



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2020 – 11:12 PM EST

PDB ID : 6XHX
Title : Crystal structure of the A2058-unmethylated *Thermus thermophilus* 70S ribosome in complex with erythromycin and protein Y (YfiA) at 2.55Å resolution
Authors : Svetlov, M.S.; Syroegin, E.A.; Aleksandrova, E.V.; Atkinson, G.C.; Gregory, S.T.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2020-06-19
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.15.1 |
| 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) | : | 2.15.1 |

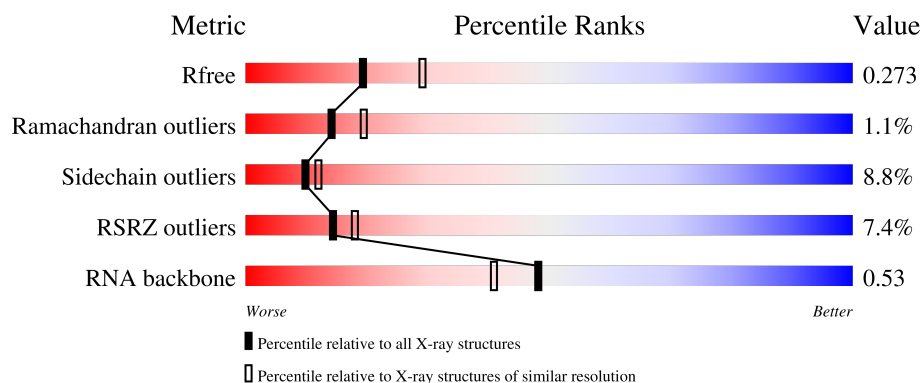
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1284 (2.56-2.52) |
| Ramachandran outliers | 138981 | 1315 (2.56-2.52) |
| Sidechain outliers | 138945 | 1315 (2.56-2.52) |
| RSRZ outliers | 127900 | 1272 (2.56-2.52) |
| RNA backbone | 3102 | 1026 (2.88-2.20) |

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 ≥ 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>81%</div> <div>16%</div> <div>..</div> </div> |
| 1 | 2A | 2915 | <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>3%</div> <div>93%</div> <div>6%</div> </div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 3 | 2D | 276 | <div> <div>16%</div> <div>93%</div> <div>7%</div> </div> |
| 4 | 1E | 206 | <div> <div>%</div> <div>92%</div> <div>7%</div> </div> |
| 4 | 2E | 206 | <div> <div>4%</div> <div>94%</div> <div>5%</div> </div> |
| 5 | 1F | 210 | <div> <div></div> <div>89%</div> <div>8%</div> </div> |
| 5 | 2F | 210 | <div> <div>5%</div> <div>90%</div> <div>7%</div> </div> |
| 6 | 1G | 182 | <div> <div>3%</div> <div>92%</div> <div>7%</div> </div> |
| 6 | 2G | 182 | <div> <div>32%</div> <div>85%</div> <div>15%</div> </div> |
| 7 | 1H | 180 | <div> <div>%</div> <div>92%</div> <div>5%</div> </div> |
| 7 | 2H | 180 | <div> <div>32%</div> <div>82%</div> <div>14%</div> </div> |
| 8 | 1I | 148 | <div> <div>4%</div> <div>85%</div> <div>14%</div> </div> |
| 8 | 2I | 148 | <div> <div>16%</div> <div>91%</div> <div>8%</div> </div> |
| 9 | 1N | 140 | <div> <div></div> <div>94%</div> <div>6%</div> </div> |
| 9 | 2N | 140 | <div> <div>6%</div> <div>93%</div> <div>7%</div> </div> |
| 10 | 1O | 122 | <div> <div></div> <div>95%</div> <div>5%</div> </div> |
| 10 | 2O | 122 | <div> <div>4%</div> <div>93%</div> <div>7%</div> </div> |
| 11 | 1P | 150 | <div> <div>%</div> <div>95%</div> <div></div> </div> |
| 11 | 2P | 150 | <div> <div>10%</div> <div>95%</div> <div>5%</div> </div> |
| 12 | 1Q | 141 | <div> <div>%</div> <div>94%</div> <div>6%</div> </div> |
| 12 | 2Q | 141 | <div> <div>9%</div> <div>96%</div> <div></div> </div> |
| 13 | 1R | 118 | <div> <div>%</div> <div>92%</div> <div>8%</div> </div> |
| 13 | 2R | 118 | <div> <div>8%</div> <div>92%</div> <div>8%</div> </div> |
| 14 | 1S | 112 | <div> <div></div> <div>89%</div> <div>8%</div> </div> |
| 14 | 2S | 112 | <div> <div>14%</div> <div>89%</div> <div>9%</div> </div> |
| 15 | 1T | 146 | <div> <div>%</div> <div>85%</div> <div>5%</div> </div> |
| 15 | 2T | 146 | <div> <div>5%</div> <div>84%</div> <div>5%</div> </div> |

Continued on next page...

Continued from previous page...

| 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 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28 | 26 | 54 | |
| 29 | 17 | 49 | |
| 29 | 27 | 49 | |
| 30 | 18 | 65 | |
| 30 | 28 | 65 | |
| 31 | 19 | 37 | |
| 31 | 29 | 37 | |
| 32 | 1a | 1521 | |
| 32 | 2a | 1521 | |
| 33 | 1b | 256 | |
| 33 | 2b | 256 | |
| 34 | 1c | 239 | |
| 34 | 2c | 239 | |
| 35 | 1d | 209 | |
| 35 | 2d | 209 | |
| 36 | 1e | 162 | |
| 36 | 2e | 162 | |
| 37 | 1f | 101 | |
| 37 | 2f | 101 | |
| 38 | 1g | 156 | |
| 38 | 2g | 156 | |
| 39 | 1h | 138 | |
| 39 | 2h | 138 | |
| 40 | 1i | 128 | |
| 40 | 2i | 128 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41 | 1j | 105 | |
| 41 | 2j | 105 | |
| 42 | 1k | 129 | |
| 42 | 2k | 129 | |
| 43 | 1l | 132 | |
| 43 | 2l | 132 | |
| 44 | 1m | 126 | |
| 44 | 2m | 126 | |
| 45 | 1n | 61 | |
| 45 | 2n | 61 | |
| 46 | 1o | 89 | |
| 46 | 2o | 89 | |
| 47 | 1p | 88 | |
| 47 | 2p | 88 | |
| 48 | 1q | 105 | |
| 48 | 2q | 105 | |
| 49 | 1r | 88 | |
| 49 | 2r | 88 | |
| 50 | 1s | 93 | |
| 50 | 2s | 93 | |
| 51 | 1t | 106 | |
| 51 | 2t | 106 | |
| 52 | 1u | 27 | |
| 52 | 2u | 27 | |
| 53 | 1y | 113 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | 2y | 113 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | 1A | 3989 | - | - | - | X |
| 54 | MG | 2A | 3024 | - | - | - | X |

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 296819 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 | | | |

Continued on next page...

Continued from previous page...

| 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 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 608 | 375 | 129 | 103 | 1 | | | |
| 22 | 20 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 608 | 375 | 129 | 103 | 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 | | | |

Continued on next page...

Continued from previous page...

| 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 | | | |

Continued on next page...

Continued from previous page...

| 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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54 | 2E | 7 | Total | Mg | 0 | 0 |
| | | | 7 | 7 | | |
| 54 | 17 | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 54 | 1T | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 54 | 1N | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 54 | 20 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 54 | 18 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 54 | 1o | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | 2W | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 54 | 1Y | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 54 | 2I | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | 13 | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 54 | 1f | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 54 | 1P | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 54 | 2B | 18 | Total | Mg | 0 | 0 |
| | | | 18 | 18 | | |
| 54 | 2a | 183 | Total | Mg | 0 | 0 |
| | | | 183 | 183 | | |
| 54 | 1E | 10 | Total | Mg | 0 | 0 |
| | | | 10 | 10 | | |
| 54 | 1b | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | 2l | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|------------|---------|---------|
| 54 | 2F | 4 | Total 4 | Mg 4 | 0 | 0 |
| 54 | 28 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 2e | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 1W | 4 | Total 4 | Mg 4 | 0 | 0 |
| 54 | 1A | 1020 | Total 1020 | Mg 1020 | 0 | 0 |
| 54 | 1t | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 1n | 3 | Total 3 | Mg 3 | 0 | 0 |
| 54 | 2P | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 1y | 3 | Total 3 | Mg 3 | 0 | 0 |
| 54 | 25 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 2T | 3 | Total 3 | Mg 3 | 0 | 0 |
| 54 | 1D | 16 | Total 16 | Mg 16 | 0 | 0 |
| 54 | 2N | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1e | 3 | Total 3 | Mg 3 | 0 | 0 |
| 54 | 2G | 3 | Total 3 | Mg 3 | 0 | 0 |
| 54 | 2f | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1V | 7 | Total 7 | Mg 7 | 0 | 0 |
| 54 | 2X | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1a | 274 | Total 274 | Mg 274 | 0 | 0 |
| 54 | 2Q | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 15 | 6 | Total 6 | Mg 6 | 0 | 0 |

Continued on next page...

Continued from previous page...

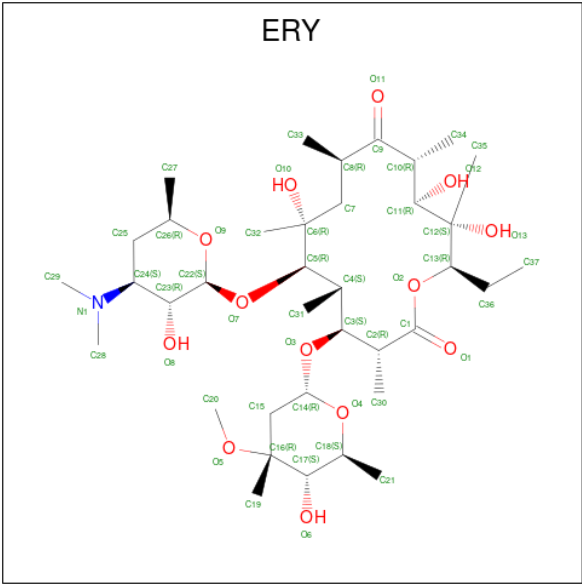
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|----------|---------|---------|
| 54 | 2j | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1R | 5 | Total 5 | Mg 5 | 0 | 0 |
| 54 | 2t | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1m | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1G | 4 | Total 4 | Mg 4 | 0 | 0 |
| 54 | 2O | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 1l | 4 | Total 4 | Mg 4 | 0 | 0 |
| 54 | 1d | 5 | Total 5 | Mg 5 | 0 | 0 |
| 54 | 2n | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1H | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 2l | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1i | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 23 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 2R | 2 | Total 2 | Mg 2 | 0 | 0 |
| 54 | 1Z | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 2D | 10 | Total 10 | Mg 10 | 0 | 0 |
| 54 | 1U | 8 | Total 8 | Mg 8 | 0 | 0 |
| 54 | 1O | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 27 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 19 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 54 | 1l | 2 | Total 2 | Mg 2 | 0 | 0 |

Continued on next page...

Continued from previous page...

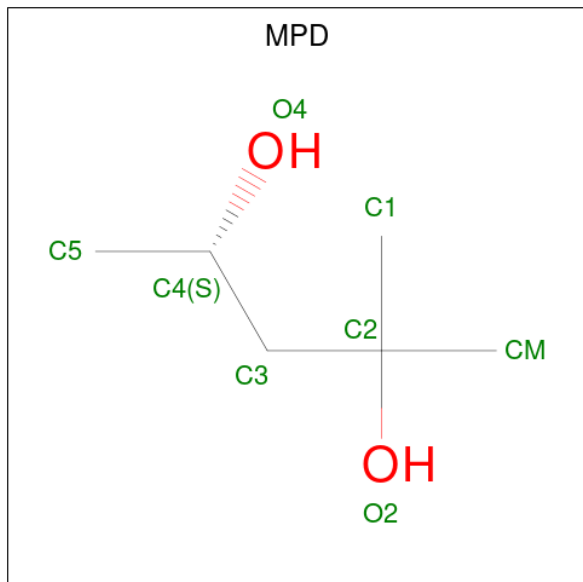
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54 | 2V | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 54 | 1F | 18 | Total | Mg | 0 | 0 |
| | | | 18 | 18 | | |
| 54 | 10 | 7 | Total | Mg | 0 | 0 |
| | | | 7 | 7 | | |
| 54 | 1g | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 54 | 2o | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | 1Q | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 54 | 2A | 733 | Total | Mg | 0 | 0 |
| | | | 733 | 733 | | |
| 54 | 1h | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 54 | 1B | 32 | Total | Mg | 0 | 0 |
| | | | 32 | 32 | | |

- Molecule 55 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C₃₇H₆₇NO₁₃).



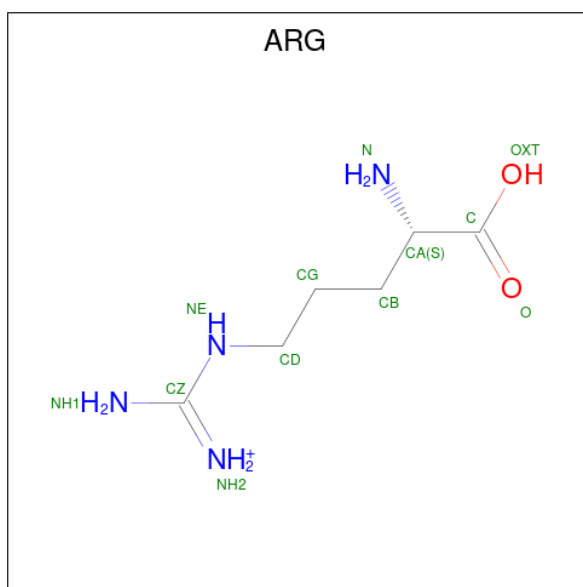
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 55 | 1A | 1 | Total | C | N | O | 0 | 0 |
| | | | 51 | 37 | 1 | 13 | | |
| 55 | 2A | 1 | Total | C | N | O | 0 | 0 |
| | | | 51 | 37 | 1 | 13 | | |

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 56 | 1A | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 56 | 1T | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 56 | 18 | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 56 | 1a | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 56 | 2A | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 56 | 2A | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 56 | 2B | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 57 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 57 | 1B | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 6 | 4 | 2 | | |
| 57 | 1F | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 6 | 4 | 2 | | |

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

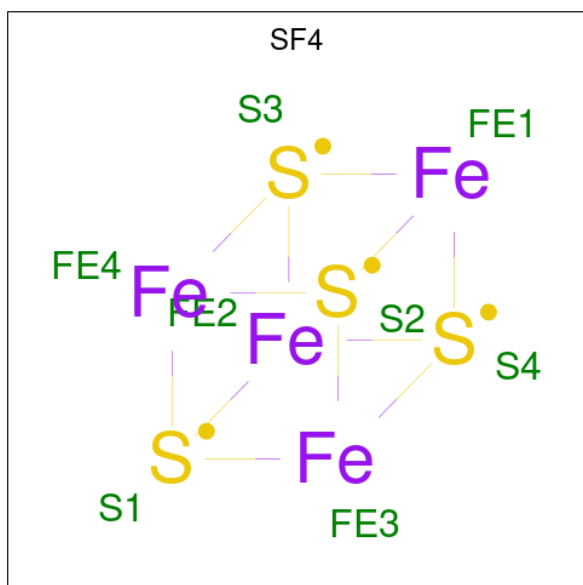
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58 | 1Y | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 14 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 1n | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 15 | 1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

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 58 | 2Y | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 58 | 16 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| 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 water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 60 | 1A | 3765 | Total | O | 0 | 0 |
| | | | 3765 | 3765 | | |
| 60 | 1B | 106 | Total | O | 0 | 0 |
| | | | 106 | 106 | | |
| 60 | 1D | 90 | Total | O | 0 | 0 |
| | | | 90 | 90 | | |
| 60 | 1E | 74 | Total | O | 0 | 0 |
| | | | 74 | 74 | | |
| 60 | 1F | 67 | Total | O | 0 | 0 |
| | | | 67 | 67 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 60 | 1G | 18 | Total 18 | O 18 | 0 | 0 |
| 60 | 1H | 14 | Total 14 | O 14 | 0 | 0 |
| 60 | 1I | 8 | Total 8 | O 8 | 0 | 0 |
| 60 | 1N | 51 | Total 51 | O 51 | 0 | 0 |
| 60 | 1O | 26 | Total 26 | O 26 | 0 | 0 |
| 60 | 1P | 57 | Total 57 | O 57 | 0 | 0 |
| 60 | 1Q | 41 | Total 41 | O 41 | 0 | 0 |
| 60 | 1R | 32 | Total 32 | O 32 | 0 | 0 |
| 60 | 1S | 14 | Total 14 | O 14 | 0 | 0 |
| 60 | 1T | 33 | Total 33 | O 33 | 0 | 0 |
| 60 | 1U | 42 | Total 42 | O 42 | 0 | 0 |
| 60 | 1V | 39 | Total 39 | O 39 | 0 | 0 |
| 60 | 1W | 27 | Total 27 | O 27 | 0 | 0 |
| 60 | 1X | 24 | Total 24 | O 24 | 0 | 0 |
| 60 | 1Y | 18 | Total 18 | O 18 | 0 | 0 |
| 60 | 1Z | 13 | Total 13 | O 13 | 0 | 0 |
| 60 | 10 | 20 | Total 20 | O 20 | 0 | 0 |
| 60 | 11 | 25 | Total 25 | O 25 | 0 | 0 |
| 60 | 12 | 12 | Total 12 | O 12 | 0 | 0 |
| 60 | 13 | 26 | Total 26 | O 26 | 0 | 0 |
| 60 | 14 | 2 | Total 2 | O 2 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 60 | 15 | 28 | Total 28 | O 28 | 0 | 0 |
| 60 | 16 | 19 | Total 19 | O 19 | 0 | 0 |
| 60 | 17 | 14 | Total 14 | O 14 | 0 | 0 |
| 60 | 18 | 28 | Total 28 | O 28 | 0 | 0 |
| 60 | 19 | 5 | Total 5 | O 5 | 0 | 0 |
| 60 | 1a | 465 | Total 465 | O 465 | 0 | 0 |
| 60 | 1d | 9 | Total 9 | O 9 | 0 | 0 |
| 60 | 1e | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 1f | 2 | Total 2 | O 2 | 0 | 0 |
| 60 | 1h | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 1i | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 1j | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 1k | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 1l | 5 | Total 5 | O 5 | 0 | 0 |
| 60 | 1m | 3 | Total 3 | O 3 | 0 | 0 |
| 60 | 1o | 3 | Total 3 | O 3 | 0 | 0 |
| 60 | 1p | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 1u | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 1y | 3 | Total 3 | O 3 | 0 | 0 |
| 60 | 2A | 1860 | Total 1860 | O 1860 | 0 | 0 |
| 60 | 2B | 53 | Total 53 | O 53 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 60 | 2D | 40 | Total 40 | O 40 | 0 | 0 |
| 60 | 2E | 19 | Total 19 | O 19 | 0 | 0 |
| 60 | 2F | 22 | Total 22 | O 22 | 0 | 0 |
| 60 | 2G | 7 | Total 7 | O 7 | 0 | 0 |
| 60 | 2H | 4 | Total 4 | O 4 | 0 | 0 |
| 60 | 2I | 4 | Total 4 | O 4 | 0 | 0 |
| 60 | 2N | 3 | Total 3 | O 3 | 0 | 0 |
| 60 | 2O | 19 | Total 19 | O 19 | 0 | 0 |
| 60 | 2P | 19 | Total 19 | O 19 | 0 | 0 |
| 60 | 2Q | 18 | Total 18 | O 18 | 0 | 0 |
| 60 | 2R | 17 | Total 17 | O 17 | 0 | 0 |
| 60 | 2S | 3 | Total 3 | O 3 | 0 | 0 |
| 60 | 2T | 8 | Total 8 | O 8 | 0 | 0 |
| 60 | 2U | 16 | Total 16 | O 16 | 0 | 0 |
| 60 | 2V | 3 | Total 3 | O 3 | 0 | 0 |
| 60 | 2W | 13 | Total 13 | O 13 | 0 | 0 |
| 60 | 2X | 6 | Total 6 | O 6 | 0 | 0 |
| 60 | 2Y | 5 | Total 5 | O 5 | 0 | 0 |
| 60 | 2Z | 7 | Total 7 | O 7 | 0 | 0 |
| 60 | 20 | 10 | Total 10 | O 10 | 0 | 0 |
| 60 | 21 | 20 | Total 20 | O 20 | 0 | 0 |

Continued on next page...

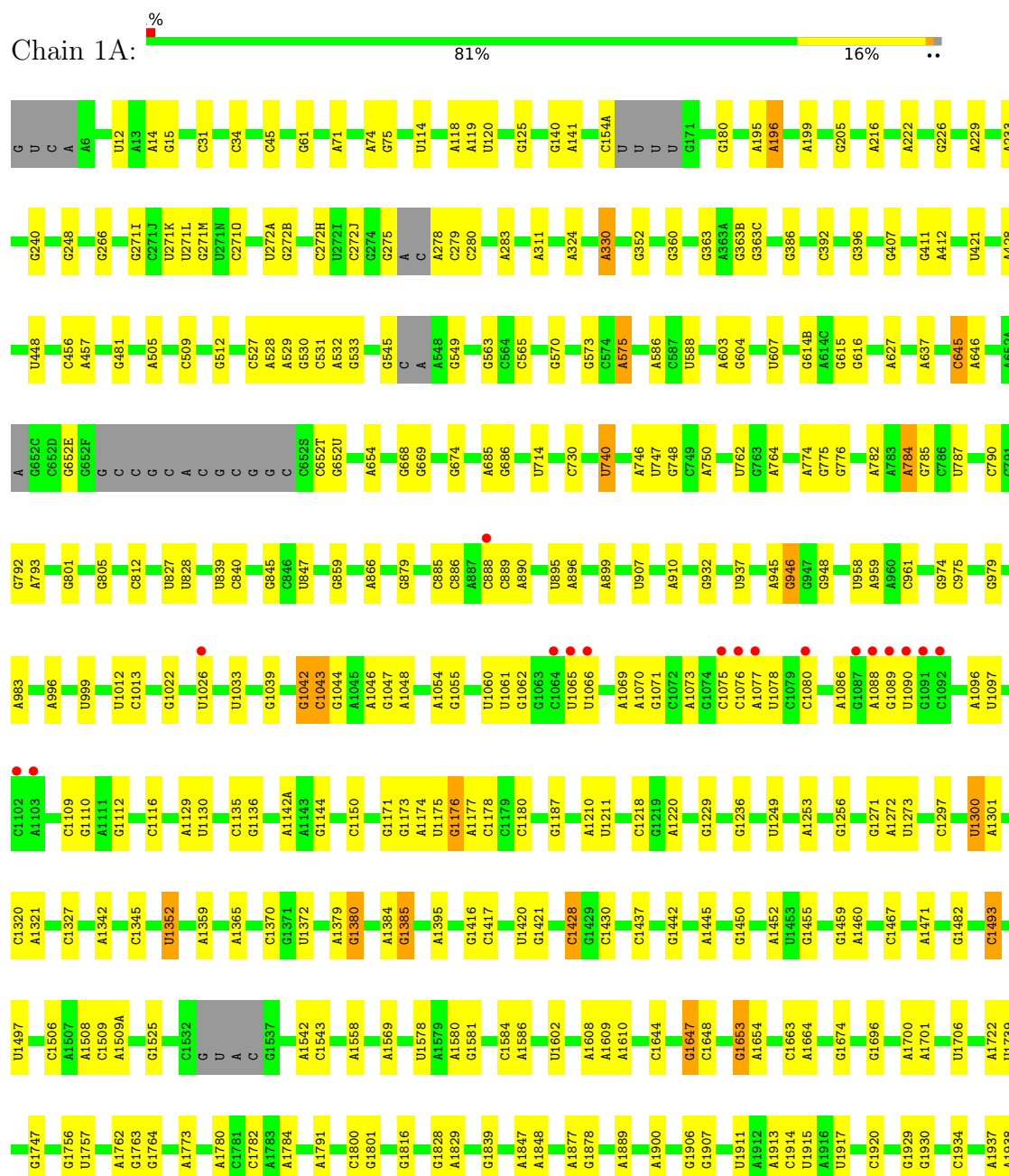
Continued from previous page...

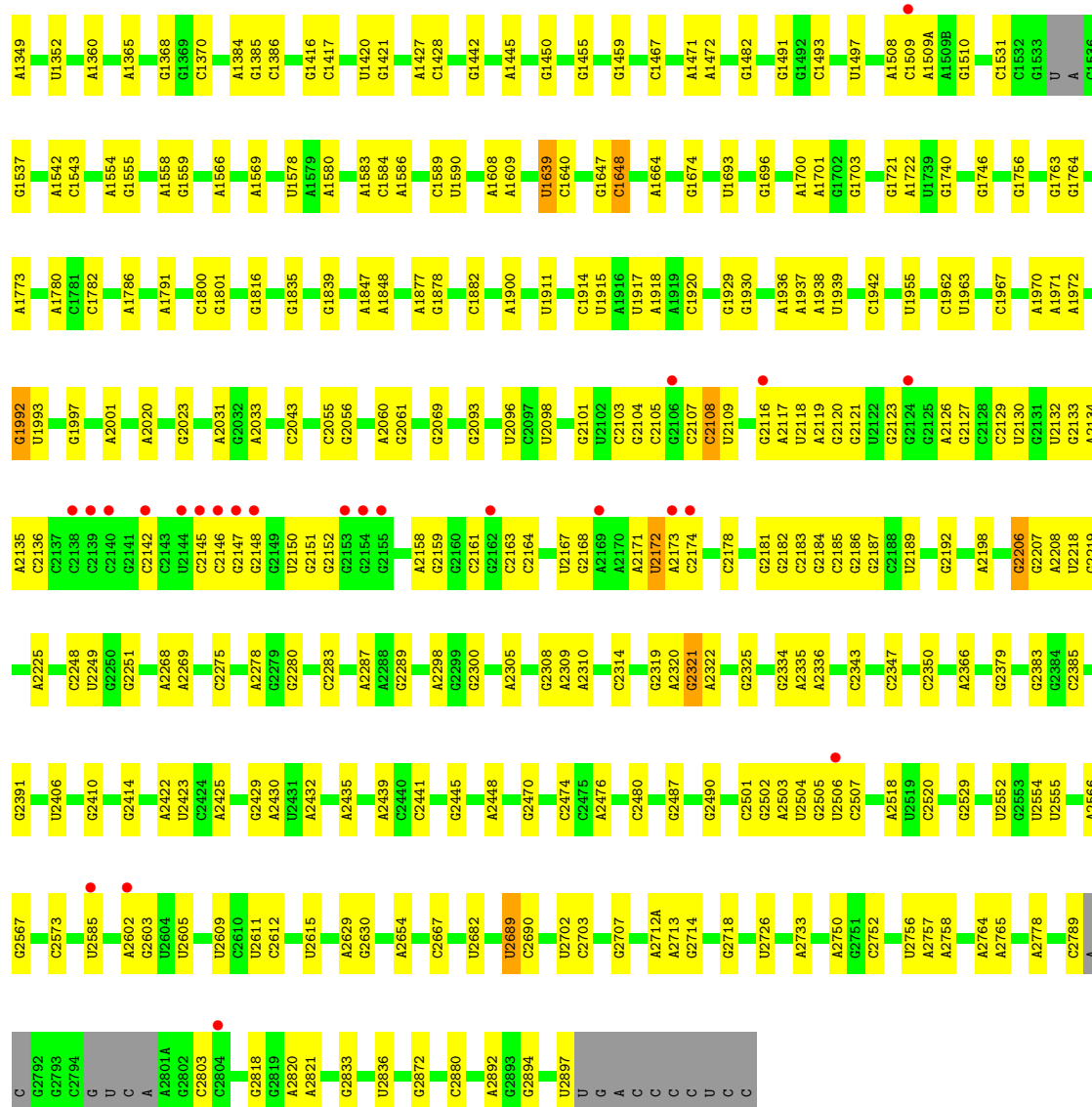
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 60 | 22 | 2 | Total 2 | O 2 | 0 | 0 |
| 60 | 23 | 3 | Total 3 | O 3 | 0 | 0 |
| 60 | 25 | 6 | Total 6 | O 6 | 0 | 0 |
| 60 | 26 | 5 | Total 5 | O 5 | 0 | 0 |
| 60 | 27 | 9 | Total 9 | O 9 | 0 | 0 |
| 60 | 28 | 9 | Total 9 | O 9 | 0 | 0 |
| 60 | 29 | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 2a | 303 | Total 303 | O 303 | 0 | 0 |
| 60 | 2d | 2 | Total 2 | O 2 | 0 | 0 |
| 60 | 2e | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 2f | 2 | Total 2 | O 2 | 0 | 0 |
| 60 | 2j | 2 | Total 2 | O 2 | 0 | 0 |
| 60 | 2l | 2 | Total 2 | O 2 | 0 | 0 |
| 60 | 2m | 3 | Total 3 | O 3 | 0 | 0 |
| 60 | 2n | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 2o | 2 | Total 2 | O 2 | 0 | 0 |
| 60 | 2p | 2 | Total 2 | O 2 | 0 | 0 |
| 60 | 2q | 1 | Total 1 | O 1 | 0 | 0 |
| 60 | 2r | 4 | Total 4 | O 4 | 0 | 0 |
| 60 | 2y | 3 | Total 3 | O 3 | 0 | 0 |

3 Residue-property plots

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

• Molecule 1: 23S Ribosomal RNA





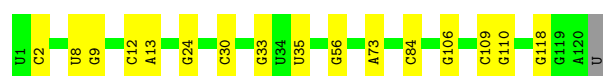
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 91% 8% .



• Molecule 2: 5S Ribosomal RNA

Chain 2B: 86% 13% .

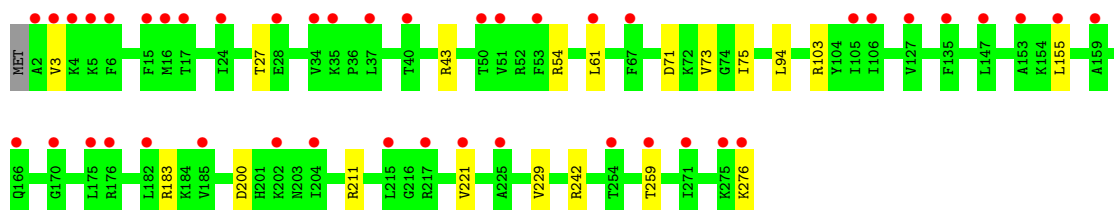


• Molecule 3: 50S ribosomal protein L2

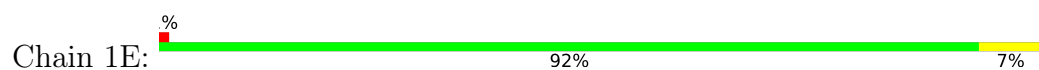
Chain 1D: 3% 93% 6% .



- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



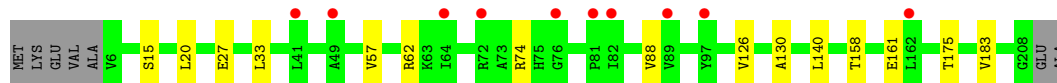
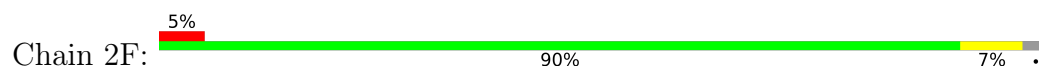
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

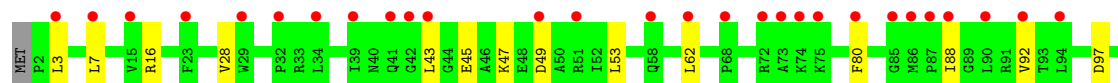
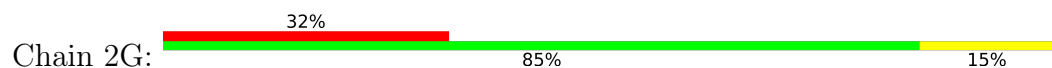


- Molecule 6: 50S ribosomal protein L5

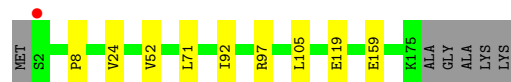
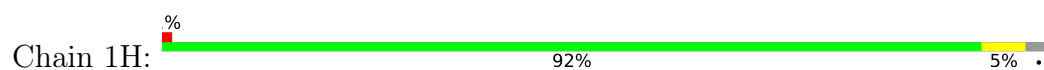




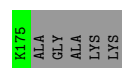
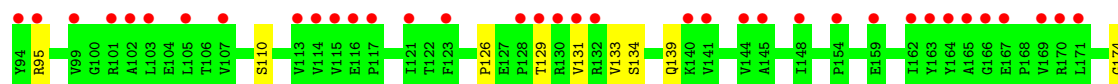
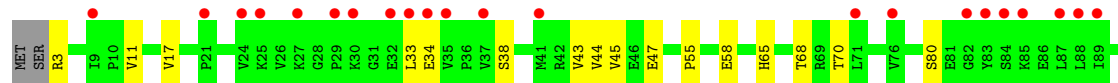
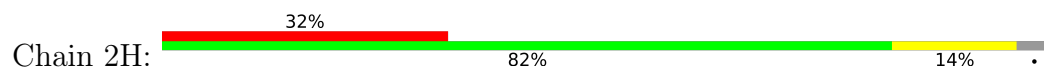
- Molecule 6: 50S ribosomal protein L5



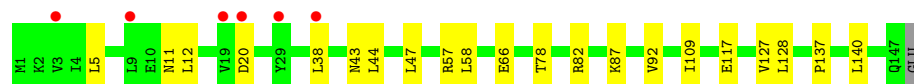
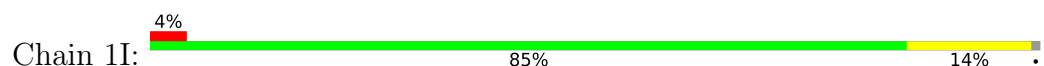
- Molecule 7: 50S ribosomal protein L6



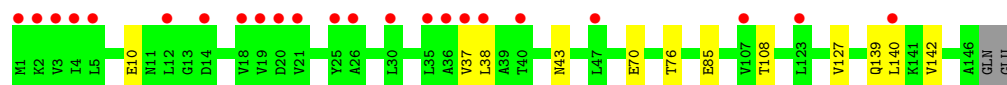
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



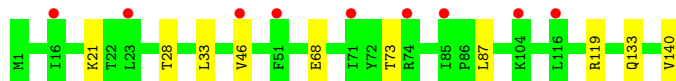
- Molecule 9: 50S ribosomal protein L13

Chain 1N:  94% 6%



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  6% 93% 7%



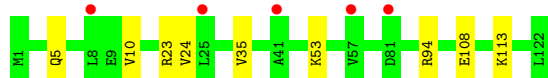
- Molecule 10: 50S ribosomal protein L14

Chain 1O:  95% 5%



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  4% 93% 7%



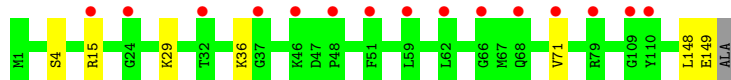
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  0% 95% 5%



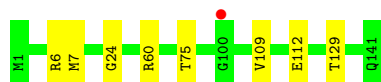
- Molecule 11: 50S ribosomal protein L15

Chain 2P:  10% 95% 5%

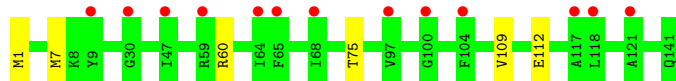


- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  0% 94% 6%



- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



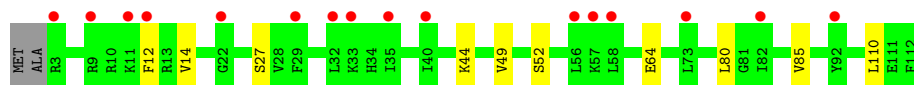
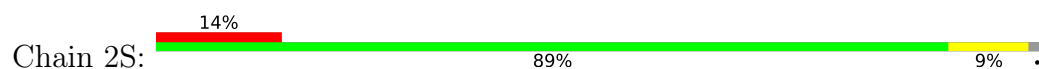
- Molecule 13: 50S ribosomal protein L17



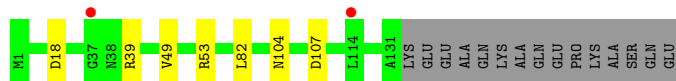
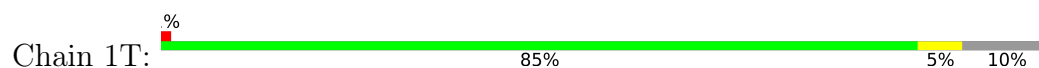
- Molecule 14: 50S ribosomal protein L18



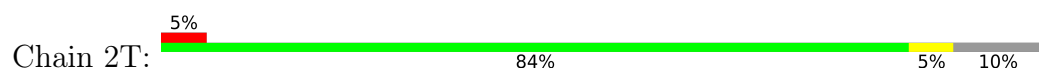
- Molecule 14: 50S ribosomal protein L18



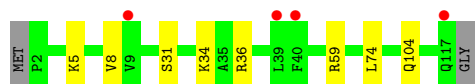
- Molecule 15: 50S ribosomal protein L19



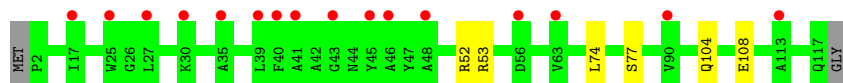
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



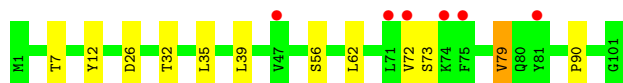
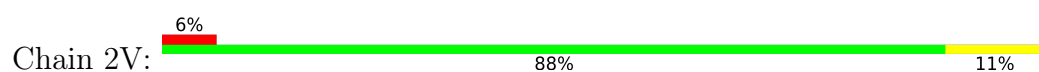
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



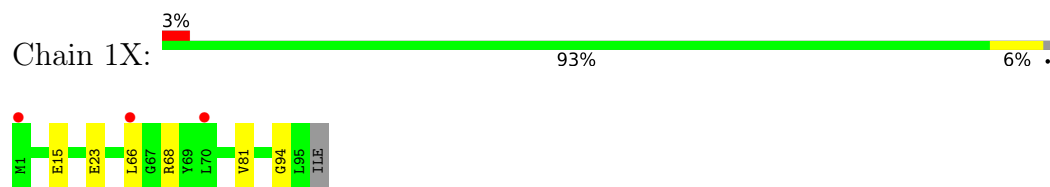
- Molecule 18: 50S ribosomal protein L22



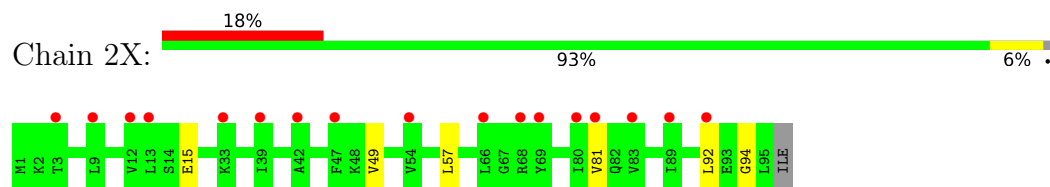
- Molecule 18: 50S ribosomal protein L22



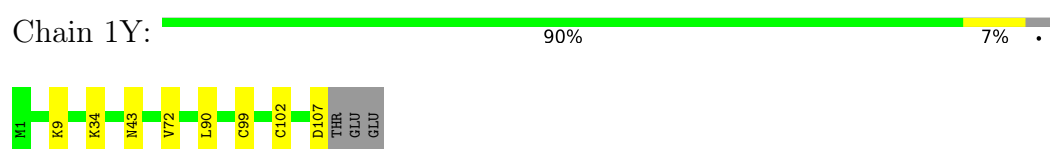
• Molecule 19: 50S ribosomal protein L23



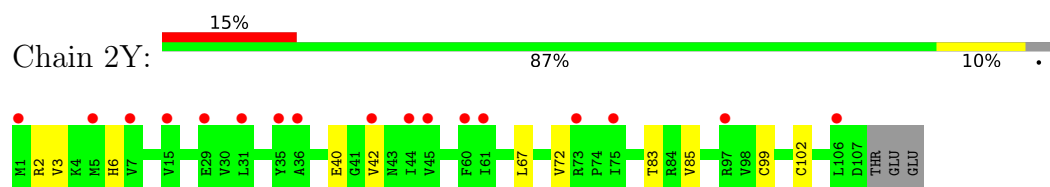
• Molecule 19: 50S ribosomal protein L23



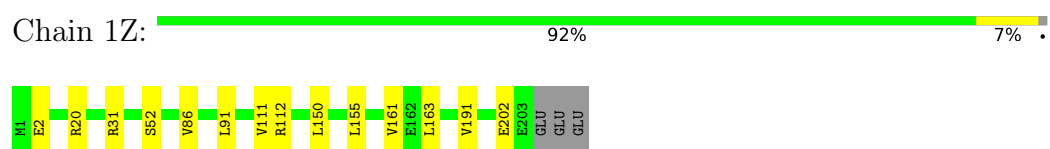
• Molecule 20: 50S ribosomal protein L24



