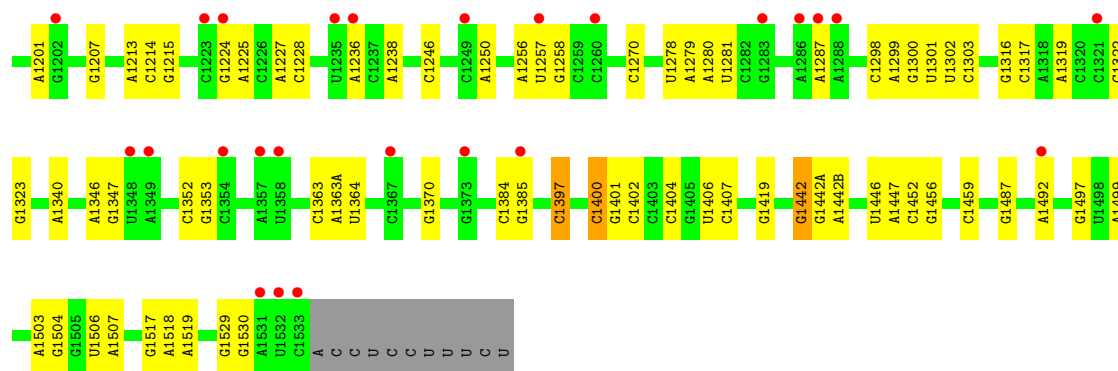
- Molecule 32: 16S Ribosomal RNA



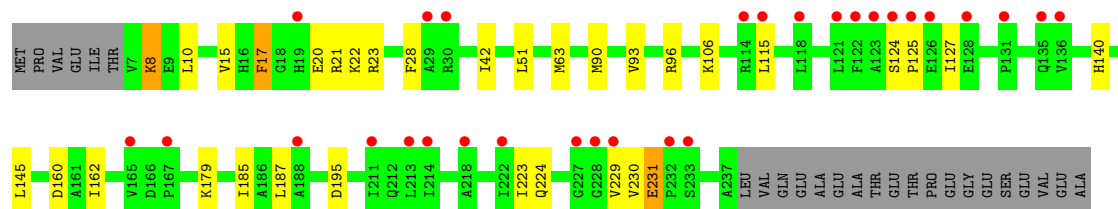
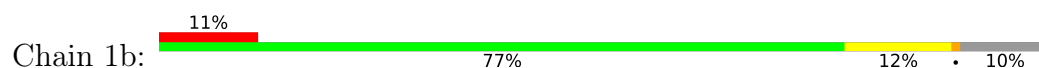


- Molecule 32: 16S Ribosomal RNA

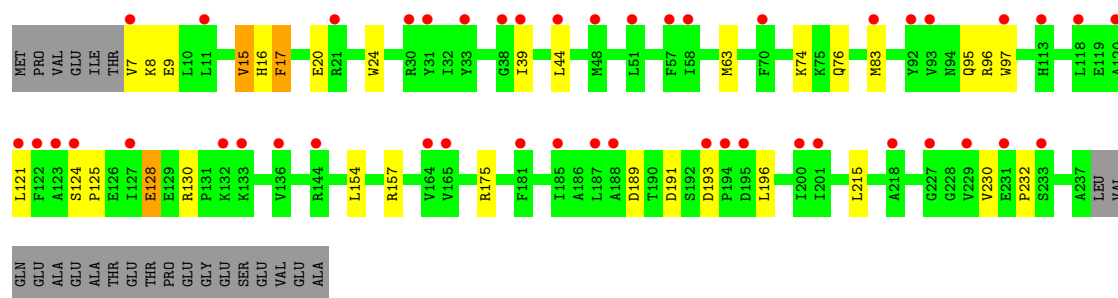
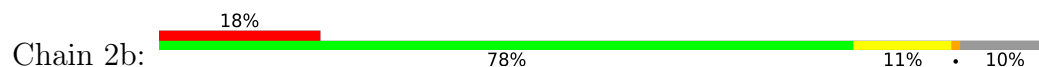




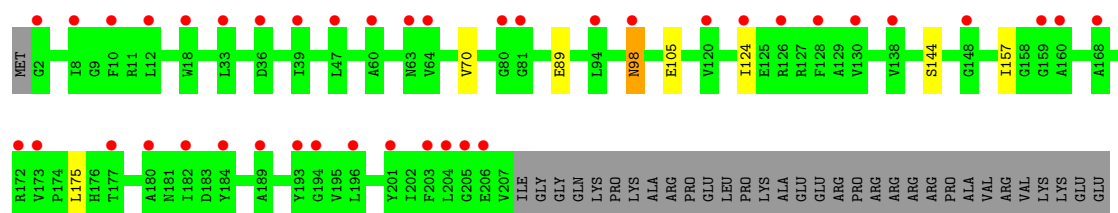
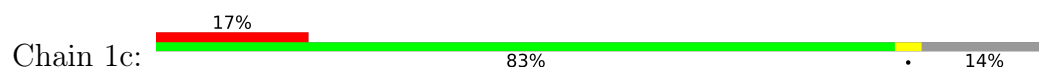
• Molecule 33: 30S ribosomal protein S2



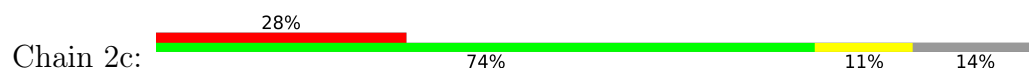
• Molecule 33: 30S ribosomal protein S2

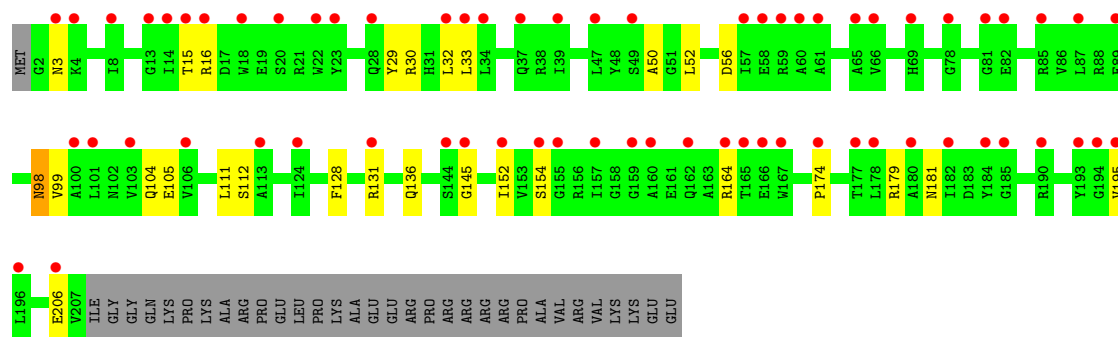


• Molecule 34: 30S ribosomal protein S3

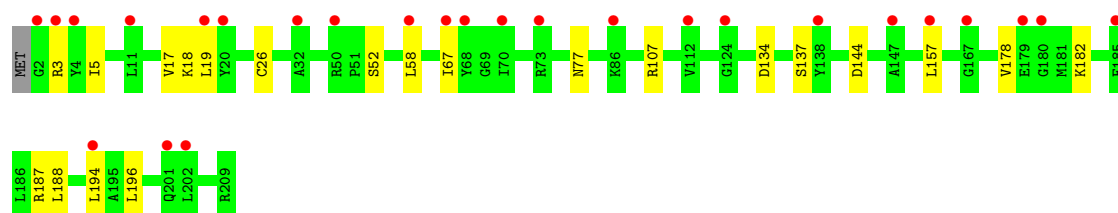
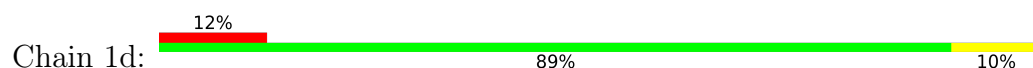


• Molecule 34: 30S ribosomal protein S3

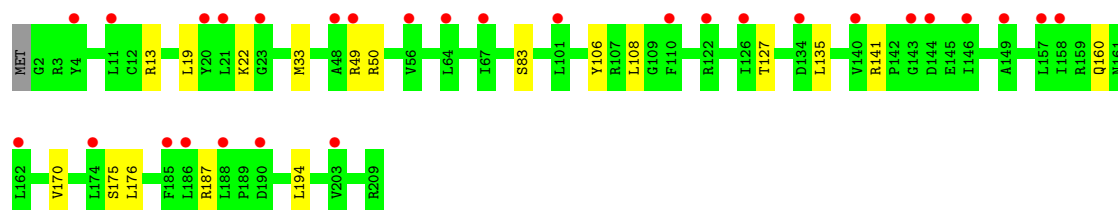




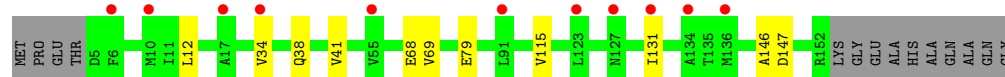
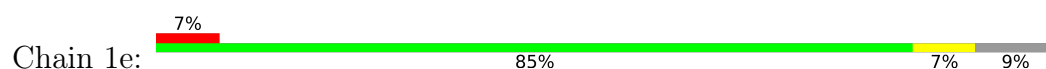
• Molecule 35: 30S ribosomal protein S4



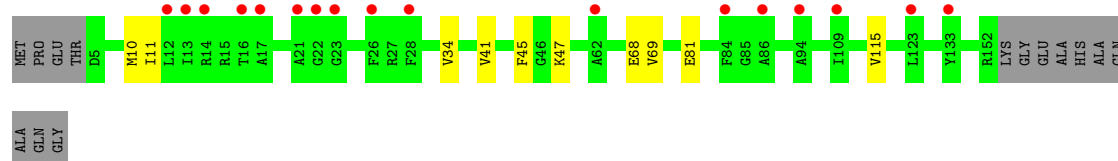
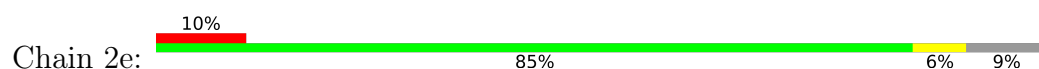
• Molecule 35: 30S ribosomal protein S4



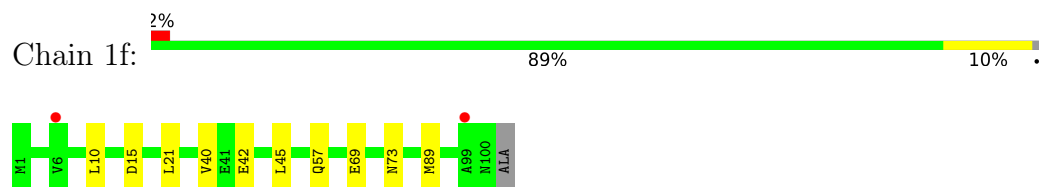
• Molecule 36: 30S ribosomal protein S5



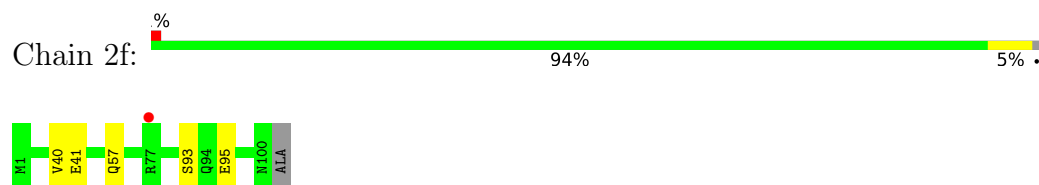
• Molecule 36: 30S ribosomal protein S5



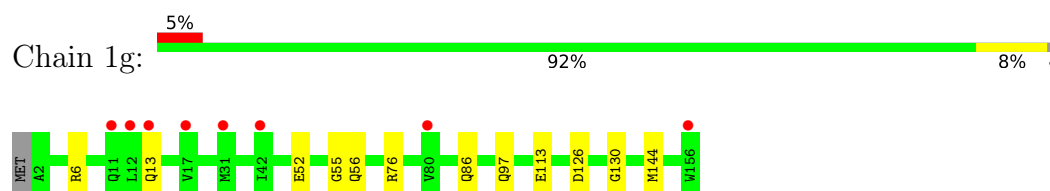
- Molecule 37: 30S ribosomal protein S6



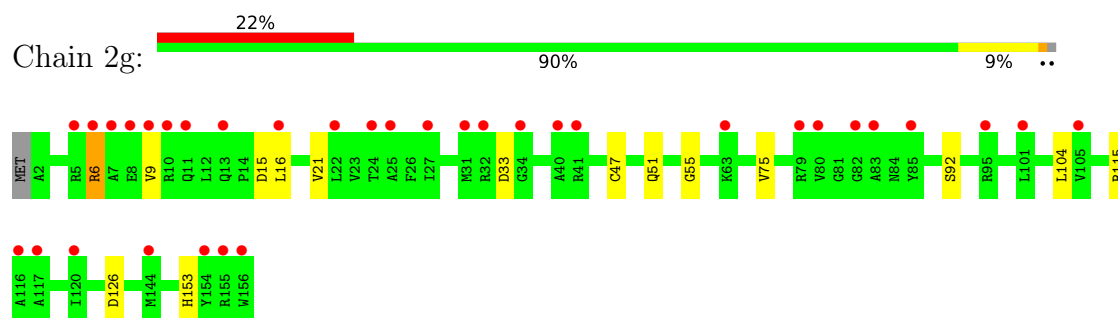
- Molecule 37: 30S ribosomal protein S6



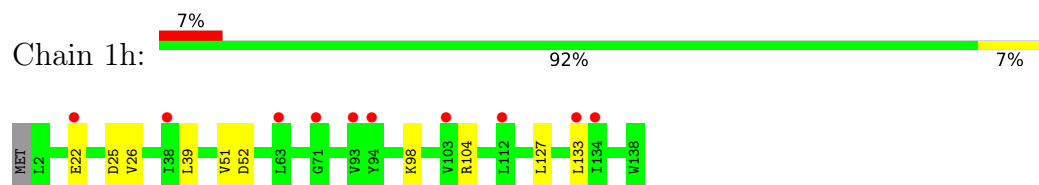
- Molecule 38: 30S ribosomal protein S7



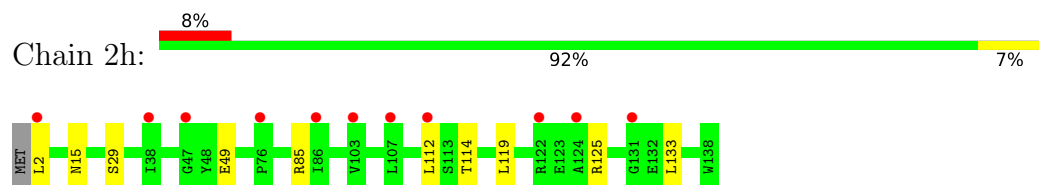
- Molecule 38: 30S ribosomal protein S7



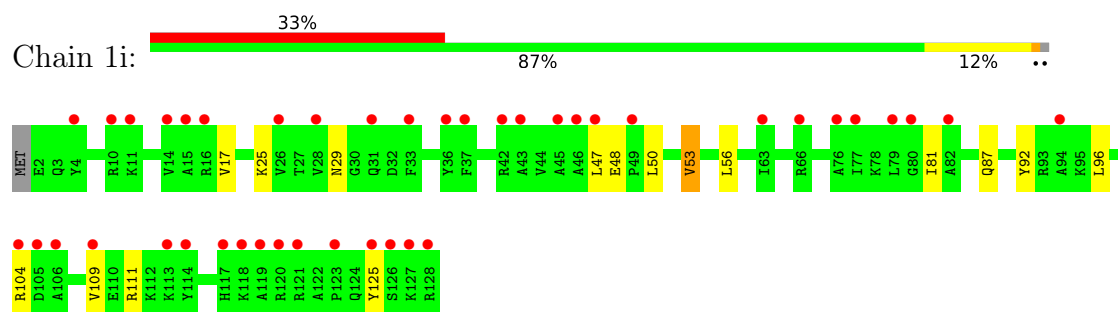
- Molecule 39: 30S ribosomal protein S8



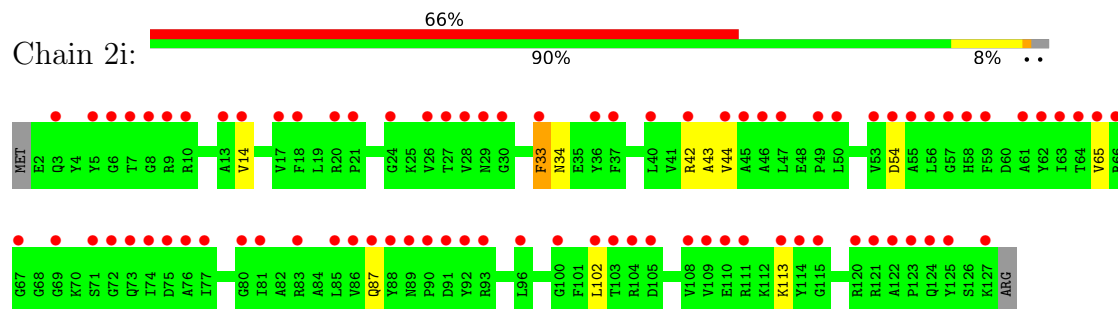
- Molecule 39: 30S ribosomal protein S8



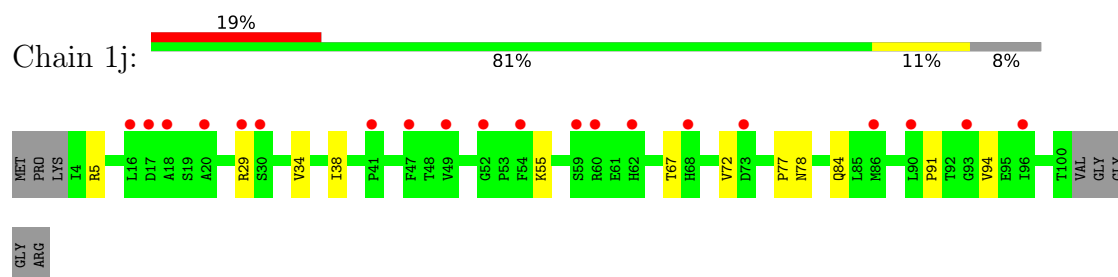
- Molecule 40: 30S ribosomal protein S9



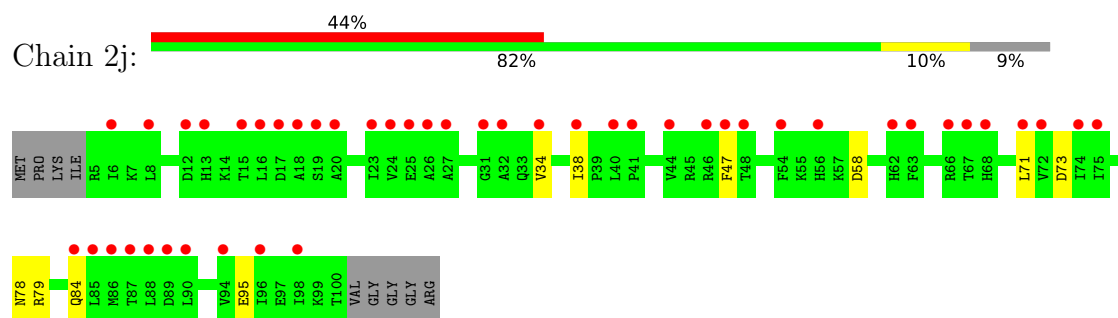
- Molecule 40: 30S ribosomal protein S9



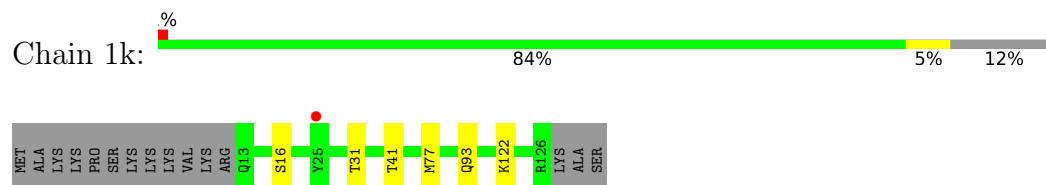
- Molecule 41: 30S ribosomal protein S10



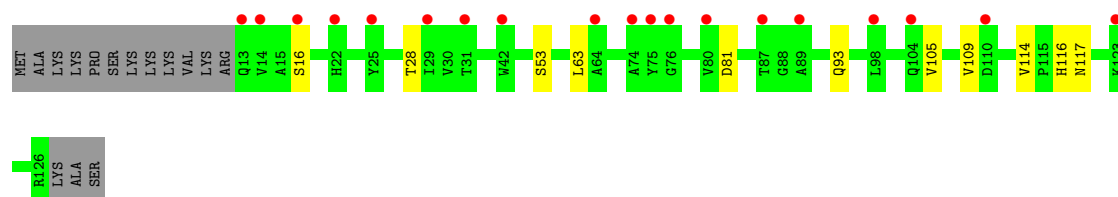
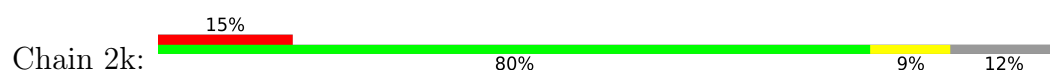
- Molecule 41: 30S ribosomal protein S10



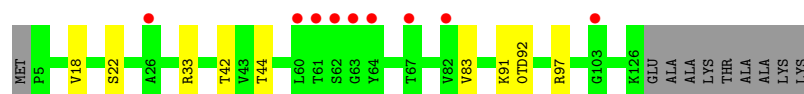
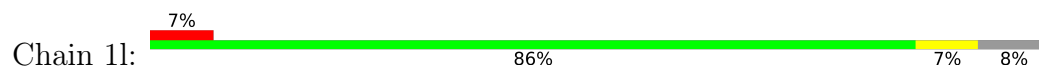
- Molecule 42: 30S ribosomal protein S11



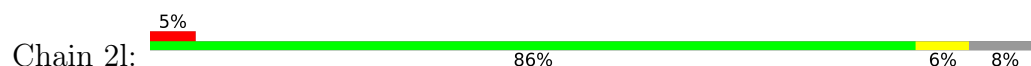
- Molecule 42: 30S ribosomal protein S11



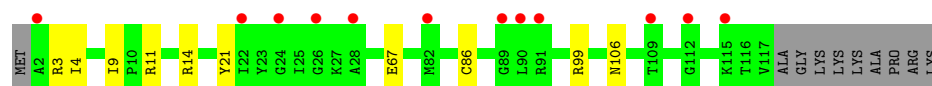
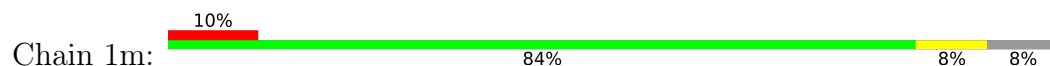
- Molecule 43: 30S ribosomal protein S12



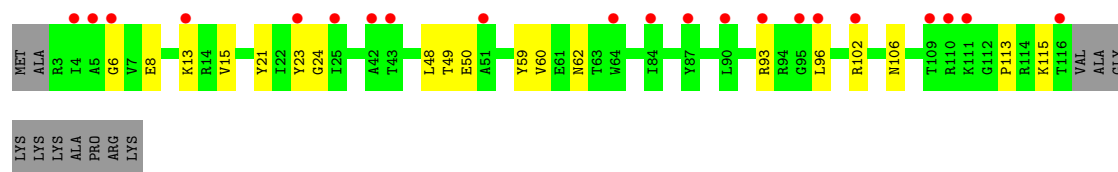
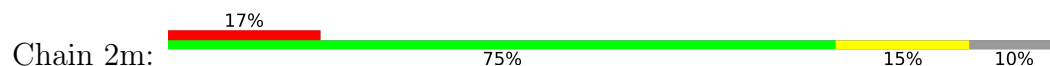
- Molecule 43: 30S ribosomal protein S12



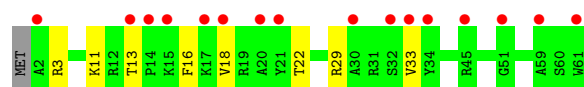
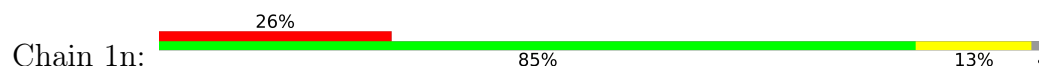
- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

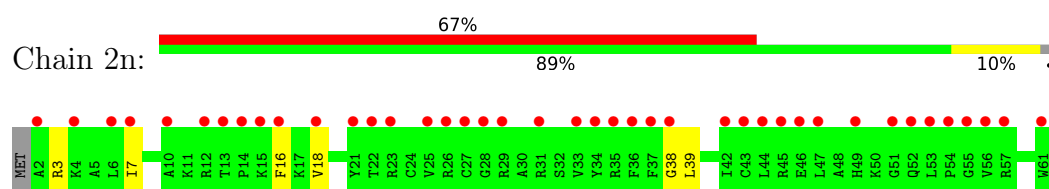


- Molecule 45: 30S ribosomal protein S14 type Z

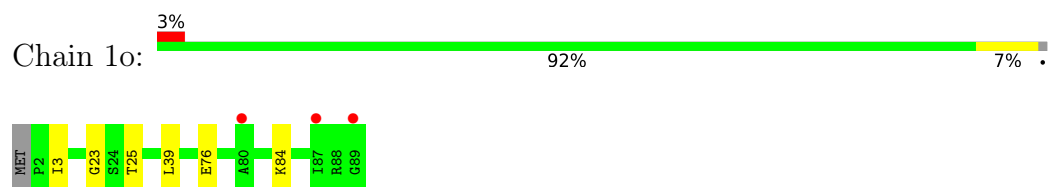


- Molecule 45: 30S ribosomal protein S14 type Z

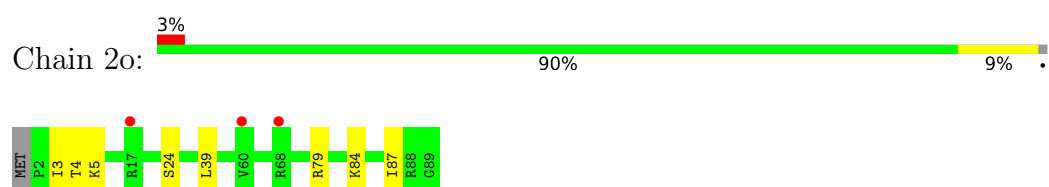




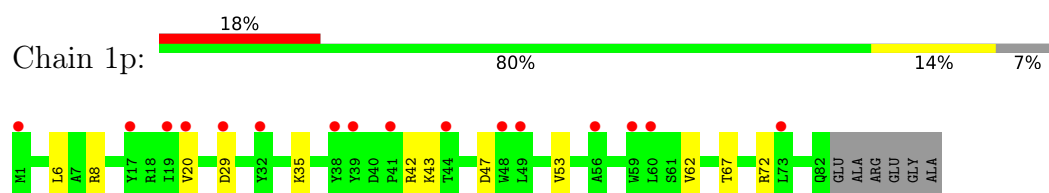
- Molecule 46: 30S ribosomal protein S15



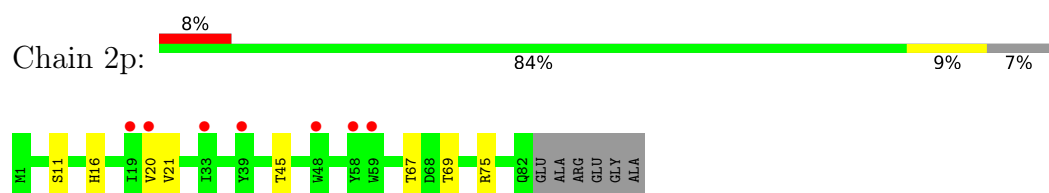
- Molecule 46: 30S ribosomal protein S15



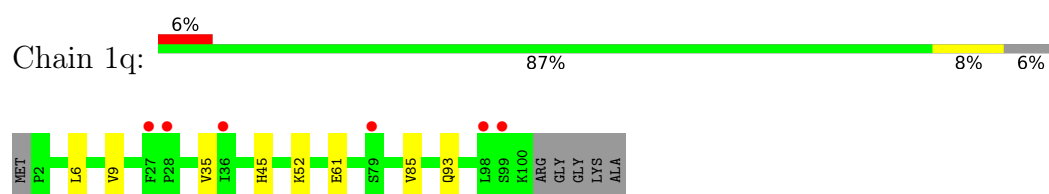
- Molecule 47: 30S ribosomal protein S16



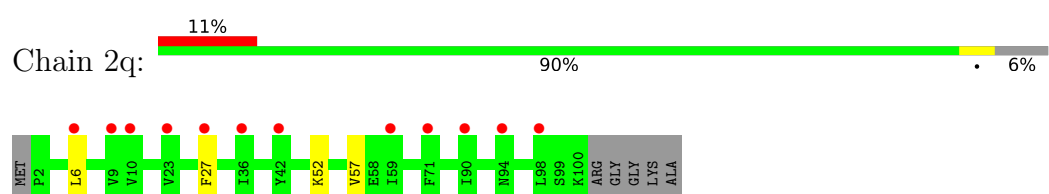
- Molecule 47: 30S ribosomal protein S16



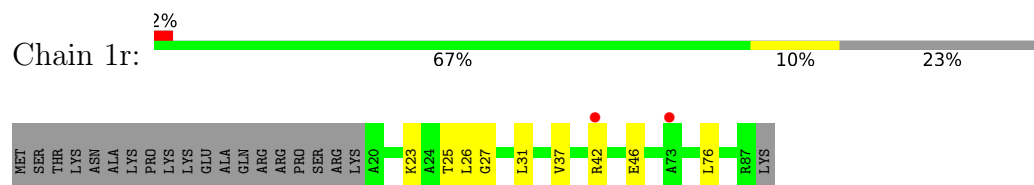
- Molecule 48: 30S ribosomal protein S17



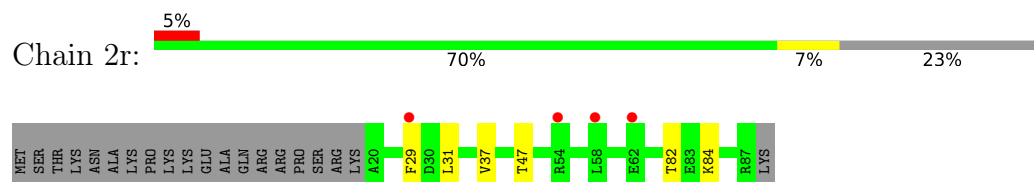
- Molecule 48: 30S ribosomal protein S17



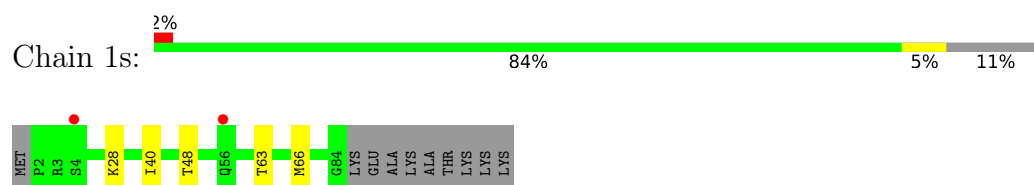
## • Molecule 49: 30S ribosomal protein S18



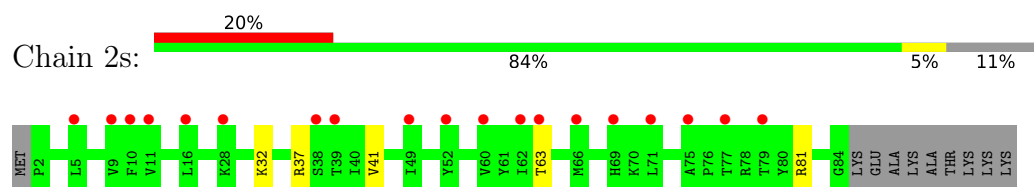
## • Molecule 49: 30S ribosomal protein S18



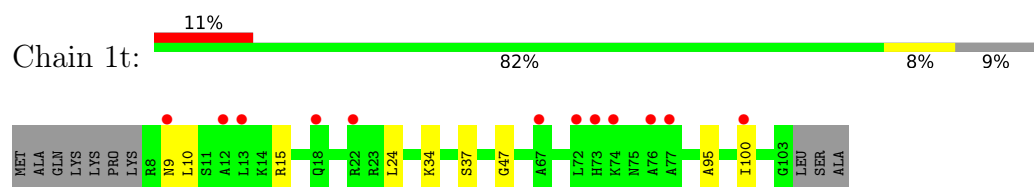
## • Molecule 50: 30S ribosomal protein S19



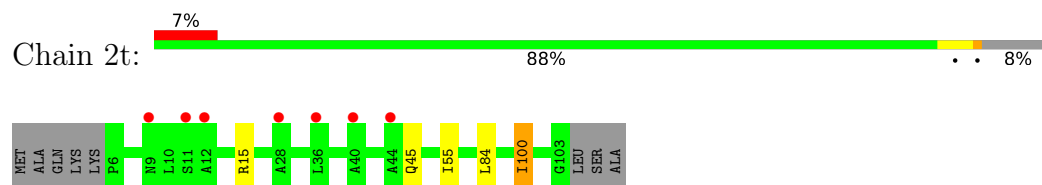
## • Molecule 50: 30S ribosomal protein S19



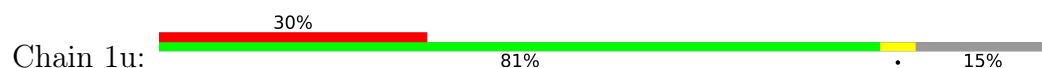
## • Molecule 51: 30S ribosomal protein S20

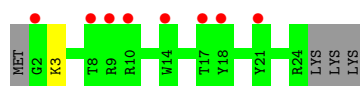


## • Molecule 51: 30S ribosomal protein S20

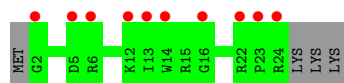
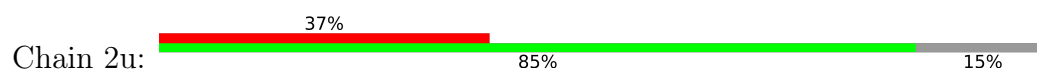


## • Molecule 52: 30S ribosomal protein Thx

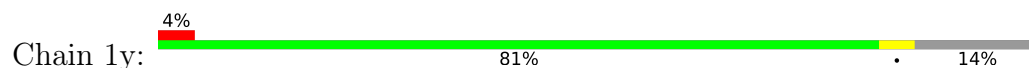




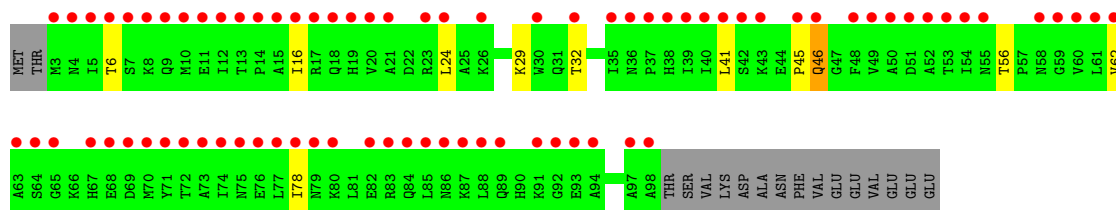
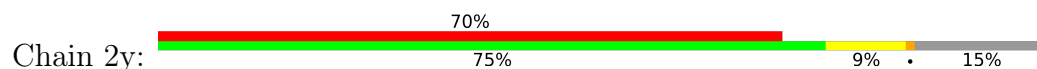
- Molecule 52: 30S ribosomal protein Thx



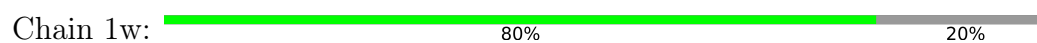
- Molecule 53: Ribosome-associated inhibitor A



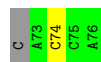
- Molecule 53: Ribosome-associated inhibitor A



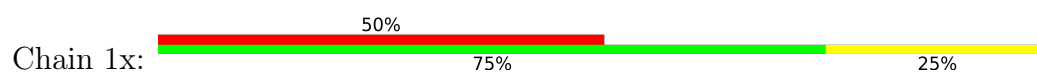
- Molecule 54: A-site Deacylated tRNA Analog



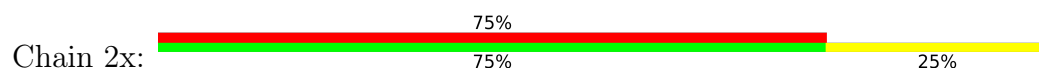
- Molecule 54: A-site Deacylated tRNA Analog



- Molecule 55: P-site Peptidyl-tRNA Analog RNA



- Molecule 55: P-site Peptidyl-tRNA Analog RNA



- Molecule 56: P-site Peptidyl-tRNA Analog Peptide



- Molecule 56: P-site Peptidyl-tRNA Analog Peptide



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.71Å 449.95Å 621.20Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 224.98 – 2.50<br>310.60 – 2.50                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.5 (224.98-2.50)<br>98.5 (310.60-2.50)                    | Depositor<br>EDS |
| $R_{merge}$   | 0.16  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.16 (at 2.52Å)   | Xtriage          |
| Refinement program  | PHENIX 1.8.2  | Depositor        |
| R, $R_{free}$   | 0.229 , 0.280<br>0.229 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set   | 98581 reflections (5.02%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 46.2  | Xtriage          |
| Anisotropy  | 0.157   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 53.0   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 297630  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 50.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: OMC, MPD, MA6, OMU, 8AN, G7M, 4OC, MG, 0TD, 2MG, CLM, SF4, OMG, 2MA, ZN, PSU, UR3, M2G, 5MC, 5MU

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   | 1A    | 0.52         | 1/69031 (0.0%) | 1.01        | 77/107754 (0.1%) |
| 1   | 2A    | 0.41         | 0/68903        | 0.90        | 51/107552 (0.0%) |
| 2   | 1B    | 0.45         | 0/2876         | 0.94        | 1/4486 (0.0%)    |
| 2   | 2B    | 0.34         | 0/2878         | 0.83        | 0/4490           |
| 3   | 1D    | 0.36         | 0/2181         | 0.57        | 0/2940           |
| 3   | 2D    | 0.32         | 0/2186         | 0.54        | 0/2944           |
| 4   | 1E    | 0.33         | 0/1592         | 0.54        | 0/2149           |
| 4   | 2E    | 0.31         | 0/1592         | 0.52        | 0/2149           |
| 5   | 1F    | 0.34         | 0/1619         | 0.56        | 0/2193           |
| 5   | 2F    | 0.31         | 0/1615         | 0.52        | 0/2188           |
| 6   | 1G    | 0.31         | 0/1451         | 0.50        | 0/1961           |
| 6   | 2G    | 0.29         | 0/1449         | 0.47        | 0/1957           |
| 7   | 1H    | 0.32         | 0/1356         | 0.50        | 0/1834           |
| 7   | 2H    | 0.29         | 0/1350         | 0.49        | 0/1826           |
| 8   | 1I    | 0.28         | 0/1109         | 0.50        | 0/1512           |
| 8   | 2I    | 1.11         | 3/1091 (0.3%)  | 0.98        | 4/1490 (0.3%)    |
| 9   | 1N    | 0.33         | 0/1148         | 0.53        | 0/1547           |
| 9   | 2N    | 0.30         | 0/1144         | 0.48        | 0/1543           |
| 10  | 1O    | 0.35         | 0/943          | 0.56        | 0/1269           |
| 10  | 2O    | 0.33         | 0/943          | 0.55        | 0/1269           |
| 11  | 1P    | 0.34         | 0/1152         | 0.56        | 0/1533           |
| 11  | 2P    | 0.30         | 0/1152         | 0.53        | 0/1533           |
| 12  | 1Q    | 0.33         | 0/1143         | 0.52        | 0/1527           |
| 12  | 2Q    | 0.32         | 0/1143         | 0.50        | 0/1527           |
| 13  | 1R    | 0.33         | 0/982          | 0.55        | 0/1312           |
| 13  | 2R    | 0.30         | 0/982          | 0.50        | 0/1312           |
| 14  | 1S    | 0.31         | 0/887          | 0.54        | 0/1180           |
| 14  | 2S    | 0.31         | 0/880          | 0.51        | 0/1172           |
| 15  | 1T    | 0.34         | 0/1105         | 0.53        | 0/1477           |
| 15  | 2T    | 0.31         | 0/1097         | 0.48        | 0/1468           |
| 16  | 1U    | 0.36         | 0/977          | 0.52        | 0/1301           |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 16  | 2U    | 0.29         | 0/977          | 0.44        | 0/1301          |
| 17  | 1V    | 0.35         | 0/786          | 0.54        | 0/1053          |
| 17  | 2V    | 0.30         | 0/782          | 0.54        | 0/1049          |
| 18  | 1W    | 0.35         | 0/897          | 0.52        | 0/1205          |
| 18  | 2W    | 0.31         | 0/897          | 0.49        | 0/1205          |
| 19  | 1X    | 0.37         | 0/764          | 0.56        | 0/1025          |
| 19  | 2X    | 0.31         | 0/764          | 0.52        | 0/1025          |
| 20  | 1Y    | 0.34         | 0/823          | 0.55        | 0/1099          |
| 20  | 2Y    | 0.32         | 0/823          | 0.52        | 0/1100          |
| 21  | 1Z    | 0.31         | 0/1620         | 0.50        | 0/2200          |
| 21  | 2Z    | 0.29         | 0/1590         | 0.48        | 0/2162          |
| 22  | 10    | 0.36         | 0/662          | 0.55        | 0/881           |
| 22  | 20    | 0.31         | 0/659          | 0.54        | 0/877           |
| 23  | 11    | 0.33         | 0/761          | 0.52        | 0/1013          |
| 23  | 21    | 0.30         | 0/766          | 0.50        | 0/1018          |
| 24  | 12    | 0.31         | 0/590          | 0.49        | 0/781           |
| 24  | 22    | 0.29         | 0/594          | 0.45        | 0/785           |
| 25  | 13    | 0.34         | 0/474          | 0.55        | 0/635           |
| 25  | 23    | 0.30         | 0/469          | 0.49        | 0/630           |
| 26  | 14    | 0.30         | 0/559          | 0.52        | 0/754           |
| 26  | 24    | 0.39         | 0/549          | 0.59        | 0/741           |
| 27  | 15    | 0.39         | 0/473          | 0.62        | 0/639           |
| 27  | 25    | 0.28         | 0/469          | 0.53        | 0/635           |
| 28  | 16    | 0.32         | 0/460          | 0.52        | 0/613           |
| 28  | 26    | 0.29         | 0/456          | 0.49        | 0/608           |
| 29  | 17    | 0.37         | 0/426          | 0.54        | 0/561           |
| 29  | 27    | 0.29         | 0/426          | 0.50        | 0/561           |
| 30  | 18    | 0.33         | 0/525          | 0.55        | 0/691           |
| 30  | 28    | 0.30         | 0/525          | 0.48        | 0/691           |
| 31  | 19    | 0.34         | 0/310          | 0.54        | 0/407           |
| 31  | 29    | 0.32         | 0/310          | 0.55        | 0/407           |
| 32  | 1a    | 0.74         | 6/35795 (0.0%) | 0.88        | 16/55864 (0.0%) |
| 32  | 2a    | 0.36         | 0/35890        | 0.88        | 24/56012 (0.0%) |
| 33  | 1b    | 0.30         | 0/1876         | 0.49        | 0/2533          |
| 33  | 2b    | 0.30         | 0/1860         | 0.50        | 0/2518          |
| 34  | 1c    | 0.29         | 0/1582         | 0.49        | 0/2137          |
| 34  | 2c    | 0.28         | 0/1566         | 0.48        | 0/2119          |
| 35  | 1d    | 0.30         | 0/1695         | 0.49        | 0/2274          |
| 35  | 2d    | 0.29         | 0/1698         | 0.47        | 0/2277          |
| 36  | 1e    | 0.29         | 0/1149         | 0.51        | 0/1548          |
| 36  | 2e    | 0.30         | 0/1149         | 0.48        | 0/1548          |
| 37  | 1f    | 0.30         | 0/827          | 0.47        | 0/1120          |
| 37  | 2f    | 0.30         | 0/829          | 0.48        | 0/1123          |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 38  | 1g    | 0.28         | 0/1254           | 0.43        | 0/1683            |
| 38  | 2g    | 0.28         | 0/1248           | 0.43        | 0/1676            |
| 39  | 1h    | 0.28         | 0/1118           | 0.49        | 0/1506            |
| 39  | 2h    | 0.28         | 0/1108           | 0.48        | 0/1494            |
| 40  | 1i    | 0.30         | 0/1005           | 0.50        | 0/1351            |
| 40  | 2i    | 0.30         | 0/985            | 0.53        | 0/1329            |
| 41  | 1j    | 0.28         | 0/732            | 0.47        | 0/993             |
| 41  | 2j    | 0.29         | 0/723            | 0.48        | 0/984             |
| 42  | 1k    | 0.28         | 0/849            | 0.48        | 0/1150            |
| 42  | 2k    | 0.28         | 0/848            | 0.49        | 0/1149            |
| 43  | 1l    | 0.29         | 0/937            | 0.49        | 0/1260            |
| 43  | 2l    | 0.29         | 0/937            | 0.49        | 0/1260            |
| 44  | 1m    | 0.28         | 0/924            | 0.46        | 0/1242            |
| 44  | 2m    | 0.30         | 0/905            | 0.48        | 0/1217            |
| 45  | 1n    | 0.30         | 0/501            | 0.47        | 0/664             |
| 45  | 2n    | 0.29         | 0/501            | 0.46        | 0/664             |
| 46  | 1o    | 0.29         | 0/739            | 0.43        | 0/985             |
| 46  | 2o    | 0.27         | 0/739            | 0.41        | 0/985             |
| 47  | 1p    | 0.28         | 0/697            | 0.51        | 0/939             |
| 47  | 2p    | 0.28         | 0/693            | 0.51        | 0/935             |
| 48  | 1q    | 0.29         | 0/836            | 0.47        | 0/1117            |
| 48  | 2q    | 0.28         | 0/836            | 0.48        | 0/1117            |
| 49  | 1r    | 0.29         | 0/560            | 0.49        | 0/746             |
| 49  | 2r    | 0.28         | 0/560            | 0.46        | 0/746             |
| 50  | 1s    | 0.27         | 0/663            | 0.47        | 0/895             |
| 50  | 2s    | 0.30         | 0/660            | 0.51        | 0/893             |
| 51  | 1t    | 0.28         | 0/734            | 0.43        | 0/969             |
| 51  | 2t    | 0.28         | 0/736            | 0.41        | 0/976             |
| 52  | 1u    | 0.28         | 0/203            | 0.46        | 0/266             |
| 52  | 2u    | 0.24         | 0/203            | 0.48        | 0/266             |
| 53  | 1y    | 0.29         | 0/776            | 0.47        | 0/1048            |
| 53  | 2y    | 0.29         | 0/761            | 0.48        | 0/1030            |
| 54  | 1w    | 0.50         | 0/69             | 0.92        | 0/106             |
| 54  | 2w    | 0.41         | 0/69             | 0.87        | 0/106             |
| 55  | 1x    | 0.59         | 0/44             | 1.30        | 0/67              |
| 55  | 2x    | 0.65         | 0/44             | 1.50        | 0/67              |
| 56  | 1v    | 0.35         | 0/22             | 0.55        | 0/28              |
| 56  | 2v    | 0.29         | 0/22             | 0.55        | 0/28              |
| All | All   | 0.46         | 10/310300 (0.0%) | 0.84        | 173/463757 (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 |
|-----|-------|---------------------|---------------------|
| 26  | 24    | 0                   | 1                   |
| 33  | 1b    | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (10) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 32  | 1a    | 368  | U    | C2-N3 | 66.62 | 1.84        | 1.37     |
| 32  | 1a    | 368  | U    | N3-C4 | 54.22 | 1.87        | 1.38     |
| 32  | 1a    | 368  | U    | N1-C2 | 45.83 | 1.79        | 1.38     |
| 32  | 1a    | 368  | U    | C4-C5 | 43.38 | 1.82        | 1.43     |
| 32  | 1a    | 368  | U    | N1-C6 | 42.86 | 1.76        | 1.38     |
| 32  | 1a    | 368  | U    | C5-C6 | 38.70 | 1.69        | 1.34     |
| 8   | 2I    | 82   | ARG  | CD-NE | 32.04 | 2.00        | 1.46     |
| 8   | 2I    | 82   | ARG  | NE-CZ | 13.15 | 1.50        | 1.33     |
| 8   | 2I    | 82   | ARG  | CG-CD | 7.51  | 1.70        | 1.51     |
| 1   | 1A    | 2790 | A    | N9-C4 | 5.17  | 1.41        | 1.37     |

All (173) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 8   | 2I    | 82   | ARG  | CD-NE-CZ   | 22.45  | 155.03      | 123.60   |
| 8   | 2I    | 82   | ARG  | NE-CZ-NH1  | 17.37  | 128.99      | 120.30   |
| 1   | 1A    | 1042 | G    | OP1-P-O3'  | -11.28 | 80.39       | 105.20   |
| 8   | 2I    | 82   | ARG  | CG-CD-NE   | 11.18  | 135.28      | 111.80   |
| 1   | 2A    | 576  | U    | O5'-P-OP1  | -10.88 | 95.91       | 105.70   |
| 1   | 2A    | 570  | G    | C5-C6-O6   | -9.37  | 122.98      | 128.60   |
| 1   | 2A    | 1092 | C    | N1-C2-O2   | 9.32   | 124.50      | 118.90   |
| 1   | 1A    | 1042 | G    | OP2-P-O3'  | -9.04  | 85.32       | 105.20   |
| 1   | 1A    | 570  | G    | C5-C6-O6   | -8.97  | 123.22      | 128.60   |
| 1   | 1A    | 751  | A    | O5'-P-OP1  | -8.78  | 97.80       | 105.70   |
| 1   | 1A    | 512  | G    | O4'-C1'-N9 | 8.75   | 115.20      | 108.20   |
| 1   | 2A    | 1092 | C    | C2-N1-C1'  | 8.70   | 128.37      | 118.80   |
| 1   | 2A    | 1648 | C    | O5'-P-OP1  | -8.69  | 97.88       | 105.70   |
| 8   | 2I    | 82   | ARG  | NE-CZ-NH2  | -8.62  | 115.99      | 120.30   |
| 1   | 2A    | 1092 | C    | N3-C2-O2   | -8.36  | 116.05      | 121.90   |
| 1   | 1A    | 801  | G    | O5'-P-OP2  | -8.32  | 98.22       | 105.70   |
| 32  | 2a    | 955  | U    | C5-C4-O4   | 8.32   | 130.89      | 125.90   |
| 32  | 2a    | 1004 | A    | O4'-C1'-N9 | 8.23   | 114.79      | 108.20   |
| 1   | 2A    | 1092 | C    | C6-N1-C2   | -8.21  | 117.02      | 120.30   |
| 1   | 1A    | 576  | U    | O5'-P-OP1  | -8.14  | 98.37       | 105.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 32  | 1a    | 558  | G    | O5'-P-OP1  | -8.11 | 98.40       | 105.70   |
| 1   | 1A    | 1372 | U    | C5-C4-O4   | -8.10 | 121.04      | 125.90   |
| 32  | 1a    | 368  | U    | C2-N3-C4   | -7.99 | 122.21      | 127.00   |
| 1   | 1A    | 1653 | G    | C8-N9-C4   | -7.81 | 103.28      | 106.40   |
| 1   | 1A    | 948  | G    | O5'-P-OP1  | -7.80 | 98.68       | 105.70   |
| 1   | 1A    | 1043 | C    | OP1-P-OP2  | 7.77  | 131.25      | 119.60   |
| 1   | 1A    | 575  | A    | O5'-P-OP1  | -7.75 | 98.72       | 105.70   |
| 1   | 2A    | 801  | G    | O5'-P-OP2  | -7.68 | 98.78       | 105.70   |
| 1   | 1A    | 570  | G    | C5-C6-N1   | 7.47  | 115.23      | 111.50   |
| 2   | 1B    | 57   | A    | N9-C4-C5   | -7.36 | 102.86      | 105.80   |
| 1   | 1A    | 1791 | A    | O5'-P-OP1  | -7.34 | 99.10       | 105.70   |
| 1   | 1A    | 1782 | C    | O5'-P-OP1  | -7.12 | 99.29       | 105.70   |
| 32  | 2a    | 1397 | C    | C2-N1-C1'  | 7.11  | 126.62      | 118.80   |
| 1   | 2A    | 570  | G    | C4-C5-N7   | 7.10  | 113.64      | 110.80   |
| 32  | 1a    | 299  | G    | C5-C6-O6   | -7.05 | 124.37      | 128.60   |
| 32  | 2a    | 266  | G    | P-O3'-C3'  | 7.04  | 128.15      | 119.70   |
| 1   | 1A    | 2074 | U    | O5'-P-OP1  | -7.04 | 99.36       | 105.70   |
| 1   | 2A    | 31   | C    | O5'-P-OP1  | -7.04 | 99.37       | 105.70   |
| 1   | 1A    | 1075 | C    | N1-C2-O2   | 7.03  | 123.12      | 118.90   |
| 1   | 2A    | 645  | C    | C2-N1-C1'  | 7.03  | 126.53      | 118.80   |
| 1   | 1A    | 570  | G    | C4-C5-N7   | 7.02  | 113.61      | 110.80   |
| 1   | 1A    | 784  | A    | P-O3'-C3'  | 6.99  | 128.09      | 119.70   |
| 1   | 1A    | 226  | G    | O4'-C1'-N9 | 6.94  | 113.75      | 108.20   |
| 1   | 1A    | 570  | G    | N9-C4-C5   | -6.89 | 102.64      | 105.40   |
| 1   | 2A    | 2598 | A    | O5'-P-OP1  | -6.84 | 99.55       | 105.70   |
| 1   | 1A    | 1372 | U    | N3-C4-O4   | 6.74  | 124.11      | 119.40   |
| 1   | 1A    | 531  | C    | O5'-P-OP2  | -6.73 | 99.64       | 105.70   |
| 1   | 1A    | 2711 | A    | O5'-P-OP2  | -6.72 | 99.65       | 105.70   |
| 32  | 2a    | 1183 | A    | P-O3'-C3'  | 6.68  | 127.72      | 119.70   |
| 1   | 1A    | 1799 | G    | C5-C6-O6   | 6.54  | 132.52      | 128.60   |
| 1   | 1A    | 845  | G    | O4'-C1'-N9 | 6.51  | 113.41      | 108.20   |
| 1   | 1A    | 1086 | A    | N1-C6-N6   | -6.47 | 114.72      | 118.60   |
| 32  | 1a    | 368  | U    | C6-N1-C2   | 6.44  | 124.86      | 121.00   |
| 1   | 1A    | 2249 | U    | N3-C4-O4   | -6.43 | 114.90      | 119.40   |
| 1   | 2A    | 2108 | C    | C2-N3-C4   | 6.43  | 123.12      | 119.90   |
| 1   | 1A    | 787  | U    | O5'-P-OP1  | -6.43 | 99.91       | 105.70   |
| 1   | 2A    | 570  | G    | N1-C6-O6   | 6.43  | 123.76      | 119.90   |
| 1   | 1A    | 1075 | C    | C2-N1-C1'  | 6.39  | 125.83      | 118.80   |
| 1   | 2A    | 568  | U    | C5-C4-O4   | -6.39 | 122.07      | 125.90   |
| 1   | 2A    | 2103 | C    | C2-N3-C4   | 6.35  | 123.08      | 119.90   |
| 1   | 1A    | 645  | C    | C2-N1-C1'  | 6.33  | 125.77      | 118.80   |
| 1   | 1A    | 1828 | G    | O5'-P-OP2  | -6.31 | 100.02      | 105.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 1A    | 645  | C    | N1-C2-O2   | 6.23  | 122.64      | 118.90   |
| 1   | 2A    | 2122 | U    | C5-C4-O4   | 6.17  | 129.60      | 125.90   |
| 1   | 2A    | 2191 | G    | C5-C6-O6   | 6.16  | 132.30      | 128.60   |
| 1   | 2A    | 1076 | C    | OP1-P-O3'  | 6.15  | 118.72      | 105.20   |
| 32  | 2a    | 754  | C    | C2-N1-C1'  | 6.15  | 125.56      | 118.80   |
| 1   | 1A    | 1653 | G    | N3-C4-C5   | -6.10 | 125.55      | 128.60   |
| 1   | 1A    | 751  | A    | O5'-P-OP2  | 6.02  | 117.92      | 110.70   |
| 1   | 1A    | 961  | C    | O5'-P-OP2  | -6.02 | 100.28      | 105.70   |
| 1   | 2A    | 570  | G    | C6-C5-N7   | -5.95 | 126.83      | 130.40   |
| 1   | 1A    | 1602 | U    | N3-C4-O4   | -5.92 | 115.25      | 119.40   |
| 1   | 1A    | 2848 | G    | O4'-C1'-N9 | 5.92  | 112.94      | 108.20   |
| 1   | 1A    | 1062 | G    | N3-C2-N2   | -5.91 | 115.76      | 119.90   |
| 1   | 1A    | 1192 | G    | C8-N9-C4   | 5.89  | 108.76      | 106.40   |
| 32  | 2a    | 754  | C    | N1-C2-O2   | 5.87  | 122.42      | 118.90   |
| 1   | 2A    | 645  | C    | N1-C2-O2   | 5.85  | 122.41      | 118.90   |
| 32  | 1a    | 1020 | U    | N1-C2-O2   | 5.83  | 126.89      | 122.80   |
| 1   | 1A    | 1614 | A    | O5'-P-OP1  | -5.83 | 100.45      | 105.70   |
| 1   | 2A    | 1992 | G    | P-O3'-C3'  | 5.83  | 126.69      | 119.70   |
| 1   | 2A    | 570  | G    | N9-C4-C5   | -5.80 | 103.08      | 105.40   |
| 1   | 1A    | 2577 | A    | O5'-P-OP1  | -5.78 | 100.50      | 105.70   |
| 1   | 2A    | 277  | C    | N1-C2-O2   | 5.78  | 122.37      | 118.90   |
| 1   | 1A    | 1428 | C    | C6-N1-C2   | 5.77  | 122.61      | 120.30   |
| 1   | 1A    | 2036 | C    | O5'-P-OP1  | -5.74 | 100.54      | 105.70   |
| 1   | 2A    | 1779 | U    | O4'-C1'-N1 | 5.74  | 112.79      | 108.20   |
| 1   | 2A    | 2248 | C    | O5'-P-OP2  | -5.72 | 100.55      | 105.70   |
| 32  | 1a    | 368  | U    | O4'-C1'-N1 | 5.72  | 112.77      | 108.20   |
| 1   | 1A    | 2689 | U    | P-O3'-C3'  | 5.71  | 126.56      | 119.70   |
| 1   | 1A    | 1052 | C    | C2-N1-C1'  | 5.70  | 125.07      | 118.80   |
| 1   | 1A    | 330  | A    | C2-N3-C4   | -5.68 | 107.76      | 110.60   |
| 1   | 1A    | 2682 | U    | O5'-P-OP2  | -5.68 | 100.59      | 105.70   |
| 1   | 1A    | 1192 | G    | N7-C8-N9   | -5.67 | 110.27      | 113.10   |
| 32  | 2a    | 1065 | U    | P-O3'-C3'  | 5.67  | 126.50      | 119.70   |
| 1   | 2A    | 845  | G    | O4'-C1'-N9 | 5.67  | 112.73      | 108.20   |
| 1   | 1A    | 2103 | C    | N1-C2-O2   | 5.66  | 122.29      | 118.90   |
| 1   | 2A    | 1313 | U    | C2-N1-C1'  | 5.64  | 124.47      | 117.70   |
| 32  | 2a    | 997  | U    | C5-C4-O4   | 5.62  | 129.27      | 125.90   |
| 1   | 2A    | 1992 | G    | C8-N9-C4   | -5.61 | 104.16      | 106.40   |
| 32  | 2a    | 1003 | G    | N3-C4-C5   | -5.60 | 125.80      | 128.60   |
| 1   | 1A    | 1493 | C    | N1-C2-O2   | 5.60  | 122.26      | 118.90   |
| 32  | 2a    | 1183 | A    | OP1-P-O3'  | 5.60  | 117.52      | 105.20   |
| 32  | 1a    | 299  | G    | C4-C5-N7   | 5.57  | 113.03      | 110.80   |
| 32  | 2a    | 266  | G    | OP2-P-O3'  | 5.57  | 117.45      | 105.20   |

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| Mol | Chain | Res    | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|-------|-------------|----------|
| 1   | 1A    | 784    | A    | OP1-P-O3'  | 5.56  | 117.44      | 105.20   |
| 1   | 2A    | 1060   | U    | C2-N1-C1'  | 5.54  | 124.35      | 117.70   |
| 32  | 2a    | 1126   | U    | N1-C2-O2   | 5.54  | 126.68      | 122.80   |
| 32  | 2a    | 687    | A    | P-O3'-C3'  | 5.54  | 126.34      | 119.70   |
| 1   | 1A    | 784    | A    | N1-C6-N6   | -5.53 | 115.28      | 118.60   |
| 1   | 1A    | 2430   | A    | C2-N3-C4   | 5.52  | 113.36      | 110.60   |
| 1   | 2A    | 2103   | C    | C5-C4-N4   | 5.51  | 124.06      | 120.20   |
| 1   | 2A    | 570    | G    | N3-C4-N9   | 5.48  | 129.29      | 126.00   |
| 1   | 2A    | 1379   | A    | OP2-P-O3'  | 5.45  | 117.20      | 105.20   |
| 1   | 2A    | 1092   | C    | C5-C6-N1   | 5.43  | 123.71      | 121.00   |
| 1   | 1A    | 330    | A    | N1-C2-N3   | 5.41  | 132.00      | 129.30   |
| 32  | 2a    | 1442   | G    | OP1-P-O3'  | 5.37  | 117.02      | 105.20   |
| 1   | 2A    | 1992   | G    | N3-C4-C5   | -5.36 | 125.92      | 128.60   |
| 1   | 1A    | 271(Y) | U    | O4'-C1'-N1 | 5.36  | 112.49      | 108.20   |
| 32  | 2a    | 1397   | C    | C6-N1-C1'  | -5.34 | 114.39      | 120.80   |
| 1   | 1A    | 961    | C    | N1-C2-O2   | -5.34 | 115.70      | 118.90   |
| 1   | 2A    | 1614   | A    | O5'-P-OP1  | -5.34 | 100.90      | 105.70   |
| 32  | 1a    | 78     | G    | C4-N9-C1'  | -5.33 | 119.58      | 126.50   |
| 1   | 2A    | 2181   | G    | C5-C6-O6   | 5.32  | 131.79      | 128.60   |
| 1   | 2A    | 2181   | G    | C6-N1-C2   | 5.32  | 128.29      | 125.10   |
| 1   | 1A    | 1416   | G    | O4'-C1'-N9 | 5.30  | 112.44      | 108.20   |
| 1   | 1A    | 961    | C    | C2-N1-C1'  | -5.28 | 112.99      | 118.80   |
| 32  | 2a    | 955    | U    | C2-N3-C4   | 5.27  | 130.16      | 127.00   |
| 1   | 2A    | 512    | G    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 1   | 1A    | 249    | C    | N1-C2-O2   | 5.26  | 122.06      | 118.90   |
| 32  | 1a    | 78     | G    | C8-N9-C1'  | 5.26  | 133.84      | 127.00   |
| 1   | 2A    | 1073   | A    | N1-C6-N6   | 5.24  | 121.74      | 118.60   |
| 1   | 1A    | 783    | A    | C2-N3-C4   | 5.24  | 113.22      | 110.60   |
| 32  | 2a    | 754    | C    | N3-C2-O2   | -5.22 | 118.25      | 121.90   |
| 1   | 1A    | 847    | U    | C2-N1-C1'  | 5.22  | 123.96      | 117.70   |
| 1   | 1A    | 2492   | U    | O5'-P-OP1  | -5.21 | 101.01      | 105.70   |
| 1   | 1A    | 2685   | G    | N1-C6-O6   | -5.21 | 116.77      | 119.90   |
| 1   | 1A    | 1190   | G    | C4-C5-N7   | -5.20 | 108.72      | 110.80   |
| 1   | 1A    | 1190   | G    | C5-N7-C8   | 5.19  | 106.89      | 104.30   |
| 1   | 1A    | 1609   | A    | C8-N9-C4   | 5.19  | 107.87      | 105.80   |
| 1   | 2A    | 1092   | C    | C6-N1-C1'  | -5.18 | 114.59      | 120.80   |
| 32  | 2a    | 1009   | G    | C5-C6-O6   | 5.18  | 131.71      | 128.60   |
| 1   | 1A    | 588    | U    | O5'-P-OP2  | -5.17 | 101.05      | 105.70   |
| 1   | 2A    | 1076   | C    | P-O3'-C3'  | 5.17  | 125.90      | 119.70   |
| 32  | 1a    | 115    | G    | P-O3'-C3'  | 5.16  | 125.89      | 119.70   |
| 32  | 2a    | 204    | U    | C2-N1-C1'  | 5.16  | 123.89      | 117.70   |
| 1   | 1A    | 1493   | C    | N3-C2-O2   | -5.16 | 118.29      | 121.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 2A    | 783  | A    | C2-N3-C4   | 5.16  | 113.18      | 110.60   |
| 1   | 2A    | 645  | C    | C6-N1-C1'  | -5.15 | 114.62      | 120.80   |
| 1   | 2A    | 1306 | C    | N1-C2-O2   | 5.15  | 121.99      | 118.90   |
| 1   | 2A    | 2689 | U    | P-O3'-C3'  | 5.15  | 125.88      | 119.70   |
| 1   | 2A    | 1111 | A    | O4'-C1'-N9 | 5.14  | 112.31      | 108.20   |
| 32  | 1a    | 365  | U    | C2-N1-C1'  | 5.14  | 123.87      | 117.70   |
| 32  | 1a    | 78   | G    | N3-C4-N9   | -5.14 | 122.92      | 126.00   |
| 32  | 1a    | 960  | U    | N1-C2-O2   | 5.12  | 126.39      | 122.80   |
| 1   | 1A    | 2571 | C    | N1-C2-O2   | -5.12 | 115.83      | 118.90   |
| 32  | 1a    | 1026 | G    | N3-C4-C5   | -5.11 | 126.04      | 128.60   |
| 1   | 2A    | 1313 | U    | N3-C2-O2   | -5.11 | 118.62      | 122.20   |
| 1   | 2A    | 192  | C    | O5'-P-OP1  | -5.11 | 101.10      | 105.70   |
| 1   | 1A    | 386  | G    | O4'-C1'-N9 | 5.11  | 112.29      | 108.20   |
| 1   | 1A    | 2501 | C    | C2-N1-C1'  | -5.10 | 113.19      | 118.80   |
| 32  | 2a    | 115  | G    | P-O3'-C3'  | 5.09  | 125.81      | 119.70   |
| 32  | 1a    | 1036 | G    | C4-N9-C1'  | 5.09  | 133.11      | 126.50   |
| 1   | 2A    | 894  | C    | N1-C2-O2   | 5.08  | 121.95      | 118.90   |
| 32  | 2a    | 1225 | A    | C6-N1-C2   | 5.08  | 121.65      | 118.60   |
| 1   | 2A    | 2108 | C    | C5-C4-N4   | 5.07  | 123.75      | 120.20   |
| 1   | 1A    | 1176 | G    | OP1-P-O3'  | 5.07  | 116.36      | 105.20   |
| 32  | 1a    | 299  | G    | N9-C4-C5   | -5.07 | 103.37      | 105.40   |
| 32  | 2a    | 1225 | A    | C5-C6-N6   | 5.06  | 127.75      | 123.70   |
| 1   | 1A    | 1102 | C    | C2-N1-C1'  | 5.04  | 124.34      | 118.80   |
| 32  | 2a    | 1126 | U    | C2-N1-C1'  | 5.03  | 123.73      | 117.70   |
| 1   | 1A    | 1799 | G    | N1-C6-O6   | -5.02 | 116.89      | 119.90   |
| 1   | 1A    | 645  | C    | C5-C6-N1   | 5.01  | 123.50      | 121.00   |
| 1   | 1A    | 2015 | A    | C8-N9-C4   | 5.00  | 107.80      | 105.80   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 33  | 1b    | 231 | GLU  | Peptide |
| 26  | 24    | 18  | CYS  | Peptide |

