



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2021 – 09:32 PM EDT

PDB ID : 7RQ8
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with iboxamycin, mRNA, deacylated A- and E-site tRNAs, and aminoacylated P-site tRNA at 2.50Å resolution
Authors : Mitcheltree, M.J.; Pisipati, A.; Syroegin, E.A.; Silvestre, K.J.; Klepacki, D.; Mason, J.D.; Terwilliger, D.W.; Testolin, G.; Pote, A.R.; Wu, K.J.Y.; Ladley, R.P.; Chatman, K.; Mankin, A.S.; Polikanov, Y.S.; Myers, A.G.
Deposited on : 2021-08-06
Resolution : 2.50 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 | : | 2.23.2 |
| 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) | : | 2.23.2 |

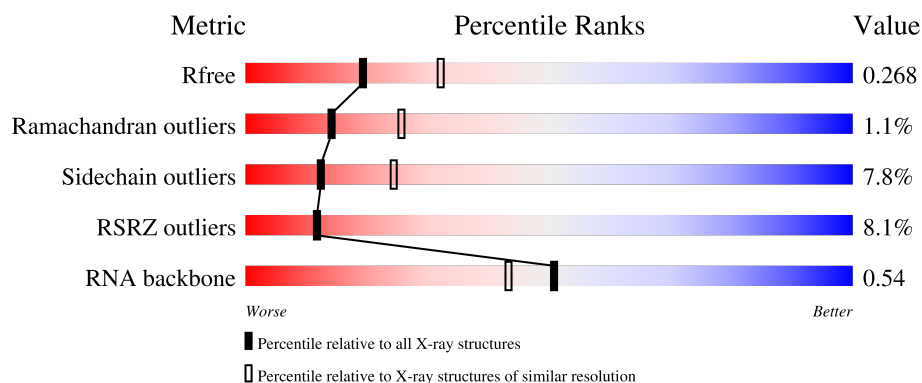
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 4661 (2.50-2.50) |
| Ramachandran outliers | 138981 | 5231 (2.50-2.50) |
| Sidechain outliers | 138945 | 5233 (2.50-2.50) |
| RSRZ outliers | 127900 | 4559 (2.50-2.50) |
| RNA backbone | 3102 | 1008 (2.84-2.16) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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>2%</div> <div>82%</div> <div>16%</div> <div>..</div> </div> |
| 1 | 2A | 2915 | <div> <div>3%</div> <div>79%</div> <div>17%</div> <div>.</div> </div> |
| 2 | 1B | 121 | <div> <div>92%</div> <div>7%</div> <div>.</div> </div> |
| 2 | 2B | 121 | <div> <div>2%</div> <div>75%</div> <div>24%</div> <div>.</div> </div> |
| 3 | 1D | 276 | <div> <div>%</div> <div>94%</div> <div>5%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | 2D | 276 | <div> <div>4%</div> <div>96%</div> <div>.</div> </div> |
| 4 | 1E | 206 | <div> <div></div> <div>92%</div> <div>7% .</div> </div> |
| 4 | 2E | 206 | <div> <div>3%</div> <div>94%</div> <div>5% .</div> </div> |
| 5 | 1F | 210 | <div> <div></div> <div>90%</div> <div>6% .</div> </div> |
| 5 | 2F | 210 | <div> <div>2%</div> <div>92%</div> <div>. .</div> </div> |
| 6 | 1G | 182 | <div> <div>2%</div> <div>92%</div> <div>7% ..</div> </div> |
| 6 | 2G | 182 | <div> <div>20%</div> <div>87%</div> <div>12% ..</div> </div> |
| 7 | 1H | 180 | <div> <div></div> <div>93%</div> <div>. .</div> </div> |
| 7 | 2H | 180 | <div> <div>53%</div> <div>88%</div> <div>8% .</div> </div> |
| 8 | 1I | 148 | <div> <div>%</div> <div>86%</div> <div>12% .</div> </div> |
| 8 | 2I | 148 | <div> <div>22%</div> <div>90%</div> <div>9% .</div> </div> |
| 9 | 1N | 140 | <div> <div></div> <div>95%</div> <div>5%</div> </div> |
| 9 | 2N | 140 | <div> <div>9%</div> <div>94%</div> <div>6%</div> </div> |
| 10 | 1O | 122 | <div> <div>%</div> <div>98%</div> <div>.</div> </div> |
| 10 | 2O | 122 | <div> <div>7%</div> <div>97%</div> <div>.</div> </div> |
| 11 | 1P | 150 | <div> <div>%</div> <div>92%</div> <div>7% .</div> </div> |
| 11 | 2P | 150 | <div> <div>8%</div> <div>91%</div> <div>8% .</div> </div> |
| 12 | 1Q | 141 | <div> <div>2%</div> <div>96%</div> <div>.</div> </div> |
| 12 | 2Q | 141 | <div> <div>23%</div> <div>95%</div> <div>5%</div> </div> |
| 13 | 1R | 118 | <div> <div></div> <div>97%</div> <div>.</div> </div> |
| 13 | 2R | 118 | <div> <div>3%</div> <div>97%</div> <div>.</div> </div> |
| 14 | 1S | 112 | <div> <div>%</div> <div>91%</div> <div>7% .</div> </div> |
| 14 | 2S | 112 | <div> <div>17%</div> <div>83%</div> <div>15% .</div> </div> |
| 15 | 1T | 146 | <div> <div>3%</div> <div>86%</div> <div>. 10%</div> </div> |
| 15 | 2T | 146 | <div> <div>4%</div> <div>85%</div> <div>5% 10%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 16 | 1U | 118 | 92% 7% |
| 16 | 2U | 118 | 93% 5% |
| 17 | 1V | 101 | 97% |
| 17 | 2V | 101 | 90% 9% |
| 18 | 1W | 113 | 96% |
| 18 | 2W | 113 | 96% |
| 19 | 1X | 96 | 95% |
| 19 | 2X | 96 | 94% 5% |
| 20 | 1Y | 110 | 93% 5% |
| 20 | 2Y | 110 | 86% 11% |
| 21 | 1Z | 206 | 69% 6% 25% |
| 21 | 2Z | 206 | 70% 8% 22% |
| 22 | 10 | 85 | 95% |
| 22 | 20 | 85 | 93% 5% |
| 23 | 11 | 98 | 97% |
| 23 | 21 | 98 | 95% |
| 24 | 12 | 72 | 92% 6% |
| 24 | 22 | 72 | 89% 8% |
| 25 | 13 | 60 | 92% 7% |
| 25 | 23 | 60 | 93% 5% |
| 26 | 14 | 71 | 83% 10% |
| 26 | 24 | 71 | 77% 18% |
| 27 | 15 | 60 | 95% |
| 27 | 25 | 60 | 93% 5% |
| 28 | 16 | 54 | 91% 7% |

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| 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 | |

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| 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 | 1v | 24 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | 2v | 24 | |
| 54 | 1w | 76 | |
| 54 | 2w | 76 | |
| 55 | 1x | 77 | |
| 55 | 2x | 77 | |
| 56 | 1y | 76 | |
| 56 | 2y | 76 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 57 | MG | 1A | 3553 | - | - | - | X |
| 57 | MG | 1E | 303 | - | - | - | X |
| 57 | MG | 1O | 201 | - | - | - | X |
| 57 | MG | 1a | 1758 | - | - | - | X |
| 57 | MG | 2A | 3544 | - | - | - | X |
| 57 | MG | 2A | 3556 | - | - | - | X |
| 57 | MG | 2a | 1616 | - | - | - | X |

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299504 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 | 2871 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61852 | 27531 | 11572 | 19878 | 2871 | | | |
| 1 | 2A | 2800 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60322 | 26848 | 11284 | 19390 | 2800 | | | |

- 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 |
| | | | 2577 | 1146 | 476 | 835 | 120 | | | |
| 2 | 2B | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2575 | 1146 | 476 | 833 | 120 | | | |

- 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 |
| | | | 2136 | 1349 | 423 | 361 | 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 |
| | | | 1423 | 913 | 253 | 253 | 4 | | | |
| 6 | 2G | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1428 | 913 | 258 | 253 | 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 | 174 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1330 | 845 | 248 | 236 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | 1I | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1097 | 701 | 191 | 204 | 1 | | | |
| 8 | 2I | 146 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1064 | 681 | 186 | 196 | 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 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |
| 9 | 2N | 140 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1117 | 719 | 207 | 187 | 4 | | | |

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14 | 1S | 110 | Total | C | N | O | 0 | 0 | 0 |
| | | | 873 | 550 | 174 | 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 |
| | | | 771 | 495 | 140 | 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 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |
| 20 | 2Y | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21 | 1Z | 154 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1240 | 795 | 222 | 220 | 3 | | | |
| 21 | 2Z | 160 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1271 | 814 | 228 | 227 | 2 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23 | 11 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |
| 23 | 21 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 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 |
| | | | 588 | 365 | 118 | 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 |
| | | | 552 | 349 | 99 | 99 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 26 | 24 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 532 | 339 | 97 | 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 |
| | | | 455 | 285 | 89 | 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 | 1503 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32327 | 14396 | 5990 | 10438 | 1503 | | | |

- 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 |
| | | | 1846 | 1179 | 331 | 331 | 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 |
| | | | 1548 | 973 | 301 | 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 |
| | | | 1655 | 1038 | 326 | 284 | 7 | | | |
| 35 | 2d | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1674 | 1050 | 333 | 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 |
| | | | 1129 | 714 | 213 | 198 | 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 |
| | | | 810 | 514 | 144 | 149 | 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 |
| | | | 1231 | 766 | 243 | 216 | 6 | | | |
| 38 | 2g | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1235 | 769 | 244 | 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 |
| | | | 1088 | 689 | 206 | 191 | 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 |
| | | | 983 | 623 | 193 | 167 | | | |
| 40 | 2i | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 978 | 619 | 190 | 169 | | | |

- 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 |
| | | | 709 | 440 | 138 | 131 | | | |
| 41 | 2j | 96 | Total | C | N | O | 0 | 0 | 0 |
| | | | 714 | 445 | 138 | 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 |
| | | | 829 | 516 | 155 | 155 | 3 | | | |

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | 1m | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 592 | 198 | 166 | 2 | | | |
| 44 | 2m | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 950 | 586 | 197 | 165 | 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 |
| | | | 652 | 417 | 120 | 113 | 2 | | | |
| 50 | 2s | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 646 | 412 | 119 | 113 | 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 |
| | | | 728 | 446 | 156 | 124 | 2 | | | |
| 51 | 2t | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 727 | 446 | 155 | 124 | 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 RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 53 | 1v | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 277 | 125 | 51 | 88 | 13 | | | |
| 53 | 2v | 13 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 277 | 125 | 51 | 88 | 13 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 54 | 1w | 71 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1530 | 685 | 274 | 498 | 71 | 2 | | |
| 54 | 2w | 69 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1482 | 662 | 267 | 482 | 69 | 2 | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 55 | 1x | 76 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1635 | 731 | 296 | 530 | 76 | 2 | | |
| 55 | 2x | 76 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1635 | 731 | 296 | 530 | 76 | 2 | | |

- Molecule 56 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 56 | 1y | 74 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1585 | 707 | 285 | 518 | 74 | 1 | | |
| 56 | 2y | 73 | Total | C | N | O | P | S | 0 | 0 |
| | | | 1565 | 698 | 283 | 510 | 73 | 1 | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 57 | 1A | 1108 | Total | Mg | 0 | 0 |
| | | | 1108 | 1108 | | |
| 57 | 1B | 36 | Total | Mg | 0 | 0 |
| | | | 36 | 36 | | |
| 57 | 1D | 12 | Total | Mg | 0 | 0 |
| | | | 12 | 12 | | |
| 57 | 1E | 16 | Total | Mg | 0 | 0 |
| | | | 16 | 16 | | |
| 57 | 1F | 12 | Total | Mg | 0 | 0 |
| | | | 12 | 12 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 57 | 1G | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | 1I | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 1N | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 1O | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 1P | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 1Q | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 1R | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | 1S | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 1T | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 1U | 9 | Total 9 | Mg 9 | 0 | 0 |
| 57 | 1V | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 1W | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 1X | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | 1Y | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | 1Z | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 10 | 8 | Total 8 | Mg 8 | 0 | 0 |
| 57 | 11 | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | 12 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 13 | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | 14 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 15 | 9 | Total 9 | Mg 9 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | 16 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 17 | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 18 | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 19 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 1a | 229 | Total 229 | Mg 229 | 0 | 0 |
| 57 | 1b | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 1d | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 1e | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 1f | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 1l | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 1m | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 1n | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 1r | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 1t | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 1v | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 1w | 5 | Total 5 | Mg 5 | 0 | 0 |
| 57 | 1x | 15 | Total 15 | Mg 15 | 0 | 0 |
| 57 | 1y | 4 | Total 4 | Mg 4 | 0 | 0 |
| 57 | 2A | 729 | Total 729 | Mg 729 | 0 | 0 |
| 57 | 2B | 18 | Total 18 | Mg 18 | 0 | 0 |
| 57 | 2D | 6 | Total 6 | Mg 6 | 0 | 0 |

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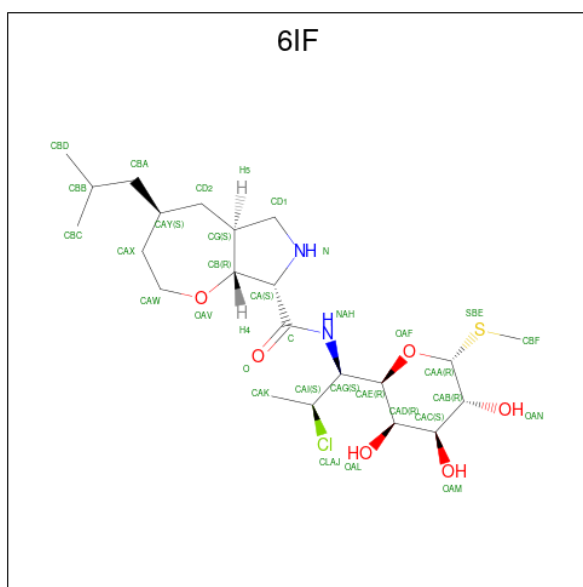
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 57 | 2E | 7 | Total 7 | Mg 7 | 0 | 0 |
| 57 | 2F | 6 | Total 6 | Mg 6 | 0 | 0 |
| 57 | 2G | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 2N | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 2O | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 2Q | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 2R | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 2T | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 2W | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 2X | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 2Y | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 2Z | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 20 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 21 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 23 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 57 | 25 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 26 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 57 | 27 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 28 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 57 | 2a | 186 | Total 186 | Mg 186 | 0 | 0 |
| 57 | 2d | 1 | Total 1 | Mg 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 57 | 2e | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | 2f | 2 | Total Mg 2 2 | 0 | 0 |
| 57 | 2l | 3 | Total Mg 3 3 | 0 | 0 |
| 57 | 2q | 3 | Total Mg 3 3 | 0 | 0 |
| 57 | 2r | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | 2t | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | 2v | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | 2w | 1 | Total Mg 1 1 | 0 | 0 |
| 57 | 2x | 5 | Total Mg 5 5 | 0 | 0 |
| 57 | 2y | 3 | Total Mg 3 3 | 0 | 0 |

- Molecule 58 is methyl 7-chloro-6,7,8-trideoxy-6-{[(4S,5aS,8S,8aR)-4-(2-methylpropyl)octahydro-2H-oxepino[2,3-c]pyrrole-8-carbonyl]amino}-1-thio-L-threo- α -D-galacto-octopyranoside (three-letter code: 6IF) (formula: $C_{22}H_{39}ClN_2O_6S$).