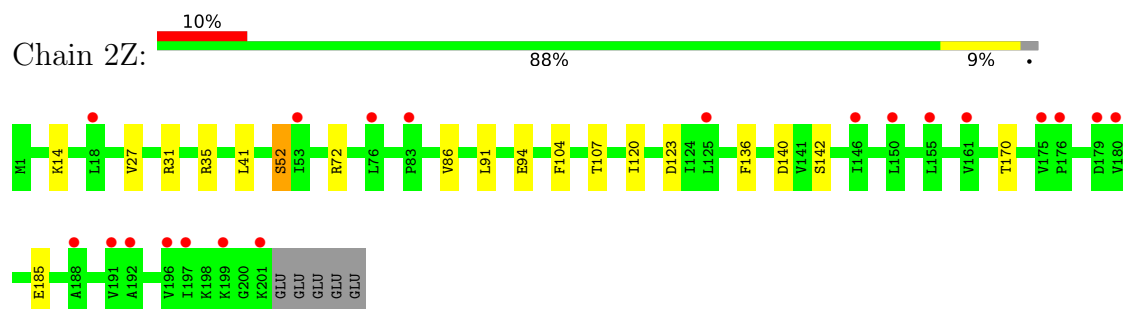
• Molecule 20: 50S ribosomal protein L24



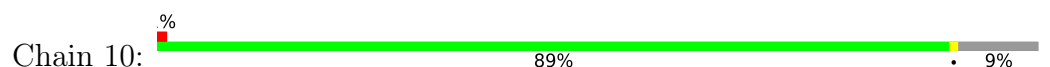
• Molecule 21: 50S ribosomal protein L25

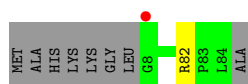


• Molecule 21: 50S ribosomal protein L25

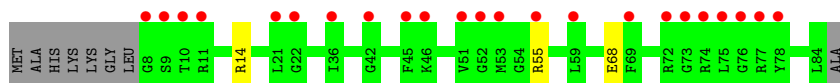
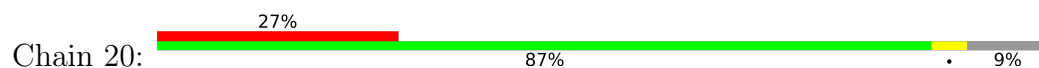


• Molecule 22: 50S ribosomal protein L27

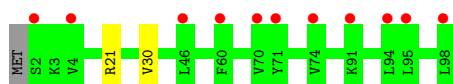




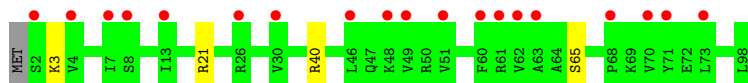
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



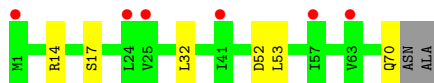
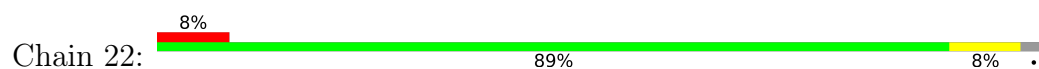
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



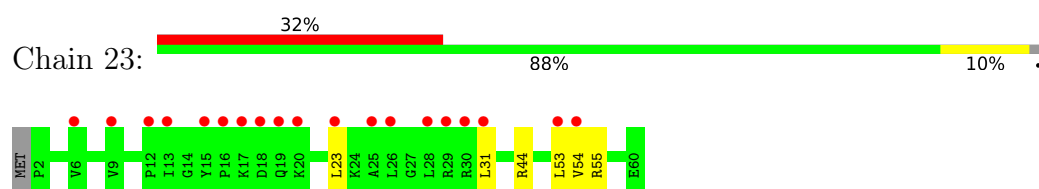
- Molecule 24: 50S ribosomal protein L29



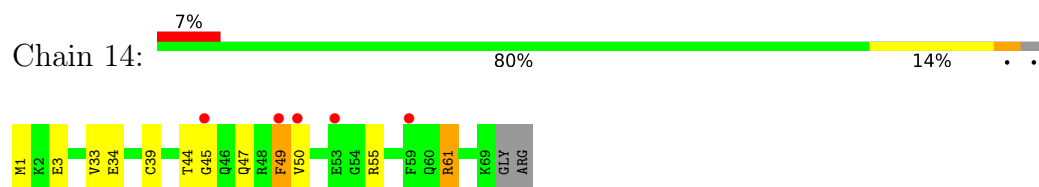
- Molecule 25: 50S ribosomal protein L30



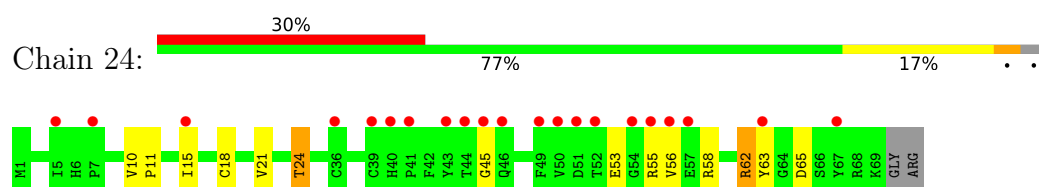
- Molecule 25: 50S ribosomal protein L30



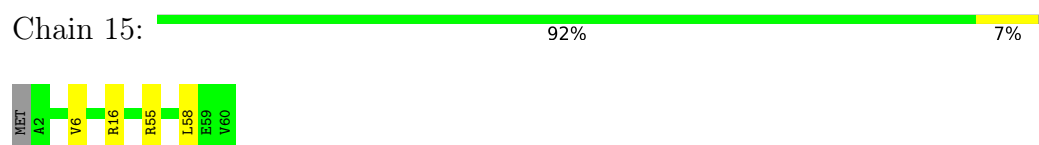
- Molecule 26: 50S ribosomal protein L31



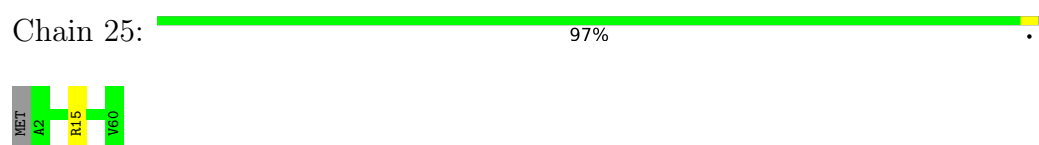
- Molecule 26: 50S ribosomal protein L31



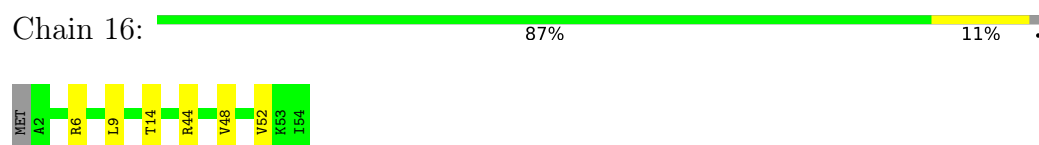
- Molecule 27: 50S ribosomal protein L32



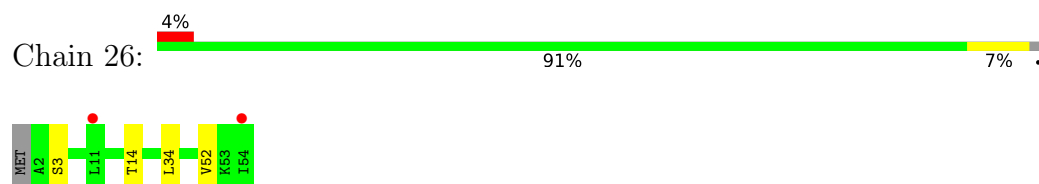
- Molecule 27: 50S ribosomal protein L32



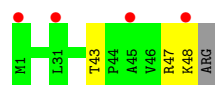
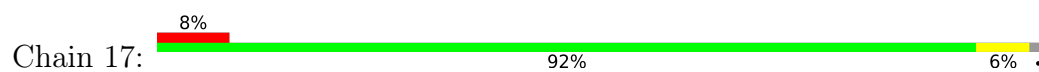
- Molecule 28: 50S ribosomal protein L33



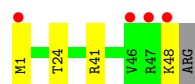
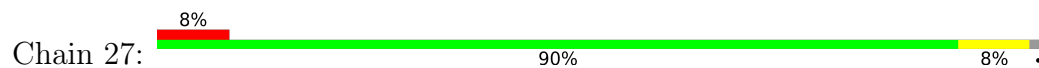
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



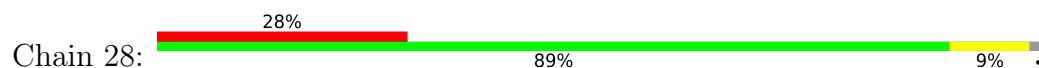
- Molecule 29: 50S ribosomal protein L34



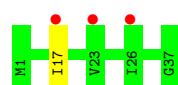
- Molecule 30: 50S ribosomal protein L35



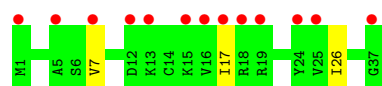
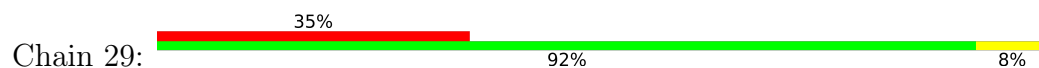
- Molecule 30: 50S ribosomal protein L35



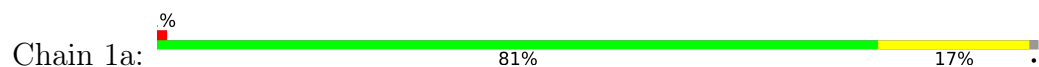
- Molecule 31: 50S ribosomal protein L36

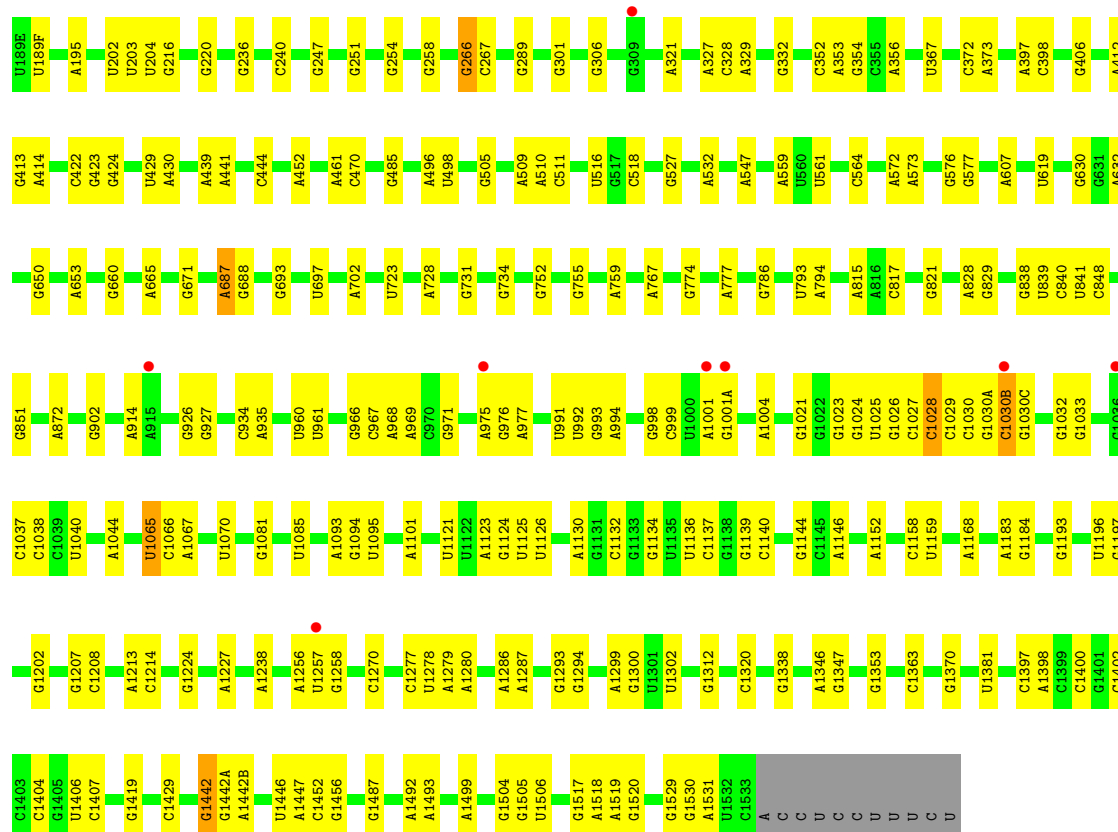


- Molecule 31: 50S ribosomal protein L36

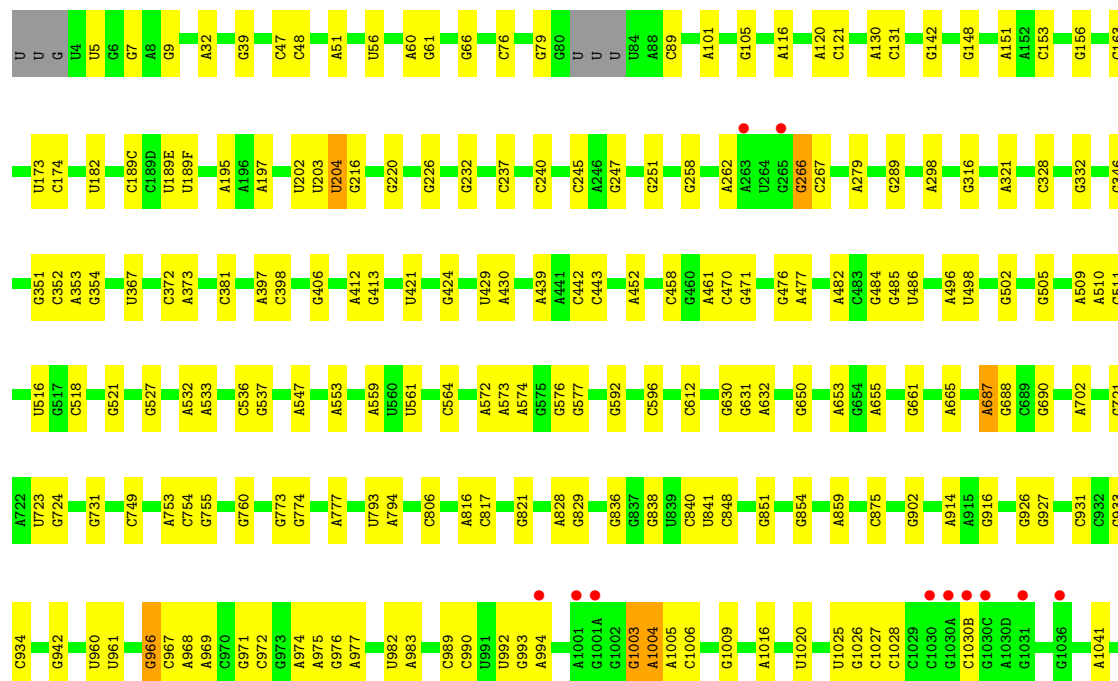
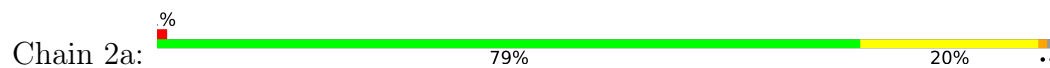


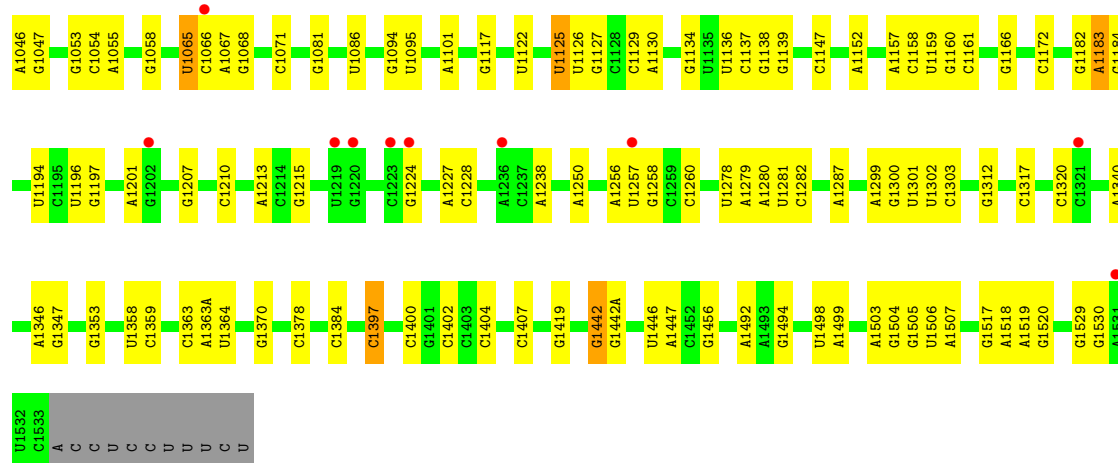
- Molecule 32: 16S Ribosomal RNA



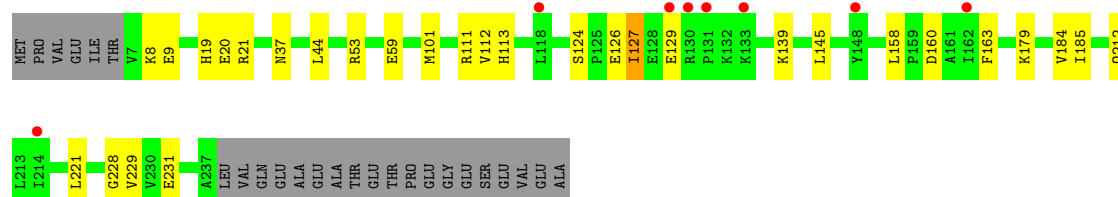
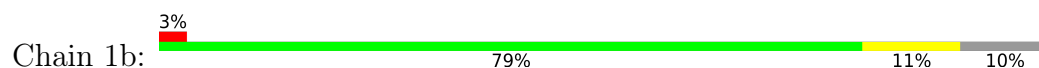


• Molecule 32: 16S Ribosomal RNA

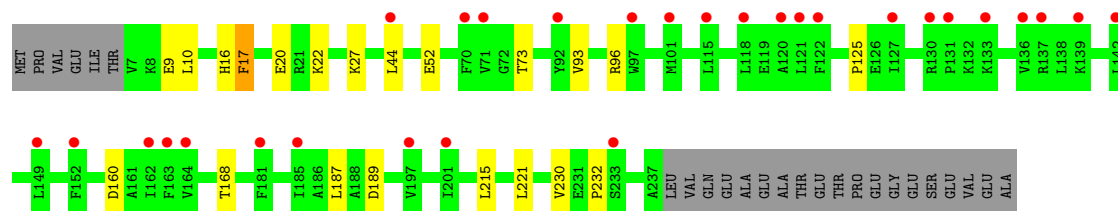
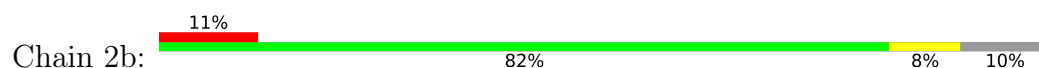




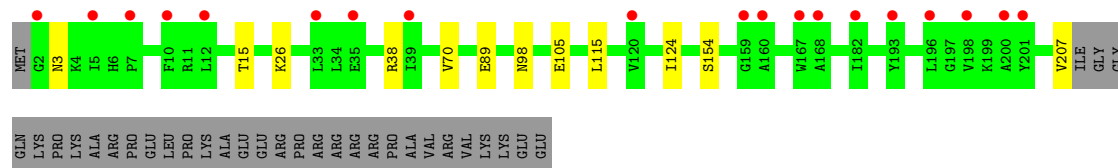
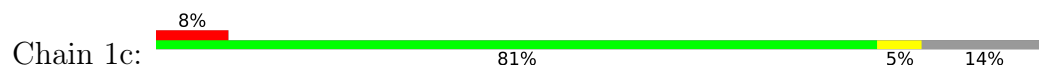
- Molecule 33: 30S ribosomal protein S2



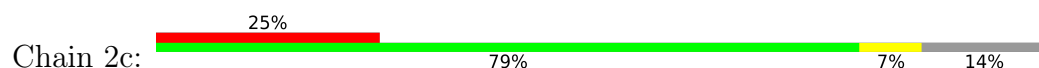
- Molecule 33: 30S ribosomal protein S2

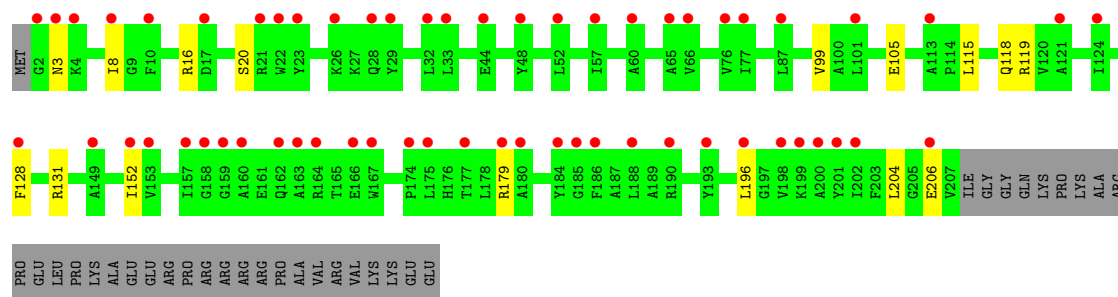


- Molecule 34: 30S ribosomal protein S3

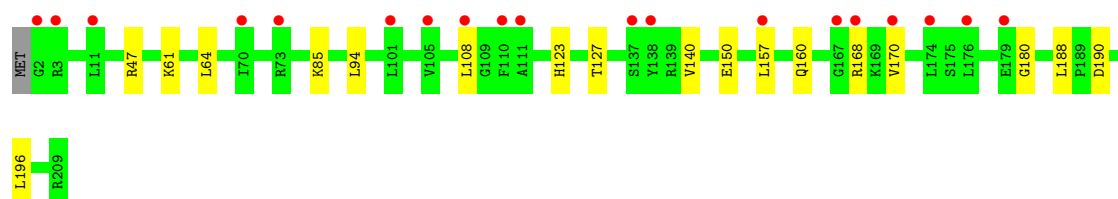
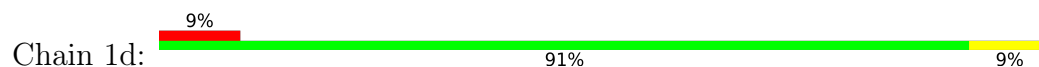


- Molecule 34: 30S ribosomal protein S3

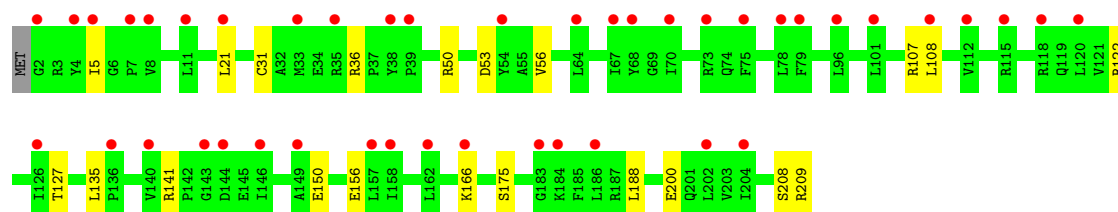
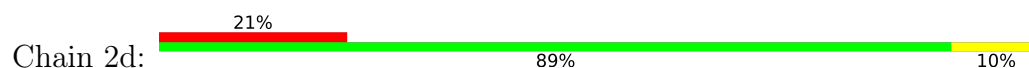




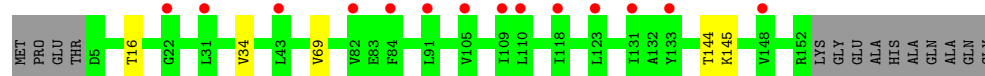
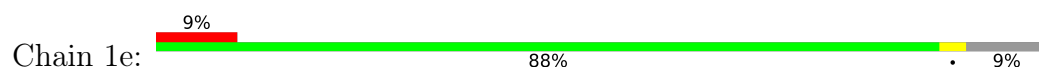
- Molecule 35: 30S ribosomal protein S4



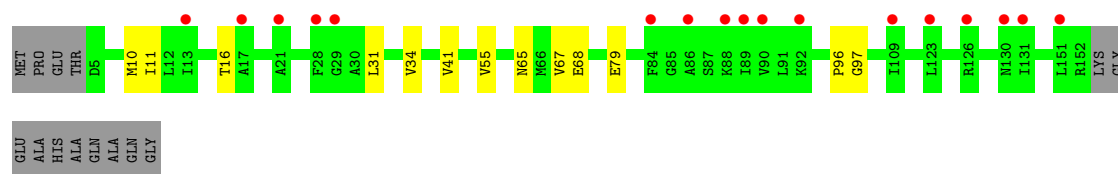
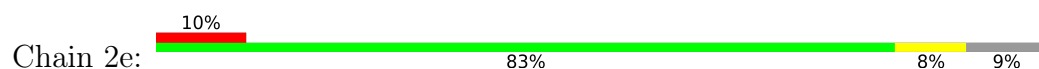
- Molecule 35: 30S ribosomal protein S4



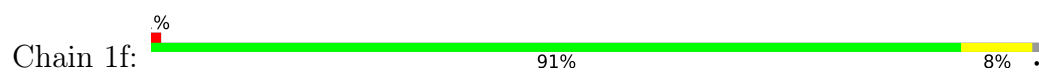
- Molecule 36: 30S ribosomal protein S5



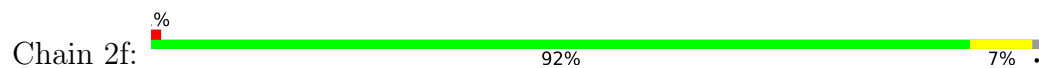
- Molecule 36: 30S ribosomal protein S5



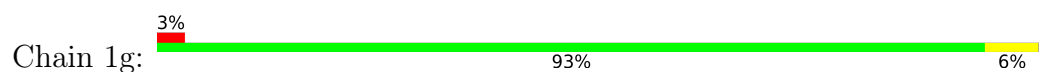
- Molecule 37: 30S ribosomal protein S6



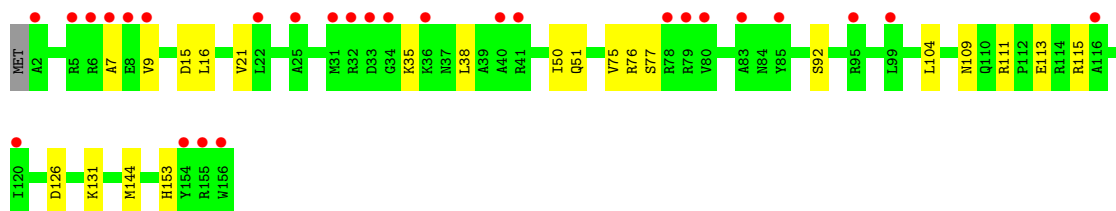
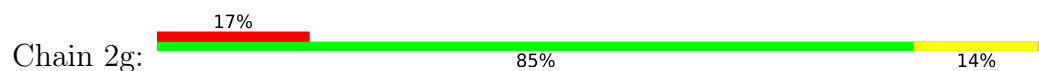
- Molecule 37: 30S ribosomal protein S6



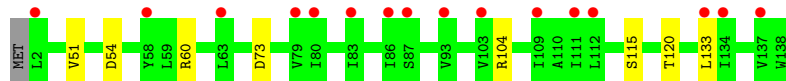
- Molecule 38: 30S ribosomal protein S7



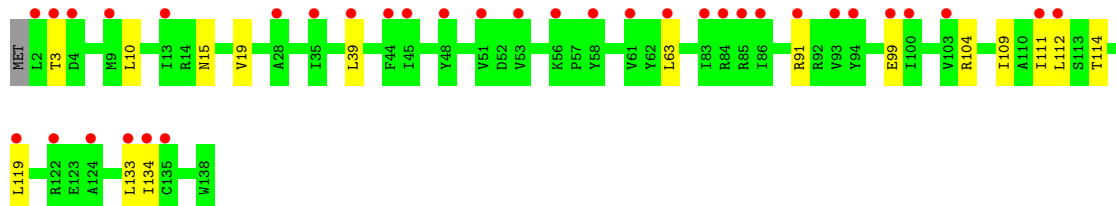
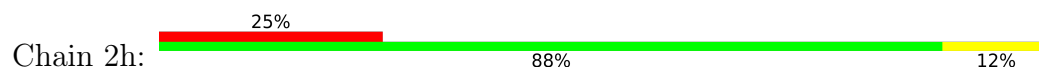
- Molecule 38: 30S ribosomal protein S7



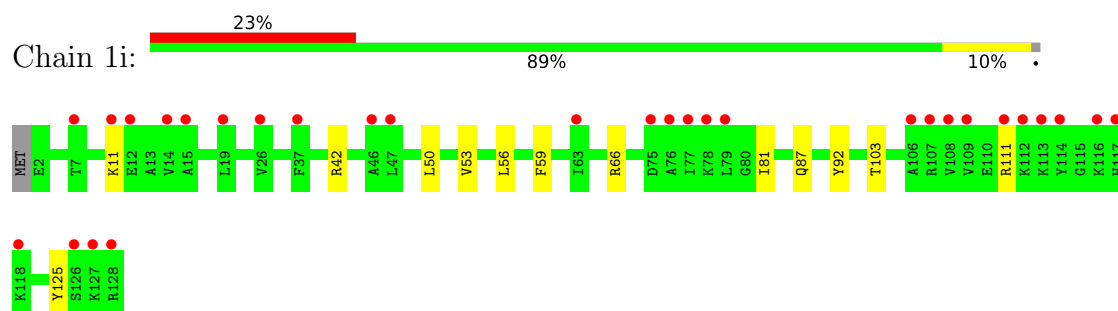
- Molecule 39: 30S ribosomal protein S8



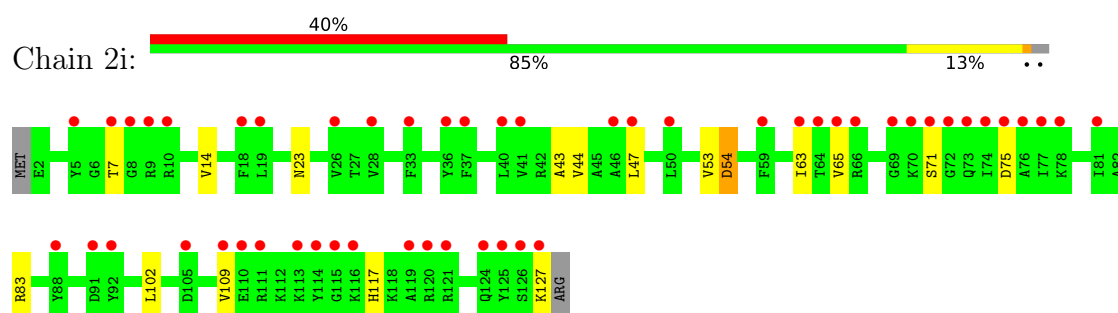
- Molecule 39: 30S ribosomal protein S8



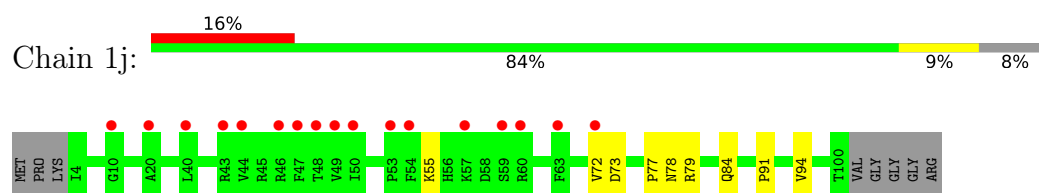
• Molecule 40: 30S ribosomal protein S9



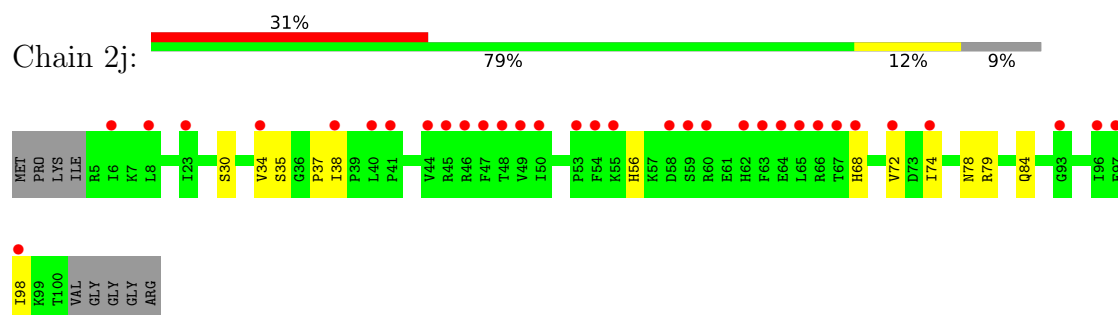
• Molecule 40: 30S ribosomal protein S9



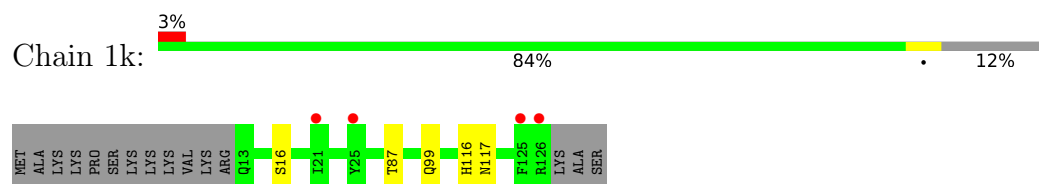
• Molecule 41: 30S ribosomal protein S10



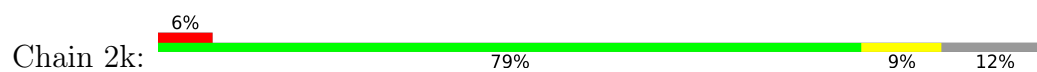
• Molecule 41: 30S ribosomal protein S10



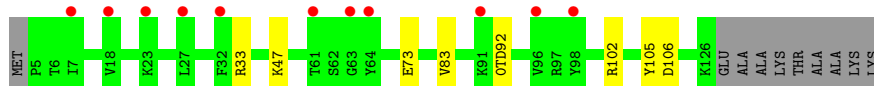
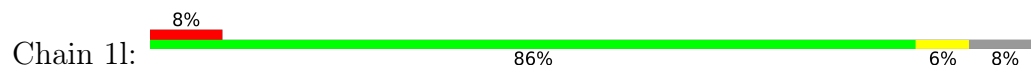
• Molecule 42: 30S ribosomal protein S11



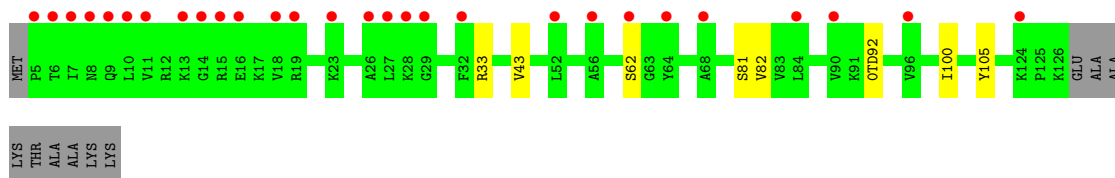
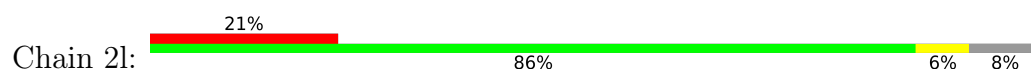
• Molecule 42: 30S ribosomal protein S11



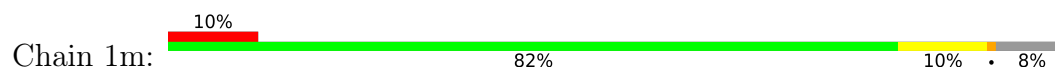
- Molecule 43: 30S ribosomal protein S12



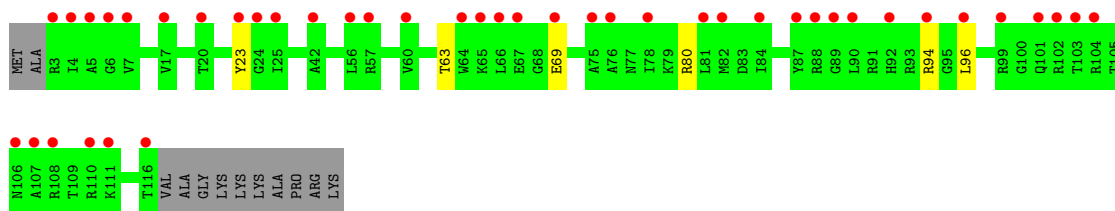
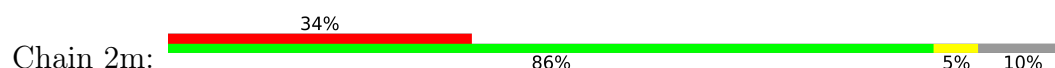
- Molecule 43: 30S ribosomal protein S12



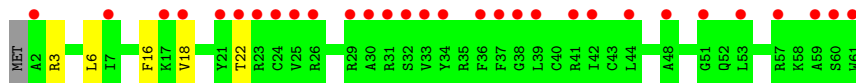
- Molecule 44: 30S ribosomal protein S13



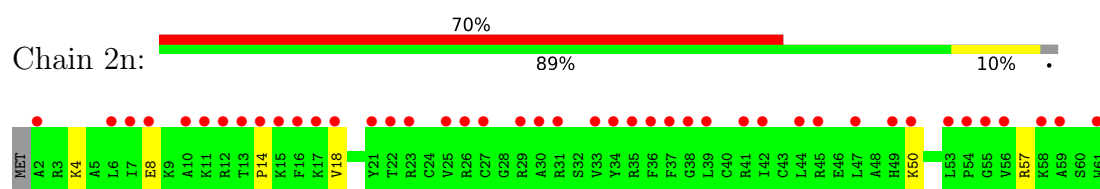
- Molecule 44: 30S ribosomal protein S13



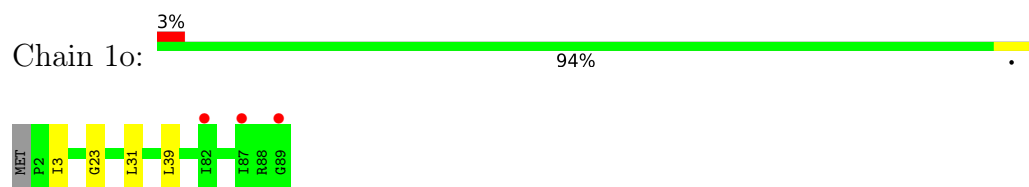
- Molecule 45: 30S ribosomal protein S14 type Z



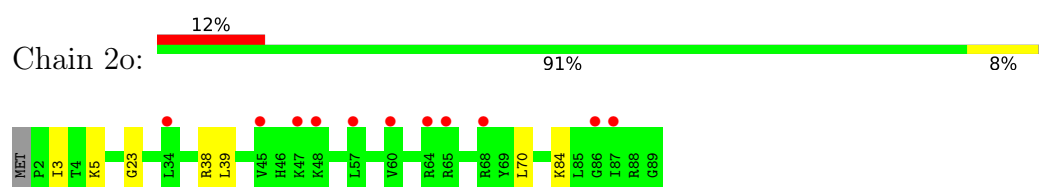
- Molecule 45: 30S ribosomal protein S14 type Z



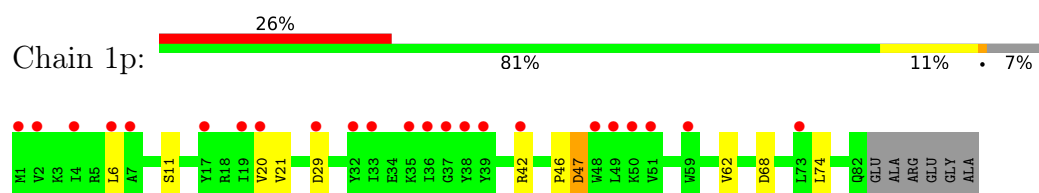
- Molecule 46: 30S ribosomal protein S15



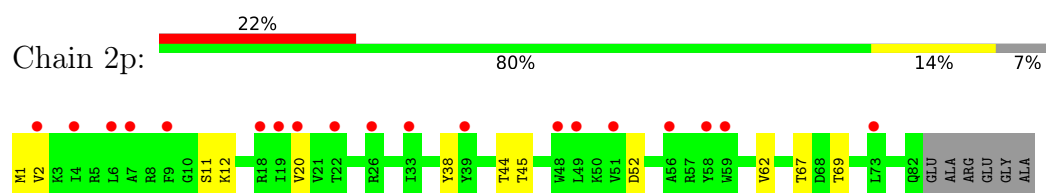
- Molecule 46: 30S ribosomal protein S15



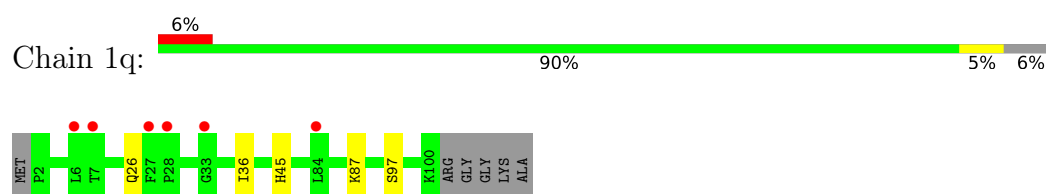
- Molecule 47: 30S ribosomal protein S16