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | 1D    | 273/276 (99%) | 258 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 3   | 2D    | 273/276 (99%) | 255 (93%) | 18 (7%)  | 0        | 100         | 100 |
| 4   | 1E    | 202/206 (98%) | 193 (96%) | 7 (4%)   | 2 (1%)   | 15          | 28  |
| 4   | 2E    | 202/206 (98%) | 187 (93%) | 14 (7%)  | 1 (0%)   | 29          | 48  |
| 5   | 1F    | 201/210 (96%) | 193 (96%) | 7 (4%)   | 1 (0%)   | 29          | 48  |
| 5   | 2F    | 201/210 (96%) | 189 (94%) | 9 (4%)   | 3 (2%)   | 10          | 18  |
| 6   | 1G    | 179/182 (98%) | 157 (88%) | 17 (10%) | 5 (3%)   | 5           | 7   |
| 6   | 2G    | 179/182 (98%) | 149 (83%) | 24 (13%) | 6 (3%)   | 3           | 5   |
| 7   | 1H    | 172/180 (96%) | 160 (93%) | 10 (6%)  | 2 (1%)   | 13          | 24  |
| 7   | 2H    | 171/180 (95%) | 138 (81%) | 31 (18%) | 2 (1%)   | 13          | 24  |
| 8   | 1I    | 145/148 (98%) | 126 (87%) | 16 (11%) | 3 (2%)   | 7           | 11  |
| 8   | 2I    | 144/148 (97%) | 126 (88%) | 13 (9%)  | 5 (4%)   | 3           | 4   |
| 9   | 1N    | 138/140 (99%) | 136 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 9   | 2N    | 138/140 (99%) | 126 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 10  | 1O    | 120/122 (98%) | 112 (93%) | 7 (6%)   | 1 (1%)   | 19          | 35  |
| 10  | 2O    | 120/122 (98%) | 112 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 11  | 1P    | 147/150 (98%) | 136 (92%) | 10 (7%)  | 1 (1%)   | 22          | 39  |
| 11  | 2P    | 147/150 (98%) | 137 (93%) | 9 (6%)   | 1 (1%)   | 22          | 39  |
| 12  | 1Q    | 139/141 (99%) | 131 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 12  | 2Q    | 139/141 (99%) | 131 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 13  | 1R    | 116/118 (98%) | 112 (97%) | 3 (3%)   | 1 (1%)   | 17          | 31  |
| 13  | 2R    | 116/118 (98%) | 110 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 14  | 1S    | 108/112 (96%) | 100 (93%) | 6 (6%)   | 2 (2%)   | 8           | 13  |
| 14  | 2S    | 108/112 (96%) | 100 (93%) | 7 (6%)   | 1 (1%)   | 17          | 31  |
| 15  | 1T    | 129/146 (88%) | 119 (92%) | 10 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 15  | 2T    | 129/146 (88%) | 121 (94%) | 7 (5%)   | 1 (1%)   | 19          | 35  |
| 16  | 1U    | 114/118 (97%) | 112 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 16  | 2U    | 114/118 (97%) | 113 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 17  | 1V    | 99/101 (98%)  | 93 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 17  | 2V    | 99/101 (98%)  | 90 (91%)  | 8 (8%)   | 1 (1%)   | 15          | 28  |
| 18  | 1W    | 110/113 (97%) | 107 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 18  | 2W    | 110/113 (97%) | 107 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 19  | 1X    | 93/96 (97%)   | 89 (96%)  | 2 (2%)   | 2 (2%)   | 6           | 10  |
| 19  | 2X    | 93/96 (97%)   | 91 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 20  | 1Y    | 105/110 (96%) | 95 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 20  | 2Y    | 105/110 (96%) | 96 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 21  | 1Z    | 201/206 (98%) | 182 (90%) | 18 (9%)  | 1 (0%)   | 29          | 48  |
| 21  | 2Z    | 199/206 (97%) | 172 (86%) | 26 (13%) | 1 (0%)   | 29          | 48  |
| 22  | 10    | 81/85 (95%)   | 78 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 22  | 20    | 81/85 (95%)   | 73 (90%)  | 8 (10%)  | 0        | 100         | 100 |
| 23  | 11    | 95/98 (97%)   | 89 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 23  | 21    | 95/98 (97%)   | 89 (94%)  | 5 (5%)   | 1 (1%)   | 14          | 26  |
| 24  | 12    | 68/72 (94%)   | 68 (100%) | 0        | 0        | 100         | 100 |
| 24  | 22    | 68/72 (94%)   | 65 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 25  | 13    | 57/60 (95%)   | 56 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 25  | 23    | 57/60 (95%)   | 53 (93%)  | 4 (7%)   | 0        | 100         | 100 |
| 26  | 14    | 67/71 (94%)   | 47 (70%)  | 17 (25%) | 3 (4%)   | 2           | 3   |
| 26  | 24    | 67/71 (94%)   | 44 (66%)  | 14 (21%) | 9 (13%)  | 0           | 0   |
| 27  | 15    | 57/60 (95%)   | 55 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 27  | 25    | 57/60 (95%)   | 56 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 28  | 16    | 51/54 (94%)   | 49 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 28  | 26    | 51/54 (94%)   | 48 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 29  | 17    | 46/49 (94%)   | 45 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 29  | 27    | 46/49 (94%)   | 46 (100%) | 0        | 0        | 100         | 100 |
| 30  | 18    | 62/65 (95%)   | 62 (100%) | 0        | 0        | 100         | 100 |
| 30  | 28    | 62/65 (95%)   | 61 (98%)  | 1 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 31  | 19    | 35/37 (95%)   | 35 (100%) | 0        | 0        | 100         | 100 |
| 31  | 29    | 35/37 (95%)   | 33 (94%)  | 2 (6%)   | 0        | 100         | 100 |
| 33  | 1b    | 229/256 (90%) | 189 (82%) | 30 (13%) | 10 (4%)  | 2           | 3   |
| 33  | 2b    | 229/256 (90%) | 182 (80%) | 37 (16%) | 10 (4%)  | 2           | 3   |
| 34  | 1c    | 204/239 (85%) | 180 (88%) | 23 (11%) | 1 (0%)   | 29          | 48  |
| 34  | 2c    | 204/239 (85%) | 160 (78%) | 37 (18%) | 7 (3%)   | 3           | 5   |
| 35  | 1d    | 206/209 (99%) | 185 (90%) | 21 (10%) | 0        | 100         | 100 |
| 35  | 2d    | 206/209 (99%) | 184 (89%) | 20 (10%) | 2 (1%)   | 15          | 28  |
| 36  | 1e    | 146/162 (90%) | 136 (93%) | 8 (6%)   | 2 (1%)   | 11          | 20  |
| 36  | 2e    | 146/162 (90%) | 134 (92%) | 12 (8%)  | 0        | 100         | 100 |
| 37  | 1f    | 98/101 (97%)  | 94 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 37  | 2f    | 98/101 (97%)  | 90 (92%)  | 8 (8%)   | 0        | 100         | 100 |
| 38  | 1g    | 153/156 (98%) | 143 (94%) | 8 (5%)   | 2 (1%)   | 12          | 21  |
| 38  | 2g    | 153/156 (98%) | 139 (91%) | 12 (8%)  | 2 (1%)   | 12          | 21  |
| 39  | 1h    | 135/138 (98%) | 126 (93%) | 9 (7%)   | 0        | 100         | 100 |
| 39  | 2h    | 135/138 (98%) | 124 (92%) | 11 (8%)  | 0        | 100         | 100 |
| 40  | 1i    | 125/128 (98%) | 111 (89%) | 11 (9%)  | 3 (2%)   | 6           | 9   |
| 40  | 2i    | 124/128 (97%) | 108 (87%) | 12 (10%) | 4 (3%)   | 4           | 5   |
| 41  | 1j    | 95/105 (90%)  | 80 (84%)  | 11 (12%) | 4 (4%)   | 3           | 3   |
| 41  | 2j    | 94/105 (90%)  | 77 (82%)  | 15 (16%) | 2 (2%)   | 7           | 11  |
| 42  | 1k    | 112/129 (87%) | 102 (91%) | 10 (9%)  | 0        | 100         | 100 |
| 42  | 2k    | 112/129 (87%) | 101 (90%) | 10 (9%)  | 1 (1%)   | 17          | 31  |
| 43  | 1l    | 119/132 (90%) | 109 (92%) | 9 (8%)   | 1 (1%)   | 19          | 35  |
| 43  | 2l    | 119/132 (90%) | 108 (91%) | 10 (8%)  | 1 (1%)   | 19          | 35  |
| 44  | 1m    | 114/126 (90%) | 100 (88%) | 11 (10%) | 3 (3%)   | 5           | 8   |
| 44  | 2m    | 112/126 (89%) | 95 (85%)  | 12 (11%) | 5 (4%)   | 2           | 3   |
| 45  | 1n    | 58/61 (95%)   | 52 (90%)  | 6 (10%)  | 0        | 100         | 100 |
| 45  | 2n    | 58/61 (95%)   | 51 (88%)  | 6 (10%)  | 1 (2%)   | 9           | 16  |
| 46  | 1o    | 86/89 (97%)   | 79 (92%)  | 6 (7%)   | 1 (1%)   | 13          | 24  |
| 46  | 2o    | 86/89 (97%)   | 78 (91%)  | 7 (8%)   | 1 (1%)   | 13          | 24  |
| 47  | 1p    | 80/88 (91%)   | 74 (92%)  | 6 (8%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 47  | 2p    | 80/88 (91%)       | 69 (86%)    | 11 (14%) | 0        | 100         | 100 |
| 48  | 1q    | 97/105 (92%)      | 88 (91%)    | 9 (9%)   | 0        | 100         | 100 |
| 48  | 2q    | 97/105 (92%)      | 90 (93%)    | 6 (6%)   | 1 (1%)   | 15          | 28  |
| 49  | 1r    | 66/88 (75%)       | 60 (91%)    | 5 (8%)   | 1 (2%)   | 10          | 18  |
| 49  | 2r    | 66/88 (75%)       | 60 (91%)    | 6 (9%)   | 0        | 100         | 100 |
| 50  | 1s    | 81/93 (87%)       | 69 (85%)    | 12 (15%) | 0        | 100         | 100 |
| 50  | 2s    | 81/93 (87%)       | 68 (84%)    | 13 (16%) | 0        | 100         | 100 |
| 51  | 1t    | 94/106 (89%)      | 83 (88%)    | 9 (10%)  | 2 (2%)   | 7           | 11  |
| 51  | 2t    | 96/106 (91%)      | 82 (85%)    | 12 (12%) | 2 (2%)   | 7           | 11  |
| 52  | 1u    | 21/27 (78%)       | 20 (95%)    | 1 (5%)   | 0        | 100         | 100 |
| 52  | 2u    | 21/27 (78%)       | 16 (76%)    | 5 (24%)  | 0        | 100         | 100 |
| 53  | 1y    | 95/113 (84%)      | 93 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 53  | 2y    | 94/113 (83%)      | 87 (93%)    | 5 (5%)   | 2 (2%)   | 7           | 11  |
| 56  | 1v    | 1/3 (33%)         | 1 (100%)    | 0        | 0        | 100         | 100 |
| 56  | 2v    | 1/3 (33%)         | 1 (100%)    | 0        | 0        | 100         | 100 |
| All | All   | 11643/12360 (94%) | 10591 (91%) | 925 (8%) | 127 (1%) | 14          | 26  |

All (127) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 1G    | 47  | LYS  |
| 8   | 1I    | 86  | THR  |
| 14  | 1S    | 59  | LYS  |
| 19  | 1X    | 94  | GLY  |
| 26  | 14    | 61  | ARG  |
| 33  | 1b    | 17  | PHE  |
| 33  | 1b    | 127 | ILE  |
| 33  | 1b    | 231 | GLU  |
| 43  | 1l    | 91  | LYS  |
| 44  | 1m    | 67  | GLU  |
| 5   | 2F    | 130 | ALA  |
| 26  | 24    | 46  | GLN  |
| 26  | 24    | 51  | ASP  |
| 33  | 2b    | 17  | PHE  |
| 40  | 2i    | 43  | ALA  |
| 40  | 2i    | 54  | ASP  |
| 43  | 2l    | 91  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 1G    | 44  | GLY  |
| 7   | 1H    | 126 | PRO  |
| 7   | 1H    | 159 | GLU  |
| 33  | 1b    | 125 | PRO  |
| 34  | 1c    | 98  | ASN  |
| 41  | 1j    | 55  | LYS  |
| 51  | 1t    | 47  | GLY  |
| 6   | 2G    | 81  | LYS  |
| 8   | 2I    | 10  | GLU  |
| 8   | 2I    | 97  | ILE  |
| 8   | 2I    | 98  | ALA  |
| 26  | 24    | 45  | GLY  |
| 26  | 24    | 48  | ARG  |
| 26  | 24    | 62  | ARG  |
| 26  | 24    | 63  | TYR  |
| 33  | 2b    | 9   | GLU  |
| 34  | 2c    | 50  | ALA  |
| 34  | 2c    | 145 | GLY  |
| 35  | 2d    | 22  | LYS  |
| 38  | 2g    | 6   | ARG  |
| 42  | 2k    | 105 | VAL  |
| 53  | 2y    | 45  | PRO  |
| 4   | 1E    | 52  | LEU  |
| 6   | 1G    | 51  | ARG  |
| 8   | 1I    | 71  | ILE  |
| 14  | 1S    | 94  | TYR  |
| 26  | 14    | 39  | CYS  |
| 33  | 1b    | 8   | LYS  |
| 33  | 1b    | 21  | ARG  |
| 33  | 1b    | 63  | MET  |
| 36  | 1e    | 38  | GLN  |
| 38  | 1g    | 55  | GLY  |
| 41  | 1j    | 77  | PRO  |
| 6   | 2G    | 124 | SER  |
| 7   | 2H    | 126 | PRO  |
| 8   | 2I    | 83  | ALA  |
| 26  | 24    | 55  | ARG  |
| 33  | 2b    | 20  | GLU  |
| 33  | 2b    | 95  | GLN  |
| 34  | 2c    | 29  | TYR  |
| 41  | 2j    | 78  | ASN  |
| 41  | 2j    | 79  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | 2m    | 21  | TYR  |
| 44  | 2m    | 23  | TYR  |
| 6   | 1G    | 49  | ASP  |
| 8   | 1I    | 105 | HIS  |
| 21  | 1Z    | 52  | SER  |
| 26  | 14    | 48  | ARG  |
| 33  | 1b    | 20  | GLU  |
| 33  | 1b    | 124 | SER  |
| 38  | 1g    | 130 | GLY  |
| 40  | 1i    | 48  | GLU  |
| 41  | 1j    | 78  | ASN  |
| 51  | 1t    | 95  | ALA  |
| 5   | 2F    | 21  | ALA  |
| 6   | 2G    | 96  | ARG  |
| 8   | 2I    | 117 | GLU  |
| 14  | 2S    | 96  | GLY  |
| 15  | 2T    | 128 | GLU  |
| 17  | 2V    | 79  | VAL  |
| 23  | 2I    | 3   | LYS  |
| 33  | 2b    | 121 | LEU  |
| 33  | 2b    | 124 | SER  |
| 33  | 2b    | 128 | GLU  |
| 34  | 2c    | 104 | GLN  |
| 35  | 2d    | 176 | LEU  |
| 40  | 2i    | 33  | PHE  |
| 40  | 2i    | 44  | VAL  |
| 44  | 2m    | 6   | GLY  |
| 46  | 2o    | 79  | ARG  |
| 53  | 2y    | 46  | GLN  |
| 4   | 1E    | 28  | ALA  |
| 36  | 1e    | 146 | ALA  |
| 40  | 1i    | 109 | VAL  |
| 4   | 2E    | 52  | LEU  |
| 5   | 2F    | 146 | ALA  |
| 6   | 2G    | 43  | LEU  |
| 6   | 2G    | 126 | ASP  |
| 11  | 2P    | 122 | PRO  |
| 21  | 2Z    | 52  | SER  |
| 26  | 24    | 49  | PHE  |
| 34  | 2c    | 98  | ASN  |
| 45  | 2n    | 38  | GLY  |
| 51  | 2t    | 45  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 1G    | 50  | ALA  |
| 10  | 1O    | 29  | ASN  |
| 11  | 1P    | 29  | LYS  |
| 13  | 1R    | 71  | GLN  |
| 33  | 1b    | 22  | LYS  |
| 40  | 1i    | 53  | VAL  |
| 41  | 1j    | 91  | PRO  |
| 44  | 1m    | 21  | TYR  |
| 44  | 1m    | 106 | ASN  |
| 34  | 2c    | 174 | PRO  |
| 48  | 2q    | 27  | PHE  |
| 19  | 1X    | 67  | GLY  |
| 46  | 1o    | 23  | GLY  |
| 7   | 2H    | 93  | GLY  |
| 33  | 2b    | 125 | PRO  |
| 38  | 2g    | 55  | GLY  |
| 51  | 2t    | 100 | ILE  |
| 49  | 1r    | 27  | GLY  |
| 5   | 1F    | 16  | GLY  |
| 6   | 2G    | 87  | PRO  |
| 26  | 24    | 50  | VAL  |
| 44  | 2m    | 24  | GLY  |
| 44  | 2m    | 113 | PRO  |
| 33  | 2b    | 15  | VAL  |
| 33  | 2b    | 232 | PRO  |
| 34  | 2c    | 99  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3   | 1D    | 214/218 (98%) | 200 (94%) | 14 (6%)  | 17          | 33 |
| 3   | 2D    | 215/218 (99%) | 192 (89%) | 23 (11%) | 6           | 13 |
| 4   | 1E    | 164/166 (99%) | 155 (94%) | 9 (6%)   | 21          | 41 |
| 4   | 2E    | 164/166 (99%) | 151 (92%) | 13 (8%)  | 12          | 24 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 5   | 1F    | 160/166 (96%)  | 149 (93%) | 11 (7%)  | 15          | 30 |
| 5   | 2F    | 159/166 (96%)  | 146 (92%) | 13 (8%)  | 11          | 22 |
| 6   | 1G    | 144/156 (92%)  | 126 (88%) | 18 (12%) | 4           | 8  |
| 6   | 2G    | 142/156 (91%)  | 127 (89%) | 15 (11%) | 6           | 13 |
| 7   | 1H    | 144/148 (97%)  | 136 (94%) | 8 (6%)   | 21          | 40 |
| 7   | 2H    | 143/148 (97%)  | 130 (91%) | 13 (9%)  | 9           | 18 |
| 8   | 1I    | 111/124 (90%)  | 91 (82%)  | 20 (18%) | 1           | 3  |
| 8   | 2I    | 108/124 (87%)  | 93 (86%)  | 15 (14%) | 3           | 6  |
| 9   | 1N    | 119/119 (100%) | 106 (89%) | 13 (11%) | 6           | 12 |
| 9   | 2N    | 118/119 (99%)  | 106 (90%) | 12 (10%) | 7           | 14 |
| 10  | 1O    | 100/100 (100%) | 95 (95%)  | 5 (5%)   | 24          | 46 |
| 10  | 2O    | 100/100 (100%) | 95 (95%)  | 5 (5%)   | 24          | 46 |
| 11  | 1P    | 115/116 (99%)  | 113 (98%) | 2 (2%)   | 60          | 82 |
| 11  | 2P    | 115/116 (99%)  | 108 (94%) | 7 (6%)   | 18          | 36 |
| 12  | 1Q    | 111/111 (100%) | 107 (96%) | 4 (4%)   | 35          | 61 |
| 12  | 2Q    | 111/111 (100%) | 104 (94%) | 7 (6%)   | 18          | 34 |
| 13  | 1R    | 101/101 (100%) | 95 (94%)  | 6 (6%)   | 19          | 37 |
| 13  | 2R    | 101/101 (100%) | 92 (91%)  | 9 (9%)   | 9           | 19 |
| 14  | 1S    | 87/88 (99%)    | 80 (92%)  | 7 (8%)   | 12          | 23 |
| 14  | 2S    | 85/88 (97%)    | 73 (86%)  | 12 (14%) | 3           | 6  |
| 15  | 1T    | 115/127 (91%)  | 107 (93%) | 8 (7%)   | 15          | 29 |
| 15  | 2T    | 113/127 (89%)  | 108 (96%) | 5 (4%)   | 28          | 52 |
| 16  | 1U    | 93/94 (99%)    | 89 (96%)  | 4 (4%)   | 29          | 53 |
| 16  | 2U    | 93/94 (99%)    | 85 (91%)  | 8 (9%)   | 10          | 20 |
| 17  | 1V    | 81/82 (99%)    | 79 (98%)  | 2 (2%)   | 47          | 73 |
| 17  | 2V    | 80/82 (98%)    | 68 (85%)  | 12 (15%) | 3           | 5  |
| 18  | 1W    | 90/92 (98%)    | 84 (93%)  | 6 (7%)   | 16          | 31 |
| 18  | 2W    | 90/92 (98%)    | 84 (93%)  | 6 (7%)   | 16          | 31 |
| 19  | 1X    | 77/78 (99%)    | 72 (94%)  | 5 (6%)   | 17          | 33 |
| 19  | 2X    | 77/78 (99%)    | 75 (97%)  | 2 (3%)   | 46          | 72 |
| 20  | 1Y    | 86/91 (94%)    | 80 (93%)  | 6 (7%)   | 15          | 29 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 20  | 2Y    | 86/91 (94%)   | 79 (92%)  | 7 (8%)   | 11          | 23 |
| 21  | 1Z    | 169/179 (94%) | 153 (90%) | 16 (10%) | 8           | 17 |
| 21  | 2Z    | 165/179 (92%) | 148 (90%) | 17 (10%) | 7           | 14 |
| 22  | 10    | 65/67 (97%)   | 61 (94%)  | 4 (6%)   | 18          | 35 |
| 22  | 20    | 64/67 (96%)   | 63 (98%)  | 1 (2%)   | 62          | 84 |
| 23  | 11    | 79/83 (95%)   | 75 (95%)  | 4 (5%)   | 24          | 45 |
| 23  | 21    | 81/83 (98%)   | 76 (94%)  | 5 (6%)   | 18          | 35 |
| 24  | 12    | 65/67 (97%)   | 60 (92%)  | 5 (8%)   | 13          | 25 |
| 24  | 22    | 66/67 (98%)   | 58 (88%)  | 8 (12%)  | 5           | 9  |
| 25  | 13    | 51/52 (98%)   | 46 (90%)  | 5 (10%)  | 8           | 15 |
| 25  | 23    | 50/52 (96%)   | 48 (96%)  | 2 (4%)   | 31          | 56 |
| 26  | 14    | 58/63 (92%)   | 51 (88%)  | 7 (12%)  | 5           | 9  |
| 26  | 24    | 54/63 (86%)   | 43 (80%)  | 11 (20%) | 1           | 2  |
| 27  | 15    | 51/52 (98%)   | 48 (94%)  | 3 (6%)   | 19          | 37 |
| 27  | 25    | 50/52 (96%)   | 47 (94%)  | 3 (6%)   | 19          | 37 |
| 28  | 16    | 51/52 (98%)   | 43 (84%)  | 8 (16%)  | 2           | 4  |
| 28  | 26    | 50/52 (96%)   | 44 (88%)  | 6 (12%)  | 5           | 9  |
| 29  | 17    | 41/42 (98%)   | 37 (90%)  | 4 (10%)  | 8           | 15 |
| 29  | 27    | 41/42 (98%)   | 34 (83%)  | 7 (17%)  | 2           | 3  |
| 30  | 18    | 54/55 (98%)   | 48 (89%)  | 6 (11%)  | 6           | 11 |
| 30  | 28    | 54/55 (98%)   | 46 (85%)  | 8 (15%)  | 3           | 5  |
| 31  | 19    | 34/34 (100%)  | 33 (97%)  | 1 (3%)   | 42          | 69 |
| 31  | 29    | 34/34 (100%)  | 32 (94%)  | 2 (6%)   | 19          | 37 |
| 33  | 1b    | 191/220 (87%) | 166 (87%) | 25 (13%) | 4           | 7  |
| 33  | 2b    | 187/220 (85%) | 162 (87%) | 25 (13%) | 4           | 7  |
| 34  | 1c    | 144/188 (77%) | 136 (94%) | 8 (6%)   | 21          | 40 |
| 34  | 2c    | 140/188 (74%) | 118 (84%) | 22 (16%) | 2           | 4  |
| 35  | 1d    | 171/181 (94%) | 150 (88%) | 21 (12%) | 4           | 9  |
| 35  | 2d    | 172/181 (95%) | 156 (91%) | 16 (9%)  | 9           | 17 |
| 36  | 1e    | 114/123 (93%) | 105 (92%) | 9 (8%)   | 12          | 24 |
| 36  | 2e    | 114/123 (93%) | 104 (91%) | 10 (9%)  | 10          | 19 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 37  | 1f    | 85/90 (94%)   | 75 (88%)  | 10 (12%) | 5           | 10 |
| 37  | 2f    | 85/90 (94%)   | 80 (94%)  | 5 (6%)   | 19          | 37 |
| 38  | 1g    | 120/127 (94%) | 110 (92%) | 10 (8%)  | 11          | 22 |
| 38  | 2g    | 119/127 (94%) | 105 (88%) | 14 (12%) | 5           | 10 |
| 39  | 1h    | 116/119 (98%) | 106 (91%) | 10 (9%)  | 10          | 20 |
| 39  | 2h    | 114/119 (96%) | 104 (91%) | 10 (9%)  | 10          | 19 |
| 40  | 1i    | 91/99 (92%)   | 77 (85%)  | 14 (15%) | 2           | 5  |
| 40  | 2i    | 88/99 (89%)   | 80 (91%)  | 8 (9%)   | 9           | 18 |
| 41  | 1j    | 68/92 (74%)   | 60 (88%)  | 8 (12%)  | 5           | 10 |
| 41  | 2j    | 68/92 (74%)   | 60 (88%)  | 8 (12%)  | 5           | 10 |
| 42  | 1k    | 83/99 (84%)   | 77 (93%)  | 6 (7%)   | 14          | 28 |
| 42  | 2k    | 83/99 (84%)   | 73 (88%)  | 10 (12%) | 5           | 9  |
| 43  | 1l    | 96/108 (89%)  | 89 (93%)  | 7 (7%)   | 14          | 27 |
| 43  | 2l    | 96/108 (89%)  | 90 (94%)  | 6 (6%)   | 18          | 34 |
| 44  | 1m    | 90/101 (89%)  | 83 (92%)  | 7 (8%)   | 12          | 24 |
| 44  | 2m    | 87/101 (86%)  | 73 (84%)  | 14 (16%) | 2           | 4  |
| 45  | 1n    | 49/50 (98%)   | 41 (84%)  | 8 (16%)  | 2           | 4  |
| 45  | 2n    | 49/50 (98%)   | 44 (90%)  | 5 (10%)  | 7           | 14 |
| 46  | 1o    | 78/80 (98%)   | 73 (94%)  | 5 (6%)   | 17          | 33 |
| 46  | 2o    | 78/80 (98%)   | 71 (91%)  | 7 (9%)   | 9           | 19 |
| 47  | 1p    | 69/74 (93%)   | 57 (83%)  | 12 (17%) | 2           | 3  |
| 47  | 2p    | 68/74 (92%)   | 60 (88%)  | 8 (12%)  | 5           | 10 |
| 48  | 1q    | 94/97 (97%)   | 86 (92%)  | 8 (8%)   | 10          | 21 |
| 48  | 2q    | 94/97 (97%)   | 91 (97%)  | 3 (3%)   | 39          | 65 |
| 49  | 1r    | 59/77 (77%)   | 51 (86%)  | 8 (14%)  | 3           | 7  |
| 49  | 2r    | 59/77 (77%)   | 53 (90%)  | 6 (10%)  | 7           | 14 |
| 50  | 1s    | 68/80 (85%)   | 63 (93%)  | 5 (7%)   | 13          | 27 |
| 50  | 2s    | 67/80 (84%)   | 62 (92%)  | 5 (8%)   | 13          | 26 |
| 51  | 1t    | 71/82 (87%)   | 64 (90%)  | 7 (10%)  | 8           | 15 |
| 51  | 2t    | 70/82 (85%)   | 66 (94%)  | 4 (6%)   | 20          | 39 |
| 52  | 1u    | 18/22 (82%)   | 17 (94%)  | 1 (6%)   | 21          | 40 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 52  | 2u    | 18/22 (82%)      | 18 (100%)  | 0        | 100         | 100 |
| 53  | 1y    | 82/98 (84%)      | 77 (94%)   | 5 (6%)   | 18          | 36  |
| 53  | 2y    | 79/98 (81%)      | 69 (87%)   | 10 (13%) | 4           | 8   |
| 56  | 1v    | 3/3 (100%)       | 2 (67%)    | 1 (33%)  | 0           | 0   |
| 56  | 2v    | 3/3 (100%)       | 2 (67%)    | 1 (33%)  | 0           | 0   |
| All | All   | 9537/10266 (93%) | 8680 (91%) | 857 (9%) | 9           | 19  |

All (857) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 39  | LYS  |
| 3   | 1D    | 94  | LEU  |
| 3   | 1D    | 111 | LEU  |
| 3   | 1D    | 112 | GLN  |
| 3   | 1D    | 141 | VAL  |
| 3   | 1D    | 171 | ASP  |
| 3   | 1D    | 193 | VAL  |
| 3   | 1D    | 211 | ARG  |
| 3   | 1D    | 217 | ARG  |
| 3   | 1D    | 221 | VAL  |
| 3   | 1D    | 229 | VAL  |
| 3   | 1D    | 242 | ARG  |
| 3   | 1D    | 259 | THR  |
| 3   | 1D    | 275 | LYS  |
| 4   | 1E    | 7   | VAL  |
| 4   | 1E    | 9   | VAL  |
| 4   | 1E    | 87  | GLU  |
| 4   | 1E    | 113 | PHE  |
| 4   | 1E    | 116 | VAL  |
| 4   | 1E    | 119 | ARG  |
| 4   | 1E    | 181 | LEU  |
| 4   | 1E    | 184 | VAL  |
| 4   | 1E    | 202 | LYS  |
| 5   | 1F    | 18  | ARG  |
| 5   | 1F    | 23  | ASP  |
| 5   | 1F    | 53  | THR  |
| 5   | 1F    | 57  | VAL  |
| 5   | 1F    | 74  | ARG  |
| 5   | 1F    | 88  | VAL  |
| 5   | 1F    | 132 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 1F    | 162 | LEU  |
| 5   | 1F    | 183 | VAL  |
| 5   | 1F    | 189 | THR  |
| 5   | 1F    | 192 | LEU  |
| 6   | 1G    | 5   | VAL  |
| 6   | 1G    | 7   | LEU  |
| 6   | 1G    | 21  | ARG  |
| 6   | 1G    | 49  | ASP  |
| 6   | 1G    | 53  | LEU  |
| 6   | 1G    | 62  | LEU  |
| 6   | 1G    | 67  | LYS  |
| 6   | 1G    | 75  | LYS  |
| 6   | 1G    | 79  | ASN  |
| 6   | 1G    | 82  | LEU  |
| 6   | 1G    | 86  | MET  |
| 6   | 1G    | 92  | VAL  |
| 6   | 1G    | 109 | VAL  |
| 6   | 1G    | 126 | ASP  |
| 6   | 1G    | 133 | LEU  |
| 6   | 1G    | 144 | ILE  |
| 6   | 1G    | 155 | MET  |
| 6   | 1G    | 175 | LEU  |
| 7   | 1H    | 23  | ARG  |
| 7   | 1H    | 24  | VAL  |
| 7   | 1H    | 44  | VAL  |
| 7   | 1H    | 58  | GLU  |
| 7   | 1H    | 101 | ARG  |
| 7   | 1H    | 107 | VAL  |
| 7   | 1H    | 111 | HIS  |
| 7   | 1H    | 124 | GLU  |
| 8   | 1I    | 9   | LEU  |
| 8   | 1I    | 14  | ASP  |
| 8   | 1I    | 20  | ASP  |
| 8   | 1I    | 38  | LEU  |
| 8   | 1I    | 42  | SER  |
| 8   | 1I    | 43  | ASN  |
| 8   | 1I    | 44  | LEU  |
| 8   | 1I    | 60  | GLU  |
| 8   | 1I    | 61  | ARG  |
| 8   | 1I    | 66  | GLU  |
| 8   | 1I    | 68  | LEU  |
| 8   | 1I    | 78  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 1I    | 87  | LYS  |
| 8   | 1I    | 92  | VAL  |
| 8   | 1I    | 96  | ASP  |
| 8   | 1I    | 102 | SER  |
| 8   | 1I    | 108 | THR  |
| 8   | 1I    | 109 | ILE  |
| 8   | 1I    | 117 | GLU  |
| 8   | 1I    | 140 | LEU  |
| 9   | 1N    | 1   | MET  |
| 9   | 1N    | 5   | VAL  |
| 9   | 1N    | 8   | GLN  |
| 9   | 1N    | 14  | VAL  |
| 9   | 1N    | 34  | LEU  |
| 9   | 1N    | 48  | MET  |
| 9   | 1N    | 62  | VAL  |
| 9   | 1N    | 67  | LEU  |
| 9   | 1N    | 73  | THR  |
| 9   | 1N    | 87  | LEU  |
| 9   | 1N    | 89  | LYS  |
| 9   | 1N    | 99  | LEU  |
| 9   | 1N    | 133 | GLN  |
| 10  | 1O    | 9   | GLU  |
| 10  | 1O    | 28  | SER  |
| 10  | 1O    | 69  | ILE  |
| 10  | 1O    | 96  | THR  |
| 10  | 1O    | 113 | LYS  |
| 11  | 1P    | 1   | MET  |
| 11  | 1P    | 95  | VAL  |
| 12  | 1Q    | 60  | ARG  |
| 12  | 1Q    | 75  | THR  |
| 12  | 1Q    | 109 | VAL  |
| 12  | 1Q    | 112 | GLU  |
| 13  | 1R    | 14  | SER  |
| 13  | 1R    | 29  | LEU  |
| 13  | 1R    | 36  | THR  |
| 13  | 1R    | 56  | LYS  |
| 13  | 1R    | 67  | LEU  |
| 13  | 1R    | 114 | VAL  |
| 14  | 1S    | 14  | VAL  |
| 14  | 1S    | 46  | VAL  |
| 14  | 1S    | 49  | VAL  |
| 14  | 1S    | 50  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | 1S    | 52  | SER  |
| 14  | 1S    | 59  | LYS  |
| 14  | 1S    | 69  | VAL  |
| 15  | 1T    | 6   | LEU  |
| 15  | 1T    | 33  | LYS  |
| 15  | 1T    | 53  | ARG  |
| 15  | 1T    | 78  | LEU  |
| 15  | 1T    | 82  | LEU  |
| 15  | 1T    | 85  | LYS  |
| 15  | 1T    | 108 | ARG  |
| 15  | 1T    | 112 | ARG  |
| 16  | 1U    | 5   | LYS  |
| 16  | 1U    | 31  | SER  |
| 16  | 1U    | 74  | LEU  |
| 16  | 1U    | 104 | GLN  |
| 17  | 1V    | 72  | VAL  |
| 17  | 1V    | 79  | VAL  |
| 18  | 1W    | 11  | ARG  |
| 18  | 1W    | 15  | ARG  |
| 18  | 1W    | 17  | VAL  |
| 18  | 1W    | 19  | LEU  |
| 18  | 1W    | 100 | THR  |
| 18  | 1W    | 107 | LEU  |
| 19  | 1X    | 35  | THR  |
| 19  | 1X    | 38  | GLU  |
| 19  | 1X    | 45  | THR  |
| 19  | 1X    | 88  | LYS  |
| 19  | 1X    | 95  | LEU  |
| 20  | 1Y    | 23  | ARG  |
| 20  | 1Y    | 31  | LEU  |
| 20  | 1Y    | 43  | ASN  |
| 20  | 1Y    | 72  | VAL  |
| 20  | 1Y    | 99  | CYS  |
| 20  | 1Y    | 107 | ASP  |
| 21  | 1Z    | 18  | LEU  |
| 21  | 1Z    | 19  | ARG  |
| 21  | 1Z    | 31  | ARG  |
| 21  | 1Z    | 50  | GLN  |
| 21  | 1Z    | 80  | ARG  |
| 21  | 1Z    | 86  | VAL  |
| 21  | 1Z    | 91  | LEU  |
| 21  | 1Z    | 98  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | 1Z    | 118 | GLN  |
| 21  | 1Z    | 132 | ASN  |
| 21  | 1Z    | 150 | LEU  |
| 21  | 1Z    | 154 | ASP  |
| 21  | 1Z    | 155 | LEU  |
| 21  | 1Z    | 161 | VAL  |
| 21  | 1Z    | 170 | THR  |
| 21  | 1Z    | 198 | LYS  |
| 22  | 10    | 10  | THR  |
| 22  | 10    | 14  | ARG  |
| 22  | 10    | 74  | ARG  |
| 22  | 10    | 82  | ARG  |
| 23  | 11    | 30  | VAL  |
| 23  | 11    | 35  | THR  |
| 23  | 11    | 40  | ARG  |
| 23  | 11    | 94  | LEU  |
| 24  | 12    | 27  | GLU  |
| 24  | 12    | 30  | ARG  |
| 24  | 12    | 32  | LEU  |
| 24  | 12    | 38  | GLN  |
| 24  | 12    | 41  | ILE  |
| 25  | 13    | 8   | LEU  |
| 25  | 13    | 32  | GLN  |
| 25  | 13    | 54  | VAL  |
| 25  | 13    | 56  | VAL  |
| 25  | 13    | 58  | VAL  |
| 26  | 14    | 27  | THR  |
| 26  | 14    | 33  | VAL  |
| 26  | 14    | 49  | PHE  |
| 26  | 14    | 56  | VAL  |
| 26  | 14    | 58  | ARG  |
| 26  | 14    | 60  | GLN  |
| 26  | 14    | 68  | ARG  |
| 27  | 15    | 6   | VAL  |
| 27  | 15    | 16  | ARG  |
| 27  | 15    | 37  | LYS  |
| 28  | 16    | 5   | VAL  |
| 28  | 16    | 6   | ARG  |
| 28  | 16    | 19  | ARG  |
| 28  | 16    | 44  | ARG  |
| 28  | 16    | 47  | THR  |
| 28  | 16    | 48  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | 16    | 49  | HIS  |
| 28  | 16    | 52  | VAL  |
| 29  | 17    | 42  | LEU  |
| 29  | 17    | 43  | THR  |
| 29  | 17    | 46  | VAL  |
| 29  | 17    | 47  | ARG  |
| 30  | 18    | 14  | VAL  |
| 30  | 18    | 23  | VAL  |
| 30  | 18    | 29  | LYS  |
| 30  | 18    | 31  | HIS  |
| 30  | 18    | 34  | TRP  |
| 30  | 18    | 58  | ILE  |
| 31  | 19    | 13  | LYS  |
| 33  | 1b    | 8   | LYS  |
| 33  | 1b    | 10  | LEU  |
| 33  | 1b    | 15  | VAL  |
| 33  | 1b    | 17  | PHE  |
| 33  | 1b    | 23  | ARG  |
| 33  | 1b    | 28  | PHE  |
| 33  | 1b    | 42  | ILE  |
| 33  | 1b    | 51  | LEU  |
| 33  | 1b    | 90  | MET  |
| 33  | 1b    | 93  | VAL  |
| 33  | 1b    | 96  | ARG  |
| 33  | 1b    | 106 | LYS  |
| 33  | 1b    | 115 | LEU  |
| 33  | 1b    | 140 | HIS  |
| 33  | 1b    | 145 | LEU  |
| 33  | 1b    | 160 | ASP  |
| 33  | 1b    | 162 | ILE  |
| 33  | 1b    | 179 | LYS  |
| 33  | 1b    | 185 | ILE  |
| 33  | 1b    | 187 | LEU  |
| 33  | 1b    | 195 | ASP  |
| 33  | 1b    | 223 | ILE  |
| 33  | 1b    | 224 | GLN  |
| 33  | 1b    | 229 | VAL  |
| 33  | 1b    | 230 | VAL  |
| 34  | 1c    | 70  | VAL  |
| 34  | 1c    | 89  | GLU  |
| 34  | 1c    | 98  | ASN  |
| 34  | 1c    | 105 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | 1c    | 124 | ILE  |
| 34  | 1c    | 144 | SER  |
| 34  | 1c    | 157 | ILE  |
| 34  | 1c    | 175 | LEU  |
| 35  | 1d    | 3   | ARG  |
| 35  | 1d    | 5   | ILE  |
| 35  | 1d    | 17  | VAL  |
| 35  | 1d    | 18  | LYS  |
| 35  | 1d    | 19  | LEU  |
| 35  | 1d    | 26  | CYS  |
| 35  | 1d    | 52  | SER  |
| 35  | 1d    | 58  | LEU  |
| 35  | 1d    | 67  | ILE  |
| 35  | 1d    | 77  | ASN  |
| 35  | 1d    | 107 | ARG  |
| 35  | 1d    | 134 | ASP  |
| 35  | 1d    | 137 | SER  |
| 35  | 1d    | 144 | ASP  |
| 35  | 1d    | 157 | LEU  |
| 35  | 1d    | 178 | VAL  |
| 35  | 1d    | 182 | LYS  |
| 35  | 1d    | 187 | ARG  |
| 35  | 1d    | 188 | LEU  |
| 35  | 1d    | 194 | LEU  |
| 35  | 1d    | 196 | LEU  |
| 36  | 1e    | 12  | LEU  |
| 36  | 1e    | 34  | VAL  |
| 36  | 1e    | 41  | VAL  |
| 36  | 1e    | 68  | GLU  |
| 36  | 1e    | 69  | VAL  |
| 36  | 1e    | 79  | GLU  |
| 36  | 1e    | 115 | VAL  |
| 36  | 1e    | 131 | ILE  |
| 36  | 1e    | 147 | ASP  |
| 37  | 1f    | 10  | LEU  |
| 37  | 1f    | 15  | ASP  |
| 37  | 1f    | 21  | LEU  |
| 37  | 1f    | 40  | VAL  |
| 37  | 1f    | 42  | GLU  |
| 37  | 1f    | 45  | LEU  |
| 37  | 1f    | 57  | GLN  |
| 37  | 1f    | 69  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | 1f    | 73  | ASN  |
| 37  | 1f    | 89  | MET  |
| 38  | 1g    | 6   | ARG  |
| 38  | 1g    | 13  | GLN  |
| 38  | 1g    | 52  | GLU  |
| 38  | 1g    | 56  | GLN  |
| 38  | 1g    | 76  | ARG  |
| 38  | 1g    | 86  | GLN  |
| 38  | 1g    | 97  | GLN  |
| 38  | 1g    | 113 | GLU  |
| 38  | 1g    | 126 | ASP  |
| 38  | 1g    | 144 | MET  |
| 39  | 1h    | 22  | GLU  |
| 39  | 1h    | 25  | ASP  |
| 39  | 1h    | 26  | VAL  |
| 39  | 1h    | 39  | LEU  |
| 39  | 1h    | 51  | VAL  |
| 39  | 1h    | 52  | ASP  |
| 39  | 1h    | 98  | LYS  |
| 39  | 1h    | 104 | ARG  |
| 39  | 1h    | 127 | LEU  |
| 39  | 1h    | 133 | LEU  |
| 40  | 1i    | 17  | VAL  |
| 40  | 1i    | 25  | LYS  |
| 40  | 1i    | 29  | ASN  |
| 40  | 1i    | 47  | LEU  |
| 40  | 1i    | 50  | LEU  |
| 40  | 1i    | 53  | VAL  |
| 40  | 1i    | 56  | LEU  |
| 40  | 1i    | 81  | ILE  |
| 40  | 1i    | 87  | GLN  |
| 40  | 1i    | 92  | TYR  |
| 40  | 1i    | 96  | LEU  |
| 40  | 1i    | 104 | ARG  |
| 40  | 1i    | 111 | ARG  |
| 40  | 1i    | 125 | TYR  |
| 41  | 1j    | 5   | ARG  |
| 41  | 1j    | 29  | ARG  |
| 41  | 1j    | 34  | VAL  |
| 41  | 1j    | 38  | ILE  |
| 41  | 1j    | 67  | THR  |
| 41  | 1j    | 72  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | 1j    | 84  | GLN  |
| 41  | 1j    | 94  | VAL  |
| 42  | 1k    | 16  | SER  |
| 42  | 1k    | 31  | THR  |
| 42  | 1k    | 41  | THR  |
| 42  | 1k    | 77  | MET  |
| 42  | 1k    | 93  | GLN  |
| 42  | 1k    | 122 | LYS  |
| 43  | 1l    | 18  | VAL  |
| 43  | 1l    | 22  | SER  |
| 43  | 1l    | 33  | ARG  |
| 43  | 1l    | 42  | THR  |
| 43  | 1l    | 44  | THR  |
| 43  | 1l    | 83  | VAL  |
| 43  | 1l    | 97  | ARG  |
| 44  | 1m    | 3   | ARG  |
| 44  | 1m    | 4   | ILE  |
| 44  | 1m    | 9   | ILE  |
| 44  | 1m    | 11  | ARG  |
| 44  | 1m    | 14  | ARG  |
| 44  | 1m    | 86  | CYS  |
| 44  | 1m    | 99  | ARG  |
| 45  | 1n    | 3   | ARG  |
| 45  | 1n    | 11  | LYS  |
| 45  | 1n    | 13  | THR  |
| 45  | 1n    | 16  | PHE  |
| 45  | 1n    | 18  | VAL  |
| 45  | 1n    | 22  | THR  |
| 45  | 1n    | 29  | ARG  |
| 45  | 1n    | 33  | VAL  |
| 46  | 1o    | 3   | ILE  |
| 46  | 1o    | 25  | THR  |
| 46  | 1o    | 39  | LEU  |
| 46  | 1o    | 76  | GLU  |
| 46  | 1o    | 84  | LYS  |
| 47  | 1p    | 6   | LEU  |
| 47  | 1p    | 8   | ARG  |
| 47  | 1p    | 20  | VAL  |
| 47  | 1p    | 29  | ASP  |
| 47  | 1p    | 35  | LYS  |
| 47  | 1p    | 42  | ARG  |
| 47  | 1p    | 43  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 1p    | 47  | ASP  |
| 47  | 1p    | 53  | VAL  |
| 47  | 1p    | 62  | VAL  |
| 47  | 1p    | 67  | THR  |
| 47  | 1p    | 72  | ARG  |
| 48  | 1q    | 6   | LEU  |
| 48  | 1q    | 9   | VAL  |
| 48  | 1q    | 35  | VAL  |
| 48  | 1q    | 45  | HIS  |
| 48  | 1q    | 52  | LYS  |
| 48  | 1q    | 61  | GLU  |
| 48  | 1q    | 85  | VAL  |
| 48  | 1q    | 93  | GLN  |
| 49  | 1r    | 23  | LYS  |
| 49  | 1r    | 25  | THR  |
| 49  | 1r    | 26  | LEU  |
| 49  | 1r    | 31  | LEU  |
| 49  | 1r    | 37  | VAL  |
| 49  | 1r    | 42  | ARG  |
| 49  | 1r    | 46  | GLU  |
| 49  | 1r    | 76  | LEU  |
| 50  | 1s    | 28  | LYS  |
| 50  | 1s    | 40  | ILE  |
| 50  | 1s    | 48  | THR  |
| 50  | 1s    | 63  | THR  |
| 50  | 1s    | 66  | MET  |
| 51  | 1t    | 9   | ASN  |
| 51  | 1t    | 10  | LEU  |
| 51  | 1t    | 15  | ARG  |
| 51  | 1t    | 24  | LEU  |
| 51  | 1t    | 34  | LYS  |
| 51  | 1t    | 37  | SER  |
| 51  | 1t    | 100 | ILE  |
| 52  | 1u    | 3   | LYS  |
| 53  | 1y    | 23  | ARG  |
| 53  | 1y    | 42  | SER  |
| 53  | 1y    | 46  | GLN  |
| 53  | 1y    | 60  | VAL  |
| 53  | 1y    | 61  | LEU  |
| 56  | 1v    | 2   | THR  |
| 3   | 2D    | 3   | VAL  |
| 3   | 2D    | 18  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2D    | 27  | THR  |
| 3   | 2D    | 38  | LYS  |
| 3   | 2D    | 61  | LEU  |
| 3   | 2D    | 71  | ASP  |
| 3   | 2D    | 75  | ILE  |
| 3   | 2D    | 94  | LEU  |
| 3   | 2D    | 103 | ARG  |
| 3   | 2D    | 113 | VAL  |
| 3   | 2D    | 134 | ARG  |
| 3   | 2D    | 141 | VAL  |
| 3   | 2D    | 155 | LEU  |
| 3   | 2D    | 173 | VAL  |
| 3   | 2D    | 183 | ARG  |
| 3   | 2D    | 211 | ARG  |
| 3   | 2D    | 221 | VAL  |
| 3   | 2D    | 229 | VAL  |
| 3   | 2D    | 242 | ARG  |
| 3   | 2D    | 259 | THR  |
| 3   | 2D    | 260 | ARG  |
| 3   | 2D    | 274 | ARG  |
| 3   | 2D    | 276 | LYS  |
| 4   | 2E    | 38  | THR  |
| 4   | 2E    | 73  | GLU  |
| 4   | 2E    | 90  | THR  |
| 4   | 2E    | 97  | LYS  |
| 4   | 2E    | 113 | PHE  |
| 4   | 2E    | 116 | VAL  |
| 4   | 2E    | 119 | ARG  |
| 4   | 2E    | 152 | LYS  |
| 4   | 2E    | 154 | LYS  |
| 4   | 2E    | 181 | LEU  |
| 4   | 2E    | 184 | VAL  |
| 4   | 2E    | 188 | VAL  |
| 4   | 2E    | 195 | LEU  |
| 5   | 2F    | 15  | SER  |
| 5   | 2F    | 17  | ARG  |
| 5   | 2F    | 27  | GLU  |
| 5   | 2F    | 33  | LEU  |
| 5   | 2F    | 57  | VAL  |
| 5   | 2F    | 74  | ARG  |
| 5   | 2F    | 140 | LEU  |
| 5   | 2F    | 158 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 2F    | 170 | LEU  |
| 5   | 2F    | 175 | THR  |
| 5   | 2F    | 179 | GLU  |
| 5   | 2F    | 192 | LEU  |
| 5   | 2F    | 197 | ASP  |
| 6   | 2G    | 3   | LEU  |
| 6   | 2G    | 9   | ARG  |
| 6   | 2G    | 28  | VAL  |
| 6   | 2G    | 43  | LEU  |
| 6   | 2G    | 51  | ARG  |
| 6   | 2G    | 53  | LEU  |
| 6   | 2G    | 58  | GLN  |
| 6   | 2G    | 62  | LEU  |
| 6   | 2G    | 78  | SER  |
| 6   | 2G    | 86  | MET  |
| 6   | 2G    | 98  | ARG  |
| 6   | 2G    | 115 | ARG  |
| 6   | 2G    | 126 | ASP  |
| 6   | 2G    | 133 | LEU  |
| 6   | 2G    | 143 | GLU  |
| 7   | 2H    | 13  | LYS  |
| 7   | 2H    | 32  | GLU  |
| 7   | 2H    | 33  | LEU  |
| 7   | 2H    | 38  | SER  |
| 7   | 2H    | 43  | VAL  |
| 7   | 2H    | 44  | VAL  |
| 7   | 2H    | 52  | VAL  |
| 7   | 2H    | 71  | LEU  |
| 7   | 2H    | 105 | LEU  |
| 7   | 2H    | 106 | THR  |
| 7   | 2H    | 114 | VAL  |
| 7   | 2H    | 130 | ARG  |
| 7   | 2H    | 152 | ARG  |
| 8   | 2I    | 7   | GLU  |
| 8   | 2I    | 38  | LEU  |
| 8   | 2I    | 47  | LEU  |
| 8   | 2I    | 54  | GLN  |
| 8   | 2I    | 58  | LEU  |
| 8   | 2I    | 64  | GLU  |
| 8   | 2I    | 70  | GLU  |
| 8   | 2I    | 74  | ASN  |
| 8   | 2I    | 76  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 2I    | 82  | ARG  |
| 8   | 2I    | 92  | VAL  |
| 8   | 2I    | 107 | VAL  |
| 8   | 2I    | 125 | GLU  |
| 8   | 2I    | 129 | THR  |
| 8   | 2I    | 142 | VAL  |
| 9   | 2N    | 9   | VAL  |
| 9   | 2N    | 12  | ARG  |
| 9   | 2N    | 15  | LEU  |
| 9   | 2N    | 28  | THR  |
| 9   | 2N    | 33  | LEU  |
| 9   | 2N    | 48  | MET  |
| 9   | 2N    | 67  | LEU  |
| 9   | 2N    | 73  | THR  |
| 9   | 2N    | 74  | ARG  |
| 9   | 2N    | 87  | LEU  |
| 9   | 2N    | 99  | LEU  |
| 9   | 2N    | 140 | VAL  |
| 10  | 2O    | 35  | VAL  |
| 10  | 2O    | 69  | ILE  |
| 10  | 2O    | 70  | LYS  |
| 10  | 2O    | 78  | ARG  |
| 10  | 2O    | 88  | ASN  |
| 11  | 2P    | 15  | ARG  |
| 11  | 2P    | 29  | LYS  |
| 11  | 2P    | 95  | VAL  |
| 11  | 2P    | 125 | VAL  |
| 11  | 2P    | 147 | LEU  |
| 11  | 2P    | 148 | LEU  |
| 11  | 2P    | 149 | GLU  |
| 12  | 2Q    | 1   | MET  |
| 12  | 2Q    | 7   | MET  |
| 12  | 2Q    | 75  | THR  |
| 12  | 2Q    | 85  | LYS  |
| 12  | 2Q    | 109 | VAL  |
| 12  | 2Q    | 124 | LYS  |
| 12  | 2Q    | 133 | ARG  |
| 13  | 2R    | 20  | LEU  |
| 13  | 2R    | 29  | LEU  |
| 13  | 2R    | 33  | ARG  |
| 13  | 2R    | 36  | THR  |
| 13  | 2R    | 67  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | 2R    | 86  | ARG  |
| 13  | 2R    | 100 | LEU  |
| 13  | 2R    | 102 | GLU  |
| 13  | 2R    | 114 | VAL  |
| 14  | 2S    | 8   | GLU  |
| 14  | 2S    | 12  | PHE  |
| 14  | 2S    | 13  | ARG  |
| 14  | 2S    | 25  | ARG  |
| 14  | 2S    | 50  | SER  |
| 14  | 2S    | 52  | SER  |
| 14  | 2S    | 53  | SER  |
| 14  | 2S    | 64  | GLU  |
| 14  | 2S    | 80  | LEU  |
| 14  | 2S    | 85  | VAL  |
| 14  | 2S    | 110 | LEU  |
| 14  | 2S    | 111 | GLU  |
| 15  | 2T    | 36  | GLU  |
| 15  | 2T    | 42  | ILE  |
| 15  | 2T    | 53  | ARG  |
| 15  | 2T    | 54  | ARG  |
| 15  | 2T    | 67  | SER  |
| 16  | 2U    | 5   | LYS  |
| 16  | 2U    | 30  | LYS  |
| 16  | 2U    | 31  | SER  |
| 16  | 2U    | 55  | ARG  |
| 16  | 2U    | 59  | ARG  |
| 16  | 2U    | 74  | LEU  |
| 16  | 2U    | 100 | VAL  |
| 16  | 2U    | 104 | GLN  |
| 17  | 2V    | 1   | MET  |
| 17  | 2V    | 5   | VAL  |
| 17  | 2V    | 26  | ASP  |
| 17  | 2V    | 32  | THR  |
| 17  | 2V    | 35  | LEU  |
| 17  | 2V    | 39  | LEU  |
| 17  | 2V    | 46  | VAL  |
| 17  | 2V    | 53  | GLU  |
| 17  | 2V    | 62  | LEU  |
| 17  | 2V    | 71  | LEU  |
| 17  | 2V    | 79  | VAL  |
| 17  | 2V    | 96  | ILE  |
| 18  | 2W    | 11  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | 2W    | 17  | VAL  |
| 18  | 2W    | 23  | LEU  |
| 18  | 2W    | 68  | ARG  |
| 18  | 2W    | 100 | THR  |
| 18  | 2W    | 107 | LEU  |
| 19  | 2X    | 81  | VAL  |
| 19  | 2X    | 95  | LEU  |
| 20  | 2Y    | 3   | VAL  |
| 20  | 2Y    | 6   | HIS  |
| 20  | 2Y    | 44  | ILE  |
| 20  | 2Y    | 55  | TYR  |
| 20  | 2Y    | 90  | LEU  |
| 20  | 2Y    | 99  | CYS  |
| 20  | 2Y    | 101 | LYS  |
| 21  | 2Z    | 2   | GLU  |
| 21  | 2Z    | 31  | ARG  |
| 21  | 2Z    | 41  | LEU  |
| 21  | 2Z    | 53  | ILE  |
| 21  | 2Z    | 67  | LEU  |
| 21  | 2Z    | 72  | ARG  |
| 21  | 2Z    | 73  | GLN  |
| 21  | 2Z    | 86  | VAL  |
| 21  | 2Z    | 107 | THR  |
| 21  | 2Z    | 121 | HIS  |
| 21  | 2Z    | 123 | ASP  |
| 21  | 2Z    | 135 | GLU  |
| 21  | 2Z    | 175 | VAL  |
| 21  | 2Z    | 182 | LYS  |
| 21  | 2Z    | 190 | GLU  |
| 21  | 2Z    | 193 | GLU  |
| 21  | 2Z    | 198 | LYS  |
| 22  | 20    | 36  | ILE  |
| 23  | 21    | 4   | VAL  |
| 23  | 21    | 21  | ARG  |
| 23  | 21    | 40  | ARG  |
| 23  | 21    | 85  | LEU  |
| 23  | 21    | 95  | LEU  |
| 24  | 22    | 1   | MET  |
| 24  | 22    | 17  | SER  |
| 24  | 22    | 31  | GLU  |
| 24  | 22    | 32  | LEU  |
| 24  | 22    | 45  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | 22    | 53  | LEU  |
| 24  | 22    | 62  | THR  |
| 24  | 22    | 64  | LEU  |
| 25  | 23    | 54  | VAL  |
| 25  | 23    | 57  | GLU  |
| 26  | 24    | 8   | LYS  |
| 26  | 24    | 9   | LEU  |
| 26  | 24    | 20  | ASN  |
| 26  | 24    | 21  | VAL  |
| 26  | 24    | 27  | THR  |
| 26  | 24    | 40  | HIS  |
| 26  | 24    | 42  | PHE  |
| 26  | 24    | 50  | VAL  |
| 26  | 24    | 52  | THR  |
| 26  | 24    | 53  | GLU  |
| 26  | 24    | 61  | ARG  |
| 27  | 25    | 29  | THR  |
| 27  | 25    | 40  | LYS  |
| 27  | 25    | 55  | ARG  |
| 28  | 26    | 14  | THR  |
| 28  | 26    | 20  | ASN  |
| 28  | 26    | 30  | THR  |
| 28  | 26    | 34  | LEU  |
| 28  | 26    | 50  | ARG  |
| 28  | 26    | 54  | ILE  |
| 29  | 27    | 10  | ARG  |
| 29  | 27    | 23  | ARG  |
| 29  | 27    | 41  | ARG  |
| 29  | 27    | 43  | THR  |
| 29  | 27    | 46  | VAL  |
| 29  | 27    | 47  | ARG  |
| 29  | 27    | 48  | LYS  |
| 30  | 28    | 14  | VAL  |
| 30  | 28    | 23  | VAL  |
| 30  | 28    | 26  | LYS  |
| 30  | 28    | 31  | HIS  |
| 30  | 28    | 34  | TRP  |
| 30  | 28    | 46  | ARG  |
| 30  | 28    | 49  | VAL  |
| 30  | 28    | 50  | LEU  |
| 31  | 29    | 4   | ARG  |
| 31  | 29    | 17  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | 2b    | 7   | VAL  |
| 33  | 2b    | 8   | LYS  |
| 33  | 2b    | 15  | VAL  |
| 33  | 2b    | 16  | HIS  |
| 33  | 2b    | 17  | PHE  |
| 33  | 2b    | 24  | TRP  |
| 33  | 2b    | 39  | ILE  |
| 33  | 2b    | 44  | LEU  |
| 33  | 2b    | 63  | MET  |
| 33  | 2b    | 74  | LYS  |
| 33  | 2b    | 76  | GLN  |
| 33  | 2b    | 83  | MET  |
| 33  | 2b    | 96  | ARG  |
| 33  | 2b    | 97  | TRP  |
| 33  | 2b    | 128 | GLU  |
| 33  | 2b    | 130 | ARG  |
| 33  | 2b    | 154 | LEU  |
| 33  | 2b    | 157 | ARG  |
| 33  | 2b    | 175 | ARG  |
| 33  | 2b    | 189 | ASP  |
| 33  | 2b    | 191 | ASP  |
| 33  | 2b    | 193 | ASP  |
| 33  | 2b    | 196 | LEU  |
| 33  | 2b    | 215 | LEU  |
| 33  | 2b    | 230 | VAL  |
| 34  | 2c    | 3   | ASN  |
| 34  | 2c    | 15  | THR  |
| 34  | 2c    | 16  | ARG  |
| 34  | 2c    | 30  | ARG  |
| 34  | 2c    | 32  | LEU  |
| 34  | 2c    | 33  | LEU  |
| 34  | 2c    | 52  | LEU  |
| 34  | 2c    | 56  | ASP  |
| 34  | 2c    | 98  | ASN  |
| 34  | 2c    | 105 | GLU  |
| 34  | 2c    | 111 | LEU  |
| 34  | 2c    | 112 | SER  |
| 34  | 2c    | 128 | PHE  |
| 34  | 2c    | 131 | ARG  |
| 34  | 2c    | 136 | GLN  |
| 34  | 2c    | 152 | ILE  |
| 34  | 2c    | 154 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | 2c    | 164 | ARG  |
| 34  | 2c    | 179 | ARG  |
| 34  | 2c    | 181 | ASN  |
| 34  | 2c    | 195 | VAL  |
| 34  | 2c    | 206 | GLU  |
| 35  | 2d    | 13  | ARG  |
| 35  | 2d    | 19  | LEU  |
| 35  | 2d    | 33  | MET  |
| 35  | 2d    | 49  | ARG  |
| 35  | 2d    | 50  | ARG  |
| 35  | 2d    | 83  | SER  |
| 35  | 2d    | 106 | TYR  |
| 35  | 2d    | 108 | LEU  |
| 35  | 2d    | 127 | THR  |
| 35  | 2d    | 135 | LEU  |
| 35  | 2d    | 141 | ARG  |
| 35  | 2d    | 160 | GLN  |
| 35  | 2d    | 170 | VAL  |
| 35  | 2d    | 175 | SER  |
| 35  | 2d    | 187 | ARG  |
| 35  | 2d    | 194 | LEU  |
| 36  | 2e    | 10  | MET  |
| 36  | 2e    | 11  | ILE  |
| 36  | 2e    | 34  | VAL  |
| 36  | 2e    | 41  | VAL  |
| 36  | 2e    | 45  | PHE  |
| 36  | 2e    | 47  | LYS  |
| 36  | 2e    | 68  | GLU  |
| 36  | 2e    | 69  | VAL  |
| 36  | 2e    | 81  | GLU  |
| 36  | 2e    | 115 | VAL  |
| 37  | 2f    | 40  | VAL  |
| 37  | 2f    | 41  | GLU  |
| 37  | 2f    | 57  | GLN  |
| 37  | 2f    | 93  | SER  |
| 37  | 2f    | 95  | GLU  |
| 38  | 2g    | 6   | ARG  |
| 38  | 2g    | 9   | VAL  |
| 38  | 2g    | 15  | ASP  |
| 38  | 2g    | 16  | LEU  |
| 38  | 2g    | 21  | VAL  |
| 38  | 2g    | 33  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 38  | 2g    | 47  | CYS  |
| 38  | 2g    | 51  | GLN  |
| 38  | 2g    | 75  | VAL  |
| 38  | 2g    | 92  | SER  |
| 38  | 2g    | 104 | LEU  |
| 38  | 2g    | 115 | ARG  |
| 38  | 2g    | 126 | ASP  |
| 38  | 2g    | 153 | HIS  |
| 39  | 2h    | 2   | LEU  |
| 39  | 2h    | 15  | ASN  |
| 39  | 2h    | 29  | SER  |
| 39  | 2h    | 49  | GLU  |
| 39  | 2h    | 85  | ARG  |
| 39  | 2h    | 112 | LEU  |
| 39  | 2h    | 114 | THR  |
| 39  | 2h    | 119 | LEU  |
| 39  | 2h    | 125 | ARG  |
| 39  | 2h    | 133 | LEU  |
| 40  | 2i    | 14  | VAL  |
| 40  | 2i    | 33  | PHE  |
| 40  | 2i    | 34  | ASN  |
| 40  | 2i    | 42  | ARG  |
| 40  | 2i    | 65  | VAL  |
| 40  | 2i    | 87  | GLN  |
| 40  | 2i    | 102 | LEU  |
| 40  | 2i    | 113 | LYS  |
| 41  | 2j    | 34  | VAL  |
| 41  | 2j    | 38  | ILE  |
| 41  | 2j    | 47  | PHE  |
| 41  | 2j    | 58  | ASP  |
| 41  | 2j    | 71  | LEU  |
| 41  | 2j    | 73  | ASP  |
| 41  | 2j    | 84  | GLN  |
| 41  | 2j    | 95  | GLU  |
| 42  | 2k    | 16  | SER  |
| 42  | 2k    | 28  | THR  |
| 42  | 2k    | 53  | SER  |
| 42  | 2k    | 63  | LEU  |
| 42  | 2k    | 81  | ASP  |
| 42  | 2k    | 93  | GLN  |
| 42  | 2k    | 109 | VAL  |
| 42  | 2k    | 114 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | 2k    | 116 | HIS  |
| 42  | 2k    | 117 | ASN  |
| 43  | 2l    | 6   | THR  |
| 43  | 2l    | 28  | LYS  |
| 43  | 2l    | 33  | ARG  |
| 43  | 2l    | 67  | THR  |
| 43  | 2l    | 79  | GLU  |
| 43  | 2l    | 89  | ARG  |
| 44  | 2m    | 8   | GLU  |
| 44  | 2m    | 13  | LYS  |
| 44  | 2m    | 15  | VAL  |
| 44  | 2m    | 48  | LEU  |
| 44  | 2m    | 49  | THR  |
| 44  | 2m    | 50  | GLU  |
| 44  | 2m    | 59  | TYR  |
| 44  | 2m    | 60  | VAL  |
| 44  | 2m    | 62  | ASN  |
| 44  | 2m    | 93  | ARG  |
| 44  | 2m    | 96  | LEU  |
| 44  | 2m    | 102 | ARG  |
| 44  | 2m    | 106 | ASN  |
| 44  | 2m    | 115 | LYS  |
| 45  | 2n    | 3   | ARG  |
| 45  | 2n    | 7   | ILE  |
| 45  | 2n    | 16  | PHE  |
| 45  | 2n    | 18  | VAL  |
| 45  | 2n    | 39  | LEU  |
| 46  | 2o    | 3   | ILE  |
| 46  | 2o    | 4   | THR  |
| 46  | 2o    | 5   | LYS  |
| 46  | 2o    | 24  | SER  |
| 46  | 2o    | 39  | LEU  |
| 46  | 2o    | 84  | LYS  |
| 46  | 2o    | 87  | ILE  |
| 47  | 2p    | 11  | SER  |
| 47  | 2p    | 16  | HIS  |
| 47  | 2p    | 20  | VAL  |
| 47  | 2p    | 21  | VAL  |
| 47  | 2p    | 45  | THR  |
| 47  | 2p    | 67  | THR  |
| 47  | 2p    | 69  | THR  |
| 47  | 2p    | 75  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | 2q    | 6   | LEU  |
| 48  | 2q    | 52  | LYS  |
| 48  | 2q    | 57  | VAL  |
| 49  | 2r    | 29  | PHE  |
| 49  | 2r    | 31  | LEU  |
| 49  | 2r    | 37  | VAL  |
| 49  | 2r    | 47  | THR  |
| 49  | 2r    | 82  | THR  |
| 49  | 2r    | 84  | LYS  |
| 50  | 2s    | 32  | LYS  |
| 50  | 2s    | 37  | ARG  |
| 50  | 2s    | 41  | VAL  |
| 50  | 2s    | 63  | THR  |
| 50  | 2s    | 81  | ARG  |
| 51  | 2t    | 15  | ARG  |
| 51  | 2t    | 55  | ILE  |
| 51  | 2t    | 84  | LEU  |
| 51  | 2t    | 100 | ILE  |
| 53  | 2y    | 6   | THR  |
| 53  | 2y    | 16  | ILE  |
| 53  | 2y    | 24  | LEU  |
| 53  | 2y    | 29  | LYS  |
| 53  | 2y    | 32  | THR  |
| 53  | 2y    | 41  | LEU  |
| 53  | 2y    | 46  | GLN  |
| 53  | 2y    | 56  | THR  |
| 53  | 2y    | 62  | VAL  |
| 53  | 2y    | 78  | ILE  |
| 56  | 2v    | 2   | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 1D    | 87  | ASN  |
| 3   | 1D    | 253 | GLN  |
| 4   | 1E    | 48  | GLN  |
| 5   | 1F    | 69  | HIS  |
| 7   | 1H    | 139 | GLN  |
| 8   | 1I    | 43  | ASN  |
| 9   | 1N    | 8   | GLN  |
| 9   | 1N    | 69  | GLN  |
| 9   | 1N    | 94  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | 1N    | 133 | GLN  |
| 10  | 1O    | 3   | GLN  |
| 10  | 1O    | 88  | ASN  |
| 11  | 1P    | 84  | ASN  |
| 14  | 1S    | 84  | GLN  |
| 15  | 1T    | 58  | ASN  |
| 15  | 1T    | 123 | GLN  |
| 16  | 1U    | 117 | GLN  |
| 19  | 1X    | 31  | HIS  |
| 20  | 1Y    | 6   | HIS  |
| 20  | 1Y    | 43  | ASN  |
| 21  | 1Z    | 50  | GLN  |
| 23  | 11    | 56  | GLN  |
| 25  | 13    | 32  | GLN  |
| 26  | 14    | 20  | ASN  |
| 33  | 1b    | 212 | GLN  |
| 34  | 1c    | 6   | HIS  |
| 34  | 1c    | 102 | ASN  |
| 34  | 1c    | 104 | GLN  |
| 34  | 1c    | 110 | ASN  |
| 35  | 1d    | 77  | ASN  |
| 35  | 1d    | 129 | ASN  |
| 36  | 1e    | 78  | HIS  |
| 37  | 1f    | 57  | GLN  |
| 37  | 1f    | 84  | ASN  |
| 38  | 1g    | 13  | GLN  |
| 38  | 1g    | 28  | ASN  |
| 38  | 1g    | 37  | ASN  |
| 38  | 1g    | 64  | GLN  |
| 38  | 1g    | 86  | GLN  |
| 38  | 1g    | 96  | GLN  |
| 40  | 1i    | 3   | GLN  |
| 40  | 1i    | 31  | GLN  |
| 40  | 1i    | 73  | GLN  |
| 40  | 1i    | 87  | GLN  |
| 40  | 1i    | 124 | GLN  |
| 41  | 1j    | 13  | HIS  |
| 41  | 1j    | 56  | HIS  |
| 41  | 1j    | 84  | GLN  |
| 42  | 1k    | 93  | GLN  |
| 42  | 1k    | 117 | ASN  |
| 43  | 1l    | 99  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | 1m    | 106 | ASN  |
| 46  | 1o    | 13  | GLN  |
| 47  | 1p    | 16  | HIS  |
| 48  | 1q    | 16  | GLN  |
| 50  | 1s    | 69  | HIS  |
| 50  | 1s    | 83  | HIS  |
| 51  | 1t    | 42  | GLN  |
| 51  | 1t    | 90  | GLN  |
| 53  | 1y    | 38  | HIS  |
| 53  | 1y    | 89  | GLN  |
| 3   | 2D    | 87  | ASN  |
| 3   | 2D    | 143 | HIS  |
| 3   | 2D    | 253 | GLN  |
| 4   | 2E    | 48  | GLN  |
| 6   | 2G    | 58  | GLN  |
| 6   | 2G    | 79  | ASN  |
| 6   | 2G    | 130 | ASN  |
| 7   | 2H    | 143 | GLN  |
| 8   | 2I    | 43  | ASN  |
| 8   | 2I    | 105 | HIS  |
| 8   | 2I    | 133 | HIS  |
| 12  | 2Q    | 123 | HIS  |
| 15  | 2T    | 38  | ASN  |
| 15  | 2T    | 58  | ASN  |
| 15  | 2T    | 123 | GLN  |
| 16  | 2U    | 104 | GLN  |
| 17  | 2V    | 64  | HIS  |
| 19  | 2X    | 31  | HIS  |
| 19  | 2X    | 82  | GLN  |
| 20  | 2Y    | 6   | HIS  |
| 21  | 2Z    | 73  | GLN  |
| 24  | 22    | 9   | GLN  |
| 26  | 24    | 60  | GLN  |
| 28  | 26    | 20  | ASN  |
| 30  | 28    | 35  | GLN  |
| 33  | 2b    | 19  | HIS  |
| 33  | 2b    | 212 | GLN  |
| 33  | 2b    | 224 | GLN  |
| 34  | 2c    | 176 | HIS  |
| 34  | 2c    | 181 | ASN  |
| 35  | 2d    | 42  | GLN  |
| 35  | 2d    | 77  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | 2d    | 116 | GLN  |
| 35  | 2d    | 123 | HIS  |
| 35  | 2d    | 160 | GLN  |
| 35  | 2d    | 161 | ASN  |
| 35  | 2d    | 201 | GLN  |
| 36  | 2e    | 141 | GLN  |
| 37  | 2f    | 100 | ASN  |
| 38  | 2g    | 13  | GLN  |
| 38  | 2g    | 28  | ASN  |
| 38  | 2g    | 56  | GLN  |
| 38  | 2g    | 64  | GLN  |
| 39  | 2h    | 15  | ASN  |
| 40  | 2i    | 58  | HIS  |
| 41  | 2j    | 62  | HIS  |
| 41  | 2j    | 84  | GLN  |
| 42  | 2k    | 62  | GLN  |
| 42  | 2k    | 116 | HIS  |
| 42  | 2k    | 117 | ASN  |
| 43  | 2l    | 99  | HIS  |
| 44  | 2m    | 62  | ASN  |
| 44  | 2m    | 77  | ASN  |
| 44  | 2m    | 92  | HIS  |
| 44  | 2m    | 106 | ASN  |
| 46  | 2o    | 9   | GLN  |
| 46  | 2o    | 13  | GLN  |
| 46  | 2o    | 37  | ASN  |
| 50  | 2s    | 14  | HIS  |
| 50  | 2s    | 23  | ASN  |
| 51  | 2t    | 90  | GLN  |
| 53  | 2y    | 46  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | 1A    | 2864/2915 (98%) | 427 (14%)         | 28 (0%)         |
| 1   | 2A    | 2857/2915 (98%) | 497 (17%)         | 35 (1%)         |
| 2   | 1B    | 119/121 (98%)   | 9 (7%)            | 0               |
| 2   | 2B    | 119/121 (98%)   | 16 (13%)          | 0               |
| 32  | 1a    | 1494/1521 (98%) | 264 (17%)         | 0               |
| 32  | 2a    | 1498/1521 (98%) | 290 (19%)         | 0               |
| 54  | 1w    | 3/5 (60%)       | 0                 | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 54  | 2w    | 3/5 (60%)       | 1 (33%)           | 0               |
| 55  | 1x    | 1/4 (25%)       | 0                 | 0               |
| 55  | 2x    | 1/4 (25%)       | 0                 | 0               |
| All | All   | 8959/9132 (98%) | 1504 (16%)        | 63 (0%)         |