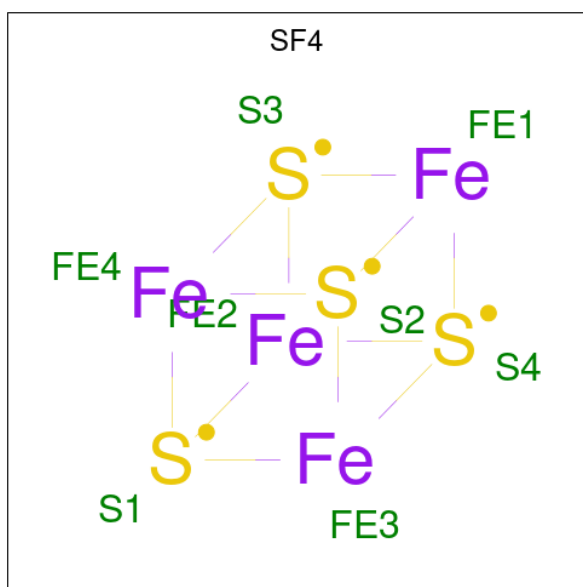


| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---|---------|---------|
| 58 | 1A | 1 | Total | C | Cl | N | O | S | 0 | 0 |
| | | | 32 | 22 | 1 | 2 | 6 | 1 | | |
| 58 | 2A | 1 | Total | C | Cl | N | O | S | 0 | 0 |
| | | | 32 | 22 | 1 | 2 | 6 | 1 | | |

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59 | 1Y | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 14 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 15 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 16 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 19 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 1n | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 2Y | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 24 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 25 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 26 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 29 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 2n | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 60 | 1d | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |
| 60 | 2d | 1 | Total | Fe | S | 0 | 0 |
| | | | 8 | 4 | 4 | | |

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 61 | 2A | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 62 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 62 | 1A | 2122 | Total | O | 0 | 0 |
| | | | 2122 | 2122 | | |
| 62 | 1B | 69 | Total | O | 0 | 0 |
| | | | 69 | 69 | | |
| 62 | 1D | 24 | Total | O | 0 | 0 |
| | | | 24 | 24 | | |
| 62 | 1E | 27 | Total | O | 0 | 0 |
| | | | 27 | 27 | | |
| 62 | 1F | 18 | Total | O | 0 | 0 |
| | | | 18 | 18 | | |
| 62 | 1G | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 62 | 1H | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 62 | 1N | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 62 | 1O | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 62 | 1P | 20 | Total | O | 0 | 0 |
| | | | 20 | 20 | | |
| 62 | 1Q | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |
| 62 | 1R | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |
| 62 | 1S | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 62 | 1T | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |
| 62 | 1U | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |
| 62 | 1V | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 62 | 1W | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 62 | 1X | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 62 | 1Y | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 62 | 1Z | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | 10 | 10 | Total | O | 0 | 0 |
| | | | 10 | 10 | | |
| 62 | 11 | 12 | Total | O | 0 | 0 |
| | | | 12 | 12 | | |
| 62 | 12 | 4 | Total | O | 0 | 0 |
| | | | 4 | 4 | | |
| 62 | 13 | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 62 | 15 | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 62 | 16 | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | 17 | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 62 | 18 | 10 | Total 10 | O 10 | 0 | 0 |
| 62 | 1a | 361 | Total 361 | O 361 | 0 | 0 |
| 62 | 1b | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1d | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1e | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1g | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1l | 4 | Total 4 | O 4 | 0 | 0 |
| 62 | 1m | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 1q | 4 | Total 4 | O 4 | 0 | 0 |
| 62 | 1u | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 1v | 5 | Total 5 | O 5 | 0 | 0 |
| 62 | 1w | 6 | Total 6 | O 6 | 0 | 0 |
| 62 | 1x | 16 | Total 16 | O 16 | 0 | 0 |
| 62 | 1y | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2A | 968 | Total 968 | O 968 | 0 | 0 |
| 62 | 2B | 15 | Total 15 | O 15 | 0 | 0 |
| 62 | 2D | 16 | Total 16 | O 16 | 0 | 0 |
| 62 | 2E | 9 | Total 9 | O 9 | 0 | 0 |
| 62 | 2F | 9 | Total 9 | O 9 | 0 | 0 |
| 62 | 2I | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2N | 1 | Total 1 | O 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 62 | 2O | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2P | 10 | Total 10 | O 10 | 0 | 0 |
| 62 | 2Q | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2R | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 2T | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 2W | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2X | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 2Y | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 20 | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 21 | 3 | Total 3 | O 3 | 0 | 0 |
| 62 | 23 | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 25 | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 26 | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 27 | 2 | Total 2 | O 2 | 0 | 0 |
| 62 | 28 | 6 | Total 6 | O 6 | 0 | 0 |
| 62 | 29 | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2a | 51 | Total 51 | O 51 | 0 | 0 |
| 62 | 2d | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2i | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2j | 1 | Total 1 | O 1 | 0 | 0 |
| 62 | 2l | 3 | Total 3 | O 3 | 0 | 0 |

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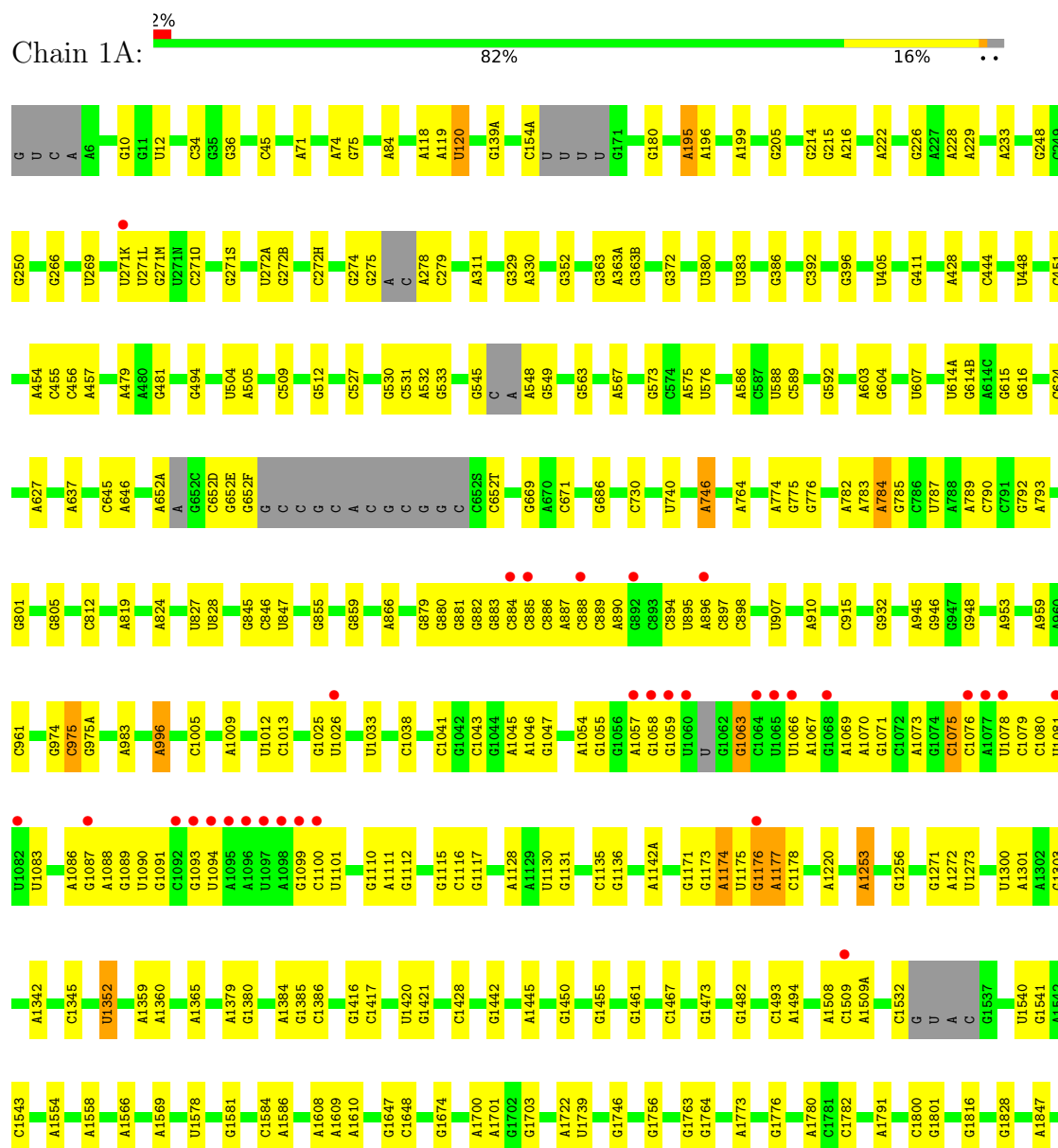
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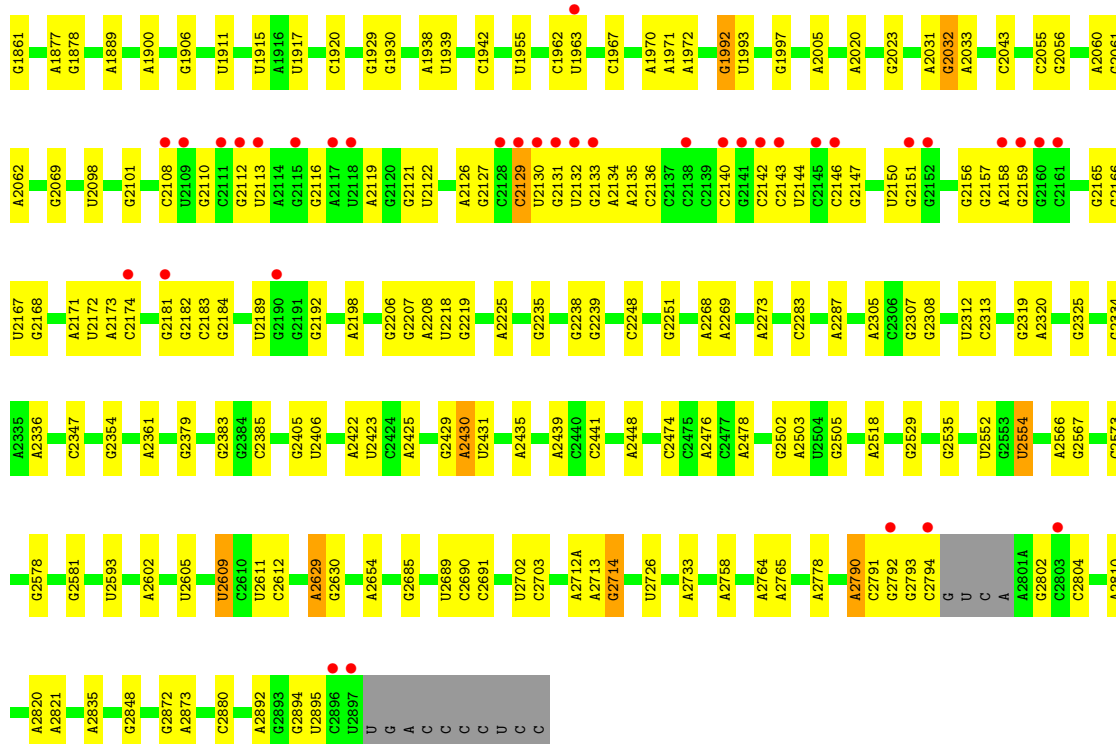
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 62 | 2p | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 62 | 2t | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 62 | 2x | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 62 | 2y | 8 | Total | O | 0 | 0 |
| | | | 8 | 8 | | |