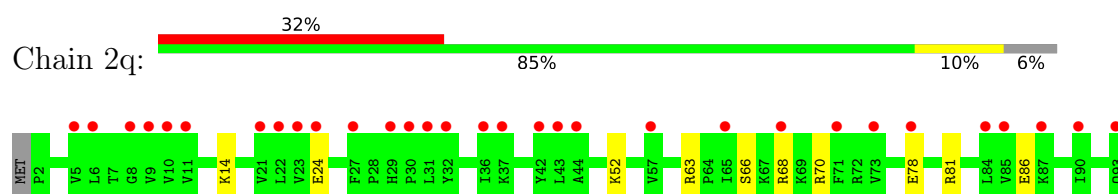
- Molecule 47: 30S ribosomal protein S16

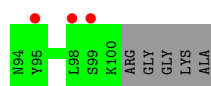


- Molecule 48: 30S ribosomal protein S17

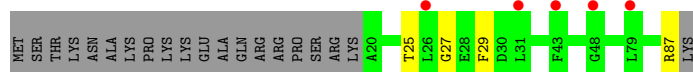
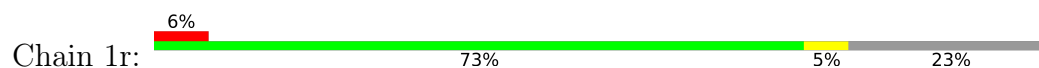


- Molecule 48: 30S ribosomal protein S17

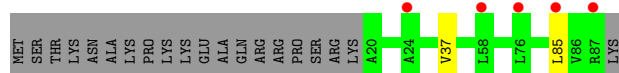




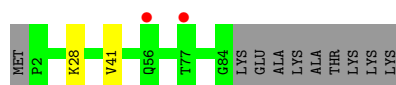
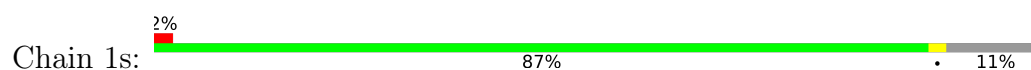
- Molecule 49: 30S ribosomal protein S18



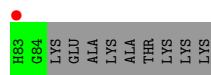
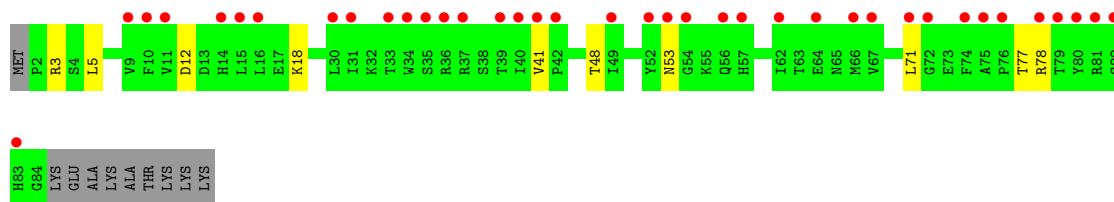
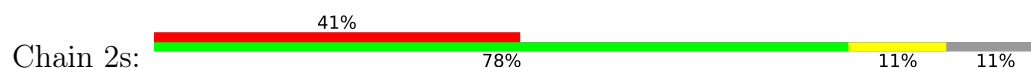
- Molecule 49: 30S ribosomal protein S18



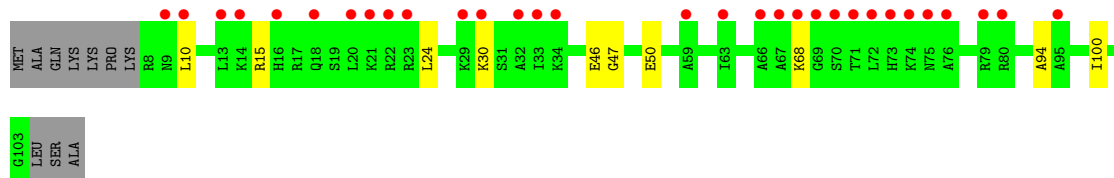
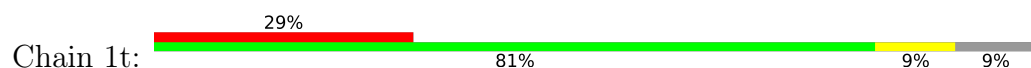
- Molecule 50: 30S ribosomal protein S19



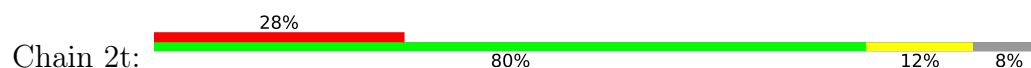
- Molecule 50: 30S ribosomal protein S19




- Molecule 51: 30S ribosomal protein S20

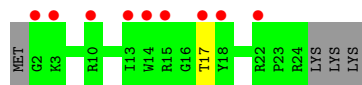


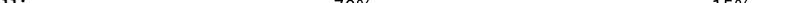
- Molecule 51: 30S ribosomal protein S20

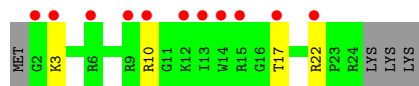


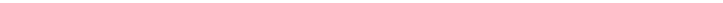


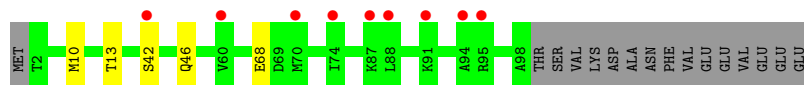
- Chain 1u: 




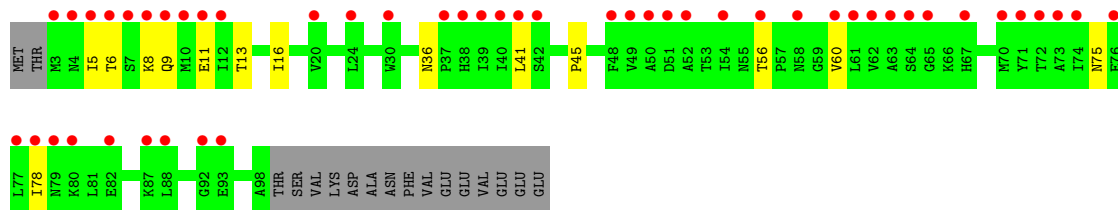
- Chain 2u: 



- Chain 1y: 



- Chain 2y: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.51Å 448.86Å 619.61Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 224.43 – 2.55 254.97 – 2.55 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (224.43-2.55) 99.9 (254.97-2.55) | Depositor EDS |
| R_{merge} | 0.26 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.15 (at 2.55Å) | Xtriage |
| Refinement program | PHENIX 1.8.2 | Depositor |
| R, R_{free} | 0.222 , 0.272 0.222 , 0.273 | Depositor DCC |
| R_{free} test set | 93828 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 53.8 | Xtriage |
| Anisotropy | 0.213 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 57.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 296819 | wwPDB-VP |
| Average B, all atoms (Å ²) | 59.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, OMG, 2MU, ZN, SF4, 0TD, MPD, ERY, 2MA, 2MG, 5MC, UR3, MA6, 4OC, M2G, 7MG, PSU

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 | 0.54 | 2/69029 (0.0%) | 1.02 | 89/107746 (0.1%) |
| 1 | 2A | 0.43 | 1/68901 (0.0%) | 0.92 | 63/107544 (0.1%) |
| 2 | 1B | 0.45 | 0/2876 | 0.95 | 0/4486 |
| 2 | 2B | 0.36 | 0/2878 | 0.87 | 0/4490 |
| 3 | 1D | 0.36 | 0/2181 | 0.60 | 0/2940 |
| 3 | 2D | 0.33 | 0/2186 | 0.52 | 0/2944 |
| 4 | 1E | 0.36 | 0/1592 | 0.56 | 0/2149 |
| 4 | 2E | 0.31 | 0/1592 | 0.51 | 0/2149 |
| 5 | 1F | 0.33 | 0/1619 | 0.53 | 0/2193 |
| 5 | 2F | 0.30 | 0/1615 | 0.52 | 0/2188 |
| 6 | 1G | 0.30 | 0/1451 | 0.50 | 0/1961 |
| 6 | 2G | 0.30 | 0/1449 | 0.49 | 0/1957 |
| 7 | 1H | 0.33 | 0/1356 | 0.51 | 0/1834 |
| 7 | 2H | 0.29 | 0/1350 | 0.48 | 0/1826 |
| 8 | 1I | 0.29 | 0/1109 | 0.49 | 0/1512 |
| 8 | 2I | 0.28 | 0/1091 | 0.50 | 0/1490 |
| 9 | 1N | 0.34 | 0/1148 | 0.52 | 0/1547 |
| 9 | 2N | 0.29 | 0/1144 | 0.47 | 0/1543 |
| 10 | 1O | 0.40 | 0/943 | 0.57 | 0/1269 |
| 10 | 2O | 0.33 | 0/943 | 0.53 | 0/1269 |
| 11 | 1P | 0.35 | 0/1152 | 0.57 | 0/1533 |
| 11 | 2P | 0.31 | 0/1152 | 0.51 | 0/1533 |
| 12 | 1Q | 0.35 | 0/1143 | 0.52 | 0/1527 |
| 12 | 2Q | 0.30 | 0/1143 | 0.48 | 0/1527 |
| 13 | 1R | 0.34 | 0/982 | 0.55 | 0/1312 |
| 13 | 2R | 0.30 | 0/982 | 0.51 | 0/1312 |
| 14 | 1S | 0.32 | 0/887 | 0.53 | 0/1180 |
| 14 | 2S | 0.29 | 0/880 | 0.51 | 0/1172 |
| 15 | 1T | 0.33 | 0/1105 | 0.53 | 0/1477 |
| 15 | 2T | 0.31 | 0/1097 | 0.49 | 0/1468 |
| 16 | 1U | 0.34 | 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 | 0.55 | 0/1053 |
| 17 | 2V | 0.31 | 0/782 | 0.55 | 0/1049 |
| 18 | 1W | 0.35 | 0/897 | 0.53 | 0/1205 |
| 18 | 2W | 0.31 | 0/897 | 0.49 | 0/1205 |
| 19 | 1X | 0.36 | 0/764 | 0.58 | 0/1025 |
| 19 | 2X | 0.31 | 0/764 | 0.50 | 0/1025 |
| 20 | 1Y | 0.39 | 0/823 | 0.55 | 0/1099 |
| 20 | 2Y | 0.32 | 0/823 | 0.53 | 0/1100 |
| 21 | 1Z | 0.32 | 0/1620 | 0.50 | 0/2200 |
| 21 | 2Z | 0.30 | 0/1590 | 0.50 | 0/2162 |
| 22 | 10 | 0.37 | 0/616 | 0.55 | 0/821 |
| 22 | 20 | 0.31 | 0/616 | 0.51 | 0/821 |
| 23 | 11 | 0.34 | 0/761 | 0.52 | 0/1013 |
| 23 | 21 | 0.33 | 0/766 | 0.52 | 0/1018 |
| 24 | 12 | 0.32 | 0/590 | 0.56 | 0/781 |
| 24 | 22 | 0.29 | 0/594 | 0.44 | 0/785 |
| 25 | 13 | 0.37 | 0/474 | 0.55 | 0/635 |
| 25 | 23 | 0.28 | 0/469 | 0.52 | 0/630 |
| 26 | 14 | 0.30 | 0/559 | 0.54 | 0/754 |
| 26 | 24 | 0.36 | 0/549 | 0.55 | 0/741 |
| 27 | 15 | 0.37 | 0/473 | 0.60 | 0/639 |
| 27 | 25 | 0.29 | 0/469 | 0.56 | 0/635 |
| 28 | 16 | 0.34 | 0/460 | 0.50 | 0/613 |
| 28 | 26 | 0.30 | 0/456 | 0.49 | 0/608 |
| 29 | 17 | 0.37 | 0/426 | 0.54 | 0/561 |
| 29 | 27 | 0.30 | 0/426 | 0.51 | 0/561 |
| 30 | 18 | 0.35 | 0/525 | 0.53 | 0/691 |
| 30 | 28 | 0.30 | 0/525 | 0.48 | 0/691 |
| 31 | 19 | 0.31 | 0/310 | 0.52 | 0/407 |
| 31 | 29 | 0.32 | 0/310 | 0.52 | 0/407 |
| 32 | 1a | 0.38 | 0/35795 | 0.90 | 12/55864 (0.0%) |
| 32 | 2a | 0.37 | 0/35890 | 0.91 | 32/56012 (0.1%) |
| 33 | 1b | 0.29 | 0/1876 | 0.48 | 0/2533 |
| 33 | 2b | 0.31 | 0/1860 | 0.51 | 0/2518 |
| 34 | 1c | 0.30 | 0/1582 | 0.47 | 0/2137 |
| 34 | 2c | 0.30 | 0/1566 | 0.47 | 0/2119 |
| 35 | 1d | 0.29 | 0/1695 | 0.50 | 0/2274 |
| 35 | 2d | 0.31 | 0/1698 | 0.49 | 0/2277 |
| 36 | 1e | 0.30 | 0/1149 | 0.51 | 0/1548 |
| 36 | 2e | 0.31 | 0/1149 | 0.48 | 0/1548 |
| 37 | 1f | 0.30 | 0/827 | 0.48 | 0/1120 |
| 37 | 2f | 0.29 | 0/829 | 0.49 | 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 | 0.42 | 0/1676 |
| 39 | 1h | 0.29 | 0/1118 | 0.49 | 0/1506 |
| 39 | 2h | 0.28 | 0/1108 | 0.48 | 0/1494 |
| 40 | 1i | 0.30 | 0/1005 | 0.49 | 0/1351 |
| 40 | 2i | 0.29 | 0/985 | 0.47 | 0/1329 |
| 41 | 1j | 0.27 | 0/732 | 0.46 | 0/993 |
| 41 | 2j | 0.29 | 0/723 | 0.50 | 0/984 |
| 42 | 1k | 0.28 | 0/849 | 0.47 | 0/1150 |
| 42 | 2k | 0.28 | 0/848 | 0.50 | 0/1149 |
| 43 | 1l | 0.29 | 0/937 | 0.50 | 0/1260 |
| 43 | 2l | 0.29 | 0/937 | 0.50 | 0/1260 |
| 44 | 1m | 0.28 | 0/924 | 0.50 | 0/1242 |
| 44 | 2m | 0.29 | 0/905 | 0.50 | 0/1217 |
| 45 | 1n | 0.29 | 0/501 | 0.47 | 0/664 |
| 45 | 2n | 0.29 | 0/501 | 0.47 | 0/664 |
| 46 | 1o | 0.29 | 0/739 | 0.45 | 0/985 |
| 46 | 2o | 0.28 | 0/739 | 0.45 | 0/985 |
| 47 | 1p | 0.28 | 0/697 | 0.50 | 0/939 |
| 47 | 2p | 0.28 | 0/693 | 0.49 | 0/935 |
| 48 | 1q | 0.31 | 0/836 | 0.51 | 0/1117 |
| 48 | 2q | 0.29 | 0/836 | 0.50 | 0/1117 |
| 49 | 1r | 0.29 | 0/560 | 0.49 | 0/746 |
| 49 | 2r | 0.30 | 0/560 | 0.49 | 0/746 |
| 50 | 1s | 0.29 | 0/663 | 0.50 | 0/895 |
| 50 | 2s | 0.30 | 0/660 | 0.49 | 0/893 |
| 51 | 1t | 0.29 | 0/734 | 0.46 | 0/969 |
| 51 | 2t | 0.28 | 0/736 | 0.43 | 0/976 |
| 52 | 1u | 0.31 | 0/203 | 0.46 | 0/266 |
| 52 | 2u | 0.25 | 0/203 | 0.51 | 0/266 |
| 53 | 1y | 0.29 | 0/776 | 0.47 | 0/1048 |
| 53 | 2y | 0.27 | 0/761 | 0.46 | 0/1030 |
| All | All | 0.41 | 3/309937 (0.0%) | 0.85 | 196/463223 (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 |
|-----|-------|---------------------|---------------------|
| 21 | 2Z | 0 | 1 |
| 26 | 24 | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 40 | 1i | 0 | 1 |
| All | All | 0 | 3 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 1 | 1A | 330 | A | N9-C4 | -7.27 | 1.33 | 1.37 |
| 1 | 1A | 330 | A | N3-C4 | -5.58 | 1.31 | 1.34 |
| 1 | 2A | 2104 | G | N1-C2 | -5.16 | 1.33 | 1.37 |

The worst 5 of 196 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1 | 2A | 2104 | G | C5-C6-O6 | 12.37 | 136.02 | 128.60 |
| 1 | 1A | 1042 | G | OP1-P-O3' | -12.06 | 78.67 | 105.20 |
| 1 | 2A | 2104 | G | N3-C2-N2 | 10.78 | 127.44 | 119.90 |
| 1 | 1A | 588 | U | O5'-P-OP2 | -10.44 | 96.31 | 105.70 |
| 1 | 1A | 330 | A | C2-N3-C4 | -10.23 | 105.48 | 110.60 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 40 | 1i | 59 | PHE | Peptide |
| 26 | 24 | 18 | CYS | Peptide |
| 21 | 2Z | 136 | PHE | Peptide |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | 1D | 273/276 (99%) | 259 (95%) | 14 (5%) | 0 | 100 | 100 |
| 3 | 2D | 273/276 (99%) | 252 (92%) | 21 (8%) | 0 | 100 | 100 |
| 4 | 1E | 202/206 (98%) | 192 (95%) | 7 (4%) | 3 (2%) | 10 | 14 |
| 4 | 2E | 202/206 (98%) | 186 (92%) | 14 (7%) | 2 (1%) | 15 | 22 |
| 5 | 1F | 201/210 (96%) | 192 (96%) | 8 (4%) | 1 (0%) | 29 | 40 |
| 5 | 2F | 201/210 (96%) | 195 (97%) | 5 (2%) | 1 (0%) | 29 | 40 |
| 6 | 1G | 179/182 (98%) | 157 (88%) | 17 (10%) | 5 (3%) | 5 | 4 |
| 6 | 2G | 179/182 (98%) | 152 (85%) | 24 (13%) | 3 (2%) | 9 | 11 |
| 7 | 1H | 172/180 (96%) | 161 (94%) | 9 (5%) | 2 (1%) | 13 | 17 |
| 7 | 2H | 171/180 (95%) | 153 (90%) | 13 (8%) | 5 (3%) | 4 | 4 |
| 8 | 1I | 145/148 (98%) | 126 (87%) | 18 (12%) | 1 (1%) | 22 | 30 |
| 8 | 2I | 144/148 (97%) | 133 (92%) | 9 (6%) | 2 (1%) | 11 | 15 |
| 9 | 1N | 138/140 (99%) | 134 (97%) | 3 (2%) | 1 (1%) | 22 | 30 |
| 9 | 2N | 138/140 (99%) | 133 (96%) | 5 (4%) | 0 | 100 | 100 |
| 10 | 1O | 120/122 (98%) | 112 (93%) | 7 (6%) | 1 (1%) | 19 | 27 |
| 10 | 2O | 120/122 (98%) | 111 (92%) | 8 (7%) | 1 (1%) | 19 | 27 |
| 11 | 1P | 147/150 (98%) | 137 (93%) | 10 (7%) | 0 | 100 | 100 |
| 11 | 2P | 147/150 (98%) | 135 (92%) | 10 (7%) | 2 (1%) | 11 | 15 |
| 12 | 1Q | 139/141 (99%) | 134 (96%) | 4 (3%) | 1 (1%) | 22 | 30 |
| 12 | 2Q | 139/141 (99%) | 126 (91%) | 13 (9%) | 0 | 100 | 100 |
| 13 | 1R | 116/118 (98%) | 113 (97%) | 3 (3%) | 0 | 100 | 100 |
| 13 | 2R | 116/118 (98%) | 112 (97%) | 4 (3%) | 0 | 100 | 100 |
| 14 | 1S | 108/112 (96%) | 99 (92%) | 8 (7%) | 1 (1%) | 17 | 24 |
| 14 | 2S | 108/112 (96%) | 95 (88%) | 13 (12%) | 0 | 100 | 100 |
| 15 | 1T | 129/146 (88%) | 122 (95%) | 7 (5%) | 0 | 100 | 100 |
| 15 | 2T | 129/146 (88%) | 119 (92%) | 10 (8%) | 0 | 100 | 100 |
| 16 | 1U | 114/118 (97%) | 112 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | 2U | 114/118 (97%) | 111 (97%) | 3 (3%) | 0 | 100 | 100 |
| 17 | 1V | 99/101 (98%) | 94 (95%) | 3 (3%) | 2 (2%) | 7 | 8 |
| 17 | 2V | 99/101 (98%) | 94 (95%) | 4 (4%) | 1 (1%) | 15 | 22 |
| 18 | 1W | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 18 | 2W | 110/113 (97%) | 106 (96%) | 4 (4%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 19 | 1X | 93/96 (97%) | 88 (95%) | 4 (4%) | 1 (1%) | 14 | 19 |
| 19 | 2X | 93/96 (97%) | 87 (94%) | 5 (5%) | 1 (1%) | 14 | 19 |
| 20 | 1Y | 105/110 (96%) | 97 (92%) | 7 (7%) | 1 (1%) | 15 | 22 |
| 20 | 2Y | 105/110 (96%) | 97 (92%) | 7 (7%) | 1 (1%) | 15 | 22 |
| 21 | 1Z | 201/206 (98%) | 185 (92%) | 15 (8%) | 1 (0%) | 29 | 40 |
| 21 | 2Z | 199/206 (97%) | 177 (89%) | 19 (10%) | 3 (2%) | 10 | 14 |
| 22 | 10 | 75/85 (88%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |
| 22 | 20 | 75/85 (88%) | 69 (92%) | 6 (8%) | 0 | 100 | 100 |
| 23 | 11 | 95/98 (97%) | 94 (99%) | 1 (1%) | 0 | 100 | 100 |
| 23 | 21 | 95/98 (97%) | 88 (93%) | 6 (6%) | 1 (1%) | 14 | 19 |
| 24 | 12 | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 24 | 22 | 68/72 (94%) | 63 (93%) | 5 (7%) | 0 | 100 | 100 |
| 25 | 13 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 25 | 23 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 26 | 14 | 67/71 (94%) | 52 (78%) | 8 (12%) | 7 (10%) | 0 | 0 |
| 26 | 24 | 67/71 (94%) | 44 (66%) | 16 (24%) | 7 (10%) | 0 | 0 |
| 27 | 15 | 57/60 (95%) | 57 (100%) | 0 | 0 | 100 | 100 |
| 27 | 25 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 28 | 16 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 28 | 26 | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |
| 29 | 17 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 29 | 27 | 46/49 (94%) | 45 (98%) | 1 (2%) | 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 |
| 31 | 19 | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 31 | 29 | 35/37 (95%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 33 | 1b | 229/256 (90%) | 191 (83%) | 28 (12%) | 10 (4%) | 2 | 1 |
| 33 | 2b | 229/256 (90%) | 197 (86%) | 27 (12%) | 5 (2%) | 6 | 7 |
| 34 | 1c | 204/239 (85%) | 186 (91%) | 18 (9%) | 0 | 100 | 100 |
| 34 | 2c | 204/239 (85%) | 175 (86%) | 27 (13%) | 2 (1%) | 15 | 22 |
| 35 | 1d | 206/209 (99%) | 193 (94%) | 12 (6%) | 1 (0%) | 29 | 40 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 35 | 2d | 206/209 (99%) | 186 (90%) | 19 (9%) | 1 (0%) | 29 | 40 |
| 36 | 1e | 146/162 (90%) | 140 (96%) | 6 (4%) | 0 | 100 | 100 |
| 36 | 2e | 146/162 (90%) | 134 (92%) | 10 (7%) | 2 (1%) | 11 | 15 |
| 37 | 1f | 98/101 (97%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 37 | 2f | 98/101 (97%) | 89 (91%) | 9 (9%) | 0 | 100 | 100 |
| 38 | 1g | 153/156 (98%) | 143 (94%) | 9 (6%) | 1 (1%) | 22 | 30 |
| 38 | 2g | 153/156 (98%) | 131 (86%) | 19 (12%) | 3 (2%) | 7 | 8 |
| 39 | 1h | 135/138 (98%) | 128 (95%) | 7 (5%) | 0 | 100 | 100 |
| 39 | 2h | 135/138 (98%) | 122 (90%) | 11 (8%) | 2 (2%) | 10 | 14 |
| 40 | 1i | 125/128 (98%) | 112 (90%) | 12 (10%) | 1 (1%) | 19 | 27 |
| 40 | 2i | 124/128 (97%) | 106 (86%) | 15 (12%) | 3 (2%) | 6 | 5 |
| 41 | 1j | 95/105 (90%) | 77 (81%) | 13 (14%) | 5 (5%) | 2 | 0 |
| 41 | 2j | 94/105 (90%) | 75 (80%) | 12 (13%) | 7 (7%) | 1 | 0 |
| 42 | 1k | 112/129 (87%) | 102 (91%) | 9 (8%) | 1 (1%) | 17 | 24 |
| 42 | 2k | 112/129 (87%) | 102 (91%) | 8 (7%) | 2 (2%) | 8 | 10 |
| 43 | 1l | 119/132 (90%) | 109 (92%) | 9 (8%) | 1 (1%) | 19 | 27 |
| 43 | 2l | 119/132 (90%) | 107 (90%) | 11 (9%) | 1 (1%) | 19 | 27 |
| 44 | 1m | 114/126 (90%) | 100 (88%) | 11 (10%) | 3 (3%) | 5 | 5 |
| 44 | 2m | 112/126 (89%) | 95 (85%) | 16 (14%) | 1 (1%) | 17 | 24 |
| 45 | 1n | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 | 100 |
| 45 | 2n | 58/61 (95%) | 50 (86%) | 7 (12%) | 1 (2%) | 9 | 11 |
| 46 | 1o | 86/89 (97%) | 81 (94%) | 4 (5%) | 1 (1%) | 13 | 17 |
| 46 | 2o | 86/89 (97%) | 81 (94%) | 4 (5%) | 1 (1%) | 13 | 17 |
| 47 | 1p | 80/88 (91%) | 71 (89%) | 6 (8%) | 3 (4%) | 3 | 2 |
| 47 | 2p | 80/88 (91%) | 67 (84%) | 12 (15%) | 1 (1%) | 12 | 16 |
| 48 | 1q | 97/105 (92%) | 88 (91%) | 9 (9%) | 0 | 100 | 100 |
| 48 | 2q | 97/105 (92%) | 88 (91%) | 8 (8%) | 1 (1%) | 15 | 22 |
| 49 | 1r | 66/88 (75%) | 64 (97%) | 1 (2%) | 1 (2%) | 10 | 14 |
| 49 | 2r | 66/88 (75%) | 61 (92%) | 5 (8%) | 0 | 100 | 100 |
| 50 | 1s | 81/93 (87%) | 71 (88%) | 10 (12%) | 0 | 100 | 100 |
| 50 | 2s | 81/93 (87%) | 70 (86%) | 11 (14%) | 0 | 100 | 100 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 51 | 1t | 94/106 (89%) | 86 (92%) | 6 (6%) | 2 (2%) | 7 | 7 |
| 51 | 2t | 96/106 (91%) | 84 (88%) | 9 (9%) | 3 (3%) | 4 | 3 |
| 52 | 1u | 21/27 (78%) | 19 (90%) | 2 (10%) | 0 | 100 | 100 |
| 52 | 2u | 21/27 (78%) | 16 (76%) | 4 (19%) | 1 (5%) | 2 | 1 |
| 53 | 1y | 95/113 (84%) | 93 (98%) | 1 (1%) | 1 (1%) | 14 | 19 |
| 53 | 2y | 94/113 (83%) | 88 (94%) | 4 (4%) | 2 (2%) | 7 | 7 |
| All | All | 11629/12354 (94%) | 10669 (92%) | 832 (7%) | 128 (1%) | 14 | 19 |

5 of 128 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 1E | 71 | GLY |
| 6 | 1G | 47 | LYS |
| 7 | 1H | 92 | ILE |
| 14 | 1S | 59 | LYS |
| 26 | 14 | 44 | THR |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3 | 1D | 214/218 (98%) | 197 (92%) | 17 (8%) | 12 | 15 |
| 3 | 2D | 215/218 (99%) | 196 (91%) | 19 (9%) | 10 | 12 |
| 4 | 1E | 164/166 (99%) | 152 (93%) | 12 (7%) | 14 | 18 |
| 4 | 2E | 164/166 (99%) | 155 (94%) | 9 (6%) | 21 | 29 |
| 5 | 1F | 160/166 (96%) | 144 (90%) | 16 (10%) | 7 | 8 |
| 5 | 2F | 159/166 (96%) | 145 (91%) | 14 (9%) | 10 | 12 |
| 6 | 1G | 144/156 (92%) | 135 (94%) | 9 (6%) | 18 | 23 |
| 6 | 2G | 142/156 (91%) | 118 (83%) | 24 (17%) | 2 | 2 |
| 7 | 1H | 144/148 (97%) | 137 (95%) | 7 (5%) | 25 | 34 |
| 7 | 2H | 143/148 (97%) | 123 (86%) | 20 (14%) | 3 | 3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 8 | 1I | 111/124 (90%) | 92 (83%) | 19 (17%) | 2 | 2 |
| 8 | 2I | 108/124 (87%) | 98 (91%) | 10 (9%) | 9 | 10 |
| 9 | 1N | 119/119 (100%) | 111 (93%) | 8 (7%) | 16 | 21 |
| 9 | 2N | 118/119 (99%) | 108 (92%) | 10 (8%) | 10 | 13 |
| 10 | 1O | 100/100 (100%) | 95 (95%) | 5 (5%) | 24 | 33 |
| 10 | 2O | 100/100 (100%) | 92 (92%) | 8 (8%) | 12 | 15 |
| 11 | 1P | 115/116 (99%) | 109 (95%) | 6 (5%) | 23 | 30 |
| 11 | 2P | 115/116 (99%) | 110 (96%) | 5 (4%) | 29 | 39 |
| 12 | 1Q | 111/111 (100%) | 104 (94%) | 7 (6%) | 18 | 23 |
| 12 | 2Q | 111/111 (100%) | 105 (95%) | 6 (5%) | 22 | 29 |
| 13 | 1R | 101/101 (100%) | 92 (91%) | 9 (9%) | 9 | 12 |
| 13 | 2R | 101/101 (100%) | 92 (91%) | 9 (9%) | 9 | 12 |
| 14 | 1S | 87/88 (99%) | 77 (88%) | 10 (12%) | 5 | 5 |
| 14 | 2S | 85/88 (97%) | 75 (88%) | 10 (12%) | 5 | 5 |
| 15 | 1T | 115/127 (91%) | 108 (94%) | 7 (6%) | 18 | 24 |
| 15 | 2T | 113/127 (89%) | 105 (93%) | 8 (7%) | 14 | 19 |
| 16 | 1U | 93/94 (99%) | 85 (91%) | 8 (9%) | 10 | 13 |
| 16 | 2U | 93/94 (99%) | 87 (94%) | 6 (6%) | 17 | 23 |
| 17 | 1V | 81/82 (99%) | 74 (91%) | 7 (9%) | 10 | 13 |
| 17 | 2V | 80/82 (98%) | 68 (85%) | 12 (15%) | 3 | 2 |
| 18 | 1W | 90/92 (98%) | 83 (92%) | 7 (8%) | 12 | 16 |
| 18 | 2W | 90/92 (98%) | 87 (97%) | 3 (3%) | 38 | 51 |
| 19 | 1X | 77/78 (99%) | 72 (94%) | 5 (6%) | 17 | 23 |
| 19 | 2X | 77/78 (99%) | 72 (94%) | 5 (6%) | 17 | 23 |
| 20 | 1Y | 86/91 (94%) | 79 (92%) | 7 (8%) | 11 | 14 |
| 20 | 2Y | 86/91 (94%) | 76 (88%) | 10 (12%) | 5 | 5 |
| 21 | 1Z | 169/179 (94%) | 156 (92%) | 13 (8%) | 13 | 16 |
| 21 | 2Z | 165/179 (92%) | 149 (90%) | 16 (10%) | 8 | 9 |
| 22 | 10 | 61/67 (91%) | 60 (98%) | 1 (2%) | 62 | 77 |
| 22 | 20 | 61/67 (91%) | 58 (95%) | 3 (5%) | 25 | 34 |
| 23 | 11 | 79/83 (95%) | 77 (98%) | 2 (2%) | 47 | 62 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 23 | 21 | 81/83 (98%) | 78 (96%) | 3 (4%) | 34 | 46 |
| 24 | 12 | 65/67 (97%) | 59 (91%) | 6 (9%) | 9 | 11 |
| 24 | 22 | 66/67 (98%) | 60 (91%) | 6 (9%) | 9 | 11 |
| 25 | 13 | 51/52 (98%) | 46 (90%) | 5 (10%) | 8 | 9 |
| 25 | 23 | 50/52 (96%) | 44 (88%) | 6 (12%) | 5 | 5 |
| 26 | 14 | 58/63 (92%) | 51 (88%) | 7 (12%) | 5 | 4 |
| 26 | 24 | 54/63 (86%) | 46 (85%) | 8 (15%) | 3 | 2 |
| 27 | 15 | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 16 |
| 27 | 25 | 50/52 (96%) | 49 (98%) | 1 (2%) | 55 | 70 |
| 28 | 16 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 5 |
| 28 | 26 | 50/52 (96%) | 46 (92%) | 4 (8%) | 12 | 15 |
| 29 | 17 | 41/42 (98%) | 38 (93%) | 3 (7%) | 14 | 18 |
| 29 | 27 | 41/42 (98%) | 37 (90%) | 4 (10%) | 8 | 9 |
| 30 | 18 | 54/55 (98%) | 49 (91%) | 5 (9%) | 9 | 10 |
| 30 | 28 | 54/55 (98%) | 48 (89%) | 6 (11%) | 6 | 6 |
| 31 | 19 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 57 |
| 31 | 29 | 34/34 (100%) | 31 (91%) | 3 (9%) | 10 | 12 |
| 33 | 1b | 191/220 (87%) | 170 (89%) | 21 (11%) | 6 | 6 |
| 33 | 2b | 187/220 (85%) | 170 (91%) | 17 (9%) | 9 | 11 |
| 34 | 1c | 144/188 (77%) | 132 (92%) | 12 (8%) | 11 | 14 |
| 34 | 2c | 140/188 (74%) | 126 (90%) | 14 (10%) | 7 | 8 |
| 35 | 1d | 171/181 (94%) | 154 (90%) | 17 (10%) | 8 | 9 |
| 35 | 2d | 172/181 (95%) | 152 (88%) | 20 (12%) | 5 | 5 |
| 36 | 1e | 114/123 (93%) | 109 (96%) | 5 (4%) | 28 | 38 |
| 36 | 2e | 114/123 (93%) | 103 (90%) | 11 (10%) | 8 | 9 |
| 37 | 1f | 85/90 (94%) | 77 (91%) | 8 (9%) | 8 | 10 |
| 37 | 2f | 85/90 (94%) | 78 (92%) | 7 (8%) | 11 | 14 |
| 38 | 1g | 120/127 (94%) | 111 (92%) | 9 (8%) | 13 | 17 |
| 38 | 2g | 119/127 (94%) | 100 (84%) | 19 (16%) | 2 | 2 |
| 39 | 1h | 116/119 (98%) | 108 (93%) | 8 (7%) | 15 | 20 |
| 39 | 2h | 114/119 (96%) | 100 (88%) | 14 (12%) | 4 | 4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 40 | 1i | 91/99 (92%) | 80 (88%) | 11 (12%) | 5 | 4 |
| 40 | 2i | 88/99 (89%) | 73 (83%) | 15 (17%) | 2 | 2 |
| 41 | 1j | 68/92 (74%) | 64 (94%) | 4 (6%) | 19 | 25 |
| 41 | 2j | 68/92 (74%) | 62 (91%) | 6 (9%) | 10 | 12 |
| 42 | 1k | 83/99 (84%) | 79 (95%) | 4 (5%) | 25 | 34 |
| 42 | 2k | 83/99 (84%) | 73 (88%) | 10 (12%) | 5 | 5 |
| 43 | 1l | 96/108 (89%) | 90 (94%) | 6 (6%) | 18 | 23 |
| 43 | 2l | 96/108 (89%) | 90 (94%) | 6 (6%) | 18 | 23 |
| 44 | 1m | 90/101 (89%) | 79 (88%) | 11 (12%) | 5 | 4 |
| 44 | 2m | 87/101 (86%) | 82 (94%) | 5 (6%) | 20 | 27 |
| 45 | 1n | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 | 8 |
| 45 | 2n | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 | 8 |
| 46 | 1o | 78/80 (98%) | 75 (96%) | 3 (4%) | 33 | 45 |
| 46 | 2o | 78/80 (98%) | 72 (92%) | 6 (8%) | 13 | 16 |
| 47 | 1p | 69/74 (93%) | 60 (87%) | 9 (13%) | 4 | 3 |
| 47 | 2p | 68/74 (92%) | 57 (84%) | 11 (16%) | 2 | 2 |
| 48 | 1q | 94/97 (97%) | 89 (95%) | 5 (5%) | 22 | 30 |
| 48 | 2q | 94/97 (97%) | 85 (90%) | 9 (10%) | 8 | 9 |
| 49 | 1r | 59/77 (77%) | 56 (95%) | 3 (5%) | 24 | 32 |
| 49 | 2r | 59/77 (77%) | 57 (97%) | 2 (3%) | 37 | 50 |
| 50 | 1s | 68/80 (85%) | 66 (97%) | 2 (3%) | 42 | 57 |
| 50 | 2s | 67/80 (84%) | 57 (85%) | 10 (15%) | 3 | 2 |
| 51 | 1t | 71/82 (87%) | 63 (89%) | 8 (11%) | 6 | 5 |
| 51 | 2t | 70/82 (85%) | 60 (86%) | 10 (14%) | 3 | 3 |
| 52 | 1u | 18/22 (82%) | 17 (94%) | 1 (6%) | 21 | 28 |
| 52 | 2u | 18/22 (82%) | 15 (83%) | 3 (17%) | 2 | 2 |
| 53 | 1y | 82/98 (84%) | 78 (95%) | 4 (5%) | 25 | 34 |
| 53 | 2y | 79/98 (81%) | 67 (85%) | 12 (15%) | 3 | 2 |
| All | All | 9524/10260 (93%) | 8689 (91%) | 835 (9%) | 10 | 12 |

5 of 835 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 2D | 43 | ARG |
| 8 | 2I | 127 | VAL |
| 45 | 2n | 57 | ARG |
| 3 | 2D | 211 | ARG |
| 6 | 2G | 62 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46 | 1o | 28 | GLN |
| 4 | 2E | 48 | GLN |
| 41 | 2j | 62 | HIS |
| 47 | 1p | 16 | HIS |
| 50 | 1s | 83 | HIS |

5.3.3 RNA [i](#)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 1A | 2862/2915 (98%) | 434 (15%) | 33 (1%) |
| 1 | 2A | 2855/2915 (97%) | 485 (16%) | 31 (1%) |
| 2 | 1B | 119/121 (98%) | 10 (8%) | 0 |
| 2 | 2B | 119/121 (98%) | 16 (13%) | 0 |
| 32 | 1a | 1494/1521 (98%) | 257 (17%) | 0 |
| 32 | 2a | 1498/1521 (98%) | 290 (19%) | 0 |
| All | All | 8947/9114 (98%) | 1492 (16%) | 64 (0%) |

5 of 1492 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1A | 12 | U |
| 1 | 1A | 14 | A |
| 1 | 1A | 15 | G |
| 1 | 1A | 34 | C |
| 1 | 1A | 45 | C |

5 of 64 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 2406 | U |
| 1 | 2A | 266 | G |
| 1 | 2A | 2321 | G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 2422 | A |
| 1 | 1A | 2893 | G |