All (1504) RNA backbone outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 15     | G    |
| 1   | 1A    | 34     | C    |
| 1   | 1A    | 45     | C    |
| 1   | 1A    | 50     | U    |
| 1   | 1A    | 71     | A    |
| 1   | 1A    | 74     | A    |
| 1   | 1A    | 75     | G    |
| 1   | 1A    | 92     | A    |
| 1   | 1A    | 118    | A    |
| 1   | 1A    | 119    | A    |
| 1   | 1A    | 120    | U    |
| 1   | 1A    | 154(A) | C    |
| 1   | 1A    | 181    | A    |
| 1   | 1A    | 196    | A    |
| 1   | 1A    | 197    | A    |
| 1   | 1A    | 199    | A    |
| 1   | 1A    | 205    | G    |
| 1   | 1A    | 215    | G    |
| 1   | 1A    | 216    | A    |
| 1   | 1A    | 219    | G    |
| 1   | 1A    | 222    | A    |
| 1   | 1A    | 229    | A    |
| 1   | 1A    | 248    | G    |
| 1   | 1A    | 271(I) | G    |
| 1   | 1A    | 271(K) | U    |
| 1   | 1A    | 271(L) | U    |
| 1   | 1A    | 271(M) | G    |
| 1   | 1A    | 271(N) | U    |
| 1   | 1A    | 271(O) | C    |
| 1   | 1A    | 271(S) | G    |
| 1   | 1A    | 272(A) | U    |
| 1   | 1A    | 272(B) | G    |
| 1   | 1A    | 272(H) | C    |
| 1   | 1A    | 275    | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 279    | C    |
| 1   | 1A    | 280    | C    |
| 1   | 1A    | 283    | A    |
| 1   | 1A    | 311    | A    |
| 1   | 1A    | 330    | A    |
| 1   | 1A    | 346    | A    |
| 1   | 1A    | 352    | G    |
| 1   | 1A    | 363    | G    |
| 1   | 1A    | 363(B) | G    |
| 1   | 1A    | 386    | G    |
| 1   | 1A    | 396    | G    |
| 1   | 1A    | 405    | U    |
| 1   | 1A    | 411    | G    |
| 1   | 1A    | 412    | A    |
| 1   | 1A    | 428    | A    |
| 1   | 1A    | 447    | A    |
| 1   | 1A    | 451    | C    |
| 1   | 1A    | 454    | A    |
| 1   | 1A    | 456    | C    |
| 1   | 1A    | 457    | A    |
| 1   | 1A    | 481    | G    |
| 1   | 1A    | 505    | A    |
| 1   | 1A    | 508    | G    |
| 1   | 1A    | 509    | C    |
| 1   | 1A    | 530    | G    |
| 1   | 1A    | 531    | C    |
| 1   | 1A    | 532    | A    |
| 1   | 1A    | 533    | G    |
| 1   | 1A    | 545    | G    |
| 1   | 1A    | 549    | G    |
| 1   | 1A    | 563    | G    |
| 1   | 1A    | 573    | G    |
| 1   | 1A    | 575    | A    |
| 1   | 1A    | 592    | G    |
| 1   | 1A    | 603    | A    |
| 1   | 1A    | 604    | G    |
| 1   | 1A    | 607    | U    |
| 1   | 1A    | 615    | G    |
| 1   | 1A    | 616    | G    |
| 1   | 1A    | 621    | A    |
| 1   | 1A    | 627    | A    |
| 1   | 1A    | 637    | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 645    | C    |
| 1   | 1A    | 646    | A    |
| 1   | 1A    | 652(E) | G    |
| 1   | 1A    | 652(U) | G    |
| 1   | 1A    | 668    | G    |
| 1   | 1A    | 669    | G    |
| 1   | 1A    | 686    | G    |
| 1   | 1A    | 730    | C    |
| 1   | 1A    | 731    | C    |
| 1   | 1A    | 775    | G    |
| 1   | 1A    | 776    | G    |
| 1   | 1A    | 782    | A    |
| 1   | 1A    | 784    | A    |
| 1   | 1A    | 785    | G    |
| 1   | 1A    | 790    | C    |
| 1   | 1A    | 792    | G    |
| 1   | 1A    | 805    | G    |
| 1   | 1A    | 812    | C    |
| 1   | 1A    | 827    | U    |
| 1   | 1A    | 828    | U    |
| 1   | 1A    | 859    | G    |
| 1   | 1A    | 866    | A    |
| 1   | 1A    | 884    | C    |
| 1   | 1A    | 886    | C    |
| 1   | 1A    | 887    | A    |
| 1   | 1A    | 888    | C    |
| 1   | 1A    | 889    | C    |
| 1   | 1A    | 890    | A    |
| 1   | 1A    | 896    | A    |
| 1   | 1A    | 897    | C    |
| 1   | 1A    | 899    | A    |
| 1   | 1A    | 900    | A    |
| 1   | 1A    | 907    | U    |
| 1   | 1A    | 910    | A    |
| 1   | 1A    | 915    | C    |
| 1   | 1A    | 932    | G    |
| 1   | 1A    | 945    | A    |
| 1   | 1A    | 946    | G    |
| 1   | 1A    | 961    | C    |
| 1   | 1A    | 974    | G    |
| 1   | 1A    | 975    | C    |
| 1   | 1A    | 983    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 996  | A    |
| 1   | 1A    | 1012 | U    |
| 1   | 1A    | 1013 | C    |
| 1   | 1A    | 1026 | U    |
| 1   | 1A    | 1033 | U    |
| 1   | 1A    | 1046 | A    |
| 1   | 1A    | 1047 | G    |
| 1   | 1A    | 1048 | A    |
| 1   | 1A    | 1054 | A    |
| 1   | 1A    | 1058 | G    |
| 1   | 1A    | 1061 | U    |
| 1   | 1A    | 1062 | G    |
| 1   | 1A    | 1063 | G    |
| 1   | 1A    | 1065 | U    |
| 1   | 1A    | 1066 | U    |
| 1   | 1A    | 1067 | A    |
| 1   | 1A    | 1070 | A    |
| 1   | 1A    | 1072 | C    |
| 1   | 1A    | 1073 | A    |
| 1   | 1A    | 1074 | G    |
| 1   | 1A    | 1075 | C    |
| 1   | 1A    | 1077 | A    |
| 1   | 1A    | 1079 | C    |
| 1   | 1A    | 1080 | C    |
| 1   | 1A    | 1088 | A    |
| 1   | 1A    | 1089 | G    |
| 1   | 1A    | 1090 | U    |
| 1   | 1A    | 1091 | G    |
| 1   | 1A    | 1096 | A    |
| 1   | 1A    | 1097 | U    |
| 1   | 1A    | 1098 | A    |
| 1   | 1A    | 1100 | C    |
| 1   | 1A    | 1101 | U    |
| 1   | 1A    | 1104 | C    |
| 1   | 1A    | 1109 | C    |
| 1   | 1A    | 1110 | G    |
| 1   | 1A    | 1112 | G    |
| 1   | 1A    | 1128 | A    |
| 1   | 1A    | 1130 | U    |
| 1   | 1A    | 1135 | C    |
| 1   | 1A    | 1136 | G    |
| 1   | 1A    | 1141 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1170 | G    |
| 1   | 1A    | 1171 | G    |
| 1   | 1A    | 1173 | G    |
| 1   | 1A    | 1174 | A    |
| 1   | 1A    | 1175 | U    |
| 1   | 1A    | 1176 | G    |
| 1   | 1A    | 1177 | A    |
| 1   | 1A    | 1178 | C    |
| 1   | 1A    | 1210 | A    |
| 1   | 1A    | 1211 | U    |
| 1   | 1A    | 1218 | C    |
| 1   | 1A    | 1220 | A    |
| 1   | 1A    | 1250 | G    |
| 1   | 1A    | 1253 | A    |
| 1   | 1A    | 1256 | G    |
| 1   | 1A    | 1271 | G    |
| 1   | 1A    | 1272 | A    |
| 1   | 1A    | 1273 | U    |
| 1   | 1A    | 1300 | U    |
| 1   | 1A    | 1301 | A    |
| 1   | 1A    | 1303 | G    |
| 1   | 1A    | 1345 | C    |
| 1   | 1A    | 1352 | U    |
| 1   | 1A    | 1359 | A    |
| 1   | 1A    | 1360 | A    |
| 1   | 1A    | 1365 | A    |
| 1   | 1A    | 1370 | C    |
| 1   | 1A    | 1380 | G    |
| 1   | 1A    | 1384 | A    |
| 1   | 1A    | 1385 | G    |
| 1   | 1A    | 1416 | G    |
| 1   | 1A    | 1417 | C    |
| 1   | 1A    | 1420 | U    |
| 1   | 1A    | 1421 | G    |
| 1   | 1A    | 1428 | C    |
| 1   | 1A    | 1437 | C    |
| 1   | 1A    | 1445 | A    |
| 1   | 1A    | 1450 | G    |
| 1   | 1A    | 1451 | C    |
| 1   | 1A    | 1455 | G    |
| 1   | 1A    | 1459 | G    |
| 1   | 1A    | 1460 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 1A    | 1467    | C    |
| 1   | 1A    | 1471    | A    |
| 1   | 1A    | 1473    | G    |
| 1   | 1A    | 1478    | G    |
| 1   | 1A    | 1482    | G    |
| 1   | 1A    | 1484    | G    |
| 1   | 1A    | 1490    | A    |
| 1   | 1A    | 1493    | C    |
| 1   | 1A    | 1505    | C    |
| 1   | 1A    | 1508    | A    |
| 1   | 1A    | 1509    | C    |
| 1   | 1A    | 1509(A) | A    |
| 1   | 1A    | 1523    | U    |
| 1   | 1A    | 1525    | G    |
| 1   | 1A    | 1529    | G    |
| 1   | 1A    | 1531    | C    |
| 1   | 1A    | 1542    | A    |
| 1   | 1A    | 1543    | C    |
| 1   | 1A    | 1558    | A    |
| 1   | 1A    | 1569    | A    |
| 1   | 1A    | 1578    | U    |
| 1   | 1A    | 1579    | A    |
| 1   | 1A    | 1580    | A    |
| 1   | 1A    | 1581    | G    |
| 1   | 1A    | 1584    | C    |
| 1   | 1A    | 1586    | A    |
| 1   | 1A    | 1608    | A    |
| 1   | 1A    | 1609    | A    |
| 1   | 1A    | 1610    | A    |
| 1   | 1A    | 1616    | A    |
| 1   | 1A    | 1634    | A    |
| 1   | 1A    | 1639    | U    |
| 1   | 1A    | 1648    | C    |
| 1   | 1A    | 1654    | A    |
| 1   | 1A    | 1664    | A    |
| 1   | 1A    | 1674    | G    |
| 1   | 1A    | 1696    | G    |
| 1   | 1A    | 1700    | A    |
| 1   | 1A    | 1701    | A    |
| 1   | 1A    | 1717    | G    |
| 1   | 1A    | 1722    | A    |
| 1   | 1A    | 1739    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 1740 | G    |
| 1   | 1A    | 1756 | G    |
| 1   | 1A    | 1757 | U    |
| 1   | 1A    | 1758 | G    |
| 1   | 1A    | 1762 | A    |
| 1   | 1A    | 1763 | G    |
| 1   | 1A    | 1764 | G    |
| 1   | 1A    | 1773 | A    |
| 1   | 1A    | 1780 | A    |
| 1   | 1A    | 1782 | C    |
| 1   | 1A    | 1791 | A    |
| 1   | 1A    | 1800 | C    |
| 1   | 1A    | 1801 | G    |
| 1   | 1A    | 1812 | A    |
| 1   | 1A    | 1816 | G    |
| 1   | 1A    | 1839 | G    |
| 1   | 1A    | 1847 | A    |
| 1   | 1A    | 1877 | A    |
| 1   | 1A    | 1878 | G    |
| 1   | 1A    | 1889 | A    |
| 1   | 1A    | 1900 | A    |
| 1   | 1A    | 1906 | G    |
| 1   | 1A    | 1913 | A    |
| 1   | 1A    | 1914 | C    |
| 1   | 1A    | 1919 | A    |
| 1   | 1A    | 1929 | G    |
| 1   | 1A    | 1930 | G    |
| 1   | 1A    | 1936 | A    |
| 1   | 1A    | 1938 | A    |
| 1   | 1A    | 1941 | C    |
| 1   | 1A    | 1955 | U    |
| 1   | 1A    | 1963 | U    |
| 1   | 1A    | 1965 | C    |
| 1   | 1A    | 1967 | C    |
| 1   | 1A    | 1970 | A    |
| 1   | 1A    | 1971 | A    |
| 1   | 1A    | 1972 | A    |
| 1   | 1A    | 1985 | G    |
| 1   | 1A    | 1993 | U    |
| 1   | 1A    | 1997 | G    |
| 1   | 1A    | 2023 | G    |
| 1   | 1A    | 2031 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2032 | G    |
| 1   | 1A    | 2033 | A    |
| 1   | 1A    | 2043 | C    |
| 1   | 1A    | 2055 | C    |
| 1   | 1A    | 2056 | G    |
| 1   | 1A    | 2060 | A    |
| 1   | 1A    | 2061 | G    |
| 1   | 1A    | 2069 | G    |
| 1   | 1A    | 2093 | G    |
| 1   | 1A    | 2103 | C    |
| 1   | 1A    | 2107 | C    |
| 1   | 1A    | 2108 | C    |
| 1   | 1A    | 2110 | G    |
| 1   | 1A    | 2111 | C    |
| 1   | 1A    | 2112 | G    |
| 1   | 1A    | 2116 | G    |
| 1   | 1A    | 2117 | A    |
| 1   | 1A    | 2119 | A    |
| 1   | 1A    | 2126 | A    |
| 1   | 1A    | 2127 | G    |
| 1   | 1A    | 2131 | G    |
| 1   | 1A    | 2132 | U    |
| 1   | 1A    | 2133 | G    |
| 1   | 1A    | 2134 | A    |
| 1   | 1A    | 2135 | A    |
| 1   | 1A    | 2137 | C    |
| 1   | 1A    | 2146 | C    |
| 1   | 1A    | 2148 | G    |
| 1   | 1A    | 2158 | A    |
| 1   | 1A    | 2159 | G    |
| 1   | 1A    | 2164 | C    |
| 1   | 1A    | 2171 | A    |
| 1   | 1A    | 2172 | U    |
| 1   | 1A    | 2181 | G    |
| 1   | 1A    | 2186 | G    |
| 1   | 1A    | 2187 | G    |
| 1   | 1A    | 2189 | U    |
| 1   | 1A    | 2190 | G    |
| 1   | 1A    | 2192 | G    |
| 1   | 1A    | 2198 | A    |
| 1   | 1A    | 2206 | G    |
| 1   | 1A    | 2207 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 1A    | 2208 | A    |
| 1   | 1A    | 2225 | A    |
| 1   | 1A    | 2238 | G    |
| 1   | 1A    | 2239 | G    |
| 1   | 1A    | 2267 | A    |
| 1   | 1A    | 2268 | A    |
| 1   | 1A    | 2269 | A    |
| 1   | 1A    | 2273 | A    |
| 1   | 1A    | 2278 | A    |
| 1   | 1A    | 2280 | G    |
| 1   | 1A    | 2283 | C    |
| 1   | 1A    | 2287 | A    |
| 1   | 1A    | 2289 | G    |
| 1   | 1A    | 2305 | A    |
| 1   | 1A    | 2307 | G    |
| 1   | 1A    | 2308 | G    |
| 1   | 1A    | 2318 | G    |
| 1   | 1A    | 2320 | A    |
| 1   | 1A    | 2321 | G    |
| 1   | 1A    | 2325 | G    |
| 1   | 1A    | 2334 | G    |
| 1   | 1A    | 2336 | A    |
| 1   | 1A    | 2347 | C    |
| 1   | 1A    | 2350 | C    |
| 1   | 1A    | 2361 | A    |
| 1   | 1A    | 2383 | G    |
| 1   | 1A    | 2385 | C    |
| 1   | 1A    | 2393 | A    |
| 1   | 1A    | 2406 | U    |
| 1   | 1A    | 2422 | A    |
| 1   | 1A    | 2423 | U    |
| 1   | 1A    | 2424 | C    |
| 1   | 1A    | 2425 | A    |
| 1   | 1A    | 2428 | G    |
| 1   | 1A    | 2429 | G    |
| 1   | 1A    | 2430 | A    |
| 1   | 1A    | 2431 | U    |
| 1   | 1A    | 2434 | A    |
| 1   | 1A    | 2435 | A    |
| 1   | 1A    | 2439 | A    |
| 1   | 1A    | 2441 | C    |
| 1   | 1A    | 2448 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 1A    | 2468    | G    |
| 1   | 1A    | 2476    | A    |
| 1   | 1A    | 2502    | G    |
| 1   | 1A    | 2504    | U    |
| 1   | 1A    | 2505    | G    |
| 1   | 1A    | 2518    | A    |
| 1   | 1A    | 2520    | C    |
| 1   | 1A    | 2529    | G    |
| 1   | 1A    | 2535    | G    |
| 1   | 1A    | 2554    | U    |
| 1   | 1A    | 2566    | A    |
| 1   | 1A    | 2567    | G    |
| 1   | 1A    | 2573    | C    |
| 1   | 1A    | 2574    | G    |
| 1   | 1A    | 2585    | U    |
| 1   | 1A    | 2602    | A    |
| 1   | 1A    | 2609    | U    |
| 1   | 1A    | 2611    | U    |
| 1   | 1A    | 2612    | C    |
| 1   | 1A    | 2629    | A    |
| 1   | 1A    | 2630    | G    |
| 1   | 1A    | 2641    | G    |
| 1   | 1A    | 2654    | A    |
| 1   | 1A    | 2662    | A    |
| 1   | 1A    | 2689    | U    |
| 1   | 1A    | 2690    | C    |
| 1   | 1A    | 2691    | C    |
| 1   | 1A    | 2702    | U    |
| 1   | 1A    | 2703    | C    |
| 1   | 1A    | 2712(A) | A    |
| 1   | 1A    | 2713    | A    |
| 1   | 1A    | 2714    | G    |
| 1   | 1A    | 2726    | U    |
| 1   | 1A    | 2733    | A    |
| 1   | 1A    | 2744    | G    |
| 1   | 1A    | 2758    | A    |
| 1   | 1A    | 2764    | A    |
| 1   | 1A    | 2765    | A    |
| 1   | 1A    | 2766    | G    |
| 1   | 1A    | 2769    | C    |
| 1   | 1A    | 2778    | A    |
| 1   | 1A    | 2790    | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 1A    | 2791   | C    |
| 1   | 1A    | 2794   | C    |
| 1   | 1A    | 2802   | G    |
| 1   | 1A    | 2805   | G    |
| 1   | 1A    | 2818   | G    |
| 1   | 1A    | 2820   | A    |
| 1   | 1A    | 2821   | A    |
| 1   | 1A    | 2833   | G    |
| 1   | 1A    | 2835   | A    |
| 1   | 1A    | 2869   | G    |
| 1   | 1A    | 2872   | G    |
| 1   | 1A    | 2892   | A    |
| 1   | 1A    | 2893   | G    |
| 1   | 1A    | 2894   | G    |
| 1   | 1A    | 2895   | U    |
| 2   | 1B    | 2      | C    |
| 2   | 1B    | 3      | C    |
| 2   | 1B    | 13     | A    |
| 2   | 1B    | 45     | A    |
| 2   | 1B    | 56     | G    |
| 2   | 1B    | 66     | A    |
| 2   | 1B    | 73     | A    |
| 2   | 1B    | 106    | G    |
| 2   | 1B    | 110    | G    |
| 32  | 1a    | 7      | G    |
| 32  | 1a    | 9      | G    |
| 32  | 1a    | 32     | A    |
| 32  | 1a    | 39     | G    |
| 32  | 1a    | 47     | C    |
| 32  | 1a    | 48     | C    |
| 32  | 1a    | 50     | A    |
| 32  | 1a    | 51     | A    |
| 32  | 1a    | 61     | G    |
| 32  | 1a    | 68     | G    |
| 32  | 1a    | 78     | G    |
| 32  | 1a    | 79     | G    |
| 32  | 1a    | 98     | G    |
| 32  | 1a    | 101    | A    |
| 32  | 1a    | 116    | A    |
| 32  | 1a    | 120    | A    |
| 32  | 1a    | 121    | C    |
| 32  | 1a    | 129(A) | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 32  | 1a    | 131    | C    |
| 32  | 1a    | 137    | C    |
| 32  | 1a    | 141    | A    |
| 32  | 1a    | 163    | C    |
| 32  | 1a    | 169    | C    |
| 32  | 1a    | 173    | U    |
| 32  | 1a    | 174    | C    |
| 32  | 1a    | 182    | U    |
| 32  | 1a    | 189(D) | C    |
| 32  | 1a    | 190    | U    |
| 32  | 1a    | 195    | A    |
| 32  | 1a    | 197    | A    |
| 32  | 1a    | 201    | C    |
| 32  | 1a    | 216    | G    |
| 32  | 1a    | 217    | C    |
| 32  | 1a    | 220    | G    |
| 32  | 1a    | 247    | G    |
| 32  | 1a    | 251    | G    |
| 32  | 1a    | 258    | G    |
| 32  | 1a    | 266    | G    |
| 32  | 1a    | 267    | C    |
| 32  | 1a    | 280    | C    |
| 32  | 1a    | 289    | G    |
| 32  | 1a    | 321    | A    |
| 32  | 1a    | 328    | C    |
| 32  | 1a    | 329    | A    |
| 32  | 1a    | 332    | G    |
| 32  | 1a    | 347    | G    |
| 32  | 1a    | 348    | G    |
| 32  | 1a    | 352    | C    |
| 32  | 1a    | 354    | G    |
| 32  | 1a    | 356    | A    |
| 32  | 1a    | 367    | U    |
| 32  | 1a    | 372    | C    |
| 32  | 1a    | 373    | A    |
| 32  | 1a    | 383    | A    |
| 32  | 1a    | 392    | G    |
| 32  | 1a    | 393    | A    |
| 32  | 1a    | 397    | A    |
| 32  | 1a    | 406    | G    |
| 32  | 1a    | 412    | A    |
| 32  | 1a    | 413    | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 423 | G    |
| 32  | 1a    | 424 | G    |
| 32  | 1a    | 429 | U    |
| 32  | 1a    | 430 | A    |
| 32  | 1a    | 439 | A    |
| 32  | 1a    | 442 | C    |
| 32  | 1a    | 444 | C    |
| 32  | 1a    | 452 | A    |
| 32  | 1a    | 461 | A    |
| 32  | 1a    | 470 | C    |
| 32  | 1a    | 477 | A    |
| 32  | 1a    | 485 | G    |
| 32  | 1a    | 487 | A    |
| 32  | 1a    | 496 | A    |
| 32  | 1a    | 498 | U    |
| 32  | 1a    | 505 | G    |
| 32  | 1a    | 509 | A    |
| 32  | 1a    | 510 | A    |
| 32  | 1a    | 511 | C    |
| 32  | 1a    | 518 | C    |
| 32  | 1a    | 519 | C    |
| 32  | 1a    | 521 | G    |
| 32  | 1a    | 524 | G    |
| 32  | 1a    | 531 | U    |
| 32  | 1a    | 532 | A    |
| 32  | 1a    | 547 | A    |
| 32  | 1a    | 559 | A    |
| 32  | 1a    | 561 | U    |
| 32  | 1a    | 562 | C    |
| 32  | 1a    | 564 | C    |
| 32  | 1a    | 572 | A    |
| 32  | 1a    | 573 | A    |
| 32  | 1a    | 575 | G    |
| 32  | 1a    | 576 | G    |
| 32  | 1a    | 577 | G    |
| 32  | 1a    | 596 | C    |
| 32  | 1a    | 607 | A    |
| 32  | 1a    | 619 | U    |
| 32  | 1a    | 630 | G    |
| 32  | 1a    | 632 | A    |
| 32  | 1a    | 633 | G    |
| 32  | 1a    | 642 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 1a    | 653 | A    |
| 32  | 1a    | 657 | G    |
| 32  | 1a    | 661 | G    |
| 32  | 1a    | 665 | A    |
| 32  | 1a    | 687 | A    |
| 32  | 1a    | 688 | G    |
| 32  | 1a    | 693 | G    |
| 32  | 1a    | 717 | C    |
| 32  | 1a    | 724 | G    |
| 32  | 1a    | 728 | A    |
| 32  | 1a    | 731 | G    |
| 32  | 1a    | 734 | G    |
| 32  | 1a    | 747 | C    |
| 32  | 1a    | 755 | G    |
| 32  | 1a    | 759 | A    |
| 32  | 1a    | 768 | A    |
| 32  | 1a    | 774 | G    |
| 32  | 1a    | 777 | A    |
| 32  | 1a    | 793 | U    |
| 32  | 1a    | 794 | A    |
| 32  | 1a    | 816 | A    |
| 32  | 1a    | 817 | C    |
| 32  | 1a    | 821 | G    |
| 32  | 1a    | 827 | U    |
| 32  | 1a    | 828 | A    |
| 32  | 1a    | 829 | G    |
| 32  | 1a    | 836 | G    |
| 32  | 1a    | 839 | U    |
| 32  | 1a    | 840 | C    |
| 32  | 1a    | 841 | U    |
| 32  | 1a    | 848 | C    |
| 32  | 1a    | 855 | G    |
| 32  | 1a    | 870 | U    |
| 32  | 1a    | 878 | G    |
| 32  | 1a    | 902 | G    |
| 32  | 1a    | 913 | A    |
| 32  | 1a    | 914 | A    |
| 32  | 1a    | 926 | G    |
| 32  | 1a    | 927 | G    |
| 32  | 1a    | 931 | C    |
| 32  | 1a    | 934 | C    |
| 32  | 1a    | 935 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 1a    | 939     | G    |
| 32  | 1a    | 940     | C    |
| 32  | 1a    | 958     | A    |
| 32  | 1a    | 960     | U    |
| 32  | 1a    | 961     | U    |
| 32  | 1a    | 968     | A    |
| 32  | 1a    | 969     | A    |
| 32  | 1a    | 971     | G    |
| 32  | 1a    | 974     | A    |
| 32  | 1a    | 975     | A    |
| 32  | 1a    | 976     | G    |
| 32  | 1a    | 977     | A    |
| 32  | 1a    | 991     | U    |
| 32  | 1a    | 992     | U    |
| 32  | 1a    | 993     | G    |
| 32  | 1a    | 996     | A    |
| 32  | 1a    | 998     | G    |
| 32  | 1a    | 999     | C    |
| 32  | 1a    | 1001(A) | G    |
| 32  | 1a    | 1004    | A    |
| 32  | 1a    | 1005    | A    |
| 32  | 1a    | 1006    | C    |
| 32  | 1a    | 1009    | G    |
| 32  | 1a    | 1017    | G    |
| 32  | 1a    | 1020    | U    |
| 32  | 1a    | 1022    | G    |
| 32  | 1a    | 1023    | G    |
| 32  | 1a    | 1024    | G    |
| 32  | 1a    | 1025    | U    |
| 32  | 1a    | 1026    | G    |
| 32  | 1a    | 1027    | C    |
| 32  | 1a    | 1028    | C    |
| 32  | 1a    | 1030    | C    |
| 32  | 1a    | 1030(A) | G    |
| 32  | 1a    | 1030(B) | C    |
| 32  | 1a    | 1031    | G    |
| 32  | 1a    | 1032    | G    |
| 32  | 1a    | 1033    | G    |
| 32  | 1a    | 1037    | C    |
| 32  | 1a    | 1044    | A    |
| 32  | 1a    | 1063    | C    |
| 32  | 1a    | 1065    | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 1a    | 1066 | C    |
| 32  | 1a    | 1067 | A    |
| 32  | 1a    | 1070 | U    |
| 32  | 1a    | 1081 | G    |
| 32  | 1a    | 1094 | G    |
| 32  | 1a    | 1095 | U    |
| 32  | 1a    | 1101 | A    |
| 32  | 1a    | 1125 | U    |
| 32  | 1a    | 1127 | G    |
| 32  | 1a    | 1133 | G    |
| 32  | 1a    | 1134 | G    |
| 32  | 1a    | 1136 | U    |
| 32  | 1a    | 1137 | C    |
| 32  | 1a    | 1139 | G    |
| 32  | 1a    | 1140 | C    |
| 32  | 1a    | 1144 | G    |
| 32  | 1a    | 1146 | A    |
| 32  | 1a    | 1152 | A    |
| 32  | 1a    | 1155 | G    |
| 32  | 1a    | 1159 | U    |
| 32  | 1a    | 1163 | C    |
| 32  | 1a    | 1168 | A    |
| 32  | 1a    | 1183 | A    |
| 32  | 1a    | 1184 | G    |
| 32  | 1a    | 1186 | G    |
| 32  | 1a    | 1196 | U    |
| 32  | 1a    | 1197 | G    |
| 32  | 1a    | 1202 | G    |
| 32  | 1a    | 1212 | U    |
| 32  | 1a    | 1213 | A    |
| 32  | 1a    | 1224 | G    |
| 32  | 1a    | 1225 | A    |
| 32  | 1a    | 1227 | A    |
| 32  | 1a    | 1238 | A    |
| 32  | 1a    | 1256 | A    |
| 32  | 1a    | 1257 | U    |
| 32  | 1a    | 1258 | G    |
| 32  | 1a    | 1260 | C    |
| 32  | 1a    | 1270 | C    |
| 32  | 1a    | 1277 | C    |
| 32  | 1a    | 1278 | U    |
| 32  | 1a    | 1279 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 1a    | 1280    | A    |
| 32  | 1a    | 1286    | A    |
| 32  | 1a    | 1287    | A    |
| 32  | 1a    | 1293    | G    |
| 32  | 1a    | 1299    | A    |
| 32  | 1a    | 1300    | G    |
| 32  | 1a    | 1320    | C    |
| 32  | 1a    | 1322    | C    |
| 32  | 1a    | 1340    | A    |
| 32  | 1a    | 1346    | A    |
| 32  | 1a    | 1347    | G    |
| 32  | 1a    | 1353    | G    |
| 32  | 1a    | 1363    | C    |
| 32  | 1a    | 1370    | G    |
| 32  | 1a    | 1397    | C    |
| 32  | 1a    | 1398    | A    |
| 32  | 1a    | 1406    | U    |
| 32  | 1a    | 1419    | G    |
| 32  | 1a    | 1442    | G    |
| 32  | 1a    | 1442(A) | G    |
| 32  | 1a    | 1447    | A    |
| 32  | 1a    | 1456    | G    |
| 32  | 1a    | 1457    | G    |
| 32  | 1a    | 1469    | G    |
| 32  | 1a    | 1492    | A    |
| 32  | 1a    | 1493    | A    |
| 32  | 1a    | 1503    | A    |
| 32  | 1a    | 1504    | G    |
| 32  | 1a    | 1505    | G    |
| 32  | 1a    | 1506    | U    |
| 32  | 1a    | 1507    | A    |
| 32  | 1a    | 1517    | G    |
| 32  | 1a    | 1520    | G    |
| 32  | 1a    | 1529    | G    |
| 32  | 1a    | 1530    | G    |
| 32  | 1a    | 1531    | A    |
| 1   | 2A    | 10      | G    |
| 1   | 2A    | 12      | U    |
| 1   | 2A    | 15      | G    |
| 1   | 2A    | 34      | C    |
| 1   | 2A    | 45      | C    |
| 1   | 2A    | 63      | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 71     | A    |
| 1   | 2A    | 74     | A    |
| 1   | 2A    | 75     | G    |
| 1   | 2A    | 84     | A    |
| 1   | 2A    | 92     | A    |
| 1   | 2A    | 102    | G    |
| 1   | 2A    | 118    | A    |
| 1   | 2A    | 119    | A    |
| 1   | 2A    | 120    | U    |
| 1   | 2A    | 131    | G    |
| 1   | 2A    | 139    | G    |
| 1   | 2A    | 139(A) | G    |
| 1   | 2A    | 141    | A    |
| 1   | 2A    | 157    | U    |
| 1   | 2A    | 181    | A    |
| 1   | 2A    | 196    | A    |
| 1   | 2A    | 199    | A    |
| 1   | 2A    | 201    | C    |
| 1   | 2A    | 205    | G    |
| 1   | 2A    | 214    | G    |
| 1   | 2A    | 215    | G    |
| 1   | 2A    | 216    | A    |
| 1   | 2A    | 221    | A    |
| 1   | 2A    | 222    | A    |
| 1   | 2A    | 223    | A    |
| 1   | 2A    | 229    | A    |
| 1   | 2A    | 230    | U    |
| 1   | 2A    | 233    | A    |
| 1   | 2A    | 248    | G    |
| 1   | 2A    | 271(D) | G    |
| 1   | 2A    | 271(E) | U    |
| 1   | 2A    | 271(K) | U    |
| 1   | 2A    | 271(L) | U    |
| 1   | 2A    | 271(M) | G    |
| 1   | 2A    | 271(N) | U    |
| 1   | 2A    | 271(O) | C    |
| 1   | 2A    | 272(A) | U    |
| 1   | 2A    | 272(B) | G    |
| 1   | 2A    | 277    | C    |
| 1   | 2A    | 278    | A    |
| 1   | 2A    | 283    | A    |
| 1   | 2A    | 302    | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2A    | 311 | A    |
| 1   | 2A    | 317 | G    |
| 1   | 2A    | 324 | A    |
| 1   | 2A    | 327 | G    |
| 1   | 2A    | 329 | G    |
| 1   | 2A    | 330 | A    |
| 1   | 2A    | 333 | G    |
| 1   | 2A    | 335 | C    |
| 1   | 2A    | 352 | G    |
| 1   | 2A    | 363 | G    |
| 1   | 2A    | 370 | G    |
| 1   | 2A    | 386 | G    |
| 1   | 2A    | 390 | A    |
| 1   | 2A    | 396 | G    |
| 1   | 2A    | 399 | G    |
| 1   | 2A    | 405 | U    |
| 1   | 2A    | 411 | G    |
| 1   | 2A    | 412 | A    |
| 1   | 2A    | 428 | A    |
| 1   | 2A    | 444 | C    |
| 1   | 2A    | 446 | G    |
| 1   | 2A    | 454 | A    |
| 1   | 2A    | 455 | C    |
| 1   | 2A    | 456 | C    |
| 1   | 2A    | 457 | A    |
| 1   | 2A    | 470 | A    |
| 1   | 2A    | 475 | U    |
| 1   | 2A    | 481 | G    |
| 1   | 2A    | 482 | A    |
| 1   | 2A    | 504 | U    |
| 1   | 2A    | 505 | A    |
| 1   | 2A    | 509 | C    |
| 1   | 2A    | 530 | G    |
| 1   | 2A    | 531 | C    |
| 1   | 2A    | 532 | A    |
| 1   | 2A    | 533 | G    |
| 1   | 2A    | 545 | G    |
| 1   | 2A    | 551 | G    |
| 1   | 2A    | 563 | G    |
| 1   | 2A    | 573 | G    |
| 1   | 2A    | 575 | A    |
| 1   | 2A    | 586 | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 2A    | 603    | A    |
| 1   | 2A    | 604    | G    |
| 1   | 2A    | 607    | U    |
| 1   | 2A    | 614(B) | G    |
| 1   | 2A    | 614(C) | A    |
| 1   | 2A    | 615    | G    |
| 1   | 2A    | 616    | G    |
| 1   | 2A    | 627    | A    |
| 1   | 2A    | 634    | C    |
| 1   | 2A    | 637    | A    |
| 1   | 2A    | 645    | C    |
| 1   | 2A    | 646    | A    |
| 1   | 2A    | 652(B) | A    |
| 1   | 2A    | 652(C) | G    |
| 1   | 2A    | 652(U) | G    |
| 1   | 2A    | 653    | A    |
| 1   | 2A    | 669    | G    |
| 1   | 2A    | 686    | G    |
| 1   | 2A    | 701    | G    |
| 1   | 2A    | 730    | C    |
| 1   | 2A    | 740    | U    |
| 1   | 2A    | 752    | A    |
| 1   | 2A    | 753    | C    |
| 1   | 2A    | 771    | G    |
| 1   | 2A    | 775    | G    |
| 1   | 2A    | 776    | G    |
| 1   | 2A    | 782    | A    |
| 1   | 2A    | 784    | A    |
| 1   | 2A    | 785    | G    |
| 1   | 2A    | 792    | G    |
| 1   | 2A    | 805    | G    |
| 1   | 2A    | 812    | C    |
| 1   | 2A    | 827    | U    |
| 1   | 2A    | 828    | U    |
| 1   | 2A    | 847    | U    |
| 1   | 2A    | 857    | C    |
| 1   | 2A    | 859    | G    |
| 1   | 2A    | 869    | G    |
| 1   | 2A    | 880    | G    |
| 1   | 2A    | 882    | G    |
| 1   | 2A    | 886    | C    |
| 1   | 2A    | 887    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 888  | C    |
| 1   | 2A    | 889  | C    |
| 1   | 2A    | 890  | A    |
| 1   | 2A    | 893  | C    |
| 1   | 2A    | 896  | A    |
| 1   | 2A    | 897  | C    |
| 1   | 2A    | 901  | A    |
| 1   | 2A    | 910  | A    |
| 1   | 2A    | 915  | C    |
| 1   | 2A    | 917  | A    |
| 1   | 2A    | 932  | G    |
| 1   | 2A    | 937  | U    |
| 1   | 2A    | 938  | G    |
| 1   | 2A    | 941  | A    |
| 1   | 2A    | 945  | A    |
| 1   | 2A    | 946  | G    |
| 1   | 2A    | 953  | A    |
| 1   | 2A    | 959  | A    |
| 1   | 2A    | 961  | C    |
| 1   | 2A    | 974  | G    |
| 1   | 2A    | 975  | C    |
| 1   | 2A    | 980  | A    |
| 1   | 2A    | 983  | A    |
| 1   | 2A    | 996  | A    |
| 1   | 2A    | 1006 | C    |
| 1   | 2A    | 1012 | U    |
| 1   | 2A    | 1013 | C    |
| 1   | 2A    | 1026 | U    |
| 1   | 2A    | 1033 | U    |
| 1   | 2A    | 1038 | C    |
| 1   | 2A    | 1044 | G    |
| 1   | 2A    | 1045 | A    |
| 1   | 2A    | 1046 | A    |
| 1   | 2A    | 1047 | G    |
| 1   | 2A    | 1048 | A    |
| 1   | 2A    | 1052 | C    |
| 1   | 2A    | 1054 | A    |
| 1   | 2A    | 1056 | G    |
| 1   | 2A    | 1060 | U    |
| 1   | 2A    | 1064 | C    |
| 1   | 2A    | 1065 | U    |
| 1   | 2A    | 1066 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1067 | A    |
| 1   | 2A    | 1068 | G    |
| 1   | 2A    | 1070 | A    |
| 1   | 2A    | 1071 | G    |
| 1   | 2A    | 1073 | A    |
| 1   | 2A    | 1074 | G    |
| 1   | 2A    | 1075 | C    |
| 1   | 2A    | 1076 | C    |
| 1   | 2A    | 1077 | A    |
| 1   | 2A    | 1079 | C    |
| 1   | 2A    | 1080 | C    |
| 1   | 2A    | 1081 | U    |
| 1   | 2A    | 1082 | U    |
| 1   | 2A    | 1083 | U    |
| 1   | 2A    | 1084 | A    |
| 1   | 2A    | 1085 | A    |
| 1   | 2A    | 1086 | A    |
| 1   | 2A    | 1088 | A    |
| 1   | 2A    | 1090 | U    |
| 1   | 2A    | 1091 | G    |
| 1   | 2A    | 1092 | C    |
| 1   | 2A    | 1093 | G    |
| 1   | 2A    | 1095 | A    |
| 1   | 2A    | 1097 | U    |
| 1   | 2A    | 1098 | A    |
| 1   | 2A    | 1106 | G    |
| 1   | 2A    | 1110 | G    |
| 1   | 2A    | 1112 | G    |
| 1   | 2A    | 1116 | C    |
| 1   | 2A    | 1117 | G    |
| 1   | 2A    | 1120 | G    |
| 1   | 2A    | 1129 | A    |
| 1   | 2A    | 1135 | C    |
| 1   | 2A    | 1136 | G    |
| 1   | 2A    | 1171 | G    |
| 1   | 2A    | 1211 | U    |
| 1   | 2A    | 1212 | G    |
| 1   | 2A    | 1220 | A    |
| 1   | 2A    | 1244 | G    |
| 1   | 2A    | 1253 | A    |
| 1   | 2A    | 1256 | G    |
| 1   | 2A    | 1271 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 1272    | A    |
| 1   | 2A    | 1273    | U    |
| 1   | 2A    | 1274    | A    |
| 1   | 2A    | 1276    | A    |
| 1   | 2A    | 1300    | U    |
| 1   | 2A    | 1301    | A    |
| 1   | 2A    | 1303    | G    |
| 1   | 2A    | 1314    | C    |
| 1   | 2A    | 1321    | A    |
| 1   | 2A    | 1342    | A    |
| 1   | 2A    | 1349    | A    |
| 1   | 2A    | 1352    | U    |
| 1   | 2A    | 1365    | A    |
| 1   | 2A    | 1368    | G    |
| 1   | 2A    | 1372    | U    |
| 1   | 2A    | 1380    | G    |
| 1   | 2A    | 1384    | A    |
| 1   | 2A    | 1385    | G    |
| 1   | 2A    | 1386    | C    |
| 1   | 2A    | 1414    | G    |
| 1   | 2A    | 1416    | G    |
| 1   | 2A    | 1417    | C    |
| 1   | 2A    | 1420    | U    |
| 1   | 2A    | 1421    | G    |
| 1   | 2A    | 1427    | A    |
| 1   | 2A    | 1428    | C    |
| 1   | 2A    | 1445    | A    |
| 1   | 2A    | 1450    | G    |
| 1   | 2A    | 1455    | G    |
| 1   | 2A    | 1459    | G    |
| 1   | 2A    | 1467    | C    |
| 1   | 2A    | 1471    | A    |
| 1   | 2A    | 1482    | G    |
| 1   | 2A    | 1493    | C    |
| 1   | 2A    | 1497    | U    |
| 1   | 2A    | 1507    | A    |
| 1   | 2A    | 1508    | A    |
| 1   | 2A    | 1509    | C    |
| 1   | 2A    | 1509(A) | A    |
| 1   | 2A    | 1511    | C    |
| 1   | 2A    | 1531    | C    |
| 1   | 2A    | 1533    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1542 | A    |
| 1   | 2A    | 1543 | C    |
| 1   | 2A    | 1558 | A    |
| 1   | 2A    | 1566 | A    |
| 1   | 2A    | 1569 | A    |
| 1   | 2A    | 1578 | U    |
| 1   | 2A    | 1580 | A    |
| 1   | 2A    | 1584 | C    |
| 1   | 2A    | 1586 | A    |
| 1   | 2A    | 1590 | U    |
| 1   | 2A    | 1593 | G    |
| 1   | 2A    | 1608 | A    |
| 1   | 2A    | 1609 | A    |
| 1   | 2A    | 1610 | A    |
| 1   | 2A    | 1613 | G    |
| 1   | 2A    | 1639 | U    |
| 1   | 2A    | 1648 | C    |
| 1   | 2A    | 1674 | G    |
| 1   | 2A    | 1696 | G    |
| 1   | 2A    | 1700 | A    |
| 1   | 2A    | 1721 | G    |
| 1   | 2A    | 1722 | A    |
| 1   | 2A    | 1740 | G    |
| 1   | 2A    | 1741 | A    |
| 1   | 2A    | 1756 | G    |
| 1   | 2A    | 1757 | U    |
| 1   | 2A    | 1762 | A    |
| 1   | 2A    | 1763 | G    |
| 1   | 2A    | 1764 | G    |
| 1   | 2A    | 1773 | A    |
| 1   | 2A    | 1780 | A    |
| 1   | 2A    | 1782 | C    |
| 1   | 2A    | 1786 | A    |
| 1   | 2A    | 1791 | A    |
| 1   | 2A    | 1800 | C    |
| 1   | 2A    | 1801 | G    |
| 1   | 2A    | 1816 | G    |
| 1   | 2A    | 1829 | A    |
| 1   | 2A    | 1834 | U    |
| 1   | 2A    | 1835 | G    |
| 1   | 2A    | 1847 | A    |
| 1   | 2A    | 1848 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1852 | C    |
| 1   | 2A    | 1877 | A    |
| 1   | 2A    | 1878 | G    |
| 1   | 2A    | 1900 | A    |
| 1   | 2A    | 1906 | G    |
| 1   | 2A    | 1914 | C    |
| 1   | 2A    | 1927 | A    |
| 1   | 2A    | 1929 | G    |
| 1   | 2A    | 1930 | G    |
| 1   | 2A    | 1937 | A    |
| 1   | 2A    | 1938 | A    |
| 1   | 2A    | 1955 | U    |
| 1   | 2A    | 1963 | U    |
| 1   | 2A    | 1967 | C    |
| 1   | 2A    | 1970 | A    |
| 1   | 2A    | 1971 | A    |
| 1   | 2A    | 1972 | A    |
| 1   | 2A    | 1984 | G    |
| 1   | 2A    | 1993 | U    |
| 1   | 2A    | 1997 | G    |
| 1   | 2A    | 2020 | A    |
| 1   | 2A    | 2023 | G    |
| 1   | 2A    | 2031 | A    |
| 1   | 2A    | 2033 | A    |
| 1   | 2A    | 2043 | C    |
| 1   | 2A    | 2055 | C    |
| 1   | 2A    | 2056 | G    |
| 1   | 2A    | 2060 | A    |
| 1   | 2A    | 2061 | G    |
| 1   | 2A    | 2069 | G    |
| 1   | 2A    | 2096 | U    |
| 1   | 2A    | 2101 | G    |
| 1   | 2A    | 2103 | C    |
| 1   | 2A    | 2105 | C    |
| 1   | 2A    | 2107 | C    |
| 1   | 2A    | 2108 | C    |
| 1   | 2A    | 2109 | U    |
| 1   | 2A    | 2110 | G    |
| 1   | 2A    | 2112 | G    |
| 1   | 2A    | 2116 | G    |
| 1   | 2A    | 2117 | A    |
| 1   | 2A    | 2118 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2119 | A    |
| 1   | 2A    | 2120 | G    |
| 1   | 2A    | 2121 | G    |
| 1   | 2A    | 2123 | G    |
| 1   | 2A    | 2126 | A    |
| 1   | 2A    | 2127 | G    |
| 1   | 2A    | 2129 | C    |
| 1   | 2A    | 2130 | U    |
| 1   | 2A    | 2132 | U    |
| 1   | 2A    | 2133 | G    |
| 1   | 2A    | 2134 | A    |
| 1   | 2A    | 2135 | A    |
| 1   | 2A    | 2136 | C    |
| 1   | 2A    | 2137 | C    |
| 1   | 2A    | 2138 | C    |
| 1   | 2A    | 2140 | C    |
| 1   | 2A    | 2141 | G    |
| 1   | 2A    | 2145 | C    |
| 1   | 2A    | 2146 | C    |
| 1   | 2A    | 2147 | G    |
| 1   | 2A    | 2148 | G    |
| 1   | 2A    | 2150 | U    |
| 1   | 2A    | 2151 | G    |
| 1   | 2A    | 2155 | G    |
| 1   | 2A    | 2158 | A    |
| 1   | 2A    | 2159 | G    |
| 1   | 2A    | 2160 | G    |
| 1   | 2A    | 2161 | C    |
| 1   | 2A    | 2164 | C    |
| 1   | 2A    | 2165 | G    |
| 1   | 2A    | 2166 | G    |
| 1   | 2A    | 2172 | U    |
| 1   | 2A    | 2173 | A    |
| 1   | 2A    | 2174 | C    |
| 1   | 2A    | 2175 | C    |
| 1   | 2A    | 2178 | C    |
| 1   | 2A    | 2182 | G    |
| 1   | 2A    | 2186 | G    |
| 1   | 2A    | 2187 | G    |
| 1   | 2A    | 2189 | U    |
| 1   | 2A    | 2192 | G    |
| 1   | 2A    | 2198 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2206 | G    |
| 1   | 2A    | 2207 | G    |
| 1   | 2A    | 2208 | A    |
| 1   | 2A    | 2225 | A    |
| 1   | 2A    | 2238 | G    |
| 1   | 2A    | 2239 | G    |
| 1   | 2A    | 2268 | A    |
| 1   | 2A    | 2269 | A    |
| 1   | 2A    | 2273 | A    |
| 1   | 2A    | 2275 | C    |
| 1   | 2A    | 2280 | G    |
| 1   | 2A    | 2283 | C    |
| 1   | 2A    | 2287 | A    |
| 1   | 2A    | 2289 | G    |
| 1   | 2A    | 2294 | C    |
| 1   | 2A    | 2300 | G    |
| 1   | 2A    | 2305 | A    |
| 1   | 2A    | 2308 | G    |
| 1   | 2A    | 2309 | A    |
| 1   | 2A    | 2310 | A    |
| 1   | 2A    | 2311 | A    |
| 1   | 2A    | 2312 | U    |
| 1   | 2A    | 2319 | G    |
| 1   | 2A    | 2320 | A    |
| 1   | 2A    | 2321 | G    |
| 1   | 2A    | 2322 | A    |
| 1   | 2A    | 2325 | G    |
| 1   | 2A    | 2327 | A    |
| 1   | 2A    | 2334 | G    |
| 1   | 2A    | 2335 | A    |
| 1   | 2A    | 2347 | C    |
| 1   | 2A    | 2350 | C    |
| 1   | 2A    | 2354 | G    |
| 1   | 2A    | 2366 | A    |
| 1   | 2A    | 2383 | G    |
| 1   | 2A    | 2385 | C    |
| 1   | 2A    | 2396 | G    |
| 1   | 2A    | 2402 | C    |
| 1   | 2A    | 2406 | U    |
| 1   | 2A    | 2410 | G    |
| 1   | 2A    | 2414 | G    |
| 1   | 2A    | 2422 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 2A    | 2423    | U    |
| 1   | 2A    | 2424    | C    |
| 1   | 2A    | 2425    | A    |
| 1   | 2A    | 2429    | G    |
| 1   | 2A    | 2430    | A    |
| 1   | 2A    | 2435    | A    |
| 1   | 2A    | 2439    | A    |
| 1   | 2A    | 2441    | C    |
| 1   | 2A    | 2445    | G    |
| 1   | 2A    | 2448    | A    |
| 1   | 2A    | 2468    | G    |
| 1   | 2A    | 2474    | C    |
| 1   | 2A    | 2476    | A    |
| 1   | 2A    | 2487    | G    |
| 1   | 2A    | 2490    | G    |
| 1   | 2A    | 2491    | U    |
| 1   | 2A    | 2498    | C    |
| 1   | 2A    | 2502    | G    |
| 1   | 2A    | 2504    | U    |
| 1   | 2A    | 2505    | G    |
| 1   | 2A    | 2518    | A    |
| 1   | 2A    | 2529    | G    |
| 1   | 2A    | 2549    | G    |
| 1   | 2A    | 2554    | U    |
| 1   | 2A    | 2556    | C    |
| 1   | 2A    | 2566    | A    |
| 1   | 2A    | 2567    | G    |
| 1   | 2A    | 2573    | C    |
| 1   | 2A    | 2582    | G    |
| 1   | 2A    | 2602    | A    |
| 1   | 2A    | 2609    | U    |
| 1   | 2A    | 2611    | U    |
| 1   | 2A    | 2612    | C    |
| 1   | 2A    | 2629    | A    |
| 1   | 2A    | 2630    | G    |
| 1   | 2A    | 2654    | A    |
| 1   | 2A    | 2663    | G    |
| 1   | 2A    | 2682    | U    |
| 1   | 2A    | 2689    | U    |
| 1   | 2A    | 2690    | C    |
| 1   | 2A    | 2703    | C    |
| 1   | 2A    | 2712(A) | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 2713 | A    |
| 1   | 2A    | 2714 | G    |
| 1   | 2A    | 2726 | U    |
| 1   | 2A    | 2733 | A    |
| 1   | 2A    | 2752 | C    |
| 1   | 2A    | 2754 | U    |
| 1   | 2A    | 2757 | A    |
| 1   | 2A    | 2758 | A    |
| 1   | 2A    | 2764 | A    |
| 1   | 2A    | 2765 | A    |
| 1   | 2A    | 2769 | C    |
| 1   | 2A    | 2778 | A    |
| 1   | 2A    | 2779 | U    |
| 1   | 2A    | 2789 | C    |
| 1   | 2A    | 2802 | G    |
| 1   | 2A    | 2803 | C    |
| 1   | 2A    | 2818 | G    |
| 1   | 2A    | 2820 | A    |
| 1   | 2A    | 2821 | A    |
| 1   | 2A    | 2833 | G    |
| 1   | 2A    | 2834 | G    |
| 1   | 2A    | 2835 | A    |
| 1   | 2A    | 2848 | G    |
| 1   | 2A    | 2872 | G    |
| 1   | 2A    | 2880 | C    |
| 1   | 2A    | 2891 | G    |
| 1   | 2A    | 2892 | A    |
| 1   | 2A    | 2894 | G    |
| 1   | 2A    | 2895 | U    |
| 2   | 2B    | 2    | C    |
| 2   | 2B    | 8    | U    |
| 2   | 2B    | 9    | G    |
| 2   | 2B    | 12   | C    |
| 2   | 2B    | 21   | G    |
| 2   | 2B    | 23   | G    |
| 2   | 2B    | 24   | G    |
| 2   | 2B    | 33   | G    |
| 2   | 2B    | 41   | U    |
| 2   | 2B    | 42   | C    |
| 2   | 2B    | 56   | G    |
| 2   | 2B    | 73   | A    |
| 2   | 2B    | 89   | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | 2B    | 90     | A    |
| 2   | 2B    | 110    | G    |
| 2   | 2B    | 116    | G    |
| 32  | 2a    | 5      | U    |
| 32  | 2a    | 6      | G    |
| 32  | 2a    | 9      | G    |
| 32  | 2a    | 22     | G    |
| 32  | 2a    | 29     | G    |
| 32  | 2a    | 30     | U    |
| 32  | 2a    | 32     | A    |
| 32  | 2a    | 39     | G    |
| 32  | 2a    | 47     | C    |
| 32  | 2a    | 48     | C    |
| 32  | 2a    | 51     | A    |
| 32  | 2a    | 60     | A    |
| 32  | 2a    | 61     | G    |
| 32  | 2a    | 78     | G    |
| 32  | 2a    | 88     | A    |
| 32  | 2a    | 89     | C    |
| 32  | 2a    | 101    | A    |
| 32  | 2a    | 102    | G    |
| 32  | 2a    | 116    | A    |
| 32  | 2a    | 121    | C    |
| 32  | 2a    | 129(A) | G    |
| 32  | 2a    | 131    | C    |
| 32  | 2a    | 142    | G    |
| 32  | 2a    | 144    | G    |
| 32  | 2a    | 156    | G    |
| 32  | 2a    | 163    | C    |
| 32  | 2a    | 173    | U    |
| 32  | 2a    | 174    | C    |
| 32  | 2a    | 182    | U    |
| 32  | 2a    | 189(B) | C    |
| 32  | 2a    | 189(C) | C    |
| 32  | 2a    | 189(D) | C    |
| 32  | 2a    | 189(F) | U    |
| 32  | 2a    | 189(G) | G    |
| 32  | 2a    | 194    | C    |
| 32  | 2a    | 195    | A    |
| 32  | 2a    | 196    | A    |
| 32  | 2a    | 201    | C    |
| 32  | 2a    | 202    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2a    | 204 | U    |
| 32  | 2a    | 216 | G    |
| 32  | 2a    | 220 | G    |
| 32  | 2a    | 223 | U    |
| 32  | 2a    | 240 | C    |
| 32  | 2a    | 247 | G    |
| 32  | 2a    | 251 | G    |
| 32  | 2a    | 258 | G    |
| 32  | 2a    | 266 | G    |
| 32  | 2a    | 267 | C    |
| 32  | 2a    | 289 | G    |
| 32  | 2a    | 306 | G    |
| 32  | 2a    | 316 | G    |
| 32  | 2a    | 319 | G    |
| 32  | 2a    | 321 | A    |
| 32  | 2a    | 328 | C    |
| 32  | 2a    | 332 | G    |
| 32  | 2a    | 345 | C    |
| 32  | 2a    | 351 | G    |
| 32  | 2a    | 352 | C    |
| 32  | 2a    | 353 | A    |
| 32  | 2a    | 354 | G    |
| 32  | 2a    | 363 | A    |
| 32  | 2a    | 367 | U    |
| 32  | 2a    | 372 | C    |
| 32  | 2a    | 373 | A    |
| 32  | 2a    | 382 | A    |
| 32  | 2a    | 392 | G    |
| 32  | 2a    | 397 | A    |
| 32  | 2a    | 398 | C    |
| 32  | 2a    | 406 | G    |
| 32  | 2a    | 409 | G    |
| 32  | 2a    | 412 | A    |
| 32  | 2a    | 413 | G    |
| 32  | 2a    | 423 | G    |
| 32  | 2a    | 429 | U    |
| 32  | 2a    | 430 | A    |
| 32  | 2a    | 439 | A    |
| 32  | 2a    | 442 | C    |
| 32  | 2a    | 452 | A    |
| 32  | 2a    | 461 | A    |
| 32  | 2a    | 470 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2a    | 471 | G    |
| 32  | 2a    | 476 | G    |
| 32  | 2a    | 477 | A    |
| 32  | 2a    | 484 | G    |
| 32  | 2a    | 485 | G    |
| 32  | 2a    | 496 | A    |
| 32  | 2a    | 498 | U    |
| 32  | 2a    | 505 | G    |
| 32  | 2a    | 508 | C    |
| 32  | 2a    | 509 | A    |
| 32  | 2a    | 510 | A    |
| 32  | 2a    | 511 | C    |
| 32  | 2a    | 518 | C    |
| 32  | 2a    | 521 | G    |
| 32  | 2a    | 532 | A    |
| 32  | 2a    | 533 | A    |
| 32  | 2a    | 547 | A    |
| 32  | 2a    | 559 | A    |
| 32  | 2a    | 562 | C    |
| 32  | 2a    | 564 | C    |
| 32  | 2a    | 572 | A    |
| 32  | 2a    | 573 | A    |
| 32  | 2a    | 574 | A    |
| 32  | 2a    | 576 | G    |
| 32  | 2a    | 577 | G    |
| 32  | 2a    | 596 | C    |
| 32  | 2a    | 630 | G    |
| 32  | 2a    | 631 | G    |
| 32  | 2a    | 632 | A    |
| 32  | 2a    | 648 | A    |
| 32  | 2a    | 651 | C    |
| 32  | 2a    | 653 | A    |
| 32  | 2a    | 665 | A    |
| 32  | 2a    | 685 | G    |
| 32  | 2a    | 687 | A    |
| 32  | 2a    | 688 | G    |
| 32  | 2a    | 702 | A    |
| 32  | 2a    | 703 | G    |
| 32  | 2a    | 712 | A    |
| 32  | 2a    | 723 | U    |
| 32  | 2a    | 731 | G    |
| 32  | 2a    | 734 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | 2a    | 735 | C    |
| 32  | 2a    | 742 | G    |
| 32  | 2a    | 746 | A    |
| 32  | 2a    | 749 | C    |
| 32  | 2a    | 753 | A    |
| 32  | 2a    | 755 | G    |
| 32  | 2a    | 777 | A    |
| 32  | 2a    | 784 | C    |
| 32  | 2a    | 793 | U    |
| 32  | 2a    | 794 | A    |
| 32  | 2a    | 802 | A    |
| 32  | 2a    | 805 | C    |
| 32  | 2a    | 817 | C    |
| 32  | 2a    | 821 | G    |
| 32  | 2a    | 828 | A    |
| 32  | 2a    | 829 | G    |
| 32  | 2a    | 840 | C    |
| 32  | 2a    | 841 | U    |
| 32  | 2a    | 851 | G    |
| 32  | 2a    | 854 | G    |
| 32  | 2a    | 859 | A    |
| 32  | 2a    | 872 | A    |
| 32  | 2a    | 902 | G    |
| 32  | 2a    | 914 | A    |
| 32  | 2a    | 916 | G    |
| 32  | 2a    | 920 | U    |
| 32  | 2a    | 926 | G    |
| 32  | 2a    | 927 | G    |
| 32  | 2a    | 931 | C    |
| 32  | 2a    | 934 | C    |
| 32  | 2a    | 939 | G    |
| 32  | 2a    | 955 | U    |
| 32  | 2a    | 960 | U    |
| 32  | 2a    | 961 | U    |
| 32  | 2a    | 966 | M2G  |
| 32  | 2a    | 968 | A    |
| 32  | 2a    | 969 | A    |
| 32  | 2a    | 971 | G    |
| 32  | 2a    | 972 | C    |
| 32  | 2a    | 974 | A    |
| 32  | 2a    | 975 | A    |
| 32  | 2a    | 976 | G    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 977     | A    |
| 32  | 2a    | 983     | A    |
| 32  | 2a    | 992     | U    |
| 32  | 2a    | 993     | G    |
| 32  | 2a    | 994     | A    |
| 32  | 2a    | 995     | C    |
| 32  | 2a    | 996     | A    |
| 32  | 2a    | 1000    | U    |
| 32  | 2a    | 1003    | G    |
| 32  | 2a    | 1004    | A    |
| 32  | 2a    | 1005    | A    |
| 32  | 2a    | 1006    | C    |
| 32  | 2a    | 1017    | G    |
| 32  | 2a    | 1020    | U    |
| 32  | 2a    | 1022    | G    |
| 32  | 2a    | 1023    | G    |
| 32  | 2a    | 1025    | U    |
| 32  | 2a    | 1026    | G    |
| 32  | 2a    | 1027    | C    |
| 32  | 2a    | 1028    | C    |
| 32  | 2a    | 1029    | C    |
| 32  | 2a    | 1030(A) | G    |
| 32  | 2a    | 1030(B) | C    |
| 32  | 2a    | 1030(C) | G    |
| 32  | 2a    | 1031    | G    |
| 32  | 2a    | 1032    | G    |
| 32  | 2a    | 1034    | G    |
| 32  | 2a    | 1041    | A    |
| 32  | 2a    | 1043    | C    |
| 32  | 2a    | 1053    | G    |
| 32  | 2a    | 1054    | C    |
| 32  | 2a    | 1065    | U    |
| 32  | 2a    | 1066    | C    |
| 32  | 2a    | 1068    | G    |
| 32  | 2a    | 1081    | G    |
| 32  | 2a    | 1094    | G    |
| 32  | 2a    | 1101    | A    |
| 32  | 2a    | 1113    | C    |
| 32  | 2a    | 1118    | C    |
| 32  | 2a    | 1122    | U    |
| 32  | 2a    | 1125    | U    |
| 32  | 2a    | 1129    | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 32  | 2a    | 1130 | A    |
| 32  | 2a    | 1134 | G    |
| 32  | 2a    | 1136 | U    |
| 32  | 2a    | 1137 | C    |
| 32  | 2a    | 1138 | G    |
| 32  | 2a    | 1139 | G    |
| 32  | 2a    | 1147 | C    |
| 32  | 2a    | 1152 | A    |
| 32  | 2a    | 1157 | A    |
| 32  | 2a    | 1158 | C    |
| 32  | 2a    | 1159 | U    |
| 32  | 2a    | 1161 | C    |
| 32  | 2a    | 1182 | G    |
| 32  | 2a    | 1183 | A    |
| 32  | 2a    | 1184 | G    |
| 32  | 2a    | 1196 | U    |
| 32  | 2a    | 1197 | G    |
| 32  | 2a    | 1201 | A    |
| 32  | 2a    | 1213 | A    |
| 32  | 2a    | 1214 | C    |
| 32  | 2a    | 1215 | G    |
| 32  | 2a    | 1224 | G    |
| 32  | 2a    | 1227 | A    |
| 32  | 2a    | 1228 | C    |
| 32  | 2a    | 1236 | A    |
| 32  | 2a    | 1238 | A    |
| 32  | 2a    | 1246 | C    |
| 32  | 2a    | 1250 | A    |
| 32  | 2a    | 1256 | A    |
| 32  | 2a    | 1257 | U    |
| 32  | 2a    | 1258 | G    |
| 32  | 2a    | 1270 | C    |
| 32  | 2a    | 1278 | U    |
| 32  | 2a    | 1279 | A    |
| 32  | 2a    | 1280 | A    |
| 32  | 2a    | 1281 | U    |
| 32  | 2a    | 1287 | A    |
| 32  | 2a    | 1298 | C    |
| 32  | 2a    | 1299 | A    |
| 32  | 2a    | 1300 | G    |
| 32  | 2a    | 1301 | U    |
| 32  | 2a    | 1302 | U    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 32  | 2a    | 1303    | C    |
| 32  | 2a    | 1316    | G    |
| 32  | 2a    | 1317    | C    |
| 32  | 2a    | 1319    | A    |
| 32  | 2a    | 1322    | C    |
| 32  | 2a    | 1323    | G    |
| 32  | 2a    | 1340    | A    |
| 32  | 2a    | 1346    | A    |
| 32  | 2a    | 1347    | G    |
| 32  | 2a    | 1352    | C    |
| 32  | 2a    | 1353    | G    |
| 32  | 2a    | 1363    | C    |
| 32  | 2a    | 1363(A) | A    |
| 32  | 2a    | 1364    | U    |
| 32  | 2a    | 1370    | G    |
| 32  | 2a    | 1384    | C    |
| 32  | 2a    | 1385    | G    |
| 32  | 2a    | 1397    | C    |
| 32  | 2a    | 1400    | 5MC  |
| 32  | 2a    | 1401    | G    |
| 32  | 2a    | 1406    | U    |
| 32  | 2a    | 1419    | G    |
| 32  | 2a    | 1442    | G    |
| 32  | 2a    | 1442(A) | G    |
| 32  | 2a    | 1442(B) | A    |
| 32  | 2a    | 1446    | U    |
| 32  | 2a    | 1447    | A    |
| 32  | 2a    | 1452    | C    |
| 32  | 2a    | 1456    | G    |
| 32  | 2a    | 1459    | C    |
| 32  | 2a    | 1487    | G    |
| 32  | 2a    | 1492    | A    |
| 32  | 2a    | 1497    | G    |
| 32  | 2a    | 1499    | A    |
| 32  | 2a    | 1503    | A    |
| 32  | 2a    | 1504    | G    |
| 32  | 2a    | 1506    | U    |
| 32  | 2a    | 1507    | A    |
| 32  | 2a    | 1517    | G    |
| 32  | 2a    | 1529    | G    |
| 32  | 2a    | 1530    | G    |
| 54  | 2w    | 74      | C    |