3 Residue-property plots [i](#)

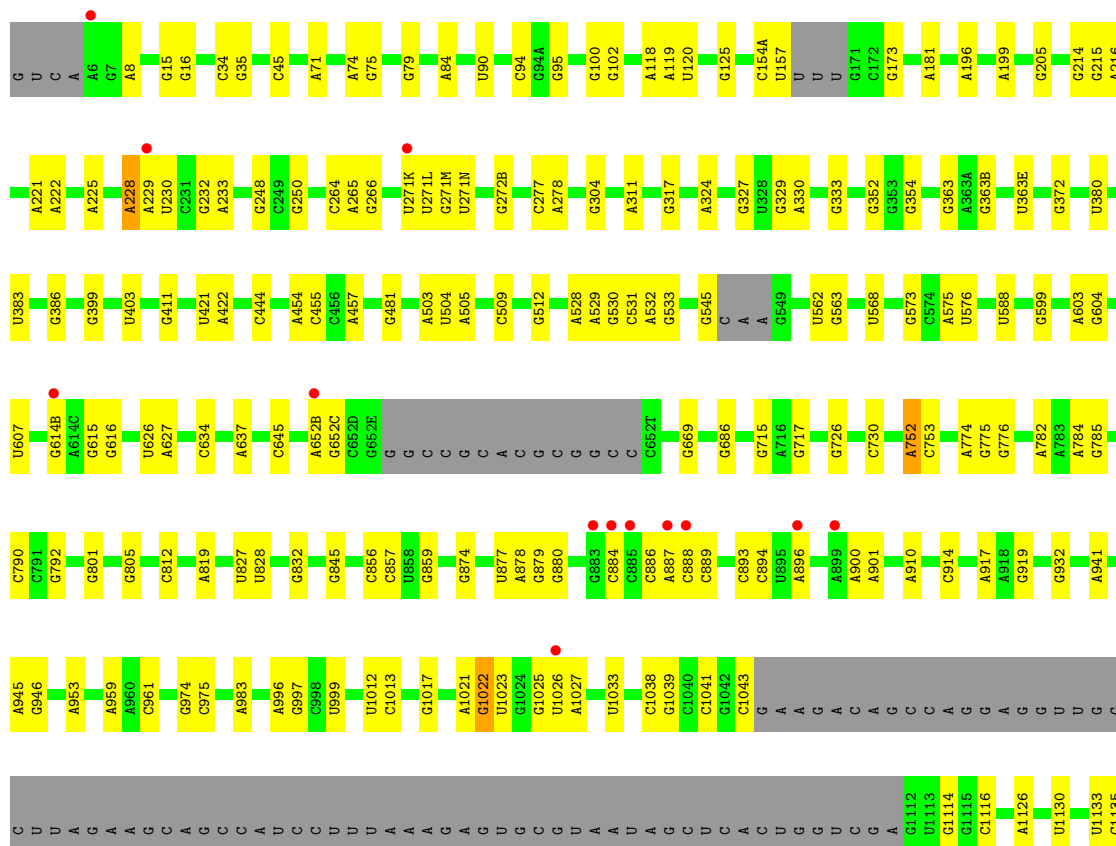
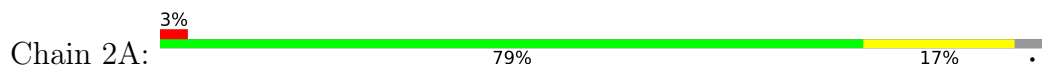
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

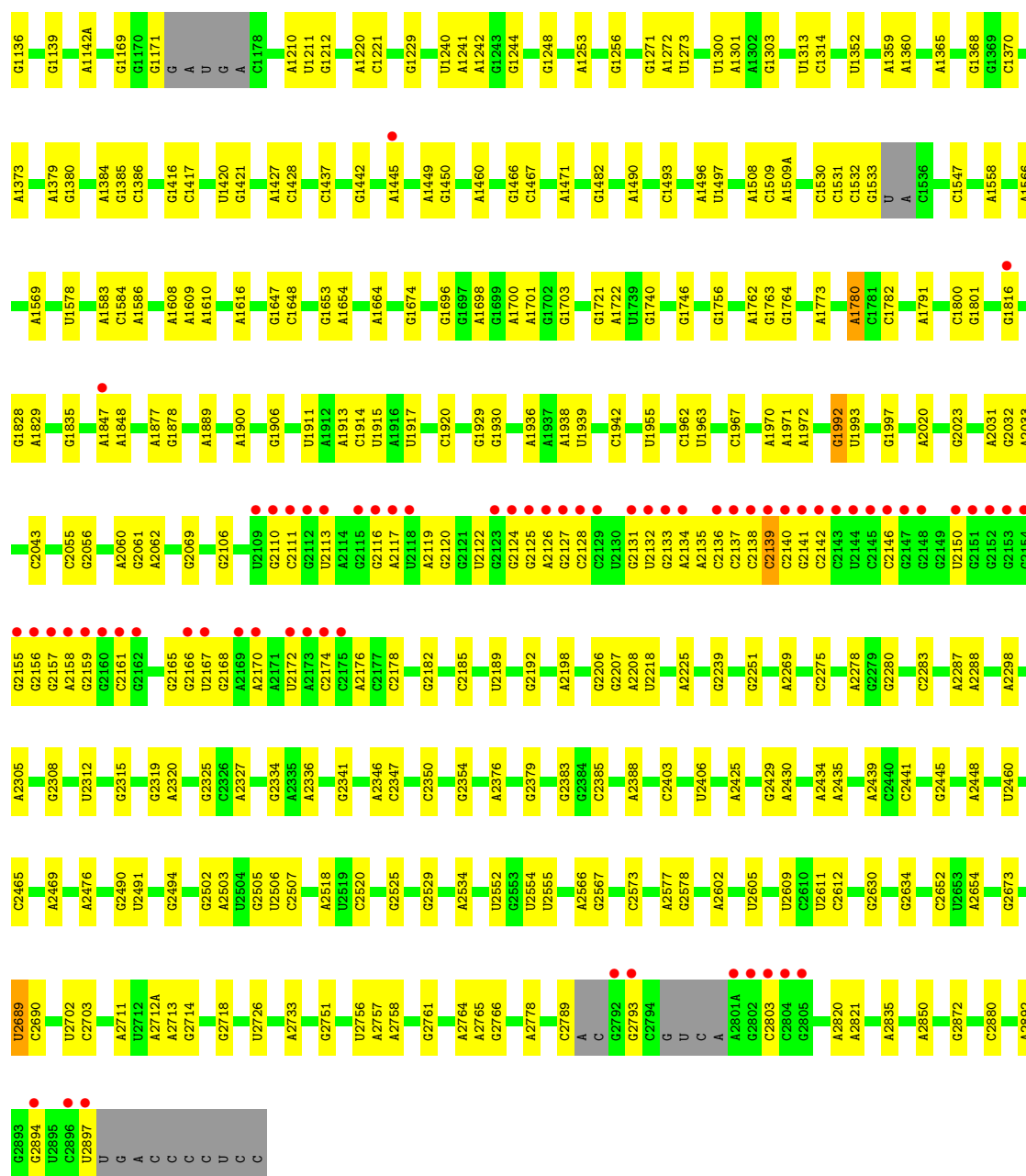
• Molecule 1: 23S Ribosomal RNA





● Molecule 1: 23S Ribosomal RNA





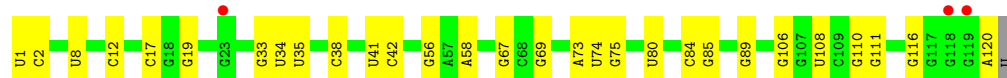
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 92% 7% .

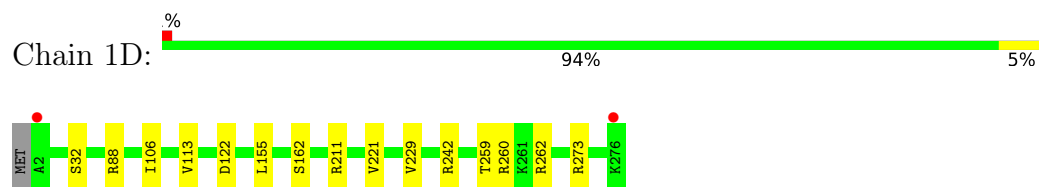


• Molecule 2: 5S Ribosomal RNA

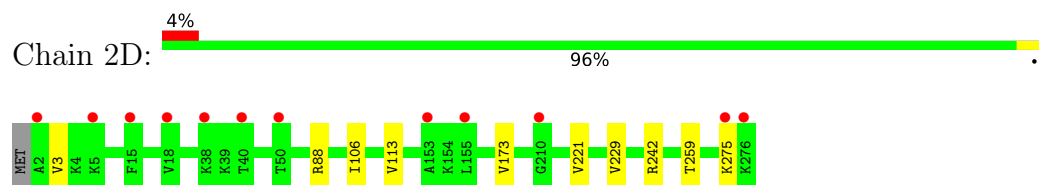
Chain 2B: 2% 75% 24% .



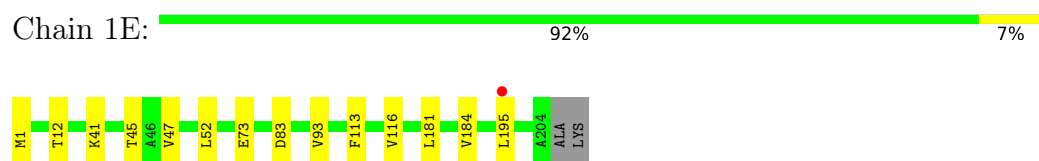
- Molecule 3: 50S ribosomal protein L2



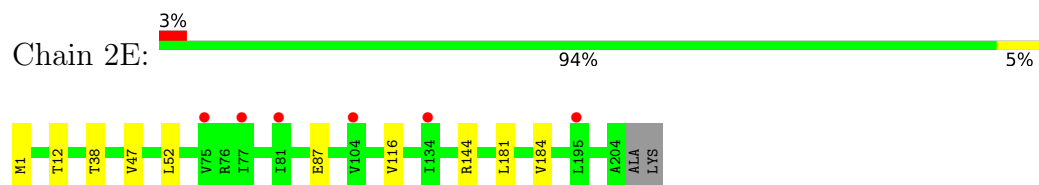
- Molecule 3: 50S ribosomal protein L2



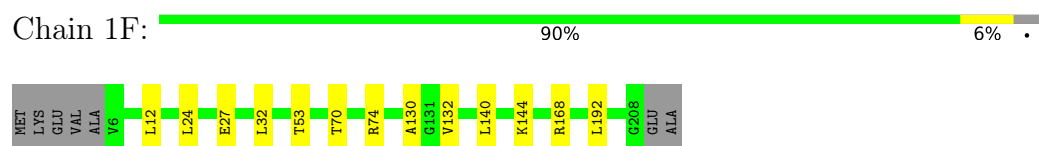
- Molecule 4: 50S ribosomal protein L3



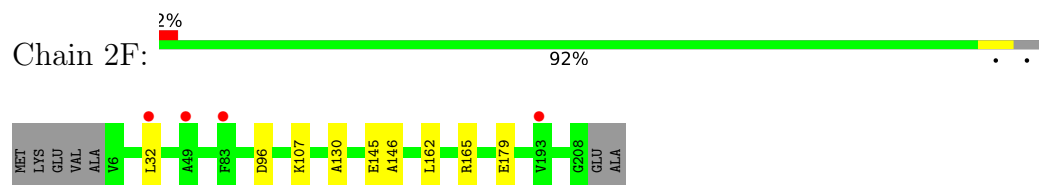
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

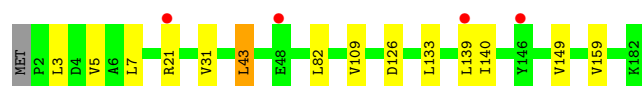


- Molecule 5: 50S ribosomal protein L4

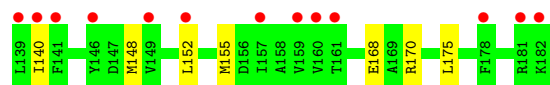
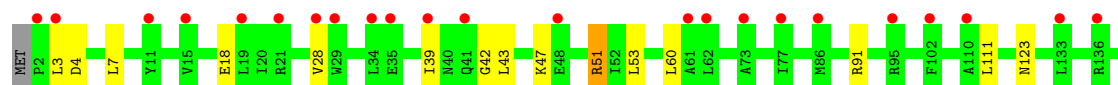
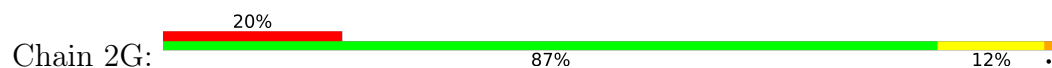


- Molecule 6: 50S ribosomal protein L5





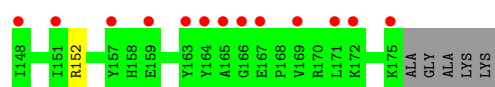
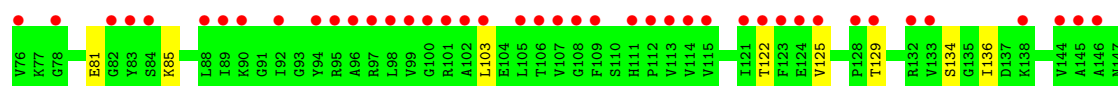
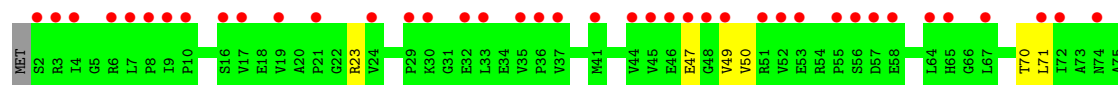
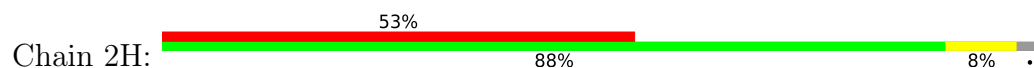
- Molecule 6: 50S ribosomal protein L5



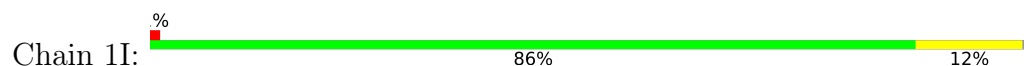
- Molecule 7: 50S ribosomal protein L6



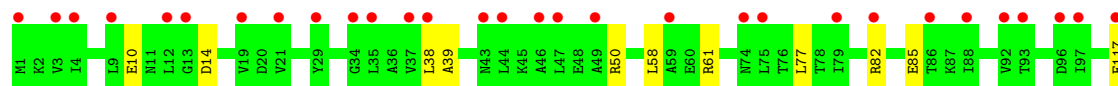
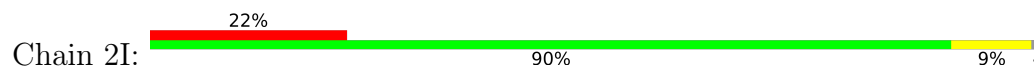
- Molecule 7: 50S ribosomal protein L6

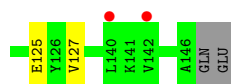


- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9





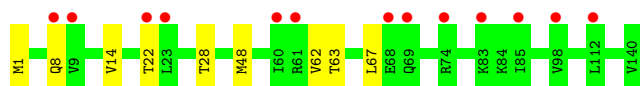
- Molecule 9: 50S ribosomal protein L13

Chain 1N: 95% 5%



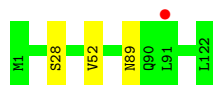
- Molecule 9: 50S ribosomal protein L13

Chain 2N: 9% 94% 6%



- Molecule 10: 50S ribosomal protein L14

Chain 1O: 0% 98% 2%



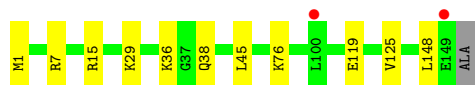
- Molecule 10: 50S ribosomal protein L14