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

48 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 | 4OC | 2a | 1402 | 32 | 16,23,24 | 0.68 | 0 | 17,32,35 | 1.25 | 1 (5%) |
| 32 | 5MC | 2a | 1404 | 32 | 15,22,23 | 1.34 | 1 (6%) | 19,32,35 | 1.40 | 3 (15%) |
| 32 | PSU | 2a | 516 | 32,54 | 17,21,22 | 1.69 | 3 (17%) | 20,30,33 | 3.07 | 7 (35%) |
| 1 | 4OC | 2A | 1920 | 1 | 15,22,24 | 0.74 | 0 | 17,31,35 | 1.35 | 1 (5%) |
| 1 | 2MA | 1A | 2503 | 1,54 | 17,25,26 | 1.28 | 2 (11%) | 19,37,40 | 1.90 | 3 (15%) |
| 1 | 5MU | 2A | 1939 | 1,54 | 15,22,23 | 1.13 | 1 (6%) | 16,32,35 | 1.79 | 2 (12%) |
| 1 | PSU | 2A | 2605 | 1 | 17,21,22 | 1.83 | 3 (17%) | 20,30,33 | 3.30 | 6 (30%) |
| 1 | 5MU | 1A | 1939 | 1 | 15,22,23 | 1.17 | 1 (6%) | 16,32,35 | 1.86 | 2 (12%) |
| 32 | UR3 | 1a | 1498 | 32 | 14,22,23 | 0.71 | 0 | 15,32,35 | 0.66 | 0 |
| 32 | 2MG | 1a | 1207 | 32,54 | 19,26,27 | 1.29 | 2 (10%) | 21,38,41 | 2.68 | 10 (47%) |
| 32 | MA6 | 1a | 1518 | 32 | 19,26,27 | 0.84 | 0 | 18,38,41 | 1.28 | 2 (11%) |
| 43 | 0TD | 1l | 92 | 43 | 4,9,10 | 3.10 | 1 (25%) | 3,11,13 | 6.44 | 1 (33%) |
| 32 | UR3 | 2a | 1498 | 32 | 14,22,23 | 0.82 | 1 (7%) | 15,32,35 | 0.78 | 1 (6%) |
| 32 | MA6 | 2a | 1519 | 32 | 19,26,27 | 0.82 | 0 | 18,38,41 | 1.53 | 2 (11%) |
| 32 | 5MC | 1a | 1407 | 32 | 15,22,23 | 1.38 | 1 (6%) | 19,32,35 | 1.33 | 1 (5%) |
| 1 | 5MU | 1A | 1915 | 1 | 15,22,23 | 1.04 | 1 (6%) | 16,32,35 | 2.02 | 1 (6%) |
| 32 | MA6 | 1a | 1519 | 32 | 19,26,27 | 0.82 | 0 | 18,38,41 | 1.52 | 2 (11%) |
| 32 | M2G | 1a | 966 | 32 | 20,27,28 | 1.33 | 3 (15%) | 22,40,43 | 2.13 | 5 (22%) |
| 1 | PSU | 2A | 1911 | 1 | 17,21,22 | 1.52 | 3 (17%) | 20,30,33 | 3.10 | 6 (30%) |
| 1 | 4OC | 1A | 1920 | 1 | 15,22,24 | 0.73 | 0 | 17,31,35 | 1.47 | 2 (11%) |
| 32 | 5MC | 2a | 967 | 32 | 15,22,23 | 1.38 | 1 (6%) | 19,32,35 | 1.29 | 2 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | OMG | 1A | 2251 | 1,54 | 18,26,27 | 1.35 | 2 (11%) | 20,38,41 | 2.33 | 6 (30%) |
| 32 | MA6 | 2a | 1518 | 32 | 19,26,27 | 0.79 | 0 | 18,38,41 | 1.39 | 2 (11%) |
| 1 | 2MA | 2A | 2503 | 1,54 | 17,25,26 | 1.38 | 2 (11%) | 19,37,40 | 2.04 | 3 (15%) |
| 32 | PSU | 1a | 516 | 32,54 | 17,21,22 | 1.47 | 4 (23%) | 20,30,33 | 3.14 | 6 (30%) |
| 1 | PSU | 2A | 1917 | 1 | 17,21,22 | 1.57 | 2 (11%) | 20,30,33 | 3.07 | 6 (30%) |
| 1 | 5MC | 2A | 1962 | 1,54 | 15,22,23 | 1.27 | 1 (6%) | 19,32,35 | 1.52 | 4 (21%) |
| 32 | 5MC | 2a | 1400 | 32 | 15,22,23 | 1.36 | 1 (6%) | 19,32,35 | 1.36 | 3 (15%) |
| 1 | 5MC | 1A | 1962 | 1 | 15,22,23 | 1.23 | 1 (6%) | 19,32,35 | 1.18 | 2 (10%) |
| 1 | PSU | 1A | 2605 | 1,54 | 17,21,22 | 1.63 | 3 (17%) | 20,30,33 | 3.28 | 6 (30%) |
| 1 | PSU | 1A | 1911 | 1 | 17,21,22 | 1.56 | 3 (17%) | 20,30,33 | 3.06 | 6 (30%) |
| 32 | 5MC | 1a | 967 | 32 | 15,22,23 | 1.29 | 1 (6%) | 19,32,35 | 1.33 | 3 (15%) |
| 1 | 2MU | 2A | 2552 | 1,54 | 14,22,24 | 0.91 | 0 | 14,31,36 | 0.75 | 1 (7%) |
| 32 | 7MG | 2a | 527 | 32 | 22,26,27 | 1.77 | 4 (18%) | 28,39,42 | 2.68 | 8 (28%) |
| 32 | 5MC | 2a | 1407 | 32 | 15,22,23 | 1.32 | 1 (6%) | 19,32,35 | 1.35 | 2 (10%) |
| 1 | OMG | 2A | 2251 | 1,54 | 18,26,27 | 1.21 | 2 (11%) | 20,38,41 | 2.18 | 6 (30%) |
| 1 | PSU | 1A | 1917 | 1 | 17,21,22 | 1.50 | 2 (11%) | 20,30,33 | 3.19 | 6 (30%) |
| 43 | 0TD | 2l | 92 | 43 | 4,9,10 | 3.03 | 1 (25%) | 3,11,13 | 7.87 | 1 (33%) |
| 1 | 5MU | 2A | 1915 | 1 | 15,22,23 | 1.06 | 1 (6%) | 16,32,35 | 2.13 | 1 (6%) |
| 32 | 7MG | 1a | 527 | 32,54 | 22,26,27 | 1.73 | 4 (18%) | 28,39,42 | 2.71 | 8 (28%) |
| 32 | 4OC | 1a | 1402 | 32 | 16,23,24 | 0.64 | 0 | 17,32,35 | 1.22 | 1 (5%) |
| 32 | 2MG | 2a | 1207 | 32 | 19,26,27 | 1.25 | 2 (10%) | 21,38,41 | 2.17 | 6 (28%) |
| 1 | 5MC | 2A | 1942 | 1 | 15,22,23 | 1.35 | 1 (6%) | 19,32,35 | 1.37 | 3 (15%) |
| 32 | M2G | 2a | 966 | 32 | 20,27,28 | 1.49 | 3 (15%) | 22,40,43 | 2.13 | 5 (22%) |
| 32 | 5MC | 1a | 1400 | 32 | 15,22,23 | 1.37 | 1 (6%) | 19,32,35 | 1.38 | 3 (15%) |
| 1 | 5MC | 1A | 1942 | 1 | 15,22,23 | 1.32 | 1 (6%) | 19,32,35 | 1.25 | 2 (10%) |
| 32 | 5MC | 1a | 1404 | 32 | 15,22,23 | 1.33 | 1 (6%) | 19,32,35 | 1.30 | 3 (15%) |
| 1 | 2MU | 1A | 2552 | 1,54 | 14,22,24 | 0.76 | 0 | 14,31,36 | 0.86 | 1 (7%) |

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 | 4OC | 2a | 1402 | 32 | - | 2/9/29/30 | 0/2/2/2 |
| 32 | 5MC | 2a | 1404 | 32 | - | 0/5/25/26 | 0/2/2/2 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|-----------|---------|
| 32 | PSU | 2a | 516 | 32,54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | 2A | 1920 | 1 | - | 1/7/27/30 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 1,54 | - | 2/3/25/26 | 0/3/3/3 |
| 1 | 5MU | 2A | 1939 | 1,54 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1939 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | UR3 | 1a | 1498 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 2MG | 1a | 1207 | 32,54 | - | 2/5/27/28 | 0/3/3/3 |
| 32 | MA6 | 1a | 1518 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 43 | 0TD | 1l | 92 | 43 | - | 1/3/12/14 | - |
| 32 | UR3 | 2a | 1498 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | MA6 | 2a | 1519 | 32 | - | 2/7/29/30 | 0/3/3/3 |
| 32 | 5MC | 1a | 1407 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1915 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1519 | 32 | - | 2/7/29/30 | 0/3/3/3 |
| 32 | M2G | 1a | 966 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | PSU | 2A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4OC | 1A | 1920 | 1 | - | 1/7/27/30 | 0/2/2/2 |
| 32 | 5MC | 2a | 967 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | OMG | 1A | 2251 | 1,54 | - | 1/5/27/28 | 0/3/3/3 |
| 32 | MA6 | 2a | 1518 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | 2MA | 2A | 2503 | 1,54 | - | 1/3/25/26 | 0/3/3/3 |
| 32 | PSU | 1a | 516 | 32,54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1917 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1962 | 1,54 | - | 2/5/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1400 | 32 | - | 2/5/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1962 | 1 | - | 2/5/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 2605 | 1,54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 967 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 2MU | 2A | 2552 | 1,54 | - | 0/7/27/28 | 0/2/2/2 |
| 32 | 7MG | 2a | 527 | 32 | - | 2/7/37/38 | 0/3/3/3 |
| 32 | 5MC | 2a | 1407 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | OMG | 2A | 2251 | 1,54 | - | 1/5/27/28 | 0/3/3/3 |
| 1 | PSU | 1A | 1917 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 43 | 0TD | 2l | 92 | 43 | - | 1/3/12/14 | - |
| 1 | 5MU | 2A | 1915 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 7MG | 1a | 527 | 32,54 | - | 2/7/37/38 | 0/3/3/3 |
| 32 | 4OC | 1a | 1402 | 32 | - | 4/9/29/30 | 0/2/2/2 |
| 32 | 2MG | 2a | 1207 | 32 | - | 2/5/27/28 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | 5MC | 2A | 1942 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | M2G | 2a | 966 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 32 | 5MC | 1a | 1400 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1942 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1404 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 2MU | 1A | 2552 | 1,54 | - | 0/7/27/28 | 0/2/2/2 |

The worst 5 of 68 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 43 | 1l | 92 | 0TD | CB-SB | -5.87 | 1.69 | 1.84 |
| 1 | 2A | 2605 | PSU | C5-C1' | -5.79 | 1.47 | 1.52 |
| 43 | 2l | 92 | 0TD | CB-SB | -5.78 | 1.70 | 1.84 |
| 32 | 2a | 967 | 5MC | C5-C4 | 5.01 | 1.49 | 1.41 |
| 32 | 2a | 1400 | 5MC | C5-C4 | 4.85 | 1.48 | 1.41 |

The worst 5 of 164 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 43 | 2l | 92 | 0TD | CSB-SB-CB | -13.56 | 75.19 | 101.85 |
| 43 | 1l | 92 | 0TD | CSB-SB-CB | -11.08 | 80.06 | 101.85 |
| 1 | 1A | 2605 | PSU | N1-C2-N3 | -8.96 | 121.31 | 128.43 |
| 1 | 1A | 1917 | PSU | N1-C2-N3 | -8.86 | 121.39 | 128.43 |
| 32 | 1a | 516 | PSU | N1-C2-N3 | -8.85 | 121.39 | 128.43 |

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 32 | 2a | 1402 | 4OC | N3-C4-N4-CM4 |
| 32 | 2a | 1402 | 4OC | C5-C4-N4-CM4 |
| 1 | 2A | 1920 | 4OC | O4'-C1'-N1-C6 |
| 32 | 1a | 1207 | 2MG | N1-C2-N2-CM2 |
| 32 | 1a | 1207 | 2MG | N3-C2-N2-CM2 |

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 2499 ligands modelled in this entry, 2486 are monoatomic - leaving 13 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 56 | MPD | 2A | 3735 | - | 7,7,7 | 0.26 | 0 | 9,10,10 | 0.22 | 0 |
| 59 | SF4 | 2d | 501 | 35 | 0,12,12 | 0.00 | - | - | | |
| 56 | MPD | 1T | 204 | - | 7,7,7 | 0.31 | 0 | 9,10,10 | 0.26 | 0 |
| 56 | MPD | 2A | 3736 | - | 7,7,7 | 0.31 | 0 | 9,10,10 | 0.32 | 0 |
| 55 | ERY | 2A | 3734 | - | 53,53,53 | 0.91 | 2 (3%) | 82,82,82 | 1.58 | 13 (15%) |
| 59 | SF4 | 1d | 306 | 35 | 0,12,12 | 0.00 | - | - | | |
| 57 | ARG | 1B | 233 | 54 | 7,11,11 | 0.24 | 0 | 6,13,13 | 0.27 | 0 |
| 57 | ARG | 1F | 319 | 54 | 7,11,11 | 0.34 | 0 | 6,13,13 | 0.37 | 0 |
| 56 | MPD | 1a | 1875 | - | 7,7,7 | 0.37 | 0 | 9,10,10 | 0.44 | 0 |
| 55 | ERY | 1A | 4021 | - | 53,53,53 | 0.91 | 2 (3%) | 82,82,82 | 1.44 | 13 (15%) |
| 56 | MPD | 2B | 219 | - | 7,7,7 | 0.29 | 0 | 9,10,10 | 0.28 | 0 |
| 56 | MPD | 1A | 4022 | 54 | 7,7,7 | 0.27 | 0 | 9,10,10 | 0.57 | 0 |
| 56 | MPD | 18 | 103 | - | 7,7,7 | 0.31 | 0 | 9,10,10 | 0.49 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|--------------|---------|
| 56 | MPD | 2A | 3735 | - | - | 2/5/5/5 | - |
| 57 | ARG | 1B | 233 | 54 | - | 2/7/11/11 | - |
| 56 | MPD | 1T | 204 | - | - | 4/5/5/5 | - |
| 56 | MPD | 2A | 3736 | - | - | 2/5/5/5 | - |
| 55 | ERY | 2A | 3734 | - | - | 7/72/107/107 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|--------------|---------|
| 59 | SF4 | 2d | 501 | 35 | - | - | 0/6/5/5 |
| 56 | MPD | 18 | 103 | - | - | 2/5/5/5 | - |
| 57 | ARG | 1F | 319 | 54 | - | 0/7/11/11 | - |
| 56 | MPD | 1a | 1875 | - | - | 3/5/5/5 | - |
| 55 | ERY | 1A | 4021 | - | - | 7/72/107/107 | 0/3/3/3 |
| 59 | SF4 | 1d | 306 | 35 | - | - | 0/6/5/5 |
| 56 | MPD | 2B | 219 | - | - | 2/5/5/5 | - |
| 56 | MPD | 1A | 4022 | 54 | - | 3/5/5/5 | - |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 55 | 2A | 3734 | ERY | O2-C1 | 4.77 | 1.45 | 1.34 |
| 55 | 1A | 4021 | ERY | O2-C1 | 4.66 | 1.45 | 1.34 |
| 55 | 1A | 4021 | ERY | O2-C13 | -2.52 | 1.42 | 1.46 |
| 55 | 2A | 3734 | ERY | O2-C13 | -2.02 | 1.42 | 1.46 |

The worst 5 of 26 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 55 | 2A | 3734 | ERY | O5-C16-C17 | 4.33 | 110.22 | 103.81 |
| 55 | 2A | 3734 | ERY | C13-O2-C1 | -4.14 | 110.81 | 118.18 |
| 55 | 1A | 4021 | ERY | O7-C5-C4 | -3.83 | 105.80 | 111.54 |
| 55 | 2A | 3734 | ERY | C6-C5-C4 | -3.82 | 108.64 | 114.05 |
| 55 | 2A | 3734 | ERY | O5-C16-C15 | -3.57 | 107.24 | 112.96 |

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

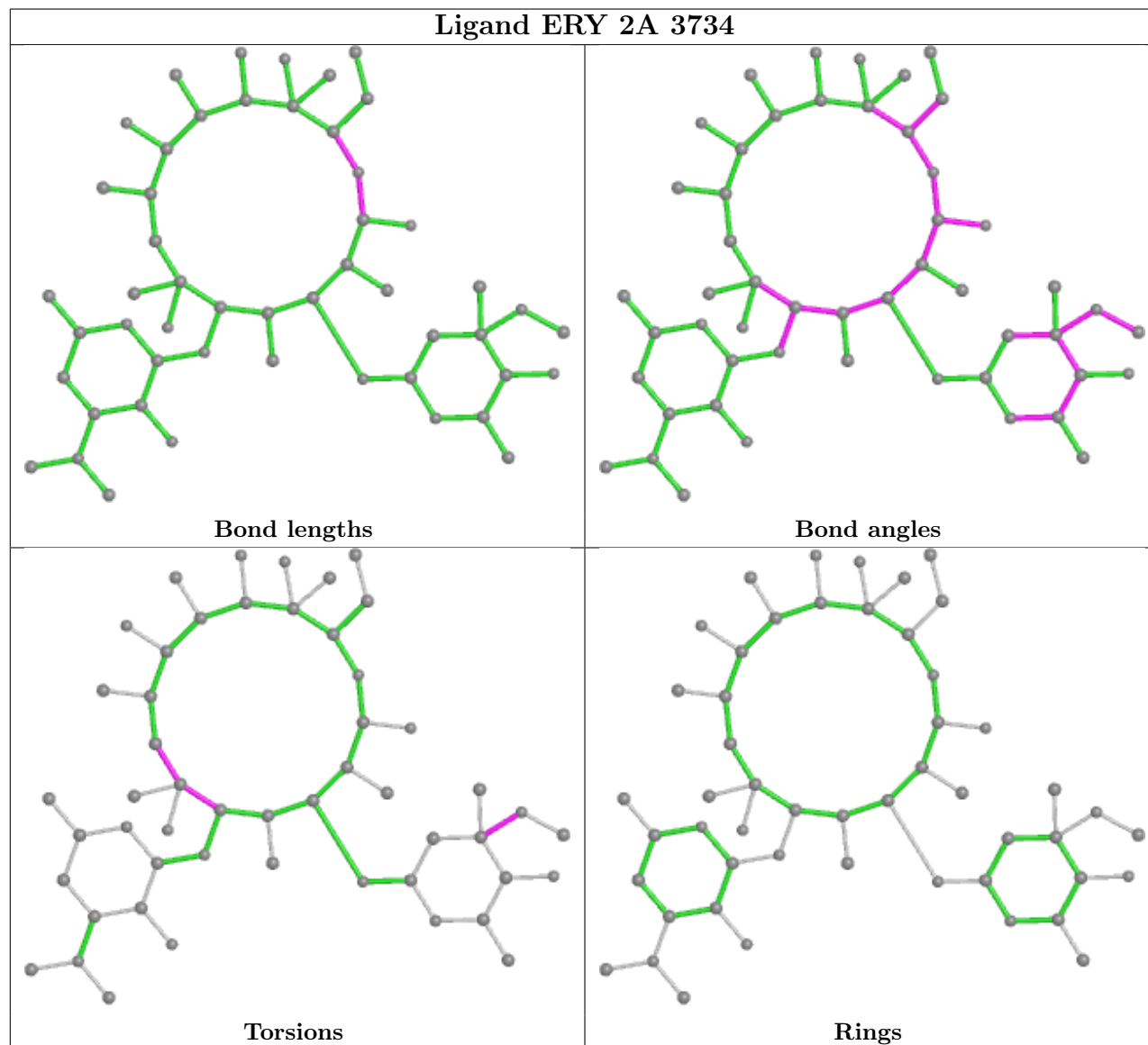
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 56 | 1A | 4022 | MPD | C1-C2-C3-C4 |
| 56 | 1A | 4022 | MPD | O2-C2-C3-C4 |
| 55 | 2A | 3734 | ERY | C32-C6-C7-C8 |
| 55 | 2A | 3734 | ERY | C15-C16-O5-C20 |
| 55 | 2A | 3734 | ERY | C17-C16-O5-C20 |

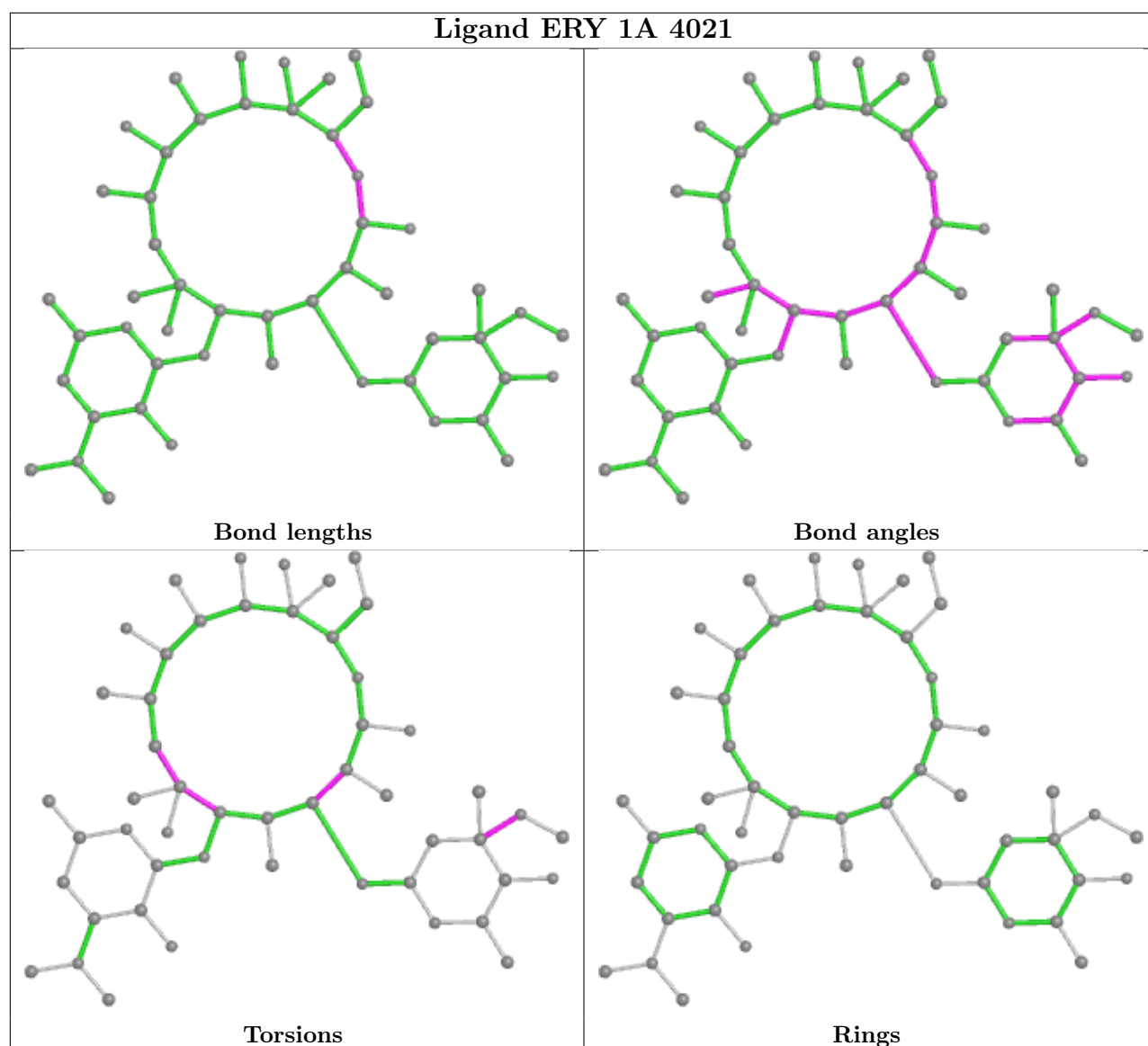
There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | 1A | 2861/2915 (98%) | 0.27 | 42 (1%) 73 79 | 22, 39, 89, 104 | 0 |
| 1 | 2A | 2856/2915 (97%) | 0.04 | 33 (1%) 79 84 | 35, 58, 91, 103 | 0 |
| 2 | 1B | 120/121 (99%) | -0.01 | 0 100 100 | 30, 52, 65, 78 | 0 |
| 2 | 2B | 120/121 (99%) | -0.34 | 0 100 100 | 60, 75, 83, 87 | 0 |
| 3 | 1D | 275/276 (99%) | 0.70 | 8 (2%) 51 59 | 25, 41, 54, 72 | 0 |
| 3 | 2D | 275/276 (99%) | 1.08 | 44 (16%) 1 2 | 36, 53, 65, 78 | 0 |
| 4 | 1E | 204/206 (99%) | 0.64 | 3 (1%) 73 79 | 23, 44, 60, 70 | 0 |
| 4 | 2E | 204/206 (99%) | 0.53 | 9 (4%) 34 41 | 32, 58, 73, 81 | 0 |
| 5 | 1F | 203/210 (96%) | 0.50 | 1 (0%) 91 94 | 22, 46, 68, 84 | 0 |
| 5 | 2F | 203/210 (96%) | 0.54 | 10 (4%) 29 35 | 36, 65, 77, 83 | 0 |
| 6 | 1G | 181/182 (99%) | 0.34 | 6 (3%) 46 53 | 47, 63, 74, 79 | 0 |
| 6 | 2G | 181/182 (99%) | 1.60 | 59 (32%) 0 0 | 70, 79, 86, 89 | 0 |
| 7 | 1H | 174/180 (96%) | 0.38 | 1 (0%) 89 92 | 38, 55, 66, 74 | 0 |
| 7 | 2H | 173/180 (96%) | 1.56 | 58 (33%) 0 0 | 66, 77, 83, 87 | 0 |
| 8 | 1I | 147/148 (99%) | 0.22 | 6 (4%) 37 44 | 46, 71, 79, 82 | 0 |
| 8 | 2I | 146/148 (98%) | 0.70 | 23 (15%) 2 2 | 60, 72, 81, 85 | 0 |
| 9 | 1N | 140/140 (100%) | 0.56 | 0 100 100 | 29, 42, 62, 79 | 0 |
| 9 | 2N | 140/140 (100%) | 0.79 | 9 (6%) 19 22 | 45, 62, 74, 80 | 0 |
| 10 | 1O | 122/122 (100%) | 0.55 | 0 100 100 | 32, 44, 58, 64 | 0 |
| 10 | 2O | 122/122 (100%) | 0.62 | 5 (4%) 37 44 | 49, 58, 68, 77 | 0 |
| 11 | 1P | 149/150 (99%) | 0.44 | 1 (0%) 87 90 | 23, 48, 66, 76 | 0 |
| 11 | 2P | 149/150 (99%) | 0.74 | 15 (10%) 7 8 | 39, 65, 77, 83 | 0 |
| 12 | 1Q | 141/141 (100%) | 0.55 | 1 (0%) 87 90 | 30, 44, 54, 65 | 0 |
| 12 | 2Q | 141/141 (100%) | 0.94 | 13 (9%) 9 10 | 47, 62, 72, 76 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 13 | 1R | 118/118 (100%) | 0.59 | 1 (0%) 86 89 | 30, 39, 53, 62 | 0 |
| 13 | 2R | 118/118 (100%) | 0.79 | 10 (8%) 10 12 | 42, 54, 63, 72 | 0 |
| 14 | 1S | 110/112 (98%) | 0.34 | 0 100 100 | 39, 51, 64, 69 | 0 |
| 14 | 2S | 110/112 (98%) | 0.75 | 16 (14%) 2 3 | 63, 70, 76, 79 | 0 |
| 15 | 1T | 131/146 (89%) | 0.54 | 2 (1%) 73 79 | 34, 48, 66, 80 | 0 |
| 15 | 2T | 131/146 (89%) | 0.58 | 8 (6%) 21 25 | 49, 60, 73, 78 | 0 |
| 16 | 1U | 116/118 (98%) | 0.85 | 4 (3%) 45 52 | 24, 35, 49, 67 | 0 |
| 16 | 2U | 116/118 (98%) | 0.88 | 16 (13%) 2 3 | 41, 59, 71, 76 | 0 |
| 17 | 1V | 101/101 (100%) | 0.64 | 1 (0%) 82 86 | 27, 44, 60, 67 | 0 |
| 17 | 2V | 101/101 (100%) | 0.43 | 6 (5%) 22 26 | 44, 65, 73, 78 | 0 |
| 18 | 1W | 112/113 (99%) | 0.60 | 0 100 100 | 26, 34, 55, 80 | 0 |
| 18 | 2W | 112/113 (99%) | 0.84 | 9 (8%) 12 15 | 39, 50, 65, 88 | 0 |
| 19 | 1X | 95/96 (98%) | 0.65 | 3 (3%) 47 55 | 30, 39, 60, 69 | 0 |
| 19 | 2X | 95/96 (98%) | 1.18 | 17 (17%) 1 1 | 48, 60, 71, 76 | 0 |
| 20 | 1Y | 107/110 (97%) | 0.43 | 0 100 100 | 35, 50, 65, 70 | 0 |
| 20 | 2Y | 107/110 (97%) | 1.11 | 17 (15%) 1 2 | 57, 67, 76, 81 | 0 |
| 21 | 1Z | 203/206 (98%) | 0.31 | 0 100 100 | 41, 58, 71, 80 | 0 |
| 21 | 2Z | 201/206 (97%) | 0.63 | 20 (9%) 7 9 | 65, 73, 79, 84 | 0 |
| 22 | 10 | 77/85 (90%) | 0.60 | 1 (1%) 77 82 | 31, 40, 56, 60 | 0 |
| 22 | 20 | 77/85 (90%) | 1.49 | 23 (29%) 0 0 | 50, 62, 70, 74 | 0 |
| 23 | 11 | 97/98 (98%) | 1.05 | 11 (11%) 5 6 | 31, 46, 65, 72 | 0 |
| 23 | 21 | 97/98 (98%) | 1.27 | 19 (19%) 1 1 | 43, 58, 72, 75 | 0 |
| 24 | 12 | 70/72 (97%) | 0.49 | 0 100 100 | 36, 50, 61, 76 | 0 |
| 24 | 22 | 70/72 (97%) | 0.70 | 6 (8%) 10 12 | 57, 66, 73, 76 | 0 |
| 25 | 13 | 59/60 (98%) | 0.48 | 0 100 100 | 30, 40, 60, 65 | 0 |
| 25 | 23 | 59/60 (98%) | 1.42 | 19 (32%) 0 0 | 50, 61, 75, 80 | 0 |
| 26 | 14 | 69/71 (97%) | 0.24 | 5 (7%) 15 18 | 55, 77, 87, 90 | 0 |
| 26 | 24 | 69/71 (97%) | 1.38 | 21 (30%) 0 0 | 74, 84, 89, 94 | 0 |
| 27 | 15 | 59/60 (98%) | 0.58 | 0 100 100 | 23, 38, 56, 63 | 0 |
| 27 | 25 | 59/60 (98%) | 0.50 | 0 100 100 | 37, 52, 66, 70 | 0 |
| 28 | 16 | 53/54 (98%) | 0.40 | 0 100 100 | 35, 46, 59, 64 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28 | 26 | 53/54 (98%) | 0.47 | 2 (3%) 40 47 | 52, 60, 68, 71 | 0 |
| 29 | 17 | 48/49 (97%) | 0.81 | 4 (8%) 11 13 | 23, 31, 55, 62 | 0 |
| 29 | 27 | 48/49 (97%) | 0.93 | 4 (8%) 11 13 | 34, 43, 63, 68 | 0 |
| 30 | 18 | 64/65 (98%) | 0.73 | 2 (3%) 49 56 | 30, 37, 45, 60 | 0 |
| 30 | 28 | 64/65 (98%) | 1.55 | 18 (28%) 0 0 | 44, 56, 64, 70 | 0 |
| 31 | 19 | 37/37 (100%) | 1.01 | 3 (8%) 12 15 | 35, 46, 62, 63 | 0 |
| 31 | 29 | 37/37 (100%) | 1.76 | 13 (35%) 0 0 | 57, 64, 76, 80 | 0 |
| 32 | 1a | 1488/1521 (97%) | -0.09 | 9 (0%) 89 92 | 42, 69, 88, 101 | 0 |
| 32 | 2a | 1492/1521 (98%) | -0.01 | 21 (1%) 75 81 | 55, 76, 91, 100 | 0 |
| 33 | 1b | 231/256 (90%) | 0.28 | 8 (3%) 44 51 | 66, 75, 82, 88 | 0 |
| 33 | 2b | 231/256 (90%) | 0.61 | 29 (12%) 3 4 | 71, 80, 86, 89 | 0 |
| 34 | 1c | 206/239 (86%) | 0.62 | 19 (9%) 9 10 | 57, 71, 78, 84 | 0 |
| 34 | 2c | 206/239 (86%) | 1.34 | 59 (28%) 0 0 | 72, 80, 86, 90 | 0 |
| 35 | 1d | 208/209 (99%) | 0.67 | 19 (9%) 9 11 | 58, 70, 77, 86 | 0 |
| 35 | 2d | 208/209 (99%) | 1.12 | 43 (20%) 1 0 | 64, 72, 79, 81 | 0 |
| 36 | 1e | 148/162 (91%) | 0.86 | 14 (9%) 8 10 | 56, 65, 73, 80 | 0 |
| 36 | 2e | 148/162 (91%) | 0.63 | 17 (11%) 4 6 | 63, 73, 80, 85 | 0 |
| 37 | 1f | 100/101 (99%) | 0.19 | 1 (1%) 82 86 | 58, 65, 73, 77 | 0 |
| 37 | 2f | 100/101 (99%) | 0.14 | 1 (1%) 82 86 | 59, 70, 76, 79 | 0 |
| 38 | 1g | 155/156 (99%) | 0.26 | 5 (3%) 47 55 | 61, 70, 77, 87 | 0 |
| 38 | 2g | 155/156 (99%) | 0.95 | 27 (17%) 1 1 | 69, 78, 83, 87 | 0 |
| 39 | 1h | 137/138 (99%) | 0.82 | 16 (11%) 4 6 | 59, 68, 74, 77 | 0 |
| 39 | 2h | 137/138 (99%) | 1.27 | 35 (25%) 0 0 | 65, 73, 78, 87 | 0 |
| 40 | 1i | 127/128 (99%) | 1.20 | 30 (23%) 0 0 | 58, 75, 81, 84 | 0 |
| 40 | 2i | 126/128 (98%) | 1.95 | 51 (40%) 0 0 | 74, 80, 84, 89 | 0 |
| 41 | 1j | 97/105 (92%) | 0.74 | 17 (17%) 1 1 | 64, 73, 83, 85 | 0 |
| 41 | 2j | 96/105 (91%) | 1.52 | 33 (34%) 0 0 | 71, 81, 86, 88 | 0 |
| 42 | 1k | 114/129 (88%) | 0.41 | 4 (3%) 44 51 | 44, 64, 71, 76 | 0 |
| 42 | 2k | 114/129 (88%) | 0.68 | 8 (7%) 16 19 | 61, 72, 79, 84 | 0 |
| 43 | 1l | 121/132 (91%) | 0.76 | 11 (9%) 9 11 | 53, 60, 69, 74 | 0 |
| 43 | 2l | 121/132 (91%) | 1.21 | 28 (23%) 0 0 | 59, 68, 76, 79 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | 1m | 116/126 (92%) | 0.70 | 13 (11%) 5 7 | 58, 72, 78, 84 | 0 |
| 44 | 2m | 114/126 (90%) | 1.80 | 43 (37%) 0 0 | 74, 80, 84, 85 | 0 |
| 45 | 1n | 60/61 (98%) | 2.25 | 30 (50%) 0 0 | 63, 69, 75, 75 | 0 |
| 45 | 2n | 60/61 (98%) | 3.24 | 43 (71%) 0 0 | 73, 80, 85, 87 | 0 |
| 46 | 1o | 88/89 (98%) | 0.45 | 3 (3%) 45 52 | 50, 65, 75, 78 | 0 |
| 46 | 2o | 88/89 (98%) | 0.85 | 11 (12%) 3 5 | 65, 73, 78, 84 | 0 |
| 47 | 1p | 82/88 (93%) | 1.56 | 23 (28%) 0 0 | 61, 70, 77, 81 | 0 |
| 47 | 2p | 82/88 (93%) | 1.25 | 19 (23%) 0 0 | 63, 71, 75, 80 | 0 |
| 48 | 1q | 99/105 (94%) | 0.85 | 6 (6%) 21 25 | 58, 66, 75, 77 | 0 |
| 48 | 2q | 99/105 (94%) | 1.61 | 34 (34%) 0 0 | 61, 70, 77, 82 | 0 |
| 49 | 1r | 68/88 (77%) | 0.54 | 5 (7%) 14 18 | 58, 65, 74, 80 | 0 |
| 49 | 2r | 68/88 (77%) | 0.60 | 5 (7%) 14 18 | 65, 73, 80, 82 | 0 |
| 50 | 1s | 83/93 (89%) | 0.37 | 2 (2%) 59 65 | 65, 73, 80, 83 | 0 |
| 50 | 2s | 83/93 (89%) | 1.76 | 38 (45%) 0 0 | 71, 81, 86, 88 | 0 |
| 51 | 1t | 96/106 (90%) | 1.36 | 31 (32%) 0 0 | 62, 69, 79, 84 | 0 |
| 51 | 2t | 98/106 (92%) | 1.39 | 30 (30%) 0 0 | 59, 69, 76, 81 | 0 |
| 52 | 1u | 23/27 (85%) | 1.82 | 9 (39%) 0 0 | 67, 72, 78, 79 | 0 |
| 52 | 2u | 23/27 (85%) | 2.12 | 11 (47%) 0 0 | 74, 78, 82, 83 | 0 |
| 53 | 1y | 97/113 (85%) | 0.75 | 9 (9%) 8 10 | 54, 63, 73, 75 | 0 |
| 53 | 2y | 96/113 (84%) | 2.28 | 49 (51%) 0 0 | 67, 76, 82, 84 | 0 |
| All | All | 20766/21468 (96%) | 0.51 | 1547 (7%) 14 18 | 22, 64, 84, 104 | 0 |

The worst 5 of 1547 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | 2n | 2 | ALA | 10.8 |
| 1 | 1A | 1087 | G | 8.2 |
| 8 | 2I | 3 | VAL | 8.0 |
| 1 | 1A | 1090 | U | 7.9 |
| 40 | 2i | 115 | GLY | 7.8 |