All (63) RNA pucker outliers are listed below:

| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | 1A    | 214     | G    |
| 1   | 1A    | 266     | G    |
| 1   | 1A    | 278     | A    |
| 1   | 1A    | 746     | A    |
| 1   | 1A    | 764     | A    |
| 1   | 1A    | 784     | A    |
| 1   | 1A    | 839     | U    |
| 1   | 1A    | 840     | C    |
| 1   | 1A    | 888     | C    |
| 1   | 1A    | 895     | U    |
| 1   | 1A    | 974     | G    |
| 1   | 1A    | 1047    | G    |
| 1   | 1A    | 1089    | G    |
| 1   | 1A    | 1142(A) | A    |
| 1   | 1A    | 1145    | C    |
| 1   | 1A    | 1175    | U    |
| 1   | 1A    | 1210    | A    |
| 1   | 1A    | 1379    | A    |
| 1   | 1A    | 1442    | G    |
| 1   | 1A    | 1608    | A    |
| 1   | 1A    | 1653    | G    |
| 1   | 1A    | 2126    | A    |
| 1   | 1A    | 2238    | G    |
| 1   | 1A    | 2406    | U    |
| 1   | 1A    | 2422    | A    |
| 1   | 1A    | 2430    | A    |
| 1   | 1A    | 2689    | U    |
| 1   | 1A    | 2893    | G    |
| 1   | 2A    | 195     | A    |
| 1   | 2A    | 196     | A    |
| 1   | 2A    | 249     | C    |
| 1   | 2A    | 266     | G    |
| 1   | 2A    | 271(M)  | G    |
| 1   | 2A    | 277     | C    |
| 1   | 2A    | 746     | A    |
| 1   | 2A    | 752     | A    |
| 1   | 2A    | 764     | A    |
| 1   | 2A    | 827     | U    |
| 1   | 2A    | 840     | C    |
| 1   | 2A    | 856     | C    |
| 1   | 2A    | 900     | A    |
| 1   | 2A    | 1047    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | 2A    | 1051 | G    |
| 1   | 2A    | 1053 | C    |
| 1   | 2A    | 1065 | U    |
| 1   | 2A    | 1067 | A    |
| 1   | 2A    | 1073 | A    |
| 1   | 2A    | 1076 | C    |
| 1   | 2A    | 1210 | A    |
| 1   | 2A    | 1275 | A    |
| 1   | 2A    | 1379 | A    |
| 1   | 2A    | 1420 | U    |
| 1   | 2A    | 1442 | G    |
| 1   | 2A    | 1491 | G    |
| 1   | 2A    | 1992 | G    |
| 1   | 2A    | 2126 | A    |
| 1   | 2A    | 2171 | A    |
| 1   | 2A    | 2172 | U    |
| 1   | 2A    | 2321 | G    |
| 1   | 2A    | 2406 | U    |
| 1   | 2A    | 2422 | A    |
| 1   | 2A    | 2689 | U    |
| 1   | 2A    | 2756 | U    |

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

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

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | 5MC  | 1a    | 1404 | 32   | 15,22,23     | 1.36 | 1 (6%)   | 19,32,35    | 1.22 | 1 (5%)   |
| 32  | 5MC  | 1a    | 1407 | 32   | 15,22,23     | 1.30 | 1 (6%)   | 19,32,35    | 1.50 | 3 (15%)  |
| 1   | PSU  | 2A    | 2605 | 1    | 17,21,22     | 1.61 | 4 (23%)  | 20,30,33    | 3.26 | 6 (30%)  |
| 32  | 5MC  | 2a    | 967  | 32   | 15,22,23     | 1.32 | 1 (6%)   | 19,32,35    | 1.33 | 3 (15%)  |
| 1   | 5MU  | 1A    | 1939 | 1    | 15,22,23     | 1.09 | 1 (6%)   | 16,32,35    | 1.97 | 2 (12%)  |
| 1   | 5MU  | 2A    | 1939 | 57,1 | 15,22,23     | 1.07 | 1 (6%)   | 16,32,35    | 1.88 | 2 (12%)  |

| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 32  | M2G  | 1a    | 966  | 32       | 20,27,28     | 1.43 | 3 (15%)  | 22,40,43    | 2.24 | 6 (27%)  |
| 1   | 5MC  | 2A    | 1942 | 1        | 15,22,23     | 1.34 | 1 (6%)   | 19,32,35    | 1.40 | 3 (15%)  |
| 32  | 4OC  | 2a    | 1402 | 32       | 16,23,24     | 0.65 | 0        | 17,32,35    | 1.30 | 1 (5%)   |
| 1   | 2MA  | 1A    | 2503 | 57,1     | 17,25,26     | 1.26 | 2 (11%)  | 19,37,40    | 2.04 | 3 (15%)  |
| 43  | 0TD  | 1l    | 92   | 43       | 4,9,10       | 3.19 | 1 (25%)  | 3,11,13     | 5.60 | 1 (33%)  |
| 1   | 2MA  | 2A    | 2503 | 57,1     | 17,25,26     | 1.36 | 2 (11%)  | 19,37,40    | 2.16 | 3 (15%)  |
| 32  | UR3  | 1a    | 1498 | 32       | 14,22,23     | 0.76 | 0        | 15,32,35    | 0.74 | 0        |
| 32  | MA6  | 2a    | 1519 | 32       | 19,26,27     | 0.83 | 0        | 18,38,41    | 1.62 | 2 (11%)  |
| 1   | PSU  | 1A    | 1911 | 1        | 17,21,22     | 1.53 | 3 (17%)  | 20,30,33    | 3.10 | 7 (35%)  |
| 1   | 5MC  | 1A    | 1942 | 57,1     | 15,22,23     | 1.15 | 1 (6%)   | 19,32,35    | 1.46 | 4 (21%)  |
| 32  | 5MC  | 2a    | 1404 | 32       | 15,22,23     | 1.33 | 1 (6%)   | 19,32,35    | 1.32 | 3 (15%)  |
| 32  | 4OC  | 1a    | 1402 | 32       | 16,23,24     | 0.59 | 0        | 17,32,35    | 1.25 | 2 (11%)  |
| 32  | PSU  | 2a    | 516  | 32,57    | 17,21,22     | 1.74 | 3 (17%)  | 20,30,33    | 3.11 | 7 (35%)  |
| 43  | 0TD  | 2l    | 92   | 43       | 4,9,10       | 2.97 | 1 (25%)  | 3,11,13     | 9.43 | 1 (33%)  |
| 32  | MA6  | 2a    | 1518 | 32       | 19,26,27     | 0.79 | 0        | 18,38,41    | 1.44 | 2 (11%)  |
| 55  | 8AN  | 2x    | 76   | 57,56,55 | 19,24,25     | 1.21 | 3 (15%)  | 13,35,38    | 1.77 | 2 (15%)  |
| 1   | PSU  | 2A    | 1911 | 1        | 17,21,22     | 1.46 | 3 (17%)  | 20,30,33    | 3.18 | 6 (30%)  |
| 1   | 5MU  | 2A    | 1915 | 1        | 15,22,23     | 1.08 | 1 (6%)   | 16,32,35    | 1.97 | 1 (6%)   |
| 32  | 5MC  | 1a    | 967  | 32       | 15,22,23     | 1.24 | 1 (6%)   | 19,32,35    | 1.37 | 2 (10%)  |
| 32  | UR3  | 2a    | 1498 | 32       | 14,22,23     | 0.72 | 0        | 15,32,35    | 0.65 | 0        |
| 1   | PSU  | 1A    | 1917 | 1        | 17,21,22     | 1.51 | 2 (11%)  | 20,30,33    | 3.15 | 6 (30%)  |
| 32  | 5MC  | 1a    | 1400 | 32       | 15,22,23     | 1.30 | 1 (6%)   | 19,32,35    | 1.37 | 3 (15%)  |
| 32  | 5MC  | 2a    | 1407 | 32       | 15,22,23     | 1.36 | 1 (6%)   | 19,32,35    | 1.39 | 2 (10%)  |
| 32  | 2MG  | 2a    | 1207 | 32       | 19,26,27     | 1.15 | 2 (10%)  | 21,38,41    | 2.18 | 7 (33%)  |
| 32  | G7M  | 1a    | 527  | 32,57    | 20,26,27     | 1.51 | 2 (10%)  | 20,39,42    | 2.02 | 4 (20%)  |
| 32  | MA6  | 1a    | 1518 | 32       | 19,26,27     | 0.80 | 0        | 18,38,41    | 1.34 | 2 (11%)  |
| 1   | OMG  | 1A    | 2251 | 1        | 18,26,27     | 1.37 | 2 (11%)  | 20,38,41    | 2.26 | 6 (30%)  |
| 32  | PSU  | 1a    | 516  | 32,57    | 17,21,22     | 1.42 | 3 (17%)  | 20,30,33    | 3.17 | 6 (30%)  |
| 55  | 8AN  | 1x    | 76   | 57,56,55 | 19,24,25     | 1.19 | 3 (15%)  | 13,35,38    | 1.79 | 1 (7%)   |
| 32  | M2G  | 2a    | 966  | 32,57    | 20,27,28     | 1.50 | 3 (15%)  | 22,40,43    | 2.18 | 5 (22%)  |
| 1   | PSU  | 2A    | 1917 | 1        | 17,21,22     | 1.57 | 4 (23%)  | 20,30,33    | 3.12 | 5 (25%)  |
| 1   | OMC  | 1A    | 1920 | 1        | 15,22,23     | 0.70 | 0        | 17,31,34    | 1.47 | 2 (11%)  |
| 32  | 5MC  | 2a    | 1400 | 32       | 15,22,23     | 1.25 | 1 (6%)   | 19,32,35    | 1.36 | 3 (15%)  |
| 1   | PSU  | 1A    | 2605 | 1        | 17,21,22     | 1.65 | 4 (23%)  | 20,30,33    | 3.13 | 6 (30%)  |
| 1   | OMU  | 2A    | 2552 | 57,1     | 14,22,23     | 0.88 | 0        | 14,31,34    | 0.75 | 1 (7%)   |

| Mol | Type | Chain | Res  | Link    | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |         | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | OMG  | 2A    | 2251 | 12,57,1 | 18,26,27     | 1.16 | 2 (11%)  | 20,38,41    | 1.96 | 6 (30%)  |
| 1   | OMC  | 2A    | 1920 | 1       | 15,22,23     | 0.69 | 0        | 17,31,34    | 1.41 | 2 (11%)  |
| 1   | 5MU  | 1A    | 1915 | 1       | 15,22,23     | 1.03 | 1 (6%)   | 16,32,35    | 2.04 | 2 (12%)  |
| 1   | 5MC  | 2A    | 1962 | 1       | 15,22,23     | 1.39 | 1 (6%)   | 19,32,35    | 1.31 | 3 (15%)  |
| 32  | G7M  | 2a    | 527  | 32      | 20,26,27     | 1.51 | 2 (10%)  | 20,39,42    | 2.06 | 4 (20%)  |
| 1   | OMU  | 1A    | 2552 | 57,1    | 14,22,23     | 0.84 | 0        | 14,31,34    | 0.83 | 1 (7%)   |
| 32  | 2MG  | 1a    | 1207 | 32      | 19,26,27     | 1.21 | 2 (10%)  | 21,38,41    | 2.49 | 9 (42%)  |
| 32  | MA6  | 1a    | 1519 | 32      | 19,26,27     | 0.82 | 0        | 18,38,41    | 1.50 | 2 (11%)  |
| 1   | 5MC  | 1A    | 1962 | 57,1    | 15,22,23     | 1.31 | 1 (6%)   | 19,32,35    | 1.21 | 2 (10%)  |

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

| Mol | Type | Chain | Res  | Link     | Chirals | Torsions  | Rings   |
|-----|------|-------|------|----------|---------|-----------|---------|
| 32  | 5MC  | 1a    | 1404 | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1407 | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 1   | PSU  | 2A    | 2605 | 1        | -       | 0/7/25/26 | 0/2/2/2 |
| 32  | 5MC  | 2a    | 967  | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1939 | 1        | -       | 0/5/25/26 | 0/2/2/2 |
| 1   | 5MU  | 2A    | 1939 | 57,1     | -       | 2/5/25/26 | 0/2/2/2 |
| 32  | M2G  | 1a    | 966  | 32       | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | 5MC  | 2A    | 1942 | 1        | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | 4OC  | 2a    | 1402 | 32       | -       | 0/9/29/30 | 0/2/2/2 |
| 1   | 2MA  | 1A    | 2503 | 57,1     | -       | 2/3/25/26 | 0/3/3/3 |
| 43  | 0TD  | 1l    | 92   | 43       | -       | 3/3/12/14 | -       |
| 1   | 2MA  | 2A    | 2503 | 57,1     | -       | 1/3/25/26 | 0/3/3/3 |
| 32  | UR3  | 1a    | 1498 | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | MA6  | 2a    | 1519 | 32       | -       | 2/7/29/30 | 0/3/3/3 |
| 1   | PSU  | 1A    | 1911 | 1        | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | 5MC  | 1A    | 1942 | 57,1     | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1404 | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | 4OC  | 1a    | 1402 | 32       | -       | 2/9/29/30 | 0/2/2/2 |
| 32  | PSU  | 2a    | 516  | 32,57    | -       | 0/7/25/26 | 0/2/2/2 |
| 43  | 0TD  | 2l    | 92   | 43       | -       | 1/3/12/14 | -       |
| 32  | MA6  | 2a    | 1518 | 32       | -       | 0/7/29/30 | 0/3/3/3 |
| 55  | 8AN  | 2x    | 76   | 57,56,55 | -       | 1/3/25/26 | 0/3/3/3 |
| 1   | PSU  | 2A    | 1911 | 1        | -       | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions  | Rings   |
|-----|------|-------|------|----------|---------|-----------|---------|
| 1   | 5MU  | 2A    | 1915 | 1        | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | 5MC  | 1a    | 967  | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | UR3  | 2a    | 1498 | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 1   | PSU  | 1A    | 1917 | 1        | -       | 1/7/25/26 | 0/2/2/2 |
| 32  | 5MC  | 1a    | 1400 | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1407 | 32       | -       | 0/5/25/26 | 0/2/2/2 |
| 32  | 2MG  | 2a    | 1207 | 32       | -       | 2/5/27/28 | 0/3/3/3 |
| 32  | G7M  | 1a    | 527  | 32,57    | -       | 1/3/25/26 | 0/3/3/3 |
| 32  | MA6  | 1a    | 1518 | 32       | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | OMG  | 1A    | 2251 | 1        | -       | 0/5/27/28 | 0/3/3/3 |
| 32  | PSU  | 1a    | 516  | 32,57    | -       | 0/7/25/26 | 0/2/2/2 |
| 55  | 8AN  | 1x    | 76   | 57,56,55 | -       | 1/3/25/26 | 0/3/3/3 |
| 32  | M2G  | 2a    | 966  | 32,57    | -       | 0/7/29/30 | 0/3/3/3 |
| 1   | PSU  | 2A    | 1917 | 1        | -       | 1/7/25/26 | 0/2/2/2 |
| 1   | OMC  | 1A    | 1920 | 1        | -       | 2/7/27/28 | 0/2/2/2 |
| 32  | 5MC  | 2a    | 1400 | 32       | -       | 4/5/25/26 | 0/2/2/2 |
| 1   | PSU  | 1A    | 2605 | 1        | -       | 0/7/25/26 | 0/2/2/2 |
| 1   | OMU  | 2A    | 2552 | 57,1     | -       | 0/7/27/28 | 0/2/2/2 |
| 1   | OMG  | 2A    | 2251 | 12,57,1  | -       | 0/5/27/28 | 0/3/3/3 |
| 1   | OMC  | 2A    | 1920 | 1        | -       | 1/7/27/28 | 0/2/2/2 |
| 1   | 5MU  | 1A    | 1915 | 1        | -       | 0/5/25/26 | 0/2/2/2 |
| 1   | 5MC  | 2A    | 1962 | 1        | -       | 2/5/25/26 | 0/2/2/2 |
| 32  | G7M  | 2a    | 527  | 32       | -       | 3/3/25/26 | 0/3/3/3 |
| 1   | OMU  | 1A    | 2552 | 57,1     | -       | 0/7/27/28 | 0/2/2/2 |
| 32  | 2MG  | 1a    | 1207 | 32       | -       | 0/5/27/28 | 0/3/3/3 |
| 32  | MA6  | 1a    | 1519 | 32       | -       | 2/7/29/30 | 0/3/3/3 |
| 1   | 5MC  | 1A    | 1962 | 57,1     | -       | 2/5/25/26 | 0/2/2/2 |

All (72) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 43  | 1l    | 92   | 0TD  | CB-SB  | -6.05 | 1.69        | 1.84     |
| 43  | 2l    | 92   | 0TD  | CB-SB  | -5.67 | 1.70        | 1.84     |
| 32  | 2a    | 516  | PSU  | C5-C1' | -5.15 | 1.47        | 1.52     |
| 1   | 2A    | 1962 | 5MC  | C5-C4  | 4.98  | 1.49        | 1.41     |
| 32  | 1a    | 527  | G7M  | C5-C4  | 4.91  | 1.46        | 1.39     |
| 32  | 1a    | 1404 | 5MC  | C5-C4  | 4.86  | 1.48        | 1.41     |
| 32  | 2a    | 1407 | 5MC  | C5-C4  | 4.79  | 1.48        | 1.41     |
| 32  | 2a    | 967  | 5MC  | C5-C4  | 4.76  | 1.48        | 1.41     |
| 1   | 2A    | 1942 | 5MC  | C5-C4  | 4.76  | 1.48        | 1.41     |
| 1   | 2A    | 2503 | 2MA  | C5-C6  | 4.75  | 1.48        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 32  | 2a    | 1404 | 5MC  | C5-C4  | 4.75  | 1.48        | 1.41     |
| 32  | 1a    | 1407 | 5MC  | C5-C4  | 4.65  | 1.48        | 1.41     |
| 32  | 2a    | 527  | G7M  | C5-C4  | 4.64  | 1.46        | 1.39     |
| 1   | 1A    | 1962 | 5MC  | C5-C4  | 4.62  | 1.48        | 1.41     |
| 32  | 1a    | 1400 | 5MC  | C5-C4  | 4.52  | 1.48        | 1.41     |
| 1   | 1A    | 2251 | OMG  | C5-C6  | 4.46  | 1.49        | 1.41     |
| 32  | 1a    | 967  | 5MC  | C5-C4  | 4.44  | 1.48        | 1.41     |
| 32  | 2a    | 1400 | 5MC  | C5-C4  | 4.37  | 1.48        | 1.41     |
| 32  | 2a    | 966  | M2G  | C5-C6  | 4.37  | 1.48        | 1.41     |
| 1   | 2A    | 2605 | PSU  | C5-C1' | -4.33 | 1.48        | 1.52     |
| 1   | 1A    | 2605 | PSU  | C5-C1' | -4.32 | 1.48        | 1.52     |
| 32  | 1a    | 966  | M2G  | C5-C6  | 4.27  | 1.48        | 1.41     |
| 32  | 1a    | 1207 | 2MG  | C5-C6  | 4.16  | 1.48        | 1.41     |
| 32  | 2a    | 527  | G7M  | C5-C6  | 4.14  | 1.48        | 1.41     |
| 1   | 1A    | 1911 | PSU  | C5-C1' | -4.09 | 1.48        | 1.52     |
| 1   | 1A    | 2503 | 2MA  | C5-C6  | 4.06  | 1.47        | 1.41     |
| 32  | 2a    | 1207 | 2MG  | C5-C6  | 4.05  | 1.48        | 1.41     |
| 1   | 1A    | 1942 | 5MC  | C5-C4  | 4.03  | 1.47        | 1.41     |
| 1   | 2A    | 1917 | PSU  | C5-C1' | -3.90 | 1.48        | 1.52     |
| 32  | 1a    | 527  | G7M  | C5-C6  | 3.85  | 1.48        | 1.41     |
| 1   | 2A    | 2251 | OMG  | C5-C6  | 3.80  | 1.47        | 1.41     |
| 1   | 1A    | 1917 | PSU  | C5-C1' | -3.78 | 1.49        | 1.52     |
| 32  | 2a    | 966  | M2G  | C2-N2  | 3.73  | 1.41        | 1.34     |
| 1   | 2A    | 1911 | PSU  | C5-C4  | 3.63  | 1.49        | 1.41     |
| 1   | 1A    | 1917 | PSU  | C5-C4  | 3.60  | 1.49        | 1.41     |
| 1   | 2A    | 1917 | PSU  | C5-C4  | 3.55  | 1.49        | 1.41     |
| 32  | 1a    | 516  | PSU  | C5-C4  | 3.50  | 1.49        | 1.41     |
| 1   | 2A    | 1915 | 5MU  | C5-C4  | 3.47  | 1.48        | 1.41     |
| 32  | 1a    | 966  | M2G  | C2-N2  | 3.43  | 1.40        | 1.34     |
| 1   | 1A    | 1939 | 5MU  | C5-C4  | 3.43  | 1.48        | 1.41     |
| 1   | 2A    | 1939 | 5MU  | C5-C4  | 3.40  | 1.48        | 1.41     |
| 32  | 2a    | 516  | PSU  | C5-C4  | 3.31  | 1.48        | 1.41     |
| 1   | 2A    | 2605 | PSU  | C5-C4  | 3.31  | 1.48        | 1.41     |
| 1   | 1A    | 1911 | PSU  | C5-C4  | 3.29  | 1.48        | 1.41     |
| 1   | 1A    | 1915 | 5MU  | C5-C4  | 3.24  | 1.48        | 1.41     |
| 1   | 1A    | 2605 | PSU  | C5-C4  | 3.24  | 1.48        | 1.41     |
| 1   | 2A    | 1911 | PSU  | C5-C1' | -3.22 | 1.49        | 1.52     |
| 32  | 1a    | 516  | PSU  | C5-C1' | -3.00 | 1.49        | 1.52     |
| 55  | 2x    | 76   | 8AN  | C5-C4  | -2.83 | 1.33        | 1.40     |
| 55  | 1x    | 76   | 8AN  | C5-C4  | -2.75 | 1.33        | 1.40     |
| 32  | 2a    | 966  | M2G  | C5-C4  | 2.65  | 1.47        | 1.40     |
| 1   | 1A    | 2605 | PSU  | C2-N3  | -2.63 | 1.32        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | 1A    | 2251 | OMG  | C5-C4   | 2.59  | 1.47        | 1.40     |
| 55  | 2x    | 76   | 8AN  | C6-C5   | -2.58 | 1.33        | 1.43     |
| 1   | 2A    | 2251 | OMG  | C5-C4   | 2.54  | 1.47        | 1.40     |
| 32  | 1a    | 966  | M2G  | C5-C4   | 2.50  | 1.47        | 1.40     |
| 55  | 1x    | 76   | 8AN  | C6-C5   | -2.40 | 1.34        | 1.43     |
| 32  | 2a    | 516  | PSU  | O4'-C1' | -2.40 | 1.41        | 1.44     |
| 32  | 2a    | 1207 | 2MG  | C5-C4   | 2.31  | 1.47        | 1.40     |
| 32  | 1a    | 1207 | 2MG  | C5-C4   | 2.23  | 1.46        | 1.40     |
| 1   | 2A    | 2503 | 2MA  | C5-C4   | 2.21  | 1.46        | 1.40     |
| 1   | 1A    | 2503 | 2MA  | C5-C4   | 2.20  | 1.46        | 1.40     |
| 1   | 2A    | 2605 | PSU  | C2-N3   | -2.19 | 1.33        | 1.38     |
| 1   | 1A    | 2605 | PSU  | C2-N1   | -2.17 | 1.33        | 1.38     |
| 55  | 1x    | 76   | 8AN  | C5-N7   | -2.15 | 1.31        | 1.39     |
| 1   | 2A    | 1911 | PSU  | C2-N3   | -2.14 | 1.33        | 1.38     |
| 32  | 1a    | 516  | PSU  | O4'-C1' | -2.14 | 1.41        | 1.44     |
| 1   | 2A    | 1917 | PSU  | C2-N1   | -2.09 | 1.34        | 1.38     |
| 1   | 1A    | 1911 | PSU  | O4'-C1' | -2.08 | 1.41        | 1.44     |
| 55  | 2x    | 76   | 8AN  | C5-N7   | -2.06 | 1.32        | 1.39     |
| 1   | 2A    | 1917 | PSU  | O4'-C1' | -2.06 | 1.41        | 1.44     |
| 1   | 2A    | 2605 | PSU  | C2-N1   | -2.01 | 1.34        | 1.38     |

All (163) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 43  | 2l    | 92   | 0TD  | CSB-SB-CB | 16.27 | 133.86      | 101.85   |
| 43  | 1l    | 92   | 0TD  | CSB-SB-CB | 9.61  | 120.76      | 101.85   |
| 32  | 1a    | 516  | PSU  | N3-C2-N1  | -9.06 | 121.23      | 128.43   |
| 1   | 2A    | 2605 | PSU  | N3-C2-N1  | -8.97 | 121.30      | 128.43   |
| 1   | 1A    | 1917 | PSU  | N3-C2-N1  | -8.80 | 121.44      | 128.43   |
| 1   | 2A    | 1911 | PSU  | N3-C2-N1  | -8.58 | 121.61      | 128.43   |
| 1   | 2A    | 1917 | PSU  | N3-C2-N1  | -8.51 | 121.66      | 128.43   |
| 1   | 1A    | 1911 | PSU  | N3-C2-N1  | -8.41 | 121.75      | 128.43   |
| 1   | 1A    | 2605 | PSU  | N3-C2-N1  | -7.94 | 122.12      | 128.43   |
| 32  | 2a    | 516  | PSU  | N3-C2-N1  | -7.90 | 122.15      | 128.43   |
| 1   | 1A    | 1915 | 5MU  | C2-N3-C4  | 7.36  | 121.35      | 115.14   |
| 1   | 2A    | 1915 | 5MU  | C2-N3-C4  | 7.23  | 121.25      | 115.14   |
| 32  | 1a    | 516  | PSU  | C2-N3-C4  | 7.12  | 121.16      | 115.14   |
| 1   | 2A    | 1917 | PSU  | C2-N3-C4  | 7.06  | 121.11      | 115.14   |
| 1   | 1A    | 1939 | 5MU  | C2-N3-C4  | 7.03  | 121.08      | 115.14   |
| 1   | 2A    | 1911 | PSU  | C2-N3-C4  | 6.79  | 120.88      | 115.14   |
| 1   | 1A    | 1917 | PSU  | C2-N3-C4  | 6.72  | 120.82      | 115.14   |
| 1   | 2A    | 1939 | 5MU  | C2-N3-C4  | 6.67  | 120.77      | 115.14   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | 1A    | 1911 | PSU  | C2-N3-C4   | 6.64  | 120.75      | 115.14   |
| 1   | 2A    | 2503 | 2MA  | C2-N3-C4   | 6.64  | 120.92      | 115.52   |
| 1   | 2A    | 2605 | PSU  | C2-N3-C4   | 6.60  | 120.72      | 115.14   |
| 32  | 2a    | 516  | PSU  | C2-N3-C4   | 6.53  | 120.65      | 115.14   |
| 1   | 1A    | 2503 | 2MA  | C2-N3-C4   | 6.51  | 120.81      | 115.52   |
| 1   | 1A    | 2605 | PSU  | C2-N3-C4   | 5.99  | 120.20      | 115.14   |
| 55  | 1x    | 76   | 8AN  | N3-C2-N1   | -5.79 | 119.63      | 128.68   |
| 32  | 2a    | 516  | PSU  | C5-C4-N3   | -5.78 | 117.91      | 125.36   |
| 1   | 2A    | 1917 | PSU  | C5-C4-N3   | -5.63 | 118.11      | 125.36   |
| 55  | 2x    | 76   | 8AN  | N3-C2-N1   | -5.54 | 120.02      | 128.68   |
| 32  | 2a    | 966  | M2G  | C2-N1-C6   | 5.53  | 122.77      | 116.18   |
| 32  | 1a    | 527  | G7M  | C5-C6-N1   | -5.53 | 115.87      | 123.43   |
| 32  | 2a    | 527  | G7M  | C5-C6-N1   | -5.31 | 116.17      | 123.43   |
| 32  | 1a    | 966  | M2G  | C2-N1-C6   | 5.28  | 122.47      | 116.18   |
| 32  | 1a    | 966  | M2G  | C2-N3-C4   | 5.20  | 121.18      | 115.28   |
| 1   | 1A    | 1911 | PSU  | C5-C4-N3   | -5.19 | 118.67      | 125.36   |
| 32  | 1a    | 516  | PSU  | C5-C4-N3   | -5.18 | 118.68      | 125.36   |
| 1   | 1A    | 2251 | OMG  | C2-N3-C4   | 5.16  | 121.25      | 115.36   |
| 1   | 1A    | 1917 | PSU  | C5-C4-N3   | -5.13 | 118.75      | 125.36   |
| 1   | 2A    | 2605 | PSU  | C5-C4-N3   | -5.03 | 118.89      | 125.36   |
| 1   | 2A    | 2251 | OMG  | C2-N3-C4   | 5.01  | 121.08      | 115.36   |
| 1   | 1A    | 2605 | PSU  | C5-C6-N1   | -4.90 | 118.42      | 124.44   |
| 1   | 2A    | 1911 | PSU  | C5-C4-N3   | -4.83 | 119.14      | 125.36   |
| 32  | 1a    | 1207 | 2MG  | C2-N3-C4   | 4.83  | 120.76      | 115.28   |
| 32  | 2a    | 1519 | MA6  | N3-C2-N1   | -4.82 | 121.14      | 128.68   |
| 1   | 1A    | 2605 | PSU  | C5-C4-N3   | -4.81 | 119.16      | 125.36   |
| 32  | 2a    | 966  | M2G  | C2-N3-C4   | 4.78  | 120.71      | 115.28   |
| 32  | 2a    | 1518 | MA6  | N3-C2-N1   | -4.76 | 121.24      | 128.68   |
| 32  | 1a    | 1518 | MA6  | N3-C2-N1   | -4.72 | 121.30      | 128.68   |
| 32  | 1a    | 1519 | MA6  | N3-C2-N1   | -4.70 | 121.33      | 128.68   |
| 1   | 2A    | 2605 | PSU  | C6-N1-C2   | 4.61  | 122.97      | 115.36   |
| 32  | 2a    | 1207 | 2MG  | C5-C6-N1   | -4.59 | 117.16      | 123.43   |
| 1   | 2A    | 2503 | 2MA  | C5-C6-N1   | -4.57 | 118.27      | 123.06   |
| 1   | 1A    | 2503 | 2MA  | C5-C6-N1   | -4.56 | 118.27      | 123.06   |
| 1   | 1A    | 2605 | PSU  | C5-C1'-C2' | -4.56 | 107.19      | 115.32   |
| 32  | 2a    | 516  | PSU  | C5-C6-N1   | -4.50 | 118.90      | 124.44   |
| 32  | 1a    | 527  | G7M  | C2-N1-C6   | 4.49  | 123.07      | 115.93   |
| 32  | 1a    | 1207 | 2MG  | C4-C5-C6   | -4.47 | 116.53      | 120.80   |
| 32  | 2a    | 527  | G7M  | C2-N3-C4   | 4.42  | 120.41      | 115.36   |
| 1   | 2A    | 2605 | PSU  | C5-C6-N1   | -4.41 | 119.01      | 124.44   |
| 1   | 1A    | 2605 | PSU  | C6-N1-C2   | 4.40  | 122.62      | 115.36   |
| 32  | 2a    | 966  | M2G  | C5-C6-N1   | -4.38 | 117.44      | 123.43   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 32  | 2a    | 1207 | 2MG  | C2-N3-C4   | 4.38  | 120.25      | 115.28   |
| 32  | 2a    | 527  | G7M  | C2-N1-C6   | 4.35  | 122.84      | 115.93   |
| 1   | 2A    | 1920 | OMC  | C4-N3-C2   | 4.31  | 120.71      | 116.34   |
| 32  | 1a    | 1207 | 2MG  | C2-N1-C6   | 4.30  | 122.88      | 115.18   |
| 1   | 1A    | 1917 | PSU  | C6-N1-C2   | 4.28  | 122.42      | 115.36   |
| 1   | 1A    | 1920 | OMC  | C4-N3-C2   | 4.25  | 120.65      | 116.34   |
| 32  | 1a    | 516  | PSU  | C6-N1-C2   | 4.24  | 122.35      | 115.36   |
| 1   | 1A    | 2251 | OMG  | C5-C6-N1   | -4.20 | 117.69      | 123.43   |
| 1   | 2A    | 1911 | PSU  | C6-N1-C2   | 4.20  | 122.29      | 115.36   |
| 32  | 2a    | 1207 | 2MG  | C2-N1-C6   | 4.19  | 122.68      | 115.18   |
| 32  | 1a    | 1207 | 2MG  | C5-C6-N1   | -4.15 | 117.76      | 123.43   |
| 1   | 2A    | 1911 | PSU  | C5-C6-N1   | -4.14 | 119.35      | 124.44   |
| 1   | 1A    | 1911 | PSU  | C5-C6-N1   | -4.12 | 119.37      | 124.44   |
| 1   | 1A    | 1911 | PSU  | C6-N1-C2   | 4.08  | 122.09      | 115.36   |
| 32  | 2a    | 516  | PSU  | C6-N1-C2   | 4.07  | 122.07      | 115.36   |
| 32  | 1a    | 966  | M2G  | C5-C6-N1   | -3.99 | 117.97      | 123.43   |
| 32  | 1a    | 966  | M2G  | C4-C5-C6   | -3.97 | 117.01      | 120.80   |
| 1   | 1A    | 1917 | PSU  | C5-C6-N1   | -3.96 | 119.57      | 124.44   |
| 32  | 2a    | 1407 | 5MC  | C4-N3-C2   | 3.95  | 120.79      | 116.02   |
| 1   | 1A    | 2251 | OMG  | C2-N1-C6   | 3.92  | 122.16      | 115.93   |
| 32  | 1a    | 1207 | 2MG  | CM2-N2-C2  | -3.90 | 118.88      | 123.59   |
| 1   | 2A    | 1917 | PSU  | C6-N1-C2   | 3.90  | 121.79      | 115.36   |
| 32  | 1a    | 527  | G7M  | C2-N3-C4   | 3.87  | 119.78      | 115.36   |
| 32  | 1a    | 516  | PSU  | C5-C6-N1   | -3.80 | 119.77      | 124.44   |
| 32  | 1a    | 967  | 5MC  | C4-N3-C2   | 3.79  | 120.60      | 116.02   |
| 1   | 2A    | 2251 | OMG  | C5-C6-N1   | -3.79 | 118.24      | 123.43   |
| 1   | 2A    | 1911 | PSU  | C5-C1'-C2' | -3.74 | 108.64      | 115.32   |
| 32  | 2a    | 1207 | 2MG  | C4-C5-C6   | -3.74 | 117.23      | 120.80   |
| 1   | 1A    | 2251 | OMG  | C4-C5-N7   | -3.71 | 105.53      | 109.40   |
| 32  | 1a    | 1404 | 5MC  | C4-N3-C2   | 3.69  | 120.47      | 116.02   |
| 32  | 1a    | 1407 | 5MC  | C4-N3-C2   | 3.66  | 120.44      | 116.02   |
| 32  | 2a    | 967  | 5MC  | C4-N3-C2   | 3.64  | 120.41      | 116.02   |
| 32  | 1a    | 1402 | 4OC  | CM4-N4-C4  | -3.62 | 119.86      | 122.97   |
| 32  | 2a    | 1519 | MA6  | C4-C5-N7   | -3.55 | 105.70      | 109.40   |
| 1   | 1A    | 1942 | 5MC  | C4-N3-C2   | 3.53  | 120.28      | 116.02   |
| 1   | 2A    | 1962 | 5MC  | C4-N3-C2   | 3.50  | 120.24      | 116.02   |
| 32  | 2a    | 1404 | 5MC  | C4-N3-C2   | 3.46  | 120.20      | 116.02   |
| 32  | 2a    | 1400 | 5MC  | C4-N3-C2   | 3.46  | 120.19      | 116.02   |
| 1   | 1A    | 2251 | OMG  | C4-C5-C6   | -3.44 | 117.51      | 120.80   |
| 32  | 1a    | 1400 | 5MC  | C4-N3-C2   | 3.43  | 120.16      | 116.02   |
| 32  | 2a    | 966  | M2G  | C4-C5-C6   | -3.40 | 117.55      | 120.80   |
| 1   | 2A    | 1917 | PSU  | C5-C6-N1   | -3.32 | 120.36      | 124.44   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1A    | 1962 | 5MC  | C4-N3-C2    | 3.31  | 120.02      | 116.02   |
| 32  | 1a    | 1519 | MA6  | C4-C5-N7    | -3.31 | 105.95      | 109.40   |
| 1   | 2A    | 2251 | OMG  | C2-N1-C6    | 3.31  | 121.19      | 115.93   |
| 1   | 2A    | 1942 | 5MC  | C4-N3-C2    | 3.30  | 120.01      | 116.02   |
| 1   | 2A    | 2605 | PSU  | C5-C1'-C2'  | -3.30 | 109.43      | 115.32   |
| 1   | 1A    | 1911 | PSU  | C5-C1'-C2'  | -3.21 | 109.60      | 115.32   |
| 32  | 2a    | 1402 | 4OC  | CM4-N4-C4   | -3.20 | 120.22      | 122.97   |
| 32  | 1a    | 1207 | 2MG  | C4-C5-N7    | -3.17 | 106.09      | 109.40   |
| 1   | 2A    | 2503 | 2MA  | C4-C5-N7    | -3.15 | 106.12      | 109.40   |
| 1   | 1A    | 2251 | OMG  | N3-C2-N1    | -3.09 | 123.11      | 127.22   |
| 32  | 2a    | 1400 | 5MC  | N4-C4-N3    | 3.04  | 121.32      | 117.03   |
| 32  | 1a    | 527  | G7M  | N3-C2-N1    | -2.99 | 123.23      | 127.22   |
| 32  | 2a    | 527  | G7M  | N3-C2-N1    | -2.97 | 123.26      | 127.22   |
| 32  | 2a    | 1518 | MA6  | C4-C5-N7    | -2.97 | 106.31      | 109.40   |
| 32  | 1a    | 1207 | 2MG  | N2-C2-N1    | 2.87  | 119.71      | 116.96   |
| 32  | 1a    | 1407 | 5MC  | N4-C4-N3    | 2.84  | 121.05      | 117.03   |
| 32  | 1a    | 966  | M2G  | C4-C5-N7    | -2.84 | 106.44      | 109.40   |
| 32  | 1a    | 967  | 5MC  | N4-C4-N3    | 2.81  | 121.00      | 117.03   |
| 32  | 1a    | 1400 | 5MC  | C5-C6-N1    | -2.78 | 119.19      | 122.19   |
| 1   | 1A    | 1942 | 5MC  | N4-C4-N3    | 2.78  | 120.97      | 117.03   |
| 1   | 2A    | 1942 | 5MC  | C5-C6-N1    | -2.78 | 119.20      | 122.19   |
| 1   | 2A    | 1962 | 5MC  | N4-C4-N3    | 2.78  | 120.96      | 117.03   |
| 32  | 2a    | 1207 | 2MG  | C4-C5-N7    | -2.72 | 106.57      | 109.40   |
| 1   | 1A    | 1917 | PSU  | C5-C1'-C2'  | -2.71 | 110.49      | 115.32   |
| 1   | 2A    | 2251 | OMG  | N3-C2-N1    | -2.70 | 123.63      | 127.22   |
| 1   | 2A    | 1942 | 5MC  | N4-C4-N3    | 2.69  | 120.84      | 117.03   |
| 32  | 1a    | 1207 | 2MG  | C1'-N9-C4   | -2.69 | 121.92      | 126.64   |
| 32  | 2a    | 1207 | 2MG  | CM2-N2-C2   | -2.68 | 120.36      | 123.59   |
| 32  | 2a    | 966  | M2G  | C4-C5-N7    | -2.65 | 106.64      | 109.40   |
| 1   | 1A    | 1920 | OMC  | N4-C4-N3    | 2.58  | 120.57      | 116.49   |
| 55  | 2x    | 76   | 8AN  | O4'-C1'-C2' | -2.58 | 103.16      | 106.93   |
| 1   | 1A    | 1962 | 5MC  | C5-C6-N1    | -2.58 | 119.42      | 122.19   |
| 1   | 2A    | 2251 | OMG  | C4-C5-N7    | -2.55 | 106.74      | 109.40   |
| 1   | 1A    | 2503 | 2MA  | C4-C5-N7    | -2.53 | 106.77      | 109.40   |
| 1   | 1A    | 1939 | 5MU  | C5-C6-N1    | -2.53 | 119.47      | 122.19   |
| 1   | 2A    | 2552 | OMU  | C5-C4-N3    | -2.52 | 117.77      | 123.31   |
| 32  | 2a    | 1404 | 5MC  | N4-C4-N3    | 2.49  | 120.56      | 117.03   |
| 32  | 1a    | 1400 | 5MC  | N4-C4-N3    | 2.46  | 120.52      | 117.03   |
| 1   | 2A    | 2251 | OMG  | C4-C5-C6    | -2.43 | 118.48      | 120.80   |
| 1   | 2A    | 1920 | OMC  | N4-C4-N3    | 2.42  | 120.32      | 116.49   |
| 32  | 2a    | 516  | PSU  | O4'-C1'-C2' | 2.42  | 108.58      | 104.66   |
| 32  | 2a    | 967  | 5MC  | N4-C4-N3    | 2.38  | 120.40      | 117.03   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 32  | 2a    | 1407 | 5MC  | N4-C4-N3    | 2.38  | 120.39      | 117.03   |
| 32  | 2a    | 1207 | 2MG  | N2-C2-N1    | 2.36  | 119.23      | 116.96   |
| 32  | 1a    | 1407 | 5MC  | CM5-C5-C4   | -2.36 | 119.34      | 121.72   |
| 32  | 2a    | 1400 | 5MC  | C5-C6-N1    | -2.35 | 119.66      | 122.19   |
| 32  | 1a    | 1207 | 2MG  | N3-C2-N1    | -2.35 | 122.52      | 126.23   |
| 1   | 1A    | 1942 | 5MC  | C5-C6-N1    | -2.32 | 119.69      | 122.19   |
| 32  | 1a    | 1518 | MA6  | C4-C5-N7    | -2.30 | 107.00      | 109.40   |
| 32  | 2a    | 967  | 5MC  | C5-C6-N1    | -2.29 | 119.73      | 122.19   |
| 1   | 1A    | 2552 | OMU  | C5-C4-N3    | -2.27 | 118.31      | 123.31   |
| 1   | 1A    | 1942 | 5MC  | CM5-C5-C4   | -2.26 | 119.44      | 121.72   |
| 32  | 2a    | 1404 | 5MC  | C5-C6-N1    | -2.26 | 119.76      | 122.19   |
| 1   | 1A    | 1915 | 5MU  | C6-N1-C1'   | -2.26 | 114.17      | 119.24   |
| 32  | 1a    | 966  | M2G  | N1-C2-N2    | 2.22  | 119.44      | 117.19   |
| 32  | 2a    | 516  | PSU  | C5-C1'-C2'  | -2.15 | 111.48      | 115.32   |
| 32  | 1a    | 1402 | 4OC  | C5-C4-N3    | -2.11 | 119.61      | 123.16   |
| 32  | 1a    | 516  | PSU  | O4'-C1'-C2' | 2.09  | 108.05      | 104.66   |
| 1   | 2A    | 1939 | 5MU  | C5-C6-N1    | -2.08 | 119.95      | 122.19   |
| 1   | 2A    | 1962 | 5MC  | C5-C6-N1    | -2.08 | 119.95      | 122.19   |
| 1   | 1A    | 1911 | PSU  | O4'-C1'-C2' | 2.08  | 108.03      | 104.66   |

There are no chirality outliers.

All (36) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 1   | 1A    | 1920 | OMC  | C2'-C1'-N1-C6   |
| 1   | 1A    | 1962 | 5MC  | O4'-C1'-N1-C6   |
| 1   | 1A    | 1962 | 5MC  | C2'-C1'-N1-C6   |
| 43  | 1l    | 92   | 0TD  | O-C-CA-CB       |
| 43  | 1l    | 92   | 0TD  | CG-CB-SB-CSB    |
| 1   | 2A    | 1939 | 5MU  | C2'-C1'-N1-C6   |
| 1   | 2A    | 1939 | 5MU  | O4'-C1'-N1-C6   |
| 1   | 2A    | 1962 | 5MC  | O4'-C1'-N1-C6   |
| 1   | 2A    | 1962 | 5MC  | C2'-C1'-N1-C6   |
| 32  | 2a    | 1207 | 2MG  | N1-C2-N2-CM2    |
| 32  | 2a    | 1207 | 2MG  | N3-C2-N2-CM2    |
| 32  | 2a    | 1400 | 5MC  | O4'-C1'-N1-C6   |
| 32  | 2a    | 1400 | 5MC  | C2'-C1'-N1-C6   |
| 43  | 2l    | 92   | 0TD  | CG-CB-SB-CSB    |
| 32  | 2a    | 1400 | 5MC  | C3'-C4'-C5'-O5' |
| 32  | 1a    | 1402 | 4OC  | O4'-C4'-C5'-O5' |
| 32  | 1a    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 32  | 2a    | 1400 | 5MC  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 55  | 1x    | 76   | 8AN  | C4'-C5'-O5'-P   |
| 32  | 1a    | 1402 | 4OC  | C3'-C4'-C5'-O5' |
| 32  | 1a    | 1519 | MA6  | C3'-C4'-C5'-O5' |
| 55  | 2x    | 76   | 8AN  | C4'-C5'-O5'-P   |
| 32  | 2a    | 527  | G7M  | C3'-C4'-C5'-O5' |
| 32  | 2a    | 1519 | MA6  | O4'-C4'-C5'-O5' |
| 32  | 1a    | 527  | G7M  | C3'-C4'-C5'-O5' |
| 1   | 2A    | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 2503 | 2MA  | C4'-C5'-O5'-P   |
| 1   | 1A    | 2503 | 2MA  | O4'-C4'-C5'-O5' |
| 1   | 1A    | 1920 | OMC  | C3'-C2'-O2'-CM2 |
| 1   | 2A    | 1920 | OMC  | C3'-C2'-O2'-CM2 |
| 43  | 1l    | 92   | 0TD  | CA-CB-SB-CSB    |
| 32  | 2a    | 527  | G7M  | C4'-C5'-O5'-P   |
| 1   | 1A    | 1917 | PSU  | C2'-C1'-C5-C6   |
| 1   | 2A    | 1917 | PSU  | C2'-C1'-C5-C6   |
| 32  | 2a    | 527  | G7M  | O4'-C4'-C5'-O5' |
| 32  | 2a    | 1519 | MA6  | C3'-C4'-C5'-O5' |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2510 ligands modelled in this entry, 2498 are monoatomic - leaving 12 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$ |
| 60  | CLM  | 2z    | 1   | -    | 19,20,20     | 0.95 | 1 (5%)      | 23,27,27    | 0.92 | 1 (4%)      |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 62  | MPD  | 1z    | 2003 | -    | 7,7,7        | 0.27 | 0        | 9,10,10     | 0.22 | 0        |
| 62  | MPD  | 2z    | 2002 | -    | 7,7,7        | 0.31 | 0        | 9,10,10     | 0.33 | 0        |
| 62  | MPD  | 2z    | 2003 | -    | 7,7,7        | 0.24 | 0        | 9,10,10     | 0.19 | 0        |
| 62  | MPD  | 1z    | 2002 | -    | 7,7,7        | 0.27 | 0        | 9,10,10     | 0.19 | 0        |
| 61  | ARG  | 1z    | 1001 | 57   | 7,11,11      | 0.27 | 0        | 6,13,13     | 0.36 | 0        |
| 62  | MPD  | 1z    | 2001 | -    | 7,7,7        | 0.26 | 0        | 9,10,10     | 0.17 | 0        |
| 61  | ARG  | 1z    | 1003 | -    | 7,11,11      | 0.28 | 0        | 6,13,13     | 0.35 | 0        |
| 62  | MPD  | 1z    | 2004 | -    | 7,7,7        | 0.37 | 0        | 9,10,10     | 0.58 | 0        |
| 59  | SF4  | 2d    | 501  | 35   | 0,12,12      | -    | -        | -           | -    | -        |
| 59  | SF4  | 1d    | 501  | 35   | 0,12,12      | -    | -        | -           | -    | -        |
| 60  | CLM  | 1z    | 1    | -    | 19,20,20     | 1.06 | 1 (5%)   | 23,27,27    | 1.21 | 3 (13%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 60  | CLM  | 2z    | 1    | -    | -       | 0/20/22/22 | 0/1/1/1 |
| 62  | MPD  | 1z    | 2003 | -    | -       | 1/5/5/5    | -       |
| 62  | MPD  | 2z    | 2002 | -    | -       | 2/5/5/5    | -       |
| 62  | MPD  | 2z    | 2003 | -    | -       | 2/5/5/5    | -       |
| 62  | MPD  | 1z    | 2002 | -    | -       | 1/5/5/5    | -       |
| 61  | ARG  | 1z    | 1001 | 57   | -       | 1/7/11/11  | -       |
| 62  | MPD  | 1z    | 2001 | -    | -       | 0/5/5/5    | -       |
| 61  | ARG  | 1z    | 1003 | -    | -       | 1/7/11/11  | -       |
| 62  | MPD  | 1z    | 2004 | -    | -       | 3/5/5/5    | -       |
| 59  | SF4  | 2d    | 501  | 35   | -       | -          | 0/6/5/5 |
| 59  | SF4  | 1d    | 501  | 35   | -       | -          | 0/6/5/5 |
| 60  | CLM  | 1z    | 1    | -    | -       | 4/20/22/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 60  | 1z    | 1   | CLM  | C6-C5 | -2.38 | 1.48        | 1.51     |
| 60  | 2z    | 1   | CLM  | C6-C5 | -2.24 | 1.48        | 1.51     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 60  | 1z    | 1   | CLM  | C10-C9-N9 | 2.93 | 121.58      | 119.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 60  | 2z    | 1   | CLM  | C8-C9-N9 | 2.29  | 121.10      | 119.38   |
| 60  | 1z    | 1   | CLM  | O5-C5-C6 | -2.19 | 106.42      | 111.19   |
| 60  | 1z    | 1   | CLM  | C3-N2-C2 | -2.18 | 119.22      | 123.07   |

There are no chirality outliers.