Chain 2O: 7% 97% 3%



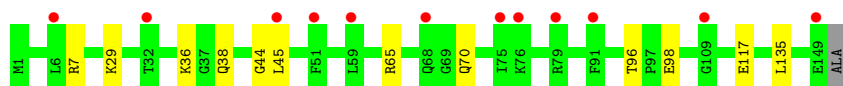
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 0% 92% 8%



- Molecule 11: 50S ribosomal protein L15

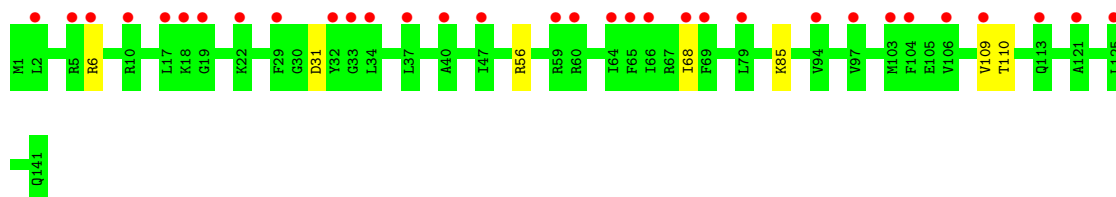
Chain 2P: 8% 91% 1%



- Molecule 12: 50S ribosomal protein L16



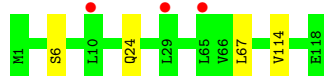
- Molecule 12: 50S ribosomal protein L16



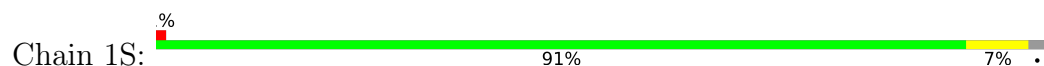
- Molecule 13: 50S ribosomal protein L17



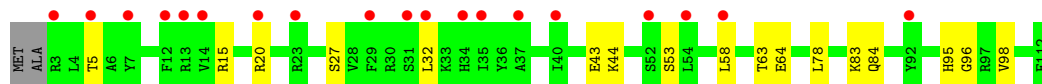
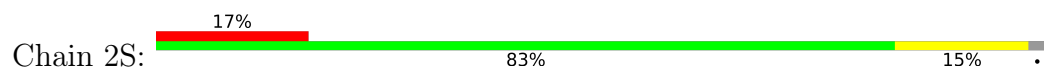
- Molecule 13: 50S ribosomal protein L17



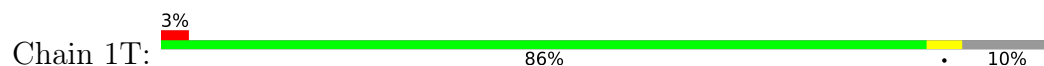
- Molecule 14: 50S ribosomal protein L18

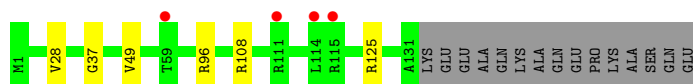


- Molecule 14: 50S ribosomal protein L18

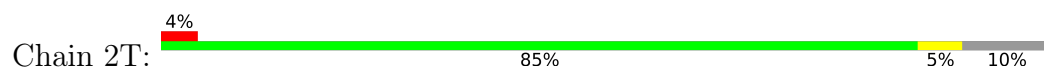


- Molecule 15: 50S ribosomal protein L19

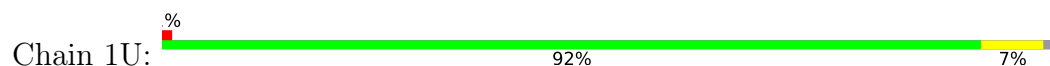




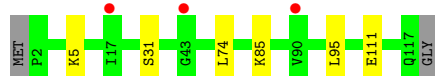
- Molecule 15: 50S ribosomal protein L19



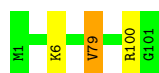
- Molecule 16: 50S ribosomal protein L20



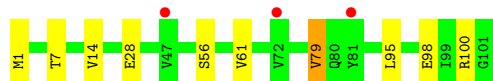
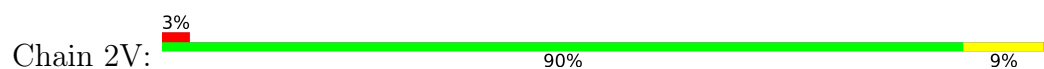
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



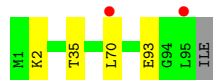
- Molecule 18: 50S ribosomal protein L22



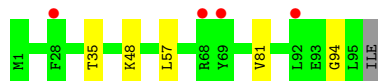
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



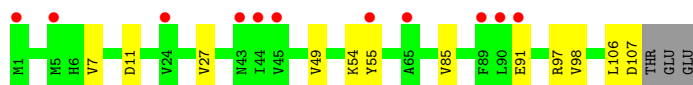
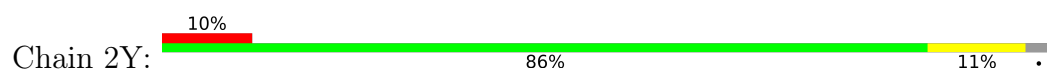
- Molecule 19: 50S ribosomal protein L23



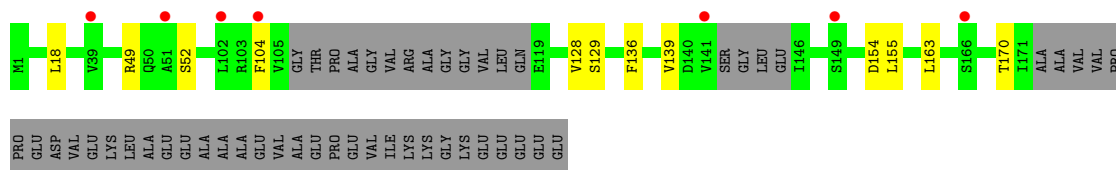
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

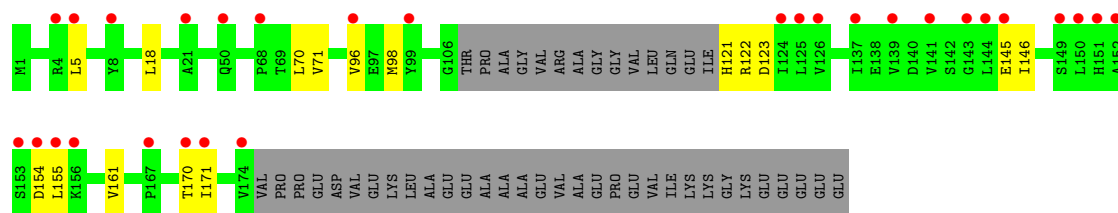


- Molecule 21: 50S ribosomal protein L25

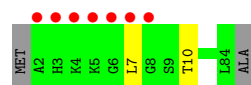


- Molecule 21: 50S ribosomal protein L25

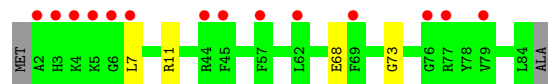
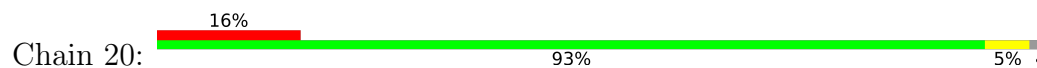




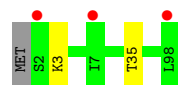
- Molecule 22: 50S ribosomal protein L27



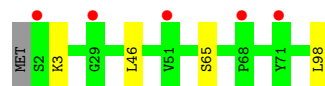
- Molecule 22: 50S ribosomal protein L27



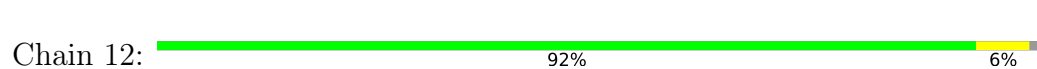
- Molecule 23: 50S ribosomal protein L28



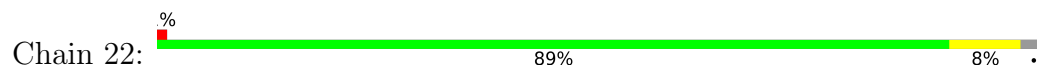
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

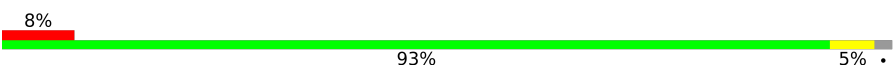


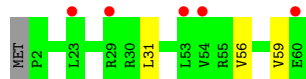
- Molecule 25: 50S ribosomal protein L30

Chain 13:  92% 7% .




- Molecule 25: 50S ribosomal protein L30

Chain 23:  8% 93% 5% .




- Molecule 26: 50S ribosomal protein L31

Chain 14:  4% 83% 10% . .



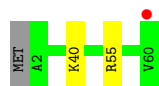
- Molecule 26: 50S ribosomal protein L31

Chain 24:  21% 77% 18% . .

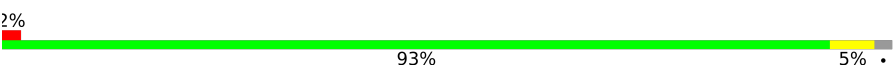


- Molecule 27: 50S ribosomal protein L32

Chain 15:  2% 95% . .



- Molecule 27: 50S ribosomal protein L32

Chain 25:  2% 93% 5% .

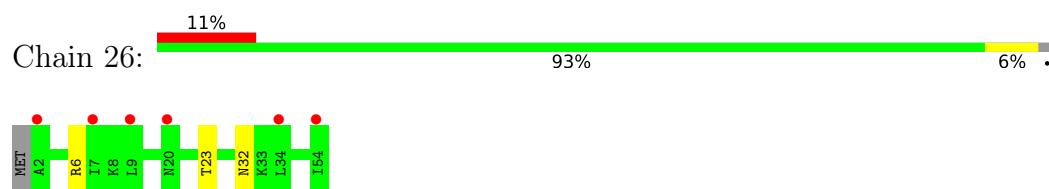


- Molecule 28: 50S ribosomal protein L33

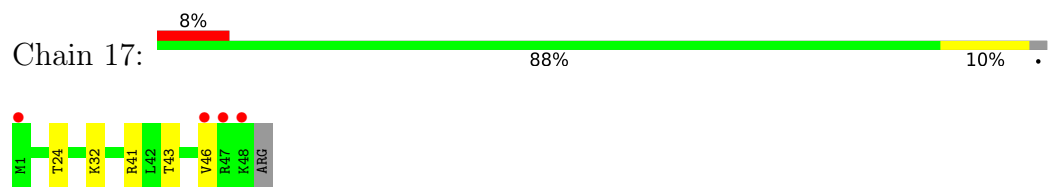
Chain 16:  91% 7% .



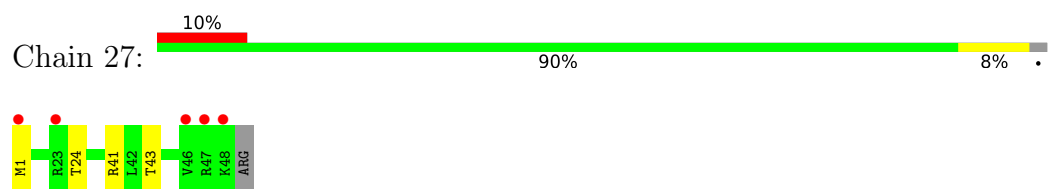
- Molecule 28: 50S ribosomal protein L33



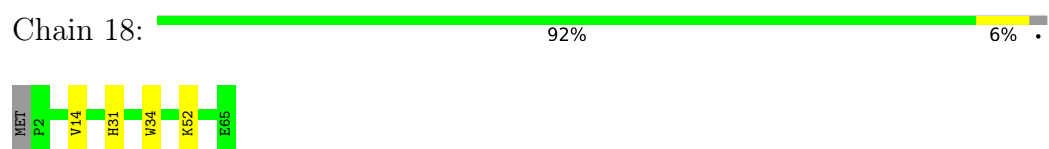
- Molecule 29: 50S ribosomal protein L34



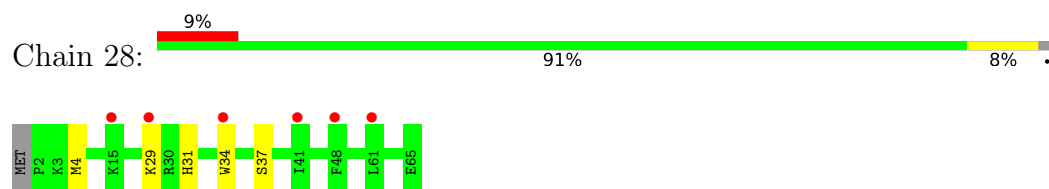
- Molecule 29: 50S ribosomal protein L34



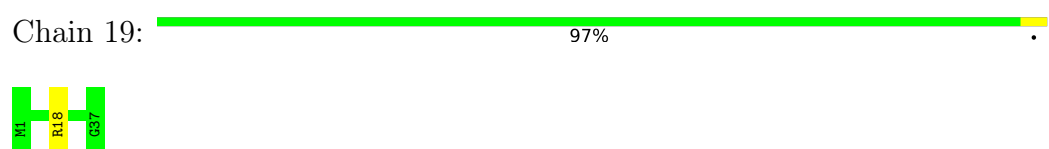
- Molecule 30: 50S ribosomal protein L35



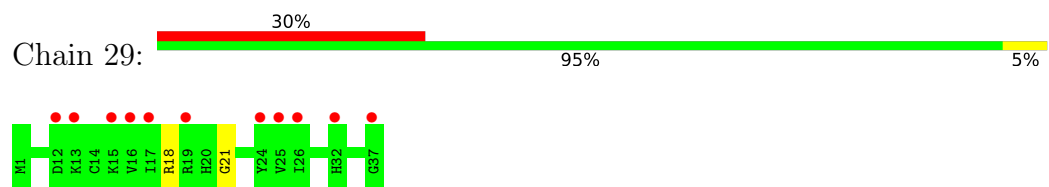
- Molecule 30: 50S ribosomal protein L35