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 32 | 5MC | 2a | 967 | 21/22 | 0.91 | 0.20 | 71,76,81,84 | 0 |
| 43 | 0TD | 2l | 92 | 10/11 | 0.91 | 0.21 | 67,70,73,81 | 0 |
| 32 | M2G | 2a | 966 | 25/26 | 0.91 | 0.20 | 69,76,86,98 | 0 |
| 1 | 5MU | 2A | 1915 | 21/22 | 0.92 | 0.11 | 80,84,88,102 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.92 | 0.12 | 73,79,95,99 | 0 |
| 32 | 4OC | 2a | 1402 | 22/23 | 0.93 | 0.18 | 62,69,73,81 | 0 |
| 32 | PSU | 2a | 516 | 20/21 | 0.93 | 0.12 | 76,79,84,89 | 0 |
| 1 | 4OC | 2A | 1920 | 21/23 | 0.93 | 0.16 | 67,70,73,76 | 0 |
| 32 | 2MG | 1a | 1207 | 24/25 | 0.93 | 0.14 | 63,72,76,80 | 0 |
| 32 | 2MG | 2a | 1207 | 24/25 | 0.93 | 0.13 | 77,85,88,97 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.93 | 0.11 | 68,74,86,88 | 0 |
| 32 | 5MC | 2a | 1404 | 21/22 | 0.94 | 0.19 | 63,68,70,73 | 0 |
| 43 | 0TD | 1l | 92 | 10/11 | 0.94 | 0.17 | 51,59,63,68 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.94 | 0.12 | 68,75,80,84 | 0 |
| 1 | PSU | 1A | 1911 | 20/21 | 0.94 | 0.14 | 61,69,76,82 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.95 | 0.13 | 65,72,76,79 | 0 |
| 32 | M2G | 1a | 966 | 25/26 | 0.96 | 0.20 | 54,65,71,77 | 0 |
| 32 | 5MC | 1a | 967 | 21/22 | 0.96 | 0.21 | 65,71,75,80 | 0 |
| 32 | 7MG | 2a | 527 | 24/25 | 0.96 | 0.15 | 64,69,71,76 | 0 |
| 32 | 5MC | 2a | 1407 | 21/22 | 0.96 | 0.16 | 60,68,72,78 | 0 |
| 32 | MA6 | 2a | 1519 | 24/25 | 0.96 | 0.21 | 62,67,71,76 | 0 |
| 32 | 5MC | 1a | 1407 | 21/22 | 0.96 | 0.19 | 46,56,62,67 | 0 |
| 32 | MA6 | 2a | 1518 | 24/25 | 0.96 | 0.23 | 63,70,73,75 | 0 |
| 32 | 7MG | 1a | 527 | 24/25 | 0.96 | 0.17 | 50,57,62,62 | 0 |
| 32 | PSU | 1a | 516 | 20/21 | 0.96 | 0.14 | 61,67,71,77 | 0 |
| 32 | UR3 | 2a | 1498 | 21/22 | 0.96 | 0.17 | 57,64,70,75 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.97 | 0.21 | 42,46,51,51 | 0 |
| 1 | 4OC | 1A | 1920 | 21/23 | 0.97 | 0.18 | 47,62,69,73 | 0 |
| 32 | 5MC | 2a | 1400 | 21/22 | 0.97 | 0.26 | 67,74,78,81 | 0 |
| 32 | MA6 | 1a | 1519 | 24/25 | 0.97 | 0.21 | 48,54,58,62 | 0 |
| 32 | MA6 | 1a | 1518 | 24/25 | 0.97 | 0.23 | 44,53,57,60 | 0 |
| 32 | 4OC | 1a | 1402 | 22/23 | 0.97 | 0.19 | 50,55,61,64 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.97 | 0.22 | 31,37,43,44 | 0 |
| 1 | PSU | 2A | 2605 | 20/21 | 0.97 | 0.23 | 37,41,48,49 | 0 |
| 32 | 5MC | 1a | 1400 | 21/22 | 0.97 | 0.21 | 43,56,64,66 | 0 |
| 32 | 5MC | 1a | 1404 | 21/22 | 0.97 | 0.17 | 49,54,59,61 | 0 |
| 1 | 5MU | 2A | 1939 | 21/22 | 0.98 | 0.19 | 39,48,50,53 | 0 |
| 1 | 2MU | 2A | 2552 | 21/23 | 0.98 | 0.18 | 40,46,51,53 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.98 | 0.16 | 44,53,56,59 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.98 | 0.17 | 29,34,38,40 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.98 | 0.16 | 43,57,62,67 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1 | 5MC | 1A | 1962 | 21/22 | 0.98 | 0.18 | 30,39,45,47 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.98 | 0.18 | 30,33,38,39 | 0 |
| 32 | UR3 | 1a | 1498 | 21/22 | 0.98 | 0.18 | 49,55,59,65 | 0 |
| 1 | 2MU | 1A | 2552 | 21/23 | 0.98 | 0.20 | 30,35,38,43 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.99 | 0.16 | 35,42,48,56 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.99 | 0.20 | 24,29,33,33 | 0 |
| 1 | 2MA | 1A | 2503 | 23/24 | 0.99 | 0.21 | 20,25,30,32 | 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2a | 3056 | 1/1 | 0.38 | 0.18 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3244 | 1/1 | 0.45 | 0.16 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3651 | 1/1 | 0.46 | 0.19 | 81,81,81,81 | 0 |
| 54 | MG | 2A | 3577 | 1/1 | 0.48 | 0.17 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3170 | 1/1 | 0.49 | 0.33 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3667 | 1/1 | 0.52 | 0.12 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3945 | 1/1 | 0.52 | 0.18 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3630 | 1/1 | 0.55 | 0.26 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3436 | 1/1 | 0.55 | 0.16 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3557 | 1/1 | 0.56 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3695 | 1/1 | 0.56 | 0.09 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3115 | 1/1 | 0.56 | 0.23 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3285 | 1/1 | 0.57 | 0.24 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3965 | 1/1 | 0.62 | 0.22 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3622 | 1/1 | 0.63 | 0.15 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3539 | 1/1 | 0.64 | 0.07 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3604 | 1/1 | 0.65 | 0.12 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3593 | 1/1 | 0.65 | 0.20 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 4010 | 1/1 | 0.66 | 0.09 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3109 | 1/1 | 0.66 | 0.32 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3917 | 1/1 | 0.67 | 0.16 | 35,35,35,35 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3613 | 1/1 | 0.67 | 0.15 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3721 | 1/1 | 0.68 | 0.19 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3870 | 1/1 | 0.69 | 0.13 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1800 | 1/1 | 0.69 | 0.14 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1604 | 1/1 | 0.69 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 2a | 3069 | 1/1 | 0.70 | 0.16 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3486 | 1/1 | 0.70 | 0.19 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3219 | 1/1 | 0.71 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3512 | 1/1 | 0.71 | 0.09 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3525 | 1/1 | 0.71 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3044 | 1/1 | 0.71 | 0.11 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3986 | 1/1 | 0.71 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | 2F | 303 | 1/1 | 0.72 | 0.14 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3475 | 1/1 | 0.72 | 0.18 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3185 | 1/1 | 0.72 | 0.14 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3150 | 1/1 | 0.72 | 0.15 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1786 | 1/1 | 0.72 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3883 | 1/1 | 0.72 | 0.08 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3566 | 1/1 | 0.72 | 0.14 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1760 | 1/1 | 0.72 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3009 | 1/1 | 0.73 | 0.23 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1775 | 1/1 | 0.73 | 0.26 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1756 | 1/1 | 0.73 | 0.23 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3385 | 1/1 | 0.73 | 0.20 | 33,33,33,33 | 0 |
| 54 | MG | 2a | 3105 | 1/1 | 0.73 | 0.18 | 71,71,71,71 | 0 |
| 54 | MG | 2B | 217 | 1/1 | 0.73 | 0.07 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3598 | 1/1 | 0.74 | 0.11 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3254 | 1/1 | 0.74 | 0.32 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1766 | 1/1 | 0.74 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3106 | 1/1 | 0.74 | 0.18 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1810 | 1/1 | 0.74 | 0.09 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3693 | 1/1 | 0.74 | 0.16 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3196 | 1/1 | 0.74 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 18 | 102 | 1/1 | 0.74 | 0.12 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1742 | 1/1 | 0.74 | 0.17 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1859 | 1/1 | 0.75 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3040 | 1/1 | 0.75 | 0.13 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3582 | 1/1 | 0.75 | 0.14 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3285 | 1/1 | 0.75 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3521 | 1/1 | 0.75 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3732 | 1/1 | 0.75 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1825 | 1/1 | 0.75 | 0.10 | 71,71,71,71 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2O | 202 | 1/1 | 0.75 | 0.19 | 80,80,80,80 | 0 |
| 54 | MG | 1a | 1844 | 1/1 | 0.76 | 0.18 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3989 | 1/1 | 0.76 | 0.69 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3321 | 1/1 | 0.76 | 0.13 | 63,63,63,63 | 0 |
| 54 | MG | 1D | 312 | 1/1 | 0.76 | 0.16 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3014 | 1/1 | 0.76 | 0.21 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3591 | 1/1 | 0.76 | 0.12 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1774 | 1/1 | 0.76 | 0.20 | 70,70,70,70 | 0 |
| 54 | MG | 2a | 3085 | 1/1 | 0.76 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3586 | 1/1 | 0.76 | 0.17 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3036 | 1/1 | 0.76 | 0.19 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3233 | 1/1 | 0.76 | 0.18 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3660 | 1/1 | 0.76 | 0.07 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3619 | 1/1 | 0.77 | 0.16 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3024 | 1/1 | 0.77 | 0.47 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3025 | 1/1 | 0.77 | 0.19 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3215 | 1/1 | 0.77 | 0.11 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3048 | 1/1 | 0.77 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 2a | 3106 | 1/1 | 0.77 | 0.24 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3547 | 1/1 | 0.77 | 0.08 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1693 | 1/1 | 0.77 | 0.17 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3288 | 1/1 | 0.77 | 0.18 | 60,60,60,60 | 0 |
| 54 | MG | 2a | 3065 | 1/1 | 0.77 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3618 | 1/1 | 0.77 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 1G | 203 | 1/1 | 0.77 | 0.19 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3093 | 1/1 | 0.77 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3295 | 1/1 | 0.77 | 0.14 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3222 | 1/1 | 0.77 | 0.12 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1746 | 1/1 | 0.77 | 0.15 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3473 | 1/1 | 0.77 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3676 | 1/1 | 0.78 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3707 | 1/1 | 0.78 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3915 | 1/1 | 0.78 | 0.08 | 50,50,50,50 | 0 |
| 54 | MG | 2a | 3141 | 1/1 | 0.78 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3679 | 1/1 | 0.78 | 0.11 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3179 | 1/1 | 0.78 | 0.12 | 60,60,60,60 | 0 |
| 54 | MG | 1Y | 202 | 1/1 | 0.78 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3062 | 1/1 | 0.78 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3172 | 1/1 | 0.78 | 0.08 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3126 | 1/1 | 0.78 | 0.08 | 65,65,65,65 | 0 |
| 54 | MG | 1b | 301 | 1/1 | 0.78 | 0.12 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3420 | 1/1 | 0.78 | 0.24 | 73,73,73,73 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 4016 | 1/1 | 0.78 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | 2B | 201 | 1/1 | 0.78 | 0.11 | 75,75,75,75 | 0 |
| 54 | MG | 2a | 3037 | 1/1 | 0.78 | 0.19 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3255 | 1/1 | 0.78 | 0.35 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1688 | 1/1 | 0.78 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3449 | 1/1 | 0.78 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3923 | 1/1 | 0.78 | 0.16 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3345 | 1/1 | 0.78 | 0.10 | 41,41,41,41 | 0 |
| 54 | MG | 1a | 1715 | 1/1 | 0.78 | 0.14 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1757 | 1/1 | 0.78 | 0.21 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3004 | 1/1 | 0.78 | 0.13 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3311 | 1/1 | 0.78 | 0.12 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1706 | 1/1 | 0.78 | 0.18 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3625 | 1/1 | 0.79 | 0.07 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3491 | 1/1 | 0.79 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3675 | 1/1 | 0.79 | 0.17 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3231 | 1/1 | 0.79 | 0.16 | 49,49,49,49 | 0 |
| 54 | MG | 20 | 102 | 1/1 | 0.79 | 0.17 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3529 | 1/1 | 0.79 | 0.34 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3017 | 1/1 | 0.79 | 0.17 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3480 | 1/1 | 0.79 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3406 | 1/1 | 0.79 | 0.15 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3997 | 1/1 | 0.79 | 0.10 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3220 | 1/1 | 0.79 | 0.19 | 66,66,66,66 | 0 |
| 54 | MG | 1h | 202 | 1/1 | 0.79 | 0.12 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1641 | 1/1 | 0.79 | 0.13 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3481 | 1/1 | 0.80 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3134 | 1/1 | 0.80 | 0.10 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1608 | 1/1 | 0.80 | 0.09 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3210 | 1/1 | 0.80 | 0.15 | 56,56,56,56 | 0 |
| 58 | ZN | 2Y | 501 | 1/1 | 0.80 | 0.15 | 84,84,84,84 | 0 |
| 54 | MG | 1a | 1621 | 1/1 | 0.80 | 0.11 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3287 | 1/1 | 0.80 | 0.13 | 69,69,69,69 | 0 |
| 54 | MG | 2a | 3019 | 1/1 | 0.80 | 0.18 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3638 | 1/1 | 0.80 | 0.07 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1865 | 1/1 | 0.80 | 0.06 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3529 | 1/1 | 0.80 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3580 | 1/1 | 0.80 | 0.20 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3283 | 1/1 | 0.80 | 0.14 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3611 | 1/1 | 0.80 | 0.50 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3473 | 1/1 | 0.80 | 0.13 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1848 | 1/1 | 0.80 | 0.11 | 70,70,70,70 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1674 | 1/1 | 0.80 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3121 | 1/1 | 0.80 | 0.25 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3589 | 1/1 | 0.80 | 0.11 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3328 | 1/1 | 0.80 | 0.21 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3091 | 1/1 | 0.80 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3378 | 1/1 | 0.80 | 0.11 | 39,39,39,39 | 0 |
| 54 | MG | 2G | 201 | 1/1 | 0.80 | 0.23 | 78,78,78,78 | 0 |
| 54 | MG | 1a | 1816 | 1/1 | 0.80 | 0.09 | 92,92,92,92 | 0 |
| 54 | MG | 2A | 3640 | 1/1 | 0.81 | 0.06 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1798 | 1/1 | 0.81 | 0.19 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3151 | 1/1 | 0.81 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3063 | 1/1 | 0.81 | 0.45 | 54,54,54,54 | 0 |
| 54 | MG | 1a | 1753 | 1/1 | 0.81 | 0.25 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3519 | 1/1 | 0.81 | 0.17 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3119 | 1/1 | 0.81 | 0.13 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3633 | 1/1 | 0.81 | 0.65 | 45,45,45,45 | 0 |
| 54 | MG | 2a | 3072 | 1/1 | 0.81 | 0.14 | 72,72,72,72 | 0 |
| 57 | ARG | 1F | 319 | 12/12 | 0.81 | 0.16 | 55,65,74,77 | 0 |
| 54 | MG | 2A | 3186 | 1/1 | 0.81 | 0.35 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1624 | 1/1 | 0.81 | 0.16 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1682 | 1/1 | 0.81 | 0.26 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3161 | 1/1 | 0.81 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3172 | 1/1 | 0.81 | 0.21 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1777 | 1/1 | 0.81 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3183 | 1/1 | 0.81 | 0.37 | 54,54,54,54 | 0 |
| 54 | MG | 1G | 202 | 1/1 | 0.81 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3588 | 1/1 | 0.81 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3722 | 1/1 | 0.81 | 0.30 | 73,73,73,73 | 0 |
| 54 | MG | 2a | 3054 | 1/1 | 0.81 | 0.10 | 70,70,70,70 | 0 |
| 54 | MG | 2a | 3020 | 1/1 | 0.81 | 0.08 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1813 | 1/1 | 0.81 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1849 | 1/1 | 0.81 | 0.21 | 85,85,85,85 | 0 |
| 54 | MG | 2A | 3401 | 1/1 | 0.82 | 0.17 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3060 | 1/1 | 0.82 | 0.13 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3413 | 1/1 | 0.82 | 0.14 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3588 | 1/1 | 0.82 | 0.27 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3435 | 1/1 | 0.82 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3990 | 1/1 | 0.82 | 0.17 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3356 | 1/1 | 0.82 | 0.10 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3363 | 1/1 | 0.82 | 0.29 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1696 | 1/1 | 0.82 | 0.13 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3235 | 1/1 | 0.82 | 0.31 | 62,62,62,62 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3944 | 1/1 | 0.82 | 0.22 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3042 | 1/1 | 0.82 | 0.13 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1689 | 1/1 | 0.82 | 0.10 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3464 | 1/1 | 0.82 | 0.07 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1857 | 1/1 | 0.82 | 0.11 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3062 | 1/1 | 0.82 | 0.11 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1668 | 1/1 | 0.82 | 0.21 | 64,64,64,64 | 0 |
| 54 | MG | 1l | 103 | 1/1 | 0.82 | 0.19 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3301 | 1/1 | 0.82 | 0.23 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3654 | 1/1 | 0.82 | 0.13 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3187 | 1/1 | 0.82 | 0.15 | 66,66,66,66 | 0 |
| 54 | MG | 2B | 214 | 1/1 | 0.82 | 0.11 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3562 | 1/1 | 0.82 | 0.12 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3032 | 1/1 | 0.83 | 0.13 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3922 | 1/1 | 0.83 | 0.09 | 43,43,43,43 | 0 |
| 54 | MG | 2a | 3090 | 1/1 | 0.83 | 0.09 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1828 | 1/1 | 0.83 | 0.13 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3166 | 1/1 | 0.83 | 0.09 | 66,66,66,66 | 0 |
| 54 | MG | 2f | 201 | 1/1 | 0.83 | 0.11 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1665 | 1/1 | 0.83 | 0.15 | 71,71,71,71 | 0 |
| 54 | MG | 10 | 105 | 1/1 | 0.83 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3469 | 1/1 | 0.83 | 0.25 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3230 | 1/1 | 0.83 | 0.26 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3494 | 1/1 | 0.83 | 0.09 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1645 | 1/1 | 0.83 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3457 | 1/1 | 0.83 | 0.14 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3072 | 1/1 | 0.83 | 0.28 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3133 | 1/1 | 0.83 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3424 | 1/1 | 0.83 | 0.12 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3272 | 1/1 | 0.83 | 0.08 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3722 | 1/1 | 0.83 | 0.08 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3131 | 1/1 | 0.83 | 0.21 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1874 | 1/1 | 0.83 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3557 | 1/1 | 0.83 | 0.07 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3059 | 1/1 | 0.83 | 0.37 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3511 | 1/1 | 0.83 | 0.17 | 38,38,38,38 | 0 |
| 54 | MG | 2a | 3089 | 1/1 | 0.83 | 0.15 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1603 | 1/1 | 0.83 | 0.19 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3528 | 1/1 | 0.83 | 0.20 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3001 | 1/1 | 0.83 | 0.22 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3817 | 1/1 | 0.83 | 0.28 | 41,41,41,41 | 0 |
| 54 | MG | 1a | 1695 | 1/1 | 0.83 | 0.09 | 54,54,54,54 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3187 | 1/1 | 0.83 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | 1B | 222 | 1/1 | 0.83 | 0.22 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3523 | 1/1 | 0.83 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3628 | 1/1 | 0.84 | 0.23 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3456 | 1/1 | 0.84 | 0.15 | 61,61,61,61 | 0 |
| 54 | MG | 2a | 3015 | 1/1 | 0.84 | 0.14 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3221 | 1/1 | 0.84 | 0.13 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3895 | 1/1 | 0.84 | 0.12 | 27,27,27,27 | 0 |
| 54 | MG | 2a | 3058 | 1/1 | 0.84 | 0.19 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 4014 | 1/1 | 0.84 | 0.17 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3002 | 1/1 | 0.84 | 0.47 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3832 | 1/1 | 0.84 | 0.08 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3830 | 1/1 | 0.84 | 0.14 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3971 | 1/1 | 0.84 | 0.19 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3190 | 1/1 | 0.84 | 0.27 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3034 | 1/1 | 0.84 | 0.17 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1870 | 1/1 | 0.84 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3615 | 1/1 | 0.84 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2E | 304 | 1/1 | 0.84 | 0.14 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1661 | 1/1 | 0.84 | 0.80 | 74,74,74,74 | 0 |
| 54 | MG | 1d | 302 | 1/1 | 0.84 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3216 | 1/1 | 0.84 | 0.30 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3510 | 1/1 | 0.84 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 2a | 3061 | 1/1 | 0.84 | 0.15 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3425 | 1/1 | 0.84 | 0.20 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1811 | 1/1 | 0.84 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3787 | 1/1 | 0.84 | 0.16 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3465 | 1/1 | 0.84 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3227 | 1/1 | 0.84 | 0.40 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3030 | 1/1 | 0.84 | 0.12 | 34,34,34,34 | 0 |
| 54 | MG | 2a | 3040 | 1/1 | 0.84 | 0.10 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3935 | 1/1 | 0.84 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3925 | 1/1 | 0.84 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3590 | 1/1 | 0.84 | 0.12 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3012 | 1/1 | 0.84 | 0.64 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1714 | 1/1 | 0.84 | 0.11 | 77,77,77,77 | 0 |
| 54 | MG | 19 | 101 | 1/1 | 0.85 | 0.14 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1657 | 1/1 | 0.85 | 0.28 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3856 | 1/1 | 0.85 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3003 | 1/1 | 0.85 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3292 | 1/1 | 0.85 | 0.17 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3047 | 1/1 | 0.85 | 0.28 | 60,60,60,60 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3417 | 1/1 | 0.85 | 0.08 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1671 | 1/1 | 0.85 | 0.06 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3443 | 1/1 | 0.85 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3721 | 1/1 | 0.85 | 0.14 | 42,42,42,42 | 0 |
| 54 | MG | 1a | 1808 | 1/1 | 0.85 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3640 | 1/1 | 0.85 | 0.27 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3835 | 1/1 | 0.85 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 1V | 206 | 1/1 | 0.85 | 0.20 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3587 | 1/1 | 0.85 | 0.09 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3278 | 1/1 | 0.85 | 0.15 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3303 | 1/1 | 0.85 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3704 | 1/1 | 0.85 | 0.13 | 52,52,52,52 | 0 |
| 54 | MG | 2a | 3007 | 1/1 | 0.85 | 0.15 | 72,72,72,72 | 0 |
| 54 | MG | 2a | 3070 | 1/1 | 0.85 | 0.12 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3772 | 1/1 | 0.85 | 0.11 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3672 | 1/1 | 0.85 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 2a | 3023 | 1/1 | 0.85 | 0.09 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3819 | 1/1 | 0.85 | 0.44 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1801 | 1/1 | 0.85 | 0.05 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3117 | 1/1 | 0.85 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3731 | 1/1 | 0.85 | 0.25 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1797 | 1/1 | 0.85 | 0.13 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3383 | 1/1 | 0.85 | 0.14 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3789 | 1/1 | 0.85 | 0.31 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3057 | 1/1 | 0.85 | 0.23 | 64,64,64,64 | 0 |
| 54 | MG | 1F | 317 | 1/1 | 0.85 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3080 | 1/1 | 0.85 | 0.10 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3296 | 1/1 | 0.85 | 0.07 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1685 | 1/1 | 0.85 | 0.32 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3602 | 1/1 | 0.85 | 0.06 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1660 | 1/1 | 0.85 | 0.31 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3748 | 1/1 | 0.85 | 0.18 | 21,21,21,21 | 0 |
| 54 | MG | 1T | 202 | 1/1 | 0.85 | 0.14 | 77,77,77,77 | 0 |
| 54 | MG | 1H | 202 | 1/1 | 0.85 | 0.13 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3035 | 1/1 | 0.85 | 0.11 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3054 | 1/1 | 0.85 | 0.13 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1731 | 1/1 | 0.85 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 1P | 204 | 1/1 | 0.85 | 0.58 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3723 | 1/1 | 0.86 | 0.10 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3180 | 1/1 | 0.86 | 0.09 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3327 | 1/1 | 0.86 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3110 | 1/1 | 0.86 | 0.26 | 57,57,57,57 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3089 | 1/1 | 0.86 | 0.15 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3857 | 1/1 | 0.86 | 0.26 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3585 | 1/1 | 0.86 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3276 | 1/1 | 0.86 | 0.20 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3865 | 1/1 | 0.86 | 0.13 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3571 | 1/1 | 0.86 | 0.15 | 23,23,23,23 | 0 |
| 54 | MG | 1A | 3097 | 1/1 | 0.86 | 0.23 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1732 | 1/1 | 0.86 | 0.10 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1802 | 1/1 | 0.86 | 0.17 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3711 | 1/1 | 0.86 | 0.26 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3183 | 1/1 | 0.86 | 0.10 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3055 | 1/1 | 0.86 | 0.12 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3458 | 1/1 | 0.86 | 0.11 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1618 | 1/1 | 0.86 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3368 | 1/1 | 0.86 | 0.12 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3177 | 1/1 | 0.86 | 0.47 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3024 | 1/1 | 0.86 | 0.18 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3022 | 1/1 | 0.86 | 0.25 | 49,49,49,49 | 0 |
| 54 | MG | 1n | 102 | 1/1 | 0.86 | 0.16 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3210 | 1/1 | 0.86 | 0.50 | 46,46,46,46 | 0 |
| 54 | MG | 15 | 106 | 1/1 | 0.86 | 0.23 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3983 | 1/1 | 0.86 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 2G | 203 | 1/1 | 0.86 | 0.07 | 70,70,70,70 | 0 |
| 58 | ZN | 24 | 501 | 1/1 | 0.86 | 0.04 | 122,122,122,122 | 0 |
| 54 | MG | 2A | 3306 | 1/1 | 0.86 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3582 | 1/1 | 0.86 | 0.10 | 83,83,83,83 | 0 |
| 54 | MG | 1a | 1652 | 1/1 | 0.86 | 0.32 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3361 | 1/1 | 0.86 | 0.21 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3193 | 1/1 | 0.86 | 0.12 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1752 | 1/1 | 0.86 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3418 | 1/1 | 0.86 | 0.44 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3994 | 1/1 | 0.86 | 0.41 | 48,48,48,48 | 0 |
| 54 | MG | 1E | 306 | 1/1 | 0.86 | 0.12 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3699 | 1/1 | 0.86 | 0.34 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3612 | 1/1 | 0.86 | 0.21 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1826 | 1/1 | 0.86 | 0.10 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3301 | 1/1 | 0.86 | 0.19 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3271 | 1/1 | 0.86 | 0.10 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3131 | 1/1 | 0.86 | 0.12 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3150 | 1/1 | 0.86 | 0.08 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3701 | 1/1 | 0.86 | 0.13 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3639 | 1/1 | 0.86 | 0.25 | 73,73,73,73 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3114 | 1/1 | 0.86 | 0.24 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3755 | 1/1 | 0.86 | 0.23 | 77,77,77,77 | 0 |
| 54 | MG | 1a | 1821 | 1/1 | 0.86 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3514 | 1/1 | 0.86 | 0.10 | 34,34,34,34 | 0 |
| 54 | MG | 1B | 209 | 1/1 | 0.87 | 0.34 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3907 | 1/1 | 0.87 | 0.07 | 37,37,37,37 | 0 |
| 54 | MG | 1t | 201 | 1/1 | 0.87 | 0.13 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3371 | 1/1 | 0.87 | 0.08 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3498 | 1/1 | 0.87 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3382 | 1/1 | 0.87 | 0.27 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 4003 | 1/1 | 0.87 | 0.15 | 90,90,90,90 | 0 |
| 56 | MPD | 2B | 219 | 8/8 | 0.87 | 0.16 | 61,71,72,75 | 0 |
| 54 | MG | 1A | 3694 | 1/1 | 0.87 | 0.26 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 4001 | 1/1 | 0.87 | 0.25 | 62,62,62,62 | 0 |
| 54 | MG | 2a | 3022 | 1/1 | 0.87 | 0.16 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3412 | 1/1 | 0.87 | 0.11 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3463 | 1/1 | 0.87 | 0.15 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3033 | 1/1 | 0.87 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 1B | 207 | 1/1 | 0.87 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3671 | 1/1 | 0.87 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3428 | 1/1 | 0.87 | 0.24 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3705 | 1/1 | 0.87 | 0.24 | 55,55,55,55 | 0 |
| 54 | MG | 2e | 201 | 1/1 | 0.87 | 0.26 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3231 | 1/1 | 0.87 | 0.28 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3196 | 1/1 | 0.87 | 0.26 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3245 | 1/1 | 0.87 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3016 | 1/1 | 0.87 | 0.19 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1719 | 1/1 | 0.87 | 0.16 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3569 | 1/1 | 0.87 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1672 | 1/1 | 0.87 | 0.28 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3454 | 1/1 | 0.87 | 0.12 | 39,39,39,39 | 0 |
| 54 | MG | 1y | 201 | 1/1 | 0.87 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3354 | 1/1 | 0.87 | 0.19 | 63,63,63,63 | 0 |
| 54 | MG | 2T | 3301 | 1/1 | 0.87 | 0.18 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3342 | 1/1 | 0.87 | 0.14 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3616 | 1/1 | 0.87 | 0.18 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3169 | 1/1 | 0.87 | 0.31 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3479 | 1/1 | 0.87 | 0.16 | 22,22,22,22 | 0 |
| 54 | MG | 2A | 3550 | 1/1 | 0.87 | 0.13 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3543 | 1/1 | 0.87 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3188 | 1/1 | 0.87 | 0.17 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3522 | 1/1 | 0.87 | 0.19 | 41,41,41,41 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3634 | 1/1 | 0.87 | 0.29 | 75,75,75,75 | 0 |
| 54 | MG | 2a | 3128 | 1/1 | 0.87 | 0.14 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3240 | 1/1 | 0.87 | 0.20 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1678 | 1/1 | 0.87 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1784 | 1/1 | 0.87 | 0.14 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3881 | 1/1 | 0.87 | 0.13 | 29,29,29,29 | 0 |
| 54 | MG | 1a | 1707 | 1/1 | 0.87 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3354 | 1/1 | 0.87 | 0.17 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3484 | 1/1 | 0.87 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 2a | 3027 | 1/1 | 0.88 | 0.26 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1680 | 1/1 | 0.88 | 0.19 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3253 | 1/1 | 0.88 | 0.07 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1794 | 1/1 | 0.88 | 0.43 | 86,86,86,86 | 0 |
| 54 | MG | 1B | 228 | 1/1 | 0.88 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3209 | 1/1 | 0.88 | 0.09 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3823 | 1/1 | 0.88 | 0.17 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3826 | 1/1 | 0.88 | 0.11 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3336 | 1/1 | 0.88 | 0.10 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3487 | 1/1 | 0.88 | 0.17 | 41,41,41,41 | 0 |
| 54 | MG | 1a | 1647 | 1/1 | 0.88 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3631 | 1/1 | 0.88 | 0.16 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3260 | 1/1 | 0.88 | 0.16 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 4002 | 1/1 | 0.88 | 0.15 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3080 | 1/1 | 0.88 | 0.26 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3063 | 1/1 | 0.88 | 0.15 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1763 | 1/1 | 0.88 | 0.20 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3745 | 1/1 | 0.88 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3221 | 1/1 | 0.88 | 0.16 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3234 | 1/1 | 0.88 | 0.55 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3927 | 1/1 | 0.88 | 0.17 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1819 | 1/1 | 0.88 | 0.16 | 75,75,75,75 | 0 |
| 54 | MG | 2a | 3133 | 1/1 | 0.88 | 0.11 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3309 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3125 | 1/1 | 0.88 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3533 | 1/1 | 0.88 | 0.12 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3220 | 1/1 | 0.88 | 0.21 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3175 | 1/1 | 0.88 | 0.13 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3534 | 1/1 | 0.88 | 0.10 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3642 | 1/1 | 0.88 | 0.30 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3882 | 1/1 | 0.88 | 0.13 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3198 | 1/1 | 0.88 | 0.48 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3951 | 1/1 | 0.88 | 0.17 | 44,44,44,44 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3718 | 1/1 | 0.88 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3388 | 1/1 | 0.88 | 0.23 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3827 | 1/1 | 0.88 | 0.26 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3057 | 1/1 | 0.88 | 0.18 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3261 | 1/1 | 0.88 | 0.10 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3578 | 1/1 | 0.88 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3516 | 1/1 | 0.88 | 0.36 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3028 | 1/1 | 0.88 | 0.08 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3924 | 1/1 | 0.88 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3728 | 1/1 | 0.88 | 0.16 | 28,28,28,28 | 0 |
| 54 | MG | 2A | 3373 | 1/1 | 0.88 | 0.19 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1610 | 1/1 | 0.88 | 0.30 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3904 | 1/1 | 0.88 | 0.18 | 37,37,37,37 | 0 |
| 54 | MG | 2F | 302 | 1/1 | 0.88 | 0.12 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3708 | 1/1 | 0.88 | 0.08 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3405 | 1/1 | 0.88 | 0.09 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3346 | 1/1 | 0.88 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3423 | 1/1 | 0.88 | 0.40 | 77,77,77,77 | 0 |
| 54 | MG | 1B | 220 | 1/1 | 0.88 | 0.16 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3575 | 1/1 | 0.88 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3531 | 1/1 | 0.88 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3136 | 1/1 | 0.88 | 0.35 | 84,84,84,84 | 0 |
| 54 | MG | 1A | 3779 | 1/1 | 0.88 | 0.15 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3507 | 1/1 | 0.88 | 0.09 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3138 | 1/1 | 0.88 | 0.16 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3660 | 1/1 | 0.88 | 0.12 | 81,81,81,81 | 0 |
| 54 | MG | 2a | 3012 | 1/1 | 0.88 | 0.14 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3451 | 1/1 | 0.88 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 2a | 3180 | 1/1 | 0.88 | 0.07 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1700 | 1/1 | 0.88 | 0.11 | 54,54,54,54 | 0 |
| 54 | MG | 2a | 3174 | 1/1 | 0.88 | 0.13 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3955 | 1/1 | 0.88 | 0.07 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3858 | 1/1 | 0.88 | 0.12 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3073 | 1/1 | 0.88 | 0.32 | 49,49,49,49 | 0 |
| 54 | MG | 1R | 205 | 1/1 | 0.88 | 0.17 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3386 | 1/1 | 0.88 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3259 | 1/1 | 0.88 | 0.14 | 55,55,55,55 | 0 |
| 54 | MG | 1B | 211 | 1/1 | 0.88 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3336 | 1/1 | 0.88 | 0.16 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3662 | 1/1 | 0.89 | 0.27 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1690 | 1/1 | 0.89 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3226 | 1/1 | 0.89 | 0.16 | 43,43,43,43 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3573 | 1/1 | 0.89 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3969 | 1/1 | 0.89 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3206 | 1/1 | 0.89 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3211 | 1/1 | 0.89 | 0.11 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3677 | 1/1 | 0.89 | 0.14 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3450 | 1/1 | 0.89 | 0.22 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3017 | 1/1 | 0.89 | 0.22 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3130 | 1/1 | 0.89 | 0.07 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3918 | 1/1 | 0.89 | 0.27 | 55,55,55,55 | 0 |
| 54 | MG | 2O | 201 | 1/1 | 0.89 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3320 | 1/1 | 0.89 | 0.18 | 41,41,41,41 | 0 |
| 54 | MG | 1B | 232 | 1/1 | 0.89 | 0.17 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3112 | 1/1 | 0.89 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 2a | 3049 | 1/1 | 0.89 | 0.24 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3256 | 1/1 | 0.89 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3314 | 1/1 | 0.89 | 0.20 | 57,57,57,57 | 0 |
| 54 | MG | 2B | 202 | 1/1 | 0.89 | 0.08 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1669 | 1/1 | 0.89 | 0.13 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3165 | 1/1 | 0.89 | 0.70 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3090 | 1/1 | 0.89 | 0.20 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3777 | 1/1 | 0.89 | 0.21 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3379 | 1/1 | 0.89 | 0.20 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3104 | 1/1 | 0.89 | 0.80 | 43,43,43,43 | 0 |
| 54 | MG | 1V | 205 | 1/1 | 0.89 | 0.40 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3570 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 1a | 1663 | 1/1 | 0.89 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3807 | 1/1 | 0.89 | 0.22 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3302 | 1/1 | 0.89 | 0.28 | 64,64,64,64 | 0 |
| 54 | MG | 1I | 104 | 1/1 | 0.89 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3459 | 1/1 | 0.89 | 0.11 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3524 | 1/1 | 0.89 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3255 | 1/1 | 0.89 | 0.13 | 51,51,51,51 | 0 |
| 54 | MG | 1B | 203 | 1/1 | 0.89 | 0.18 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1662 | 1/1 | 0.89 | 0.14 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3898 | 1/1 | 0.89 | 0.15 | 61,61,61,61 | 0 |
| 56 | MPD | 2A | 3735 | 8/8 | 0.89 | 0.41 | 50,57,60,64 | 0 |
| 54 | MG | 2A | 3364 | 1/1 | 0.89 | 0.16 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3444 | 1/1 | 0.89 | 0.11 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3467 | 1/1 | 0.89 | 0.18 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3168 | 1/1 | 0.89 | 0.20 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3786 | 1/1 | 0.89 | 0.19 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3440 | 1/1 | 0.89 | 0.13 | 74,74,74,74 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3584 | 1/1 | 0.89 | 0.07 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3683 | 1/1 | 0.89 | 0.10 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3941 | 1/1 | 0.89 | 0.21 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3058 | 1/1 | 0.89 | 0.22 | 41,41,41,41 | 0 |
| 54 | MG | 1E | 305 | 1/1 | 0.89 | 0.06 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3575 | 1/1 | 0.89 | 0.18 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3552 | 1/1 | 0.89 | 0.09 | 39,39,39,39 | 0 |
| 54 | MG | 2a | 3046 | 1/1 | 0.89 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3113 | 1/1 | 0.89 | 0.27 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1631 | 1/1 | 0.89 | 0.21 | 51,51,51,51 | 0 |
| 54 | MG | 2a | 3031 | 1/1 | 0.89 | 0.11 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3920 | 1/1 | 0.89 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3012 | 1/1 | 0.89 | 0.21 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1803 | 1/1 | 0.89 | 0.22 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3056 | 1/1 | 0.89 | 0.16 | 62,62,62,62 | 0 |
| 54 | MG | 2a | 3086 | 1/1 | 0.89 | 0.08 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3583 | 1/1 | 0.89 | 0.08 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3050 | 1/1 | 0.89 | 0.41 | 46,46,46,46 | 0 |
| 54 | MG | 1B | 210 | 1/1 | 0.89 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3244 | 1/1 | 0.89 | 0.30 | 39,39,39,39 | 0 |
| 54 | MG | 1P | 205 | 1/1 | 0.89 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3514 | 1/1 | 0.89 | 0.20 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3548 | 1/1 | 0.89 | 0.30 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3892 | 1/1 | 0.89 | 0.21 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3348 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 1a | 1767 | 1/1 | 0.89 | 0.16 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3477 | 1/1 | 0.89 | 0.27 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3064 | 1/1 | 0.89 | 0.16 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3081 | 1/1 | 0.89 | 0.21 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3698 | 1/1 | 0.89 | 0.55 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3261 | 1/1 | 0.89 | 0.14 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3770 | 1/1 | 0.89 | 0.15 | 32,32,32,32 | 0 |
| 54 | MG | 1a | 1720 | 1/1 | 0.89 | 0.17 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3238 | 1/1 | 0.89 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3501 | 1/1 | 0.89 | 0.12 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3664 | 1/1 | 0.89 | 0.18 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1636 | 1/1 | 0.89 | 0.19 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3802 | 1/1 | 0.89 | 0.13 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3053 | 1/1 | 0.89 | 0.08 | 49,49,49,49 | 0 |
| 54 | MG | 2a | 3043 | 1/1 | 0.89 | 0.20 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3389 | 1/1 | 0.89 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3781 | 1/1 | 0.90 | 0.07 | 33,33,33,33 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1y | 203 | 1/1 | 0.90 | 0.18 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1697 | 1/1 | 0.90 | 0.10 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3708 | 1/1 | 0.90 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3956 | 1/1 | 0.90 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3470 | 1/1 | 0.90 | 0.10 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3324 | 1/1 | 0.90 | 0.23 | 49,49,49,49 | 0 |
| 54 | MG | 1B | 223 | 1/1 | 0.90 | 0.17 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3281 | 1/1 | 0.90 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1842 | 1/1 | 0.90 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3981 | 1/1 | 0.90 | 0.16 | 46,46,46,46 | 0 |
| 54 | MG | 2a | 3124 | 1/1 | 0.90 | 0.13 | 56,56,56,56 | 0 |
| 54 | MG | 1B | 226 | 1/1 | 0.90 | 0.19 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3002 | 1/1 | 0.90 | 0.10 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3005 | 1/1 | 0.90 | 0.14 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3723 | 1/1 | 0.90 | 0.12 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3194 | 1/1 | 0.90 | 0.26 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3098 | 1/1 | 0.90 | 0.09 | 57,57,57,57 | 0 |
| 54 | MG | 1B | 224 | 1/1 | 0.90 | 0.06 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3505 | 1/1 | 0.90 | 0.13 | 61,61,61,61 | 0 |
| 54 | MG | 2E | 307 | 1/1 | 0.90 | 0.17 | 63,63,63,63 | 0 |
| 54 | MG | 1D | 309 | 1/1 | 0.90 | 0.59 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3041 | 1/1 | 0.90 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3440 | 1/1 | 0.90 | 0.14 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3712 | 1/1 | 0.90 | 0.22 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1643 | 1/1 | 0.90 | 0.27 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3475 | 1/1 | 0.90 | 0.15 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3476 | 1/1 | 0.90 | 0.17 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3439 | 1/1 | 0.90 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3331 | 1/1 | 0.90 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3767 | 1/1 | 0.90 | 0.15 | 28,28,28,28 | 0 |
| 54 | MG | 2P | 201 | 1/1 | 0.90 | 0.34 | 45,45,45,45 | 0 |
| 54 | MG | 2a | 3094 | 1/1 | 0.90 | 0.10 | 82,82,82,82 | 0 |
| 54 | MG | 1a | 1837 | 1/1 | 0.90 | 0.08 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3467 | 1/1 | 0.90 | 0.07 | 60,60,60,60 | 0 |
| 54 | MG | 2a | 3144 | 1/1 | 0.90 | 0.15 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3335 | 1/1 | 0.90 | 0.13 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3087 | 1/1 | 0.90 | 0.20 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3069 | 1/1 | 0.90 | 0.37 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3293 | 1/1 | 0.90 | 0.16 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1781 | 1/1 | 0.90 | 0.13 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3304 | 1/1 | 0.90 | 0.07 | 84,84,84,84 | 0 |
| 54 | MG | 2A | 3153 | 1/1 | 0.90 | 0.11 | 45,45,45,45 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1716 | 1/1 | 0.90 | 0.32 | 75,75,75,75 | 0 |
| 54 | MG | 2a | 3142 | 1/1 | 0.90 | 0.09 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3013 | 1/1 | 0.90 | 0.07 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3576 | 1/1 | 0.90 | 0.48 | 44,44,44,44 | 0 |
| 54 | MG | 1a | 1824 | 1/1 | 0.90 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3804 | 1/1 | 0.90 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 1f | 201 | 1/1 | 0.90 | 0.20 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3572 | 1/1 | 0.90 | 0.09 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3861 | 1/1 | 0.90 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3092 | 1/1 | 0.90 | 0.39 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3135 | 1/1 | 0.90 | 0.12 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1634 | 1/1 | 0.90 | 0.13 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3714 | 1/1 | 0.90 | 0.58 | 53,53,53,53 | 0 |
| 54 | MG | 2a | 3084 | 1/1 | 0.90 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3016 | 1/1 | 0.90 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3670 | 1/1 | 0.90 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3821 | 1/1 | 0.90 | 0.13 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3348 | 1/1 | 0.90 | 0.15 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3453 | 1/1 | 0.90 | 0.22 | 23,23,23,23 | 0 |
| 54 | MG | 2a | 3055 | 1/1 | 0.90 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3410 | 1/1 | 0.90 | 0.18 | 25,25,25,25 | 0 |
| 54 | MG | 2A | 3623 | 1/1 | 0.90 | 0.10 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1850 | 1/1 | 0.90 | 0.23 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3194 | 1/1 | 0.90 | 0.21 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3377 | 1/1 | 0.90 | 0.16 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3934 | 1/1 | 0.90 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3181 | 1/1 | 0.90 | 0.24 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1771 | 1/1 | 0.90 | 0.11 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3395 | 1/1 | 0.90 | 0.15 | 24,24,24,24 | 0 |
| 54 | MG | 1B | 230 | 1/1 | 0.90 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3150 | 1/1 | 0.90 | 0.39 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3149 | 1/1 | 0.90 | 0.16 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 4019 | 1/1 | 0.90 | 0.39 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1780 | 1/1 | 0.90 | 0.14 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3246 | 1/1 | 0.90 | 0.16 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3893 | 1/1 | 0.90 | 0.14 | 46,46,46,46 | 0 |
| 54 | MG | 2a | 3160 | 1/1 | 0.90 | 0.12 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3996 | 1/1 | 0.90 | 0.16 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3987 | 1/1 | 0.90 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 2N | 201 | 1/1 | 0.90 | 0.27 | 76,76,76,76 | 0 |
| 54 | MG | 1G | 204 | 1/1 | 0.90 | 0.14 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3620 | 1/1 | 0.90 | 0.14 | 50,50,50,50 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3626 | 1/1 | 0.90 | 0.17 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3563 | 1/1 | 0.90 | 0.13 | 44,44,44,44 | 0 |
| 54 | MG | 1a | 1867 | 1/1 | 0.90 | 0.10 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3011 | 1/1 | 0.90 | 0.17 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3109 | 1/1 | 0.90 | 0.24 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3248 | 1/1 | 0.90 | 0.15 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3018 | 1/1 | 0.90 | 0.20 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3027 | 1/1 | 0.90 | 0.09 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3280 | 1/1 | 0.90 | 0.27 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3625 | 1/1 | 0.90 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 1F | 312 | 1/1 | 0.90 | 0.15 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3275 | 1/1 | 0.90 | 0.16 | 56,56,56,56 | 0 |
| 56 | MPD | 1T | 204 | 8/8 | 0.90 | 0.17 | 61,65,73,74 | 0 |
| 54 | MG | 1A | 3107 | 1/1 | 0.90 | 0.15 | 44,44,44,44 | 0 |
| 54 | MG | 1a | 1625 | 1/1 | 0.90 | 0.13 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3349 | 1/1 | 0.90 | 0.10 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1843 | 1/1 | 0.90 | 0.23 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3595 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3160 | 1/1 | 0.90 | 0.41 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3416 | 1/1 | 0.90 | 0.15 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3201 | 1/1 | 0.90 | 0.16 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3539 | 1/1 | 0.90 | 0.16 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3533 | 1/1 | 0.90 | 0.16 | 49,49,49,49 | 0 |
| 54 | MG | 2a | 3001 | 1/1 | 0.90 | 0.28 | 56,56,56,56 | 0 |
| 54 | MG | 2j | 201 | 1/1 | 0.90 | 0.11 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3962 | 1/1 | 0.90 | 0.24 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3035 | 1/1 | 0.90 | 0.21 | 43,43,43,43 | 0 |
| 54 | MG | 2B | 208 | 1/1 | 0.90 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3535 | 1/1 | 0.90 | 0.18 | 43,43,43,43 | 0 |
| 54 | MG | 1a | 1853 | 1/1 | 0.90 | 0.06 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3757 | 1/1 | 0.91 | 0.19 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3733 | 1/1 | 0.91 | 0.10 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3224 | 1/1 | 0.91 | 0.31 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3369 | 1/1 | 0.91 | 0.11 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3127 | 1/1 | 0.91 | 0.41 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3659 | 1/1 | 0.91 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3556 | 1/1 | 0.91 | 0.18 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3495 | 1/1 | 0.91 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3366 | 1/1 | 0.91 | 0.21 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3399 | 1/1 | 0.91 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1725 | 1/1 | 0.91 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1639 | 1/1 | 0.91 | 0.22 | 75,75,75,75 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1675 | 1/1 | 0.91 | 0.15 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3266 | 1/1 | 0.91 | 0.18 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3236 | 1/1 | 0.91 | 0.41 | 43,43,43,43 | 0 |
| 54 | MG | 25 | 101 | 1/1 | 0.91 | 0.50 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3137 | 1/1 | 0.91 | 0.13 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3025 | 1/1 | 0.91 | 0.17 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1664 | 1/1 | 0.91 | 0.39 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3191 | 1/1 | 0.91 | 0.17 | 40,40,40,40 | 0 |
| 54 | MG | 10 | 101 | 1/1 | 0.91 | 0.21 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3171 | 1/1 | 0.91 | 0.46 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3528 | 1/1 | 0.91 | 0.18 | 45,45,45,45 | 0 |
| 54 | MG | 2B | 203 | 1/1 | 0.91 | 0.09 | 83,83,83,83 | 0 |
| 54 | MG | 1A | 3565 | 1/1 | 0.91 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3617 | 1/1 | 0.91 | 0.23 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3067 | 1/1 | 0.91 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3209 | 1/1 | 0.91 | 0.22 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3192 | 1/1 | 0.91 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3100 | 1/1 | 0.91 | 0.17 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1609 | 1/1 | 0.91 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3429 | 1/1 | 0.91 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3313 | 1/1 | 0.91 | 0.15 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3599 | 1/1 | 0.91 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3850 | 1/1 | 0.91 | 0.10 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3307 | 1/1 | 0.91 | 0.15 | 38,38,38,38 | 0 |
| 54 | MG | 1B | 214 | 1/1 | 0.91 | 0.20 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3189 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | 2a | 3109 | 1/1 | 0.91 | 0.06 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3618 | 1/1 | 0.91 | 0.23 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3628 | 1/1 | 0.91 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3499 | 1/1 | 0.91 | 0.16 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3086 | 1/1 | 0.91 | 0.21 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3614 | 1/1 | 0.91 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3436 | 1/1 | 0.91 | 0.13 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3037 | 1/1 | 0.91 | 0.22 | 43,43,43,43 | 0 |
| 54 | MG | 2a | 3146 | 1/1 | 0.91 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3178 | 1/1 | 0.91 | 0.11 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3655 | 1/1 | 0.91 | 0.16 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3375 | 1/1 | 0.91 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1686 | 1/1 | 0.91 | 0.15 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3390 | 1/1 | 0.91 | 0.23 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1638 | 1/1 | 0.91 | 0.10 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3257 | 1/1 | 0.91 | 0.10 | 57,57,57,57 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1782 | 1/1 | 0.91 | 0.14 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3462 | 1/1 | 0.91 | 0.21 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3066 | 1/1 | 0.91 | 0.13 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3118 | 1/1 | 0.91 | 0.23 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3429 | 1/1 | 0.91 | 0.57 | 63,63,63,63 | 0 |
| 54 | MG | 2a | 3091 | 1/1 | 0.91 | 0.11 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3592 | 1/1 | 0.91 | 0.17 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3638 | 1/1 | 0.91 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3538 | 1/1 | 0.91 | 0.10 | 34,34,34,34 | 0 |
| 54 | MG | 1a | 1721 | 1/1 | 0.91 | 0.32 | 80,80,80,80 | 0 |
| 54 | MG | 1a | 1772 | 1/1 | 0.91 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3358 | 1/1 | 0.91 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3166 | 1/1 | 0.91 | 0.16 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3203 | 1/1 | 0.91 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3273 | 1/1 | 0.91 | 0.09 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1869 | 1/1 | 0.91 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3104 | 1/1 | 0.91 | 0.21 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3679 | 1/1 | 0.91 | 0.11 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3979 | 1/1 | 0.91 | 0.13 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3134 | 1/1 | 0.91 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3688 | 1/1 | 0.91 | 0.20 | 58,58,58,58 | 0 |
| 54 | MG | 1F | 307 | 1/1 | 0.91 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3794 | 1/1 | 0.91 | 0.07 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3489 | 1/1 | 0.91 | 0.08 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3288 | 1/1 | 0.91 | 0.10 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3353 | 1/1 | 0.91 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1834 | 1/1 | 0.91 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3909 | 1/1 | 0.91 | 0.53 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3585 | 1/1 | 0.91 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1795 | 1/1 | 0.91 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3678 | 1/1 | 0.91 | 0.13 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3116 | 1/1 | 0.91 | 0.22 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3606 | 1/1 | 0.91 | 0.35 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3977 | 1/1 | 0.91 | 0.16 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3549 | 1/1 | 0.91 | 0.10 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3633 | 1/1 | 0.91 | 0.07 | 66,66,66,66 | 0 |