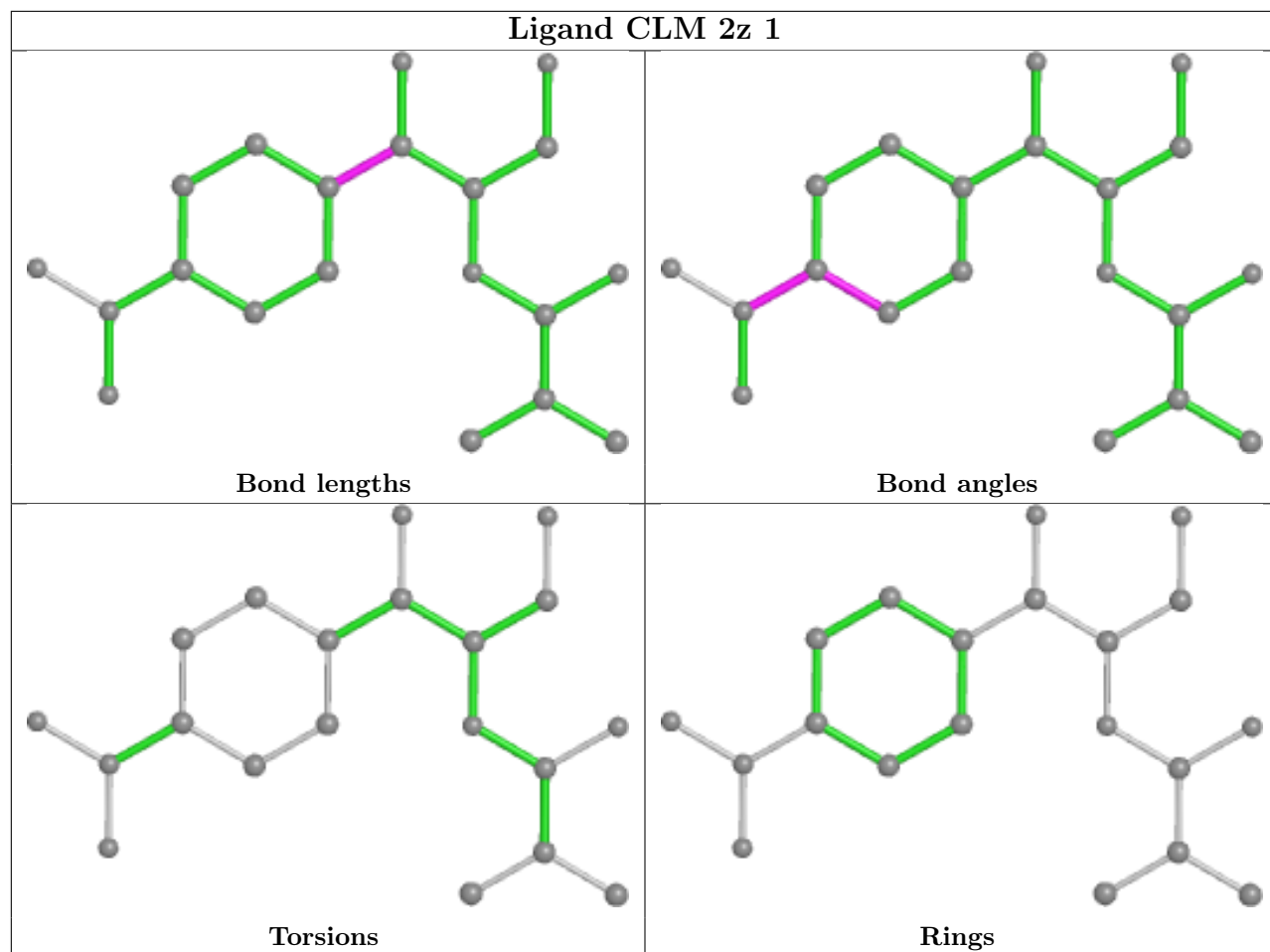
All (15) torsion outliers are listed below:

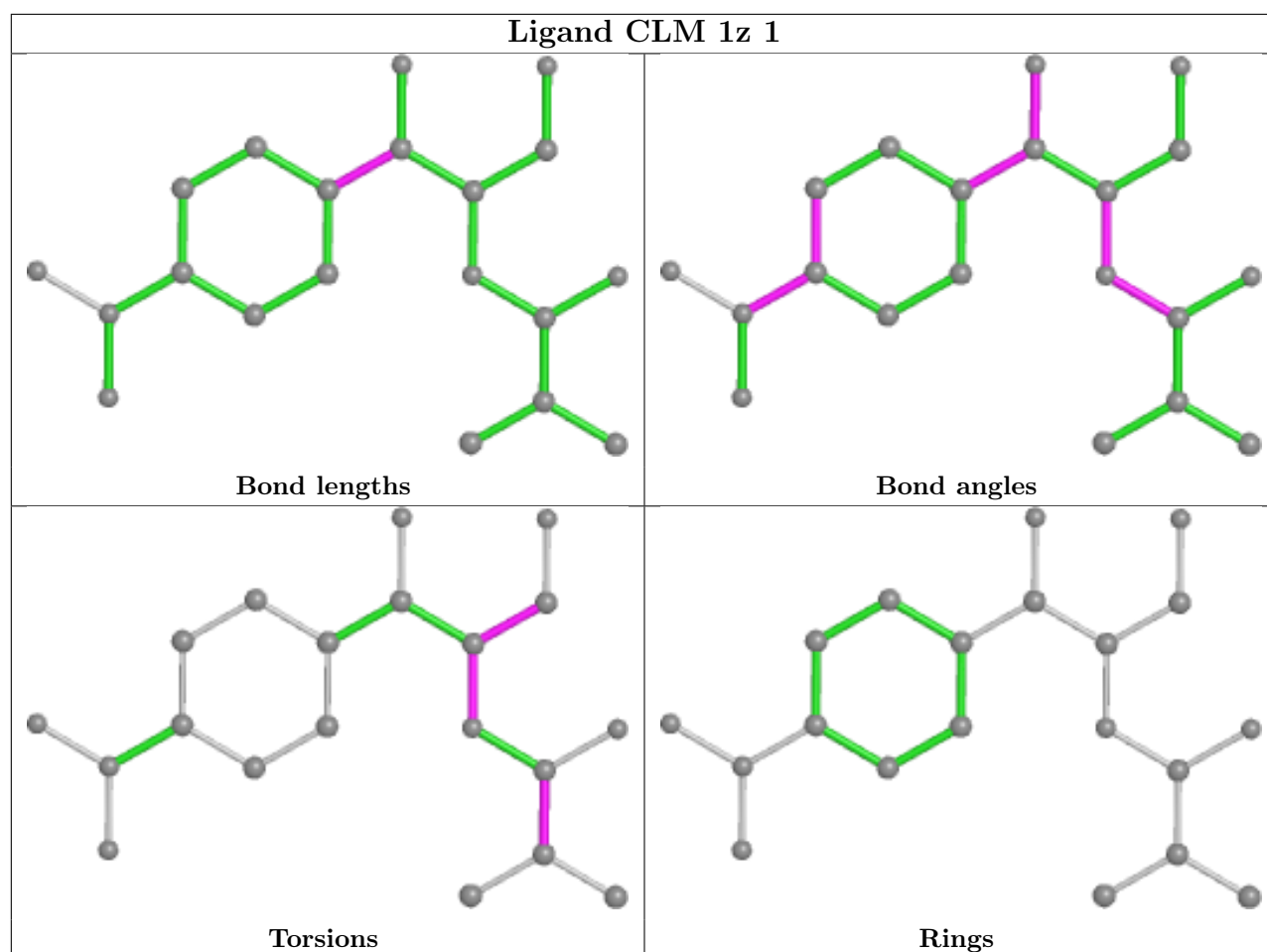
| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 60  | 1z    | 1    | CLM  | C5-C3-N2-C2  |
| 61  | 1z    | 1003 | ARG  | CA-CB-CG-CD  |
| 60  | 1z    | 1    | CLM  | C5-C3-C4-O4  |
| 60  | 1z    | 1    | CLM  | N2-C3-C4-O4  |
| 60  | 1z    | 1    | CLM  | CL2-C1-C2-N2 |
| 61  | 1z    | 1001 | ARG  | CA-CB-CG-CD  |
| 62  | 1z    | 2004 | MPD  | O2-C2-C3-C4  |
| 62  | 1z    | 2003 | MPD  | C2-C3-C4-C5  |
| 62  | 2z    | 2002 | MPD  | C2-C3-C4-C5  |
| 62  | 2z    | 2003 | MPD  | O2-C2-C3-C4  |
| 62  | 1z    | 2002 | MPD  | C2-C3-C4-C5  |
| 62  | 1z    | 2004 | MPD  | C2-C3-C4-C5  |
| 62  | 2z    | 2003 | MPD  | C2-C3-C4-C5  |
| 62  | 1z    | 2004 | MPD  | C2-C3-C4-O4  |
| 62  | 2z    | 2002 | MPD  | C2-C3-C4-O4  |

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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   | 1A    | 2861/2915 (98%) | 0.68   | 86 (3%)   | 50  | 53  | 15, 32, 79, 90        | 0       |
| 1   | 2A    | 2856/2915 (97%) | 0.53   | 99 (3%)   | 44  | 47  | 27, 48, 81, 90        | 0       |
| 2   | 1B    | 120/121 (99%)   | 0.36   | 0         | 100 | 100 | 24, 43, 54, 68        | 0       |
| 2   | 2B    | 120/121 (99%)   | 0.28   | 0         | 100 | 100 | 49, 64, 71, 75        | 0       |
| 3   | 1D    | 275/276 (99%)   | 0.76   | 4 (1%)    | 73  | 75  | 18, 33, 44, 58        | 0       |
| 3   | 2D    | 275/276 (99%)   | 0.77   | 7 (2%)    | 57  | 61  | 27, 43, 54, 67        | 0       |
| 4   | 1E    | 204/206 (99%)   | 0.75   | 2 (0%)    | 82  | 84  | 16, 36, 52, 64        | 0       |
| 4   | 2E    | 204/206 (99%)   | 0.71   | 3 (1%)    | 73  | 75  | 25, 48, 62, 68        | 0       |
| 5   | 1F    | 203/210 (96%)   | 0.69   | 3 (1%)    | 73  | 75  | 14, 36, 58, 74        | 0       |
| 5   | 2F    | 203/210 (96%)   | 0.64   | 7 (3%)    | 45  | 48  | 28, 55, 65, 73        | 0       |
| 6   | 1G    | 181/182 (99%)   | 0.47   | 6 (3%)    | 46  | 50  | 40, 56, 66, 72        | 0       |
| 6   | 2G    | 181/182 (99%)   | 1.15   | 33 (18%)  | 1   | 1   | 58, 68, 74, 77        | 0       |
| 7   | 1H    | 174/180 (96%)   | 0.49   | 1 (0%)    | 89  | 90  | 30, 45, 55, 58        | 0       |
| 7   | 2H    | 173/180 (96%)   | 0.82   | 19 (10%)  | 5   | 5   | 58, 66, 72, 76        | 0       |
| 8   | 1I    | 147/148 (99%)   | 0.36   | 1 (0%)    | 87  | 89  | 37, 61, 70, 76        | 0       |
| 8   | 2I    | 146/148 (98%)   | 0.66   | 15 (10%)  | 6   | 6   | 46, 64, 72, 76        | 0       |
| 9   | 1N    | 140/140 (100%)  | 0.69   | 0         | 100 | 100 | 22, 32, 48, 65        | 0       |
| 9   | 2N    | 140/140 (100%)  | 0.65   | 5 (3%)    | 42  | 46  | 39, 52, 62, 70        | 0       |
| 10  | 1O    | 122/122 (100%)  | 0.63   | 0         | 100 | 100 | 23, 35, 50, 57        | 0       |
| 10  | 2O    | 122/122 (100%)  | 0.58   | 0         | 100 | 100 | 38, 47, 59, 64        | 0       |
| 11  | 1P    | 149/150 (99%)   | 0.63   | 2 (1%)    | 77  | 79  | 15, 40, 58, 63        | 0       |
| 11  | 2P    | 149/150 (99%)   | 0.79   | 9 (6%)    | 21  | 22  | 31, 55, 67, 72        | 0       |
| 12  | 1Q    | 141/141 (100%)  | 0.69   | 0         | 100 | 100 | 22, 34, 45, 51        | 0       |
| 12  | 2Q    | 141/141 (100%)  | 0.73   | 11 (7%)   | 13  | 13  | 37, 52, 61, 68        | 0       |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13  | 1R    | 118/118 (100%) | 0.67   | 0 100 100    | 21, 30, 43, 50        | 0     |
| 13  | 2R    | 118/118 (100%) | 0.62   | 2 (1%) 70 72 | 33, 44, 52, 58        | 0     |
| 14  | 1S    | 110/112 (98%)  | 0.49   | 0 100 100    | 32, 43, 54, 58        | 0     |
| 14  | 2S    | 110/112 (98%)  | 0.65   | 7 (6%) 19 20 | 52, 59, 63, 68        | 0     |
| 15  | 1T    | 131/146 (89%)  | 0.58   | 0 100 100    | 28, 38, 57, 70        | 0     |
| 15  | 2T    | 131/146 (89%)  | 0.55   | 5 (3%) 40 43 | 39, 50, 63, 68        | 0     |
| 16  | 1U    | 116/118 (98%)  | 0.80   | 1 (0%) 84 86 | 17, 26, 40, 51        | 0     |
| 16  | 2U    | 116/118 (98%)  | 0.88   | 6 (5%) 27 29 | 33, 48, 61, 68        | 0     |
| 17  | 1V    | 101/101 (100%) | 0.63   | 0 100 100    | 16, 35, 49, 54        | 0     |
| 17  | 2V    | 101/101 (100%) | 0.56   | 1 (0%) 82 84 | 38, 57, 63, 67        | 0     |
| 18  | 1W    | 112/113 (99%)  | 0.77   | 0 100 100    | 18, 26, 45, 62        | 0     |
| 18  | 2W    | 112/113 (99%)  | 0.65   | 1 (0%) 84 86 | 32, 42, 57, 76        | 0     |
| 19  | 1X    | 95/96 (98%)    | 0.74   | 3 (3%) 47 51 | 22, 33, 52, 63        | 0     |
| 19  | 2X    | 95/96 (98%)    | 0.91   | 7 (7%) 14 15 | 38, 52, 64, 69        | 0     |
| 20  | 1Y    | 107/110 (97%)  | 0.61   | 2 (1%) 66 69 | 32, 42, 55, 63        | 0     |
| 20  | 2Y    | 107/110 (97%)  | 0.75   | 9 (8%) 11 11 | 45, 57, 66, 72        | 0     |
| 21  | 1Z    | 203/206 (98%)  | 0.44   | 3 (1%) 73 75 | 32, 49, 61, 71        | 0     |
| 21  | 2Z    | 201/206 (97%)  | 0.52   | 6 (2%) 50 53 | 50, 62, 69, 77        | 0     |
| 22  | 10    | 83/85 (97%)    | 0.95   | 7 (8%) 11 11 | 23, 32, 58, 68        | 0     |
| 22  | 20    | 83/85 (97%)    | 1.25   | 13 (15%) 2 1 | 40, 51, 62, 69        | 0     |
| 23  | 11    | 97/98 (98%)    | 0.81   | 4 (4%) 37 40 | 24, 39, 59, 61        | 0     |
| 23  | 21    | 97/98 (98%)    | 0.75   | 8 (8%) 11 11 | 35, 48, 63, 68        | 0     |
| 24  | 12    | 70/72 (97%)    | 0.59   | 1 (1%) 75 77 | 30, 43, 51, 62        | 0     |
| 24  | 22    | 70/72 (97%)    | 0.48   | 0 100 100    | 46, 58, 62, 65        | 0     |
| 25  | 13    | 59/60 (98%)    | 0.67   | 1 (1%) 70 72 | 22, 31, 49, 56        | 0     |
| 25  | 23    | 59/60 (98%)    | 1.00   | 6 (10%) 6 6  | 41, 49, 63, 72        | 0     |
| 26  | 14    | 69/71 (97%)    | 0.77   | 7 (10%) 7 6  | 50, 68, 75, 79        | 0     |
| 26  | 24    | 69/71 (97%)    | 1.49   | 19 (27%) 0 0 | 67, 73, 79, 81        | 0     |
| 27  | 15    | 59/60 (98%)    | 0.88   | 1 (1%) 70 72 | 17, 28, 44, 55        | 0     |
| 27  | 25    | 59/60 (98%)    | 0.62   | 0 100 100    | 27, 42, 55, 65        | 0     |
| 28  | 16    | 53/54 (98%)    | 0.43   | 0 100 100    | 27, 36, 49, 51        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28  | 26    | 53/54 (98%)     | 0.62   | 2 (3%) 40 43  | 44, 51, 59, 63        | 0     |
| 29  | 17    | 48/49 (97%)     | 0.91   | 2 (4%) 36 39  | 16, 23, 48, 51        | 0     |
| 29  | 27    | 48/49 (97%)     | 0.88   | 2 (4%) 36 39  | 29, 36, 51, 62        | 0     |
| 30  | 18    | 64/65 (98%)     | 0.77   | 1 (1%) 72 74  | 22, 29, 36, 50        | 0     |
| 30  | 28    | 64/65 (98%)     | 1.06   | 8 (12%) 3 3   | 36, 45, 50, 59        | 0     |
| 31  | 19    | 37/37 (100%)    | 0.78   | 0 100 100     | 26, 35, 50, 53        | 0     |
| 31  | 29    | 37/37 (100%)    | 1.02   | 3 (8%) 12 12  | 46, 54, 64, 66        | 0     |
| 32  | 1a    | 1488/1521 (97%) | 0.44   | 41 (2%) 53 56 | 33, 60, 78, 90        | 0     |
| 32  | 2a    | 1492/1521 (98%) | 0.53   | 72 (4%) 30 32 | 41, 65, 80, 90        | 0     |
| 33  | 1b    | 231/256 (90%)   | 0.83   | 29 (12%) 3 3  | 56, 66, 73, 79        | 0     |
| 33  | 2b    | 231/256 (90%)   | 1.12   | 46 (19%) 1 1  | 59, 69, 75, 80        | 0     |
| 34  | 1c    | 206/239 (86%)   | 1.16   | 41 (19%) 1 1  | 52, 63, 71, 74        | 0     |
| 34  | 2c    | 206/239 (86%)   | 1.45   | 66 (32%) 0 0  | 57, 69, 74, 80        | 0     |
| 35  | 1d    | 208/209 (99%)   | 1.00   | 26 (12%) 3 3  | 48, 61, 69, 73        | 0     |
| 35  | 2d    | 208/209 (99%)   | 1.02   | 29 (13%) 2 2  | 49, 61, 67, 70        | 0     |
| 36  | 1e    | 148/162 (91%)   | 0.74   | 11 (7%) 14 15 | 42, 57, 64, 69        | 0     |
| 36  | 2e    | 148/162 (91%)   | 0.93   | 17 (11%) 4 4  | 51, 61, 69, 74        | 0     |
| 37  | 1f    | 100/101 (99%)   | 0.51   | 2 (2%) 65 68  | 46, 58, 65, 67        | 0     |
| 37  | 2f    | 100/101 (99%)   | 0.43   | 1 (1%) 82 84  | 48, 60, 65, 67        | 0     |
| 38  | 1g    | 155/156 (99%)   | 0.54   | 8 (5%) 27 29  | 52, 62, 67, 72        | 0     |
| 38  | 2g    | 155/156 (99%)   | 1.08   | 34 (21%) 0 0  | 59, 67, 71, 75        | 0     |
| 39  | 1h    | 137/138 (99%)   | 0.76   | 10 (7%) 15 15 | 47, 59, 64, 67        | 0     |
| 39  | 2h    | 137/138 (99%)   | 0.83   | 11 (8%) 12 12 | 54, 61, 66, 68        | 0     |
| 40  | 1i    | 127/128 (99%)   | 1.52   | 42 (33%) 0 0  | 56, 66, 72, 74        | 0     |
| 40  | 2i    | 126/128 (98%)   | 2.67   | 84 (66%) 0 0  | 61, 70, 75, 79        | 0     |
| 41  | 1j    | 97/105 (92%)    | 1.27   | 20 (20%) 1 0  | 55, 66, 73, 78        | 0     |
| 41  | 2j    | 96/105 (91%)    | 1.93   | 46 (47%) 0 0  | 61, 70, 75, 77        | 0     |
| 42  | 1k    | 114/129 (88%)   | 0.57   | 1 (0%) 84 86  | 40, 55, 64, 67        | 0     |
| 42  | 2k    | 114/129 (88%)   | 1.04   | 19 (16%) 1 1  | 49, 61, 68, 71        | 0     |
| 43  | 1l    | 121/132 (91%)   | 0.86   | 9 (7%) 14 15  | 45, 53, 60, 63        | 0     |
| 43  | 2l    | 121/132 (91%)   | 0.69   | 7 (5%) 23 24  | 44, 56, 63, 70        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44  | 1m    | 116/126 (92%)     | 0.82   | 12 (10%) 6 6    | 54, 65, 70, 77        | 0     |
| 44  | 2m    | 114/126 (90%)     | 1.17   | 21 (18%) 1 1    | 61, 69, 73, 76        | 0     |
| 45  | 1n    | 60/61 (98%)       | 1.58   | 16 (26%) 0 0    | 54, 61, 66, 71        | 0     |
| 45  | 2n    | 60/61 (98%)       | 2.56   | 41 (68%) 0 0    | 60, 68, 73, 79        | 0     |
| 46  | 1o    | 88/89 (98%)       | 0.62   | 3 (3%) 45 48    | 38, 55, 66, 72        | 0     |
| 46  | 2o    | 88/89 (98%)       | 0.77   | 3 (3%) 45 48    | 51, 61, 67, 74        | 0     |
| 47  | 1p    | 82/88 (93%)       | 1.13   | 16 (19%) 1 1    | 50, 61, 67, 74        | 0     |
| 47  | 2p    | 82/88 (93%)       | 0.91   | 7 (8%) 10 10    | 54, 60, 66, 70        | 0     |
| 48  | 1q    | 99/105 (94%)      | 0.82   | 6 (6%) 21 22    | 45, 58, 64, 69        | 0     |
| 48  | 2q    | 99/105 (94%)      | 0.92   | 12 (12%) 4 4    | 47, 59, 66, 70        | 0     |
| 49  | 1r    | 68/88 (77%)       | 0.44   | 2 (2%) 51 55    | 48, 57, 66, 73        | 0     |
| 49  | 2r    | 68/88 (77%)       | 0.72   | 4 (5%) 22 23    | 52, 61, 69, 74        | 0     |
| 50  | 1s    | 83/93 (89%)       | 0.58   | 2 (2%) 59 62    | 56, 65, 70, 76        | 0     |
| 50  | 2s    | 83/93 (89%)       | 1.38   | 19 (22%) 0 0    | 59, 70, 74, 78        | 0     |
| 51  | 1t    | 96/106 (90%)      | 0.94   | 12 (12%) 3 3    | 53, 61, 68, 70        | 0     |
| 51  | 2t    | 98/106 (92%)      | 0.79   | 7 (7%) 16 16    | 50, 60, 66, 71        | 0     |
| 52  | 1u    | 23/27 (85%)       | 1.68   | 8 (34%) 0 0     | 59, 62, 66, 69        | 0     |
| 52  | 2u    | 23/27 (85%)       | 2.04   | 10 (43%) 0 0    | 62, 68, 70, 71        | 0     |
| 53  | 1y    | 97/113 (85%)      | 0.83   | 5 (5%) 27 29    | 47, 56, 67, 71        | 0     |
| 53  | 2y    | 96/113 (84%)      | 3.68   | 79 (82%) 0 0    | 66, 74, 80, 82        | 0     |
| 54  | 1w    | 4/5 (80%)         | 0.46   | 0 100 100       | 45, 49, 56, 71        | 0     |
| 54  | 2w    | 4/5 (80%)         | 0.71   | 0 100 100       | 50, 58, 65, 72        | 0     |
| 55  | 1x    | 3/4 (75%)         | 3.58   | 2 (66%) 0 0     | 61, 61, 67, 73        | 0     |
| 55  | 2x    | 3/4 (75%)         | 5.30   | 3 (100%) 0 0    | 65, 65, 69, 77        | 0     |
| 56  | 1v    | 3/3 (100%)        | 7.20   | 3 (100%) 0 0    | 50, 50, 59, 61        | 0     |
| 56  | 2v    | 3/3 (100%)        | 7.38   | 3 (100%) 0 0    | 58, 58, 66, 67        | 0     |
| All | All   | 20798/21492 (96%) | 0.73   | 1419 (6%) 17 17 | 14, 54, 74, 90        | 0     |

All (1419) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 56  | 1v    | 1   | MET  | 10.3 |
| 55  | 2x    | 73  | A    | 9.4  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 53  | 2y    | 88      | LEU  | 9.3  |
| 21  | 2Z    | 192     | ALA  | 9.3  |
| 53  | 2y    | 40      | ILE  | 9.0  |
| 56  | 2v    | 2       | THR  | 8.7  |
| 56  | 2v    | 1       | MET  | 8.4  |
| 34  | 2c    | 157     | ILE  | 8.4  |
| 53  | 2y    | 41      | LEU  | 8.4  |
| 53  | 2y    | 50      | ALA  | 7.8  |
| 1   | 1A    | 1087    | G    | 7.3  |
| 53  | 2y    | 78      | ILE  | 7.3  |
| 53  | 2y    | 12      | ILE  | 7.0  |
| 1   | 2A    | 2153    | G    | 7.0  |
| 53  | 2y    | 48      | PHE  | 7.0  |
| 32  | 2a    | 1030(A) | G    | 6.5  |
| 1   | 1A    | 1076    | C    | 6.4  |
| 45  | 2n    | 2       | ALA  | 6.4  |
| 22  | 10    | 7       | LEU  | 6.3  |
| 45  | 2n    | 13      | THR  | 6.2  |
| 1   | 2A    | 2142    | C    | 6.2  |
| 53  | 2y    | 10      | MET  | 6.1  |
| 41  | 2j    | 67      | THR  | 6.0  |
| 53  | 2y    | 51      | ASP  | 6.0  |
| 32  | 2a    | 1030(B) | C    | 6.0  |
| 53  | 2y    | 52      | ALA  | 6.0  |
| 1   | 2A    | 2139    | C    | 6.0  |
| 1   | 2A    | 2132    | U    | 6.0  |
| 56  | 1v    | 2       | THR  | 6.0  |
| 40  | 2i    | 75      | ASP  | 5.9  |
| 1   | 2A    | 2140    | C    | 5.9  |
| 40  | 2i    | 76      | ALA  | 5.9  |
| 40  | 2i    | 42      | ARG  | 5.8  |
| 1   | 2A    | 2138    | C    | 5.8  |
| 53  | 2y    | 64      | SER  | 5.8  |
| 1   | 1A    | 1091    | G    | 5.8  |
| 40  | 2i    | 108     | VAL  | 5.8  |
| 34  | 2c    | 177     | THR  | 5.7  |
| 1   | 2A    | 2125    | G    | 5.7  |
| 1   | 2A    | 2147    | G    | 5.7  |
| 45  | 1n    | 51      | GLY  | 5.6  |
| 53  | 2y    | 77      | LEU  | 5.6  |
| 32  | 1a    | 1030(B) | C    | 5.6  |
| 55  | 1x    | 75      | C    | 5.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 53         | 2y           | 42         | SER         | 5.6         |
| 1          | 1A           | 1090       | U           | 5.6         |
| 53         | 2y           | 71         | TYR         | 5.6         |
| 40         | 2i           | 36         | TYR         | 5.5         |
| 1          | 1A           | 2141       | G           | 5.5         |
| 40         | 2i           | 18         | PHE         | 5.5         |
| 53         | 2y           | 39         | ILE         | 5.4         |
| 22         | 20           | 3          | HIS         | 5.3         |
| 56         | 1v           | 3          | ILE         | 5.3         |
| 1          | 1A           | 1068       | G           | 5.3         |
| 53         | 2y           | 49         | VAL         | 5.3         |
| 40         | 2i           | 63         | ILE         | 5.3         |
| 53         | 2y           | 79         | ASN         | 5.3         |
| 44         | 2m           | 116        | THR         | 5.3         |
| 19         | 2X           | 92         | LEU         | 5.3         |
| 53         | 2y           | 74         | ILE         | 5.2         |
| 1          | 2A           | 2141       | G           | 5.2         |
| 53         | 2y           | 63         | ALA         | 5.2         |
| 40         | 2i           | 72         | GLY         | 5.2         |
| 40         | 1i           | 14         | VAL         | 5.2         |
| 53         | 2y           | 38         | HIS         | 5.2         |
| 22         | 10           | 2          | ALA         | 5.2         |
| 1          | 1A           | 1089       | G           | 5.1         |
| 1          | 2A           | 2124       | G           | 5.1         |
| 1          | 2A           | 2802       | G           | 5.1         |
| 20         | 2Y           | 1          | MET         | 5.1         |
| 32         | 1a           | 1001       | A           | 5.1         |
| 56         | 2v           | 3          | ILE         | 5.1         |
| 41         | 2j           | 34         | VAL         | 5.0         |
| 34         | 2c           | 152        | ILE         | 5.0         |
| 32         | 1a           | 1257       | U           | 5.0         |
| 32         | 2a           | 1001       | A           | 5.0         |
| 44         | 1m           | 2          | ALA         | 5.0         |
| 53         | 2y           | 70         | MET         | 5.0         |
| 32         | 2a           | 1257       | U           | 5.0         |
| 23         | 11           | 2          | SER         | 4.9         |
| 21         | 2Z           | 191        | VAL         | 4.9         |
| 40         | 2i           | 8          | GLY         | 4.9         |
| 40         | 2i           | 30         | GLY         | 4.9         |
| 53         | 2y           | 11         | GLU         | 4.9         |
| 45         | 2n           | 44         | LEU         | 4.9         |
| 1          | 1A           | 1072       | C           | 4.9         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | 2n    | 12   | ARG  | 4.9  |
| 26  | 24    | 51   | ASP  | 4.8  |
| 53  | 2y    | 67   | HIS  | 4.8  |
| 33  | 2b    | 39   | ILE  | 4.8  |
| 53  | 2y    | 9    | GLN  | 4.8  |
| 1   | 1A    | 2132 | U    | 4.8  |
| 41  | 2j    | 26   | ALA  | 4.8  |
| 6   | 2G    | 87   | PRO  | 4.8  |
| 40  | 2i    | 103  | THR  | 4.8  |
| 22  | 20    | 2    | ALA  | 4.8  |
| 1   | 1A    | 1063 | G    | 4.8  |
| 40  | 2i    | 102  | LEU  | 4.8  |
| 40  | 2i    | 109  | VAL  | 4.8  |
| 1   | 2A    | 2146 | C    | 4.7  |
| 41  | 2j    | 27   | ALA  | 4.7  |
| 1   | 1A    | 1092 | C    | 4.7  |
| 45  | 2n    | 25   | VAL  | 4.7  |
| 53  | 2y    | 73   | ALA  | 4.6  |
| 39  | 2h    | 2    | LEU  | 4.6  |
| 26  | 24    | 52   | THR  | 4.6  |
| 36  | 2e    | 12   | LEU  | 4.6  |
| 34  | 2c    | 124  | ILE  | 4.6  |
| 32  | 2a    | 1036 | G    | 4.6  |
| 32  | 1a    | 1030 | C    | 4.6  |
| 40  | 1i    | 63   | ILE  | 4.6  |
| 53  | 2y    | 5    | ILE  | 4.6  |
| 53  | 2y    | 69   | ASP  | 4.6  |
| 53  | 2y    | 62   | VAL  | 4.6  |
| 41  | 2j    | 96   | ILE  | 4.6  |
| 26  | 24    | 45   | GLY  | 4.5  |
| 1   | 1A    | 2805 | G    | 4.5  |
| 32  | 2a    | 1033 | G    | 4.5  |
| 34  | 2c    | 8    | ILE  | 4.5  |
| 53  | 2y    | 53   | THR  | 4.5  |
| 1   | 1A    | 1064 | C    | 4.5  |
| 32  | 1a    | 1029 | C    | 4.5  |
| 41  | 1j    | 29   | ARG  | 4.5  |
| 40  | 2i    | 62   | TYR  | 4.5  |
| 1   | 1A    | 2792 | G    | 4.5  |
| 1   | 1A    | 1065 | U    | 4.5  |
| 53  | 2y    | 87   | LYS  | 4.5  |
| 55  | 1x    | 74   | C    | 4.5  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 26  | 24    | 49      | PHE  | 4.5  |
| 1   | 2A    | 2174    | C    | 4.5  |
| 33  | 1b    | 118     | LEU  | 4.5  |
| 7   | 2H    | 93      | GLY  | 4.5  |
| 40  | 2i    | 69      | GLY  | 4.5  |
| 1   | 2A    | 2106    | G    | 4.4  |
| 50  | 2s    | 66      | MET  | 4.4  |
| 40  | 2i    | 26      | VAL  | 4.4  |
| 1   | 1A    | 1080    | C    | 4.4  |
| 1   | 2A    | 2136    | C    | 4.4  |
| 32  | 1a    | 1001(A) | G    | 4.4  |
| 6   | 2G    | 135     | LEU  | 4.4  |
| 45  | 1n    | 34      | TYR  | 4.4  |
| 34  | 2c    | 159     | GLY  | 4.4  |
| 40  | 2i    | 61      | ALA  | 4.4  |
| 40  | 2i    | 21      | PRO  | 4.4  |
| 40  | 2i    | 66      | ARG  | 4.4  |
| 41  | 2j    | 72      | VAL  | 4.3  |
| 53  | 2y    | 84      | GLN  | 4.3  |
| 31  | 29    | 16      | VAL  | 4.3  |
| 34  | 1c    | 194     | GLY  | 4.3  |
| 53  | 2y    | 19      | HIS  | 4.3  |
| 32  | 2a    | 1286    | A    | 4.3  |
| 23  | 21    | 2       | SER  | 4.3  |
| 45  | 2n    | 61      | TRP  | 4.3  |
| 1   | 2A    | 2152    | G    | 4.3  |
| 26  | 14    | 18      | CYS  | 4.3  |
| 32  | 1a    | 1031    | G    | 4.3  |
| 50  | 2s    | 10      | PHE  | 4.3  |
| 7   | 2H    | 102     | ALA  | 4.2  |
| 36  | 2e    | 109     | ILE  | 4.2  |
| 53  | 2y    | 92      | GLY  | 4.2  |
| 1   | 2A    | 1509    | C    | 4.2  |
| 33  | 2b    | 136     | VAL  | 4.2  |
| 34  | 1c    | 204     | LEU  | 4.2  |
| 38  | 1g    | 156     | TRP  | 4.2  |
| 44  | 1m    | 24      | GLY  | 4.2  |
| 1   | 1A    | 2794    | C    | 4.2  |
| 1   | 2A    | 2107    | C    | 4.2  |
| 1   | 1A    | 1074    | G    | 4.2  |
| 53  | 2y    | 58      | ASN  | 4.2  |
| 53  | 2y    | 35      | ILE  | 4.2  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 1   | 2A    | 2169    | A    | 4.2  |
| 34  | 2c    | 155     | GLY  | 4.2  |
| 1   | 2A    | 2151    | G    | 4.2  |
| 1   | 1A    | 1509    | C    | 4.2  |
| 1   | 1A    | 2116    | G    | 4.1  |
| 1   | 1A    | 2793    | G    | 4.1  |
| 50  | 1s    | 4       | SER  | 4.1  |
| 1   | 1A    | 1176    | G    | 4.1  |
| 1   | 2A    | 2793    | G    | 4.1  |
| 44  | 2m    | 6       | GLY  | 4.1  |
| 1   | 1A    | 1067    | A    | 4.1  |
| 1   | 2A    | 2173    | A    | 4.1  |
| 53  | 2y    | 37      | PRO  | 4.1  |
| 6   | 2G    | 73      | ALA  | 4.1  |
| 7   | 2H    | 101     | ARG  | 4.1  |
| 32  | 1a    | 1030(D) | A    | 4.1  |
| 34  | 2c    | 164     | ARG  | 4.1  |
| 1   | 2A    | 2131    | G    | 4.1  |
| 22  | 10    | 6       | GLY  | 4.1  |
| 36  | 2e    | 13      | ILE  | 4.1  |
| 42  | 2k    | 75      | TYR  | 4.1  |
| 40  | 1i    | 28      | VAL  | 4.1  |
| 52  | 2u    | 2       | GLY  | 4.1  |
| 1   | 2A    | 2191    | G    | 4.0  |
| 29  | 27    | 47      | ARG  | 4.0  |
| 34  | 1c    | 80      | GLY  | 4.0  |
| 53  | 2y    | 65      | GLY  | 4.0  |
| 38  | 2g    | 154     | TYR  | 4.0  |
| 1   | 1A    | 2804    | C    | 4.0  |
| 32  | 2a    | 1029    | C    | 4.0  |
| 39  | 1h    | 134     | ILE  | 4.0  |
| 1   | 1A    | 1083    | U    | 4.0  |
| 8   | 2I    | 46      | ALA  | 4.0  |
| 1   | 1A    | 1075    | C    | 4.0  |
| 1   | 2A    | 2159    | G    | 4.0  |
| 34  | 1c    | 148     | GLY  | 4.0  |
| 32  | 1a    | 1030(C) | G    | 4.0  |
| 1   | 2A    | 2801(A) | A    | 4.0  |
| 53  | 2y    | 82      | GLU  | 4.0  |
| 52  | 2u    | 16      | GLY  | 4.0  |
| 40  | 2i    | 115     | GLY  | 3.9  |
| 1   | 1A    | 1175    | U    | 3.9  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 7   | 2H    | 165     | ALA  | 3.9  |
| 1   | 2A    | 2123    | G    | 3.9  |
| 41  | 2j    | 48      | THR  | 3.9  |
| 35  | 1d    | 2       | GLY  | 3.9  |
| 26  | 24    | 50      | VAL  | 3.9  |
| 1   | 1A    | 1093    | G    | 3.9  |
| 1   | 2A    | 2110    | G    | 3.9  |
| 32  | 2a    | 1031    | G    | 3.9  |
| 40  | 2i    | 67      | GLY  | 3.9  |
| 1   | 2A    | 2896    | C    | 3.9  |
| 22  | 20    | 4       | LYS  | 3.9  |
| 1   | 2A    | 1085    | A    | 3.9  |
| 40  | 1i    | 37      | PHE  | 3.9  |
| 40  | 2i    | 56      | LEU  | 3.9  |
| 50  | 2s    | 69      | HIS  | 3.8  |
| 26  | 24    | 18      | CYS  | 3.8  |
| 48  | 1q    | 98      | LEU  | 3.8  |
| 53  | 2y    | 4       | ASN  | 3.8  |
| 41  | 2j    | 23      | ILE  | 3.8  |
| 43  | 2l    | 18      | VAL  | 3.8  |
| 32  | 2a    | 1026    | G    | 3.8  |
| 40  | 2i    | 74      | ILE  | 3.8  |
| 53  | 2y    | 61      | LEU  | 3.8  |
| 35  | 2d    | 146     | ILE  | 3.8  |
| 16  | 2U    | 73      | GLY  | 3.8  |
| 40  | 2i    | 5       | TYR  | 3.8  |
| 1   | 1A    | 888     | C    | 3.8  |
| 34  | 1c    | 63      | ASN  | 3.8  |
| 20  | 2Y    | 42      | VAL  | 3.8  |
| 32  | 2a    | 1531    | A    | 3.8  |
| 53  | 2y    | 18      | GLN  | 3.8  |
| 35  | 1d    | 3       | ARG  | 3.7  |
| 45  | 2n    | 10      | ALA  | 3.7  |
| 32  | 1a    | 1028    | C    | 3.7  |
| 1   | 2A    | 2805    | G    | 3.7  |
| 38  | 1g    | 12      | LEU  | 3.7  |
| 34  | 1c    | 94      | LEU  | 3.7  |
| 32  | 1a    | 1030(A) | G    | 3.7  |
| 40  | 1i    | 106     | ALA  | 3.7  |
| 53  | 2y    | 15      | ALA  | 3.7  |
| 51  | 1t    | 18      | GLN  | 3.7  |
| 26  | 24    | 63      | TYR  | 3.7  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 11  | 2P    | 79      | ARG  | 3.7  |
| 38  | 2g    | 5       | ARG  | 3.7  |
| 55  | 2x    | 74      | C    | 3.7  |
| 22  | 20    | 7       | LEU  | 3.7  |
| 45  | 1n    | 14      | PRO  | 3.7  |
| 34  | 1c    | 81      | GLY  | 3.7  |
| 1   | 2A    | 2133    | G    | 3.7  |
| 44  | 2m    | 5       | ALA  | 3.7  |
| 47  | 1p    | 48      | TRP  | 3.7  |
| 1   | 1A    | 2140    | C    | 3.7  |
| 41  | 2j    | 19      | SER  | 3.7  |
| 22  | 20    | 76      | GLY  | 3.7  |
| 40  | 2i    | 28      | VAL  | 3.7  |
| 53  | 2y    | 8       | LYS  | 3.7  |
| 53  | 2y    | 21      | ALA  | 3.7  |
| 26  | 14    | 49      | PHE  | 3.7  |
| 1   | 1A    | 1066    | U    | 3.7  |
| 32  | 1a    | 1286    | A    | 3.7  |
| 8   | 2I    | 89      | TYR  | 3.7  |
| 33  | 2b    | 118     | LEU  | 3.7  |
| 1   | 1A    | 2115    | G    | 3.7  |
| 53  | 2y    | 7       | SER  | 3.7  |
| 43  | 2l    | 19      | ARG  | 3.7  |
| 23  | 21    | 70      | VAL  | 3.7  |
| 36  | 2e    | 16      | THR  | 3.7  |
| 33  | 2b    | 218     | ALA  | 3.7  |
| 42  | 2k    | 74      | ALA  | 3.7  |
| 22  | 10    | 5       | LYS  | 3.6  |
| 40  | 2i    | 92      | TYR  | 3.6  |
| 32  | 2a    | 1030(D) | A    | 3.6  |
| 1   | 2A    | 2803    | C    | 3.6  |
| 1   | 1A    | 1082    | U    | 3.6  |
| 40  | 2i    | 90      | PRO  | 3.6  |
| 33  | 2b    | 44      | LEU  | 3.6  |
| 34  | 2c    | 33      | LEU  | 3.6  |
| 40  | 2i    | 88      | TYR  | 3.6  |
| 52  | 2u    | 13      | ILE  | 3.6  |
| 40  | 2i    | 105     | ASP  | 3.6  |
| 41  | 2j    | 62      | HIS  | 3.6  |
| 1   | 2A    | 229     | A    | 3.6  |
| 1   | 2A    | 2804    | C    | 3.6  |
| 7   | 1H    | 2       | SER  | 3.6  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 50  | 2s    | 79      | THR  | 3.6  |
| 40  | 1i    | 109     | VAL  | 3.6  |
| 33  | 1b    | 214     | ILE  | 3.6  |
| 40  | 2i    | 111     | ARG  | 3.6  |
| 41  | 2j    | 16      | LEU  | 3.6  |
| 53  | 2y    | 24      | LEU  | 3.6  |
| 6   | 1G    | 146     | TYR  | 3.6  |
| 35  | 1d    | 32      | ALA  | 3.6  |
| 40  | 2i    | 122     | ALA  | 3.6  |
| 1   | 2A    | 2162    | G    | 3.6  |
| 32  | 2a    | 1030(C) | G    | 3.6  |
| 48  | 1q    | 27      | PHE  | 3.5  |
| 33  | 1b    | 121     | LEU  | 3.5  |
| 38  | 2g    | 34      | GLY  | 3.5  |
| 38  | 2g    | 82      | GLY  | 3.5  |
| 34  | 2c    | 23      | TYR  | 3.5  |
| 1   | 1A    | 1103    | A    | 3.5  |
| 34  | 2c    | 160     | ALA  | 3.5  |
| 40  | 2i    | 14      | VAL  | 3.5  |
| 6   | 2G    | 152     | LEU  | 3.5  |
| 48  | 2q    | 98      | LEU  | 3.5  |
| 38  | 2g    | 83      | ALA  | 3.5  |
| 34  | 1c    | 130     | VAL  | 3.5  |
| 34  | 2c    | 66      | VAL  | 3.5  |
| 25  | 23    | 15      | TYR  | 3.5  |
| 1   | 1A    | 2113    | U    | 3.5  |
| 45  | 2n    | 55      | GLY  | 3.5  |
| 40  | 2i    | 45      | ALA  | 3.5  |
| 40  | 1i    | 26      | VAL  | 3.5  |
| 45  | 2n    | 56      | VAL  | 3.5  |
| 40  | 2i    | 114     | TYR  | 3.5  |
| 52  | 2u    | 6       | ARG  | 3.5  |
| 41  | 2j    | 31      | GLY  | 3.5  |
| 6   | 2G    | 43      | LEU  | 3.5  |
| 53  | 2y    | 80      | LYS  | 3.5  |
| 44  | 2m    | 102     | ARG  | 3.5  |
| 48  | 2q    | 71      | PHE  | 3.5  |
| 53  | 2y    | 46      | GLN  | 3.5  |
| 1   | 2A    | 2154    | G    | 3.5  |
| 35  | 1d    | 180     | GLY  | 3.5  |
| 38  | 1g    | 80      | VAL  | 3.5  |
| 38  | 2g    | 80      | VAL  | 3.5  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 41  | 2j    | 6       | ILE  | 3.4  |
| 35  | 2d    | 149     | ALA  | 3.4  |
| 44  | 2m    | 43      | THR  | 3.4  |
| 53  | 2y    | 13      | THR  | 3.4  |
| 40  | 2i    | 49      | PRO  | 3.4  |
| 19  | 2X    | 68      | ARG  | 3.4  |
| 53  | 2y    | 85      | LEU  | 3.4  |
| 33  | 1b    | 29      | ALA  | 3.4  |
| 42  | 2k    | 89      | ALA  | 3.4  |
| 35  | 1d    | 179     | GLU  | 3.4  |
| 1   | 2A    | 2897    | U    | 3.4  |
| 26  | 24    | 56      | VAL  | 3.4  |
| 33  | 2b    | 93      | VAL  | 3.4  |
| 45  | 1n    | 33      | VAL  | 3.4  |
| 6   | 2G    | 157     | ILE  | 3.4  |
| 47  | 1p    | 19      | ILE  | 3.4  |
| 40  | 1i    | 10      | ARG  | 3.4  |
| 48  | 2q    | 9       | VAL  | 3.4  |
| 1   | 1A    | 2144    | U    | 3.4  |
| 52  | 1u    | 18      | TYR  | 3.4  |
| 34  | 2c    | 165     | THR  | 3.4  |
| 53  | 2y    | 45      | PRO  | 3.4  |
| 1   | 2A    | 2177    | C    | 3.4  |
| 45  | 2n    | 51      | GLY  | 3.4  |
| 7   | 2H    | 105     | LEU  | 3.4  |
| 33  | 2b    | 124     | SER  | 3.4  |
| 32  | 2a    | 1001(A) | G    | 3.4  |
| 26  | 24    | 66      | SER  | 3.3  |
| 40  | 2i    | 40      | LEU  | 3.3  |
| 40  | 2i    | 50      | LEU  | 3.3  |
| 41  | 1j    | 90      | LEU  | 3.3  |
| 45  | 2n    | 47      | LEU  | 3.3  |
| 34  | 1c    | 180     | ALA  | 3.3  |
| 43  | 1l    | 61      | THR  | 3.3  |
| 1   | 1A    | 1079    | C    | 3.3  |
| 1   | 1A    | 2107    | C    | 3.3  |
| 32  | 2a    | 1249    | C    | 3.3  |
| 1   | 2A    | 2120    | G    | 3.3  |
| 35  | 1d    | 70      | ILE  | 3.3  |
| 52  | 2u    | 14      | TRP  | 3.3  |
| 26  | 24    | 64      | GLY  | 3.3  |
| 41  | 1j    | 49      | VAL  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | 2n    | 28   | GLY  | 3.3  |
| 53  | 1y    | 49   | VAL  | 3.3  |
| 1   | 2A    | 2126 | A    | 3.3  |
| 32  | 1a    | 1036 | G    | 3.3  |
| 46  | 2o    | 68   | ARG  | 3.3  |
| 53  | 2y    | 17   | ARG  | 3.3  |
| 7   | 2H    | 113  | VAL  | 3.3  |
| 27  | 15    | 60   | VAL  | 3.3  |
| 1   | 2A    | 1046 | A    | 3.3  |
| 51  | 1t    | 13   | LEU  | 3.3  |
| 1   | 1A    | 1081 | U    | 3.3  |
| 32  | 1a    | 1000 | U    | 3.3  |
| 51  | 1t    | 67   | ALA  | 3.3  |
| 1   | 2A    | 2168 | G    | 3.3  |
| 33  | 1b    | 165  | VAL  | 3.3  |
| 6   | 2G    | 82   | LEU  | 3.3  |
| 1   | 2A    | 2176 | A    | 3.3  |
| 41  | 1j    | 86   | MET  | 3.3  |
| 33  | 2b    | 30   | ARG  | 3.3  |
| 48  | 2q    | 23   | VAL  | 3.3  |
| 40  | 2i    | 47   | LEU  | 3.3  |
| 50  | 2s    | 75   | ALA  | 3.3  |
| 53  | 2y    | 16   | ILE  | 3.3  |
| 53  | 2y    | 72   | THR  | 3.3  |
| 53  | 2y    | 94   | ALA  | 3.3  |
| 1   | 2A    | 1076 | C    | 3.3  |
| 6   | 1G    | 48   | GLU  | 3.3  |
| 32  | 2a    | 1030 | C    | 3.3  |
| 6   | 2G    | 86   | MET  | 3.3  |
| 40  | 2i    | 91   | ASP  | 3.3  |
| 42  | 2k    | 25   | TYR  | 3.3  |
| 43  | 1l    | 64   | TYR  | 3.3  |
| 32  | 1a    | 1033 | G    | 3.2  |
| 34  | 2c    | 60   | ALA  | 3.2  |
| 35  | 2d    | 144  | ASP  | 3.2  |
| 44  | 1m    | 115  | LYS  | 3.2  |
| 40  | 2i    | 73   | GLN  | 3.2  |
| 42  | 1k    | 25   | TYR  | 3.2  |
| 45  | 2n    | 18   | VAL  | 3.2  |
| 47  | 2p    | 20   | VAL  | 3.2  |
| 14  | 2S    | 54   | LEU  | 3.2  |
| 41  | 2j    | 68   | HIS  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | 24    | 44   | THR  | 3.2  |
| 40  | 2i    | 27   | THR  | 3.2  |
| 33  | 1b    | 128  | GLU  | 3.2  |
| 6   | 2G    | 65   | GLY  | 3.2  |
| 14  | 2S    | 22   | GLY  | 3.2  |
| 44  | 1m    | 112  | GLY  | 3.2  |
| 45  | 2n    | 36   | PHE  | 3.2  |
| 1   | 1A    | 2142 | C    | 3.2  |
| 1   | 2A    | 888  | C    | 3.2  |
| 40  | 2i    | 127  | LYS  | 3.2  |
| 33  | 2b    | 31   | TYR  | 3.2  |
| 7   | 2H    | 19   | VAL  | 3.2  |
| 40  | 2i    | 85   | LEU  | 3.2  |
| 34  | 2c    | 61   | ALA  | 3.2  |
| 50  | 2s    | 63   | THR  | 3.2  |
| 53  | 1y    | 95   | ARG  | 3.2  |
| 40  | 2i    | 125  | TYR  | 3.2  |
| 1   | 2A    | 2118 | U    | 3.2  |
| 29  | 17    | 46   | VAL  | 3.2  |
| 41  | 2j    | 44   | VAL  | 3.2  |
| 41  | 2j    | 87   | THR  | 3.2  |
| 36  | 2e    | 84   | PHE  | 3.2  |
| 34  | 1c    | 18   | TRP  | 3.2  |
| 42  | 2k    | 13   | GLN  | 3.2  |
| 45  | 2n    | 14   | PRO  | 3.2  |
| 33  | 2b    | 165  | VAL  | 3.2  |
| 38  | 2g    | 41   | ARG  | 3.2  |
| 19  | 2X    | 69   | TYR  | 3.1  |
| 35  | 2d    | 158  | ILE  | 3.1  |
| 11  | 2P    | 34   | GLY  | 3.1  |
| 22  | 20    | 42   | GLY  | 3.1  |
| 40  | 2i    | 6    | GLY  | 3.1  |
| 53  | 2y    | 83   | ARG  | 3.1  |
| 33  | 2b    | 231  | GLU  | 3.1  |
| 34  | 2c    | 87   | LEU  | 3.1  |
| 40  | 2i    | 7    | THR  | 3.1  |
| 1   | 1A    | 1097 | U    | 3.1  |
| 6   | 2G    | 39   | ILE  | 3.1  |
| 7   | 2H    | 92   | ILE  | 3.1  |
| 36  | 2e    | 28   | PHE  | 3.1  |
| 32  | 1a    | 1026 | G    | 3.1  |
| 32  | 2a    | 1373 | G    | 3.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 33  | 2b    | 113    | HIS  | 3.1  |
| 38  | 2g    | 155    | ARG  | 3.1  |
| 45  | 2n    | 35     | ARG  | 3.1  |
| 26  | 24    | 39     | CYS  | 3.1  |
| 3   | 2D    | 2      | ALA  | 3.1  |
| 41  | 2j    | 15     | THR  | 3.1  |
| 45  | 1n    | 30     | ALA  | 3.1  |
| 40  | 2i    | 57     | GLY  | 3.1  |
| 51  | 2t    | 9      | ASN  | 3.1  |
| 15  | 2T    | 111    | ARG  | 3.1  |
| 30  | 28    | 58     | ILE  | 3.1  |
| 1   | 2A    | 2137   | C    | 3.1  |
| 40  | 1i    | 49     | PRO  | 3.1  |
| 14  | 2S    | 21     | THR  | 3.1  |
| 33  | 2b    | 164    | VAL  | 3.1  |
| 40  | 1i    | 46     | ALA  | 3.1  |
| 40  | 2i    | 65     | VAL  | 3.1  |
| 5   | 2F    | 166    | ALA  | 3.1  |
| 33  | 1b    | 213    | LEU  | 3.1  |
| 38  | 2g    | 22     | LEU  | 3.1  |
| 6   | 2G    | 85     | GLY  | 3.1  |
| 45  | 2n    | 22     | THR  | 3.1  |
| 6   | 2G    | 117    | PHE  | 3.1  |
| 7   | 2H    | 21     | PRO  | 3.1  |
| 33  | 1b    | 122    | PHE  | 3.1  |
| 34  | 1c    | 203    | PHE  | 3.1  |
| 41  | 2j    | 47     | PHE  | 3.1  |
| 50  | 2s    | 62     | ILE  | 3.1  |
| 1   | 2A    | 652(B) | A    | 3.1  |
| 1   | 1A    | 2893   | G    | 3.1  |
| 45  | 2n    | 43     | CYS  | 3.1  |
| 52  | 1u    | 14     | TRP  | 3.1  |
| 47  | 2p    | 19     | ILE  | 3.1  |
| 48  | 2q    | 27     | PHE  | 3.1  |
| 1   | 2A    | 2181   | G    | 3.0  |
| 1   | 2A    | 2179   | C    | 3.0  |
| 19  | 2X    | 84     | ALA  | 3.0  |
| 22  | 10    | 3      | HIS  | 3.0  |
| 25  | 23    | 26     | LEU  | 3.0  |
| 33  | 1b    | 188    | ALA  | 3.0  |
| 45  | 2n    | 53     | LEU  | 3.0  |
| 34  | 1c    | 2      | GLY  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | 2y    | 75   | ASN  | 3.0  |
| 1   | 2A    | 2108 | C    | 3.0  |
| 50  | 2s    | 11   | VAL  | 3.0  |
| 53  | 2y    | 20   | VAL  | 3.0  |
| 35  | 1d    | 4    | TYR  | 3.0  |
| 35  | 1d    | 138  | TYR  | 3.0  |
| 32  | 2a    | 998  | G    | 3.0  |
| 1   | 2A    | 2178 | C    | 3.0  |
| 53  | 2y    | 3    | MET  | 3.0  |
| 34  | 1c    | 39   | ILE  | 3.0  |
| 26  | 14    | 46   | GLN  | 3.0  |
| 6   | 2G    | 94   | LEU  | 3.0  |
| 32  | 2a    | 1321 | C    | 3.0  |
| 35  | 2d    | 67   | ILE  | 3.0  |
| 33  | 2b    | 187  | LEU  | 3.0  |
| 40  | 2i    | 13   | ALA  | 3.0  |
| 53  | 2y    | 60   | VAL  | 3.0  |
| 1   | 1A    | 2147 | G    | 3.0  |
| 1   | 1A    | 2152 | G    | 3.0  |
| 41  | 1j    | 73   | ASP  | 3.0  |
| 51  | 1t    | 73   | HIS  | 3.0  |
| 45  | 2n    | 21   | TYR  | 3.0  |
| 1   | 1A    | 2176 | A    | 3.0  |
| 3   | 2D    | 37   | LEU  | 3.0  |
| 35  | 1d    | 11   | LEU  | 3.0  |
| 38  | 2g    | 40   | ALA  | 3.0  |
| 40  | 1i    | 76   | ALA  | 3.0  |
| 7   | 2H    | 115  | VAL  | 2.9  |
| 34  | 2c    | 89   | GLU  | 2.9  |
| 53  | 2y    | 76   | GLU  | 2.9  |
| 1   | 2A    | 1075 | C    | 2.9  |
| 32  | 2a    | 1114 | C    | 2.9  |
| 32  | 2a    | 1202 | G    | 2.9  |
| 33  | 2b    | 132  | LYS  | 2.9  |
| 12  | 2Q    | 59   | ARG  | 2.9  |
| 33  | 2b    | 92   | TYR  | 2.9  |
| 40  | 2i    | 121  | ARG  | 2.9  |
| 43  | 2l    | 89   | ARG  | 2.9  |
| 52  | 1u    | 9    | ARG  | 2.9  |
| 23  | 2l    | 62   | VAL  | 2.9  |
| 34  | 1c    | 138  | VAL  | 2.9  |
| 1   | 2A    | 2150 | U    | 2.9  |