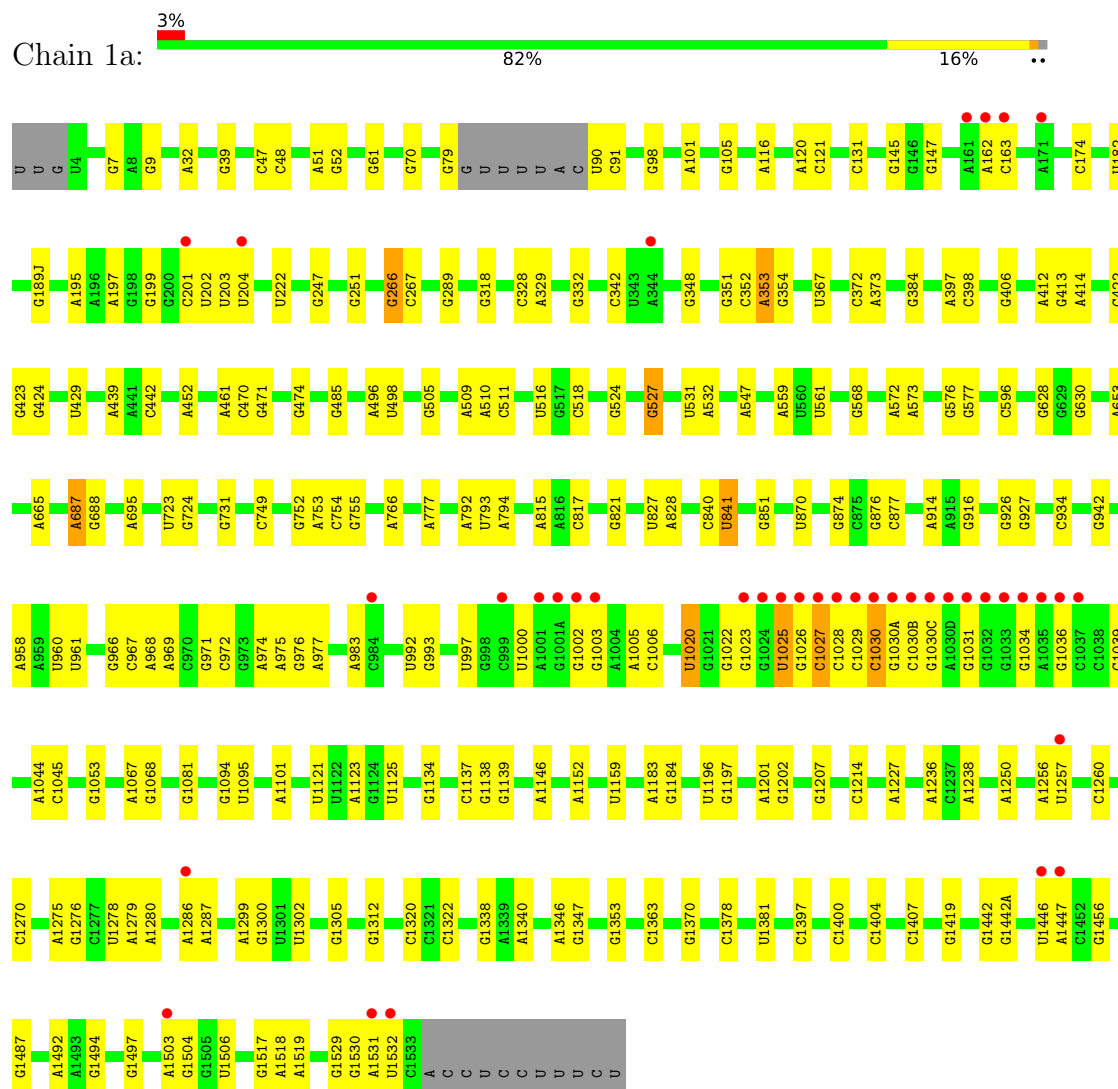
- Molecule 31: 50S ribosomal protein L36



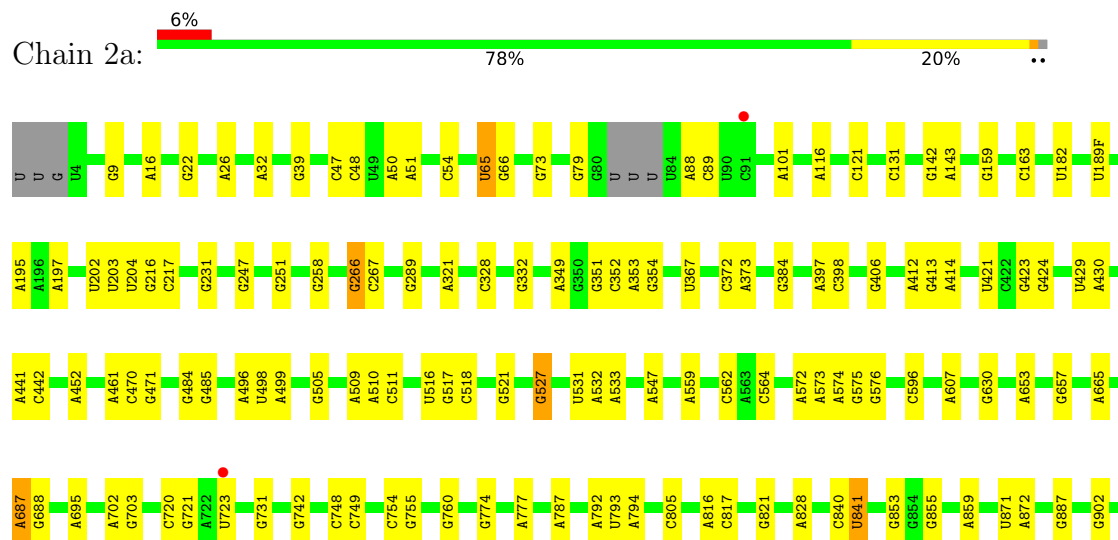
- Molecule 31: 50S ribosomal protein L36

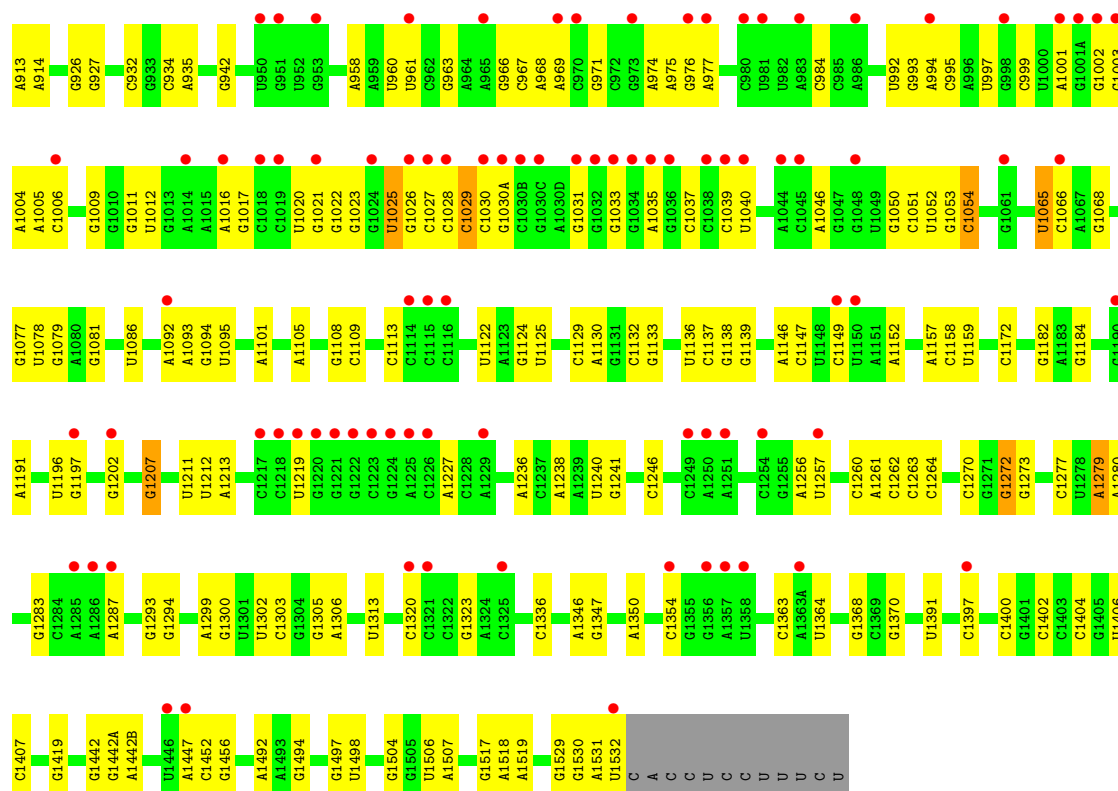


• Molecule 32: 16S Ribosomal RNA

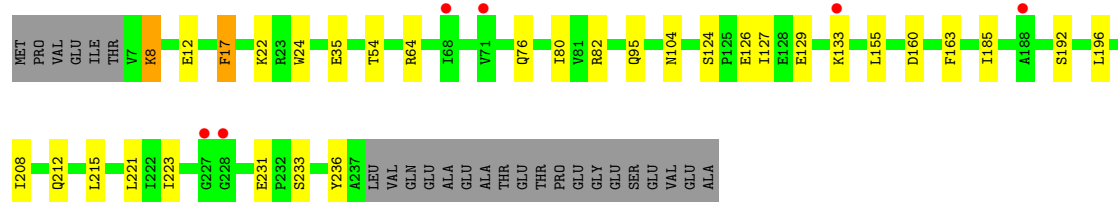
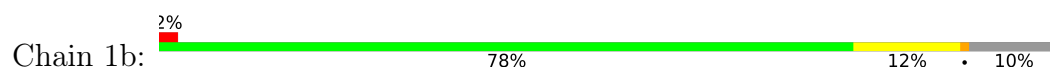


• Molecule 32: 16S Ribosomal RNA

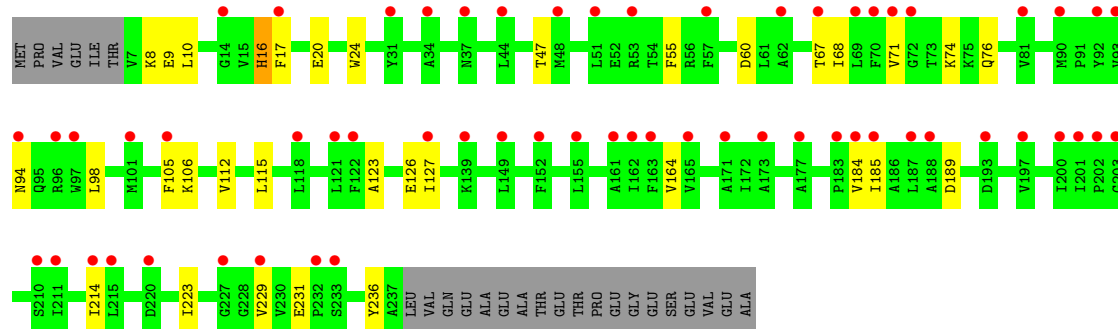
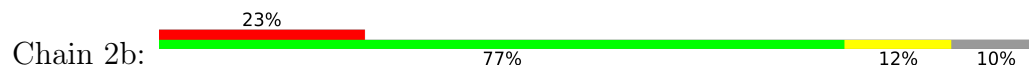




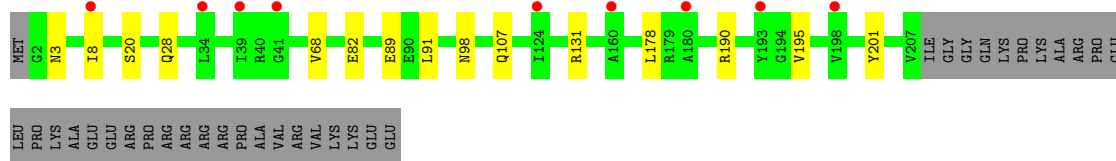
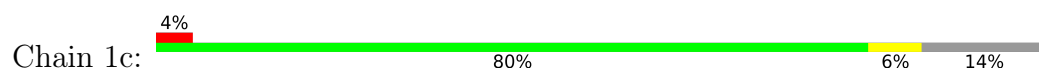
- Molecule 33: 30S ribosomal protein S2



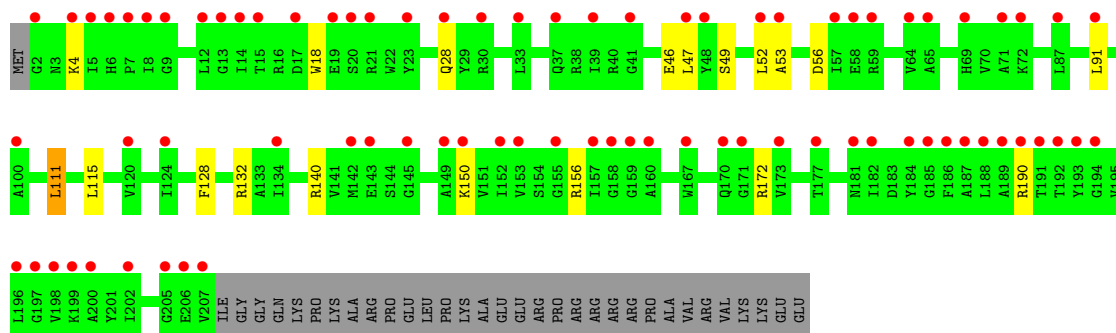
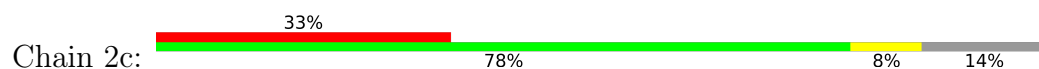
- Molecule 33: 30S ribosomal protein S2