| 54 | MG | 2D | 307 | 1/1 | 0.91 | 0.29 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3648 | 1/1 | 0.91 | 0.10 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3545 | 1/1 | 0.91 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3498 | 1/1 | 0.91 | 0.12 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3581 | 1/1 | 0.91 | 0.12 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3809 | 1/1 | 0.91 | 0.22 | 57,57,57,57 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3954 | 1/1 | 0.91 | 0.05 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3685 | 1/1 | 0.91 | 0.06 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3060 | 1/1 | 0.91 | 0.22 | 49,49,49,49 | 0 |
| 54 | MG | 2a | 3129 | 1/1 | 0.91 | 0.23 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3609 | 1/1 | 0.91 | 0.41 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3950 | 1/1 | 0.91 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | 1B | 208 | 1/1 | 0.91 | 0.21 | 47,47,47,47 | 0 |
| 54 | MG | 2a | 3162 | 1/1 | 0.91 | 0.07 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1778 | 1/1 | 0.91 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3937 | 1/1 | 0.91 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3162 | 1/1 | 0.91 | 0.27 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3200 | 1/1 | 0.91 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3758 | 1/1 | 0.91 | 0.08 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3852 | 1/1 | 0.91 | 0.15 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3634 | 1/1 | 0.91 | 0.20 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3921 | 1/1 | 0.91 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 1G | 201 | 1/1 | 0.91 | 0.10 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1796 | 1/1 | 0.91 | 0.22 | 71,71,71,71 | 0 |
| 54 | MG | 17 | 104 | 1/1 | 0.91 | 0.17 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3074 | 1/1 | 0.91 | 0.07 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3808 | 1/1 | 0.91 | 0.21 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3215 | 1/1 | 0.91 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3352 | 1/1 | 0.91 | 0.15 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3976 | 1/1 | 0.91 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3879 | 1/1 | 0.91 | 0.15 | 27,27,27,27 | 0 |
| 54 | MG | 2A | 3572 | 1/1 | 0.91 | 0.16 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3766 | 1/1 | 0.91 | 0.17 | 47,47,47,47 | 0 |
| 54 | MG | 2a | 3177 | 1/1 | 0.91 | 0.09 | 74,74,74,74 | 0 |
| 54 | MG | 2a | 3053 | 1/1 | 0.91 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3103 | 1/1 | 0.91 | 0.09 | 85,85,85,85 | 0 |
| 54 | MG | 1A | 3849 | 1/1 | 0.91 | 0.14 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3438 | 1/1 | 0.91 | 0.09 | 54,54,54,54 | 0 |
| 54 | MG | 2a | 3044 | 1/1 | 0.91 | 0.07 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3647 | 1/1 | 0.91 | 0.15 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3877 | 1/1 | 0.91 | 0.08 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3059 | 1/1 | 0.91 | 0.18 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3389 | 1/1 | 0.91 | 0.10 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3524 | 1/1 | 0.91 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3373 | 1/1 | 0.91 | 0.18 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3520 | 1/1 | 0.91 | 0.15 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1761 | 1/1 | 0.91 | 0.14 | 84,84,84,84 | 0 |
| 54 | MG | 1D | 313 | 1/1 | 0.91 | 0.11 | 57,57,57,57 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1629 | 1/1 | 0.91 | 0.13 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3394 | 1/1 | 0.91 | 0.18 | 22,22,22,22 | 0 |
| 54 | MG | 2A | 3154 | 1/1 | 0.91 | 0.26 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3121 | 1/1 | 0.91 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3503 | 1/1 | 0.91 | 0.10 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3186 | 1/1 | 0.91 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1O | 201 | 1/1 | 0.91 | 0.32 | 50,50,50,50 | 0 |
| 54 | MG | 1a | 1666 | 1/1 | 0.92 | 0.45 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3932 | 1/1 | 0.92 | 0.08 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3324 | 1/1 | 0.92 | 0.13 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3559 | 1/1 | 0.92 | 0.19 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3641 | 1/1 | 0.92 | 0.21 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3325 | 1/1 | 0.92 | 0.16 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3277 | 1/1 | 0.92 | 0.10 | 73,73,73,73 | 0 |
| 57 | ARG | 1B | 233 | 12/12 | 0.92 | 0.20 | 36,52,59,62 | 0 |
| 54 | MG | 1A | 3412 | 1/1 | 0.92 | 0.07 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3872 | 1/1 | 0.92 | 0.19 | 35,35,35,35 | 0 |
| 54 | MG | 2D | 305 | 1/1 | 0.92 | 0.21 | 38,38,38,38 | 0 |
| 54 | MG | 1g | 202 | 1/1 | 0.92 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3148 | 1/1 | 0.92 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3558 | 1/1 | 0.92 | 0.12 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1726 | 1/1 | 0.92 | 0.21 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3632 | 1/1 | 0.92 | 0.16 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1807 | 1/1 | 0.92 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3384 | 1/1 | 0.92 | 0.15 | 32,32,32,32 | 0 |
| 54 | MG | 2a | 3158 | 1/1 | 0.92 | 0.23 | 69,69,69,69 | 0 |
| 54 | MG | 2a | 3083 | 1/1 | 0.92 | 0.23 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3905 | 1/1 | 0.92 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3208 | 1/1 | 0.92 | 0.52 | 59,59,59,59 | 0 |
| 54 | MG | 1N | 204 | 1/1 | 0.92 | 0.06 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3079 | 1/1 | 0.92 | 0.13 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3658 | 1/1 | 0.92 | 0.08 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3527 | 1/1 | 0.92 | 0.26 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3197 | 1/1 | 0.92 | 0.42 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3942 | 1/1 | 0.92 | 0.16 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3472 | 1/1 | 0.92 | 0.07 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3906 | 1/1 | 0.92 | 0.16 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3362 | 1/1 | 0.92 | 0.22 | 53,53,53,53 | 0 |
| 54 | MG | 2a | 3153 | 1/1 | 0.92 | 0.09 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1872 | 1/1 | 0.92 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1617 | 1/1 | 0.92 | 0.06 | 73,73,73,73 | 0 |
| 54 | MG | 1B | 225 | 1/1 | 0.92 | 0.07 | 49,49,49,49 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3287 | 1/1 | 0.92 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 2R | 202 | 1/1 | 0.92 | 0.21 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3163 | 1/1 | 0.92 | 0.21 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3141 | 1/1 | 0.92 | 0.18 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3853 | 1/1 | 0.92 | 0.11 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3689 | 1/1 | 0.92 | 0.10 | 40,40,40,40 | 0 |
| 54 | MG | 1d | 305 | 1/1 | 0.92 | 0.08 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3102 | 1/1 | 0.92 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3592 | 1/1 | 0.92 | 0.06 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3607 | 1/1 | 0.92 | 0.06 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3077 | 1/1 | 0.92 | 0.14 | 72,72,72,72 | 0 |
| 54 | MG | 2a | 3034 | 1/1 | 0.92 | 0.08 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3088 | 1/1 | 0.92 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1724 | 1/1 | 0.92 | 0.14 | 40,40,40,40 | 0 |
| 54 | MG | 2a | 3026 | 1/1 | 0.92 | 0.11 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3218 | 1/1 | 0.92 | 0.22 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3663 | 1/1 | 0.92 | 0.14 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1846 | 1/1 | 0.92 | 0.13 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3369 | 1/1 | 0.92 | 0.15 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3457 | 1/1 | 0.92 | 0.17 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3715 | 1/1 | 0.92 | 0.15 | 64,64,64,64 | 0 |
| 54 | MG | 10 | 104 | 1/1 | 0.92 | 0.09 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3242 | 1/1 | 0.92 | 0.36 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1622 | 1/1 | 0.92 | 0.14 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3551 | 1/1 | 0.92 | 0.10 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3391 | 1/1 | 0.92 | 0.08 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3899 | 1/1 | 0.92 | 0.09 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 4006 | 1/1 | 0.92 | 0.29 | 57,57,57,57 | 0 |
| 54 | MG | 1e | 202 | 1/1 | 0.92 | 0.24 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3249 | 1/1 | 0.92 | 0.44 | 44,44,44,44 | 0 |
| 54 | MG | 2a | 3078 | 1/1 | 0.92 | 0.08 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1858 | 1/1 | 0.92 | 0.20 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3810 | 1/1 | 0.92 | 0.27 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3560 | 1/1 | 0.92 | 0.12 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1692 | 1/1 | 0.92 | 0.17 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3724 | 1/1 | 0.92 | 0.37 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1851 | 1/1 | 0.92 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3696 | 1/1 | 0.92 | 0.21 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3102 | 1/1 | 0.92 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3300 | 1/1 | 0.92 | 0.27 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3697 | 1/1 | 0.92 | 0.10 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3797 | 1/1 | 0.92 | 0.09 | 41,41,41,41 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3661 | 1/1 | 0.92 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 10 | 102 | 1/1 | 0.92 | 0.26 | 37,37,37,37 | 0 |
| 54 | MG | 1a | 1814 | 1/1 | 0.92 | 0.08 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1601 | 1/1 | 0.92 | 0.13 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3426 | 1/1 | 0.92 | 0.10 | 40,40,40,40 | 0 |
| 54 | MG | 2a | 3052 | 1/1 | 0.92 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3714 | 1/1 | 0.92 | 0.06 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3583 | 1/1 | 0.92 | 0.18 | 42,42,42,42 | 0 |
| 54 | MG | 2a | 3063 | 1/1 | 0.92 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3251 | 1/1 | 0.92 | 0.35 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3471 | 1/1 | 0.92 | 0.17 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3803 | 1/1 | 0.92 | 0.14 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3343 | 1/1 | 0.92 | 0.15 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3170 | 1/1 | 0.92 | 0.15 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3241 | 1/1 | 0.92 | 0.23 | 67,67,67,67 | 0 |
| 54 | MG | 1B | 217 | 1/1 | 0.92 | 0.25 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3788 | 1/1 | 0.92 | 0.18 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3008 | 1/1 | 0.92 | 0.20 | 42,42,42,42 | 0 |
| 54 | MG | 1W | 201 | 1/1 | 0.92 | 0.32 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3653 | 1/1 | 0.92 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3785 | 1/1 | 0.92 | 0.24 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3799 | 1/1 | 0.92 | 0.08 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3765 | 1/1 | 0.92 | 0.19 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1602 | 1/1 | 0.92 | 0.19 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3993 | 1/1 | 0.92 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3087 | 1/1 | 0.92 | 0.07 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3527 | 1/1 | 0.92 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3031 | 1/1 | 0.92 | 0.14 | 19,19,19,19 | 0 |
| 54 | MG | 2a | 3127 | 1/1 | 0.92 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1790 | 1/1 | 0.92 | 0.08 | 80,80,80,80 | 0 |
| 54 | MG | 1D | 307 | 1/1 | 0.92 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1701 | 1/1 | 0.92 | 0.15 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3715 | 1/1 | 0.92 | 0.71 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3505 | 1/1 | 0.92 | 0.16 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3959 | 1/1 | 0.92 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3224 | 1/1 | 0.92 | 0.21 | 48,48,48,48 | 0 |
| 54 | MG | 1B | 216 | 1/1 | 0.92 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1P | 203 | 1/1 | 0.92 | 0.50 | 36,36,36,36 | 0 |
| 54 | MG | 1B | 231 | 1/1 | 0.92 | 0.18 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3669 | 1/1 | 0.92 | 0.07 | 71,71,71,71 | 0 |
| 54 | MG | 2a | 3042 | 1/1 | 0.92 | 0.09 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1768 | 1/1 | 0.92 | 0.10 | 60,60,60,60 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3393 | 1/1 | 0.92 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3448 | 1/1 | 0.92 | 0.12 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3171 | 1/1 | 0.92 | 0.11 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3223 | 1/1 | 0.92 | 0.21 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3077 | 1/1 | 0.92 | 0.25 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3596 | 1/1 | 0.92 | 0.07 | 34,34,34,34 | 0 |
| 54 | MG | 1a | 1860 | 1/1 | 0.92 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3768 | 1/1 | 0.92 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3340 | 1/1 | 0.92 | 0.11 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3650 | 1/1 | 0.92 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3952 | 1/1 | 0.92 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3447 | 1/1 | 0.92 | 0.13 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3705 | 1/1 | 0.92 | 0.07 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3469 | 1/1 | 0.92 | 0.16 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3656 | 1/1 | 0.92 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3199 | 1/1 | 0.92 | 0.20 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 4007 | 1/1 | 0.92 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3542 | 1/1 | 0.92 | 0.07 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1847 | 1/1 | 0.92 | 0.13 | 68,68,68,68 | 0 |
| 56 | MPD | 1a | 1875 | 8/8 | 0.92 | 0.21 | 60,64,68,69 | 0 |
| 54 | MG | 2A | 3615 | 1/1 | 0.93 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1736 | 1/1 | 0.93 | 0.24 | 62,62,62,62 | 0 |
| 54 | MG | 1F | 316 | 1/1 | 0.93 | 0.17 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3257 | 1/1 | 0.93 | 0.16 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3426 | 1/1 | 0.93 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3014 | 1/1 | 0.93 | 0.23 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3026 | 1/1 | 0.93 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3128 | 1/1 | 0.93 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3065 | 1/1 | 0.93 | 0.08 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1754 | 1/1 | 0.93 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3930 | 1/1 | 0.93 | 0.04 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3626 | 1/1 | 0.93 | 0.14 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1632 | 1/1 | 0.93 | 0.09 | 55,55,55,55 | 0 |
| 54 | MG | 2a | 3114 | 1/1 | 0.93 | 0.13 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3195 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3727 | 1/1 | 0.93 | 0.28 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3674 | 1/1 | 0.93 | 0.18 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3033 | 1/1 | 0.93 | 0.23 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3146 | 1/1 | 0.93 | 0.39 | 34,34,34,34 | 0 |
| 54 | MG | 1a | 1856 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3509 | 1/1 | 0.93 | 0.30 | 63,63,63,63 | 0 |
| 54 | MG | 1D | 315 | 1/1 | 0.93 | 0.16 | 49,49,49,49 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1619 | 1/1 | 0.93 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3377 | 1/1 | 0.93 | 0.11 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3643 | 1/1 | 0.93 | 0.21 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3749 | 1/1 | 0.93 | 0.10 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3270 | 1/1 | 0.93 | 0.56 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3339 | 1/1 | 0.93 | 0.17 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 4018 | 1/1 | 0.93 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3322 | 1/1 | 0.93 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3006 | 1/1 | 0.93 | 0.13 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3242 | 1/1 | 0.93 | 0.19 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3425 | 1/1 | 0.93 | 0.16 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3316 | 1/1 | 0.93 | 0.11 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3840 | 1/1 | 0.93 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3126 | 1/1 | 0.93 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3495 | 1/1 | 0.93 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1687 | 1/1 | 0.93 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 2a | 3108 | 1/1 | 0.93 | 0.19 | 79,79,79,79 | 0 |
| 54 | MG | 13 | 103 | 1/1 | 0.93 | 0.10 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3864 | 1/1 | 0.93 | 0.13 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3088 | 1/1 | 0.93 | 0.27 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3671 | 1/1 | 0.93 | 0.09 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3124 | 1/1 | 0.93 | 0.12 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3407 | 1/1 | 0.93 | 0.20 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3142 | 1/1 | 0.93 | 0.19 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1642 | 1/1 | 0.93 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3036 | 1/1 | 0.93 | 0.10 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3980 | 1/1 | 0.93 | 0.07 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3568 | 1/1 | 0.93 | 0.06 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3197 | 1/1 | 0.93 | 0.19 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3276 | 1/1 | 0.93 | 0.17 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3341 | 1/1 | 0.93 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3801 | 1/1 | 0.93 | 0.12 | 44,44,44,44 | 0 |
| 54 | MG | 1B | 206 | 1/1 | 0.93 | 0.33 | 43,43,43,43 | 0 |
| 54 | MG | 1a | 1673 | 1/1 | 0.93 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 17 | 103 | 1/1 | 0.93 | 0.34 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3478 | 1/1 | 0.93 | 0.20 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3431 | 1/1 | 0.93 | 0.16 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3886 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3247 | 1/1 | 0.93 | 0.37 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3071 | 1/1 | 0.93 | 0.72 | 57,57,57,57 | 0 |
| 54 | MG | 1d | 304 | 1/1 | 0.93 | 0.25 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3203 | 1/1 | 0.93 | 0.21 | 72,72,72,72 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3700 | 1/1 | 0.93 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3648 | 1/1 | 0.93 | 0.13 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3596 | 1/1 | 0.93 | 0.07 | 53,53,53,53 | 0 |
| 54 | MG | 2B | 207 | 1/1 | 0.93 | 0.18 | 63,63,63,63 | 0 |
| 54 | MG | 2a | 3082 | 1/1 | 0.93 | 0.18 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3214 | 1/1 | 0.93 | 0.17 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3125 | 1/1 | 0.93 | 0.21 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3030 | 1/1 | 0.93 | 0.22 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3838 | 1/1 | 0.93 | 0.14 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3158 | 1/1 | 0.93 | 0.47 | 37,37,37,37 | 0 |
| 54 | MG | 2a | 3048 | 1/1 | 0.93 | 0.25 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3720 | 1/1 | 0.93 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 1l | 202 | 1/1 | 0.93 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3096 | 1/1 | 0.93 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3584 | 1/1 | 0.93 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1627 | 1/1 | 0.93 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3729 | 1/1 | 0.93 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3961 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3395 | 1/1 | 0.93 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3687 | 1/1 | 0.93 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3698 | 1/1 | 0.93 | 0.08 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3903 | 1/1 | 0.93 | 0.17 | 28,28,28,28 | 0 |
| 54 | MG | 2A | 3213 | 1/1 | 0.93 | 0.14 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3704 | 1/1 | 0.93 | 0.35 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3380 | 1/1 | 0.93 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3033 | 1/1 | 0.93 | 0.66 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3432 | 1/1 | 0.93 | 0.05 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3600 | 1/1 | 0.93 | 0.18 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3264 | 1/1 | 0.93 | 0.28 | 27,27,27,27 | 0 |
| 54 | MG | 1n | 103 | 1/1 | 0.93 | 0.15 | 63,63,63,63 | 0 |
| 54 | MG | 1F | 302 | 1/1 | 0.93 | 0.62 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3145 | 1/1 | 0.93 | 0.25 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3546 | 1/1 | 0.93 | 0.19 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3400 | 1/1 | 0.93 | 0.14 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3277 | 1/1 | 0.93 | 0.13 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3466 | 1/1 | 0.93 | 0.16 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3659 | 1/1 | 0.93 | 0.16 | 22,22,22,22 | 0 |
| 54 | MG | 1A | 3083 | 1/1 | 0.93 | 0.14 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3594 | 1/1 | 0.93 | 0.17 | 41,41,41,41 | 0 |
| 54 | MG | 1a | 1635 | 1/1 | 0.93 | 0.16 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3386 | 1/1 | 0.93 | 0.15 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3998 | 1/1 | 0.93 | 0.27 | 48,48,48,48 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3217 | 1/1 | 0.93 | 0.19 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3556 | 1/1 | 0.93 | 0.18 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3553 | 1/1 | 0.93 | 0.06 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3676 | 1/1 | 0.93 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3427 | 1/1 | 0.93 | 0.09 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3140 | 1/1 | 0.93 | 0.31 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1873 | 1/1 | 0.93 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1630 | 1/1 | 0.93 | 0.07 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3050 | 1/1 | 0.93 | 0.14 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3624 | 1/1 | 0.93 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 2a | 3165 | 1/1 | 0.93 | 0.11 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3978 | 1/1 | 0.93 | 0.07 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3065 | 1/1 | 0.93 | 0.18 | 44,44,44,44 | 0 |
| 54 | MG | 2D | 309 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1841 | 1/1 | 0.93 | 0.21 | 61,61,61,61 | 0 |
| 54 | MG | 1t | 202 | 1/1 | 0.93 | 0.18 | 62,62,62,62 | 0 |
| 54 | MG | 2a | 3006 | 1/1 | 0.93 | 0.17 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3831 | 1/1 | 0.93 | 0.15 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3776 | 1/1 | 0.93 | 0.17 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3342 | 1/1 | 0.93 | 0.09 | 57,57,57,57 | 0 |
| 54 | MG | 1U | 204 | 1/1 | 0.93 | 0.48 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3175 | 1/1 | 0.93 | 0.22 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3684 | 1/1 | 0.93 | 0.09 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3173 | 1/1 | 0.93 | 0.24 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3357 | 1/1 | 0.93 | 0.18 | 21,21,21,21 | 0 |
| 54 | MG | 1N | 203 | 1/1 | 0.93 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3101 | 1/1 | 0.93 | 0.09 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1605 | 1/1 | 0.93 | 0.18 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3661 | 1/1 | 0.93 | 0.18 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3597 | 1/1 | 0.93 | 0.11 | 36,36,36,36 | 0 |
| 54 | MG | 1g | 201 | 1/1 | 0.93 | 0.18 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3142 | 1/1 | 0.93 | 0.17 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3670 | 1/1 | 0.93 | 0.13 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3088 | 1/1 | 0.93 | 0.10 | 35,35,35,35 | 0 |
| 54 | MG | 2X | 101 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 1B | 227 | 1/1 | 0.93 | 0.10 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3313 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3157 | 1/1 | 0.93 | 0.12 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3507 | 1/1 | 0.93 | 0.18 | 43,43,43,43 | 0 |
| 54 | MG | 1d | 301 | 1/1 | 0.93 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3204 | 1/1 | 0.93 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3619 | 1/1 | 0.93 | 0.20 | 38,38,38,38 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3474 | 1/1 | 0.93 | 0.13 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3437 | 1/1 | 0.93 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3525 | 1/1 | 0.93 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3677 | 1/1 | 0.93 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3068 | 1/1 | 0.93 | 0.17 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3271 | 1/1 | 0.93 | 0.16 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3601 | 1/1 | 0.93 | 0.27 | 32,32,32,32 | 0 |
| 54 | MG | 1a | 1738 | 1/1 | 0.93 | 0.15 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3686 | 1/1 | 0.93 | 0.20 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3608 | 1/1 | 0.93 | 0.12 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3709 | 1/1 | 0.93 | 0.06 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3773 | 1/1 | 0.93 | 0.24 | 21,21,21,21 | 0 |
| 54 | MG | 1a | 1791 | 1/1 | 0.93 | 0.11 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1863 | 1/1 | 0.93 | 0.11 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3848 | 1/1 | 0.93 | 0.10 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1812 | 1/1 | 0.93 | 0.09 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3068 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3182 | 1/1 | 0.93 | 0.54 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3291 | 1/1 | 0.93 | 0.14 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3055 | 1/1 | 0.93 | 0.22 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3474 | 1/1 | 0.93 | 0.21 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3262 | 1/1 | 0.93 | 0.14 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3975 | 1/1 | 0.93 | 0.13 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3518 | 1/1 | 0.93 | 0.08 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3603 | 1/1 | 0.93 | 0.18 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3691 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3448 | 1/1 | 0.93 | 0.11 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3662 | 1/1 | 0.93 | 0.15 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3933 | 1/1 | 0.93 | 0.23 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3649 | 1/1 | 0.93 | 0.09 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3133 | 1/1 | 0.93 | 0.42 | 37,37,37,37 | 0 |
| 54 | MG | 1a | 1681 | 1/1 | 0.93 | 0.28 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3957 | 1/1 | 0.93 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1644 | 1/1 | 0.93 | 0.13 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3202 | 1/1 | 0.93 | 0.16 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3143 | 1/1 | 0.93 | 0.17 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3199 | 1/1 | 0.93 | 0.29 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3995 | 1/1 | 0.93 | 0.04 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3916 | 1/1 | 0.93 | 0.08 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3674 | 1/1 | 0.93 | 0.12 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3394 | 1/1 | 0.94 | 0.07 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3356 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3267 | 1/1 | 0.94 | 0.25 | 53,53,53,53 | 0 |
| 54 | MG | 10 | 107 | 1/1 | 0.94 | 0.17 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3383 | 1/1 | 0.94 | 0.13 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3571 | 1/1 | 0.94 | 0.07 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3496 | 1/1 | 0.94 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3250 | 1/1 | 0.94 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 2a | 3159 | 1/1 | 0.94 | 0.12 | 66,66,66,66 | 0 |
| 54 | MG | 1l | 201 | 1/1 | 0.94 | 0.16 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3939 | 1/1 | 0.94 | 0.12 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3299 | 1/1 | 0.94 | 0.15 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3074 | 1/1 | 0.94 | 0.16 | 42,42,42,42 | 0 |
| 54 | MG | 2a | 3126 | 1/1 | 0.94 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3335 | 1/1 | 0.94 | 0.16 | 35,35,35,35 | 0 |
| 54 | MG | 1a | 1835 | 1/1 | 0.94 | 0.08 | 75,75,75,75 | 0 |
| 54 | MG | 2a | 3120 | 1/1 | 0.94 | 0.16 | 68,68,68,68 | 0 |
| 54 | MG | 13 | 101 | 1/1 | 0.94 | 0.16 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3084 | 1/1 | 0.94 | 0.22 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3701 | 1/1 | 0.94 | 0.17 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3300 | 1/1 | 0.94 | 0.31 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3605 | 1/1 | 0.94 | 0.11 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3703 | 1/1 | 0.94 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3719 | 1/1 | 0.94 | 0.12 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3579 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |
| 54 | MG | 1a | 1822 | 1/1 | 0.94 | 0.14 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3408 | 1/1 | 0.94 | 0.16 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3402 | 1/1 | 0.94 | 0.18 | 17,17,17,17 | 0 |
| 54 | MG | 2A | 3404 | 1/1 | 0.94 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3280 | 1/1 | 0.94 | 0.10 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3616 | 1/1 | 0.94 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3590 | 1/1 | 0.94 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3546 | 1/1 | 0.94 | 0.18 | 44,44,44,44 | 0 |
| 54 | MG | 2Q | 201 | 1/1 | 0.94 | 0.08 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3010 | 1/1 | 0.94 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3289 | 1/1 | 0.94 | 0.14 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3636 | 1/1 | 0.94 | 0.09 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3029 | 1/1 | 0.94 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3241 | 1/1 | 0.94 | 0.36 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 4013 | 1/1 | 0.94 | 0.16 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3999 | 1/1 | 0.94 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1U | 201 | 1/1 | 0.94 | 0.32 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3860 | 1/1 | 0.94 | 0.17 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3484 | 1/1 | 0.94 | 0.09 | 56,56,56,56 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3683 | 1/1 | 0.94 | 0.20 | 35,35,35,35 | 0 |
| 54 | MG | 20 | 101 | 1/1 | 0.94 | 0.50 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3433 | 1/1 | 0.94 | 0.17 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3370 | 1/1 | 0.94 | 0.30 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3360 | 1/1 | 0.94 | 0.07 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3747 | 1/1 | 0.94 | 0.23 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3699 | 1/1 | 0.94 | 0.20 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3482 | 1/1 | 0.94 | 0.17 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3706 | 1/1 | 0.94 | 0.10 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3958 | 1/1 | 0.94 | 0.16 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3839 | 1/1 | 0.94 | 0.26 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3264 | 1/1 | 0.94 | 0.09 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3263 | 1/1 | 0.94 | 0.19 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3682 | 1/1 | 0.94 | 0.10 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3093 | 1/1 | 0.94 | 0.18 | 41,41,41,41 | 0 |
| 54 | MG | 1F | 314 | 1/1 | 0.94 | 0.45 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3159 | 1/1 | 0.94 | 0.28 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3279 | 1/1 | 0.94 | 0.20 | 42,42,42,42 | 0 |
| 54 | MG | 1H | 201 | 1/1 | 0.94 | 0.21 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3908 | 1/1 | 0.94 | 0.17 | 21,21,21,21 | 0 |
| 54 | MG | 1a | 1653 | 1/1 | 0.94 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3761 | 1/1 | 0.94 | 0.09 | 28,28,28,28 | 0 |
| 54 | MG | 2a | 3064 | 1/1 | 0.94 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3645 | 1/1 | 0.94 | 0.25 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3526 | 1/1 | 0.94 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3249 | 1/1 | 0.94 | 0.68 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3103 | 1/1 | 0.94 | 0.16 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3323 | 1/1 | 0.94 | 0.16 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3009 | 1/1 | 0.94 | 0.11 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3418 | 1/1 | 0.94 | 0.20 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3123 | 1/1 | 0.94 | 0.16 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3019 | 1/1 | 0.94 | 0.50 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3431 | 1/1 | 0.94 | 0.64 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3693 | 1/1 | 0.94 | 0.20 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3837 | 1/1 | 0.94 | 0.16 | 35,35,35,35 | 0 |
| 54 | MG | 1B | 202 | 1/1 | 0.94 | 0.23 | 50,50,50,50 | 0 |
| 54 | MG | 1B | 201 | 1/1 | 0.94 | 0.27 | 51,51,51,51 | 0 |
| 54 | MG | 1Z | 301 | 1/1 | 0.94 | 0.22 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3567 | 1/1 | 0.94 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3081 | 1/1 | 0.94 | 0.26 | 41,41,41,41 | 0 |
| 54 | MG | 2a | 3035 | 1/1 | 0.94 | 0.18 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3668 | 1/1 | 0.94 | 0.15 | 44,44,44,44 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3542 | 1/1 | 0.94 | 0.19 | 40,40,40,40 | 0 |
| 54 | MG | 2I | 201 | 1/1 | 0.94 | 0.16 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3366 | 1/1 | 0.94 | 0.05 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3833 | 1/1 | 0.94 | 0.19 | 34,34,34,34 | 0 |
| 54 | MG | 2a | 3008 | 1/1 | 0.94 | 0.11 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3228 | 1/1 | 0.94 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3736 | 1/1 | 0.94 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3322 | 1/1 | 0.94 | 0.15 | 29,29,29,29 | 0 |
| 54 | MG | 1a | 1817 | 1/1 | 0.94 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3002 | 1/1 | 0.94 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3415 | 1/1 | 0.94 | 0.23 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3417 | 1/1 | 0.94 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3658 | 1/1 | 0.94 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3034 | 1/1 | 0.94 | 0.21 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3724 | 1/1 | 0.94 | 0.12 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3541 | 1/1 | 0.94 | 0.06 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3341 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3700 | 1/1 | 0.94 | 0.26 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3492 | 1/1 | 0.94 | 0.13 | 44,44,44,44 | 0 |
| 54 | MG | 1a | 1628 | 1/1 | 0.94 | 0.33 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3459 | 1/1 | 0.94 | 0.14 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3657 | 1/1 | 0.94 | 0.15 | 16,16,16,16 | 0 |
| 54 | MG | 2a | 3151 | 1/1 | 0.94 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3710 | 1/1 | 0.94 | 0.10 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3156 | 1/1 | 0.94 | 0.42 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 4015 | 1/1 | 0.94 | 0.18 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3076 | 1/1 | 0.94 | 0.27 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3173 | 1/1 | 0.94 | 0.18 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3269 | 1/1 | 0.94 | 0.32 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3610 | 1/1 | 0.94 | 0.24 | 49,49,49,49 | 0 |
| 54 | MG | 25 | 102 | 1/1 | 0.94 | 0.51 | 42,42,42,42 | 0 |
| 54 | MG | 2a | 3092 | 1/1 | 0.94 | 0.13 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3680 | 1/1 | 0.94 | 0.24 | 60,60,60,60 | 0 |
| 54 | MG | 2a | 3132 | 1/1 | 0.94 | 0.07 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3321 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 2E | 305 | 1/1 | 0.94 | 0.09 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3470 | 1/1 | 0.94 | 0.16 | 23,23,23,23 | 0 |
| 54 | MG | 2T | 3303 | 1/1 | 0.94 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3206 | 1/1 | 0.94 | 0.19 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3274 | 1/1 | 0.94 | 0.09 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3984 | 1/1 | 0.94 | 0.07 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3119 | 1/1 | 0.94 | 0.28 | 33,33,33,33 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1762 | 1/1 | 0.94 | 0.20 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3885 | 1/1 | 0.94 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3381 | 1/1 | 0.94 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3117 | 1/1 | 0.94 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3491 | 1/1 | 0.94 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3463 | 1/1 | 0.94 | 0.07 | 38,38,38,38 | 0 |
| 54 | MG | 1T | 201 | 1/1 | 0.94 | 0.07 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3703 | 1/1 | 0.94 | 0.07 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3602 | 1/1 | 0.94 | 0.07 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3230 | 1/1 | 0.94 | 0.24 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3039 | 1/1 | 0.94 | 0.13 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3184 | 1/1 | 0.94 | 0.19 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3889 | 1/1 | 0.94 | 0.14 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3843 | 1/1 | 0.94 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3333 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 56 | MPD | 2A | 3736 | 8/8 | 0.94 | 0.26 | 52,56,60,62 | 0 |
| 54 | MG | 2B | 218 | 1/1 | 0.94 | 0.11 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3919 | 1/1 | 0.94 | 0.13 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3940 | 1/1 | 0.94 | 0.18 | 36,36,36,36 | 0 |
| 54 | MG | 2a | 3101 | 1/1 | 0.94 | 0.18 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3130 | 1/1 | 0.94 | 0.56 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3480 | 1/1 | 0.94 | 0.08 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3208 | 1/1 | 0.94 | 0.47 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3368 | 1/1 | 0.94 | 0.16 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3869 | 1/1 | 0.94 | 0.15 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3038 | 1/1 | 0.94 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3046 | 1/1 | 0.94 | 0.20 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3452 | 1/1 | 0.94 | 0.10 | 69,69,69,69 | 0 |
| 54 | MG | 2a | 3051 | 1/1 | 0.94 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3435 | 1/1 | 0.94 | 0.13 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3744 | 1/1 | 0.94 | 0.21 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1831 | 1/1 | 0.94 | 0.15 | 69,69,69,69 | 0 |
| 54 | MG | 1E | 301 | 1/1 | 0.94 | 0.33 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3310 | 1/1 | 0.94 | 0.82 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3968 | 1/1 | 0.94 | 0.10 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3099 | 1/1 | 0.94 | 0.15 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3319 | 1/1 | 0.94 | 0.19 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3593 | 1/1 | 0.94 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3202 | 1/1 | 0.94 | 0.23 | 52,52,52,52 | 0 |
| 54 | MG | 2B | 206 | 1/1 | 0.94 | 0.09 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3741 | 1/1 | 0.94 | 0.24 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3461 | 1/1 | 0.94 | 0.07 | 56,56,56,56 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1691 | 1/1 | 0.94 | 0.15 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3158 | 1/1 | 0.94 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3591 | 1/1 | 0.94 | 0.07 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3083 | 1/1 | 0.94 | 0.41 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1613 | 1/1 | 0.94 | 0.08 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3029 | 1/1 | 0.94 | 0.21 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3023 | 1/1 | 0.94 | 0.20 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3115 | 1/1 | 0.94 | 0.29 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3798 | 1/1 | 0.94 | 0.14 | 47,47,47,47 | 0 |
| 54 | MG | 2a | 3041 | 1/1 | 0.94 | 0.10 | 73,73,73,73 | 0 |
| 54 | MG | 1T | 203 | 1/1 | 0.94 | 0.17 | 57,57,57,57 | 0 |
| 54 | MG | 2W | 202 | 1/1 | 0.94 | 0.67 | 61,61,61,61 | 0 |
| 54 | MG | 2n | 101 | 1/1 | 0.94 | 0.11 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3605 | 1/1 | 0.94 | 0.30 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3274 | 1/1 | 0.94 | 0.13 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3312 | 1/1 | 0.94 | 0.40 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3154 | 1/1 | 0.94 | 0.16 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3399 | 1/1 | 0.94 | 0.13 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3297 | 1/1 | 0.94 | 0.12 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3461 | 1/1 | 0.94 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3212 | 1/1 | 0.94 | 0.11 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3654 | 1/1 | 0.94 | 0.13 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3190 | 1/1 | 0.94 | 0.27 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3176 | 1/1 | 0.94 | 0.10 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3066 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3146 | 1/1 | 0.94 | 0.11 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3795 | 1/1 | 0.94 | 0.09 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3207 | 1/1 | 0.94 | 0.21 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3595 | 1/1 | 0.94 | 0.11 | 44,44,44,44 | 0 |
| 54 | MG | 2a | 3045 | 1/1 | 0.94 | 0.24 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3144 | 1/1 | 0.94 | 0.28 | 41,41,41,41 | 0 |
| 54 | MG | 2T | 3302 | 1/1 | 0.94 | 0.16 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3323 | 1/1 | 0.94 | 0.07 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1651 | 1/1 | 0.94 | 0.17 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3195 | 1/1 | 0.94 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1830 | 1/1 | 0.94 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 1e | 203 | 1/1 | 0.94 | 0.11 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3666 | 1/1 | 0.94 | 0.14 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3107 | 1/1 | 0.94 | 0.17 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3455 | 1/1 | 0.94 | 0.17 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3884 | 1/1 | 0.94 | 0.27 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3100 | 1/1 | 0.94 | 0.55 | 38,38,38,38 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3468 | 1/1 | 0.94 | 0.16 | 26,26,26,26 | 0 |
| 54 | MG | 2A | 3334 | 1/1 | 0.94 | 0.17 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3414 | 1/1 | 0.94 | 0.76 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3949 | 1/1 | 0.94 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3688 | 1/1 | 0.94 | 0.09 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3790 | 1/1 | 0.94 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 1D | 311 | 1/1 | 0.94 | 0.27 | 39,39,39,39 | 0 |
| 54 | MG | 1g | 203 | 1/1 | 0.94 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3075 | 1/1 | 0.94 | 0.11 | 44,44,44,44 | 0 |
| 54 | MG | 2a | 3156 | 1/1 | 0.94 | 0.09 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3307 | 1/1 | 0.94 | 0.19 | 57,57,57,57 | 0 |
| 54 | MG | 28 | 102 | 1/1 | 0.94 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3521 | 1/1 | 0.94 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3938 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3815 | 1/1 | 0.95 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3726 | 1/1 | 0.95 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 2P | 202 | 1/1 | 0.95 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3751 | 1/1 | 0.95 | 0.18 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3259 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 54 | MG | 1a | 1871 | 1/1 | 0.95 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 2a | 3167 | 1/1 | 0.95 | 0.22 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3216 | 1/1 | 0.95 | 0.27 | 37,37,37,37 | 0 |
| 54 | MG | 2a | 3107 | 1/1 | 0.95 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3687 | 1/1 | 0.95 | 0.16 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3982 | 1/1 | 0.95 | 0.15 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3332 | 1/1 | 0.95 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1614 | 1/1 | 0.95 | 0.22 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3349 | 1/1 | 0.95 | 0.17 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3750 | 1/1 | 0.95 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3193 | 1/1 | 0.95 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3223 | 1/1 | 0.95 | 0.18 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3733 | 1/1 | 0.95 | 0.12 | 49,49,49,49 | 0 |
| 54 | MG | 2a | 3157 | 1/1 | 0.95 | 0.15 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3258 | 1/1 | 0.95 | 0.28 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3682 | 1/1 | 0.95 | 0.09 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3778 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3251 | 1/1 | 0.95 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3170 | 1/1 | 0.95 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1755 | 1/1 | 0.95 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3162 | 1/1 | 0.95 | 0.19 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3080 | 1/1 | 0.95 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1737 | 1/1 | 0.95 | 0.12 | 59,59,59,59 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3534 | 1/1 | 0.95 | 0.10 | 25,25,25,25 | 0 |
| 54 | MG | 1a | 1836 | 1/1 | 0.95 | 0.06 | 55,55,55,55 | 0 |
| 54 | MG | 2a | 3161 | 1/1 | 0.95 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3896 | 1/1 | 0.95 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3106 | 1/1 | 0.95 | 0.27 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3735 | 1/1 | 0.95 | 0.14 | 37,37,37,37 | 0 |
| 54 | MG | 1a | 1839 | 1/1 | 0.95 | 0.08 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3621 | 1/1 | 0.95 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3253 | 1/1 | 0.95 | 0.19 | 37,37,37,37 | 0 |
| 54 | MG | 1a | 1718 | 1/1 | 0.95 | 0.09 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3970 | 1/1 | 0.95 | 0.11 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3445 | 1/1 | 0.95 | 0.25 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3140 | 1/1 | 0.95 | 0.18 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3442 | 1/1 | 0.95 | 0.09 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3205 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3680 | 1/1 | 0.95 | 0.24 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3168 | 1/1 | 0.95 | 0.05 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1730 | 1/1 | 0.95 | 0.33 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3812 | 1/1 | 0.95 | 0.12 | 45,45,45,45 | 0 |
| 54 | MG | 15 | 101 | 1/1 | 0.95 | 0.47 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3565 | 1/1 | 0.95 | 0.10 | 41,41,41,41 | 0 |
| 54 | MG | 28 | 101 | 1/1 | 0.95 | 0.12 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3617 | 1/1 | 0.95 | 0.20 | 23,23,23,23 | 0 |
| 54 | MG | 1B | 219 | 1/1 | 0.95 | 0.16 | 52,52,52,52 | 0 |
| 54 | MG | 2a | 3095 | 1/1 | 0.95 | 0.06 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3256 | 1/1 | 0.95 | 0.10 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3523 | 1/1 | 0.95 | 0.11 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3712 | 1/1 | 0.95 | 0.43 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3409 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3697 | 1/1 | 0.95 | 0.15 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3719 | 1/1 | 0.95 | 0.19 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1646 | 1/1 | 0.95 | 0.19 | 51,51,51,51 | 0 |
| 54 | MG | 2a | 3066 | 1/1 | 0.95 | 0.18 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3631 | 1/1 | 0.95 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3873 | 1/1 | 0.95 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3562 | 1/1 | 0.95 | 0.24 | 43,43,43,43 | 0 |
| 54 | MG | 2a | 3068 | 1/1 | 0.95 | 0.23 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3398 | 1/1 | 0.95 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1773 | 1/1 | 0.95 | 0.17 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3064 | 1/1 | 0.95 | 0.15 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3094 | 1/1 | 0.95 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 2l | 201 | 1/1 | 0.95 | 0.13 | 63,63,63,63 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3663 | 1/1 | 0.95 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 1a | 1633 | 1/1 | 0.95 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3269 | 1/1 | 0.95 | 0.43 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3555 | 1/1 | 0.95 | 0.11 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3152 | 1/1 | 0.95 | 0.15 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3563 | 1/1 | 0.95 | 0.17 | 21,21,21,21 | 0 |
| 54 | MG | 2A | 3292 | 1/1 | 0.95 | 0.08 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3027 | 1/1 | 0.95 | 0.28 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3780 | 1/1 | 0.95 | 0.19 | 40,40,40,40 | 0 |
| 54 | MG | 1E | 302 | 1/1 | 0.95 | 0.58 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3580 | 1/1 | 0.95 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3433 | 1/1 | 0.95 | 0.08 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3229 | 1/1 | 0.95 | 0.45 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3312 | 1/1 | 0.95 | 0.14 | 50,50,50,50 | 0 |
| 54 | MG | 1B | 218 | 1/1 | 0.95 | 0.46 | 63,63,63,63 | 0 |
| 54 | MG | 1V | 204 | 1/1 | 0.95 | 0.20 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3854 | 1/1 | 0.95 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3178 | 1/1 | 0.95 | 0.22 | 48,48,48,48 | 0 |
| 54 | MG | 2G | 202 | 1/1 | 0.95 | 0.05 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3147 | 1/1 | 0.95 | 0.62 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3254 | 1/1 | 0.95 | 0.18 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3238 | 1/1 | 0.95 | 0.31 | 39,39,39,39 | 0 |
| 54 | MG | 2a | 3073 | 1/1 | 0.95 | 0.15 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3283 | 1/1 | 0.95 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3564 | 1/1 | 0.95 | 0.09 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3339 | 1/1 | 0.95 | 0.19 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3082 | 1/1 | 0.95 | 0.36 | 34,34,34,34 | 0 |
| 54 | MG | 2B | 204 | 1/1 | 0.95 | 0.18 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3517 | 1/1 | 0.95 | 0.35 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3279 | 1/1 | 0.95 | 0.08 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3326 | 1/1 | 0.95 | 0.16 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3419 | 1/1 | 0.95 | 0.15 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1854 | 1/1 | 0.95 | 0.11 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3518 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3363 | 1/1 | 0.95 | 0.17 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3673 | 1/1 | 0.95 | 0.21 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3225 | 1/1 | 0.95 | 0.08 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3086 | 1/1 | 0.95 | 0.23 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3079 | 1/1 | 0.95 | 0.19 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3225 | 1/1 | 0.95 | 0.14 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3912 | 1/1 | 0.95 | 0.13 | 20,20,20,20 | 0 |
| 54 | MG | 2a | 3135 | 1/1 | 0.95 | 0.07 | 67,67,67,67 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3401 | 1/1 | 0.95 | 0.15 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1654 | 1/1 | 0.95 | 0.08 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3560 | 1/1 | 0.95 | 0.05 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3087 | 1/1 | 0.95 | 0.17 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3695 | 1/1 | 0.95 | 0.36 | 33,33,33,33 | 0 |
| 54 | MG | 1d | 303 | 1/1 | 0.95 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3123 | 1/1 | 0.95 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3118 | 1/1 | 0.95 | 0.28 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3020 | 1/1 | 0.95 | 0.40 | 39,39,39,39 | 0 |
| 54 | MG | 1R | 204 | 1/1 | 0.95 | 0.12 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3007 | 1/1 | 0.95 | 0.13 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3992 | 1/1 | 0.95 | 0.16 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3483 | 1/1 | 0.95 | 0.16 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3367 | 1/1 | 0.95 | 0.16 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3691 | 1/1 | 0.95 | 0.19 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3179 | 1/1 | 0.95 | 0.09 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3725 | 1/1 | 0.95 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 2a | 3003 | 1/1 | 0.95 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1792 | 1/1 | 0.95 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1684 | 1/1 | 0.95 | 0.29 | 53,53,53,53 | 0 |
| 54 | MG | 10 | 103 | 1/1 | 0.95 | 0.10 | 40,40,40,40 | 0 |
| 54 | MG | 1B | 204 | 1/1 | 0.95 | 0.34 | 52,52,52,52 | 0 |
| 54 | MG | 1E | 304 | 1/1 | 0.95 | 0.11 | 24,24,24,24 | 0 |
| 54 | MG | 2a | 3021 | 1/1 | 0.95 | 0.08 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3148 | 1/1 | 0.95 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2a | 3149 | 1/1 | 0.95 | 0.08 | 71,71,71,71 | 0 |
| 54 | MG | 1y | 202 | 1/1 | 0.95 | 0.13 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3361 | 1/1 | 0.95 | 0.11 | 27,27,27,27 | 0 |
| 54 | MG | 17 | 101 | 1/1 | 0.95 | 0.12 | 28,28,28,28 | 0 |
| 54 | MG | 2A | 3293 | 1/1 | 0.95 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3052 | 1/1 | 0.95 | 0.11 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1626 | 1/1 | 0.95 | 0.09 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3329 | 1/1 | 0.95 | 0.18 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3378 | 1/1 | 0.95 | 0.13 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3479 | 1/1 | 0.95 | 0.15 | 31,31,31,31 | 0 |
| 54 | MG | 2a | 3096 | 1/1 | 0.95 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3311 | 1/1 | 0.95 | 0.24 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3635 | 1/1 | 0.95 | 0.37 | 34,34,34,34 | 0 |
| 54 | MG | 2a | 3010 | 1/1 | 0.95 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3742 | 1/1 | 0.95 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3544 | 1/1 | 0.95 | 0.23 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3272 | 1/1 | 0.95 | 0.23 | 43,43,43,43 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3910 | 1/1 | 0.95 | 0.22 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3468 | 1/1 | 0.95 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1739 | 1/1 | 0.95 | 0.17 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3738 | 1/1 | 0.95 | 0.11 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3891 | 1/1 | 0.95 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3167 | 1/1 | 0.95 | 0.65 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3718 | 1/1 | 0.95 | 0.12 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3536 | 1/1 | 0.95 | 0.11 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3846 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3290 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3775 | 1/1 | 0.95 | 0.19 | 34,34,34,34 | 0 |
| 54 | MG | 2a | 3074 | 1/1 | 0.95 | 0.20 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3769 | 1/1 | 0.95 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1679 | 1/1 | 0.95 | 0.24 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3403 | 1/1 | 0.95 | 0.07 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3013 | 1/1 | 0.95 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1750 | 1/1 | 0.95 | 0.09 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3656 | 1/1 | 0.95 | 0.11 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3608 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3213 | 1/1 | 0.95 | 0.30 | 43,43,43,43 | 0 |
| 54 | MG | 2a | 3075 | 1/1 | 0.95 | 0.21 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3318 | 1/1 | 0.95 | 0.18 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3624 | 1/1 | 0.95 | 0.08 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3095 | 1/1 | 0.95 | 0.16 | 53,53,53,53 | 0 |
| 54 | MG | 1m | 201 | 1/1 | 0.95 | 0.10 | 68,68,68,68 | 0 |
| 56 | MPD | 18 | 103 | 8/8 | 0.95 | 0.31 | 33,41,46,48 | 0 |
| 54 | MG | 2A | 3045 | 1/1 | 0.95 | 0.12 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1637 | 1/1 | 0.95 | 0.12 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3281 | 1/1 | 0.95 | 0.34 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3127 | 1/1 | 0.95 | 0.27 | 56,56,56,56 | 0 |
| 54 | MG | 1P | 202 | 1/1 | 0.95 | 0.37 | 29,29,29,29 | 0 |
| 54 | MG | 1D | 314 | 1/1 | 0.95 | 0.09 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3430 | 1/1 | 0.95 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1789 | 1/1 | 0.95 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3553 | 1/1 | 0.95 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 2D | 308 | 1/1 | 0.95 | 0.42 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3232 | 1/1 | 0.95 | 0.28 | 30,30,30,30 | 0 |
| 54 | MG | 1a | 1741 | 1/1 | 0.95 | 0.17 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3669 | 1/1 | 0.95 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3009 | 1/1 | 0.95 | 0.22 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3732 | 1/1 | 0.95 | 0.13 | 32,32,32,32 | 0 |
| 54 | MG | 1a | 1615 | 1/1 | 0.95 | 0.18 | 60,60,60,60 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3270 | 1/1 | 0.95 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3239 | 1/1 | 0.95 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3613 | 1/1 | 0.95 | 0.10 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3430 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3350 | 1/1 | 0.95 | 0.10 | 32,32,32,32 | 0 |
| 54 | MG | 1W | 202 | 1/1 | 0.95 | 0.23 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3579 | 1/1 | 0.95 | 0.27 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3330 | 1/1 | 0.95 | 0.05 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1655 | 1/1 | 0.95 | 0.18 | 58,58,58,58 | 0 |
| 56 | MPD | 1A | 4022 | 8/8 | 0.95 | 0.14 | 46,53,56,59 | 0 |
| 54 | MG | 2B | 209 | 1/1 | 0.95 | 0.18 | 72,72,72,72 | 0 |
| 54 | MG | 2a | 3183 | 1/1 | 0.95 | 0.14 | 86,86,86,86 | 0 |