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| Mol | Chain | Res     | Type | RSRZ |
|-----|-------|---------|------|------|
| 40  | 2i    | 81      | ILE  | 2.9  |
| 33  | 2b    | 233     | SER  | 2.9  |
| 41  | 1j    | 30      | SER  | 2.9  |
| 26  | 24    | 68      | ARG  | 2.9  |
| 35  | 1d    | 50      | ARG  | 2.9  |
| 40  | 2i    | 3       | GLN  | 2.9  |
| 50  | 1s    | 56      | GLN  | 2.9  |
| 4   | 1E    | 28      | ALA  | 2.9  |
| 34  | 1c    | 196     | LEU  | 2.9  |
| 36  | 1e    | 134     | ALA  | 2.9  |
| 36  | 2e    | 22      | GLY  | 2.9  |
| 29  | 17    | 1       | MET  | 2.9  |
| 33  | 2b    | 21      | ARG  | 2.9  |
| 40  | 2i    | 10      | ARG  | 2.9  |
| 6   | 2G    | 140     | ILE  | 2.9  |
| 8   | 1I    | 85      | GLU  | 2.9  |
| 48  | 2q    | 90      | ILE  | 2.9  |
| 49  | 2r    | 58      | LEU  | 2.9  |
| 51  | 1t    | 76      | ALA  | 2.9  |
| 1   | 2A    | 2145    | C    | 2.9  |
| 1   | 1A    | 2801(A) | A    | 2.9  |
| 1   | 2A    | 2170    | A    | 2.9  |
| 40  | 2i    | 71      | SER  | 2.9  |
| 44  | 2m    | 64      | TRP  | 2.9  |
| 34  | 2c    | 81      | GLY  | 2.9  |
| 33  | 2b    | 123     | ALA  | 2.9  |
| 45  | 1n    | 59      | ALA  | 2.9  |
| 51  | 1t    | 72      | LEU  | 2.9  |
| 23  | 2l    | 26      | ARG  | 2.9  |
| 45  | 2n    | 26      | ARG  | 2.9  |
| 50  | 2s    | 52      | TYR  | 2.9  |
| 1   | 2A    | 2148    | G    | 2.9  |
| 20  | 1Y    | 1       | MET  | 2.9  |
| 1   | 2A    | 6       | A    | 2.9  |
| 26  | 14    | 17      | GLY  | 2.9  |
| 34  | 2c    | 3       | ASN  | 2.9  |
| 38  | 2g    | 156     | TRP  | 2.9  |
| 7   | 2H    | 45      | VAL  | 2.9  |
| 32  | 2a    | 1287    | A    | 2.9  |
| 11  | 2P    | 134     | ALA  | 2.9  |
| 39  | 1h    | 133     | LEU  | 2.9  |
| 41  | 1j    | 20      | ALA  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | 2j    | 20   | ALA  | 2.9  |
| 45  | 1n    | 61   | TRP  | 2.9  |
| 26  | 24    | 67   | TYR  | 2.9  |
| 35  | 2d    | 20   | TYR  | 2.9  |
| 44  | 2m    | 87   | TYR  | 2.9  |
| 8   | 2l    | 107  | VAL  | 2.8  |
| 32  | 2a    | 1006 | C    | 2.8  |
| 40  | 2i    | 29   | ASN  | 2.8  |
| 40  | 1i    | 66   | ARG  | 2.8  |
| 45  | 2n    | 52   | GLN  | 2.8  |
| 1   | 2A    | 1067 | A    | 2.8  |
| 6   | 1G    | 82   | LEU  | 2.8  |
| 35  | 2d    | 188  | LEU  | 2.8  |
| 39  | 2h    | 112  | LEU  | 2.8  |
| 40  | 1i    | 128  | ARG  | 2.8  |
| 40  | 2i    | 17   | VAL  | 2.8  |
| 45  | 1n    | 18   | VAL  | 2.8  |
| 3   | 2D    | 38   | LYS  | 2.8  |
| 32  | 2a    | 1116 | C    | 2.8  |
| 53  | 2y    | 89   | GLN  | 2.8  |
| 55  | 2x    | 75   | C    | 2.8  |
| 1   | 1A    | 2167 | U    | 2.8  |
| 40  | 1i    | 117  | HIS  | 2.8  |
| 3   | 2D    | 215  | LEU  | 2.8  |
| 11  | 2P    | 99   | LEU  | 2.8  |
| 32  | 2a    | 1035 | A    | 2.8  |
| 11  | 2P    | 37   | GLY  | 2.8  |
| 40  | 1i    | 104  | ARG  | 2.8  |
| 48  | 1q    | 79   | SER  | 2.8  |
| 53  | 2y    | 43   | LYS  | 2.8  |
| 34  | 1c    | 201  | TYR  | 2.8  |
| 25  | 23    | 21   | ALA  | 2.8  |
| 40  | 2i    | 64   | THR  | 2.8  |
| 34  | 1c    | 205  | GLY  | 2.8  |
| 51  | 2t    | 11   | SER  | 2.8  |
| 22  | 20    | 45   | PHE  | 2.8  |
| 33  | 2b    | 185  | ILE  | 2.8  |
| 52  | 1u    | 2    | GLY  | 2.8  |
| 33  | 2b    | 7    | VAL  | 2.8  |
| 1   | 1A    | 2155 | G    | 2.8  |
| 20  | 1Y    | 23   | ARG  | 2.8  |
| 33  | 2b    | 120  | ALA  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 1A    | 2146 | C    | 2.8  |
| 8   | 2I    | 34   | GLY  | 2.8  |
| 34  | 2c    | 178  | LEU  | 2.8  |
| 35  | 2d    | 157  | LEU  | 2.8  |
| 45  | 2n    | 46   | GLU  | 2.8  |
| 41  | 2j    | 13   | HIS  | 2.8  |
| 41  | 2j    | 94   | VAL  | 2.8  |
| 50  | 2s    | 60   | VAL  | 2.8  |
| 1   | 1A    | 2114 | A    | 2.8  |
| 1   | 2A    | 2109 | U    | 2.8  |
| 35  | 2d    | 48   | ALA  | 2.8  |
| 1   | 1A    | 889  | C    | 2.8  |
| 34  | 2c    | 16   | ARG  | 2.8  |
| 40  | 2i    | 20   | ARG  | 2.8  |
| 38  | 2g    | 31   | MET  | 2.8  |
| 8   | 2I    | 92   | VAL  | 2.7  |
| 53  | 2y    | 68   | GLU  | 2.7  |
| 1   | 2A    | 1066 | U    | 2.7  |
| 35  | 1d    | 124  | GLY  | 2.7  |
| 33  | 2b    | 201  | ILE  | 2.7  |
| 44  | 2m    | 51   | ALA  | 2.7  |
| 35  | 2d    | 64   | LEU  | 2.7  |
| 38  | 2g    | 101  | LEU  | 2.7  |
| 41  | 2j    | 90   | LEU  | 2.7  |
| 40  | 2i    | 120  | ARG  | 2.7  |
| 32  | 1a    | 1024 | G    | 2.7  |
| 1   | 2A    | 2111 | C    | 2.7  |
| 26  | 14    | 57   | GLU  | 2.7  |
| 11  | 2P    | 110  | TYR  | 2.7  |
| 32  | 2a    | 1348 | U    | 2.7  |
| 35  | 1d    | 67   | ILE  | 2.7  |
| 42  | 2k    | 31   | THR  | 2.7  |
| 43  | 2l    | 32   | PHE  | 2.7  |
| 6   | 2G    | 3    | LEU  | 2.7  |
| 44  | 2m    | 90   | LEU  | 2.7  |
| 34  | 2c    | 82   | GLU  | 2.7  |
| 53  | 2y    | 93   | GLU  | 2.7  |
| 32  | 1a    | 1032 | G    | 2.7  |
| 25  | 23    | 59   | VAL  | 2.7  |
| 34  | 1c    | 159  | GLY  | 2.7  |
| 21  | 1Z    | 188  | ALA  | 2.7  |
| 34  | 2c    | 58   | GLU  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | 2c    | 180  | ALA  | 2.7  |
| 30  | 28    | 50   | LEU  | 2.7  |
| 36  | 2e    | 133  | TYR  | 2.7  |
| 47  | 1p    | 59   | TRP  | 2.7  |
| 1   | 1A    | 1077 | A    | 2.7  |
| 40  | 2i    | 123  | PRO  | 2.7  |
| 41  | 2j    | 41   | PRO  | 2.7  |
| 36  | 2e    | 23   | GLY  | 2.7  |
| 6   | 2G    | 57   | ALA  | 2.7  |
| 32  | 1a    | 841  | U    | 2.7  |
| 33  | 1b    | 123  | ALA  | 2.7  |
| 33  | 2b    | 193  | ASP  | 2.7  |
| 40  | 1i    | 118  | LYS  | 2.7  |
| 47  | 1p    | 44   | THR  | 2.7  |
| 52  | 2u    | 12   | LYS  | 2.7  |
| 35  | 2d    | 11   | LEU  | 2.7  |
| 45  | 2n    | 16   | PHE  | 2.7  |
| 44  | 2m    | 23   | TYR  | 2.7  |
| 33  | 1b    | 19   | HIS  | 2.7  |
| 1   | 1A    | 2602 | A    | 2.7  |
| 1   | 1A    | 2803 | C    | 2.7  |
| 1   | 2A    | 2161 | C    | 2.7  |
| 50  | 2s    | 9    | VAL  | 2.7  |
| 34  | 2c    | 162  | GLN  | 2.7  |
| 1   | 1A    | 2807 | G    | 2.7  |
| 1   | 2A    | 2160 | G    | 2.7  |
| 34  | 2c    | 39   | ILE  | 2.7  |
| 36  | 1e    | 91   | LEU  | 2.7  |
| 41  | 2j    | 63   | PHE  | 2.7  |
| 45  | 2n    | 54   | PRO  | 2.7  |
| 16  | 1U    | 9    | VAL  | 2.7  |
| 34  | 2c    | 106  | VAL  | 2.7  |
| 41  | 2j    | 24   | VAL  | 2.7  |
| 32  | 2a    | 1149 | C    | 2.7  |
| 53  | 2y    | 23   | ARG  | 2.7  |
| 34  | 2c    | 145  | GLY  | 2.7  |
| 36  | 1e    | 127  | ASN  | 2.7  |
| 1   | 2A    | 2792 | G    | 2.7  |
| 15  | 2T    | 66   | VAL  | 2.6  |
| 16  | 2U    | 41   | ALA  | 2.6  |
| 33  | 2b    | 200  | ILE  | 2.6  |
| 34  | 1c    | 47   | LEU  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | 1e    | 131  | ILE  | 2.6  |
| 41  | 1j    | 16   | LEU  | 2.6  |
| 33  | 1b    | 126  | GLU  | 2.6  |
| 7   | 2H    | 106  | THR  | 2.6  |
| 34  | 2c    | 15   | THR  | 2.6  |
| 41  | 2j    | 18   | ALA  | 2.6  |
| 32  | 2a    | 1358 | U    | 2.6  |
| 32  | 2a    | 1532 | U    | 2.6  |
| 39  | 2h    | 107  | LEU  | 2.6  |
| 40  | 2i    | 100  | GLY  | 2.6  |
| 53  | 2y    | 86   | ASN  | 2.6  |
| 33  | 2b    | 70   | PHE  | 2.6  |
| 34  | 1c    | 8    | ILE  | 2.6  |
| 41  | 1j    | 96   | ILE  | 2.6  |
| 41  | 2j    | 75   | ILE  | 2.6  |
| 1   | 1A    | 2143 | C    | 2.6  |
| 41  | 2j    | 89   | ASP  | 2.6  |
| 45  | 2n    | 34   | TYR  | 2.6  |
| 40  | 2i    | 93   | ARG  | 2.6  |
| 1   | 1A    | 2153 | G    | 2.6  |
| 32  | 2a    | 1021 | G    | 2.6  |
| 33  | 1b    | 136  | VAL  | 2.6  |
| 36  | 1e    | 17   | ALA  | 2.6  |
| 43  | 1l    | 26   | ALA  | 2.6  |
| 22  | 10    | 42   | GLY  | 2.6  |
| 1   | 1A    | 1078 | U    | 2.6  |
| 8   | 2I    | 47   | LEU  | 2.6  |
| 32  | 2a    | 1349 | A    | 2.6  |
| 34  | 1c    | 206  | GLU  | 2.6  |
| 41  | 2j    | 98   | ILE  | 2.6  |
| 42  | 2k    | 110  | ASP  | 2.6  |
| 14  | 2S    | 20   | ARG  | 2.6  |
| 1   | 2A    | 889  | C    | 2.6  |
| 40  | 1i    | 114  | TYR  | 2.6  |
| 40  | 2i    | 110  | GLU  | 2.6  |
| 40  | 2i    | 53   | VAL  | 2.6  |
| 41  | 1j    | 93   | GLY  | 2.6  |
| 1   | 1A    | 2159 | G    | 2.6  |
| 1   | 2A    | 2182 | G    | 2.6  |
| 32  | 1a    | 1003 | G    | 2.6  |
| 32  | 2a    | 1040 | U    | 2.6  |
| 35  | 2d    | 162  | LEU  | 2.6  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 39  | 2h    | 122    | ARG  | 2.6  |
| 51  | 1t    | 22     | ARG  | 2.6  |
| 1   | 2A    | 2117   | A    | 2.6  |
| 6   | 2G    | 146    | TYR  | 2.6  |
| 32  | 2a    | 979    | C    | 2.6  |
| 17  | 2V    | 5      | VAL  | 2.6  |
| 34  | 1c    | 60     | ALA  | 2.6  |
| 36  | 2e    | 21     | ALA  | 2.6  |
| 45  | 2n    | 6      | LEU  | 2.6  |
| 52  | 2u    | 23     | PRO  | 2.6  |
| 30  | 28    | 48     | PHE  | 2.6  |
| 44  | 2m    | 84     | ILE  | 2.6  |
| 1   | 2A    | 2894   | G    | 2.6  |
| 32  | 1a    | 1492   | A    | 2.6  |
| 45  | 1n    | 21     | TYR  | 2.6  |
| 13  | 2R    | 84     | ALA  | 2.6  |
| 33  | 1b    | 218    | ALA  | 2.6  |
| 35  | 1d    | 147    | ALA  | 2.6  |
| 38  | 1g    | 17     | VAL  | 2.6  |
| 38  | 2g    | 24     | THR  | 2.6  |
| 53  | 2y    | 98     | ALA  | 2.6  |
| 34  | 1c    | 33     | LEU  | 2.6  |
| 1   | 1A    | 271(K) | U    | 2.6  |
| 40  | 1i    | 77     | ILE  | 2.6  |
| 40  | 2i    | 59     | PHE  | 2.6  |
| 30  | 28    | 7      | HIS  | 2.6  |
| 33  | 2b    | 48     | MET  | 2.6  |
| 1   | 2A    | 1103   | A    | 2.6  |
| 1   | 2A    | 2116   | G    | 2.6  |
| 20  | 2Y    | 73     | ARG  | 2.6  |
| 32  | 2a    | 1023   | G    | 2.6  |
| 35  | 1d    | 167    | GLY  | 2.6  |
| 41  | 1j    | 68     | HIS  | 2.6  |
| 45  | 2n    | 57     | ARG  | 2.6  |
| 47  | 2p    | 39     | TYR  | 2.6  |
| 1   | 1A    | 1102   | C    | 2.6  |
| 26  | 24    | 27     | THR  | 2.5  |
| 36  | 2e    | 17     | ALA  | 2.5  |
| 38  | 2g    | 25     | ALA  | 2.5  |
| 40  | 1i    | 82     | ALA  | 2.5  |
| 51  | 2t    | 40     | ALA  | 2.5  |
| 28  | 26    | 52     | VAL  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 52  | 1u    | 17   | THR  | 2.5  |
| 11  | 1P    | 135  | LEU  | 2.5  |
| 33  | 2b    | 51   | LEU  | 2.5  |
| 35  | 1d    | 202  | LEU  | 2.5  |
| 40  | 2i    | 113  | LYS  | 2.5  |
| 20  | 2Y    | 75   | ILE  | 2.5  |
| 33  | 1b    | 135  | GLN  | 2.5  |
| 48  | 1q    | 36   | ILE  | 2.5  |
| 8   | 2I    | 82   | ARG  | 2.5  |
| 33  | 1b    | 227  | GLY  | 2.5  |
| 33  | 2b    | 227  | GLY  | 2.5  |
| 34  | 2c    | 18   | TRP  | 2.5  |
| 1   | 2A    | 2157 | G    | 2.5  |
| 32  | 2a    | 80   | G    | 2.5  |
| 32  | 2a    | 886  | G    | 2.5  |
| 34  | 1c    | 184  | TYR  | 2.5  |
| 38  | 2g    | 85   | TYR  | 2.5  |
| 40  | 1i    | 125  | TYR  | 2.5  |
| 16  | 2U    | 113  | ALA  | 2.5  |
| 21  | 1Z    | 51   | ALA  | 2.5  |
| 37  | 1f    | 99   | ALA  | 2.5  |
| 41  | 1j    | 18   | ALA  | 2.5  |
| 50  | 2s    | 28   | LYS  | 2.5  |
| 8   | 2I    | 30   | LEU  | 2.5  |
| 19  | 2X    | 83   | VAL  | 2.5  |
| 32  | 1a    | 999  | C    | 2.5  |
| 52  | 1u    | 8    | THR  | 2.5  |
| 39  | 1h    | 93   | VAL  | 2.5  |
| 33  | 1b    | 211  | ILE  | 2.5  |
| 8   | 2I    | 20   | ASP  | 2.5  |
| 22  | 10    | 4    | LYS  | 2.5  |
| 6   | 2G    | 29   | TRP  | 2.5  |
| 6   | 2G    | 58   | GLN  | 2.5  |
| 34  | 2c    | 65   | ALA  | 2.5  |
| 38  | 2g    | 13   | GLN  | 2.5  |
| 44  | 2m    | 42   | ALA  | 2.5  |
| 1   | 1A    | 2112 | G    | 2.5  |
| 30  | 28    | 22   | VAL  | 2.5  |
| 35  | 2d    | 203  | VAL  | 2.5  |
| 1   | 1A    | 2175 | C    | 2.5  |
| 50  | 2s    | 5    | LEU  | 2.5  |
| 11  | 2P    | 22   | GLY  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 34  | 1c    | 182  | ILE  | 2.5  |
| 34  | 2c    | 14   | ILE  | 2.5  |
| 39  | 2h    | 131  | GLY  | 2.5  |
| 45  | 2n    | 38   | GLY  | 2.5  |
| 46  | 1o    | 89   | GLY  | 2.5  |
| 47  | 2p    | 48   | TRP  | 2.5  |
| 45  | 1n    | 2    | ALA  | 2.5  |
| 1   | 1A    | 2062 | A    | 2.5  |
| 1   | 1A    | 2892 | A    | 2.5  |
| 32  | 1a    | 1349 | A    | 2.5  |
| 33  | 2b    | 195  | ASP  | 2.5  |
| 34  | 1c    | 12   | LEU  | 2.5  |
| 43  | 1l    | 60   | LEU  | 2.5  |
| 5   | 1F    | 16   | GLY  | 2.5  |
| 32  | 1a    | 1020 | U    | 2.5  |
| 39  | 1h    | 38   | ILE  | 2.5  |
| 38  | 1g    | 13   | GLN  | 2.5  |
| 35  | 2d    | 49   | ARG  | 2.5  |
| 3   | 1D    | 275  | LYS  | 2.5  |
| 33  | 2b    | 194  | PRO  | 2.5  |
| 33  | 1b    | 229  | VAL  | 2.5  |
| 40  | 2i    | 44   | VAL  | 2.5  |
| 1   | 1A    | 2169 | A    | 2.5  |
| 1   | 2A    | 2310 | A    | 2.5  |
| 32  | 2a    | 1150 | U    | 2.5  |
| 8   | 2I    | 88   | ILE  | 2.5  |
| 7   | 2H    | 95   | ARG  | 2.5  |
| 34  | 2c    | 206  | GLU  | 2.5  |
| 36  | 2e    | 26   | PHE  | 2.5  |
| 49  | 1r    | 42   | ARG  | 2.5  |
| 1   | 1A    | 2123 | G    | 2.5  |
| 32  | 2a    | 1034 | G    | 2.5  |
| 53  | 2y    | 6    | THR  | 2.5  |
| 35  | 2d    | 23   | GLY  | 2.5  |
| 26  | 14    | 56   | VAL  | 2.5  |
| 33  | 2b    | 97   | TRP  | 2.5  |
| 34  | 2c    | 47   | LEU  | 2.5  |
| 47  | 1p    | 49   | LEU  | 2.5  |
| 38  | 2g    | 8    | GLU  | 2.5  |
| 42  | 2k    | 104  | GLN  | 2.5  |
| 20  | 2Y    | 52   | SER  | 2.5  |
| 30  | 28    | 46   | ARG  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 35  | 2d    | 122  | ARG  | 2.5  |
| 45  | 2n    | 29   | ARG  | 2.5  |
| 1   | 2A    | 2135 | A    | 2.5  |
| 32  | 1a    | 1035 | A    | 2.5  |
| 32  | 2a    | 1041 | A    | 2.5  |
| 45  | 2n    | 42   | ILE  | 2.5  |
| 53  | 2y    | 26   | LYS  | 2.5  |
| 1   | 2A    | 1064 | C    | 2.5  |
| 1   | 2A    | 2127 | G    | 2.5  |
| 22  | 20    | 6    | GLY  | 2.5  |
| 23  | 21    | 24   | ALA  | 2.5  |
| 50  | 2s    | 39   | THR  | 2.5  |
| 21  | 2Z    | 125  | LEU  | 2.4  |
| 38  | 2g    | 10   | ARG  | 2.4  |
| 6   | 2G    | 159  | VAL  | 2.4  |
| 39  | 1h    | 103  | VAL  | 2.4  |
| 45  | 2n    | 33   | VAL  | 2.4  |
| 28  | 26    | 42   | TRP  | 2.4  |
| 32  | 1a    | 1136 | U    | 2.4  |
| 48  | 1q    | 99   | SER  | 2.4  |
| 53  | 1y    | 42   | SER  | 2.4  |
| 33  | 2b    | 127  | ILE  | 2.4  |
| 35  | 1d    | 185  | PHE  | 2.4  |
| 36  | 1e    | 6    | PHE  | 2.4  |
| 39  | 2h    | 38   | ILE  | 2.4  |
| 53  | 1y    | 35   | ILE  | 2.4  |
| 32  | 2a    | 1236 | A    | 2.4  |
| 1   | 1A    | 2174 | C    | 2.4  |
| 32  | 2a    | 1354 | C    | 2.4  |
| 34  | 2c    | 174  | PRO  | 2.4  |
| 48  | 2q    | 94   | ASN  | 2.4  |
| 34  | 1c    | 172  | ARG  | 2.4  |
| 45  | 2n    | 4    | LYS  | 2.4  |
| 32  | 2a    | 1385 | G    | 2.4  |
| 12  | 2Q    | 35   | VAL  | 2.4  |
| 12  | 2Q    | 97   | VAL  | 2.4  |
| 34  | 1c    | 120  | VAL  | 2.4  |
| 47  | 1p    | 38   | TYR  | 2.4  |
| 34  | 2c    | 182  | ILE  | 2.4  |
| 39  | 2h    | 86   | ILE  | 2.4  |
| 47  | 2p    | 59   | TRP  | 2.4  |
| 9   | 2N    | 104  | LYS  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | 2a    | 1111 | A    | 2.4  |
| 33  | 1b    | 114  | ARG  | 2.4  |
| 45  | 2n    | 31   | ARG  | 2.4  |
| 1   | 1A    | 2896 | C    | 2.4  |
| 16  | 2U    | 21   | ALA  | 2.4  |
| 39  | 2h    | 124  | ALA  | 2.4  |
| 7   | 2H    | 103  | LEU  | 2.4  |
| 12  | 2Q    | 34   | LEU  | 2.4  |
| 33  | 1b    | 115  | LEU  | 2.4  |
| 34  | 2c    | 196  | LEU  | 2.4  |
| 47  | 1p    | 20   | VAL  | 2.4  |
| 48  | 2q    | 10   | VAL  | 2.4  |
| 41  | 2j    | 12   | ASP  | 2.4  |
| 1   | 1A    | 2130 | U    | 2.4  |
| 1   | 2A    | 1816 | G    | 2.4  |
| 40  | 1i    | 127  | LYS  | 2.4  |
| 33  | 2b    | 122  | PHE  | 2.4  |
| 36  | 2e    | 14   | ARG  | 2.4  |
| 40  | 2i    | 104  | ARG  | 2.4  |
| 26  | 24    | 19   | GLY  | 2.4  |
| 34  | 2c    | 185  | GLY  | 2.4  |
| 44  | 2m    | 95   | GLY  | 2.4  |
| 7   | 2H    | 128  | PRO  | 2.4  |
| 6   | 2G    | 64   | THR  | 2.4  |
| 1   | 2A    | 1102 | C    | 2.4  |
| 32  | 2a    | 1151 | A    | 2.4  |
| 40  | 2i    | 96   | LEU  | 2.4  |
| 35  | 2d    | 56   | VAL  | 2.4  |
| 44  | 1m    | 91   | ARG  | 2.4  |
| 14  | 2S    | 36   | TYR  | 2.4  |
| 14  | 2S    | 92   | TYR  | 2.4  |
| 47  | 2p    | 58   | TYR  | 2.4  |
| 41  | 1j    | 47   | PHE  | 2.4  |
| 1   | 1A    | 2124 | G    | 2.4  |
| 32  | 2a    | 1061 | G    | 2.4  |
| 41  | 1j    | 41   | PRO  | 2.4  |
| 4   | 1E    | 163  | GLU  | 2.4  |
| 34  | 2c    | 22   | TRP  | 2.4  |
| 34  | 1c    | 177  | THR  | 2.4  |
| 42  | 2k    | 87   | THR  | 2.4  |
| 47  | 1p    | 60   | LEU  | 2.4  |
| 37  | 2f    | 77   | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 32  | 2a    | 1235 | U    | 2.4  |
| 40  | 2i    | 24   | GLY  | 2.4  |
| 35  | 1d    | 86   | LYS  | 2.4  |
| 33  | 2b    | 188  | ALA  | 2.4  |
| 40  | 2i    | 54   | ASP  | 2.4  |
| 42  | 2k    | 42   | TRP  | 2.4  |
| 45  | 2n    | 27   | CYS  | 2.4  |
| 51  | 2t    | 12   | ALA  | 2.4  |
| 32  | 1a    | 1021 | G    | 2.4  |
| 5   | 2F    | 62   | ARG  | 2.4  |
| 34  | 2c    | 59   | ARG  | 2.4  |
| 42  | 2k    | 98   | LEU  | 2.4  |
| 50  | 2s    | 38   | SER  | 2.4  |
| 1   | 2A    | 887  | A    | 2.4  |
| 33  | 1b    | 228  | GLY  | 2.4  |
| 36  | 1e    | 34   | VAL  | 2.4  |
| 43  | 2l    | 13   | LYS  | 2.4  |
| 36  | 1e    | 10   | MET  | 2.4  |
| 47  | 1p    | 1    | MET  | 2.4  |
| 52  | 2u    | 5    | ASP  | 2.4  |
| 50  | 2s    | 77   | THR  | 2.4  |
| 31  | 29    | 11   | CYS  | 2.4  |
| 34  | 2c    | 34   | LEU  | 2.4  |
| 41  | 2j    | 40   | LEU  | 2.4  |
| 32  | 1a    | 1034 | G    | 2.3  |
| 44  | 2m    | 111  | LYS  | 2.3  |
| 45  | 1n    | 17   | LYS  | 2.3  |
| 15  | 2T    | 70   | VAL  | 2.3  |
| 46  | 2o    | 60   | VAL  | 2.3  |
| 1   | 2A    | 1118 | C    | 2.3  |
| 1   | 2A    | 2119 | A    | 2.3  |
| 1   | 2A    | 2130 | U    | 2.3  |
| 1   | 2A    | 2144 | U    | 2.3  |
| 13  | 2R    | 68   | ARG  | 2.3  |
| 19  | 2X    | 39   | ILE  | 2.3  |
| 40  | 2i    | 37   | PHE  | 2.3  |
| 41  | 2j    | 46   | ARG  | 2.3  |
| 48  | 2q    | 36   | ILE  | 2.3  |
| 36  | 2e    | 94   | ALA  | 2.3  |
| 3   | 2D    | 50   | THR  | 2.3  |
| 53  | 2y    | 91   | LYS  | 2.3  |
| 16  | 2U    | 74   | LEU  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | 2m    | 96   | LEU  | 2.3  |
| 53  | 2y    | 36   | ASN  | 2.3  |
| 1   | 2A    | 2156 | G    | 2.3  |
| 32  | 2a    | 976  | G    | 2.3  |
| 32  | 2a    | 1032 | G    | 2.3  |
| 5   | 2F    | 81   | PRO  | 2.3  |
| 6   | 2G    | 142  | PRO  | 2.3  |
| 34  | 2c    | 190  | ARG  | 2.3  |
| 40  | 1i    | 121  | ARG  | 2.3  |
| 47  | 1p    | 29   | ASP  | 2.3  |
| 32  | 2a    | 1157 | A    | 2.3  |
| 38  | 2g    | 120  | ILE  | 2.3  |
| 3   | 2D    | 272  | ALA  | 2.3  |
| 12  | 2Q    | 136  | ALA  | 2.3  |
| 40  | 1i    | 36   | TYR  | 2.3  |
| 22  | 20    | 8    | GLY  | 2.3  |
| 38  | 2g    | 79   | ARG  | 2.3  |
| 53  | 2y    | 30   | TRP  | 2.3  |
| 7   | 2H    | 35   | VAL  | 2.3  |
| 40  | 1i    | 31   | GLN  | 2.3  |
| 1   | 1A    | 2127 | G    | 2.3  |
| 22  | 20    | 57   | PHE  | 2.3  |
| 32  | 2a    | 1002 | G    | 2.3  |
| 32  | 2a    | 1003 | G    | 2.3  |
| 32  | 2a    | 1027 | C    | 2.3  |
| 33  | 2b    | 57   | PHE  | 2.3  |
| 12  | 2Q    | 114  | ALA  | 2.3  |
| 24  | 12    | 13   | ALA  | 2.3  |
| 34  | 1c    | 189  | ALA  | 2.3  |
| 34  | 2c    | 113  | ALA  | 2.3  |
| 40  | 1i    | 126  | SER  | 2.3  |
| 20  | 2Y    | 80   | GLY  | 2.3  |
| 43  | 1l    | 67   | THR  | 2.3  |
| 23  | 11    | 95   | LEU  | 2.3  |
| 34  | 1c    | 126  | ARG  | 2.3  |
| 40  | 1i    | 79   | LEU  | 2.3  |
| 40  | 2i    | 83   | ARG  | 2.3  |
| 41  | 2j    | 17   | ASP  | 2.3  |
| 4   | 2E    | 116  | VAL  | 2.3  |
| 9   | 2N    | 9    | VAL  | 2.3  |
| 9   | 2N    | 42   | TRP  | 2.3  |
| 29  | 27    | 46   | VAL  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 47  | 1p    | 41   | PRO  | 2.3  |
| 44  | 1m    | 82   | MET  | 2.3  |
| 6   | 2G    | 177  | GLY  | 2.3  |
| 12  | 2Q    | 36   | ALA  | 2.3  |
| 40  | 1i    | 43   | ALA  | 2.3  |
| 40  | 1i    | 45   | ALA  | 2.3  |
| 41  | 1j    | 59   | SER  | 2.3  |
| 43  | 1l    | 63   | GLY  | 2.3  |
| 44  | 1m    | 89   | GLY  | 2.3  |
| 32  | 1a    | 1023 | G    | 2.3  |
| 35  | 1d    | 20   | TYR  | 2.3  |
| 15  | 2T    | 105  | LEU  | 2.3  |
| 33  | 2b    | 121  | LEU  | 2.3  |
| 40  | 1i    | 47   | LEU  | 2.3  |
| 43  | 2l    | 124  | LYS  | 2.3  |
| 44  | 1m    | 90   | LEU  | 2.3  |
| 35  | 2d    | 140  | VAL  | 2.3  |
| 40  | 2i    | 89   | ASN  | 2.3  |
| 53  | 1y    | 82   | GLU  | 2.3  |
| 41  | 2j    | 38   | ILE  | 2.3  |
| 45  | 2n    | 23   | ARG  | 2.3  |
| 53  | 2y    | 55   | ASN  | 2.3  |
| 34  | 2c    | 144  | SER  | 2.3  |
| 40  | 2i    | 33   | PHE  | 2.3  |
| 41  | 2j    | 54   | PHE  | 2.3  |
| 45  | 1n    | 20   | ALA  | 2.3  |
| 5   | 1F    | 53   | THR  | 2.3  |
| 40  | 2i    | 124  | GLN  | 2.3  |
| 44  | 1m    | 109  | THR  | 2.3  |
| 19  | 2X    | 66   | LEU  | 2.3  |
| 1   | 1A    | 1071 | G    | 2.3  |
| 1   | 1A    | 1088 | A    | 2.3  |
| 35  | 1d    | 19   | LEU  | 2.3  |
| 1   | 1A    | 2156 | G    | 2.3  |
| 33  | 2b    | 229  | VAL  | 2.3  |
| 34  | 1c    | 173  | VAL  | 2.3  |
| 1   | 1A    | 2150 | U    | 2.3  |
| 32  | 1a    | 1532 | U    | 2.3  |
| 32  | 2a    | 841  | U    | 2.3  |
| 36  | 1e    | 136  | MET  | 2.3  |
| 51  | 1t    | 74   | LYS  | 2.3  |
| 26  | 24    | 54   | GLY  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | 1j    | 52   | GLY  | 2.3  |
| 38  | 2g    | 7    | ALA  | 2.3  |
| 40  | 1i    | 33   | PHE  | 2.3  |
| 6   | 2G    | 62   | LEU  | 2.3  |
| 19  | 1X    | 69   | TYR  | 2.3  |
| 34  | 2c    | 32   | LEU  | 2.3  |
| 35  | 1d    | 157  | LEU  | 2.3  |
| 35  | 1d    | 194  | LEU  | 2.3  |
| 47  | 1p    | 17   | TYR  | 2.3  |
| 21  | 2Z    | 80   | ARG  | 2.2  |
| 33  | 1b    | 131  | PRO  | 2.2  |
| 38  | 2g    | 63   | LYS  | 2.2  |
| 39  | 2h    | 76   | PRO  | 2.2  |
| 44  | 2m    | 93   | ARG  | 2.2  |
| 52  | 2u    | 24   | ARG  | 2.2  |
| 32  | 1a    | 998  | G    | 2.2  |
| 32  | 1a    | 1002 | G    | 2.2  |
| 5   | 2F    | 57   | VAL  | 2.2  |
| 51  | 1t    | 9    | ASN  | 2.2  |
| 34  | 2c    | 78   | GLY  | 2.2  |
| 35  | 2d    | 143  | GLY  | 2.2  |
| 41  | 2j    | 84   | GLN  | 2.2  |
| 30  | 18    | 37   | SER  | 2.2  |
| 33  | 1b    | 124  | SER  | 2.2  |
| 34  | 2c    | 20   | SER  | 2.2  |
| 50  | 2s    | 49   | ILE  | 2.2  |
| 41  | 1j    | 54   | PHE  | 2.2  |
| 51  | 1t    | 12   | ALA  | 2.2  |
| 12  | 2Q    | 37   | LEU  | 2.2  |
| 34  | 2c    | 85   | ARG  | 2.2  |
| 35  | 1d    | 58   | LEU  | 2.2  |
| 41  | 2j    | 8    | LEU  | 2.2  |
| 44  | 2m    | 110  | ARG  | 2.2  |
| 33  | 1b    | 125  | PRO  | 2.2  |
| 39  | 1h    | 71   | GLY  | 2.2  |
| 35  | 2d    | 134  | ASP  | 2.2  |
| 40  | 1i    | 105  | ASP  | 2.2  |
| 32  | 1a    | 1040 | U    | 2.2  |
| 33  | 2b    | 58   | ILE  | 2.2  |
| 34  | 1c    | 124  | ILE  | 2.2  |
| 44  | 1m    | 22   | ILE  | 2.2  |
| 14  | 2S    | 12   | PHE  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 26  | 24    | 59   | PHE  | 2.2  |
| 34  | 2c    | 4    | LYS  | 2.2  |
| 46  | 2o    | 17   | ARG  | 2.2  |
| 1   | 2A    | 2175 | C    | 2.2  |
| 32  | 2a    | 783  | C    | 2.2  |
| 34  | 1c    | 36   | ASP  | 2.2  |
| 39  | 1h    | 22   | GLU  | 2.2  |
| 7   | 2H    | 37   | VAL  | 2.2  |
| 34  | 2c    | 103  | VAL  | 2.2  |
| 42  | 2k    | 14   | VAL  | 2.2  |
| 45  | 1n    | 32   | SER  | 2.2  |
| 1   | 1A    | 1070 | A    | 2.2  |
| 1   | 1A    | 1085 | A    | 2.2  |
| 32  | 2a    | 1492 | A    | 2.2  |
| 3   | 1D    | 199  | ALA  | 2.2  |
| 40  | 2i    | 46   | ALA  | 2.2  |
| 6   | 2G    | 80   | PHE  | 2.2  |
| 45  | 2n    | 37   | PHE  | 2.2  |
| 1   | 2A    | 2155 | G    | 2.2  |
| 40  | 2i    | 87   | GLN  | 2.2  |
| 48  | 2q    | 6    | LEU  | 2.2  |
| 50  | 2s    | 71   | LEU  | 2.2  |
| 3   | 1D    | 47   | GLY  | 2.2  |
| 35  | 1d    | 68   | TYR  | 2.2  |
| 40  | 1i    | 113  | LYS  | 2.2  |
| 1   | 1A    | 1053 | C    | 2.2  |
| 1   | 2A    | 2143 | C    | 2.2  |
| 32  | 2a    | 174  | C    | 2.2  |
| 32  | 2a    | 848  | C    | 2.2  |
| 42  | 2k    | 80   | VAL  | 2.2  |
| 43  | 1l    | 82   | VAL  | 2.2  |
| 6   | 2G    | 61   | ALA  | 2.2  |
| 23  | 2l    | 63   | ALA  | 2.2  |
| 40  | 1i    | 94   | ALA  | 2.2  |
| 47  | 1p    | 56   | ALA  | 2.2  |
| 5   | 1F    | 85   | GLY  | 2.2  |
| 19  | 1X    | 66   | LEU  | 2.2  |
| 22  | 20    | 52   | GLY  | 2.2  |
| 41  | 2j    | 85   | LEU  | 2.2  |
| 22  | 20    | 77   | ARG  | 2.2  |
| 8   | 2I    | 3    | VAL  | 2.2  |
| 39  | 2h    | 103  | VAL  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | 2j    | 86   | MET  | 2.2  |
| 1   | 2A    | 645  | C    | 2.2  |
| 21  | 1Z    | 192  | ALA  | 2.2  |
| 51  | 2t    | 28   | ALA  | 2.2  |
| 6   | 2G    | 93   | THR  | 2.2  |
| 53  | 2y    | 32   | THR  | 2.2  |
| 32  | 2a    | 1180 | A    | 2.2  |
| 34  | 1c    | 10   | PHE  | 2.2  |
| 33  | 1b    | 232  | PRO  | 2.2  |
| 41  | 2j    | 71   | LEU  | 2.2  |
| 52  | 1u    | 10   | ARG  | 2.2  |
| 32  | 2a    | 1156 | G    | 2.2  |
| 33  | 1b    | 233  | SER  | 2.2  |
| 48  | 2q    | 42   | TYR  | 2.2  |
| 49  | 2r    | 62   | GLU  | 2.2  |
| 1   | 2A    | 2172 | U    | 2.2  |
| 11  | 2P    | 71   | VAL  | 2.2  |
| 12  | 2Q    | 102  | VAL  | 2.2  |
| 33  | 2b    | 83   | MET  | 2.2  |
| 34  | 1c    | 64   | VAL  | 2.2  |
| 34  | 2c    | 28   | GLN  | 2.2  |
| 4   | 2E    | 157  | ALA  | 2.2  |
| 36  | 2e    | 62   | ALA  | 2.2  |
| 1   | 2A    | 1079 | C    | 2.2  |
| 32  | 2a    | 1260 | C    | 2.2  |
| 32  | 2a    | 1533 | C    | 2.2  |
| 34  | 2c    | 57   | ILE  | 2.2  |
| 41  | 2j    | 74   | ILE  | 2.2  |
| 44  | 2m    | 25   | ILE  | 2.2  |
| 45  | 1n    | 13   | THR  | 2.2  |
| 18  | 2W    | 92   | ARG  | 2.2  |
| 23  | 21    | 60   | PHE  | 2.2  |
| 30  | 28    | 38   | GLY  | 2.2  |
| 34  | 2c    | 13   | GLY  | 2.2  |
| 40  | 1i    | 16   | ARG  | 2.2  |
| 40  | 1i    | 120  | ARG  | 2.2  |
| 42  | 2k    | 76   | GLY  | 2.2  |
| 53  | 2y    | 59   | GLY  | 2.2  |
| 35  | 2d    | 174  | LEU  | 2.2  |
| 35  | 2d    | 186  | LEU  | 2.2  |
| 25  | 23    | 60   | GLU  | 2.2  |
| 41  | 1j    | 62   | HIS  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2A    | 2149 | G    | 2.1  |
| 1   | 2A    | 2165 | G    | 2.1  |
| 4   | 2E    | 120  | TRP  | 2.1  |
| 38  | 2g    | 144  | MET  | 2.1  |
| 32  | 2a    | 1138 | G    | 2.1  |
| 37  | 1f    | 6    | VAL  | 2.1  |
| 38  | 2g    | 117  | ALA  | 2.1  |
| 40  | 2i    | 55   | ALA  | 2.1  |
| 41  | 1j    | 17   | ASP  | 2.1  |
| 41  | 2j    | 32   | ALA  | 2.1  |
| 42  | 2k    | 64   | ALA  | 2.1  |
| 34  | 2c    | 194  | GLY  | 2.1  |
| 38  | 2g    | 32   | ARG  | 2.1  |
| 47  | 2p    | 33   | ILE  | 2.1  |
| 51  | 1t    | 100  | ILE  | 2.1  |
| 35  | 2d    | 185  | PHE  | 2.1  |
| 48  | 1q    | 28   | PRO  | 2.1  |
| 3   | 2D    | 155  | LEU  | 2.1  |
| 33  | 2b    | 11   | LEU  | 2.1  |
| 42  | 2k    | 123  | LYS  | 2.1  |
| 34  | 2c    | 131  | ARG  | 2.1  |
| 34  | 2c    | 195  | VAL  | 2.1  |
| 38  | 2g    | 6    | ARG  | 2.1  |
| 39  | 1h    | 94   | TYR  | 2.1  |
| 47  | 1p    | 39   | TYR  | 2.1  |
| 6   | 1G    | 73   | ALA  | 2.1  |
| 33  | 2b    | 38   | GLY  | 2.1  |
| 34  | 2c    | 167  | TRP  | 2.1  |
| 40  | 1i    | 80   | GLY  | 2.1  |
| 1   | 2A    | 2206 | G    | 2.1  |
| 1   | 2A    | 2319 | G    | 2.1  |
| 15  | 2T    | 110  | ILE  | 2.1  |
| 33  | 2b    | 133  | LYS  | 2.1  |
| 44  | 2m    | 4    | ILE  | 2.1  |
| 46  | 1o    | 87   | ILE  | 2.1  |
| 33  | 2b    | 181  | PHE  | 2.1  |
| 36  | 1e    | 123  | LEU  | 2.1  |
| 32  | 1a    | 1037 | C    | 2.1  |
| 32  | 2a    | 1007 | C    | 2.1  |
| 32  | 2a    | 1223 | C    | 2.1  |
| 45  | 2n    | 49   | HIS  | 2.1  |
| 32  | 1a    | 1044 | A    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 33  | 2b    | 144  | ARG  | 2.1  |
| 45  | 1n    | 45   | ARG  | 2.1  |
| 52  | 2u    | 22   | ARG  | 2.1  |
| 44  | 2m    | 13   | LYS  | 2.1  |
| 9   | 2N    | 43   | THR  | 2.1  |
| 44  | 2m    | 109  | THR  | 2.1  |
| 5   | 2F    | 65   | TRP  | 2.1  |
| 5   | 2F    | 78   | ILE  | 2.1  |
| 20  | 2Y    | 44   | ILE  | 2.1  |
| 35  | 1d    | 201  | GLN  | 2.1  |
| 38  | 2g    | 27   | ILE  | 2.1  |
| 40  | 2i    | 77   | ILE  | 2.1  |
| 8   | 2I    | 35   | LEU  | 2.1  |
| 38  | 2g    | 16   | LEU  | 2.1  |
| 1   | 1A    | 2125 | G    | 2.1  |
| 32  | 1a    | 1233 | G    | 2.1  |
| 32  | 2a    | 1155 | G    | 2.1  |
| 32  | 2a    | 1224 | G    | 2.1  |
| 23  | 2l    | 75   | GLU  | 2.1  |
| 33  | 1b    | 30   | ARG  | 2.1  |
| 34  | 2c    | 69   | HIS  | 2.1  |
| 1   | 1A    | 2145 | C    | 2.1  |
| 34  | 2c    | 166  | GLU  | 2.1  |
| 40  | 1i    | 42   | ARG  | 2.1  |
| 45  | 1n    | 15   | LYS  | 2.1  |
| 19  | 1X    | 67   | GLY  | 2.1  |
| 32  | 2a    | 768  | A    | 2.1  |
| 38  | 1g    | 31   | MET  | 2.1  |
| 8   | 2I    | 18   | VAL  | 2.1  |
| 35  | 1d    | 112  | VAL  | 2.1  |
| 35  | 2d    | 4    | TYR  | 2.1  |
| 36  | 1e    | 55   | VAL  | 2.1  |
| 46  | 1o    | 80   | ALA  | 2.1  |
| 47  | 1p    | 32   | TYR  | 2.1  |
| 40  | 1i    | 123  | PRO  | 2.1  |
| 53  | 2y    | 14   | PRO  | 2.1  |
| 45  | 2n    | 7    | ILE  | 2.1  |
| 6   | 2G    | 139  | LEU  | 2.1  |
| 34  | 2c    | 101  | LEU  | 2.1  |
| 39  | 1h    | 112  | LEU  | 2.1  |
| 45  | 2n    | 45   | ARG  | 2.1  |
| 50  | 2s    | 16   | LEU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | 20    | 5    | LYS  | 2.1  |
| 26  | 24    | 40   | HIS  | 2.1  |
| 45  | 2n    | 15   | LYS  | 2.1  |
| 32  | 2a    | 1283 | G    | 2.1  |
| 43  | 1l    | 103  | GLY  | 2.1  |
| 1   | 1A    | 1095 | A    | 2.1  |
| 1   | 2A    | 1026 | U    | 2.1  |
| 3   | 1D    | 10   | THR  | 2.1  |
| 23  | 11    | 53   | VAL  | 2.1  |
| 38  | 2g    | 9    | VAL  | 2.1  |
| 44  | 1m    | 28   | ALA  | 2.1  |
| 53  | 2y    | 97   | ALA  | 2.1  |
| 6   | 2G    | 136  | ARG  | 2.1  |
| 9   | 2N    | 74   | ARG  | 2.1  |
| 34  | 1c    | 193  | TYR  | 2.1  |
| 34  | 2c    | 184  | TYR  | 2.1  |
| 40  | 1i    | 4    | TYR  | 2.1  |
| 40  | 1i    | 11   | LYS  | 2.1  |
| 23  | 11    | 46   | LEU  | 2.1  |
| 39  | 1h    | 63   | LEU  | 2.1  |
| 41  | 2j    | 56   | HIS  | 2.1  |
| 41  | 2j    | 88   | LEU  | 2.1  |
| 51  | 2t    | 36   | LEU  | 2.1  |
| 39  | 2h    | 47   | GLY  | 2.1  |
| 40  | 2i    | 80   | GLY  | 2.1  |
| 1   | 1A    | 2129 | C    | 2.1  |
| 6   | 2G    | 160  | VAL  | 2.1  |
| 7   | 2H    | 29   | PRO  | 2.1  |
| 32  | 1a    | 1361 | G    | 2.1  |
| 34  | 1c    | 168  | ALA  | 2.1  |
| 40  | 1i    | 119  | ALA  | 2.1  |
| 51  | 2t    | 44   | ALA  | 2.1  |
| 16  | 2U    | 9    | VAL  | 2.1  |
| 32  | 1a    | 202  | U    | 2.1  |
| 1   | 1A    | 229  | A    | 2.1  |
| 11  | 1P    | 35   | HIS  | 2.1  |
| 53  | 2y    | 54   | ILE  | 2.1  |
| 8   | 2I    | 72   | LEU  | 2.1  |
| 34  | 2c    | 154  | SER  | 2.1  |
| 43  | 1l    | 62   | SER  | 2.1  |
| 47  | 1p    | 73   | LEU  | 2.1  |
| 31  | 29    | 14   | CYS  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | 1G    | 21   | ARG  | 2.1  |
| 40  | 2i    | 9    | ARG  | 2.1  |
| 7   | 2H    | 20   | ALA  | 2.0  |
| 32  | 1a    | 217  | C    | 2.0  |
| 32  | 2a    | 1195 | C    | 2.0  |
| 38  | 2g    | 116  | ALA  | 2.0  |
| 49  | 1r    | 73   | ALA  | 2.0  |
| 40  | 2i    | 86   | VAL  | 2.0  |
| 1   | 1A    | 1059 | G    | 2.0  |
| 40  | 2i    | 58   | HIS  | 2.0  |
| 12  | 2Q    | 127  | ILE  | 2.0  |
| 26  | 14    | 63   | TYR  | 2.0  |
| 34  | 2c    | 49   | SER  | 2.0  |
| 52  | 1u    | 21   | TYR  | 2.0  |
| 1   | 1A    | 2790 | A    | 2.0  |
| 1   | 2A    | 1095 | A    | 2.0  |
| 5   | 2F    | 90   | PHE  | 2.0  |
| 6   | 1G    | 139  | LEU  | 2.0  |
| 34  | 2c    | 37   | GLN  | 2.0  |
| 35  | 2d    | 101  | LEU  | 2.0  |
| 35  | 2d    | 110  | PHE  | 2.0  |
| 43  | 2l    | 16   | GLU  | 2.0  |
| 49  | 2r    | 29   | PHE  | 2.0  |
| 49  | 2r    | 54   | ARG  | 2.0  |
| 6   | 2G    | 151  | ALA  | 2.0  |
| 6   | 2G    | 158  | ALA  | 2.0  |
| 36  | 2e    | 86   | ALA  | 2.0  |
| 40  | 1i    | 15   | ALA  | 2.0  |
| 20  | 2Y    | 24   | VAL  | 2.0  |
| 32  | 1a    | 1027 | C    | 2.0  |
| 32  | 2a    | 1367 | C    | 2.0  |
| 38  | 1g    | 11   | GLN  | 2.0  |
| 6   | 2G    | 51   | ARG  | 2.0  |
| 8   | 2I    | 12   | LEU  | 2.0  |
| 33  | 1b    | 222  | ILE  | 2.0  |
| 33  | 2b    | 33   | TYR  | 2.0  |
| 36  | 2e    | 123  | LEU  | 2.0  |
| 38  | 1g    | 42   | ILE  | 2.0  |
| 42  | 2k    | 29   | ILE  | 2.0  |
| 48  | 2q    | 59   | ILE  | 2.0  |
| 38  | 2g    | 95   | ARG  | 2.0  |
| 41  | 2j    | 66   | ARG  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | 2A    | 2190 | G    | 2.0  |
| 1   | 2A    | 2807 | G    | 2.0  |
| 32  | 2a    | 1357 | A    | 2.0  |
| 33  | 1b    | 167  | PRO  | 2.0  |
| 34  | 1c    | 160  | ALA  | 2.0  |
| 34  | 2c    | 100  | ALA  | 2.0  |
| 51  | 1t    | 77   | ALA  | 2.0  |
| 11  | 2P    | 57   | THR  | 2.0  |
| 12  | 2Q    | 110  | THR  | 2.0  |
| 42  | 2k    | 22   | HIS  | 2.0  |
| 21  | 2Z    | 128  | VAL  | 2.0  |
| 34  | 1c    | 98   | ASN  | 2.0  |
| 38  | 2g    | 105  | VAL  | 2.0  |
| 35  | 1d    | 73   | ARG  | 2.0  |
| 41  | 1j    | 60   | ARG  | 2.0  |
| 42  | 2k    | 16   | SER  | 2.0  |
| 44  | 1m    | 26   | GLY  | 2.0  |
| 21  | 2Z    | 183  | LEU  | 2.0  |
| 25  | 13    | 31   | LEU  | 2.0  |
| 25  | 23    | 53   | LEU  | 2.0  |
| 30  | 28    | 61   | LEU  | 2.0  |
| 35  | 2d    | 21   | LEU  | 2.0  |
| 35  | 2d    | 126  | ILE  | 2.0  |
| 20  | 2Y    | 20   | TYR  | 2.0  |
| 34  | 1c    | 128  | PHE  | 2.0  |
| 34  | 2c    | 193  | TYR  | 2.0  |
| 35  | 2d    | 190  | ASP  | 2.0  |
| 41  | 2j    | 25   | GLU  | 2.0  |
| 32  | 1a    | 1360 | A    | 2.0  |
| 32  | 2a    | 1288 | A    | 2.0  |
| 38  | 2g    | 11   | GLN  | 2.0  |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 1   | 5MU  | 2A    | 1915 | 21/22 | 0.79 | 0.19 | 63,76,78,90                | 0     |
| 1   | PSU  | 2A    | 1911 | 20/21 | 0.84 | 0.17 | 62,67,77,78                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55  | 8AN  | 1x    | 76   | 22/23 | 0.87 | 0.50 | 42,60,70,72                 | 0     |
| 32  | M2G  | 2a    | 966  | 25/26 | 0.88 | 0.20 | 57,64,74,84                 | 0     |
| 32  | 2MG  | 2a    | 1207 | 24/25 | 0.88 | 0.22 | 67,73,77,83                 | 0     |
| 1   | PSU  | 2A    | 1917 | 20/21 | 0.88 | 0.19 | 63,70,85,92                 | 0     |
| 55  | 8AN  | 2x    | 76   | 22/23 | 0.88 | 0.42 | 49,64,72,84                 | 0     |
| 32  | 5MC  | 1a    | 967  | 21/22 | 0.89 | 0.20 | 57,62,69,73                 | 0     |
| 43  | 0TD  | 2l    | 92   | 10/11 | 0.89 | 0.16 | 53,60,62,62                 | 0     |
| 1   | 5MU  | 1A    | 1915 | 21/22 | 0.90 | 0.17 | 54,65,69,74                 | 0     |
| 32  | 5MC  | 2a    | 1404 | 21/22 | 0.91 | 0.21 | 51,55,58,60                 | 0     |
| 1   | OMC  | 2A    | 1920 | 21/22 | 0.92 | 0.19 | 52,60,66,69                 | 0     |
| 32  | 5MC  | 2a    | 967  | 21/22 | 0.92 | 0.20 | 60,65,71,72                 | 0     |
| 32  | MA6  | 2a    | 1518 | 24/25 | 0.92 | 0.18 | 52,58,61,64                 | 0     |
| 32  | 4OC  | 2a    | 1402 | 22/23 | 0.93 | 0.21 | 53,59,65,67                 | 0     |
| 1   | PSU  | 1A    | 1911 | 20/21 | 0.93 | 0.17 | 49,57,64,68                 | 0     |
| 32  | 2MG  | 1a    | 1207 | 24/25 | 0.93 | 0.20 | 54,65,69,72                 | 0     |
| 43  | 0TD  | 1l    | 92   | 10/11 | 0.93 | 0.17 | 45,52,57,58                 | 0     |
| 1   | PSU  | 1A    | 1917 | 20/21 | 0.93 | 0.17 | 54,62,70,72                 | 0     |
| 32  | M2G  | 1a    | 966  | 25/26 | 0.93 | 0.19 | 46,54,61,62                 | 0     |
| 32  | PSU  | 2a    | 516  | 20/21 | 0.94 | 0.14 | 63,68,75,76                 | 0     |
| 32  | G7M  | 2a    | 527  | 24/25 | 0.94 | 0.17 | 53,57,60,66                 | 0     |
| 32  | 5MC  | 1a    | 1407 | 21/22 | 0.94 | 0.17 | 40,50,54,58                 | 0     |
| 32  | PSU  | 1a    | 516  | 20/21 | 0.94 | 0.18 | 54,60,67,78                 | 0     |
| 32  | 5MC  | 1a    | 1404 | 21/22 | 0.94 | 0.19 | 40,47,50,53                 | 0     |
| 32  | 5MC  | 2a    | 1400 | 21/22 | 0.94 | 0.33 | 51,68,74,76                 | 0     |
| 32  | MA6  | 2a    | 1519 | 24/25 | 0.95 | 0.27 | 46,55,60,63                 | 0     |
| 32  | MA6  | 1a    | 1518 | 24/25 | 0.95 | 0.22 | 36,43,49,55                 | 0     |
| 1   | OMU  | 2A    | 2552 | 21/22 | 0.95 | 0.20 | 28,37,42,43                 | 0     |
| 1   | PSU  | 2A    | 2605 | 20/21 | 0.95 | 0.25 | 26,36,43,44                 | 0     |
| 1   | OMG  | 2A    | 2251 | 24/25 | 0.96 | 0.20 | 33,37,42,46                 | 0     |
| 32  | MA6  | 1a    | 1519 | 24/25 | 0.96 | 0.21 | 40,43,49,50                 | 0     |
| 32  | 4OC  | 1a    | 1402 | 22/23 | 0.96 | 0.18 | 47,49,53,62                 | 0     |
| 32  | 5MC  | 2a    | 1407 | 21/22 | 0.96 | 0.16 | 50,59,63,67                 | 0     |
| 32  | G7M  | 1a    | 527  | 24/25 | 0.96 | 0.17 | 44,51,55,57                 | 0     |
| 1   | OMC  | 1A    | 1920 | 21/22 | 0.96 | 0.20 | 41,51,58,59                 | 0     |
| 32  | UR3  | 1a    | 1498 | 21/22 | 0.96 | 0.19 | 38,46,49,62                 | 0     |
| 32  | 5MC  | 1a    | 1400 | 21/22 | 0.96 | 0.20 | 42,50,61,61                 | 0     |
| 1   | 5MC  | 2A    | 1962 | 21/22 | 0.96 | 0.18 | 32,41,47,52                 | 0     |
| 1   | 5MC  | 1A    | 1942 | 21/22 | 0.97 | 0.19 | 28,33,38,42                 | 0     |
| 32  | UR3  | 2a    | 1498 | 21/22 | 0.97 | 0.22 | 52,56,60,63                 | 0     |
| 1   | 2MA  | 2A    | 2503 | 23/24 | 0.97 | 0.20 | 23,29,34,35                 | 0     |
| 1   | 5MC  | 1A    | 1962 | 21/22 | 0.97 | 0.21 | 26,30,35,38                 | 0     |
| 1   | 5MU  | 2A    | 1939 | 21/22 | 0.97 | 0.19 | 32,38,43,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1   | 5MC  | 2A    | 1942 | 21/22 | 0.97 | 0.18 | 39,46,52,58                 | 0     |
| 1   | PSU  | 1A    | 2605 | 20/21 | 0.97 | 0.20 | 18,26,29,29                 | 0     |
| 1   | 5MU  | 1A    | 1939 | 21/22 | 0.98 | 0.20 | 19,24,27,28                 | 0     |
| 1   | OMG  | 1A    | 2251 | 24/25 | 0.98 | 0.20 | 15,21,32,36                 | 0     |
| 1   | 2MA  | 1A    | 2503 | 23/24 | 0.98 | 0.23 | 14,19,22,23                 | 0     |
| 1   | OMU  | 1A    | 2552 | 21/22 | 0.98 | 0.21 | 20,28,33,34                 | 0     |