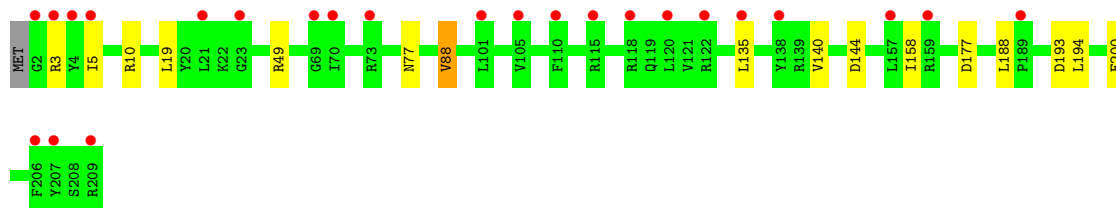
- Molecule 34: 30S ribosomal protein S3



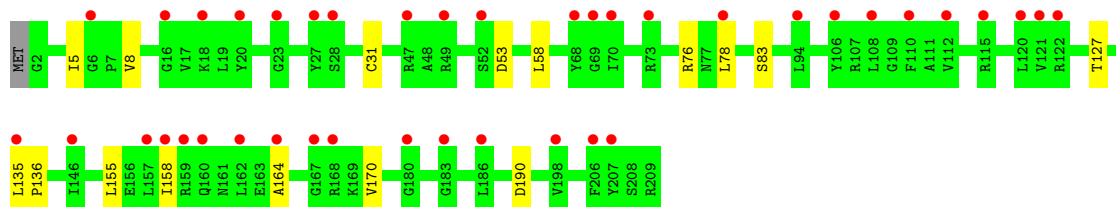
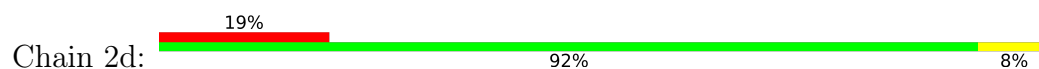
• Molecule 34: 30S ribosomal protein S3



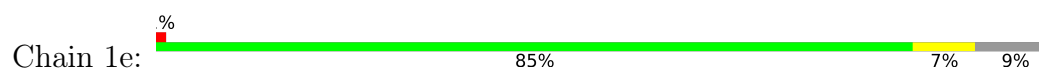
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

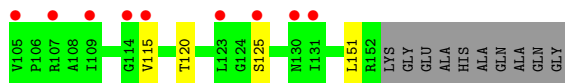
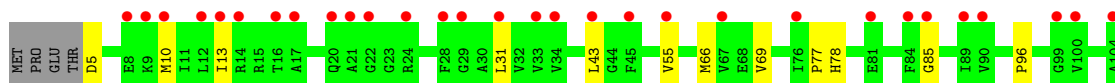
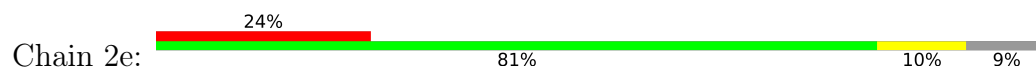


• Molecule 36: 30S ribosomal protein S5





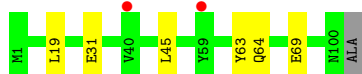
- Molecule 36: 30S ribosomal protein S5



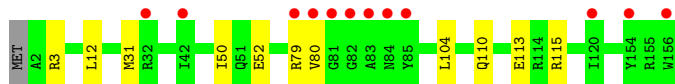
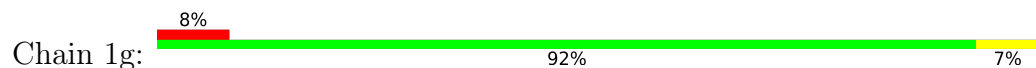
- Molecule 37: 30S ribosomal protein S6



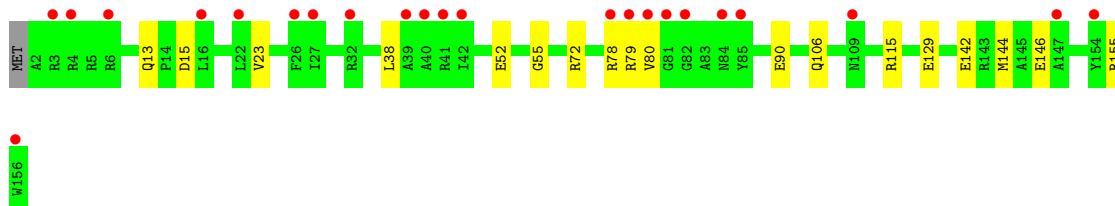
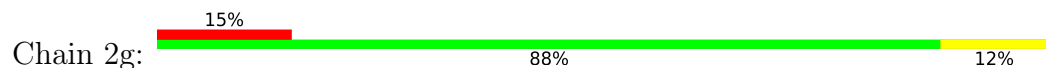
- Molecule 37: 30S ribosomal protein S6



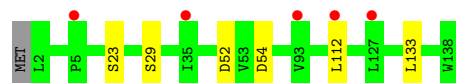
- Molecule 38: 30S ribosomal protein S7



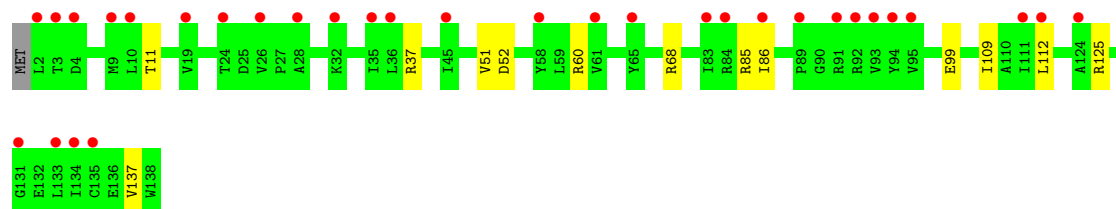
- Molecule 38: 30S ribosomal protein S7



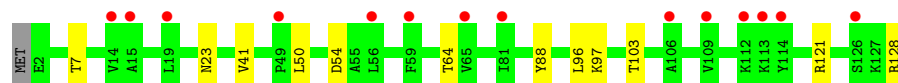
- Molecule 39: 30S ribosomal protein S8



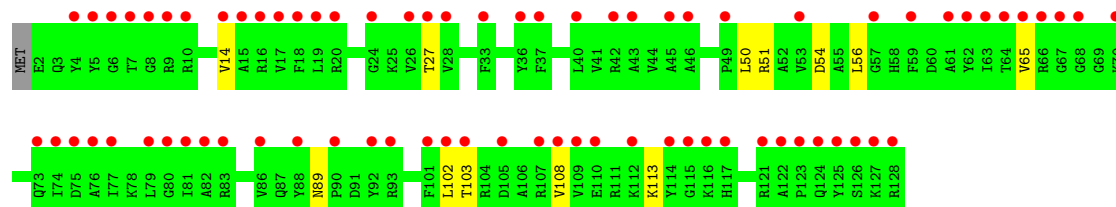
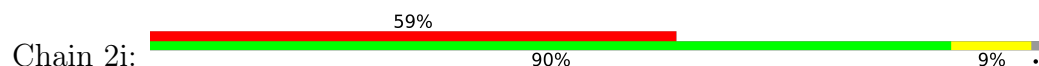
- Molecule 39: 30S ribosomal protein S8



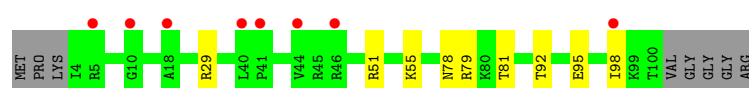
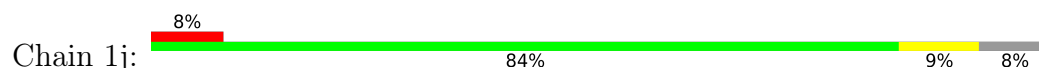
- Molecule 40: 30S ribosomal protein S9



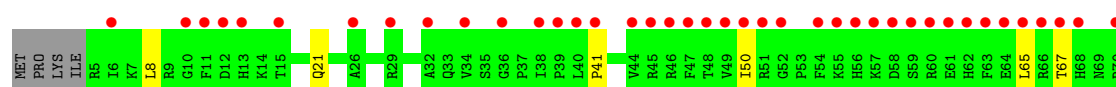
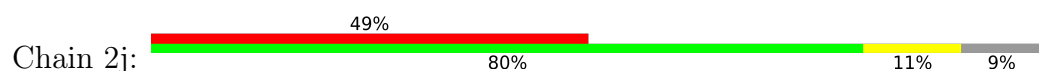
- Molecule 40: 30S ribosomal protein S9

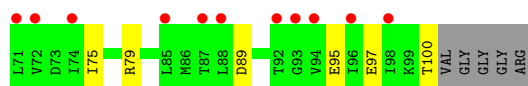


- Molecule 41: 30S ribosomal protein S10

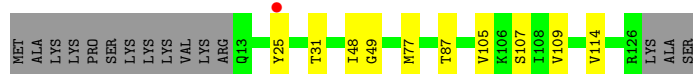
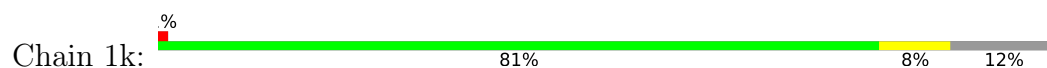


- Molecule 41: 30S ribosomal protein S10

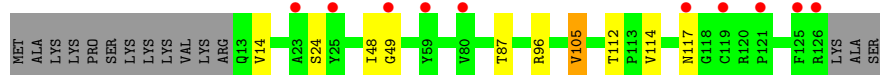
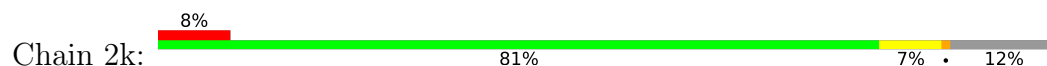




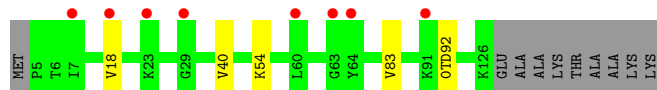
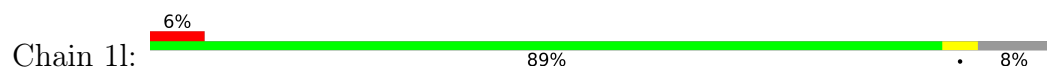
- Molecule 42: 30S ribosomal protein S11



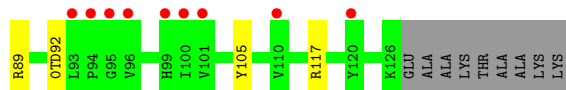
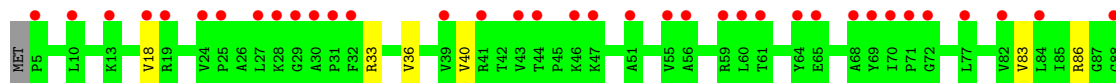
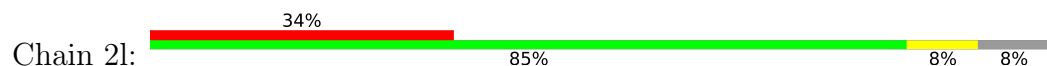
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



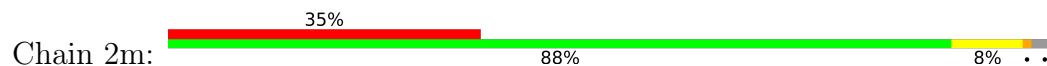
- Molecule 43: 30S ribosomal protein S12

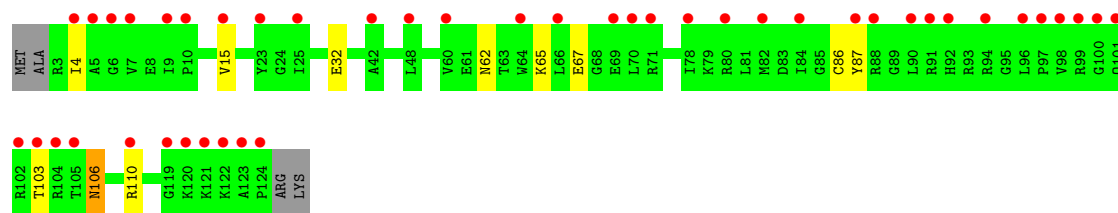


- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

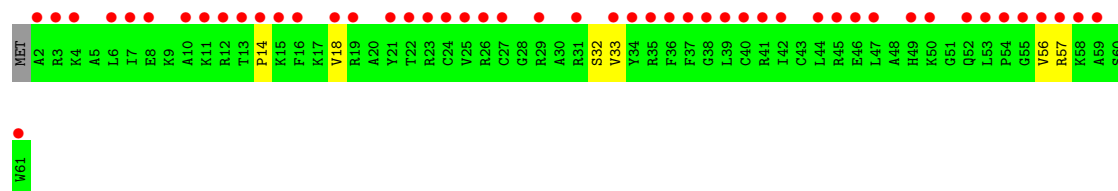
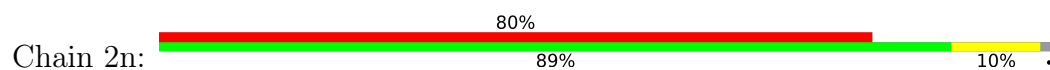




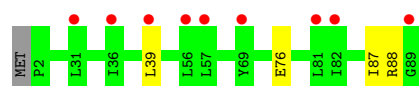
- Molecule 45: 30S ribosomal protein S14 type Z



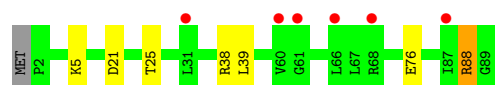
- Molecule 45: 30S ribosomal protein S14 type Z



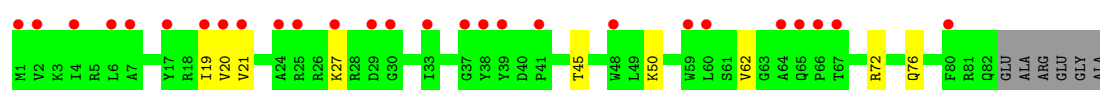
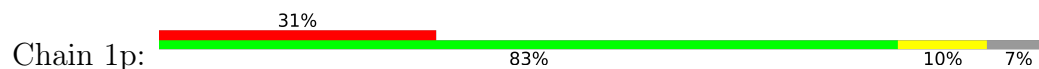
- Molecule 46: 30S ribosomal protein S15



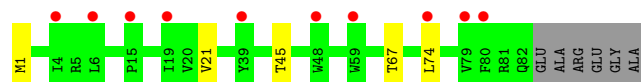
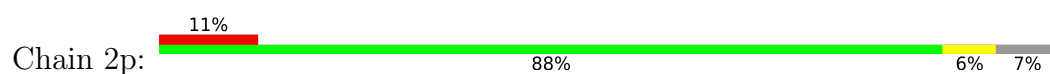
- Molecule 46: 30S ribosomal protein S15