| 54 | MG | 2a | 3039 | 1/1 | 0.95 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1868 | 1/1 | 0.95 | 0.11 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3039 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3991 | 1/1 | 0.95 | 0.14 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3515 | 1/1 | 0.95 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 4009 | 1/1 | 0.95 | 0.12 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3115 | 1/1 | 0.95 | 0.22 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3388 | 1/1 | 0.95 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1640 | 1/1 | 0.95 | 0.10 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3947 | 1/1 | 0.95 | 0.16 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3612 | 1/1 | 0.95 | 0.08 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3043 | 1/1 | 0.95 | 0.14 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3627 | 1/1 | 0.95 | 0.16 | 68,68,68,68 | 0 |
| 54 | MG | 1F | 318 | 1/1 | 0.95 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3201 | 1/1 | 0.95 | 0.08 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1820 | 1/1 | 0.95 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 1D | 303 | 1/1 | 0.95 | 0.11 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3252 | 1/1 | 0.95 | 0.32 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3316 | 1/1 | 0.95 | 0.16 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3816 | 1/1 | 0.95 | 0.12 | 27,27,27,27 | 0 |
| 54 | MG | 2A | 3561 | 1/1 | 0.95 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3291 | 1/1 | 0.95 | 0.47 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3652 | 1/1 | 0.95 | 0.55 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3122 | 1/1 | 0.95 | 0.16 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3672 | 1/1 | 0.95 | 0.07 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3019 | 1/1 | 0.95 | 0.37 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3153 | 1/1 | 0.95 | 0.18 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3351 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1699 | 1/1 | 0.95 | 0.19 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3564 | 1/1 | 0.95 | 0.18 | 39,39,39,39 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3060 | 1/1 | 0.95 | 0.14 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3645 | 1/1 | 0.95 | 0.17 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3145 | 1/1 | 0.95 | 0.30 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3586 | 1/1 | 0.95 | 0.08 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3549 | 1/1 | 0.95 | 0.08 | 59,59,59,59 | 0 |
| 54 | MG | 1f | 202 | 1/1 | 0.95 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1740 | 1/1 | 0.95 | 0.11 | 76,76,76,76 | 0 |
| 54 | MG | 10 | 106 | 1/1 | 0.95 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3139 | 1/1 | 0.95 | 0.25 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3120 | 1/1 | 0.95 | 0.59 | 54,54,54,54 | 0 |
| 54 | MG | 1a | 1606 | 1/1 | 0.95 | 0.12 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1805 | 1/1 | 0.95 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1799 | 1/1 | 0.95 | 0.10 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3305 | 1/1 | 0.95 | 0.16 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3811 | 1/1 | 0.95 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3791 | 1/1 | 0.95 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3622 | 1/1 | 0.95 | 0.12 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3541 | 1/1 | 0.95 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3372 | 1/1 | 0.95 | 0.18 | 63,63,63,63 | 0 |
| 54 | MG | 1i | 201 | 1/1 | 0.95 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3929 | 1/1 | 0.95 | 0.10 | 38,38,38,38 | 0 |
| 54 | MG | 1a | 1818 | 1/1 | 0.95 | 0.11 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3759 | 1/1 | 0.95 | 0.43 | 59,59,59,59 | 0 |
| 54 | MG | 1Q | 204 | 1/1 | 0.95 | 0.13 | 47,47,47,47 | 0 |
| 54 | MG | 2a | 3071 | 1/1 | 0.96 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3076 | 1/1 | 0.96 | 0.06 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3867 | 1/1 | 0.96 | 0.14 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3343 | 1/1 | 0.96 | 0.12 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3477 | 1/1 | 0.96 | 0.19 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1751 | 1/1 | 0.96 | 0.12 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3544 | 1/1 | 0.96 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3359 | 1/1 | 0.96 | 0.13 | 38,38,38,38 | 0 |
| 54 | MG | 2a | 3139 | 1/1 | 0.96 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3092 | 1/1 | 0.96 | 0.15 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1815 | 1/1 | 0.96 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3408 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3988 | 1/1 | 0.96 | 0.13 | 21,21,21,21 | 0 |
| 54 | MG | 2A | 3710 | 1/1 | 0.96 | 0.23 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3061 | 1/1 | 0.96 | 0.11 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3007 | 1/1 | 0.96 | 0.45 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3048 | 1/1 | 0.96 | 0.28 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1733 | 1/1 | 0.96 | 0.12 | 43,43,43,43 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3345 | 1/1 | 0.96 | 0.15 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3644 | 1/1 | 0.96 | 0.14 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3428 | 1/1 | 0.96 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3091 | 1/1 | 0.96 | 0.14 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3876 | 1/1 | 0.96 | 0.17 | 30,30,30,30 | 0 |
| 58 | ZN | 29 | 501 | 1/1 | 0.96 | 0.11 | 81,81,81,81 | 0 |
| 54 | MG | 1Y | 201 | 1/1 | 0.96 | 0.14 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3135 | 1/1 | 0.96 | 0.29 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3488 | 1/1 | 0.96 | 0.08 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3578 | 1/1 | 0.96 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | 2V | 202 | 1/1 | 0.96 | 0.47 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3260 | 1/1 | 0.96 | 0.15 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3319 | 1/1 | 0.96 | 0.17 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3222 | 1/1 | 0.96 | 0.44 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3228 | 1/1 | 0.96 | 0.61 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3637 | 1/1 | 0.96 | 0.20 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3362 | 1/1 | 0.96 | 0.18 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3946 | 1/1 | 0.96 | 0.08 | 24,24,24,24 | 0 |
| 54 | MG | 2A | 3129 | 1/1 | 0.96 | 0.10 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3502 | 1/1 | 0.96 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3028 | 1/1 | 0.96 | 0.07 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3537 | 1/1 | 0.96 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 2a | 3154 | 1/1 | 0.96 | 0.18 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3771 | 1/1 | 0.96 | 0.09 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3178 | 1/1 | 0.96 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3372 | 1/1 | 0.96 | 0.11 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3452 | 1/1 | 0.96 | 0.20 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3376 | 1/1 | 0.96 | 0.09 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3182 | 1/1 | 0.96 | 0.14 | 43,43,43,43 | 0 |
| 54 | MG | 1a | 1683 | 1/1 | 0.96 | 0.10 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3298 | 1/1 | 0.96 | 0.15 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3601 | 1/1 | 0.96 | 0.04 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3124 | 1/1 | 0.96 | 0.18 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3646 | 1/1 | 0.96 | 0.06 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1717 | 1/1 | 0.96 | 0.11 | 54,54,54,54 | 0 |
| 54 | MG | 1R | 202 | 1/1 | 0.96 | 0.13 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3297 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 4004 | 1/1 | 0.96 | 0.38 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3914 | 1/1 | 0.96 | 0.33 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3235 | 1/1 | 0.96 | 0.38 | 36,36,36,36 | 0 |
| 54 | MG | 1a | 1759 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3382 | 1/1 | 0.96 | 0.15 | 31,31,31,31 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1U | 207 | 1/1 | 0.96 | 0.75 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3793 | 1/1 | 0.96 | 0.23 | 61,61,61,61 | 0 |
| 54 | MG | 2a | 3138 | 1/1 | 0.96 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1779 | 1/1 | 0.96 | 0.23 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3636 | 1/1 | 0.96 | 0.16 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3265 | 1/1 | 0.96 | 0.10 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3455 | 1/1 | 0.96 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3099 | 1/1 | 0.96 | 0.13 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3441 | 1/1 | 0.96 | 0.17 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3547 | 1/1 | 0.96 | 0.24 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3445 | 1/1 | 0.96 | 0.14 | 27,27,27,27 | 0 |
| 54 | MG | 2A | 3326 | 1/1 | 0.96 | 0.13 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3960 | 1/1 | 0.96 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 2a | 3032 | 1/1 | 0.96 | 0.16 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3568 | 1/1 | 0.96 | 0.12 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3155 | 1/1 | 0.96 | 0.12 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3422 | 1/1 | 0.96 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3084 | 1/1 | 0.96 | 0.13 | 43,43,43,43 | 0 |
| 54 | MG | 1a | 1785 | 1/1 | 0.96 | 0.13 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1852 | 1/1 | 0.96 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3437 | 1/1 | 0.96 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3245 | 1/1 | 0.96 | 0.40 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3818 | 1/1 | 0.96 | 0.18 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1743 | 1/1 | 0.96 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1788 | 1/1 | 0.96 | 0.09 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3090 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |
| 54 | MG | 1a | 1748 | 1/1 | 0.96 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3182 | 1/1 | 0.96 | 0.13 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3266 | 1/1 | 0.96 | 0.65 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3200 | 1/1 | 0.96 | 0.22 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3647 | 1/1 | 0.96 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3482 | 1/1 | 0.96 | 0.09 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1670 | 1/1 | 0.96 | 0.52 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3031 | 1/1 | 0.96 | 0.09 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3502 | 1/1 | 0.96 | 0.17 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1694 | 1/1 | 0.96 | 0.17 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1729 | 1/1 | 0.96 | 0.06 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3421 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 54 | MG | 1n | 101 | 1/1 | 0.96 | 0.17 | 72,72,72,72 | 0 |
| 54 | MG | 27 | 101 | 1/1 | 0.96 | 0.23 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3743 | 1/1 | 0.96 | 0.18 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3664 | 1/1 | 0.96 | 0.06 | 42,42,42,42 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3082 | 1/1 | 0.96 | 0.08 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3466 | 1/1 | 0.96 | 0.05 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3344 | 1/1 | 0.96 | 0.07 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3265 | 1/1 | 0.96 | 0.21 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3049 | 1/1 | 0.96 | 0.29 | 39,39,39,39 | 0 |
| 54 | MG | 2D | 302 | 1/1 | 0.96 | 0.84 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3657 | 1/1 | 0.96 | 0.14 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3543 | 1/1 | 0.96 | 0.16 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3569 | 1/1 | 0.96 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3900 | 1/1 | 0.96 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 1a | 1827 | 1/1 | 0.96 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3497 | 1/1 | 0.96 | 0.12 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3096 | 1/1 | 0.96 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3376 | 1/1 | 0.96 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3504 | 1/1 | 0.96 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3610 | 1/1 | 0.96 | 0.17 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3192 | 1/1 | 0.96 | 0.13 | 60,60,60,60 | 0 |
| 58 | ZN | 14 | 501 | 1/1 | 0.96 | 0.07 | 110,110,110,110 | 0 |
| 54 | MG | 1a | 1829 | 1/1 | 0.96 | 0.23 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3456 | 1/1 | 0.96 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 1F | 308 | 1/1 | 0.96 | 0.18 | 24,24,24,24 | 0 |
| 54 | MG | 2B | 213 | 1/1 | 0.96 | 0.16 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1776 | 1/1 | 0.96 | 0.21 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3232 | 1/1 | 0.96 | 0.18 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3690 | 1/1 | 0.96 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1749 | 1/1 | 0.96 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3390 | 1/1 | 0.96 | 0.15 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3243 | 1/1 | 0.96 | 0.30 | 67,67,67,67 | 0 |
| 54 | MG | 1a | 1806 | 1/1 | 0.96 | 0.10 | 69,69,69,69 | 0 |
| 54 | MG | 1B | 205 | 1/1 | 0.96 | 0.11 | 41,41,41,41 | 0 |
| 54 | MG | 2I | 101 | 1/1 | 0.96 | 0.11 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3558 | 1/1 | 0.96 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1727 | 1/1 | 0.96 | 0.12 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3181 | 1/1 | 0.96 | 0.12 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3782 | 1/1 | 0.96 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3497 | 1/1 | 0.96 | 0.07 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3639 | 1/1 | 0.96 | 0.30 | 69,69,69,69 | 0 |
| 54 | MG | 2F | 301 | 1/1 | 0.96 | 0.44 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3548 | 1/1 | 0.96 | 0.16 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3702 | 1/1 | 0.96 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3774 | 1/1 | 0.96 | 0.21 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3650 | 1/1 | 0.96 | 0.13 | 55,55,55,55 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3813 | 1/1 | 0.96 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3038 | 1/1 | 0.96 | 0.12 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3754 | 1/1 | 0.96 | 0.17 | 37,37,37,37 | 0 |
| 54 | MG | 2a | 3131 | 1/1 | 0.96 | 0.13 | 61,61,61,61 | 0 |
| 54 | MG | 1V | 207 | 1/1 | 0.96 | 0.13 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3016 | 1/1 | 0.96 | 0.51 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3022 | 1/1 | 0.96 | 0.51 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3673 | 1/1 | 0.96 | 0.06 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3355 | 1/1 | 0.96 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3129 | 1/1 | 0.96 | 0.12 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3472 | 1/1 | 0.96 | 0.13 | 25,25,25,25 | 0 |
| 54 | MG | 2A | 3678 | 1/1 | 0.96 | 0.13 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3478 | 1/1 | 0.96 | 0.19 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3868 | 1/1 | 0.96 | 0.18 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1728 | 1/1 | 0.96 | 0.07 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3111 | 1/1 | 0.96 | 0.26 | 36,36,36,36 | 0 |
| 54 | MG | 1a | 1616 | 1/1 | 0.96 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3156 | 1/1 | 0.96 | 0.25 | 58,58,58,58 | 0 |
| 54 | MG | 2B | 216 | 1/1 | 0.96 | 0.11 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3655 | 1/1 | 0.96 | 0.13 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3559 | 1/1 | 0.96 | 0.12 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3711 | 1/1 | 0.96 | 0.07 | 20,20,20,20 | 0 |
| 54 | MG | 2A | 3067 | 1/1 | 0.96 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3149 | 1/1 | 0.96 | 0.27 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3015 | 1/1 | 0.96 | 0.20 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3756 | 1/1 | 0.96 | 0.16 | 32,32,32,32 | 0 |
| 54 | MG | 1a | 1745 | 1/1 | 0.96 | 0.08 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3132 | 1/1 | 0.96 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1623 | 1/1 | 0.96 | 0.26 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3393 | 1/1 | 0.96 | 0.18 | 20,20,20,20 | 0 |
| 54 | MG | 1A | 3511 | 1/1 | 0.96 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3240 | 1/1 | 0.96 | 0.19 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3911 | 1/1 | 0.96 | 0.08 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1864 | 1/1 | 0.96 | 0.12 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1723 | 1/1 | 0.96 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3485 | 1/1 | 0.96 | 0.08 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3609 | 1/1 | 0.96 | 0.11 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3406 | 1/1 | 0.96 | 0.05 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3416 | 1/1 | 0.96 | 0.17 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3684 | 1/1 | 0.96 | 0.09 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3286 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3875 | 1/1 | 0.96 | 0.17 | 39,39,39,39 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3148 | 1/1 | 0.96 | 0.08 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3404 | 1/1 | 0.96 | 0.25 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3508 | 1/1 | 0.96 | 0.09 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3011 | 1/1 | 0.96 | 0.12 | 35,35,35,35 | 0 |
| 54 | MG | 1a | 1607 | 1/1 | 0.96 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3492 | 1/1 | 0.96 | 0.06 | 40,40,40,40 | 0 |
| 54 | MG | 2a | 3038 | 1/1 | 0.96 | 0.16 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3762 | 1/1 | 0.96 | 0.16 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3792 | 1/1 | 0.96 | 0.17 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3053 | 1/1 | 0.96 | 0.43 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3471 | 1/1 | 0.96 | 0.08 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3897 | 1/1 | 0.96 | 0.05 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1744 | 1/1 | 0.96 | 0.15 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3407 | 1/1 | 0.96 | 0.16 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3446 | 1/1 | 0.96 | 0.20 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3122 | 1/1 | 0.96 | 0.20 | 74,74,74,74 | 0 |
| 54 | MG | 2B | 215 | 1/1 | 0.96 | 0.13 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3101 | 1/1 | 0.96 | 0.37 | 33,33,33,33 | 0 |
| 54 | MG | 2o | 101 | 1/1 | 0.96 | 0.08 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3140 | 1/1 | 0.96 | 0.16 | 67,67,67,67 | 0 |
| 54 | MG | 1a | 1705 | 1/1 | 0.96 | 0.08 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3692 | 1/1 | 0.96 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3734 | 1/1 | 0.96 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3021 | 1/1 | 0.96 | 0.43 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3414 | 1/1 | 0.96 | 0.07 | 63,63,63,63 | 0 |
| 54 | MG | 1B | 215 | 1/1 | 0.96 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3163 | 1/1 | 0.96 | 0.13 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3298 | 1/1 | 0.96 | 0.21 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3842 | 1/1 | 0.96 | 0.14 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3315 | 1/1 | 0.96 | 0.15 | 27,27,27,27 | 0 |
| 54 | MG | 2A | 3375 | 1/1 | 0.96 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3574 | 1/1 | 0.96 | 0.15 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3783 | 1/1 | 0.96 | 0.21 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3004 | 1/1 | 0.96 | 0.08 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1667 | 1/1 | 0.96 | 0.22 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3894 | 1/1 | 0.96 | 0.16 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3204 | 1/1 | 0.96 | 0.17 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3462 | 1/1 | 0.96 | 0.25 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3442 | 1/1 | 0.96 | 0.10 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3665 | 1/1 | 0.96 | 0.15 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3871 | 1/1 | 0.96 | 0.14 | 28,28,28,28 | 0 |
| 54 | MG | 2D | 304 | 1/1 | 0.96 | 0.61 | 44,44,44,44 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2R | 201 | 1/1 | 0.96 | 0.19 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3729 | 1/1 | 0.96 | 0.26 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3716 | 1/1 | 0.96 | 0.06 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1713 | 1/1 | 0.96 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3145 | 1/1 | 0.96 | 0.07 | 60,60,60,60 | 0 |
| 54 | MG | 2a | 3014 | 1/1 | 0.96 | 0.10 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3644 | 1/1 | 0.96 | 0.14 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3108 | 1/1 | 0.96 | 0.24 | 34,34,34,34 | 0 |
| 54 | MG | 2a | 3005 | 1/1 | 0.96 | 0.15 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3653 | 1/1 | 0.96 | 0.09 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3306 | 1/1 | 0.96 | 0.17 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3320 | 1/1 | 0.96 | 0.18 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3374 | 1/1 | 0.96 | 0.09 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3513 | 1/1 | 0.96 | 0.16 | 21,21,21,21 | 0 |
| 54 | MG | 1F | 309 | 1/1 | 0.96 | 0.31 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 4011 | 1/1 | 0.96 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3327 | 1/1 | 0.96 | 0.13 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3764 | 1/1 | 0.96 | 0.09 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3268 | 1/1 | 0.96 | 0.44 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3964 | 1/1 | 0.96 | 0.17 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3077 | 1/1 | 0.96 | 0.20 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3057 | 1/1 | 0.96 | 0.14 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3026 | 1/1 | 0.96 | 0.35 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3567 | 1/1 | 0.96 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3128 | 1/1 | 0.96 | 0.42 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3554 | 1/1 | 0.96 | 0.11 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3500 | 1/1 | 0.96 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3427 | 1/1 | 0.96 | 0.12 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3973 | 1/1 | 0.96 | 0.11 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3874 | 1/1 | 0.96 | 0.17 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3075 | 1/1 | 0.96 | 0.16 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3078 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3396 | 1/1 | 0.96 | 0.10 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3966 | 1/1 | 0.96 | 0.10 | 43,43,43,43 | 0 |
| 54 | MG | 18 | 101 | 1/1 | 0.96 | 0.22 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3561 | 1/1 | 0.96 | 0.05 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3006 | 1/1 | 0.96 | 0.17 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3880 | 1/1 | 0.96 | 0.16 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3506 | 1/1 | 0.96 | 0.17 | 20,20,20,20 | 0 |
| 54 | MG | 2A | 3103 | 1/1 | 0.96 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3184 | 1/1 | 0.96 | 0.28 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3392 | 1/1 | 0.96 | 0.14 | 37,37,37,37 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3021 | 1/1 | 0.96 | 0.18 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3685 | 1/1 | 0.96 | 0.12 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3392 | 1/1 | 0.96 | 0.17 | 24,24,24,24 | 0 |
| 54 | MG | 1A | 3250 | 1/1 | 0.96 | 0.24 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3296 | 1/1 | 0.96 | 0.11 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3134 | 1/1 | 0.96 | 0.23 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3105 | 1/1 | 0.96 | 0.09 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3247 | 1/1 | 0.96 | 0.41 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3515 | 1/1 | 0.96 | 0.22 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3713 | 1/1 | 0.96 | 0.41 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3554 | 1/1 | 0.97 | 0.10 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3023 | 1/1 | 0.97 | 0.16 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3859 | 1/1 | 0.97 | 0.11 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3111 | 1/1 | 0.97 | 0.06 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3003 | 1/1 | 0.97 | 0.16 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3931 | 1/1 | 0.97 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3890 | 1/1 | 0.97 | 0.13 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3878 | 1/1 | 0.97 | 0.19 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3219 | 1/1 | 0.97 | 0.15 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3598 | 1/1 | 0.97 | 0.14 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3506 | 1/1 | 0.97 | 0.15 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3630 | 1/1 | 0.97 | 0.06 | 40,40,40,40 | 0 |
| 54 | MG | 2B | 212 | 1/1 | 0.97 | 0.12 | 80,80,80,80 | 0 |
| 54 | MG | 2E | 303 | 1/1 | 0.97 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3337 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 54 | MG | 1E | 309 | 1/1 | 0.97 | 0.14 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3252 | 1/1 | 0.97 | 0.19 | 36,36,36,36 | 0 |
| 54 | MG | 1E | 310 | 1/1 | 0.97 | 0.09 | 58,58,58,58 | 0 |
| 54 | MG | 2E | 306 | 1/1 | 0.97 | 0.13 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3863 | 1/1 | 0.97 | 0.15 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3123 | 1/1 | 0.97 | 0.31 | 32,32,32,32 | 0 |
| 54 | MG | 1a | 1709 | 1/1 | 0.97 | 0.16 | 35,35,35,35 | 0 |
| 54 | MG | 1D | 301 | 1/1 | 0.97 | 0.41 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3403 | 1/1 | 0.97 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3689 | 1/1 | 0.97 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3310 | 1/1 | 0.97 | 0.14 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3121 | 1/1 | 0.97 | 0.20 | 35,35,35,35 | 0 |
| 54 | MG | 2a | 3112 | 1/1 | 0.97 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3248 | 1/1 | 0.97 | 0.15 | 39,39,39,39 | 0 |
| 54 | MG | 13 | 102 | 1/1 | 0.97 | 0.15 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3411 | 1/1 | 0.97 | 0.15 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3085 | 1/1 | 0.97 | 0.44 | 50,50,50,50 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2a | 3125 | 1/1 | 0.97 | 0.08 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3574 | 1/1 | 0.97 | 0.20 | 33,33,33,33 | 0 |
| 54 | MG | 1W | 204 | 1/1 | 0.97 | 0.31 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3036 | 1/1 | 0.97 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3052 | 1/1 | 0.97 | 0.23 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3062 | 1/1 | 0.97 | 0.14 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3413 | 1/1 | 0.97 | 0.06 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3621 | 1/1 | 0.97 | 0.10 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3070 | 1/1 | 0.97 | 0.28 | 27,27,27,27 | 0 |
| 54 | MG | 1a | 1649 | 1/1 | 0.97 | 0.13 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3159 | 1/1 | 0.97 | 0.13 | 29,29,29,29 | 0 |
| 54 | MG | 2B | 205 | 1/1 | 0.97 | 0.12 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3237 | 1/1 | 0.97 | 0.33 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3008 | 1/1 | 0.97 | 0.51 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3490 | 1/1 | 0.97 | 0.19 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3606 | 1/1 | 0.97 | 0.37 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3113 | 1/1 | 0.97 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3665 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3681 | 1/1 | 0.97 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3577 | 1/1 | 0.97 | 0.17 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3268 | 1/1 | 0.97 | 0.14 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3040 | 1/1 | 0.97 | 0.06 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3513 | 1/1 | 0.97 | 0.17 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3499 | 1/1 | 0.97 | 0.14 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3550 | 1/1 | 0.97 | 0.17 | 43,43,43,43 | 0 |
| 54 | MG | 2a | 3147 | 1/1 | 0.97 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1677 | 1/1 | 0.97 | 0.21 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3236 | 1/1 | 0.97 | 0.24 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3531 | 1/1 | 0.97 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3347 | 1/1 | 0.97 | 0.14 | 35,35,35,35 | 0 |
| 54 | MG | 2D | 301 | 1/1 | 0.97 | 0.51 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3049 | 1/1 | 0.97 | 0.09 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3379 | 1/1 | 0.97 | 0.07 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3329 | 1/1 | 0.97 | 0.12 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3398 | 1/1 | 0.97 | 0.13 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3117 | 1/1 | 0.97 | 0.17 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3820 | 1/1 | 0.97 | 0.46 | 27,27,27,27 | 0 |
| 54 | MG | 1a | 1787 | 1/1 | 0.97 | 0.10 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3483 | 1/1 | 0.97 | 0.11 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3675 | 1/1 | 0.97 | 0.21 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1866 | 1/1 | 0.97 | 0.06 | 44,44,44,44 | 0 |
| 54 | MG | 1F | 313 | 1/1 | 0.97 | 0.52 | 48,48,48,48 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3061 | 1/1 | 0.97 | 0.26 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3355 | 1/1 | 0.97 | 0.13 | 18,18,18,18 | 0 |
| 54 | MG | 1A | 3098 | 1/1 | 0.97 | 0.19 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3411 | 1/1 | 0.97 | 0.22 | 25,25,25,25 | 0 |
| 54 | MG | 1B | 213 | 1/1 | 0.97 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3508 | 1/1 | 0.97 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 17 | 105 | 1/1 | 0.97 | 0.22 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3913 | 1/1 | 0.97 | 0.06 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3496 | 1/1 | 0.97 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1832 | 1/1 | 0.97 | 0.27 | 52,52,52,52 | 0 |
| 54 | MG | 1U | 205 | 1/1 | 0.97 | 0.28 | 36,36,36,36 | 0 |
| 54 | MG | 1a | 1704 | 1/1 | 0.97 | 0.14 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3211 | 1/1 | 0.97 | 0.30 | 46,46,46,46 | 0 |
| 54 | MG | 2a | 3113 | 1/1 | 0.97 | 0.08 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3017 | 1/1 | 0.97 | 0.20 | 36,36,36,36 | 0 |
| 54 | MG | 2a | 3163 | 1/1 | 0.97 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3845 | 1/1 | 0.97 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3520 | 1/1 | 0.97 | 0.37 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3752 | 1/1 | 0.97 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3299 | 1/1 | 0.97 | 0.26 | 38,38,38,38 | 0 |
| 54 | MG | 2a | 3097 | 1/1 | 0.97 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3094 | 1/1 | 0.97 | 0.18 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3649 | 1/1 | 0.97 | 0.29 | 40,40,40,40 | 0 |
| 55 | ERY | 2A | 3734 | 51/51 | 0.97 | 0.31 | 32,46,59,66 | 0 |
| 54 | MG | 2A | 3010 | 1/1 | 0.97 | 0.19 | 60,60,60,60 | 0 |
| 54 | MG | 15 | 102 | 1/1 | 0.97 | 0.24 | 25,25,25,25 | 0 |
| 54 | MG | 2a | 3059 | 1/1 | 0.97 | 0.11 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3155 | 1/1 | 0.97 | 0.28 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3635 | 1/1 | 0.97 | 0.12 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3095 | 1/1 | 0.97 | 0.14 | 18,18,18,18 | 0 |
| 54 | MG | 2A | 3020 | 1/1 | 0.97 | 0.35 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3243 | 1/1 | 0.97 | 0.27 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3629 | 1/1 | 0.97 | 0.15 | 46,46,46,46 | 0 |
| 54 | MG | 2E | 301 | 1/1 | 0.97 | 0.44 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3151 | 1/1 | 0.97 | 0.20 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3464 | 1/1 | 0.97 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3067 | 1/1 | 0.97 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1698 | 1/1 | 0.97 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 2a | 3176 | 1/1 | 0.97 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1658 | 1/1 | 0.97 | 0.06 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3566 | 1/1 | 0.97 | 0.14 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3099 | 1/1 | 0.97 | 0.14 | 42,42,42,42 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2V | 203 | 1/1 | 0.97 | 0.12 | 47,47,47,47 | 0 |
| 54 | MG | 2Q | 202 | 1/1 | 0.97 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3611 | 1/1 | 0.97 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3347 | 1/1 | 0.97 | 0.17 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3453 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3024 | 1/1 | 0.97 | 0.16 | 19,19,19,19 | 0 |
| 54 | MG | 1A | 3112 | 1/1 | 0.97 | 0.15 | 39,39,39,39 | 0 |
| 54 | MG | 2a | 3171 | 1/1 | 0.97 | 0.07 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3866 | 1/1 | 0.97 | 0.11 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3078 | 1/1 | 0.97 | 0.21 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3046 | 1/1 | 0.97 | 0.17 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1793 | 1/1 | 0.97 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3073 | 1/1 | 0.97 | 0.10 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3438 | 1/1 | 0.97 | 0.16 | 44,44,44,44 | 0 |
| 54 | MG | 1a | 1758 | 1/1 | 0.97 | 0.08 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3652 | 1/1 | 0.97 | 0.16 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3308 | 1/1 | 0.97 | 0.19 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3746 | 1/1 | 0.97 | 0.10 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3164 | 1/1 | 0.97 | 0.14 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3176 | 1/1 | 0.97 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3114 | 1/1 | 0.97 | 0.18 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3836 | 1/1 | 0.97 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | 1B | 229 | 1/1 | 0.97 | 0.08 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3396 | 1/1 | 0.97 | 0.17 | 47,47,47,47 | 0 |
| 58 | ZN | 1n | 104 | 1/1 | 0.97 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3481 | 1/1 | 0.97 | 0.16 | 27,27,27,27 | 0 |
| 54 | MG | 1a | 1770 | 1/1 | 0.97 | 0.09 | 69,69,69,69 | 0 |
| 54 | MG | 1U | 203 | 1/1 | 0.97 | 0.21 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3072 | 1/1 | 0.97 | 0.15 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3157 | 1/1 | 0.97 | 0.20 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3740 | 1/1 | 0.97 | 0.20 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1809 | 1/1 | 0.97 | 0.15 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3037 | 1/1 | 0.97 | 0.34 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3570 | 1/1 | 0.97 | 0.09 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3517 | 1/1 | 0.97 | 0.17 | 53,53,53,53 | 0 |
| 54 | MG | 1N | 201 | 1/1 | 0.97 | 0.14 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3974 | 1/1 | 0.97 | 0.13 | 52,52,52,52 | 0 |
| 54 | MG | 1V | 202 | 1/1 | 0.97 | 0.33 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3730 | 1/1 | 0.97 | 0.12 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1620 | 1/1 | 0.97 | 0.20 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3391 | 1/1 | 0.97 | 0.17 | 18,18,18,18 | 0 |
| 54 | MG | 2A | 3402 | 1/1 | 0.97 | 0.15 | 37,37,37,37 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3174 | 1/1 | 0.97 | 0.27 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3189 | 1/1 | 0.97 | 0.19 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3308 | 1/1 | 0.97 | 0.14 | 23,23,23,23 | 0 |
| 54 | MG | 1e | 201 | 1/1 | 0.97 | 0.22 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 4017 | 1/1 | 0.97 | 0.26 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3668 | 1/1 | 0.97 | 0.10 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3070 | 1/1 | 0.97 | 0.16 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3353 | 1/1 | 0.97 | 0.08 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3214 | 1/1 | 0.97 | 0.71 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3449 | 1/1 | 0.97 | 0.09 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3753 | 1/1 | 0.97 | 0.08 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3530 | 1/1 | 0.97 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1769 | 1/1 | 0.97 | 0.21 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3537 | 1/1 | 0.97 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 1P | 201 | 1/1 | 0.97 | 0.61 | 36,36,36,36 | 0 |
| 54 | MG | 1a | 1711 | 1/1 | 0.97 | 0.15 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3160 | 1/1 | 0.97 | 0.67 | 36,36,36,36 | 0 |
| 54 | MG | 2a | 3029 | 1/1 | 0.97 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3686 | 1/1 | 0.97 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3111 | 1/1 | 0.97 | 0.13 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3217 | 1/1 | 0.97 | 0.10 | 38,38,38,38 | 0 |
| 54 | MG | 2B | 210 | 1/1 | 0.97 | 0.07 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3552 | 1/1 | 0.97 | 0.07 | 51,51,51,51 | 0 |
| 55 | ERY | 1A | 4021 | 51/51 | 0.97 | 0.28 | 23,35,44,46 | 0 |
| 54 | MG | 2A | 3138 | 1/1 | 0.97 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3643 | 1/1 | 0.97 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3136 | 1/1 | 0.97 | 0.14 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3535 | 1/1 | 0.97 | 0.13 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3737 | 1/1 | 0.97 | 0.16 | 28,28,28,28 | 0 |
| 54 | MG | 1a | 1656 | 1/1 | 0.97 | 0.19 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3185 | 1/1 | 0.97 | 0.23 | 44,44,44,44 | 0 |
| 54 | MG | 1R | 203 | 1/1 | 0.97 | 0.26 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3181 | 1/1 | 0.97 | 0.29 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3147 | 1/1 | 0.97 | 0.37 | 32,32,32,32 | 0 |
| 54 | MG | 1D | 305 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3576 | 1/1 | 0.97 | 0.60 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3458 | 1/1 | 0.97 | 0.06 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3487 | 1/1 | 0.97 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 1h | 201 | 1/1 | 0.97 | 0.16 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1855 | 1/1 | 0.97 | 0.15 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3397 | 1/1 | 0.97 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3522 | 1/1 | 0.97 | 0.18 | 63,63,63,63 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3174 | 1/1 | 0.97 | 0.19 | 45,45,45,45 | 0 |
| 54 | MG | 2a | 3011 | 1/1 | 0.97 | 0.16 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3284 | 1/1 | 0.97 | 0.11 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3164 | 1/1 | 0.97 | 0.23 | 48,48,48,48 | 0 |
| 54 | MG | 2D | 310 | 1/1 | 0.97 | 0.33 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3725 | 1/1 | 0.97 | 0.10 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3352 | 1/1 | 0.97 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3139 | 1/1 | 0.97 | 0.14 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3888 | 1/1 | 0.97 | 0.54 | 38,38,38,38 | 0 |
| 54 | MG | 2a | 3169 | 1/1 | 0.97 | 0.17 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3130 | 1/1 | 0.97 | 0.17 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3503 | 1/1 | 0.97 | 0.13 | 19,19,19,19 | 0 |
| 54 | MG | 2A | 3370 | 1/1 | 0.97 | 0.20 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3834 | 1/1 | 0.97 | 0.16 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3294 | 1/1 | 0.97 | 0.06 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3581 | 1/1 | 0.97 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3953 | 1/1 | 0.97 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3599 | 1/1 | 0.97 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3118 | 1/1 | 0.97 | 0.22 | 56,56,56,56 | 0 |
| 54 | MG | 1E | 307 | 1/1 | 0.97 | 0.18 | 23,23,23,23 | 0 |
| 54 | MG | 1B | 221 | 1/1 | 0.97 | 0.18 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3632 | 1/1 | 0.97 | 0.08 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3512 | 1/1 | 0.97 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1845 | 1/1 | 0.97 | 0.29 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3948 | 1/1 | 0.97 | 0.12 | 27,27,27,27 | 0 |
| 54 | MG | 1D | 308 | 1/1 | 0.97 | 0.25 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3450 | 1/1 | 0.97 | 0.15 | 45,45,45,45 | 0 |
| 54 | MG | 2B | 211 | 1/1 | 0.97 | 0.13 | 59,59,59,59 | 0 |
| 54 | MG | 2V | 201 | 1/1 | 0.97 | 0.20 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3420 | 1/1 | 0.97 | 0.19 | 28,28,28,28 | 0 |
| 54 | MG | 2A | 3079 | 1/1 | 0.97 | 0.15 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3540 | 1/1 | 0.97 | 0.05 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3364 | 1/1 | 0.97 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3294 | 1/1 | 0.97 | 0.16 | 29,29,29,29 | 0 |
| 54 | MG | 2a | 3050 | 1/1 | 0.97 | 0.18 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3717 | 1/1 | 0.97 | 0.16 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3284 | 1/1 | 0.97 | 0.32 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3239 | 1/1 | 0.97 | 0.34 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3365 | 1/1 | 0.97 | 0.10 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3191 | 1/1 | 0.97 | 0.21 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3212 | 1/1 | 0.97 | 0.30 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3314 | 1/1 | 0.97 | 0.14 | 62,62,62,62 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3177 | 1/1 | 0.97 | 0.29 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3381 | 1/1 | 0.97 | 0.14 | 31,31,31,31 | 0 |
| 54 | MG | 1a | 1703 | 1/1 | 0.97 | 0.18 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3340 | 1/1 | 0.97 | 0.20 | 28,28,28,28 | 0 |
| 54 | MG | 1D | 302 | 1/1 | 0.97 | 0.17 | 50,50,50,50 | 0 |
| 54 | MG | 1F | 311 | 1/1 | 0.97 | 0.12 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3706 | 1/1 | 0.97 | 0.07 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1702 | 1/1 | 0.97 | 0.09 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3179 | 1/1 | 0.97 | 0.34 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3295 | 1/1 | 0.97 | 0.19 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3614 | 1/1 | 0.97 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3385 | 1/1 | 0.97 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3694 | 1/1 | 0.97 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3415 | 1/1 | 0.97 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3516 | 1/1 | 0.97 | 0.18 | 22,22,22,22 | 0 |
| 54 | MG | 1A | 3805 | 1/1 | 0.97 | 0.17 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3717 | 1/1 | 0.97 | 0.18 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3198 | 1/1 | 0.97 | 0.26 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3275 | 1/1 | 0.97 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3155 | 1/1 | 0.97 | 0.10 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3681 | 1/1 | 0.97 | 0.45 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3855 | 1/1 | 0.97 | 0.13 | 47,47,47,47 | 0 |
| 54 | MG | 1F | 304 | 1/1 | 0.97 | 0.34 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3454 | 1/1 | 0.97 | 0.07 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3410 | 1/1 | 0.97 | 0.12 | 58,58,58,58 | 0 |
| 54 | MG | 1V | 203 | 1/1 | 0.97 | 0.15 | 45,45,45,45 | 0 |
| 54 | MG | 1B | 212 | 1/1 | 0.97 | 0.29 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3589 | 1/1 | 0.97 | 0.10 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3405 | 1/1 | 0.97 | 0.14 | 29,29,29,29 | 0 |
| 54 | MG | 2A | 3051 | 1/1 | 0.97 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3317 | 1/1 | 0.97 | 0.17 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3360 | 1/1 | 0.97 | 0.12 | 32,32,32,32 | 0 |
| 54 | MG | 1F | 310 | 1/1 | 0.97 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3013 | 1/1 | 0.97 | 0.16 | 22,22,22,22 | 0 |
| 54 | MG | 1A | 3692 | 1/1 | 0.98 | 0.15 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3043 | 1/1 | 0.98 | 0.15 | 28,28,28,28 | 0 |
| 54 | MG | 1F | 301 | 1/1 | 0.98 | 0.14 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3071 | 1/1 | 0.98 | 0.25 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3486 | 1/1 | 0.98 | 0.13 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3318 | 1/1 | 0.98 | 0.13 | 50,50,50,50 | 0 |
| 54 | MG | 2a | 3104 | 1/1 | 0.98 | 0.19 | 68,68,68,68 | 0 |
| 54 | MG | 2a | 3102 | 1/1 | 0.98 | 0.04 | 70,70,70,70 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1Q | 203 | 1/1 | 0.98 | 0.14 | 41,41,41,41 | 0 |
| 54 | MG | 1a | 1710 | 1/1 | 0.98 | 0.19 | 49,49,49,49 | 0 |
| 54 | MG | 1E | 308 | 1/1 | 0.98 | 0.10 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 4008 | 1/1 | 0.98 | 0.12 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3290 | 1/1 | 0.98 | 0.17 | 21,21,21,21 | 0 |
| 54 | MG | 2A | 3166 | 1/1 | 0.98 | 0.22 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3397 | 1/1 | 0.98 | 0.20 | 22,22,22,22 | 0 |
| 54 | MG | 1A | 3371 | 1/1 | 0.98 | 0.09 | 31,31,31,31 | 0 |
| 54 | MG | 2a | 3093 | 1/1 | 0.98 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 2a | 3152 | 1/1 | 0.98 | 0.10 | 71,71,71,71 | 0 |
| 54 | MG | 2a | 3047 | 1/1 | 0.98 | 0.18 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3085 | 1/1 | 0.98 | 0.27 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3620 | 1/1 | 0.98 | 0.14 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1862 | 1/1 | 0.98 | 0.11 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3443 | 1/1 | 0.98 | 0.18 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3331 | 1/1 | 0.98 | 0.13 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3076 | 1/1 | 0.98 | 0.51 | 54,54,54,54 | 0 |
| 54 | MG | 1U | 206 | 1/1 | 0.98 | 0.40 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3165 | 1/1 | 0.98 | 0.21 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3304 | 1/1 | 0.98 | 0.10 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3707 | 1/1 | 0.98 | 0.19 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3233 | 1/1 | 0.98 | 0.52 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3226 | 1/1 | 0.98 | 0.30 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3806 | 1/1 | 0.98 | 0.14 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3143 | 1/1 | 0.98 | 0.17 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3069 | 1/1 | 0.98 | 0.33 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3152 | 1/1 | 0.98 | 0.45 | 36,36,36,36 | 0 |
| 54 | MG | 1a | 1804 | 1/1 | 0.98 | 0.09 | 47,47,47,47 | 0 |
| 54 | MG | 1N | 202 | 1/1 | 0.98 | 0.15 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3936 | 1/1 | 0.98 | 0.08 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3847 | 1/1 | 0.98 | 0.15 | 39,39,39,39 | 0 |
| 54 | MG | 2t | 201 | 1/1 | 0.98 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 1a | 1708 | 1/1 | 0.98 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 1F | 315 | 1/1 | 0.98 | 0.11 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3357 | 1/1 | 0.98 | 0.17 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3540 | 1/1 | 0.98 | 0.17 | 34,34,34,34 | 0 |
| 54 | MG | 13 | 104 | 1/1 | 0.98 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 1F | 306 | 1/1 | 0.98 | 0.30 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3338 | 1/1 | 0.98 | 0.10 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3739 | 1/1 | 0.98 | 0.13 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3018 | 1/1 | 0.98 | 0.44 | 41,41,41,41 | 0 |
| 54 | MG | 1Q | 202 | 1/1 | 0.98 | 0.13 | 29,29,29,29 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3597 | 1/1 | 0.98 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 2a | 3164 | 1/1 | 0.98 | 0.03 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 4005 | 1/1 | 0.98 | 0.14 | 15,15,15,15 | 0 |
| 54 | MG | 1A | 3460 | 1/1 | 0.98 | 0.12 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3555 | 1/1 | 0.98 | 0.17 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3338 | 1/1 | 0.98 | 0.11 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3727 | 1/1 | 0.98 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3841 | 1/1 | 0.98 | 0.10 | 23,23,23,23 | 0 |
| 54 | MG | 1A | 3367 | 1/1 | 0.98 | 0.09 | 26,26,26,26 | 0 |
| 54 | MG | 2A | 3551 | 1/1 | 0.98 | 0.07 | 44,44,44,44 | 0 |
| 58 | ZN | 25 | 103 | 1/1 | 0.98 | 0.19 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3926 | 1/1 | 0.98 | 0.16 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3604 | 1/1 | 0.98 | 0.25 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3227 | 1/1 | 0.98 | 0.20 | 31,31,31,31 | 0 |
| 54 | MG | 2D | 303 | 1/1 | 0.98 | 0.38 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3493 | 1/1 | 0.98 | 0.15 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3282 | 1/1 | 0.98 | 0.43 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3365 | 1/1 | 0.98 | 0.14 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3350 | 1/1 | 0.98 | 0.16 | 32,32,32,32 | 0 |
| 54 | MG | 2a | 3168 | 1/1 | 0.98 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1l | 102 | 1/1 | 0.98 | 0.13 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3545 | 1/1 | 0.98 | 0.22 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3387 | 1/1 | 0.98 | 0.15 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3629 | 1/1 | 0.98 | 0.12 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3180 | 1/1 | 0.98 | 0.10 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3262 | 1/1 | 0.98 | 0.38 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3025 | 1/1 | 0.98 | 0.33 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1764 | 1/1 | 0.98 | 0.17 | 39,39,39,39 | 0 |
| 54 | MG | 2a | 3110 | 1/1 | 0.98 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3400 | 1/1 | 0.98 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3519 | 1/1 | 0.98 | 0.11 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3465 | 1/1 | 0.98 | 0.12 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3972 | 1/1 | 0.98 | 0.14 | 19,19,19,19 | 0 |
| 54 | MG | 2A | 3600 | 1/1 | 0.98 | 0.07 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3218 | 1/1 | 0.98 | 0.52 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1838 | 1/1 | 0.98 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3796 | 1/1 | 0.98 | 0.18 | 32,32,32,32 | 0 |
| 54 | MG | 1a | 1833 | 1/1 | 0.98 | 0.19 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3603 | 1/1 | 0.98 | 0.18 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3344 | 1/1 | 0.98 | 0.13 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3132 | 1/1 | 0.98 | 0.57 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3844 | 1/1 | 0.98 | 0.09 | 35,35,35,35 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3409 | 1/1 | 0.98 | 0.15 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3032 | 1/1 | 0.98 | 0.10 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3800 | 1/1 | 0.98 | 0.22 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3237 | 1/1 | 0.98 | 0.21 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3594 | 1/1 | 0.98 | 0.19 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3504 | 1/1 | 0.98 | 0.13 | 22,22,22,22 | 0 |
| 54 | MG | 2a | 3098 | 1/1 | 0.98 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3501 | 1/1 | 0.98 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3374 | 1/1 | 0.98 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3489 | 1/1 | 0.98 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3573 | 1/1 | 0.98 | 0.19 | 29,29,29,29 | 0 |
| 54 | MG | 2A | 3229 | 1/1 | 0.98 | 0.21 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3423 | 1/1 | 0.98 | 0.20 | 41,41,41,41 | 0 |
| 54 | MG | 15 | 103 | 1/1 | 0.98 | 0.31 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3122 | 1/1 | 0.98 | 0.19 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3646 | 1/1 | 0.98 | 0.05 | 73,73,73,73 | 0 |
| 58 | ZN | 15 | 107 | 1/1 | 0.98 | 0.20 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3042 | 1/1 | 0.98 | 0.14 | 24,24,24,24 | 0 |
| 54 | MG | 1a | 1765 | 1/1 | 0.98 | 0.17 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3666 | 1/1 | 0.98 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3081 | 1/1 | 0.98 | 0.15 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3726 | 1/1 | 0.98 | 0.17 | 24,24,24,24 | 0 |
| 54 | MG | 1A | 3424 | 1/1 | 0.98 | 0.12 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3054 | 1/1 | 0.98 | 0.26 | 24,24,24,24 | 0 |
| 54 | MG | 2A | 3451 | 1/1 | 0.98 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 15 | 104 | 1/1 | 0.98 | 0.14 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3289 | 1/1 | 0.98 | 0.18 | 25,25,25,25 | 0 |
| 54 | MG | 1a | 1676 | 1/1 | 0.98 | 0.24 | 68,68,68,68 | 0 |
| 54 | MG | 1U | 202 | 1/1 | 0.98 | 0.27 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3538 | 1/1 | 0.98 | 0.09 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3494 | 1/1 | 0.98 | 0.11 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3784 | 1/1 | 0.98 | 0.10 | 29,29,29,29 | 0 |
| 54 | MG | 2a | 3173 | 1/1 | 0.98 | 0.08 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1823 | 1/1 | 0.98 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3731 | 1/1 | 0.98 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3432 | 1/1 | 0.98 | 0.12 | 18,18,18,18 | 0 |
| 54 | MG | 1A | 3120 | 1/1 | 0.98 | 0.22 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3488 | 1/1 | 0.98 | 0.10 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 4020 | 1/1 | 0.98 | 0.12 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3207 | 1/1 | 0.98 | 0.33 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3500 | 1/1 | 0.98 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3967 | 1/1 | 0.98 | 0.09 | 27,27,27,27 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 17 | 102 | 1/1 | 0.98 | 0.14 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3359 | 1/1 | 0.98 | 0.18 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3510 | 1/1 | 0.98 | 0.13 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3380 | 1/1 | 0.98 | 0.15 | 19,19,19,19 | 0 |
| 54 | MG | 1A | 3105 | 1/1 | 0.98 | 0.18 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3188 | 1/1 | 0.98 | 0.11 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3728 | 1/1 | 0.98 | 0.07 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3824 | 1/1 | 0.98 | 0.17 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1747 | 1/1 | 0.98 | 0.18 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3814 | 1/1 | 0.98 | 0.09 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3526 | 1/1 | 0.98 | 0.15 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3169 | 1/1 | 0.98 | 0.46 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3044 | 1/1 | 0.98 | 0.18 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3346 | 1/1 | 0.98 | 0.16 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3702 | 1/1 | 0.98 | 0.35 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3317 | 1/1 | 0.98 | 0.16 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3485 | 1/1 | 0.98 | 0.11 | 36,36,36,36 | 0 |
| 54 | MG | 1a | 1650 | 1/1 | 0.98 | 0.18 | 55,55,55,55 | 0 |
| 54 | MG | 15 | 105 | 1/1 | 0.98 | 0.11 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3051 | 1/1 | 0.98 | 0.49 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3446 | 1/1 | 0.98 | 0.06 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3985 | 1/1 | 0.98 | 0.20 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3278 | 1/1 | 0.98 | 0.21 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3447 | 1/1 | 0.98 | 0.11 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3041 | 1/1 | 0.98 | 0.21 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3258 | 1/1 | 0.98 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3387 | 1/1 | 0.98 | 0.21 | 24,24,24,24 | 0 |
| 54 | MG | 1F | 303 | 1/1 | 0.98 | 0.27 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3309 | 1/1 | 0.98 | 0.23 | 35,35,35,35 | 0 |
| 54 | MG | 1F | 305 | 1/1 | 0.98 | 0.26 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3460 | 1/1 | 0.98 | 0.15 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3690 | 1/1 | 0.98 | 0.16 | 38,38,38,38 | 0 |
| 54 | MG | 1a | 1712 | 1/1 | 0.98 | 0.15 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3716 | 1/1 | 0.98 | 0.24 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3097 | 1/1 | 0.98 | 0.07 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3637 | 1/1 | 0.98 | 0.05 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3422 | 1/1 | 0.98 | 0.10 | 20,20,20,20 | 0 |
| 54 | MG | 1P | 206 | 1/1 | 0.98 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3334 | 1/1 | 0.98 | 0.10 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3696 | 1/1 | 0.98 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1612 | 1/1 | 0.98 | 0.15 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3536 | 1/1 | 0.98 | 0.12 | 28,28,28,28 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3862 | 1/1 | 0.98 | 0.14 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3509 | 1/1 | 0.98 | 0.20 | 23,23,23,23 | 0 |
| 54 | MG | 2A | 3532 | 1/1 | 0.98 | 0.20 | 50,50,50,50 | 0 |
| 58 | ZN | 1Y | 203 | 1/1 | 0.98 | 0.18 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3172 | 1/1 | 0.98 | 0.13 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3651 | 1/1 | 0.98 | 0.32 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3305 | 1/1 | 0.98 | 0.16 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3205 | 1/1 | 0.98 | 0.12 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3108 | 1/1 | 0.98 | 0.13 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3328 | 1/1 | 0.98 | 0.16 | 15,15,15,15 | 0 |
| 54 | MG | 1I | 101 | 1/1 | 0.98 | 0.20 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3047 | 1/1 | 0.98 | 0.16 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3110 | 1/1 | 0.98 | 0.31 | 31,31,31,31 | 0 |
| 58 | ZN | 2n | 102 | 1/1 | 0.98 | 0.07 | 93,93,93,93 | 0 |
| 54 | MG | 1a | 1783 | 1/1 | 0.98 | 0.23 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3167 | 1/1 | 0.98 | 0.16 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3623 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | 1Q | 201 | 1/1 | 0.98 | 0.15 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3444 | 1/1 | 0.98 | 0.16 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3161 | 1/1 | 0.98 | 0.16 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3263 | 1/1 | 0.98 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3332 | 1/1 | 0.98 | 0.16 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1659 | 1/1 | 0.98 | 0.27 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3337 | 1/1 | 0.98 | 0.13 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3116 | 1/1 | 0.98 | 0.16 | 50,50,50,50 | 0 |
| 54 | MG | 1D | 316 | 1/1 | 0.98 | 0.24 | 32,32,32,32 | 0 |
| 54 | MG | 1D | 304 | 1/1 | 0.98 | 0.09 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3642 | 1/1 | 0.98 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3928 | 1/1 | 0.98 | 0.22 | 54,54,54,54 | 0 |
| 54 | MG | 2W | 201 | 1/1 | 0.98 | 0.27 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3421 | 1/1 | 0.98 | 0.16 | 30,30,30,30 | 0 |
| 54 | MG | 2W | 203 | 1/1 | 0.98 | 0.09 | 61,61,61,61 | 0 |
| 54 | MG | 1U | 208 | 1/1 | 0.98 | 0.35 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3587 | 1/1 | 0.98 | 0.15 | 25,25,25,25 | 0 |
| 54 | MG | 1o | 101 | 1/1 | 0.98 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3286 | 1/1 | 0.98 | 0.12 | 37,37,37,37 | 0 |
| 54 | MG | 2a | 3143 | 1/1 | 0.98 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3303 | 1/1 | 0.98 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3730 | 1/1 | 0.98 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1840 | 1/1 | 0.98 | 0.14 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3358 | 1/1 | 0.98 | 0.11 | 20,20,20,20 | 0 |
| 54 | MG | 1A | 3963 | 1/1 | 0.98 | 0.17 | 51,51,51,51 | 0 |