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 4021 | 1/1   | -0.11 | 0.32 | 74,74,74,74                 | 0     |
| 57  | MG   | 1A    | 4160 | 1/1   | 0.29  | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 3010 | 1/1   | 0.33  | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3602 | 1/1   | 0.37  | 0.12 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3700 | 1/1   | 0.42  | 0.22 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3633 | 1/1   | 0.42  | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 3119 | 1/1   | 0.43  | 0.37 | 73,73,73,73                 | 0     |
| 57  | MG   | 2a    | 3025 | 1/1   | 0.45  | 0.24 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3173 | 1/1   | 0.45  | 0.23 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3787 | 1/1   | 0.46  | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3661 | 1/1   | 0.50  | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 4061 | 1/1   | 0.51  | 0.18 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 4091 | 1/1   | 0.53  | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3617 | 1/1   | 0.54  | 0.16 | 67,67,67,67                 | 0     |
| 57  | MG   | 1a    | 3292 | 1/1   | 0.56  | 0.12 | 75,75,75,75                 | 0     |
| 57  | MG   | 1A    | 4020 | 1/1   | 0.57  | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3212 | 1/1   | 0.57  | 0.54 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3002 | 1/1   | 0.58  | 0.57 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3738 | 1/1   | 0.59  | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3164 | 1/1   | 0.60  | 0.18 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 3187 | 1/1   | 0.60  | 0.06 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3678 | 1/1   | 0.61  | 0.23 | 70,70,70,70                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3995 | 1/1   | 0.62 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 4004 | 1/1   | 0.62 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3229 | 1/1   | 0.62 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 3090 | 1/1   | 0.63 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3527 | 1/1   | 0.63 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3907 | 1/1   | 0.63 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3124 | 1/1   | 0.64 | 0.14 | 73,73,73,73                 | 0     |
| 57  | MG   | 1a    | 3274 | 1/1   | 0.64 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3780 | 1/1   | 0.64 | 0.15 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3067 | 1/1   | 0.65 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 4048 | 1/1   | 0.65 | 0.24 | 68,68,68,68                 | 0     |
| 57  | MG   | 2a    | 3153 | 1/1   | 0.65 | 0.07 | 62,62,62,62                 | 0     |
| 57  | MG   | 2a    | 3155 | 1/1   | 0.65 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3200 | 1/1   | 0.65 | 0.17 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 3192 | 1/1   | 0.65 | 0.16 | 82,82,82,82                 | 0     |
| 57  | MG   | 1A    | 4170 | 1/1   | 0.66 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3253 | 1/1   | 0.66 | 0.19 | 72,72,72,72                 | 0     |
| 57  | MG   | 1A    | 3830 | 1/1   | 0.66 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3060 | 1/1   | 0.67 | 0.13 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 4129 | 1/1   | 0.67 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3314 | 1/1   | 0.67 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3606 | 1/1   | 0.67 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3765 | 1/1   | 0.67 | 0.12 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3577 | 1/1   | 0.67 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3079 | 1/1   | 0.67 | 0.25 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 4154 | 1/1   | 0.68 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3379 | 1/1   | 0.68 | 0.28 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3549 | 1/1   | 0.68 | 0.19 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3452 | 1/1   | 0.68 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3772 | 1/1   | 0.68 | 0.70 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 3143 | 1/1   | 0.68 | 0.16 | 72,72,72,72                 | 0     |
| 57  | MG   | 1a    | 3209 | 1/1   | 0.68 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3333 | 1/1   | 0.68 | 0.23 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3345 | 1/1   | 0.68 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3278 | 1/1   | 0.68 | 0.09 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3268 | 1/1   | 0.69 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 4152 | 1/1   | 0.69 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3264 | 1/1   | 0.69 | 0.20 | 74,74,74,74                 | 0     |
| 57  | MG   | 1A    | 3752 | 1/1   | 0.69 | 0.10 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3113 | 1/1   | 0.69 | 0.31 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 4076 | 1/1   | 0.69 | 0.21 | 82,82,82,82                 | 0     |
| 57  | MG   | 2A    | 3264 | 1/1   | 0.69 | 0.14 | 54,54,54,54                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 61  | ARG  | 1z    | 1003 | 12/12 | 0.69 | 0.27 | 43,60,64,64                 | 0     |
| 57  | MG   | 1a    | 3078 | 1/1   | 0.70 | 0.28 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 4006 | 1/1   | 0.70 | 0.08 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3092 | 1/1   | 0.70 | 0.29 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3281 | 1/1   | 0.70 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3641 | 1/1   | 0.70 | 0.13 | 71,71,71,71                 | 0     |
| 57  | MG   | 2A    | 3242 | 1/1   | 0.70 | 0.16 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3027 | 1/1   | 0.70 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3685 | 1/1   | 0.70 | 0.10 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3929 | 1/1   | 0.70 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3733 | 1/1   | 0.70 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3119 | 1/1   | 0.70 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3968 | 1/1   | 0.71 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3860 | 1/1   | 0.71 | 0.28 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3082 | 1/1   | 0.71 | 0.25 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3060 | 1/1   | 0.71 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3025 | 1/1   | 0.71 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3213 | 1/1   | 0.71 | 0.18 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3774 | 1/1   | 0.71 | 0.13 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 3210 | 1/1   | 0.71 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3509 | 1/1   | 0.71 | 0.24 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3365 | 1/1   | 0.72 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3183 | 1/1   | 0.72 | 0.21 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3004 | 1/1   | 0.72 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 3036 | 1/1   | 0.72 | 0.12 | 70,70,70,70                 | 0     |
| 57  | MG   | 1A    | 3998 | 1/1   | 0.72 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3222 | 1/1   | 0.72 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3087 | 1/1   | 0.72 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3257 | 1/1   | 0.72 | 0.27 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3678 | 1/1   | 0.72 | 0.23 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3213 | 1/1   | 0.72 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3183 | 1/1   | 0.72 | 0.07 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3135 | 1/1   | 0.72 | 0.13 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3745 | 1/1   | 0.72 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3061 | 1/1   | 0.72 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3721 | 1/1   | 0.73 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3645 | 1/1   | 0.73 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 3039 | 1/1   | 0.73 | 0.18 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3233 | 1/1   | 0.73 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4059 | 1/1   | 0.73 | 0.09 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3946 | 1/1   | 0.73 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3455 | 1/1   | 0.73 | 0.18 | 63,63,63,63                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3711 | 1/1   | 0.73 | 0.07 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3480 | 1/1   | 0.73 | 0.12 | 76,76,76,76                 | 0     |
| 57  | MG   | 2A    | 3483 | 1/1   | 0.73 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 4068 | 1/1   | 0.73 | 0.35 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3898 | 1/1   | 0.73 | 0.65 | 36,36,36,36                 | 0     |
| 58  | ZN   | 24    | 501  | 1/1   | 0.73 | 0.16 | 127,127,127,127             | 0     |
| 57  | MG   | 1A    | 3986 | 1/1   | 0.73 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 2a    | 3012 | 1/1   | 0.74 | 0.21 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3281 | 1/1   | 0.74 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3199 | 1/1   | 0.74 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3695 | 1/1   | 0.74 | 0.18 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 3041 | 1/1   | 0.74 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3380 | 1/1   | 0.74 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 3068 | 1/1   | 0.74 | 0.09 | 69,69,69,69                 | 0     |
| 57  | MG   | 2a    | 3072 | 1/1   | 0.74 | 0.11 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3396 | 1/1   | 0.74 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3690 | 1/1   | 0.74 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3539 | 1/1   | 0.74 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3171 | 1/1   | 0.74 | 0.17 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3030 | 1/1   | 0.74 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3504 | 1/1   | 0.74 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3033 | 1/1   | 0.74 | 0.21 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3195 | 1/1   | 0.74 | 0.34 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3782 | 1/1   | 0.74 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3197 | 1/1   | 0.74 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3060 | 1/1   | 0.75 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3095 | 1/1   | 0.75 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3925 | 1/1   | 0.75 | 0.23 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3026 | 1/1   | 0.75 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3667 | 1/1   | 0.75 | 0.25 | 66,66,66,66                 | 0     |
| 57  | MG   | 2a    | 3061 | 1/1   | 0.75 | 0.26 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3819 | 1/1   | 0.75 | 0.14 | 74,74,74,74                 | 0     |
| 57  | MG   | 2A    | 3630 | 1/1   | 0.75 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 3021 | 1/1   | 0.75 | 0.14 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 4128 | 1/1   | 0.76 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 4029 | 1/1   | 0.76 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3532 | 1/1   | 0.76 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3906 | 1/1   | 0.76 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3247 | 1/1   | 0.76 | 0.17 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3959 | 1/1   | 0.76 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3486 | 1/1   | 0.76 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 3082 | 1/1   | 0.76 | 0.19 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3503 | 1/1   | 0.76 | 0.09 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3659 | 1/1   | 0.76 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3524 | 1/1   | 0.76 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3165 | 1/1   | 0.76 | 0.39 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3534 | 1/1   | 0.76 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3542 | 1/1   | 0.76 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3868 | 1/1   | 0.76 | 0.12 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3580 | 1/1   | 0.76 | 0.20 | 64,64,64,64                 | 0     |
| 58  | ZN   | 14    | 501  | 1/1   | 0.76 | 0.07 | 104,104,104,104             | 0     |
| 57  | MG   | 1a    | 3040 | 1/1   | 0.76 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3992 | 1/1   | 0.76 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3425 | 1/1   | 0.77 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3536 | 1/1   | 0.77 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3387 | 1/1   | 0.77 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3215 | 1/1   | 0.77 | 0.29 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3566 | 1/1   | 0.77 | 0.11 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3444 | 1/1   | 0.77 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3584 | 1/1   | 0.77 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3288 | 1/1   | 0.77 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3911 | 1/1   | 0.77 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 3176 | 1/1   | 0.77 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3972 | 1/1   | 0.77 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3075 | 1/1   | 0.77 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3919 | 1/1   | 0.77 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3668 | 1/1   | 0.77 | 0.20 | 54,54,54,54                 | 0     |
| 58  | ZN   | 2Y    | 501  | 1/1   | 0.77 | 0.12 | 81,81,81,81                 | 0     |
| 57  | MG   | 1A    | 3227 | 1/1   | 0.77 | 0.33 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3944 | 1/1   | 0.77 | 0.08 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3502 | 1/1   | 0.78 | 0.34 | 72,72,72,72                 | 0     |
| 57  | MG   | 2A    | 3776 | 1/1   | 0.78 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3202 | 1/1   | 0.78 | 0.28 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3126 | 1/1   | 0.78 | 0.32 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3218 | 1/1   | 0.78 | 0.14 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3289 | 1/1   | 0.78 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3046 | 1/1   | 0.78 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3137 | 1/1   | 0.78 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3144 | 1/1   | 0.78 | 0.27 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3666 | 1/1   | 0.78 | 0.07 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3544 | 1/1   | 0.78 | 0.19 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3178 | 1/1   | 0.78 | 0.09 | 73,73,73,73                 | 0     |
| 57  | MG   | 1a    | 3184 | 1/1   | 0.78 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3593 | 1/1   | 0.78 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3206 | 1/1   | 0.78 | 0.15 | 77,77,77,77                 | 0     |
| 57  | MG   | 2A    | 3326 | 1/1   | 0.78 | 0.21 | 61,61,61,61                 | 0     |
| 57  | MG   | 2a    | 3093 | 1/1   | 0.78 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 3101 | 1/1   | 0.78 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3082 | 1/1   | 0.78 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3207 | 1/1   | 0.78 | 0.21 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 4171 | 1/1   | 0.78 | 0.27 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3306 | 1/1   | 0.78 | 0.19 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3426 | 1/1   | 0.78 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3036 | 1/1   | 0.78 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3094 | 1/1   | 0.78 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3462 | 1/1   | 0.78 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3266 | 1/1   | 0.78 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 4074 | 1/1   | 0.78 | 0.07 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3763 | 1/1   | 0.78 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3121 | 1/1   | 0.78 | 0.14 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3910 | 1/1   | 0.79 | 0.24 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3010 | 1/1   | 0.79 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 4062 | 1/1   | 0.79 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3252 | 1/1   | 0.79 | 0.26 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3293 | 1/1   | 0.79 | 0.18 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3115 | 1/1   | 0.79 | 0.19 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 3261 | 1/1   | 0.79 | 0.29 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3344 | 1/1   | 0.79 | 0.13 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 3052 | 1/1   | 0.79 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3448 | 1/1   | 0.79 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3205 | 1/1   | 0.79 | 0.23 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 3066 | 1/1   | 0.79 | 0.24 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3856 | 1/1   | 0.79 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3621 | 1/1   | 0.79 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3278 | 1/1   | 0.79 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 3084 | 1/1   | 0.79 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3631 | 1/1   | 0.79 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3467 | 1/1   | 0.79 | 0.18 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3198 | 1/1   | 0.79 | 0.16 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3746 | 1/1   | 0.79 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 3134 | 1/1   | 0.79 | 0.21 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3067 | 1/1   | 0.79 | 0.27 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3476 | 1/1   | 0.79 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3170 | 1/1   | 0.79 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3214 | 1/1   | 0.79 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3713 | 1/1   | 0.79 | 0.14 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3300 | 1/1   | 0.79 | 0.17 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3565 | 1/1   | 0.79 | 0.13 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 4130 | 1/1   | 0.79 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3485 | 1/1   | 0.79 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3523 | 1/1   | 0.79 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3587 | 1/1   | 0.79 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3341 | 1/1   | 0.80 | 0.22 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 4094 | 1/1   | 0.80 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3218 | 1/1   | 0.80 | 0.34 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3205 | 1/1   | 0.80 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3926 | 1/1   | 0.80 | 0.08 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3458 | 1/1   | 0.80 | 0.16 | 20,20,20,20                 | 0     |
| 57  | MG   | 2A    | 3048 | 1/1   | 0.80 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 3026 | 1/1   | 0.80 | 0.18 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3547 | 1/1   | 0.80 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3657 | 1/1   | 0.80 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3304 | 1/1   | 0.80 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3312 | 1/1   | 0.80 | 0.26 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3309 | 1/1   | 0.80 | 0.16 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 3235 | 1/1   | 0.80 | 0.21 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3247 | 1/1   | 0.80 | 0.10 | 75,75,75,75                 | 0     |
| 57  | MG   | 2A    | 3608 | 1/1   | 0.80 | 0.07 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3612 | 1/1   | 0.80 | 0.13 | 62,62,62,62                 | 0     |
| 57  | MG   | 1a    | 3111 | 1/1   | 0.80 | 0.11 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3386 | 1/1   | 0.80 | 0.22 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3625 | 1/1   | 0.80 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3258 | 1/1   | 0.80 | 0.24 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3174 | 1/1   | 0.80 | 0.30 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3638 | 1/1   | 0.80 | 0.07 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 4052 | 1/1   | 0.80 | 0.14 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3431 | 1/1   | 0.80 | 0.19 | 71,71,71,71                 | 0     |
| 57  | MG   | 1a    | 3120 | 1/1   | 0.80 | 0.10 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3446 | 1/1   | 0.80 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3904 | 1/1   | 0.80 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3270 | 1/1   | 0.80 | 0.07 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3019 | 1/1   | 0.80 | 0.22 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3767 | 1/1   | 0.80 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3220 | 1/1   | 0.80 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3594 | 1/1   | 0.80 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3672 | 1/1   | 0.80 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3996 | 1/1   | 0.80 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3220 | 1/1   | 0.81 | 0.29 | 51,51,51,51                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 4063 | 1/1   | 0.81 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3642 | 1/1   | 0.81 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3240 | 1/1   | 0.81 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3658 | 1/1   | 0.81 | 0.20 | 72,72,72,72                 | 0     |
| 57  | MG   | 1a    | 3047 | 1/1   | 0.81 | 0.17 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 3065 | 1/1   | 0.81 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3243 | 1/1   | 0.81 | 0.25 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3196 | 1/1   | 0.81 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3545 | 1/1   | 0.81 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3203 | 1/1   | 0.81 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4054 | 1/1   | 0.81 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3557 | 1/1   | 0.81 | 0.15 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3559 | 1/1   | 0.81 | 0.20 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3139 | 1/1   | 0.81 | 0.16 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3758 | 1/1   | 0.81 | 0.14 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3761 | 1/1   | 0.81 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3824 | 1/1   | 0.81 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3473 | 1/1   | 0.81 | 0.17 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3783 | 1/1   | 0.81 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3167 | 1/1   | 0.81 | 0.15 | 78,78,78,78                 | 0     |
| 57  | MG   | 1a    | 3226 | 1/1   | 0.81 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3797 | 1/1   | 0.81 | 0.14 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3644 | 1/1   | 0.81 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3237 | 1/1   | 0.81 | 0.07 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3097 | 1/1   | 0.81 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3100 | 1/1   | 0.81 | 0.22 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3508 | 1/1   | 0.81 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3601 | 1/1   | 0.82 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3862 | 1/1   | 0.82 | 0.20 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3260 | 1/1   | 0.82 | 0.30 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3769 | 1/1   | 0.82 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3116 | 1/1   | 0.82 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3696 | 1/1   | 0.82 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 4003 | 1/1   | 0.82 | 0.31 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3934 | 1/1   | 0.82 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 3004 | 1/1   | 0.82 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 3009 | 1/1   | 0.82 | 0.21 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3104 | 1/1   | 0.82 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3107 | 1/1   | 0.82 | 0.24 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3310 | 1/1   | 0.82 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3116 | 1/1   | 0.82 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3267 | 1/1   | 0.82 | 0.31 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2a    | 3031 | 1/1   | 0.82 | 0.17 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3120 | 1/1   | 0.82 | 0.27 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3254 | 1/1   | 0.82 | 0.11 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3130 | 1/1   | 0.82 | 0.29 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3147 | 1/1   | 0.82 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 4013 | 1/1   | 0.82 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3734 | 1/1   | 0.82 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3406 | 1/1   | 0.82 | 0.14 | 77,77,77,77                 | 0     |
| 57  | MG   | 1A    | 4096 | 1/1   | 0.82 | 0.09 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3155 | 1/1   | 0.82 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3443 | 1/1   | 0.82 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3164 | 1/1   | 0.82 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 4099 | 1/1   | 0.82 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3065 | 1/1   | 0.82 | 0.22 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 3091 | 1/1   | 0.82 | 0.21 | 69,69,69,69                 | 0     |
| 57  | MG   | 1a    | 3076 | 1/1   | 0.82 | 0.24 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3336 | 1/1   | 0.82 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3663 | 1/1   | 0.82 | 0.28 | 51,51,51,51                 | 0     |
| 57  | MG   | 2a    | 3122 | 1/1   | 0.82 | 0.13 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3686 | 1/1   | 0.82 | 0.37 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3080 | 1/1   | 0.82 | 0.17 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3687 | 1/1   | 0.82 | 0.09 | 70,70,70,70                 | 0     |
| 57  | MG   | 1a    | 3189 | 1/1   | 0.82 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3974 | 1/1   | 0.82 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3701 | 1/1   | 0.82 | 0.08 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3224 | 1/1   | 0.82 | 0.20 | 71,71,71,71                 | 0     |
| 57  | MG   | 1a    | 3090 | 1/1   | 0.82 | 0.22 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3731 | 1/1   | 0.82 | 0.19 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3692 | 1/1   | 0.82 | 0.19 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 4158 | 1/1   | 0.82 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3857 | 1/1   | 0.82 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3729 | 1/1   | 0.83 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3003 | 1/1   | 0.83 | 0.12 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3477 | 1/1   | 0.83 | 0.48 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3216 | 1/1   | 0.83 | 0.19 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3550 | 1/1   | 0.83 | 0.16 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3960 | 1/1   | 0.83 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3038 | 1/1   | 0.83 | 0.22 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3415 | 1/1   | 0.83 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3110 | 1/1   | 0.83 | 0.26 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3770 | 1/1   | 0.83 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3039 | 1/1   | 0.83 | 0.15 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3718 | 1/1   | 0.83 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3244 | 1/1   | 0.83 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3219 | 1/1   | 0.83 | 0.13 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3809 | 1/1   | 0.83 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 3007 | 1/1   | 0.83 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3017 | 1/1   | 0.83 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3988 | 1/1   | 0.83 | 0.06 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3099 | 1/1   | 0.83 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 3015 | 1/1   | 0.83 | 0.21 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3025 | 1/1   | 0.83 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3991 | 1/1   | 0.83 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3291 | 1/1   | 0.83 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3031 | 1/1   | 0.83 | 0.25 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3115 | 1/1   | 0.83 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3131 | 1/1   | 0.83 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3117 | 1/1   | 0.83 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3818 | 1/1   | 0.83 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3102 | 1/1   | 0.83 | 0.21 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3337 | 1/1   | 0.83 | 0.33 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3338 | 1/1   | 0.83 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3530 | 1/1   | 0.83 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3828 | 1/1   | 0.83 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3373 | 1/1   | 0.83 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 3074 | 1/1   | 0.83 | 0.24 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 3079 | 1/1   | 0.83 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3137 | 1/1   | 0.83 | 0.24 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3382 | 1/1   | 0.83 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 3089 | 1/1   | 0.83 | 0.17 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 3147 | 1/1   | 0.83 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3999 | 1/1   | 0.83 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3399 | 1/1   | 0.83 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3656 | 1/1   | 0.83 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3065 | 1/1   | 0.83 | 0.19 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3064 | 1/1   | 0.83 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3537 | 1/1   | 0.83 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 3139 | 1/1   | 0.83 | 0.07 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3665 | 1/1   | 0.83 | 0.13 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3667 | 1/1   | 0.83 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3307 | 1/1   | 0.83 | 0.14 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3683 | 1/1   | 0.83 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3760 | 1/1   | 0.83 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 4017 | 1/1   | 0.83 | 0.18 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3087 | 1/1   | 0.83 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 3196 | 1/1   | 0.83 | 0.12 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3460 | 1/1   | 0.83 | 0.17 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3301 | 1/1   | 0.83 | 0.23 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3470 | 1/1   | 0.83 | 0.43 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 3306 | 1/1   | 0.83 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3342 | 1/1   | 0.84 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3343 | 1/1   | 0.84 | 0.11 | 71,71,71,71                 | 0     |
| 57  | MG   | 1a    | 3132 | 1/1   | 0.84 | 0.25 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3357 | 1/1   | 0.84 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3790 | 1/1   | 0.84 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3564 | 1/1   | 0.84 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 3228 | 1/1   | 0.84 | 0.19 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3340 | 1/1   | 0.84 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3582 | 1/1   | 0.84 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3037 | 1/1   | 0.84 | 0.29 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 4169 | 1/1   | 0.84 | 0.43 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3208 | 1/1   | 0.84 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 3019 | 1/1   | 0.84 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4083 | 1/1   | 0.84 | 0.12 | 83,83,83,83                 | 0     |
| 57  | MG   | 2a    | 3024 | 1/1   | 0.84 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3011 | 1/1   | 0.84 | 0.31 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3174 | 1/1   | 0.84 | 0.30 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 3027 | 1/1   | 0.84 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3410 | 1/1   | 0.84 | 0.08 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 3033 | 1/1   | 0.84 | 0.12 | 71,71,71,71                 | 0     |
| 57  | MG   | 2A    | 3622 | 1/1   | 0.84 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3935 | 1/1   | 0.84 | 0.19 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3751 | 1/1   | 0.84 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3230 | 1/1   | 0.84 | 0.20 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3635 | 1/1   | 0.84 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3231 | 1/1   | 0.84 | 0.41 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 3063 | 1/1   | 0.84 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 1a    | 3262 | 1/1   | 0.84 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3452 | 1/1   | 0.84 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3647 | 1/1   | 0.84 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3029 | 1/1   | 0.84 | 0.30 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3562 | 1/1   | 0.84 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3105 | 1/1   | 0.84 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3173 | 1/1   | 0.84 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 4124 | 1/1   | 0.84 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3239 | 1/1   | 0.84 | 0.27 | 32,32,32,32                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3608 | 1/1   | 0.84 | 0.12 | 71,71,71,71                 | 0     |
| 57  | MG   | 2A    | 3265 | 1/1   | 0.84 | 0.23 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3481 | 1/1   | 0.84 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3114 | 1/1   | 0.84 | 0.30 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3688 | 1/1   | 0.84 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3042 | 1/1   | 0.84 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 3129 | 1/1   | 0.84 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3492 | 1/1   | 0.84 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3962 | 1/1   | 0.84 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3623 | 1/1   | 0.84 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3161 | 1/1   | 0.84 | 0.22 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3300 | 1/1   | 0.84 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3051 | 1/1   | 0.84 | 0.21 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 3216 | 1/1   | 0.84 | 0.14 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3626 | 1/1   | 0.84 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3006 | 1/1   | 0.84 | 0.51 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3187 | 1/1   | 0.84 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3192 | 1/1   | 0.84 | 0.13 | 72,72,72,72                 | 0     |
| 57  | MG   | 1A    | 3725 | 1/1   | 0.84 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3767 | 1/1   | 0.84 | 0.30 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3546 | 1/1   | 0.84 | 0.18 | 65,65,65,65                 | 0     |
| 62  | MPD  | 1z    | 2002 | 8/8   | 0.84 | 0.18 | 46,51,56,64                 | 0     |
| 57  | MG   | 1A    | 3104 | 1/1   | 0.85 | 0.19 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3519 | 1/1   | 0.85 | 0.10 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3871 | 1/1   | 0.85 | 0.24 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3083 | 1/1   | 0.85 | 0.16 | 78,78,78,78                 | 0     |
| 57  | MG   | 1A    | 3747 | 1/1   | 0.85 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3533 | 1/1   | 0.85 | 0.15 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3780 | 1/1   | 0.85 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3105 | 1/1   | 0.85 | 0.31 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3785 | 1/1   | 0.85 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3905 | 1/1   | 0.85 | 0.21 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3567 | 1/1   | 0.85 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3798 | 1/1   | 0.85 | 0.18 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3543 | 1/1   | 0.85 | 0.19 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3296 | 1/1   | 0.85 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 3008 | 1/1   | 0.85 | 0.10 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3107 | 1/1   | 0.85 | 0.29 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3135 | 1/1   | 0.85 | 0.22 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3245 | 1/1   | 0.85 | 0.07 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3399 | 1/1   | 0.85 | 0.26 | 24,24,24,24                 | 0     |
| 57  | MG   | 1a    | 3250 | 1/1   | 0.85 | 0.16 | 60,60,60,60                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3518 | 1/1   | 0.85 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3335 | 1/1   | 0.85 | 0.29 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3676 | 1/1   | 0.85 | 0.18 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3781 | 1/1   | 0.85 | 0.25 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3024 | 1/1   | 0.85 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3006 | 1/1   | 0.85 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3154 | 1/1   | 0.85 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3421 | 1/1   | 0.85 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3360 | 1/1   | 0.85 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3015 | 1/1   | 0.85 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 4030 | 1/1   | 0.85 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 3053 | 1/1   | 0.85 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 4038 | 1/1   | 0.85 | 0.31 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3050 | 1/1   | 0.85 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3614 | 1/1   | 0.85 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3190 | 1/1   | 0.85 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3622 | 1/1   | 0.85 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3400 | 1/1   | 0.85 | 0.12 | 27,27,27,27                 | 0     |
| 57  | MG   | 2a    | 3070 | 1/1   | 0.85 | 0.25 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 3071 | 1/1   | 0.85 | 0.41 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3820 | 1/1   | 0.85 | 0.23 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3707 | 1/1   | 0.85 | 0.19 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3291 | 1/1   | 0.85 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3149 | 1/1   | 0.85 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3433 | 1/1   | 0.85 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3205 | 1/1   | 0.85 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3540 | 1/1   | 0.85 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3837 | 1/1   | 0.85 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 4072 | 1/1   | 0.85 | 0.26 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3670 | 1/1   | 0.85 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4073 | 1/1   | 0.85 | 0.26 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3054 | 1/1   | 0.85 | 0.17 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3970 | 1/1   | 0.85 | 0.19 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3471 | 1/1   | 0.85 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3063 | 1/1   | 0.85 | 0.10 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 3142 | 1/1   | 0.85 | 0.24 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3037 | 1/1   | 0.85 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3694 | 1/1   | 0.85 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 4079 | 1/1   | 0.85 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 3160 | 1/1   | 0.85 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3172 | 1/1   | 0.85 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3232 | 1/1   | 0.85 | 0.12 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3034 | 1/1   | 0.85 | 0.23 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3730 | 1/1   | 0.85 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3273 | 1/1   | 0.85 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3487 | 1/1   | 0.85 | 0.22 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3557 | 1/1   | 0.85 | 0.19 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3498 | 1/1   | 0.85 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3864 | 1/1   | 0.85 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3061 | 1/1   | 0.85 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3064 | 1/1   | 0.85 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3527 | 1/1   | 0.86 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3282 | 1/1   | 0.86 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3475 | 1/1   | 0.86 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3214 | 1/1   | 0.86 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3200 | 1/1   | 0.86 | 0.21 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 4086 | 1/1   | 0.86 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3297 | 1/1   | 0.86 | 0.14 | 70,70,70,70                 | 0     |
| 57  | MG   | 1A    | 4090 | 1/1   | 0.86 | 0.13 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3224 | 1/1   | 0.86 | 0.09 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3029 | 1/1   | 0.86 | 0.20 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3489 | 1/1   | 0.86 | 0.10 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3672 | 1/1   | 0.86 | 0.24 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 4009 | 1/1   | 0.86 | 0.36 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3123 | 1/1   | 0.86 | 0.11 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3325 | 1/1   | 0.86 | 0.24 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3670 | 1/1   | 0.86 | 0.30 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3128 | 1/1   | 0.86 | 0.25 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3748 | 1/1   | 0.86 | 0.28 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3159 | 1/1   | 0.86 | 0.18 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3343 | 1/1   | 0.86 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3055 | 1/1   | 0.86 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3295 | 1/1   | 0.86 | 0.19 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3215 | 1/1   | 0.86 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3718 | 1/1   | 0.86 | 0.08 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3057 | 1/1   | 0.86 | 0.96 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 4031 | 1/1   | 0.86 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3369 | 1/1   | 0.86 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3464 | 1/1   | 0.86 | 0.17 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3184 | 1/1   | 0.86 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3228 | 1/1   | 0.86 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 3118 | 1/1   | 0.86 | 0.25 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3385 | 1/1   | 0.86 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3386 | 1/1   | 0.86 | 0.18 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3627 | 1/1   | 0.86 | 0.08 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3469 | 1/1   | 0.86 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 4056 | 1/1   | 0.86 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3716 | 1/1   | 0.86 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3801 | 1/1   | 0.86 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3001 | 1/1   | 0.86 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3419 | 1/1   | 0.86 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3478 | 1/1   | 0.86 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3993 | 1/1   | 0.86 | 0.17 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3480 | 1/1   | 0.86 | 0.28 | 71,71,71,71                 | 0     |
| 57  | MG   | 2A    | 3129 | 1/1   | 0.86 | 0.21 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3723 | 1/1   | 0.86 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | 2a    | 3190 | 1/1   | 0.86 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 3191 | 1/1   | 0.86 | 0.22 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3229 | 1/1   | 0.86 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3084 | 1/1   | 0.86 | 0.31 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3267 | 1/1   | 0.86 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3137 | 1/1   | 0.86 | 0.24 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3463 | 1/1   | 0.86 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3634 | 1/1   | 0.86 | 0.33 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3157 | 1/1   | 0.86 | 0.19 | 53,53,53,53                 | 0     |
| 62  | MPD  | 2z    | 2002 | 8/8   | 0.86 | 0.17 | 44,53,60,60                 | 0     |
| 57  | MG   | 1a    | 3099 | 1/1   | 0.87 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3021 | 1/1   | 0.87 | 0.58 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3648 | 1/1   | 0.87 | 0.06 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3655 | 1/1   | 0.87 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3272 | 1/1   | 0.87 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3322 | 1/1   | 0.87 | 0.26 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3221 | 1/1   | 0.87 | 0.26 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3691 | 1/1   | 0.87 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3582 | 1/1   | 0.87 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3496 | 1/1   | 0.87 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4065 | 1/1   | 0.87 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3909 | 1/1   | 0.87 | 0.13 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3204 | 1/1   | 0.87 | 0.19 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3460 | 1/1   | 0.87 | 0.13 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3280 | 1/1   | 0.87 | 0.29 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3915 | 1/1   | 0.87 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3055 | 1/1   | 0.87 | 0.23 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 3069 | 1/1   | 0.87 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3702 | 1/1   | 0.87 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3920 | 1/1   | 0.87 | 0.13 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3829 | 1/1   | 0.87 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3759 | 1/1   | 0.87 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 3076 | 1/1   | 0.87 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 3246 | 1/1   | 0.87 | 0.21 | 62,62,62,62                 | 0     |
| 57  | MG   | 1a    | 3130 | 1/1   | 0.87 | 0.23 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4088 | 1/1   | 0.87 | 0.24 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3544 | 1/1   | 0.87 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3422 | 1/1   | 0.87 | 0.10 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3933 | 1/1   | 0.87 | 0.30 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 3092 | 1/1   | 0.87 | 0.22 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3012 | 1/1   | 0.87 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3427 | 1/1   | 0.87 | 0.18 | 20,20,20,20                 | 0     |
| 57  | MG   | 1a    | 3140 | 1/1   | 0.87 | 0.30 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3937 | 1/1   | 0.87 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3146 | 1/1   | 0.87 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 4122 | 1/1   | 0.87 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3943 | 1/1   | 0.87 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3439 | 1/1   | 0.87 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3431 | 1/1   | 0.87 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3592 | 1/1   | 0.87 | 0.26 | 56,56,56,56                 | 0     |
| 57  | MG   | 2a    | 3148 | 1/1   | 0.87 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3777 | 1/1   | 0.87 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3380 | 1/1   | 0.87 | 0.19 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3141 | 1/1   | 0.87 | 0.25 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 3169 | 1/1   | 0.87 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3451 | 1/1   | 0.87 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3454 | 1/1   | 0.87 | 0.21 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3140 | 1/1   | 0.87 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3791 | 1/1   | 0.87 | 0.10 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 4156 | 1/1   | 0.87 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3875 | 1/1   | 0.87 | 0.08 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3629 | 1/1   | 0.87 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3292 | 1/1   | 0.87 | 0.22 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3794 | 1/1   | 0.87 | 0.17 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3182 | 1/1   | 0.87 | 0.13 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 4163 | 1/1   | 0.87 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 2a    | 3016 | 1/1   | 0.87 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4055 | 1/1   | 0.87 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3902 | 1/1   | 0.87 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3222 | 1/1   | 0.88 | 0.24 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3075 | 1/1   | 0.88 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3526 | 1/1   | 0.88 | 0.11 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3257 | 1/1   | 0.88 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3408 | 1/1   | 0.88 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3090 | 1/1   | 0.88 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3092 | 1/1   | 0.88 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 3154 | 1/1   | 0.88 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4015 | 1/1   | 0.88 | 0.17 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3433 | 1/1   | 0.88 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3029 | 1/1   | 0.88 | 0.15 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 4077 | 1/1   | 0.88 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3633 | 1/1   | 0.88 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 3032 | 1/1   | 0.88 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 4078 | 1/1   | 0.88 | 0.07 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3004 | 1/1   | 0.88 | 0.30 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 3038 | 1/1   | 0.88 | 0.21 | 62,62,62,62                 | 0     |
| 57  | MG   | 1a    | 3273 | 1/1   | 0.88 | 0.47 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3640 | 1/1   | 0.88 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 3045 | 1/1   | 0.88 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 3049 | 1/1   | 0.88 | 0.26 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3097 | 1/1   | 0.88 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3263 | 1/1   | 0.88 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3671 | 1/1   | 0.88 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3101 | 1/1   | 0.88 | 0.19 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3266 | 1/1   | 0.88 | 0.22 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 4025 | 1/1   | 0.88 | 0.14 | 21,21,21,21                 | 0     |
| 57  | MG   | 1a    | 3020 | 1/1   | 0.88 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3272 | 1/1   | 0.88 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3572 | 1/1   | 0.88 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3280 | 1/1   | 0.88 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3246 | 1/1   | 0.88 | 0.41 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3145 | 1/1   | 0.88 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3685 | 1/1   | 0.88 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3676 | 1/1   | 0.88 | 0.24 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 3304 | 1/1   | 0.88 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3035 | 1/1   | 0.88 | 0.23 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3158 | 1/1   | 0.88 | 0.19 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 4046 | 1/1   | 0.88 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3162 | 1/1   | 0.88 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 3211 | 1/1   | 0.88 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3166 | 1/1   | 0.88 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3923 | 1/1   | 0.88 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3013 | 1/1   | 0.88 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 3114 | 1/1   | 0.88 | 0.28 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3316 | 1/1   | 0.88 | 0.25 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3320 | 1/1   | 0.88 | 0.29 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 4051 | 1/1   | 0.88 | 0.16 | 21,21,21,21                 | 0     |
| 57  | MG   | 2a    | 3126 | 1/1   | 0.88 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3217 | 1/1   | 0.88 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3271 | 1/1   | 0.88 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3526 | 1/1   | 0.88 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3329 | 1/1   | 0.88 | 0.21 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3530 | 1/1   | 0.88 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3147 | 1/1   | 0.88 | 0.21 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3866 | 1/1   | 0.88 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | 2a    | 3152 | 1/1   | 0.88 | 0.07 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3193 | 1/1   | 0.88 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3050 | 1/1   | 0.88 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3740 | 1/1   | 0.88 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 3161 | 1/1   | 0.88 | 0.07 | 63,63,63,63                 | 0     |
| 57  | MG   | 2a    | 3168 | 1/1   | 0.88 | 0.19 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3505 | 1/1   | 0.88 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 4142 | 1/1   | 0.88 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3038 | 1/1   | 0.88 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 2a    | 3178 | 1/1   | 0.88 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3054 | 1/1   | 0.88 | 0.42 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 3186 | 1/1   | 0.88 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3880 | 1/1   | 0.88 | 0.08 | 73,73,73,73                 | 0     |
| 57  | MG   | 2A    | 3054 | 1/1   | 0.88 | 0.27 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3232 | 1/1   | 0.88 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3663 | 1/1   | 0.88 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3381 | 1/1   | 0.88 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 3198 | 1/1   | 0.88 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3796 | 1/1   | 0.88 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3522 | 1/1   | 0.88 | 0.22 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3757 | 1/1   | 0.88 | 0.06 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3799 | 1/1   | 0.88 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3219 | 1/1   | 0.88 | 0.21 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3948 | 1/1   | 0.88 | 0.18 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3053 | 1/1   | 0.89 | 0.18 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 4082 | 1/1   | 0.89 | 0.40 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3298 | 1/1   | 0.89 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3138 | 1/1   | 0.89 | 0.09 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3941 | 1/1   | 0.89 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3307 | 1/1   | 0.89 | 0.23 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 4087 | 1/1   | 0.89 | 0.14 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3443 | 1/1   | 0.89 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3791 | 1/1   | 0.89 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3795 | 1/1   | 0.89 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | 1a    | 3277 | 1/1   | 0.89 | 0.22 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3043 | 1/1   | 0.89 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3417 | 1/1   | 0.89 | 0.09 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3872 | 1/1   | 0.89 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3540 | 1/1   | 0.89 | 0.08 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3165 | 1/1   | 0.89 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3420 | 1/1   | 0.89 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3172 | 1/1   | 0.89 | 0.35 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3955 | 1/1   | 0.89 | 0.16 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3336 | 1/1   | 0.89 | 0.26 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3736 | 1/1   | 0.89 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3162 | 1/1   | 0.89 | 0.15 | 62,62,62,62                 | 0     |
| 57  | MG   | 2a    | 3017 | 1/1   | 0.89 | 0.24 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 4101 | 1/1   | 0.89 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3056 | 1/1   | 0.89 | 0.10 | 62,62,62,62                 | 0     |
| 57  | MG   | 1a    | 3058 | 1/1   | 0.89 | 0.20 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3356 | 1/1   | 0.89 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3569 | 1/1   | 0.89 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3573 | 1/1   | 0.89 | 0.21 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 4113 | 1/1   | 0.89 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3538 | 1/1   | 0.89 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3961 | 1/1   | 0.89 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3588 | 1/1   | 0.89 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3012 | 1/1   | 0.89 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3243 | 1/1   | 0.89 | 0.18 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3375 | 1/1   | 0.89 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 3043 | 1/1   | 0.89 | 0.17 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3607 | 1/1   | 0.89 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 3047 | 1/1   | 0.89 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3376 | 1/1   | 0.89 | 0.23 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3610 | 1/1   | 0.89 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3072 | 1/1   | 0.89 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 3055 | 1/1   | 0.89 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 3057 | 1/1   | 0.89 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3639 | 1/1   | 0.89 | 0.17 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 4049 | 1/1   | 0.89 | 0.22 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3196 | 1/1   | 0.89 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3198 | 1/1   | 0.89 | 0.23 | 75,75,75,75                 | 0     |
| 57  | MG   | 1a    | 3077 | 1/1   | 0.89 | 0.20 | 40,40,40,40                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3395 | 1/1   | 0.89 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3063 | 1/1   | 0.89 | 0.23 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3217 | 1/1   | 0.89 | 0.18 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3589 | 1/1   | 0.89 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3647 | 1/1   | 0.89 | 0.16 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3980 | 1/1   | 0.89 | 0.05 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3044 | 1/1   | 0.89 | 0.25 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3411 | 1/1   | 0.89 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3417 | 1/1   | 0.89 | 0.21 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 3088 | 1/1   | 0.89 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3213 | 1/1   | 0.89 | 0.15 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3430 | 1/1   | 0.89 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3653 | 1/1   | 0.89 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3175 | 1/1   | 0.89 | 0.22 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3832 | 1/1   | 0.89 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 4167 | 1/1   | 0.89 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3658 | 1/1   | 0.89 | 0.21 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 3116 | 1/1   | 0.89 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3843 | 1/1   | 0.89 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3450 | 1/1   | 0.89 | 0.09 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3671 | 1/1   | 0.89 | 0.18 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3078 | 1/1   | 0.89 | 0.31 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3852 | 1/1   | 0.89 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 3131 | 1/1   | 0.89 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 3132 | 1/1   | 0.89 | 0.08 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 4066 | 1/1   | 0.89 | 0.09 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3233 | 1/1   | 0.89 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 3140 | 1/1   | 0.89 | 0.15 | 64,64,64,64                 | 0     |
| 57  | MG   | 1a    | 3004 | 1/1   | 0.89 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3854 | 1/1   | 0.89 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3007 | 1/1   | 0.89 | 0.13 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 4071 | 1/1   | 0.89 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3693 | 1/1   | 0.89 | 0.11 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3013 | 1/1   | 0.89 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3595 | 1/1   | 0.89 | 0.10 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3113 | 1/1   | 0.89 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3707 | 1/1   | 0.89 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3714 | 1/1   | 0.89 | 0.23 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3273 | 1/1   | 0.89 | 0.17 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3717 | 1/1   | 0.89 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 4001 | 1/1   | 0.89 | 0.26 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 3177 | 1/1   | 0.89 | 0.35 | 73,73,73,73                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3723 | 1/1   | 0.89 | 0.19 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3724 | 1/1   | 0.89 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3727 | 1/1   | 0.89 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3858 | 1/1   | 0.89 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3118 | 1/1   | 0.89 | 0.27 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3255 | 1/1   | 0.89 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3284 | 1/1   | 0.89 | 0.58 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3751 | 1/1   | 0.89 | 0.19 | 73,73,73,73                 | 0     |
| 57  | MG   | 2A    | 3753 | 1/1   | 0.89 | 0.13 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3287 | 1/1   | 0.89 | 0.41 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3493 | 1/1   | 0.89 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3022 | 1/1   | 0.89 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3298 | 1/1   | 0.89 | 0.18 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3500 | 1/1   | 0.89 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3555 | 1/1   | 0.89 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 4057 | 1/1   | 0.90 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3361 | 1/1   | 0.90 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3571 | 1/1   | 0.90 | 0.47 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3199 | 1/1   | 0.90 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3574 | 1/1   | 0.90 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3536 | 1/1   | 0.90 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3028 | 1/1   | 0.90 | 0.16 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3616 | 1/1   | 0.90 | 0.21 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3207 | 1/1   | 0.90 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3208 | 1/1   | 0.90 | 0.20 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3210 | 1/1   | 0.90 | 0.23 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3595 | 1/1   | 0.90 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3182 | 1/1   | 0.90 | 0.21 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3978 | 1/1   | 0.90 | 0.22 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3899 | 1/1   | 0.90 | 0.18 | 25,25,25,25                 | 0     |
| 57  | MG   | 1a    | 3212 | 1/1   | 0.90 | 0.17 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3040 | 1/1   | 0.90 | 0.28 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3042 | 1/1   | 0.90 | 0.22 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3618 | 1/1   | 0.90 | 0.35 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3075 | 1/1   | 0.90 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3903 | 1/1   | 0.90 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3103 | 1/1   | 0.90 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3697 | 1/1   | 0.90 | 0.19 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3225 | 1/1   | 0.90 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3106 | 1/1   | 0.90 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3792 | 1/1   | 0.90 | 0.21 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3793 | 1/1   | 0.90 | 0.17 | 21,21,21,21                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3189 | 1/1   | 0.90 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3069 | 1/1   | 0.90 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 4075 | 1/1   | 0.90 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 3229 | 1/1   | 0.90 | 0.09 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3437 | 1/1   | 0.90 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3389 | 1/1   | 0.90 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3391 | 1/1   | 0.90 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3654 | 1/1   | 0.90 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3246 | 1/1   | 0.90 | 0.13 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3445 | 1/1   | 0.90 | 0.57 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3084 | 1/1   | 0.90 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3089 | 1/1   | 0.90 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3259 | 1/1   | 0.90 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3395 | 1/1   | 0.90 | 0.15 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3717 | 1/1   | 0.90 | 0.24 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 4080 | 1/1   | 0.90 | 0.24 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3098 | 1/1   | 0.90 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3397 | 1/1   | 0.90 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3465 | 1/1   | 0.90 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3719 | 1/1   | 0.90 | 0.25 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 3083 | 1/1   | 0.90 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3681 | 1/1   | 0.90 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 2a    | 3086 | 1/1   | 0.90 | 0.33 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3398 | 1/1   | 0.90 | 0.25 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3139 | 1/1   | 0.90 | 0.25 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3686 | 1/1   | 0.90 | 0.12 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3401 | 1/1   | 0.90 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3654 | 1/1   | 0.90 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 3096 | 1/1   | 0.90 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3133 | 1/1   | 0.90 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 3103 | 1/1   | 0.90 | 0.11 | 67,67,67,67                 | 0     |
| 57  | MG   | 2a    | 3109 | 1/1   | 0.90 | 0.24 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3691 | 1/1   | 0.90 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 3115 | 1/1   | 0.90 | 0.11 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3932 | 1/1   | 0.90 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3136 | 1/1   | 0.90 | 0.31 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3283 | 1/1   | 0.90 | 0.15 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3252 | 1/1   | 0.90 | 0.21 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3416 | 1/1   | 0.90 | 0.14 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3049 | 1/1   | 0.90 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3573 | 1/1   | 0.90 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3715 | 1/1   | 0.90 | 0.15 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3575 | 1/1   | 0.90 | 0.15 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 4106 | 1/1   | 0.90 | 0.22 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3327 | 1/1   | 0.90 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 4114 | 1/1   | 0.90 | 0.14 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3150 | 1/1   | 0.90 | 0.25 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3328 | 1/1   | 0.90 | 0.36 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 3287 | 1/1   | 0.90 | 0.06 | 62,62,62,62                 | 0     |
| 57  | MG   | 2a    | 3149 | 1/1   | 0.90 | 0.16 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 4032 | 1/1   | 0.90 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3743 | 1/1   | 0.90 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3744 | 1/1   | 0.90 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3262 | 1/1   | 0.90 | 0.28 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3093 | 1/1   | 0.90 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3163 | 1/1   | 0.90 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3317 | 1/1   | 0.90 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 3170 | 1/1   | 0.90 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3592 | 1/1   | 0.90 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3069 | 1/1   | 0.90 | 0.11 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3764 | 1/1   | 0.90 | 0.15 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3524 | 1/1   | 0.90 | 0.28 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 3179 | 1/1   | 0.90 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3127 | 1/1   | 0.90 | 0.19 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3768 | 1/1   | 0.90 | 0.16 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3867 | 1/1   | 0.90 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3129 | 1/1   | 0.90 | 0.23 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3177 | 1/1   | 0.90 | 0.19 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3055 | 1/1   | 0.90 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3186 | 1/1   | 0.90 | 0.12 | 69,69,69,69                 | 0     |
| 57  | MG   | 1a    | 3188 | 1/1   | 0.90 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3011 | 1/1   | 0.90 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3017 | 1/1   | 0.90 | 0.17 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 4161 | 1/1   | 0.90 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3083 | 1/1   | 0.90 | 0.16 | 54,54,54,54                 | 0     |
| 62  | MPD  | 1z    | 2001 | 8/8   | 0.90 | 0.16 | 56,60,62,64                 | 0     |
| 57  | MG   | 2A    | 3358 | 1/1   | 0.90 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3359 | 1/1   | 0.90 | 0.09 | 34,34,34,34                 | 0     |
| 62  | MPD  | 2z    | 2003 | 8/8   | 0.90 | 0.21 | 50,53,58,58                 | 0     |
| 57  | MG   | 2A    | 3787 | 1/1   | 0.91 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3942 | 1/1   | 0.91 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3125 | 1/1   | 0.91 | 0.26 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3520 | 1/1   | 0.91 | 0.10 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 4053 | 1/1   | 0.91 | 0.15 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3855 | 1/1   | 0.91 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3945 | 1/1   | 0.91 | 0.15 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3115 | 1/1   | 0.91 | 0.16 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3804 | 1/1   | 0.91 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 3003 | 1/1   | 0.91 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3591 | 1/1   | 0.91 | 0.33 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3953 | 1/1   | 0.91 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 4060 | 1/1   | 0.91 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3296 | 1/1   | 0.91 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3179 | 1/1   | 0.91 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3581 | 1/1   | 0.91 | 0.15 | 70,70,70,70                 | 0     |
| 57  | MG   | 1A    | 3957 | 1/1   | 0.91 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3387 | 1/1   | 0.91 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3188 | 1/1   | 0.91 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3435 | 1/1   | 0.91 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3248 | 1/1   | 0.91 | 0.54 | 31,31,31,31                 | 0     |
| 57  | MG   | 2a    | 3022 | 1/1   | 0.91 | 0.21 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3756 | 1/1   | 0.91 | 0.19 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3596 | 1/1   | 0.91 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3597 | 1/1   | 0.91 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3599 | 1/1   | 0.91 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3965 | 1/1   | 0.91 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3604 | 1/1   | 0.91 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3967 | 1/1   | 0.91 | 0.19 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3445 | 1/1   | 0.91 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3159 | 1/1   | 0.91 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3758 | 1/1   | 0.91 | 0.13 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3971 | 1/1   | 0.91 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3125 | 1/1   | 0.91 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3255 | 1/1   | 0.91 | 0.14 | 60,60,60,60                 | 0     |
| 57  | MG   | 2A    | 3206 | 1/1   | 0.91 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 3048 | 1/1   | 0.91 | 0.13 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3764 | 1/1   | 0.91 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 3050 | 1/1   | 0.91 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3628 | 1/1   | 0.91 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3879 | 1/1   | 0.91 | 0.20 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3981 | 1/1   | 0.91 | 0.18 | 18,18,18,18                 | 0     |
| 57  | MG   | 1a    | 3176 | 1/1   | 0.91 | 0.07 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 3059 | 1/1   | 0.91 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3690 | 1/1   | 0.91 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3308 | 1/1   | 0.91 | 0.22 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3778 | 1/1   | 0.91 | 0.14 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3256 | 1/1   | 0.91 | 0.37 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3059 | 1/1   | 0.91 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3693 | 1/1   | 0.91 | 0.16 | 20,20,20,20                 | 0     |
| 57  | MG   | 2A    | 3427 | 1/1   | 0.91 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3429 | 1/1   | 0.91 | 0.25 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3194 | 1/1   | 0.91 | 0.15 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3179 | 1/1   | 0.91 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 3073 | 1/1   | 0.91 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3400 | 1/1   | 0.91 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3434 | 1/1   | 0.91 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3069 | 1/1   | 0.91 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3551 | 1/1   | 0.91 | 0.19 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3662 | 1/1   | 0.91 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 3071 | 1/1   | 0.91 | 0.27 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3706 | 1/1   | 0.91 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3083 | 1/1   | 0.91 | 0.27 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3475 | 1/1   | 0.91 | 0.14 | 14,14,14,14                 | 0     |
| 57  | MG   | 2A    | 3073 | 1/1   | 0.91 | 0.16 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4111 | 1/1   | 0.91 | 0.07 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3133 | 1/1   | 0.91 | 0.16 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3677 | 1/1   | 0.91 | 0.19 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3917 | 1/1   | 0.91 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3457 | 1/1   | 0.91 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 3107 | 1/1   | 0.91 | 0.35 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4121 | 1/1   | 0.91 | 0.18 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 3111 | 1/1   | 0.91 | 0.32 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3645 | 1/1   | 0.91 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3087 | 1/1   | 0.91 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3084 | 1/1   | 0.91 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3218 | 1/1   | 0.91 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3091 | 1/1   | 0.91 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3086 | 1/1   | 0.91 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3158 | 1/1   | 0.91 | 0.18 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3652 | 1/1   | 0.91 | 0.19 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 3130 | 1/1   | 0.91 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3924 | 1/1   | 0.91 | 0.23 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3478 | 1/1   | 0.91 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3133 | 1/1   | 0.91 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3081 | 1/1   | 0.91 | 0.20 | 25,25,25,25                 | 0     |
| 57  | MG   | 2a    | 3135 | 1/1   | 0.91 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3708 | 1/1   | 0.91 | 0.10 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 4023 | 1/1   | 0.91 | 0.12 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 4144 | 1/1   | 0.91 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3111 | 1/1   | 0.91 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3487 | 1/1   | 0.91 | 0.12 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 4026 | 1/1   | 0.91 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3722 | 1/1   | 0.91 | 0.34 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 4155 | 1/1   | 0.91 | 0.10 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3104 | 1/1   | 0.91 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3726 | 1/1   | 0.91 | 0.07 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 3158 | 1/1   | 0.91 | 0.07 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3284 | 1/1   | 0.91 | 0.10 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 4157 | 1/1   | 0.91 | 0.42 | 39,39,39,39                 | 0     |
| 57  | MG   | 2a    | 3162 | 1/1   | 0.91 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3293 | 1/1   | 0.91 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3122 | 1/1   | 0.91 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3735 | 1/1   | 0.91 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3294 | 1/1   | 0.91 | 0.20 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3517 | 1/1   | 0.91 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3735 | 1/1   | 0.91 | 0.23 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3512 | 1/1   | 0.91 | 0.16 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3842 | 1/1   | 0.91 | 0.15 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3135 | 1/1   | 0.91 | 0.22 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3303 | 1/1   | 0.91 | 0.30 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 4040 | 1/1   | 0.91 | 0.21 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3294 | 1/1   | 0.91 | 0.18 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3529 | 1/1   | 0.91 | 0.09 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3144 | 1/1   | 0.91 | 0.23 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3940 | 1/1   | 0.91 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3313 | 1/1   | 0.91 | 0.22 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3148 | 1/1   | 0.91 | 0.10 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3117 | 1/1   | 0.91 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3541 | 1/1   | 0.91 | 0.27 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3152 | 1/1   | 0.91 | 0.33 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3153 | 1/1   | 0.91 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3737 | 1/1   | 0.91 | 0.26 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3784 | 1/1   | 0.91 | 0.33 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 4174 | 1/1   | 0.91 | 0.26 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3062 | 1/1   | 0.92 | 0.26 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3241 | 1/1   | 0.92 | 0.21 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3056 | 1/1   | 0.92 | 0.17 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3059 | 1/1   | 0.92 | 0.21 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3484 | 1/1   | 0.92 | 0.23 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 4105 | 1/1   | 0.92 | 0.16 | 49,49,49,49                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3756 | 1/1   | 0.92 | 0.07 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3193 | 1/1   | 0.92 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3488 | 1/1   | 0.92 | 0.07 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 4011 | 1/1   | 0.92 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3508 | 1/1   | 0.92 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 4014 | 1/1   | 0.92 | 0.09 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3495 | 1/1   | 0.92 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3199 | 1/1   | 0.92 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3262 | 1/1   | 0.92 | 0.25 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3499 | 1/1   | 0.92 | 0.16 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3202 | 1/1   | 0.92 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3501 | 1/1   | 0.92 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3290 | 1/1   | 0.92 | 0.27 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3080 | 1/1   | 0.92 | 0.26 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4118 | 1/1   | 0.92 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4120 | 1/1   | 0.92 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3509 | 1/1   | 0.92 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3806 | 1/1   | 0.92 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3515 | 1/1   | 0.92 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3511 | 1/1   | 0.92 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4123 | 1/1   | 0.92 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3814 | 1/1   | 0.92 | 0.26 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3515 | 1/1   | 0.92 | 0.14 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3930 | 1/1   | 0.92 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3528 | 1/1   | 0.92 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3096 | 1/1   | 0.92 | 0.30 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3211 | 1/1   | 0.92 | 0.24 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3215 | 1/1   | 0.92 | 0.09 | 68,68,68,68                 | 0     |
| 57  | MG   | 2a    | 3005 | 1/1   | 0.92 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3354 | 1/1   | 0.92 | 0.33 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 4143 | 1/1   | 0.92 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3537 | 1/1   | 0.92 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3101 | 1/1   | 0.92 | 0.11 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 3011 | 1/1   | 0.92 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3102 | 1/1   | 0.92 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3709 | 1/1   | 0.92 | 0.30 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 4145 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 4147 | 1/1   | 0.92 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3112 | 1/1   | 0.92 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 3020 | 1/1   | 0.92 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3223 | 1/1   | 0.92 | 0.18 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 4150 | 1/1   | 0.92 | 0.16 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3548 | 1/1   | 0.92 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3225 | 1/1   | 0.92 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3552 | 1/1   | 0.92 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3555 | 1/1   | 0.92 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 3028 | 1/1   | 0.92 | 0.20 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3305 | 1/1   | 0.92 | 0.28 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3096 | 1/1   | 0.92 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3309 | 1/1   | 0.92 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3712 | 1/1   | 0.92 | 0.22 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 4153 | 1/1   | 0.92 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3358 | 1/1   | 0.92 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3362 | 1/1   | 0.92 | 0.28 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3831 | 1/1   | 0.92 | 0.16 | 26,26,26,26                 | 0     |
| 57  | MG   | 2a    | 3044 | 1/1   | 0.92 | 0.25 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3126 | 1/1   | 0.92 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3318 | 1/1   | 0.92 | 0.33 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3241 | 1/1   | 0.92 | 0.21 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3523 | 1/1   | 0.92 | 0.17 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3587 | 1/1   | 0.92 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3134 | 1/1   | 0.92 | 0.19 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3836 | 1/1   | 0.92 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3136 | 1/1   | 0.92 | 0.16 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3331 | 1/1   | 0.92 | 0.19 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3373 | 1/1   | 0.92 | 0.28 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3377 | 1/1   | 0.92 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3598 | 1/1   | 0.92 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3142 | 1/1   | 0.92 | 0.24 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3601 | 1/1   | 0.92 | 0.15 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3183 | 1/1   | 0.92 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 3067 | 1/1   | 0.92 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3630 | 1/1   | 0.92 | 0.07 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3950 | 1/1   | 0.92 | 0.13 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3033 | 1/1   | 0.92 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3151 | 1/1   | 0.92 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3381 | 1/1   | 0.92 | 0.12 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3616 | 1/1   | 0.92 | 0.14 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3534 | 1/1   | 0.92 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3119 | 1/1   | 0.92 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3620 | 1/1   | 0.92 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3643 | 1/1   | 0.92 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3119 | 1/1   | 0.92 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3265 | 1/1   | 0.92 | 0.17 | 56,56,56,56                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3449 | 1/1   | 0.92 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 3087 | 1/1   | 0.92 | 0.36 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3268 | 1/1   | 0.92 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3374 | 1/1   | 0.92 | 0.15 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3120 | 1/1   | 0.92 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | 1a    | 3271 | 1/1   | 0.92 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3008 | 1/1   | 0.92 | 0.24 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3127 | 1/1   | 0.92 | 0.12 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3160 | 1/1   | 0.92 | 0.18 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3260 | 1/1   | 0.92 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 3104 | 1/1   | 0.92 | 0.17 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3176 | 1/1   | 0.92 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3644 | 1/1   | 0.92 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3008 | 1/1   | 0.92 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3389 | 1/1   | 0.92 | 0.14 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 4067 | 1/1   | 0.92 | 0.11 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3548 | 1/1   | 0.92 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3397 | 1/1   | 0.92 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3462 | 1/1   | 0.92 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3657 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3222 | 1/1   | 0.92 | 0.32 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3016 | 1/1   | 0.92 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 1a    | 3299 | 1/1   | 0.92 | 0.33 | 72,72,72,72                 | 0     |
| 57  | MG   | 1A    | 3206 | 1/1   | 0.92 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3558 | 1/1   | 0.92 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3414 | 1/1   | 0.92 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3143 | 1/1   | 0.92 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3891 | 1/1   | 0.92 | 0.21 | 22,22,22,22                 | 0     |
| 57  | MG   | 2a    | 3136 | 1/1   | 0.92 | 0.14 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 3137 | 1/1   | 0.92 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3423 | 1/1   | 0.92 | 0.15 | 70,70,70,70                 | 0     |
| 57  | MG   | 2A    | 3673 | 1/1   | 0.92 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3675 | 1/1   | 0.92 | 0.18 | 28,28,28,28                 | 0     |
| 57  | MG   | 1a    | 3032 | 1/1   | 0.92 | 0.19 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3984 | 1/1   | 0.92 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3559 | 1/1   | 0.92 | 0.14 | 20,20,20,20                 | 0     |
| 57  | MG   | 2A    | 3680 | 1/1   | 0.92 | 0.07 | 67,67,67,67                 | 0     |
| 57  | MG   | 1a    | 3150 | 1/1   | 0.92 | 0.19 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3151 | 1/1   | 0.92 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3038 | 1/1   | 0.92 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3472 | 1/1   | 0.92 | 0.17 | 11,11,11,11                 | 0     |
| 57  | MG   | 1a    | 3157 | 1/1   | 0.92 | 0.08 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3140 | 1/1   | 0.92 | 0.17 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3335 | 1/1   | 0.92 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3276 | 1/1   | 0.92 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3775 | 1/1   | 0.92 | 0.17 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3482 | 1/1   | 0.92 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3066 | 1/1   | 0.92 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3209 | 1/1   | 0.92 | 0.22 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3704 | 1/1   | 0.92 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3453 | 1/1   | 0.92 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3491 | 1/1   | 0.92 | 0.16 | 64,64,64,64                 | 0     |
| 57  | MG   | 2A    | 3221 | 1/1   | 0.92 | 0.08 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3712 | 1/1   | 0.92 | 0.08 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3175 | 1/1   | 0.92 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3714 | 1/1   | 0.92 | 0.09 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3458 | 1/1   | 0.92 | 0.20 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3418 | 1/1   | 0.92 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 3195 | 1/1   | 0.92 | 0.24 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3506 | 1/1   | 0.92 | 0.14 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3226 | 1/1   | 0.92 | 0.18 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 4098 | 1/1   | 0.92 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3045 | 1/1   | 0.92 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3725 | 1/1   | 0.92 | 0.15 | 65,65,65,65                 | 0     |
| 57  | MG   | 1A    | 3507 | 1/1   | 0.92 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3051 | 1/1   | 0.92 | 0.14 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3694 | 1/1   | 0.92 | 0.21 | 20,20,20,20                 | 0     |
| 62  | MPD  | 1z    | 2004 | 8/8   | 0.92 | 0.26 | 49,51,53,60                 | 0     |
| 57  | MG   | 2A    | 3236 | 1/1   | 0.92 | 0.14 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3238 | 1/1   | 0.92 | 0.59 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3826 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3239 | 1/1   | 0.93 | 0.22 | 51,51,51,51                 | 0     |
| 57  | MG   | 1a    | 3177 | 1/1   | 0.93 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3254 | 1/1   | 0.93 | 0.13 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3057 | 1/1   | 0.93 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3058 | 1/1   | 0.93 | 0.28 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3737 | 1/1   | 0.93 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3103 | 1/1   | 0.93 | 0.20 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3048 | 1/1   | 0.93 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | 1a    | 3187 | 1/1   | 0.93 | 0.28 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3748 | 1/1   | 0.93 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3749 | 1/1   | 0.93 | 0.38 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3750 | 1/1   | 0.93 | 0.35 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3255 | 1/1   | 0.93 | 0.51 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3070 | 1/1   | 0.93 | 0.16 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3754 | 1/1   | 0.93 | 0.26 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3073 | 1/1   | 0.93 | 0.37 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3070 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3833 | 1/1   | 0.93 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3052 | 1/1   | 0.93 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3077 | 1/1   | 0.93 | 0.23 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 4085 | 1/1   | 0.93 | 0.20 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3766 | 1/1   | 0.93 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3599 | 1/1   | 0.93 | 0.23 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3112 | 1/1   | 0.93 | 0.22 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3602 | 1/1   | 0.93 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 4089 | 1/1   | 0.93 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3086 | 1/1   | 0.93 | 0.20 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3507 | 1/1   | 0.93 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3277 | 1/1   | 0.93 | 0.23 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3778 | 1/1   | 0.93 | 0.28 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3214 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3607 | 1/1   | 0.93 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3514 | 1/1   | 0.93 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3113 | 1/1   | 0.93 | 0.34 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3786 | 1/1   | 0.93 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3613 | 1/1   | 0.93 | 0.18 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3788 | 1/1   | 0.93 | 0.30 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3521 | 1/1   | 0.93 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3217 | 1/1   | 0.93 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3793 | 1/1   | 0.93 | 0.14 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3794 | 1/1   | 0.93 | 0.13 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3356 | 1/1   | 0.93 | 0.21 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3286 | 1/1   | 0.93 | 0.21 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3357 | 1/1   | 0.93 | 0.15 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3186 | 1/1   | 0.93 | 0.20 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3073 | 1/1   | 0.93 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3727 | 1/1   | 0.93 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4110 | 1/1   | 0.93 | 0.08 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3438 | 1/1   | 0.93 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3103 | 1/1   | 0.93 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3865 | 1/1   | 0.93 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3538 | 1/1   | 0.93 | 0.13 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3994 | 1/1   | 0.93 | 0.07 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3302 | 1/1   | 0.93 | 0.21 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3085 | 1/1   | 0.93 | 0.21 | 24,24,24,24                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3082 | 1/1   | 0.93 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3444 | 1/1   | 0.93 | 0.19 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3114 | 1/1   | 0.93 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3997 | 1/1   | 0.93 | 0.10 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 3018 | 1/1   | 0.93 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3191 | 1/1   | 0.93 | 0.11 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3041 | 1/1   | 0.93 | 0.25 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3378 | 1/1   | 0.93 | 0.28 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3739 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3554 | 1/1   | 0.93 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3315 | 1/1   | 0.93 | 0.31 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3556 | 1/1   | 0.93 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3197 | 1/1   | 0.93 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3558 | 1/1   | 0.93 | 0.10 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 3030 | 1/1   | 0.93 | 0.32 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3091 | 1/1   | 0.93 | 0.18 | 29,29,29,29                 | 0     |
| 57  | MG   | 1a    | 3238 | 1/1   | 0.93 | 0.09 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3319 | 1/1   | 0.93 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3567 | 1/1   | 0.93 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 4138 | 1/1   | 0.93 | 0.21 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 4141 | 1/1   | 0.93 | 0.24 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3572 | 1/1   | 0.93 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3323 | 1/1   | 0.93 | 0.30 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3098 | 1/1   | 0.93 | 0.26 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3578 | 1/1   | 0.93 | 0.28 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3579 | 1/1   | 0.93 | 0.08 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3132 | 1/1   | 0.93 | 0.39 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3327 | 1/1   | 0.93 | 0.29 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 4007 | 1/1   | 0.93 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 3051 | 1/1   | 0.93 | 0.26 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3890 | 1/1   | 0.93 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3586 | 1/1   | 0.93 | 0.25 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3334 | 1/1   | 0.93 | 0.21 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3455 | 1/1   | 0.93 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3591 | 1/1   | 0.93 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3124 | 1/1   | 0.93 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3138 | 1/1   | 0.93 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3650 | 1/1   | 0.93 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 2a    | 3064 | 1/1   | 0.93 | 0.11 | 69,69,69,69                 | 0     |
| 57  | MG   | 2A    | 3341 | 1/1   | 0.93 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3141 | 1/1   | 0.93 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4148 | 1/1   | 0.93 | 0.12 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3202 | 1/1   | 0.93 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3347 | 1/1   | 0.93 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3352 | 1/1   | 0.93 | 0.21 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3603 | 1/1   | 0.93 | 0.13 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3353 | 1/1   | 0.93 | 0.15 | 68,68,68,68                 | 0     |
| 57  | MG   | 2A    | 3606 | 1/1   | 0.93 | 0.11 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3355 | 1/1   | 0.93 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3146 | 1/1   | 0.93 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3108 | 1/1   | 0.93 | 0.33 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3260 | 1/1   | 0.93 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 4151 | 1/1   | 0.93 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3755 | 1/1   | 0.93 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3461 | 1/1   | 0.93 | 0.17 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3545 | 1/1   | 0.93 | 0.17 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3237 | 1/1   | 0.93 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3299 | 1/1   | 0.93 | 0.11 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3623 | 1/1   | 0.93 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3908 | 1/1   | 0.93 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 1a    | 3118 | 1/1   | 0.93 | 0.98 | 81,81,81,81                 | 0     |
| 57  | MG   | 1A    | 3203 | 1/1   | 0.93 | 0.31 | 33,33,33,33                 | 0     |
| 57  | MG   | 2a    | 3097 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3761 | 1/1   | 0.93 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3275 | 1/1   | 0.93 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3763 | 1/1   | 0.93 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3383 | 1/1   | 0.93 | 0.16 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3660 | 1/1   | 0.93 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3636 | 1/1   | 0.93 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 3112 | 1/1   | 0.93 | 0.36 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3168 | 1/1   | 0.93 | 0.19 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3765 | 1/1   | 0.93 | 0.28 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3282 | 1/1   | 0.93 | 0.26 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3390 | 1/1   | 0.93 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3391 | 1/1   | 0.93 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3284 | 1/1   | 0.93 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3553 | 1/1   | 0.93 | 0.14 | 23,23,23,23                 | 0     |
| 57  | MG   | 2a    | 3128 | 1/1   | 0.93 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3651 | 1/1   | 0.93 | 0.16 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3652 | 1/1   | 0.93 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3664 | 1/1   | 0.93 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3468 | 1/1   | 0.93 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 4172 | 1/1   | 0.93 | 0.15 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3777 | 1/1   | 0.93 | 0.67 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3407 | 1/1   | 0.93 | 0.18 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3659 | 1/1   | 0.93 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3296 | 1/1   | 0.93 | 0.17 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3204 | 1/1   | 0.93 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3003 | 1/1   | 0.93 | 0.18 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3078 | 1/1   | 0.93 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3415 | 1/1   | 0.93 | 0.20 | 21,21,21,21                 | 0     |
| 57  | MG   | 2a    | 3145 | 1/1   | 0.93 | 0.14 | 58,58,58,58                 | 0     |
| 57  | MG   | 1a    | 3302 | 1/1   | 0.93 | 0.10 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3068 | 1/1   | 0.93 | 0.07 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3318 | 1/1   | 0.93 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 2a    | 3150 | 1/1   | 0.93 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3324 | 1/1   | 0.93 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3673 | 1/1   | 0.93 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | 1a    | 3012 | 1/1   | 0.93 | 0.20 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3010 | 1/1   | 0.93 | 0.19 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3165 | 1/1   | 0.93 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3432 | 1/1   | 0.93 | 0.21 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3483 | 1/1   | 0.93 | 0.30 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 3167 | 1/1   | 0.93 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3679 | 1/1   | 0.93 | 0.12 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3209 | 1/1   | 0.93 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3019 | 1/1   | 0.93 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3938 | 1/1   | 0.93 | 0.17 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3795 | 1/1   | 0.93 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3797 | 1/1   | 0.93 | 0.09 | 62,62,62,62                 | 0     |
| 57  | MG   | 1a    | 3024 | 1/1   | 0.93 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3800 | 1/1   | 0.93 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3451 | 1/1   | 0.93 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3028 | 1/1   | 0.93 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3484 | 1/1   | 0.93 | 0.17 | 15,15,15,15                 | 0     |
| 57  | MG   | 2A    | 3703 | 1/1   | 0.93 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3406 | 1/1   | 0.93 | 0.20 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3035 | 1/1   | 0.93 | 0.18 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3687 | 1/1   | 0.93 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3410 | 1/1   | 0.93 | 0.08 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3459 | 1/1   | 0.93 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3413 | 1/1   | 0.93 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 3169 | 1/1   | 0.93 | 0.20 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3583 | 1/1   | 0.93 | 0.18 | 14,14,14,14                 | 0     |
| 60  | CLM  | 2z    | 1    | 20/20 | 0.93 | 0.27 | 33,38,57,59                 | 0     |
| 57  | MG   | 2A    | 3464 | 1/1   | 0.93 | 0.11 | 38,38,38,38                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3037 | 1/1   | 0.93 | 0.13 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3172 | 1/1   | 0.93 | 0.12 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3586 | 1/1   | 0.93 | 0.15 | 10,10,10,10                 | 0     |
| 57  | MG   | 2A    | 3049 | 1/1   | 0.93 | 0.08 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3503 | 1/1   | 0.93 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3014 | 1/1   | 0.94 | 0.14 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3015 | 1/1   | 0.94 | 0.34 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3734 | 1/1   | 0.94 | 0.23 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 4164 | 1/1   | 0.94 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3736 | 1/1   | 0.94 | 0.17 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3479 | 1/1   | 0.94 | 0.29 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3738 | 1/1   | 0.94 | 0.21 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3741 | 1/1   | 0.94 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3742 | 1/1   | 0.94 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 4166 | 1/1   | 0.94 | 0.25 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3566 | 1/1   | 0.94 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 4168 | 1/1   | 0.94 | 0.32 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3747 | 1/1   | 0.94 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3502 | 1/1   | 0.94 | 0.18 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3237 | 1/1   | 0.94 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4027 | 1/1   | 0.94 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 4028 | 1/1   | 0.94 | 0.22 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3142 | 1/1   | 0.94 | 0.24 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3432 | 1/1   | 0.94 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3101 | 1/1   | 0.94 | 0.11 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3757 | 1/1   | 0.94 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3145 | 1/1   | 0.94 | 0.23 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3759 | 1/1   | 0.94 | 0.28 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 4175 | 1/1   | 0.94 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3762 | 1/1   | 0.94 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3325 | 1/1   | 0.94 | 0.23 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3769 | 1/1   | 0.94 | 0.24 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3252 | 1/1   | 0.94 | 0.34 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 4033 | 1/1   | 0.94 | 0.15 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 4034 | 1/1   | 0.94 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3669 | 1/1   | 0.94 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3774 | 1/1   | 0.94 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3047 | 1/1   | 0.94 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3771 | 1/1   | 0.94 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3773 | 1/1   | 0.94 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3187 | 1/1   | 0.94 | 0.24 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3775 | 1/1   | 0.94 | 0.10 | 59,59,59,59                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3580 | 1/1   | 0.94 | 0.14 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3510 | 1/1   | 0.94 | 0.11 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3511 | 1/1   | 0.94 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3439 | 1/1   | 0.94 | 0.31 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3918 | 1/1   | 0.94 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3016 | 1/1   | 0.94 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3517 | 1/1   | 0.94 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3383 | 1/1   | 0.94 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3270 | 1/1   | 0.94 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3522 | 1/1   | 0.94 | 0.15 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3168 | 1/1   | 0.94 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3674 | 1/1   | 0.94 | 0.14 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3792 | 1/1   | 0.94 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3274 | 1/1   | 0.94 | 0.20 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3584 | 1/1   | 0.94 | 0.15 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3785 | 1/1   | 0.94 | 0.21 | 21,21,21,21                 | 0     |
| 57  | MG   | 1a    | 3023 | 1/1   | 0.94 | 0.10 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3066 | 1/1   | 0.94 | 0.44 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3385 | 1/1   | 0.94 | 0.21 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3068 | 1/1   | 0.94 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3535 | 1/1   | 0.94 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3513 | 1/1   | 0.94 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3285 | 1/1   | 0.94 | 0.17 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3026 | 1/1   | 0.94 | 0.19 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3071 | 1/1   | 0.94 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3514 | 1/1   | 0.94 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3292 | 1/1   | 0.94 | 0.17 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3181 | 1/1   | 0.94 | 0.07 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3931 | 1/1   | 0.94 | 0.18 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3079 | 1/1   | 0.94 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3013 | 1/1   | 0.94 | 0.24 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3331 | 1/1   | 0.94 | 0.20 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3081 | 1/1   | 0.94 | 0.12 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3185 | 1/1   | 0.94 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3166 | 1/1   | 0.94 | 0.27 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3034 | 1/1   | 0.94 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3334 | 1/1   | 0.94 | 0.14 | 76,76,76,76                 | 0     |
| 57  | MG   | 1A    | 3598 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3190 | 1/1   | 0.94 | 0.19 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3308 | 1/1   | 0.94 | 0.19 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3936 | 1/1   | 0.94 | 0.22 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3521 | 1/1   | 0.94 | 0.15 | 41,41,41,41                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3561 | 1/1   | 0.94 | 0.09 | 61,61,61,61                 | 0     |
| 57  | MG   | 1a    | 3195 | 1/1   | 0.94 | 0.07 | 65,65,65,65                 | 0     |
| 57  | MG   | 1a    | 3039 | 1/1   | 0.94 | 0.20 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3167 | 1/1   | 0.94 | 0.71 | 38,38,38,38                 | 0     |
| 57  | MG   | 1a    | 3041 | 1/1   | 0.94 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3807 | 1/1   | 0.94 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3171 | 1/1   | 0.94 | 0.24 | 19,19,19,19                 | 0     |
| 57  | MG   | 1a    | 3044 | 1/1   | 0.94 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3811 | 1/1   | 0.94 | 0.11 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3576 | 1/1   | 0.94 | 0.12 | 27,27,27,27                 | 0     |
| 57  | MG   | 2a    | 3042 | 1/1   | 0.94 | 0.19 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3604 | 1/1   | 0.94 | 0.27 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3337 | 1/1   | 0.94 | 0.35 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3106 | 1/1   | 0.94 | 0.23 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 3046 | 1/1   | 0.94 | 0.07 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3698 | 1/1   | 0.94 | 0.16 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3701 | 1/1   | 0.94 | 0.14 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3822 | 1/1   | 0.94 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3585 | 1/1   | 0.94 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3044 | 1/1   | 0.94 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3825 | 1/1   | 0.94 | 0.14 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3266 | 1/1   | 0.94 | 0.29 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3198 | 1/1   | 0.94 | 0.12 | 32,32,32,32                 | 0     |
| 57  | MG   | 1a    | 3057 | 1/1   | 0.94 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3463 | 1/1   | 0.94 | 0.14 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3533 | 1/1   | 0.94 | 0.18 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3340 | 1/1   | 0.94 | 0.13 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 3062 | 1/1   | 0.94 | 0.19 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3617 | 1/1   | 0.94 | 0.16 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3061 | 1/1   | 0.94 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3715 | 1/1   | 0.94 | 0.20 | 59,59,59,59                 | 0     |
| 57  | MG   | 2A    | 3600 | 1/1   | 0.94 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3618 | 1/1   | 0.94 | 0.23 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3835 | 1/1   | 0.94 | 0.21 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3349 | 1/1   | 0.94 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3066 | 1/1   | 0.94 | 0.32 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3605 | 1/1   | 0.94 | 0.05 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 4092 | 1/1   | 0.94 | 0.19 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3133 | 1/1   | 0.94 | 0.14 | 57,57,57,57                 | 0     |
| 57  | MG   | 1a    | 3230 | 1/1   | 0.94 | 0.06 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3231 | 1/1   | 0.94 | 0.09 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3611 | 1/1   | 0.94 | 0.12 | 52,52,52,52                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2a    | 3081 | 1/1   | 0.94 | 0.13 | 66,66,66,66                 | 0     |
| 57  | MG   | 1A    | 3302 | 1/1   | 0.94 | 0.19 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 4095 | 1/1   | 0.94 | 0.07 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3236 | 1/1   | 0.94 | 0.15 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3969 | 1/1   | 0.94 | 0.11 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3535 | 1/1   | 0.94 | 0.10 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 3088 | 1/1   | 0.94 | 0.07 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3366 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3239 | 1/1   | 0.94 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3624 | 1/1   | 0.94 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3145 | 1/1   | 0.94 | 0.25 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3242 | 1/1   | 0.94 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | 1a    | 3244 | 1/1   | 0.94 | 0.08 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3378 | 1/1   | 0.94 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 3098 | 1/1   | 0.94 | 0.27 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 4100 | 1/1   | 0.94 | 0.10 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 3102 | 1/1   | 0.94 | 0.26 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3347 | 1/1   | 0.94 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 4102 | 1/1   | 0.94 | 0.23 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 4104 | 1/1   | 0.94 | 0.15 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3305 | 1/1   | 0.94 | 0.28 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3975 | 1/1   | 0.94 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 4109 | 1/1   | 0.94 | 0.26 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 3113 | 1/1   | 0.94 | 0.36 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3976 | 1/1   | 0.94 | 0.15 | 22,22,22,22                 | 0     |
| 57  | MG   | 1a    | 3256 | 1/1   | 0.94 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3628 | 1/1   | 0.94 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3152 | 1/1   | 0.94 | 0.22 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3155 | 1/1   | 0.94 | 0.13 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 4116 | 1/1   | 0.94 | 0.60 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 3123 | 1/1   | 0.94 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3637 | 1/1   | 0.94 | 0.09 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 3127 | 1/1   | 0.94 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3056 | 1/1   | 0.94 | 0.22 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3401 | 1/1   | 0.94 | 0.09 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3405 | 1/1   | 0.94 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3095 | 1/1   | 0.94 | 0.10 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3542 | 1/1   | 0.94 | 0.16 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3642 | 1/1   | 0.94 | 0.21 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3660 | 1/1   | 0.94 | 0.08 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3360 | 1/1   | 0.94 | 0.17 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3035 | 1/1   | 0.94 | 0.18 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3413 | 1/1   | 0.94 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3364 | 1/1   | 0.94 | 0.09 | 63,63,63,63                 | 0     |
| 57  | MG   | 2A    | 3666 | 1/1   | 0.94 | 0.21 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3180 | 1/1   | 0.94 | 0.17 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3669 | 1/1   | 0.94 | 0.20 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3181 | 1/1   | 0.94 | 0.16 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3182 | 1/1   | 0.94 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3744 | 1/1   | 0.94 | 0.73 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3370 | 1/1   | 0.94 | 0.10 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3648 | 1/1   | 0.94 | 0.20 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3423 | 1/1   | 0.94 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3191 | 1/1   | 0.94 | 0.20 | 60,60,60,60                 | 0     |
| 57  | MG   | 2a    | 3154 | 1/1   | 0.94 | 0.27 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 3098 | 1/1   | 0.94 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3876 | 1/1   | 0.94 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 3159 | 1/1   | 0.94 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3878 | 1/1   | 0.94 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3196 | 1/1   | 0.94 | 0.22 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3319 | 1/1   | 0.94 | 0.21 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3438 | 1/1   | 0.94 | 0.16 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 4146 | 1/1   | 0.94 | 0.28 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3441 | 1/1   | 0.94 | 0.12 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3442 | 1/1   | 0.94 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 4005 | 1/1   | 0.94 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3320 | 1/1   | 0.94 | 0.08 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3886 | 1/1   | 0.94 | 0.08 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 3293 | 1/1   | 0.94 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1a    | 3294 | 1/1   | 0.94 | 0.14 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3889 | 1/1   | 0.94 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3298 | 1/1   | 0.94 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 4010 | 1/1   | 0.94 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3492 | 1/1   | 0.94 | 0.14 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 4012 | 1/1   | 0.94 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3493 | 1/1   | 0.94 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 3194 | 1/1   | 0.94 | 0.18 | 68,68,68,68                 | 0     |
| 57  | MG   | 1a    | 3122 | 1/1   | 0.94 | 0.29 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3892 | 1/1   | 0.94 | 0.14 | 28,28,28,28                 | 0     |
| 57  | MG   | 2a    | 3197 | 1/1   | 0.94 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3001 | 1/1   | 0.94 | 0.19 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3002 | 1/1   | 0.94 | 0.24 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3896 | 1/1   | 0.94 | 0.09 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3494 | 1/1   | 0.94 | 0.24 | 19,19,19,19                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 4159 | 1/1   | 0.94 | 0.13 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3466 | 1/1   | 0.94 | 0.10 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3495 | 1/1   | 0.94 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3223 | 1/1   | 0.94 | 0.10 | 49,49,49,49                 | 0     |
| 62  | MPD  | 1z    | 2003 | 8/8   | 0.94 | 0.20 | 25,28,37,43                 | 0     |
| 57  | MG   | 1A    | 3901 | 1/1   | 0.94 | 0.06 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3662 | 1/1   | 0.94 | 0.17 | 16,16,16,16                 | 0     |
| 57  | MG   | 2A    | 3730 | 1/1   | 0.94 | 0.12 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3338 | 1/1   | 0.95 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3772 | 1/1   | 0.95 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3330 | 1/1   | 0.95 | 0.23 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3153 | 1/1   | 0.95 | 0.14 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3332 | 1/1   | 0.95 | 0.29 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3333 | 1/1   | 0.95 | 0.27 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3877 | 1/1   | 0.95 | 0.12 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3156 | 1/1   | 0.95 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3779 | 1/1   | 0.95 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3453 | 1/1   | 0.95 | 0.10 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3553 | 1/1   | 0.95 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3396 | 1/1   | 0.95 | 0.17 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3159 | 1/1   | 0.95 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3160 | 1/1   | 0.95 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3990 | 1/1   | 0.95 | 0.20 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 4097 | 1/1   | 0.95 | 0.16 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3789 | 1/1   | 0.95 | 0.23 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3163 | 1/1   | 0.95 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3560 | 1/1   | 0.95 | 0.37 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3456 | 1/1   | 0.95 | 0.20 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3305 | 1/1   | 0.95 | 0.30 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3036 | 1/1   | 0.95 | 0.28 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3887 | 1/1   | 0.95 | 0.14 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3568 | 1/1   | 0.95 | 0.07 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3169 | 1/1   | 0.95 | 0.21 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3045 | 1/1   | 0.95 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3888 | 1/1   | 0.95 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3800 | 1/1   | 0.95 | 0.23 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3802 | 1/1   | 0.95 | 0.22 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3803 | 1/1   | 0.95 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 1A    | 3770 | 1/1   | 0.95 | 0.10 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 3001 | 1/1   | 0.95 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | 2a    | 3002 | 1/1   | 0.95 | 0.20 | 57,57,57,57                 | 0     |
| 57  | MG   | 2A    | 3175 | 1/1   | 0.95 | 0.17 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3090 | 1/1   | 0.95 | 0.31 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3007 | 1/1   | 0.95 | 0.13 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 3006 | 1/1   | 0.95 | 0.21 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3009 | 1/1   | 0.95 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3363 | 1/1   | 0.95 | 0.07 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3116 | 1/1   | 0.95 | 0.18 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3597 | 1/1   | 0.95 | 0.22 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3583 | 1/1   | 0.95 | 0.08 | 53,53,53,53                 | 0     |
| 57  | MG   | 1a    | 3174 | 1/1   | 0.95 | 0.22 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3370 | 1/1   | 0.95 | 0.21 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 4107 | 1/1   | 0.95 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3344 | 1/1   | 0.95 | 0.23 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3016 | 1/1   | 0.95 | 0.17 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3589 | 1/1   | 0.95 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3189 | 1/1   | 0.95 | 0.10 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3377 | 1/1   | 0.95 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4000 | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3594 | 1/1   | 0.95 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3525 | 1/1   | 0.95 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3180 | 1/1   | 0.95 | 0.09 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 4002 | 1/1   | 0.95 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3680 | 1/1   | 0.95 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3183 | 1/1   | 0.95 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3900 | 1/1   | 0.95 | 0.18 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 4117 | 1/1   | 0.95 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3600 | 1/1   | 0.95 | 0.14 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3151 | 1/1   | 0.95 | 0.14 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 3035 | 1/1   | 0.95 | 0.22 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3403 | 1/1   | 0.95 | 0.29 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3392 | 1/1   | 0.95 | 0.22 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3394 | 1/1   | 0.95 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3203 | 1/1   | 0.95 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3786 | 1/1   | 0.95 | 0.20 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3466 | 1/1   | 0.95 | 0.23 | 18,18,18,18                 | 0     |
| 57  | MG   | 1a    | 3191 | 1/1   | 0.95 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3789 | 1/1   | 0.95 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3615 | 1/1   | 0.95 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 4127 | 1/1   | 0.95 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3402 | 1/1   | 0.95 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3531 | 1/1   | 0.95 | 0.18 | 17,17,17,17                 | 0     |
| 57  | MG   | 2A    | 3211 | 1/1   | 0.95 | 0.09 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3212 | 1/1   | 0.95 | 0.15 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3304 | 1/1   | 0.95 | 0.17 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3409 | 1/1   | 0.95 | 0.07 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3349 | 1/1   | 0.95 | 0.34 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 4133 | 1/1   | 0.95 | 0.10 | 27,27,27,27                 | 0     |
| 57  | MG   | 1a    | 3200 | 1/1   | 0.95 | 0.09 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 3074 | 1/1   | 0.95 | 0.26 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3259 | 1/1   | 0.95 | 0.27 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 4139 | 1/1   | 0.95 | 0.18 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3118 | 1/1   | 0.95 | 0.17 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3420 | 1/1   | 0.95 | 0.15 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3421 | 1/1   | 0.95 | 0.12 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3615 | 1/1   | 0.95 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3058 | 1/1   | 0.95 | 0.26 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3208 | 1/1   | 0.95 | 0.14 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3428 | 1/1   | 0.95 | 0.12 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3051 | 1/1   | 0.95 | 0.19 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3157 | 1/1   | 0.95 | 0.14 | 21,21,21,21                 | 0     |
| 57  | MG   | 1a    | 3081 | 1/1   | 0.95 | 0.64 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3227 | 1/1   | 0.95 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3065 | 1/1   | 0.95 | 0.36 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3804 | 1/1   | 0.95 | 0.16 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3479 | 1/1   | 0.95 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 2a    | 3080 | 1/1   | 0.95 | 0.17 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3921 | 1/1   | 0.95 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3620 | 1/1   | 0.95 | 0.21 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3440 | 1/1   | 0.95 | 0.13 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3233 | 1/1   | 0.95 | 0.26 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 3085 | 1/1   | 0.95 | 0.26 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3092 | 1/1   | 0.95 | 0.24 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3481 | 1/1   | 0.95 | 0.14 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3121 | 1/1   | 0.95 | 0.13 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3710 | 1/1   | 0.95 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3076 | 1/1   | 0.95 | 0.14 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3447 | 1/1   | 0.95 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3448 | 1/1   | 0.95 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3093 | 1/1   | 0.95 | 0.25 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3076 | 1/1   | 0.95 | 0.17 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3366 | 1/1   | 0.95 | 0.17 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 4035 | 1/1   | 0.95 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 3099 | 1/1   | 0.95 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 4036 | 1/1   | 0.95 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3227 | 1/1   | 0.95 | 0.06 | 57,57,57,57                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3007 | 1/1   | 0.95 | 0.26 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3253 | 1/1   | 0.95 | 0.12 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 3105 | 1/1   | 0.95 | 0.21 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 4039 | 1/1   | 0.95 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3629 | 1/1   | 0.95 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 2a    | 3110 | 1/1   | 0.95 | 0.29 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3258 | 1/1   | 0.95 | 0.20 | 28,28,28,28                 | 0     |
| 57  | MG   | 1a    | 3102 | 1/1   | 0.95 | 0.19 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3088 | 1/1   | 0.95 | 0.26 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3261 | 1/1   | 0.95 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3486 | 1/1   | 0.95 | 0.18 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3275 | 1/1   | 0.95 | 0.19 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3634 | 1/1   | 0.95 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3472 | 1/1   | 0.95 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3490 | 1/1   | 0.95 | 0.20 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3375 | 1/1   | 0.95 | 0.20 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3696 | 1/1   | 0.95 | 0.33 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3698 | 1/1   | 0.95 | 0.20 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3699 | 1/1   | 0.95 | 0.12 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3640 | 1/1   | 0.95 | 0.21 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3556 | 1/1   | 0.95 | 0.18 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3428 | 1/1   | 0.95 | 0.18 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 3243 | 1/1   | 0.95 | 0.12 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3834 | 1/1   | 0.95 | 0.10 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3079 | 1/1   | 0.95 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3275 | 1/1   | 0.95 | 0.09 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3009 | 1/1   | 0.95 | 0.20 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3560 | 1/1   | 0.95 | 0.15 | 19,19,19,19                 | 0     |
| 57  | MG   | 2a    | 3138 | 1/1   | 0.95 | 0.15 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3105 | 1/1   | 0.95 | 0.24 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3281 | 1/1   | 0.95 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3949 | 1/1   | 0.95 | 0.21 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3108 | 1/1   | 0.95 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3719 | 1/1   | 0.95 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3720 | 1/1   | 0.95 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3563 | 1/1   | 0.95 | 0.13 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3649 | 1/1   | 0.95 | 0.22 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3853 | 1/1   | 0.95 | 0.20 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3564 | 1/1   | 0.95 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3289 | 1/1   | 0.95 | 0.21 | 20,20,20,20                 | 0     |
| 57  | MG   | 1a    | 3009 | 1/1   | 0.95 | 0.29 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3728 | 1/1   | 0.95 | 0.19 | 36,36,36,36                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3010 | 1/1   | 0.95 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3958 | 1/1   | 0.95 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3497 | 1/1   | 0.95 | 0.19 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3330 | 1/1   | 0.95 | 0.25 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3505 | 1/1   | 0.95 | 0.07 | 54,54,54,54                 | 0     |
| 57  | MG   | 2a    | 3163 | 1/1   | 0.95 | 0.08 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3168 | 1/1   | 0.95 | 0.14 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3656 | 1/1   | 0.95 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3571 | 1/1   | 0.95 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3301 | 1/1   | 0.95 | 0.66 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3332 | 1/1   | 0.95 | 0.17 | 53,53,53,53                 | 0     |
| 57  | MG   | 2a    | 3173 | 1/1   | 0.95 | 0.08 | 48,48,48,48                 | 0     |
| 57  | MG   | 2a    | 3174 | 1/1   | 0.95 | 0.17 | 61,61,61,61                 | 0     |
| 57  | MG   | 2A    | 3127 | 1/1   | 0.95 | 0.17 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3513 | 1/1   | 0.95 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 1a    | 3269 | 1/1   | 0.95 | 0.12 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3134 | 1/1   | 0.95 | 0.34 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3182 | 1/1   | 0.95 | 0.06 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3306 | 1/1   | 0.95 | 0.41 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3131 | 1/1   | 0.95 | 0.20 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3753 | 1/1   | 0.95 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 3189 | 1/1   | 0.95 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 1a    | 3272 | 1/1   | 0.95 | 0.08 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3440 | 1/1   | 0.95 | 0.10 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3752 | 1/1   | 0.95 | 0.10 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3384 | 1/1   | 0.95 | 0.37 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3525 | 1/1   | 0.95 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3017 | 1/1   | 0.95 | 0.16 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 4081 | 1/1   | 0.95 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3042 | 1/1   | 0.95 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3973 | 1/1   | 0.95 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3869 | 1/1   | 0.95 | 0.07 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3022 | 1/1   | 0.95 | 0.36 | 33,33,33,33                 | 0     |
| 58  | ZN   | 2n    | 501  | 1/1   | 0.95 | 0.10 | 73,73,73,73                 | 0     |
| 57  | MG   | 1a    | 3285 | 1/1   | 0.95 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3047 | 1/1   | 0.95 | 0.20 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3874 | 1/1   | 0.95 | 0.15 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3148 | 1/1   | 0.95 | 0.22 | 55,55,55,55                 | 0     |
| 57  | MG   | 1a    | 3290 | 1/1   | 0.95 | 0.15 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3979 | 1/1   | 0.95 | 0.19 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3086 | 1/1   | 0.95 | 0.18 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3328 | 1/1   | 0.95 | 0.12 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3181 | 1/1   | 0.96 | 0.38 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3142 | 1/1   | 0.96 | 0.42 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3516 | 1/1   | 0.96 | 0.30 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 4084 | 1/1   | 0.96 | 0.07 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3799 | 1/1   | 0.96 | 0.15 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3144 | 1/1   | 0.96 | 0.23 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3263 | 1/1   | 0.96 | 0.15 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3097 | 1/1   | 0.96 | 0.19 | 21,21,21,21                 | 0     |
| 57  | MG   | 1a    | 3064 | 1/1   | 0.96 | 0.27 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3409 | 1/1   | 0.96 | 0.21 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3574 | 1/1   | 0.96 | 0.16 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3677 | 1/1   | 0.96 | 0.26 | 20,20,20,20                 | 0     |
| 57  | MG   | 1a    | 3068 | 1/1   | 0.96 | 0.12 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3951 | 1/1   | 0.96 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3109 | 1/1   | 0.96 | 0.18 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3070 | 1/1   | 0.96 | 0.12 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3489 | 1/1   | 0.96 | 0.23 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3813 | 1/1   | 0.96 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3956 | 1/1   | 0.96 | 0.14 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3149 | 1/1   | 0.96 | 0.19 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3578 | 1/1   | 0.96 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3783 | 1/1   | 0.96 | 0.22 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3681 | 1/1   | 0.96 | 0.19 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3682 | 1/1   | 0.96 | 0.20 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3412 | 1/1   | 0.96 | 0.12 | 41,41,41,41                 | 0     |
| 57  | MG   | 1a    | 3240 | 1/1   | 0.96 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3270 | 1/1   | 0.96 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3414 | 1/1   | 0.96 | 0.17 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3125 | 1/1   | 0.96 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3321 | 1/1   | 0.96 | 0.28 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3688 | 1/1   | 0.96 | 0.34 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3827 | 1/1   | 0.96 | 0.15 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3550 | 1/1   | 0.96 | 0.20 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3128 | 1/1   | 0.96 | 0.21 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3072 | 1/1   | 0.96 | 0.19 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3099 | 1/1   | 0.96 | 0.14 | 27,27,27,27                 | 0     |
| 57  | MG   | 1a    | 3085 | 1/1   | 0.96 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3249 | 1/1   | 0.96 | 0.13 | 68,68,68,68                 | 0     |
| 57  | MG   | 1A    | 3153 | 1/1   | 0.96 | 0.23 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3251 | 1/1   | 0.96 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3588 | 1/1   | 0.96 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3498 | 1/1   | 0.96 | 0.19 | 23,23,23,23                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1a    | 3089 | 1/1   | 0.96 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3500 | 1/1   | 0.96 | 0.15 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3339 | 1/1   | 0.96 | 0.36 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3593 | 1/1   | 0.96 | 0.23 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3193 | 1/1   | 0.96 | 0.14 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 4119 | 1/1   | 0.96 | 0.25 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3570 | 1/1   | 0.96 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3699 | 1/1   | 0.96 | 0.16 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3839 | 1/1   | 0.96 | 0.10 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3840 | 1/1   | 0.96 | 0.11 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3841 | 1/1   | 0.96 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3575 | 1/1   | 0.96 | 0.18 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3149 | 1/1   | 0.96 | 0.25 | 29,29,29,29                 | 0     |
| 57  | MG   | 1a    | 3100 | 1/1   | 0.96 | 0.24 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3122 | 1/1   | 0.96 | 0.33 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 4126 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3354 | 1/1   | 0.96 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3342 | 1/1   | 0.96 | 0.28 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3844 | 1/1   | 0.96 | 0.12 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3847 | 1/1   | 0.96 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3848 | 1/1   | 0.96 | 0.22 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 4131 | 1/1   | 0.96 | 0.20 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 4132 | 1/1   | 0.96 | 0.11 | 59,59,59,59                 | 0     |
| 57  | MG   | 1a    | 3276 | 1/1   | 0.96 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1a    | 3109 | 1/1   | 0.96 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3590 | 1/1   | 0.96 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3364 | 1/1   | 0.96 | 0.17 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3849 | 1/1   | 0.96 | 0.19 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 4136 | 1/1   | 0.96 | 0.17 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3367 | 1/1   | 0.96 | 0.19 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3034 | 1/1   | 0.96 | 0.13 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3703 | 1/1   | 0.96 | 0.15 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3277 | 1/1   | 0.96 | 0.15 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3371 | 1/1   | 0.96 | 0.18 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 4140 | 1/1   | 0.96 | 0.15 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3167 | 1/1   | 0.96 | 0.15 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3424 | 1/1   | 0.96 | 0.09 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3279 | 1/1   | 0.96 | 0.18 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3170 | 1/1   | 0.96 | 0.07 | 67,67,67,67                 | 0     |
| 57  | MG   | 2A    | 3171 | 1/1   | 0.96 | 0.10 | 59,59,59,59                 | 0     |
| 57  | MG   | 1A    | 3224 | 1/1   | 0.96 | 0.23 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3062 | 1/1   | 0.96 | 0.18 | 21,21,21,21                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3603 | 1/1   | 0.96 | 0.25 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3228 | 1/1   | 0.96 | 0.23 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3384 | 1/1   | 0.96 | 0.19 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3609 | 1/1   | 0.96 | 0.17 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3289 | 1/1   | 0.96 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3516 | 1/1   | 0.96 | 0.24 | 26,26,26,26                 | 0     |
| 57  | MG   | 2a    | 3054 | 1/1   | 0.96 | 0.19 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3015 | 1/1   | 0.96 | 0.17 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 3056 | 1/1   | 0.96 | 0.15 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3297 | 1/1   | 0.96 | 0.15 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3612 | 1/1   | 0.96 | 0.17 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3434 | 1/1   | 0.96 | 0.14 | 10,10,10,10                 | 0     |
| 57  | MG   | 1A    | 3722 | 1/1   | 0.96 | 0.12 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3186 | 1/1   | 0.96 | 0.22 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 4008 | 1/1   | 0.96 | 0.07 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3291 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3724 | 1/1   | 0.96 | 0.19 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3126 | 1/1   | 0.96 | 0.21 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3626 | 1/1   | 0.96 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3726 | 1/1   | 0.96 | 0.20 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3043 | 1/1   | 0.96 | 0.23 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3361 | 1/1   | 0.96 | 0.20 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3403 | 1/1   | 0.96 | 0.07 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3632 | 1/1   | 0.96 | 0.13 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3404 | 1/1   | 0.96 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3194 | 1/1   | 0.96 | 0.21 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3732 | 1/1   | 0.96 | 0.11 | 45,45,45,45                 | 0     |
| 57  | MG   | 2a    | 3078 | 1/1   | 0.96 | 0.11 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4016 | 1/1   | 0.96 | 0.12 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3637 | 1/1   | 0.96 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3005 | 1/1   | 0.96 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3639 | 1/1   | 0.96 | 0.18 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3441 | 1/1   | 0.96 | 0.14 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3141 | 1/1   | 0.96 | 0.29 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 4018 | 1/1   | 0.96 | 0.19 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 4019 | 1/1   | 0.96 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3442 | 1/1   | 0.96 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3235 | 1/1   | 0.96 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3883 | 1/1   | 0.96 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3418 | 1/1   | 0.96 | 0.24 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 4024 | 1/1   | 0.96 | 0.24 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3207 | 1/1   | 0.96 | 0.30 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3885 | 1/1   | 0.96 | 0.11 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 3094 | 1/1   | 0.96 | 0.19 | 50,50,50,50                 | 0     |
| 57  | MG   | 2a    | 3095 | 1/1   | 0.96 | 0.18 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3422 | 1/1   | 0.96 | 0.26 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3236 | 1/1   | 0.96 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3018 | 1/1   | 0.96 | 0.18 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3529 | 1/1   | 0.96 | 0.28 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3020 | 1/1   | 0.96 | 0.30 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3201 | 1/1   | 0.96 | 0.19 | 63,63,63,63                 | 0     |
| 57  | MG   | 1a    | 3002 | 1/1   | 0.96 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | 2A    | 3664 | 1/1   | 0.96 | 0.07 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3089 | 1/1   | 0.96 | 0.44 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3371 | 1/1   | 0.96 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3450 | 1/1   | 0.96 | 0.15 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3158 | 1/1   | 0.96 | 0.14 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3435 | 1/1   | 0.96 | 0.18 | 53,53,53,53                 | 0     |
| 57  | MG   | 2A    | 3030 | 1/1   | 0.96 | 0.08 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3031 | 1/1   | 0.96 | 0.21 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3242 | 1/1   | 0.96 | 0.23 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3631 | 1/1   | 0.96 | 0.15 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3032 | 1/1   | 0.96 | 0.21 | 36,36,36,36                 | 0     |
| 57  | MG   | 2a    | 3117 | 1/1   | 0.96 | 0.24 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3036 | 1/1   | 0.96 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3244 | 1/1   | 0.96 | 0.20 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3635 | 1/1   | 0.96 | 0.18 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 4037 | 1/1   | 0.96 | 0.10 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3682 | 1/1   | 0.96 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3636 | 1/1   | 0.96 | 0.18 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3684 | 1/1   | 0.96 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | 1a    | 3014 | 1/1   | 0.96 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3245 | 1/1   | 0.96 | 0.15 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3449 | 1/1   | 0.96 | 0.20 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3110 | 1/1   | 0.96 | 0.26 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3046 | 1/1   | 0.96 | 0.15 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 4042 | 1/1   | 0.96 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3234 | 1/1   | 0.96 | 0.25 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3247 | 1/1   | 0.96 | 0.31 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3695 | 1/1   | 0.96 | 0.11 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3046 | 1/1   | 0.96 | 0.21 | 16,16,16,16                 | 0     |
| 57  | MG   | 1a    | 3021 | 1/1   | 0.96 | 0.18 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3053 | 1/1   | 0.96 | 0.16 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3541 | 1/1   | 0.96 | 0.08 | 33,33,33,33                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 4050 | 1/1   | 0.96 | 0.12 | 19,19,19,19                 | 0     |
| 57  | MG   | 2A    | 3702 | 1/1   | 0.96 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3382 | 1/1   | 0.96 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3543 | 1/1   | 0.96 | 0.20 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3705 | 1/1   | 0.96 | 0.14 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3706 | 1/1   | 0.96 | 0.18 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3251 | 1/1   | 0.96 | 0.29 | 35,35,35,35                 | 0     |
| 57  | MG   | 1a    | 3027 | 1/1   | 0.96 | 0.23 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3646 | 1/1   | 0.96 | 0.20 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3251 | 1/1   | 0.96 | 0.28 | 42,42,42,42                 | 0     |
| 57  | MG   | 2a    | 3157 | 1/1   | 0.96 | 0.22 | 67,67,67,67                 | 0     |
| 57  | MG   | 1A    | 3766 | 1/1   | 0.96 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3062 | 1/1   | 0.96 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3254 | 1/1   | 0.96 | 0.44 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3716 | 1/1   | 0.96 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3474 | 1/1   | 0.96 | 0.12 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3063 | 1/1   | 0.96 | 0.12 | 44,44,44,44                 | 0     |
| 57  | MG   | 2A    | 3256 | 1/1   | 0.96 | 0.29 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3310 | 1/1   | 0.96 | 0.16 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3721 | 1/1   | 0.96 | 0.11 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3546 | 1/1   | 0.96 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 4058 | 1/1   | 0.96 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3315 | 1/1   | 0.96 | 0.26 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3549 | 1/1   | 0.96 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | 2a    | 3175 | 1/1   | 0.96 | 0.11 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3482 | 1/1   | 0.96 | 0.15 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3773 | 1/1   | 0.96 | 0.11 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3023 | 1/1   | 0.96 | 0.20 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3040 | 1/1   | 0.96 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 3181 | 1/1   | 0.96 | 0.10 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 4064 | 1/1   | 0.96 | 0.16 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3552 | 1/1   | 0.96 | 0.14 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 3185 | 1/1   | 0.96 | 0.11 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3388 | 1/1   | 0.96 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3490 | 1/1   | 0.96 | 0.24 | 48,48,48,48                 | 0     |
| 57  | MG   | 1a    | 3197 | 1/1   | 0.96 | 0.14 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3554 | 1/1   | 0.96 | 0.17 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3018 | 1/1   | 0.96 | 0.20 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 4070 | 1/1   | 0.96 | 0.28 | 35,35,35,35                 | 0     |
| 57  | MG   | 2a    | 3193 | 1/1   | 0.96 | 0.10 | 65,65,65,65                 | 0     |
| 57  | MG   | 2A    | 3497 | 1/1   | 0.96 | 0.08 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3390 | 1/1   | 0.96 | 0.29 | 35,35,35,35                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3474 | 1/1   | 0.96 | 0.14 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3276 | 1/1   | 0.96 | 0.07 | 69,69,69,69                 | 0     |
| 57  | MG   | 1A    | 3661 | 1/1   | 0.96 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 3200 | 1/1   | 0.96 | 0.08 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3322 | 1/1   | 0.96 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3279 | 1/1   | 0.96 | 0.16 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3788 | 1/1   | 0.96 | 0.27 | 29,29,29,29                 | 0     |
| 58  | ZN   | 26    | 501  | 1/1   | 0.96 | 0.16 | 56,56,56,56                 | 0     |
| 58  | ZN   | 29    | 501  | 1/1   | 0.96 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3477 | 1/1   | 0.96 | 0.15 | 40,40,40,40                 | 0     |
| 60  | CLM  | 1z    | 1    | 20/20 | 0.96 | 0.24 | 18,30,47,48                 | 0     |
| 57  | MG   | 2A    | 3506 | 1/1   | 0.96 | 0.10 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3323 | 1/1   | 0.96 | 0.21 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3096 | 1/1   | 0.96 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3257 | 1/1   | 0.96 | 0.28 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3939 | 1/1   | 0.96 | 0.07 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3258 | 1/1   | 0.96 | 0.35 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3093 | 1/1   | 0.96 | 0.30 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3094 | 1/1   | 0.96 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3392 | 1/1   | 0.97 | 0.15 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3394 | 1/1   | 0.97 | 0.18 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3632 | 1/1   | 0.97 | 0.10 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3052 | 1/1   | 0.97 | 0.08 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3329 | 1/1   | 0.97 | 0.16 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3195 | 1/1   | 0.97 | 0.59 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3801 | 1/1   | 0.97 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3728 | 1/1   | 0.97 | 0.28 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3846 | 1/1   | 0.97 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3128 | 1/1   | 0.97 | 0.26 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3204 | 1/1   | 0.97 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3731 | 1/1   | 0.97 | 0.20 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3278 | 1/1   | 0.97 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3850 | 1/1   | 0.97 | 0.19 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3733 | 1/1   | 0.97 | 0.18 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3005 | 1/1   | 0.97 | 0.16 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3476 | 1/1   | 0.97 | 0.16 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3985 | 1/1   | 0.97 | 0.22 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3130 | 1/1   | 0.97 | 0.22 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 4112 | 1/1   | 0.97 | 0.16 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3131 | 1/1   | 0.97 | 0.21 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3416 | 1/1   | 0.97 | 0.16 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3989 | 1/1   | 0.97 | 0.18 | 26,26,26,26                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2a    | 3014 | 1/1   | 0.97 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 4115 | 1/1   | 0.97 | 0.18 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3402 | 1/1   | 0.97 | 0.12 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3613 | 1/1   | 0.97 | 0.09 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3282 | 1/1   | 0.97 | 0.18 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3404 | 1/1   | 0.97 | 0.20 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3220 | 1/1   | 0.97 | 0.12 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3221 | 1/1   | 0.97 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3619 | 1/1   | 0.97 | 0.14 | 41,41,41,41                 | 0     |
| 57  | MG   | 2a    | 3023 | 1/1   | 0.97 | 0.13 | 58,58,58,58                 | 0     |
| 57  | MG   | 2A    | 3424 | 1/1   | 0.97 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3861 | 1/1   | 0.97 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3741 | 1/1   | 0.97 | 0.24 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3743 | 1/1   | 0.97 | 0.10 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3624 | 1/1   | 0.97 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3405 | 1/1   | 0.97 | 0.20 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3283 | 1/1   | 0.97 | 0.13 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3408 | 1/1   | 0.97 | 0.17 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 4125 | 1/1   | 0.97 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 2A    | 3249 | 1/1   | 0.97 | 0.37 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3085 | 1/1   | 0.97 | 0.17 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3132 | 1/1   | 0.97 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3750 | 1/1   | 0.97 | 0.22 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 3285 | 1/1   | 0.97 | 0.09 | 40,40,40,40                 | 0     |
| 57  | MG   | 2a    | 3040 | 1/1   | 0.97 | 0.09 | 74,74,74,74                 | 0     |
| 57  | MG   | 1a    | 3232 | 1/1   | 0.97 | 0.13 | 63,63,63,63                 | 0     |
| 57  | MG   | 1A    | 3286 | 1/1   | 0.97 | 0.28 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3873 | 1/1   | 0.97 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3651 | 1/1   | 0.97 | 0.40 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3287 | 1/1   | 0.97 | 0.25 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3241 | 1/1   | 0.97 | 0.25 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3095 | 1/1   | 0.97 | 0.26 | 41,41,41,41                 | 0     |
| 57  | MG   | 2A    | 3643 | 1/1   | 0.97 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3161 | 1/1   | 0.97 | 0.12 | 64,64,64,64                 | 0     |
| 57  | MG   | 1A    | 4137 | 1/1   | 0.97 | 0.24 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3646 | 1/1   | 0.97 | 0.13 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3655 | 1/1   | 0.97 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3570 | 1/1   | 0.97 | 0.15 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3649 | 1/1   | 0.97 | 0.09 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3650 | 1/1   | 0.97 | 0.23 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3164 | 1/1   | 0.97 | 0.22 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3881 | 1/1   | 0.97 | 0.15 | 15,15,15,15                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2a    | 3058 | 1/1   | 0.97 | 0.04 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3882 | 1/1   | 0.97 | 0.18 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3269 | 1/1   | 0.97 | 0.22 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3006 | 1/1   | 0.97 | 0.15 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3762 | 1/1   | 0.97 | 0.20 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3248 | 1/1   | 0.97 | 0.07 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3346 | 1/1   | 0.97 | 0.26 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3134 | 1/1   | 0.97 | 0.22 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3348 | 1/1   | 0.97 | 0.18 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3461 | 1/1   | 0.97 | 0.10 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3576 | 1/1   | 0.97 | 0.20 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 4149 | 1/1   | 0.97 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3114 | 1/1   | 0.97 | 0.23 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3499 | 1/1   | 0.97 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3352 | 1/1   | 0.97 | 0.20 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3467 | 1/1   | 0.97 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3893 | 1/1   | 0.97 | 0.15 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3771 | 1/1   | 0.97 | 0.48 | 40,40,40,40                 | 0     |
| 57  | MG   | 1a    | 3112 | 1/1   | 0.97 | 0.23 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3897 | 1/1   | 0.97 | 0.14 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3674 | 1/1   | 0.97 | 0.09 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3581 | 1/1   | 0.97 | 0.22 | 15,15,15,15                 | 0     |
| 57  | MG   | 1a    | 3263 | 1/1   | 0.97 | 0.23 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3288 | 1/1   | 0.97 | 0.24 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3501 | 1/1   | 0.97 | 0.12 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3679 | 1/1   | 0.97 | 0.15 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3290 | 1/1   | 0.97 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3123 | 1/1   | 0.97 | 0.56 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3136 | 1/1   | 0.97 | 0.13 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3021 | 1/1   | 0.97 | 0.29 | 20,20,20,20                 | 0     |
| 57  | MG   | 1a    | 3267 | 1/1   | 0.97 | 0.20 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3295 | 1/1   | 0.97 | 0.26 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3776 | 1/1   | 0.97 | 0.09 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3585 | 1/1   | 0.97 | 0.16 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3426 | 1/1   | 0.97 | 0.14 | 15,15,15,15                 | 0     |
| 57  | MG   | 2A    | 3299 | 1/1   | 0.97 | 0.17 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3249 | 1/1   | 0.97 | 0.18 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3692 | 1/1   | 0.97 | 0.14 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 4165 | 1/1   | 0.97 | 0.13 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3172 | 1/1   | 0.97 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 2a    | 3100 | 1/1   | 0.97 | 0.17 | 47,47,47,47                 | 0     |
| 57  | MG   | 1a    | 3124 | 1/1   | 0.97 | 0.25 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3494 | 1/1   | 0.97 | 0.12 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3697 | 1/1   | 0.97 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3782 | 1/1   | 0.97 | 0.11 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3429 | 1/1   | 0.97 | 0.18 | 20,20,20,20                 | 0     |
| 57  | MG   | 2a    | 3106 | 1/1   | 0.97 | 0.31 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3590 | 1/1   | 0.97 | 0.16 | 16,16,16,16                 | 0     |
| 57  | MG   | 2a    | 3108 | 1/1   | 0.97 | 0.33 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3359 | 1/1   | 0.97 | 0.18 | 23,23,23,23                 | 0     |
| 57  | MG   | 1a    | 3129 | 1/1   | 0.97 | 0.15 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3139 | 1/1   | 0.97 | 0.20 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3300 | 1/1   | 0.97 | 0.12 | 19,19,19,19                 | 0     |
| 57  | MG   | 1a    | 3283 | 1/1   | 0.97 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3912 | 1/1   | 0.97 | 0.18 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3143 | 1/1   | 0.97 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 4173 | 1/1   | 0.97 | 0.10 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3710 | 1/1   | 0.97 | 0.16 | 24,24,24,24                 | 0     |
| 57  | MG   | 1a    | 3286 | 1/1   | 0.97 | 0.11 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 4041 | 1/1   | 0.97 | 0.12 | 46,46,46,46                 | 0     |
| 57  | MG   | 2a    | 3121 | 1/1   | 0.97 | 0.17 | 62,62,62,62                 | 0     |
| 57  | MG   | 1A    | 3914 | 1/1   | 0.97 | 0.18 | 46,46,46,46                 | 0     |
| 57  | MG   | 1A    | 4044 | 1/1   | 0.97 | 0.14 | 25,25,25,25                 | 0     |
| 57  | MG   | 2a    | 3124 | 1/1   | 0.97 | 0.20 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 4045 | 1/1   | 0.97 | 0.06 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3067 | 1/1   | 0.97 | 0.10 | 31,31,31,31                 | 0     |
| 57  | MG   | 1a    | 3138 | 1/1   | 0.97 | 0.24 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3088 | 1/1   | 0.97 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3177 | 1/1   | 0.97 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3596 | 1/1   | 0.97 | 0.15 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3155 | 1/1   | 0.97 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3436 | 1/1   | 0.97 | 0.17 | 13,13,13,13                 | 0     |
| 57  | MG   | 2A    | 3518 | 1/1   | 0.97 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3059 | 1/1   | 0.97 | 0.11 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3369 | 1/1   | 0.97 | 0.27 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3796 | 1/1   | 0.97 | 0.09 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3080 | 1/1   | 0.97 | 0.22 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3798 | 1/1   | 0.97 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | 1a    | 3303 | 1/1   | 0.97 | 0.06 | 52,52,52,52                 | 0     |
| 57  | MG   | 2a    | 3141 | 1/1   | 0.97 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3039 | 1/1   | 0.97 | 0.10 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3216 | 1/1   | 0.97 | 0.17 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3374 | 1/1   | 0.97 | 0.24 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 3146 | 1/1   | 0.97 | 0.06 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3045 | 1/1   | 0.97 | 0.29 | 46,46,46,46                 | 0     |
| 57  | MG   | 2A    | 3339 | 1/1   | 0.97 | 0.06 | 56,56,56,56                 | 0     |
| 57  | MG   | 2A    | 3531 | 1/1   | 0.97 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 1a    | 3018 | 1/1   | 0.97 | 0.15 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3805 | 1/1   | 0.97 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3605 | 1/1   | 0.97 | 0.14 | 46,46,46,46                 | 0     |
| 57  | MG   | 1a    | 3156 | 1/1   | 0.97 | 0.21 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3311 | 1/1   | 0.97 | 0.19 | 16,16,16,16                 | 0     |
| 57  | MG   | 2a    | 3156 | 1/1   | 0.97 | 0.06 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3447 | 1/1   | 0.97 | 0.13 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3348 | 1/1   | 0.97 | 0.16 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3746 | 1/1   | 0.97 | 0.18 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3313 | 1/1   | 0.97 | 0.18 | 31,31,31,31                 | 0     |
| 57  | MG   | 2A    | 3351 | 1/1   | 0.97 | 0.13 | 36,36,36,36                 | 0     |
| 57  | MG   | 1a    | 3161 | 1/1   | 0.97 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3812 | 1/1   | 0.97 | 0.21 | 15,15,15,15                 | 0     |
| 57  | MG   | 2a    | 3164 | 1/1   | 0.97 | 0.16 | 32,32,32,32                 | 0     |
| 57  | MG   | 2a    | 3165 | 1/1   | 0.97 | 0.11 | 57,57,57,57                 | 0     |
| 57  | MG   | 2a    | 3166 | 1/1   | 0.97 | 0.15 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3610 | 1/1   | 0.97 | 0.15 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3700 | 1/1   | 0.97 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3178 | 1/1   | 0.97 | 0.11 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 4069 | 1/1   | 0.97 | 0.22 | 24,24,24,24                 | 0     |
| 57  | MG   | 2a    | 3171 | 1/1   | 0.97 | 0.11 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3755 | 1/1   | 0.97 | 0.18 | 40,40,40,40                 | 0     |
| 57  | MG   | 1A    | 3815 | 1/1   | 0.97 | 0.13 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3611 | 1/1   | 0.97 | 0.17 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3314 | 1/1   | 0.97 | 0.17 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3123 | 1/1   | 0.97 | 0.22 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3760 | 1/1   | 0.97 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3185 | 1/1   | 0.97 | 0.12 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3704 | 1/1   | 0.97 | 0.07 | 49,49,49,49                 | 0     |
| 57  | MG   | 2a    | 3180 | 1/1   | 0.97 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 1a    | 3033 | 1/1   | 0.97 | 0.12 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3024 | 1/1   | 0.97 | 0.52 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3823 | 1/1   | 0.97 | 0.19 | 14,14,14,14                 | 0     |
| 57  | MG   | 2a    | 3184 | 1/1   | 0.97 | 0.11 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3368 | 1/1   | 0.97 | 0.13 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3316 | 1/1   | 0.97 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3317 | 1/1   | 0.97 | 0.15 | 30,30,30,30                 | 0     |
| 57  | MG   | 2a    | 3188 | 1/1   | 0.97 | 0.08 | 62,62,62,62                 | 0     |
| 57  | MG   | 2A    | 3562 | 1/1   | 0.97 | 0.10 | 43,43,43,43                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3708 | 1/1   | 0.97 | 0.26 | 35,35,35,35                 | 0     |
| 57  | MG   | 2A    | 3372 | 1/1   | 0.97 | 0.18 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3185 | 1/1   | 0.97 | 0.09 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3148 | 1/1   | 0.97 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3025 | 1/1   | 0.97 | 0.19 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3268 | 1/1   | 0.97 | 0.23 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3459 | 1/1   | 0.97 | 0.13 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3106 | 1/1   | 0.97 | 0.27 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3379 | 1/1   | 0.97 | 0.13 | 44,44,44,44                 | 0     |
| 57  | MG   | 2a    | 3199 | 1/1   | 0.97 | 0.16 | 57,57,57,57                 | 0     |
| 57  | MG   | 1A    | 3225 | 1/1   | 0.97 | 0.46 | 30,30,30,30                 | 0     |
| 58  | ZN   | 1Y    | 501  | 1/1   | 0.97 | 0.17 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 3109 | 1/1   | 0.97 | 0.23 | 25,25,25,25                 | 0     |
| 58  | ZN   | 1n    | 501  | 1/1   | 0.97 | 0.10 | 66,66,66,66                 | 0     |
| 57  | MG   | 2A    | 3781 | 1/1   | 0.97 | 0.14 | 55,55,55,55                 | 0     |
| 57  | MG   | 1A    | 3192 | 1/1   | 0.97 | 0.34 | 39,39,39,39                 | 0     |
| 57  | MG   | 2A    | 3577 | 1/1   | 0.97 | 0.12 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3094 | 1/1   | 0.97 | 0.13 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3964 | 1/1   | 0.97 | 0.22 | 29,29,29,29                 | 0     |
| 57  | MG   | 2A    | 3041 | 1/1   | 0.97 | 0.23 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3465 | 1/1   | 0.97 | 0.18 | 12,12,12,12                 | 0     |
| 61  | ARG  | 1z    | 1001 | 12/12 | 0.97 | 0.22 | 26,36,46,51                 | 0     |
| 57  | MG   | 2A    | 3043 | 1/1   | 0.97 | 0.12 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3388 | 1/1   | 0.97 | 0.10 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3966 | 1/1   | 0.97 | 0.08 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3838 | 1/1   | 0.97 | 0.21 | 52,52,52,52                 | 0     |
| 57  | MG   | 1A    | 4093 | 1/1   | 0.97 | 0.12 | 28,28,28,28                 | 0     |
| 57  | MG   | 1a    | 3053 | 1/1   | 0.97 | 0.13 | 52,52,52,52                 | 0     |
| 57  | MG   | 2A    | 3393 | 1/1   | 0.97 | 0.14 | 24,24,24,24                 | 0     |
| 57  | MG   | 2A    | 3565 | 1/1   | 0.98 | 0.13 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3894 | 1/1   | 0.98 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3519 | 1/1   | 0.98 | 0.18 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3163 | 1/1   | 0.98 | 0.30 | 32,32,32,32                 | 0     |
| 57  | MG   | 1A    | 3355 | 1/1   | 0.98 | 0.21 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3407 | 1/1   | 0.98 | 0.18 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3808 | 1/1   | 0.98 | 0.15 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3019 | 1/1   | 0.98 | 0.16 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3810 | 1/1   | 0.98 | 0.21 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3226 | 1/1   | 0.98 | 0.39 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3269 | 1/1   | 0.98 | 0.15 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3411 | 1/1   | 0.98 | 0.22 | 22,22,22,22                 | 0     |
| 57  | MG   | 1a    | 3234 | 1/1   | 0.98 | 0.15 | 45,45,45,45                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2a    | 3075 | 1/1   | 0.98 | 0.07 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3194 | 1/1   | 0.98 | 0.13 | 24,24,24,24                 | 0     |
| 57  | MG   | 2a    | 3077 | 1/1   | 0.98 | 0.21 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3528 | 1/1   | 0.98 | 0.20 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3816 | 1/1   | 0.98 | 0.25 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3111 | 1/1   | 0.98 | 0.24 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3732 | 1/1   | 0.98 | 0.17 | 33,33,33,33                 | 0     |
| 57  | MG   | 2A    | 3050 | 1/1   | 0.98 | 0.09 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3143 | 1/1   | 0.98 | 0.23 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3470 | 1/1   | 0.98 | 0.12 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3020 | 1/1   | 0.98 | 0.17 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3913 | 1/1   | 0.98 | 0.21 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 4108 | 1/1   | 0.98 | 0.08 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3739 | 1/1   | 0.98 | 0.28 | 38,38,38,38                 | 0     |
| 57  | MG   | 2A    | 3740 | 1/1   | 0.98 | 0.09 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3473 | 1/1   | 0.98 | 0.19 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3363 | 1/1   | 0.98 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3274 | 1/1   | 0.98 | 0.21 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3665 | 1/1   | 0.98 | 0.19 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3060 | 1/1   | 0.98 | 0.13 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3367 | 1/1   | 0.98 | 0.14 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3311 | 1/1   | 0.98 | 0.49 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3742 | 1/1   | 0.98 | 0.17 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3922 | 1/1   | 0.98 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3234 | 1/1   | 0.98 | 0.24 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3169 | 1/1   | 0.98 | 0.21 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 4022 | 1/1   | 0.98 | 0.20 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3321 | 1/1   | 0.98 | 0.24 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3170 | 1/1   | 0.98 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3456 | 1/1   | 0.98 | 0.10 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3927 | 1/1   | 0.98 | 0.22 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3027 | 1/1   | 0.98 | 0.19 | 27,27,27,27                 | 0     |
| 57  | MG   | 1a    | 3259 | 1/1   | 0.98 | 0.15 | 48,48,48,48                 | 0     |
| 57  | MG   | 2A    | 3072 | 1/1   | 0.98 | 0.58 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3749 | 1/1   | 0.98 | 0.15 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3324 | 1/1   | 0.98 | 0.28 | 51,51,51,51                 | 0     |
| 57  | MG   | 2A    | 3074 | 1/1   | 0.98 | 0.17 | 20,20,20,20                 | 0     |
| 57  | MG   | 1a    | 3152 | 1/1   | 0.98 | 0.27 | 48,48,48,48                 | 0     |
| 57  | MG   | 1A    | 3074 | 1/1   | 0.98 | 0.23 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3240 | 1/1   | 0.98 | 0.33 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3675 | 1/1   | 0.98 | 0.14 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3469 | 1/1   | 0.98 | 0.10 | 39,39,39,39                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 2A    | 3201 | 1/1   | 0.98 | 0.28 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3326 | 1/1   | 0.98 | 0.16 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3754 | 1/1   | 0.98 | 0.24 | 15,15,15,15                 | 0     |
| 57  | MG   | 2a    | 3120 | 1/1   | 0.98 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3609 | 1/1   | 0.98 | 0.10 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3173 | 1/1   | 0.98 | 0.34 | 29,29,29,29                 | 0     |
| 57  | MG   | 1a    | 3160 | 1/1   | 0.98 | 0.16 | 61,61,61,61                 | 0     |
| 57  | MG   | 1A    | 3430 | 1/1   | 0.98 | 0.14 | 14,14,14,14                 | 0     |
| 57  | MG   | 2a    | 3125 | 1/1   | 0.98 | 0.14 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3488 | 1/1   | 0.98 | 0.17 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 4134 | 1/1   | 0.98 | 0.12 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 4135 | 1/1   | 0.98 | 0.20 | 38,38,38,38                 | 0     |
| 57  | MG   | 1A    | 3150 | 1/1   | 0.98 | 0.17 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3627 | 1/1   | 0.98 | 0.14 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3166 | 1/1   | 0.98 | 0.17 | 56,56,56,56                 | 0     |
| 57  | MG   | 1A    | 3028 | 1/1   | 0.98 | 0.21 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3683 | 1/1   | 0.98 | 0.22 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3684 | 1/1   | 0.98 | 0.11 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3485 | 1/1   | 0.98 | 0.11 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3345 | 1/1   | 0.98 | 0.16 | 45,45,45,45                 | 0     |
| 57  | MG   | 2A    | 3346 | 1/1   | 0.98 | 0.12 | 26,26,26,26                 | 0     |
| 57  | MG   | 1a    | 3279 | 1/1   | 0.98 | 0.14 | 44,44,44,44                 | 0     |
| 57  | MG   | 1a    | 3280 | 1/1   | 0.98 | 0.19 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3176 | 1/1   | 0.98 | 0.19 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3491 | 1/1   | 0.98 | 0.14 | 27,27,27,27                 | 0     |
| 57  | MG   | 2A    | 3350 | 1/1   | 0.98 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3851 | 1/1   | 0.98 | 0.12 | 24,24,24,24                 | 0     |
| 57  | MG   | 2a    | 3144 | 1/1   | 0.98 | 0.19 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 4043 | 1/1   | 0.98 | 0.18 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3001 | 1/1   | 0.98 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3178 | 1/1   | 0.98 | 0.16 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3030 | 1/1   | 0.98 | 0.21 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 4047 | 1/1   | 0.98 | 0.17 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3689 | 1/1   | 0.98 | 0.14 | 26,26,26,26                 | 0     |
| 57  | MG   | 2a    | 3151 | 1/1   | 0.98 | 0.10 | 53,53,53,53                 | 0     |
| 57  | MG   | 1A    | 3768 | 1/1   | 0.98 | 0.14 | 30,30,30,30                 | 0     |
| 57  | MG   | 1a    | 3179 | 1/1   | 0.98 | 0.14 | 39,39,39,39                 | 0     |
| 57  | MG   | 1A    | 3210 | 1/1   | 0.98 | 0.37 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3954 | 1/1   | 0.98 | 0.18 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3362 | 1/1   | 0.98 | 0.15 | 28,28,28,28                 | 0     |
| 57  | MG   | 2A    | 3653 | 1/1   | 0.98 | 0.11 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3496 | 1/1   | 0.98 | 0.24 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3154 | 1/1   | 0.98 | 0.14 | 17,17,17,17                 | 0     |
| 57  | MG   | 1a    | 3295 | 1/1   | 0.98 | 0.13 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3110 | 1/1   | 0.98 | 0.16 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3031 | 1/1   | 0.98 | 0.18 | 26,26,26,26                 | 0     |
| 57  | MG   | 2A    | 3235 | 1/1   | 0.98 | 0.33 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3625 | 1/1   | 0.98 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3156 | 1/1   | 0.98 | 0.13 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3561 | 1/1   | 0.98 | 0.11 | 26,26,26,26                 | 0     |
| 57  | MG   | 1A    | 3253 | 1/1   | 0.98 | 0.43 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3013 | 1/1   | 0.98 | 0.26 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3963 | 1/1   | 0.98 | 0.23 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3003 | 1/1   | 0.98 | 0.16 | 20,20,20,20                 | 0     |
| 57  | MG   | 1a    | 3192 | 1/1   | 0.98 | 0.13 | 43,43,43,43                 | 0     |
| 57  | MG   | 2A    | 3668 | 1/1   | 0.98 | 0.08 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3779 | 1/1   | 0.98 | 0.15 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3245 | 1/1   | 0.98 | 0.13 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3121 | 1/1   | 0.98 | 0.13 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 4162 | 1/1   | 0.98 | 0.13 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3248 | 1/1   | 0.98 | 0.33 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3393 | 1/1   | 0.98 | 0.16 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3250 | 1/1   | 0.98 | 0.15 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3297 | 1/1   | 0.98 | 0.21 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3107 | 1/1   | 0.98 | 0.19 | 44,44,44,44                 | 0     |
| 57  | MG   | 1A    | 3568 | 1/1   | 0.98 | 0.17 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 3784 | 1/1   | 0.98 | 0.08 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3108 | 1/1   | 0.98 | 0.14 | 34,34,34,34                 | 0     |
| 57  | MG   | 2A    | 3532 | 1/1   | 0.98 | 0.13 | 21,21,21,21                 | 0     |
| 57  | MG   | 2a    | 3029 | 1/1   | 0.98 | 0.11 | 52,52,52,52                 | 0     |
| 57  | MG   | 1a    | 3201 | 1/1   | 0.98 | 0.11 | 50,50,50,50                 | 0     |
| 57  | MG   | 2A    | 3008 | 1/1   | 0.98 | 0.14 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3705 | 1/1   | 0.98 | 0.18 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3188 | 1/1   | 0.98 | 0.16 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3011 | 1/1   | 0.98 | 0.18 | 51,51,51,51                 | 0     |
| 57  | MG   | 1A    | 3034 | 1/1   | 0.98 | 0.12 | 25,25,25,25                 | 0     |
| 57  | MG   | 2A    | 3539 | 1/1   | 0.98 | 0.11 | 37,37,37,37                 | 0     |
| 57  | MG   | 2a    | 3037 | 1/1   | 0.98 | 0.14 | 31,31,31,31                 | 0     |
| 57  | MG   | 1A    | 3638 | 1/1   | 0.98 | 0.16 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3303 | 1/1   | 0.98 | 0.18 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3512 | 1/1   | 0.98 | 0.13 | 21,21,21,21                 | 0     |
| 57  | MG   | 2A    | 3398 | 1/1   | 0.98 | 0.24 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3711 | 1/1   | 0.98 | 0.17 | 21,21,21,21                 | 0     |
| 57  | MG   | 1A    | 4176 | 1/1   | 0.98 | 0.13 | 44,44,44,44                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3884 | 1/1   | 0.98 | 0.35 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3190 | 1/1   | 0.98 | 0.16 | 26,26,26,26                 | 0     |
| 58  | ZN   | 15    | 501  | 1/1   | 0.98 | 0.18 | 37,37,37,37                 | 0     |
| 58  | ZN   | 19    | 501  | 1/1   | 0.98 | 0.20 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3982 | 1/1   | 0.98 | 0.11 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3713 | 1/1   | 0.98 | 0.28 | 37,37,37,37                 | 0     |
| 57  | MG   | 2A    | 3271 | 1/1   | 0.98 | 0.59 | 40,40,40,40                 | 0     |
| 57  | MG   | 2A    | 3023 | 1/1   | 0.98 | 0.11 | 33,33,33,33                 | 0     |
| 57  | MG   | 1a    | 3005 | 1/1   | 0.98 | 0.14 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3162 | 1/1   | 0.98 | 0.09 | 41,41,41,41                 | 0     |
| 59  | SF4  | 1d    | 501  | 8/8   | 0.98 | 0.12 | 52,62,71,75                 | 0     |
| 59  | SF4  | 2d    | 501  | 8/8   | 0.98 | 0.12 | 58,67,74,76                 | 0     |
| 57  | MG   | 1A    | 3223 | 1/1   | 0.98 | 0.27 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3987 | 1/1   | 0.98 | 0.18 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3457 | 1/1   | 0.98 | 0.15 | 15,15,15,15                 | 0     |
| 57  | MG   | 2A    | 3412 | 1/1   | 0.98 | 0.19 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3579 | 1/1   | 0.98 | 0.08 | 43,43,43,43                 | 0     |
| 57  | MG   | 1A    | 3351 | 1/1   | 0.98 | 0.25 | 41,41,41,41                 | 0     |
| 57  | MG   | 1A    | 3264 | 1/1   | 0.98 | 0.23 | 36,36,36,36                 | 0     |
| 57  | MG   | 2A    | 3032 | 1/1   | 0.98 | 0.18 | 22,22,22,22                 | 0     |
| 57  | MG   | 2A    | 3563 | 1/1   | 0.98 | 0.11 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3803 | 1/1   | 0.98 | 0.16 | 49,49,49,49                 | 0     |
| 57  | MG   | 1A    | 3446 | 1/1   | 0.99 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3619 | 1/1   | 0.99 | 0.18 | 54,54,54,54                 | 0     |
| 57  | MG   | 2A    | 3551 | 1/1   | 0.99 | 0.05 | 49,49,49,49                 | 0     |
| 57  | MG   | 2A    | 3184 | 1/1   | 0.99 | 0.17 | 55,55,55,55                 | 0     |
| 57  | MG   | 2A    | 3425 | 1/1   | 0.99 | 0.13 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3821 | 1/1   | 0.99 | 0.09 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3870 | 1/1   | 0.99 | 0.17 | 23,23,23,23                 | 0     |
| 57  | MG   | 2A    | 3689 | 1/1   | 0.99 | 0.11 | 54,54,54,54                 | 0     |
| 57  | MG   | 1A    | 3547 | 1/1   | 0.99 | 0.19 | 13,13,13,13                 | 0     |
| 57  | MG   | 1A    | 3977 | 1/1   | 0.99 | 0.14 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3621 | 1/1   | 0.99 | 0.16 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3077 | 1/1   | 0.99 | 0.20 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3071 | 1/1   | 0.99 | 0.19 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3419 | 1/1   | 0.99 | 0.20 | 22,22,22,22                 | 0     |
| 57  | MG   | 1A    | 3365 | 1/1   | 0.99 | 0.21 | 8,8,8,8                     | 0     |
| 57  | MG   | 1A    | 3983 | 1/1   | 0.99 | 0.15 | 11,11,11,11                 | 0     |
| 57  | MG   | 2A    | 3436 | 1/1   | 0.99 | 0.18 | 29,29,29,29                 | 0     |
| 57  | MG   | 1a    | 3091 | 1/1   | 0.99 | 0.08 | 60,60,60,60                 | 0     |
| 57  | MG   | 1A    | 3928 | 1/1   | 0.99 | 0.18 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3100 | 1/1   | 0.99 | 0.19 | 12,12,12,12                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3117 | 1/1   | 0.99 | 0.18 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3368 | 1/1   | 0.99 | 0.20 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3022 | 1/1   | 0.99 | 0.30 | 37,37,37,37                 | 0     |
| 57  | MG   | 1A    | 3745 | 1/1   | 0.99 | 0.36 | 33,33,33,33                 | 0     |
| 57  | MG   | 1A    | 3454 | 1/1   | 0.99 | 0.15 | 45,45,45,45                 | 0     |
| 57  | MG   | 1A    | 3014 | 1/1   | 0.99 | 0.30 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 4103 | 1/1   | 0.99 | 0.19 | 12,12,12,12                 | 0     |
| 57  | MG   | 2A    | 3709 | 1/1   | 0.99 | 0.17 | 32,32,32,32                 | 0     |
| 57  | MG   | 2A    | 3641 | 1/1   | 0.99 | 0.06 | 50,50,50,50                 | 0     |
| 57  | MG   | 1A    | 3261 | 1/1   | 0.99 | 0.26 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3790 | 1/1   | 0.99 | 0.18 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3301 | 1/1   | 0.99 | 0.22 | 30,30,30,30                 | 0     |
| 57  | MG   | 1A    | 3372 | 1/1   | 0.99 | 0.38 | 29,29,29,29                 | 0     |
| 57  | MG   | 1A    | 3146 | 1/1   | 0.99 | 0.24 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3180 | 1/1   | 0.99 | 0.28 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3230 | 1/1   | 0.99 | 0.18 | 12,12,12,12                 | 0     |
| 57  | MG   | 1A    | 3376 | 1/1   | 0.99 | 0.15 | 16,16,16,16                 | 0     |
| 57  | MG   | 1A    | 3265 | 1/1   | 0.99 | 0.22 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3231 | 1/1   | 0.99 | 0.14 | 15,15,15,15                 | 0     |
| 57  | MG   | 2A    | 3520 | 1/1   | 0.99 | 0.12 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3147 | 1/1   | 0.99 | 0.33 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3845 | 1/1   | 0.99 | 0.16 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3947 | 1/1   | 0.99 | 0.14 | 20,20,20,20                 | 0     |
| 57  | MG   | 1A    | 3895 | 1/1   | 0.99 | 0.23 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3353 | 1/1   | 0.99 | 0.28 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3052 | 1/1   | 0.99 | 0.13 | 42,42,42,42                 | 0     |
| 57  | MG   | 1A    | 3802 | 1/1   | 0.99 | 0.17 | 19,19,19,19                 | 0     |
| 57  | MG   | 1A    | 3952 | 1/1   | 0.99 | 0.20 | 23,23,23,23                 | 0     |
| 57  | MG   | 1A    | 3569 | 1/1   | 0.99 | 0.20 | 28,28,28,28                 | 0     |
| 57  | MG   | 1A    | 3720 | 1/1   | 0.99 | 0.20 | 28,28,28,28                 | 0     |
| 58  | ZN   | 16    | 501  | 1/1   | 0.99 | 0.21 | 35,35,35,35                 | 0     |
| 57  | MG   | 1A    | 3437 | 1/1   | 0.99 | 0.17 | 18,18,18,18                 | 0     |
| 57  | MG   | 2A    | 3468 | 1/1   | 0.99 | 0.10 | 36,36,36,36                 | 0     |
| 57  | MG   | 1A    | 3288 | 1/1   | 0.99 | 0.25 | 24,24,24,24                 | 0     |
| 57  | MG   | 1A    | 3250 | 1/1   | 0.99 | 0.14 | 27,27,27,27                 | 0     |
| 58  | ZN   | 25    | 501  | 1/1   | 0.99 | 0.20 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3471 | 1/1   | 0.99 | 0.18 | 17,17,17,17                 | 0     |
| 57  | MG   | 1A    | 3504 | 1/1   | 0.99 | 0.18 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3219 | 1/1   | 0.99 | 0.31 | 34,34,34,34                 | 0     |
| 57  | MG   | 1A    | 3312 | 1/1   | 0.99 | 0.19 | 8,8,8,8                     | 0     |
| 57  | MG   | 1A    | 3048 | 1/1   | 0.99 | 0.15 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3859 | 1/1   | 0.99 | 0.18 | 15,15,15,15                 | 0     |