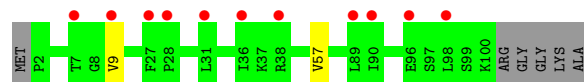
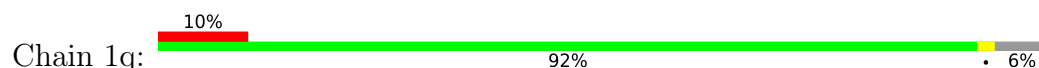
- Molecule 47: 30S ribosomal protein S16



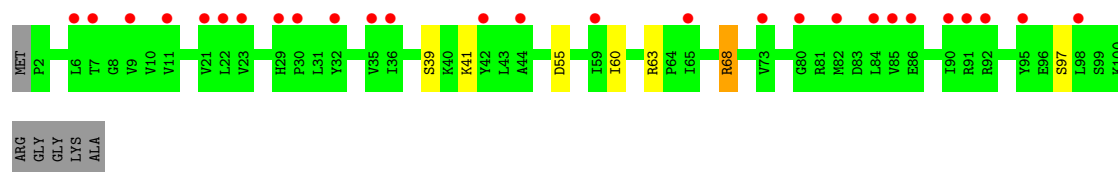
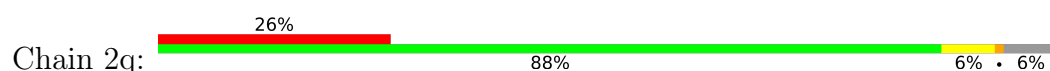
- Molecule 47: 30S ribosomal protein S16



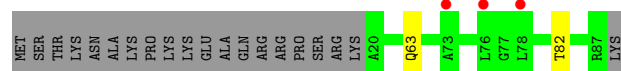
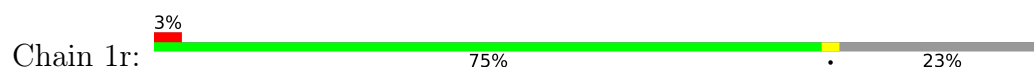
- Molecule 48: 30S ribosomal protein S17



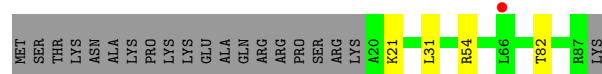
- Molecule 48: 30S ribosomal protein S17



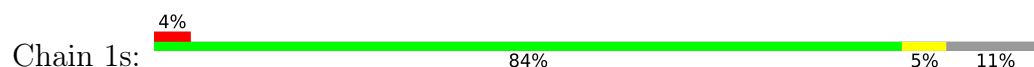
- Molecule 49: 30S ribosomal protein S18



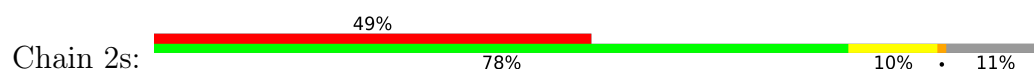
- Molecule 49: 30S ribosomal protein S18

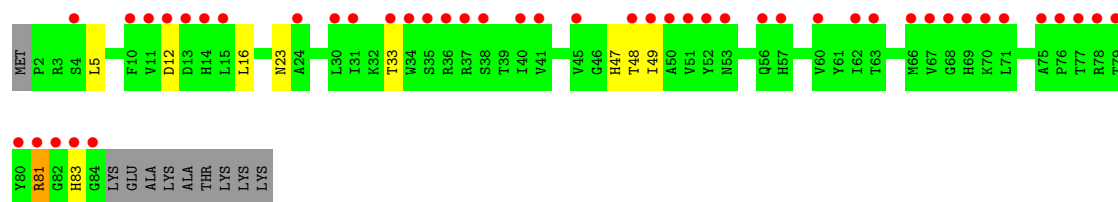


- Molecule 50: 30S ribosomal protein S19

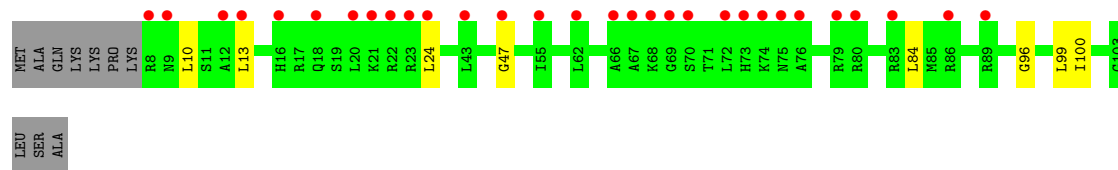
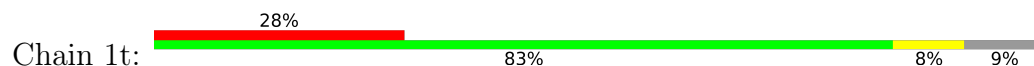


- Molecule 50: 30S ribosomal protein S19

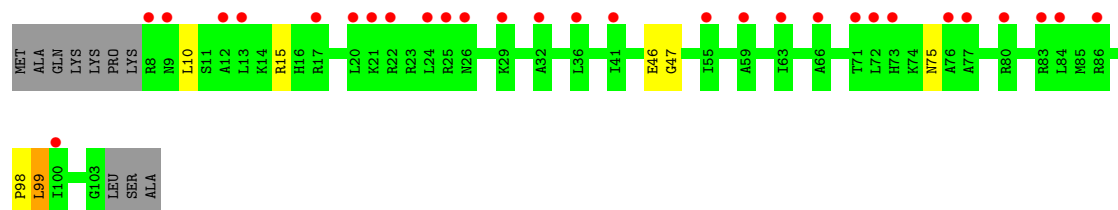
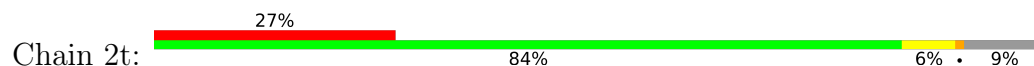




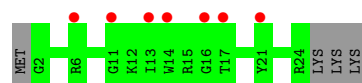
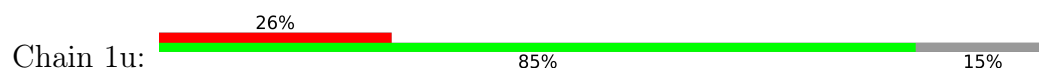
- Molecule 51: 30S ribosomal protein S20



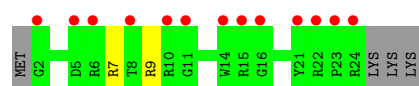
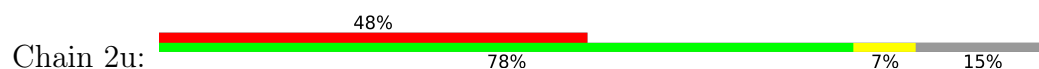
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



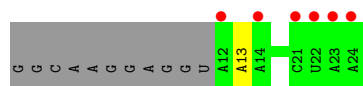
- Molecule 52: 30S ribosomal protein Thx



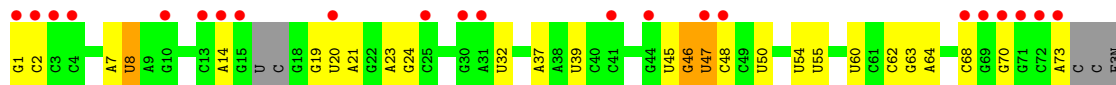
- Molecule 53: mRNA



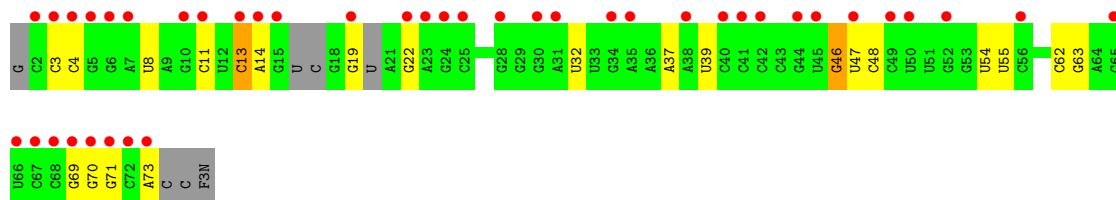
- Molecule 53: mRNA



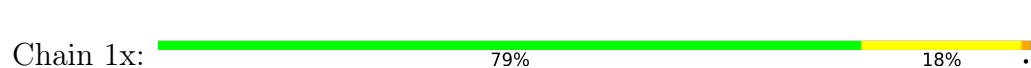
- Molecule 54: A-site tRNA



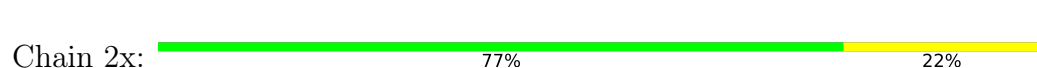
- Molecule 54: A-site tRNA



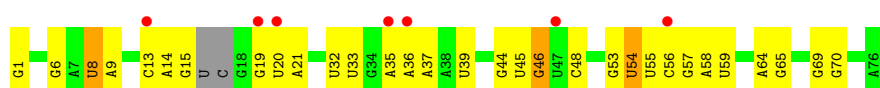
- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA

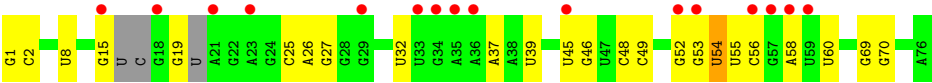


- Molecule 56: E-site tRNA



- Molecule 56: E-site tRNA





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.86Å 449.80Å 621.81Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 198.84 – 2.50 198.84 – 2.50 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (198.84-2.50) 99.8 (198.84-2.50) | Depositor EDS |
| R_{merge} | 0.20 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.26 (at 2.52Å) | Xtriage |
| Refinement program | PHENIX 1.8.2 | Depositor |
| R, R_{free} | 0.224 , 0.268 0.224 , 0.268 | Depositor DCC |
| R_{free} test set | 100061 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 51.2 | Xtriage |
| Anisotropy | 0.157 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.28 , 53.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 299504 | 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 1.58% 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: MG, 5MU, OMG, 4SU, OMU, ZN, 0TD, UR3, 31H, 7MG, K, 5MC, 2MA, MA6, 4OC, 6IF, SF4, MIA, PSU, OMC, 2MG, M2G