Continued on next page...

Continued from previous page...

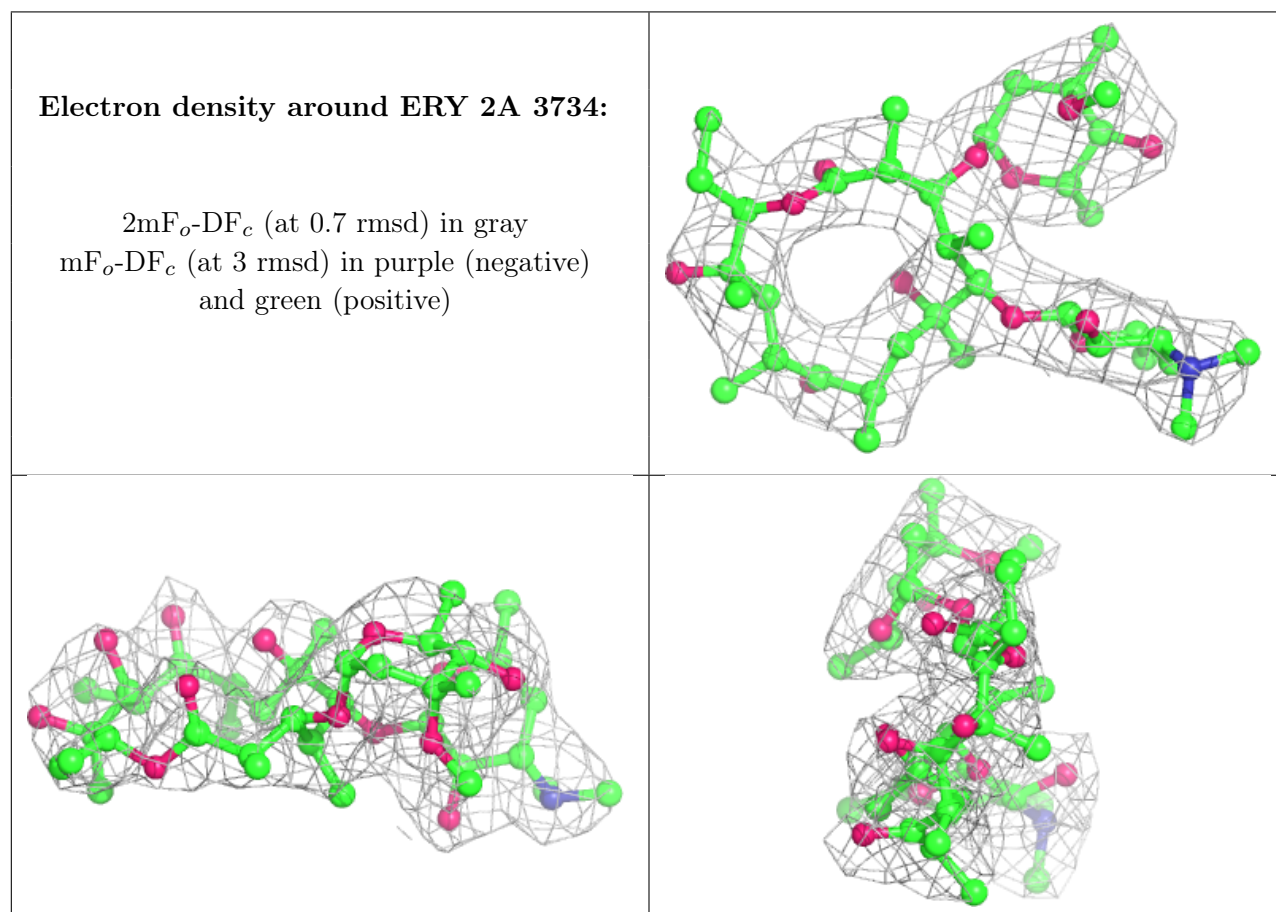
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3441 | 1/1 | 0.98 | 0.15 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3763 | 1/1 | 0.98 | 0.20 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3119 | 1/1 | 0.98 | 0.19 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3434 | 1/1 | 0.98 | 0.12 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3273 | 1/1 | 0.98 | 0.23 | 26,26,26,26 | 0 |
| 54 | MG | 2A | 3030 | 1/1 | 0.98 | 0.19 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3439 | 1/1 | 0.98 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 4012 | 1/1 | 0.99 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3018 | 1/1 | 0.99 | 0.21 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3828 | 1/1 | 0.99 | 0.19 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3144 | 1/1 | 0.99 | 0.20 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3004 | 1/1 | 0.99 | 0.12 | 40,40,40,40 | 0 |
| 54 | MG | 2e | 202 | 1/1 | 0.99 | 0.13 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3709 | 1/1 | 0.99 | 0.11 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3902 | 1/1 | 0.99 | 0.10 | 31,31,31,31 | 0 |
| 54 | MG | 1V | 201 | 1/1 | 0.99 | 0.45 | 29,29,29,29 | 0 |
| 54 | MG | 1a | 1861 | 1/1 | 0.99 | 0.13 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3141 | 1/1 | 0.99 | 0.15 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3419 | 1/1 | 0.99 | 0.24 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3943 | 1/1 | 0.99 | 0.08 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3136 | 1/1 | 0.99 | 0.21 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3267 | 1/1 | 0.99 | 0.23 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3246 | 1/1 | 0.99 | 0.27 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3005 | 1/1 | 0.99 | 0.20 | 22,22,22,22 | 0 |
| 54 | MG | 1a | 1735 | 1/1 | 0.99 | 0.11 | 54,54,54,54 | 0 |
| 54 | MG | 23 | 101 | 1/1 | 0.99 | 0.46 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3760 | 1/1 | 0.99 | 0.26 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1648 | 1/1 | 0.99 | 0.21 | 61,61,61,61 | 0 |
| 54 | MG | 1R | 201 | 1/1 | 0.99 | 0.20 | 29,29,29,29 | 0 |
| 54 | MG | 1D | 306 | 1/1 | 0.99 | 0.12 | 16,16,16,16 | 0 |
| 54 | MG | 1A | 3901 | 1/1 | 0.99 | 0.18 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3490 | 1/1 | 0.99 | 0.14 | 29,29,29,29 | 0 |
| 54 | MG | 2A | 3137 | 1/1 | 0.99 | 0.13 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3607 | 1/1 | 0.99 | 0.17 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3887 | 1/1 | 0.99 | 0.20 | 37,37,37,37 | 0 |
| 59 | SF4 | 2d | 501 | 8/8 | 0.99 | 0.14 | 70,71,85,85 | 0 |
| 54 | MG | 1A | 3713 | 1/1 | 0.99 | 0.16 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3825 | 1/1 | 0.99 | 0.13 | 18,18,18,18 | 0 |
| 54 | MG | 1a | 1611 | 1/1 | 0.99 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3137 | 1/1 | 0.99 | 0.17 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3100 | 1/1 | 0.99 | 0.10 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3325 | 1/1 | 0.99 | 0.14 | 25,25,25,25 | 0 |

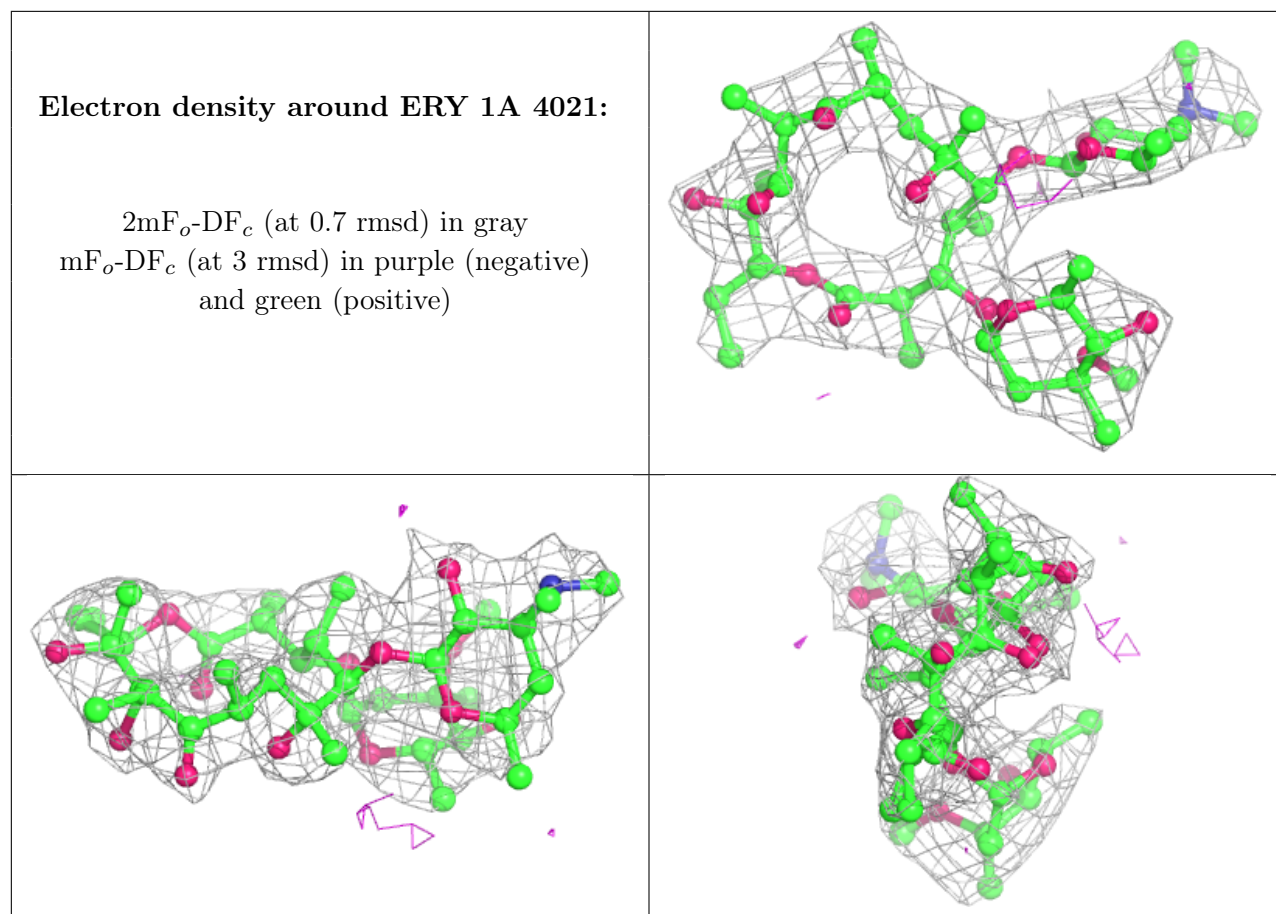
Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2E | 302 | 1/1 | 0.99 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3330 | 1/1 | 0.99 | 0.19 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 4000 | 1/1 | 0.99 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3627 | 1/1 | 0.99 | 0.16 | 23,23,23,23 | 0 |
| 54 | MG | 2A | 3282 | 1/1 | 0.99 | 0.10 | 21,21,21,21 | 0 |
| 54 | MG | 2A | 3530 | 1/1 | 0.99 | 0.09 | 51,51,51,51 | 0 |
| 59 | SF4 | 1d | 306 | 8/8 | 0.99 | 0.17 | 61,69,73,74 | 0 |
| 54 | MG | 1A | 3851 | 1/1 | 0.99 | 0.25 | 46,46,46,46 | 0 |
| 58 | ZN | 26 | 501 | 1/1 | 0.99 | 0.20 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3001 | 1/1 | 0.99 | 0.11 | 33,33,33,33 | 0 |
| 54 | MG | 1D | 310 | 1/1 | 0.99 | 0.29 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3384 | 1/1 | 0.99 | 0.16 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3315 | 1/1 | 0.99 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3058 | 1/1 | 0.99 | 0.17 | 24,24,24,24 | 0 |
| 58 | ZN | 16 | 501 | 1/1 | 0.99 | 0.24 | 46,46,46,46 | 0 |
| 54 | MG | 1W | 203 | 1/1 | 0.99 | 0.10 | 28,28,28,28 | 0 |
| 54 | MG | 1E | 303 | 1/1 | 0.99 | 0.21 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3333 | 1/1 | 0.99 | 0.14 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3667 | 1/1 | 0.99 | 0.25 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3056 | 1/1 | 0.99 | 0.15 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3822 | 1/1 | 0.99 | 0.12 | 19,19,19,19 | 0 |
| 54 | MG | 1A | 3829 | 1/1 | 0.99 | 0.16 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3351 | 1/1 | 0.99 | 0.11 | 22,22,22,22 | 0 |
| 54 | MG | 2A | 3234 | 1/1 | 0.99 | 0.44 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3434 | 1/1 | 0.99 | 0.15 | 35,35,35,35 | 0 |
| 54 | MG | 2F | 304 | 1/1 | 0.99 | 0.22 | 42,42,42,42 | 0 |
| 54 | MG | 1a | 1722 | 1/1 | 0.99 | 0.13 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3045 | 1/1 | 0.99 | 0.17 | 14,14,14,14 | 0 |
| 54 | MG | 2D | 306 | 1/1 | 0.99 | 0.36 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3641 | 1/1 | 0.99 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3302 | 1/1 | 0.99 | 0.18 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3116 | 1/1 | 0.99 | 0.25 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3493 | 1/1 | 0.99 | 0.09 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3015 | 1/1 | 0.99 | 0.17 | 38,38,38,38 | 0 |
| 54 | MG | 1a | 1734 | 1/1 | 0.99 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3720 | 1/1 | 0.99 | 0.14 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3175 | 1/1 | 0.99 | 0.17 | 22,22,22,22 | 0 |
| 54 | MG | 1A | 3089 | 1/1 | 0.99 | 0.15 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3028 | 1/1 | 0.99 | 0.32 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3532 | 1/1 | 0.99 | 0.60 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3476 | 1/1 | 0.99 | 0.09 | 42,42,42,42 | 0 |
| 58 | ZN | 19 | 102 | 1/1 | 1.00 | 0.21 | 49,49,49,49 | 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.