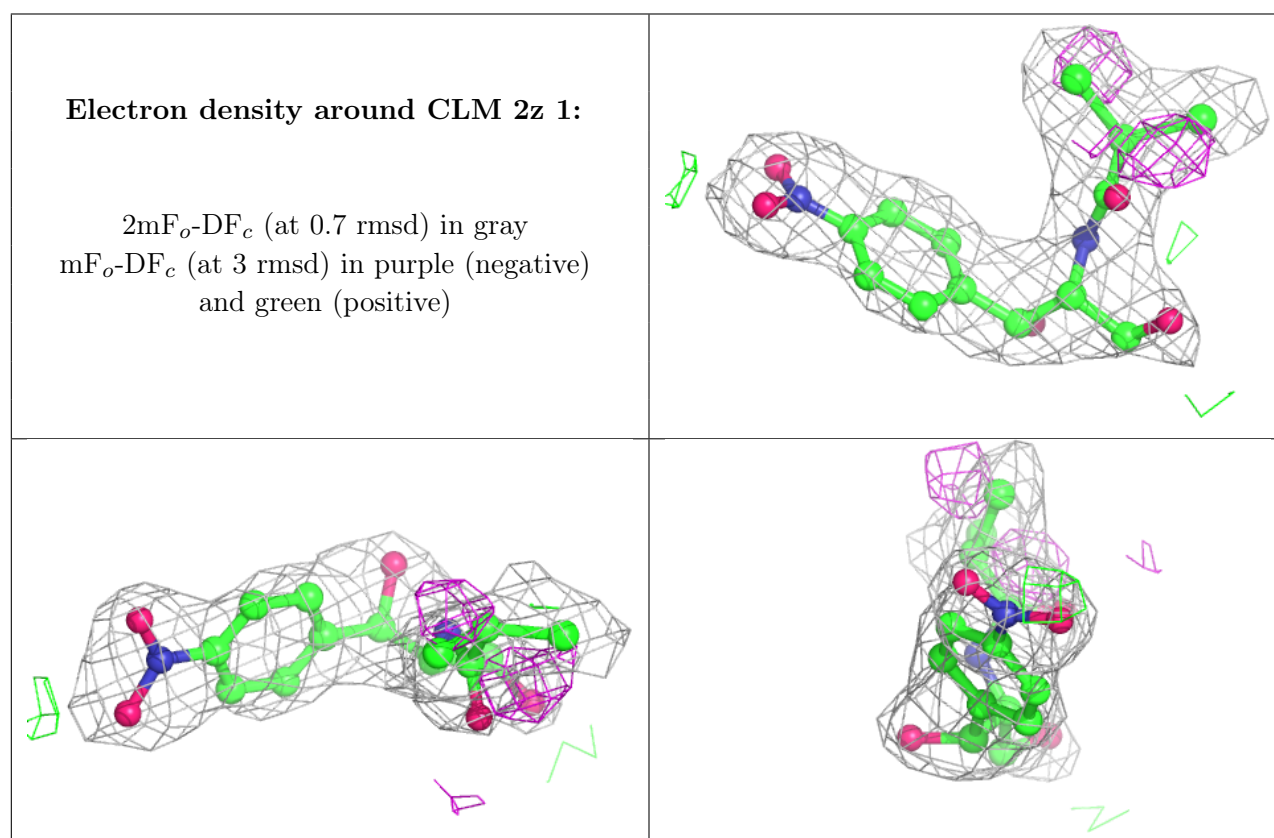
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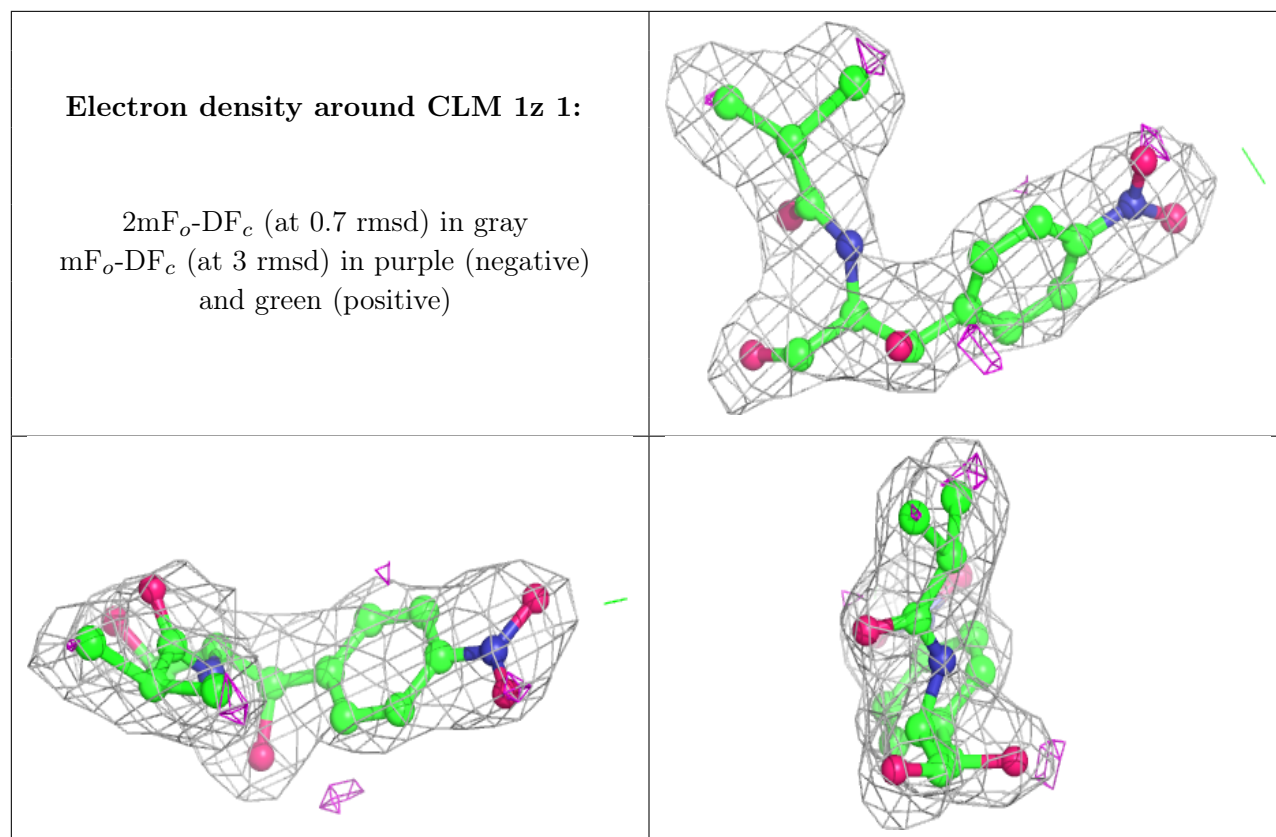


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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57  | MG   | 1A    | 3729 | 1/1   | 0.99 | 0.16 | 25,25,25,25                 | 0     |
| 57  | MG   | 1A    | 3049 | 1/1   | 0.99 | 0.12 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3026 | 1/1   | 0.99 | 0.18 | 15,15,15,15                 | 0     |
| 57  | MG   | 1A    | 3863 | 1/1   | 0.99 | 0.16 | 27,27,27,27                 | 0     |
| 57  | MG   | 1A    | 3510 | 1/1   | 0.99 | 0.13 | 9,9,9,9                     | 0     |
| 57  | MG   | 1A    | 3817 | 1/1   | 0.99 | 0.12 | 47,47,47,47                 | 0     |
| 57  | MG   | 1A    | 3916 | 1/1   | 0.99 | 0.18 | 14,14,14,14                 | 0     |
| 57  | MG   | 1A    | 3238 | 1/1   | 0.99 | 0.14 | 30,30,30,30                 | 0     |
| 57  | MG   | 2A    | 3614 | 1/1   | 0.99 | 0.17 | 18,18,18,18                 | 0     |
| 57  | MG   | 1A    | 3350 | 1/1   | 1.00 | 0.15 | 13,13,13,13                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.