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 | 0.50 | 0/69011 | 0.98 | 74/107720 (0.1%) |
| 1 | 2A | 0.38 | 0/67295 | 0.86 | 20/105042 (0.0%) |
| 2 | 1B | 0.44 | 1/2882 (0.0%) | 0.88 | 0/4494 |
| 2 | 2B | 0.42 | 1/2879 (0.0%) | 0.87 | 1/4487 (0.0%) |
| 3 | 1D | 0.35 | 0/2186 | 0.57 | 0/2944 |
| 3 | 2D | 0.31 | 0/2186 | 0.51 | 0/2944 |
| 4 | 1E | 0.35 | 0/1592 | 0.54 | 0/2149 |
| 4 | 2E | 0.31 | 0/1592 | 0.51 | 0/2149 |
| 5 | 1F | 0.33 | 0/1619 | 0.54 | 1/2193 (0.0%) |
| 5 | 2F | 0.29 | 0/1615 | 0.49 | 0/2188 |
| 6 | 1G | 0.30 | 0/1448 | 0.52 | 0/1957 |
| 6 | 2G | 0.30 | 0/1453 | 0.46 | 0/1963 |
| 7 | 1H | 0.31 | 0/1356 | 0.49 | 0/1834 |
| 7 | 2H | 0.29 | 0/1356 | 0.46 | 0/1834 |
| 8 | 1I | 0.27 | 0/1112 | 0.49 | 0/1514 |
| 8 | 2I | 0.27 | 0/1079 | 0.50 | 0/1475 |
| 9 | 1N | 0.32 | 0/1144 | 0.50 | 0/1543 |
| 9 | 2N | 0.31 | 0/1144 | 0.46 | 0/1543 |
| 10 | 1O | 0.33 | 0/943 | 0.53 | 0/1269 |
| 10 | 2O | 0.30 | 0/943 | 0.51 | 0/1269 |
| 11 | 1P | 0.33 | 0/1152 | 0.57 | 0/1533 |
| 11 | 2P | 0.30 | 0/1152 | 0.53 | 0/1533 |
| 12 | 1Q | 0.35 | 0/1143 | 0.52 | 0/1527 |
| 12 | 2Q | 0.30 | 0/1143 | 0.48 | 0/1527 |
| 13 | 1R | 0.33 | 0/982 | 0.54 | 0/1312 |
| 13 | 2R | 0.27 | 0/982 | 0.49 | 0/1312 |
| 14 | 1S | 0.30 | 0/883 | 0.52 | 0/1176 |
| 14 | 2S | 0.30 | 0/880 | 0.51 | 0/1172 |
| 15 | 1T | 0.33 | 0/1105 | 0.52 | 0/1477 |
| 15 | 2T | 0.29 | 0/1097 | 0.49 | 0/1468 |
| 16 | 1U | 0.37 | 0/977 | 0.53 | 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 | 0/782 | 0.57 | 0/1049 |
| 17 | 2V | 0.29 | 0/782 | 0.50 | 0/1049 |
| 18 | 1W | 0.36 | 0/897 | 0.53 | 0/1205 |
| 18 | 2W | 0.30 | 0/897 | 0.47 | 0/1205 |
| 19 | 1X | 0.35 | 0/764 | 0.54 | 0/1025 |
| 19 | 2X | 0.30 | 0/764 | 0.53 | 0/1025 |
| 20 | 1Y | 0.33 | 0/819 | 0.53 | 0/1095 |
| 20 | 2Y | 0.29 | 0/819 | 0.52 | 0/1095 |
| 21 | 1Z | 0.32 | 0/1267 | 0.51 | 0/1717 |
| 21 | 2Z | 0.29 | 0/1299 | 0.49 | 0/1763 |
| 22 | 10 | 0.35 | 0/662 | 0.54 | 0/881 |
| 22 | 20 | 0.32 | 0/662 | 0.50 | 0/881 |
| 23 | 11 | 0.32 | 0/762 | 0.50 | 0/1014 |
| 23 | 21 | 0.30 | 0/762 | 0.52 | 0/1014 |
| 24 | 12 | 0.30 | 0/590 | 0.46 | 0/781 |
| 24 | 22 | 0.28 | 0/590 | 0.42 | 0/781 |
| 25 | 13 | 0.30 | 0/474 | 0.54 | 0/635 |
| 25 | 23 | 0.28 | 0/469 | 0.43 | 0/630 |
| 26 | 14 | 0.32 | 0/565 | 0.54 | 0/761 |
| 26 | 24 | 0.30 | 0/545 | 0.55 | 1/737 (0.1%) |
| 27 | 15 | 0.34 | 0/469 | 0.58 | 0/635 |
| 27 | 25 | 0.30 | 0/469 | 0.49 | 0/635 |
| 28 | 16 | 0.33 | 0/460 | 0.51 | 0/613 |
| 28 | 26 | 0.28 | 0/456 | 0.50 | 0/608 |
| 29 | 17 | 0.34 | 0/426 | 0.50 | 0/561 |
| 29 | 27 | 0.27 | 0/426 | 0.47 | 0/561 |
| 30 | 18 | 0.32 | 0/525 | 0.54 | 0/691 |
| 30 | 28 | 0.27 | 0/525 | 0.48 | 0/691 |
| 31 | 19 | 0.32 | 0/310 | 0.52 | 0/407 |
| 31 | 29 | 0.29 | 0/310 | 0.51 | 0/407 |
| 32 | 1a | 0.37 | 0/35795 | 0.88 | 29/55864 (0.1%) |
| 32 | 2a | 0.36 | 2/35886 (0.0%) | 0.90 | 38/56005 (0.1%) |
| 33 | 1b | 0.29 | 0/1881 | 0.49 | 0/2542 |
| 33 | 2b | 0.31 | 0/1860 | 0.49 | 0/2518 |
| 34 | 1c | 0.28 | 0/1572 | 0.46 | 0/2126 |
| 34 | 2c | 0.30 | 0/1566 | 0.50 | 0/2119 |
| 35 | 1d | 0.28 | 0/1685 | 0.47 | 0/2262 |
| 35 | 2d | 0.28 | 0/1704 | 0.47 | 0/2284 |
| 36 | 1e | 0.29 | 0/1145 | 0.51 | 0/1543 |
| 36 | 2e | 0.29 | 0/1149 | 0.49 | 0/1548 |
| 37 | 1f | 0.28 | 0/823 | 0.48 | 0/1115 |
| 37 | 2f | 0.29 | 0/829 | 0.47 | 0/1123 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | 1g | 0.27 | 0/1250 | 0.44 | 0/1679 |
| 38 | 2g | 0.28 | 0/1254 | 0.44 | 0/1683 |
| 39 | 1h | 0.29 | 0/1108 | 0.47 | 0/1494 |
| 39 | 2h | 0.27 | 0/1108 | 0.45 | 0/1494 |
| 40 | 1i | 0.29 | 0/1002 | 0.51 | 0/1346 |
| 40 | 2i | 0.30 | 0/997 | 0.49 | 0/1343 |
| 41 | 1j | 0.27 | 0/722 | 0.48 | 0/982 |
| 41 | 2j | 0.29 | 0/727 | 0.51 | 0/988 |
| 42 | 1k | 0.28 | 0/844 | 0.47 | 0/1145 |
| 42 | 2k | 0.27 | 0/848 | 0.47 | 0/1149 |
| 43 | 1l | 0.29 | 0/937 | 0.50 | 0/1260 |
| 43 | 2l | 0.29 | 0/937 | 0.47 | 0/1260 |
| 44 | 1m | 0.29 | 0/969 | 0.49 | 0/1302 |
| 44 | 2m | 0.29 | 0/961 | 0.49 | 0/1291 |
| 45 | 1n | 0.30 | 0/501 | 0.47 | 0/664 |
| 45 | 2n | 0.30 | 0/501 | 0.48 | 0/664 |
| 46 | 1o | 0.27 | 0/739 | 0.43 | 0/985 |
| 46 | 2o | 0.26 | 0/739 | 0.43 | 0/985 |
| 47 | 1p | 0.28 | 0/697 | 0.50 | 0/939 |
| 47 | 2p | 0.27 | 0/693 | 0.51 | 0/935 |
| 48 | 1q | 0.29 | 0/836 | 0.47 | 0/1117 |
| 48 | 2q | 0.29 | 0/836 | 0.49 | 0/1117 |
| 49 | 1r | 0.28 | 0/560 | 0.51 | 0/746 |
| 49 | 2r | 0.27 | 0/560 | 0.49 | 0/746 |
| 50 | 1s | 0.26 | 0/667 | 0.53 | 0/900 |
| 50 | 2s | 0.30 | 0/661 | 0.56 | 0/893 |
| 51 | 1t | 0.27 | 0/730 | 0.44 | 0/965 |
| 51 | 2t | 0.26 | 0/729 | 0.42 | 0/965 |
| 52 | 1u | 0.25 | 0/203 | 0.43 | 0/266 |
| 52 | 2u | 0.27 | 0/203 | 0.46 | 0/266 |
| 53 | 1v | 0.42 | 0/310 | 0.93 | 0/480 |
| 53 | 2v | 0.38 | 0/310 | 0.83 | 0/480 |
| 54 | 1w | 0.52 | 1/1537 (0.1%) | 1.08 | 6/2390 (0.3%) |
| 54 | 2w | 0.50 | 0/1487 | 1.09 | 2/2311 (0.1%) |
| 55 | 1x | 0.53 | 3/1700 (0.2%) | 1.15 | 18/2650 (0.7%) |
| 55 | 2x | 0.45 | 0/1700 | 1.01 | 8/2650 (0.3%) |
| 56 | 1y | 0.51 | 1/1606 (0.1%) | 1.07 | 5/2497 (0.2%) |
| 56 | 2y | 0.49 | 1/1583 (0.1%) | 0.99 | 0/2459 |
| All | All | 0.39 | 10/316502 (0.0%) | 0.83 | 203/473837 (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 |
|-----|-------|---------------------|---------------------|
| 51 | 1t | 0 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 56 | 2y | 1 | G | OP3-P | -10.24 | 1.48 | 1.61 |
| 54 | 1w | 1 | G | OP3-P | -10.23 | 1.48 | 1.61 |
| 2 | 2B | 1 | U | OP3-P | -10.19 | 1.49 | 1.61 |
| 2 | 1B | 1 | U | OP3-P | -10.11 | 1.49 | 1.61 |
| 56 | 1y | 1 | G | OP3-P | -10.10 | 1.49 | 1.61 |

The worst 5 of 203 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 32 | 2a | 1272 | G | N3-C2-N2 | 20.12 | 133.99 | 119.90 |
| 32 | 2a | 1263 | C | N1-C2-O2 | 20.03 | 130.92 | 118.90 |
| 32 | 2a | 1272 | G | C5-C6-O6 | 16.86 | 138.72 | 128.60 |
| 32 | 2a | 1272 | G | N1-C2-N2 | -16.35 | 101.48 | 116.20 |
| 32 | 2a | 1272 | G | C6-N1-C2 | 12.00 | 132.30 | 125.10 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 51 | 1t | 99 | LEU | 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%) | 258 (94%) | 14 (5%) | 1 (0%) | 34 | 54 |
| 3 | 2D | 273/276 (99%) | 253 (93%) | 20 (7%) | 0 | 100 | 100 |
| 4 | 1E | 202/206 (98%) | 194 (96%) | 7 (4%) | 1 (0%) | 29 | 48 |
| 4 | 2E | 202/206 (98%) | 186 (92%) | 15 (7%) | 1 (0%) | 29 | 48 |
| 5 | 1F | 201/210 (96%) | 195 (97%) | 5 (2%) | 1 (0%) | 29 | 48 |
| 5 | 2F | 201/210 (96%) | 187 (93%) | 12 (6%) | 2 (1%) | 15 | 28 |
| 6 | 1G | 179/182 (98%) | 166 (93%) | 12 (7%) | 1 (1%) | 25 | 43 |
| 6 | 2G | 179/182 (98%) | 154 (86%) | 22 (12%) | 3 (2%) | 9 | 16 |
| 7 | 1H | 172/180 (96%) | 162 (94%) | 10 (6%) | 0 | 100 | 100 |
| 7 | 2H | 172/180 (96%) | 156 (91%) | 15 (9%) | 1 (1%) | 25 | 43 |
| 8 | 1I | 144/148 (97%) | 132 (92%) | 12 (8%) | 0 | 100 | 100 |
| 8 | 2I | 144/148 (97%) | 123 (85%) | 19 (13%) | 2 (1%) | 11 | 20 |
| 9 | 1N | 138/140 (99%) | 131 (95%) | 7 (5%) | 0 | 100 | 100 |
| 9 | 2N | 138/140 (99%) | 129 (94%) | 8 (6%) | 1 (1%) | 22 | 39 |
| 10 | 1O | 120/122 (98%) | 111 (92%) | 9 (8%) | 0 | 100 | 100 |
| 10 | 2O | 120/122 (98%) | 111 (92%) | 9 (8%) | 0 | 100 | 100 |
| 11 | 1P | 147/150 (98%) | 135 (92%) | 9 (6%) | 3 (2%) | 7 | 12 |
| 11 | 2P | 147/150 (98%) | 127 (86%) | 15 (10%) | 5 (3%) | 3 | 5 |
| 12 | 1Q | 139/141 (99%) | 134 (96%) | 5 (4%) | 0 | 100 | 100 |
| 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%) | 103 (95%) | 5 (5%) | 0 | 100 | 100 |
| 14 | 2S | 108/112 (96%) | 96 (89%) | 8 (7%) | 4 (4%) | 3 | 4 |
| 15 | 1T | 129/146 (88%) | 121 (94%) | 7 (5%) | 1 (1%) | 19 | 35 |
| 15 | 2T | 129/146 (88%) | 123 (95%) | 6 (5%) | 0 | 100 | 100 |
| 16 | 1U | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 16 | 2U | 114/118 (97%) | 110 (96%) | 4 (4%) | 0 | 100 | 100 |
| 17 | 1V | 99/101 (98%) | 93 (94%) | 5 (5%) | 1 (1%) | 15 | 28 |
| 17 | 2V | 99/101 (98%) | 92 (93%) | 6 (6%) | 1 (1%) | 15 | 28 |
| 18 | 1W | 110/113 (97%) | 109 (99%) | 1 (1%) | 0 | 100 | 100 |
| 18 | 2W | 110/113 (97%) | 107 (97%) | 3 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 19 | 1X | 93/96 (97%) | 88 (95%) | 3 (3%) | 2 (2%) | 6 | 10 |
| 19 | 2X | 93/96 (97%) | 88 (95%) | 4 (4%) | 1 (1%) | 14 | 26 |
| 20 | 1Y | 105/110 (96%) | 97 (92%) | 7 (7%) | 1 (1%) | 15 | 28 |
| 20 | 2Y | 105/110 (96%) | 99 (94%) | 3 (3%) | 3 (3%) | 4 | 6 |
| 21 | 1Z | 148/206 (72%) | 125 (84%) | 21 (14%) | 2 (1%) | 11 | 20 |
| 21 | 2Z | 156/206 (76%) | 122 (78%) | 33 (21%) | 1 (1%) | 25 | 43 |
| 22 | 10 | 81/85 (95%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 22 | 20 | 81/85 (95%) | 73 (90%) | 7 (9%) | 1 (1%) | 13 | 24 |
| 23 | 11 | 95/98 (97%) | 92 (97%) | 2 (2%) | 1 (1%) | 14 | 26 |
| 23 | 21 | 95/98 (97%) | 92 (97%) | 2 (2%) | 1 (1%) | 14 | 26 |
| 24 | 12 | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 24 | 22 | 68/72 (94%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 25 | 13 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | 23 | 57/60 (95%) | 52 (91%) | 4 (7%) | 1 (2%) | 8 | 14 |
| 26 | 14 | 67/71 (94%) | 54 (81%) | 8 (12%) | 5 (8%) | 1 | 1 |
| 26 | 24 | 67/71 (94%) | 47 (70%) | 17 (25%) | 3 (4%) | 2 | 3 |
| 27 | 15 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 27 | 25 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 28 | 16 | 51/54 (94%) | 51 (100%) | 0 | 0 | 100 | 100 |
| 28 | 26 | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |
| 29 | 17 | 46/49 (94%) | 45 (98%) | 1 (2%) | 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%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 31 | 29 | 35/37 (95%) | 33 (94%) | 1 (3%) | 1 (3%) | 4 | 6 |
| 33 | 1b | 229/256 (90%) | 190 (83%) | 31 (14%) | 8 (4%) | 3 | 4 |
| 33 | 2b | 229/256 (90%) | 180 (79%) | 40 (18%) | 9 (4%) | 3 | 4 |
| 34 | 1c | 204/239 (85%) | 180 (88%) | 23 (11%) | 1 (0%) | 29 | 48 |
| 34 | 2c | 204/239 (85%) | 169 (83%) | 31 (15%) | 4 (2%) | 7 | 12 |
| 35 | 1d | 206/209 (99%) | 187 (91%) | 18 (9%) | 1 (0%) | 29 | 48 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 35 | 2d | 206/209 (99%) | 187 (91%) | 17 (8%) | 2 (1%) | 15 | 28 |
| 36 | 1e | 146/162 (90%) | 133 (91%) | 12 (8%) | 1 (1%) | 22 | 39 |
| 36 | 2e | 146/162 (90%) | 125 (86%) | 17 (12%) | 4 (3%) | 5 | 7 |
| 37 | 1f | 98/101 (97%) | 91 (93%) | 7 (7%) | 0 | 100 | 100 |
| 37 | 2f | 98/101 (97%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 38 | 1g | 153/156 (98%) | 139 (91%) | 12 (8%) | 2 (1%) | 12 | 21 |
| 38 | 2g | 153/156 (98%) | 135 (88%) | 16 (10%) | 2 (1%) | 12 | 21 |
| 39 | 1h | 135/138 (98%) | 126 (93%) | 9 (7%) | 0 | 100 | 100 |
| 39 | 2h | 135/138 (98%) | 122 (90%) | 12 (9%) | 1 (1%) | 22 | 39 |
| 40 | 1i | 125/128 (98%) | 112 (90%) | 12 (10%) | 1 (1%) | 19 | 35 |
| 40 | 2i | 125/128 (98%) | 101 (81%) | 23 (18%) | 1 (1%) | 19 | 35 |
| 41 | 1j | 95/105 (90%) | 81 (85%) | 11 (12%) | 3 (3%) | 4 | 5 |
| 41 | 2j | 94/105 (90%) | 76 (81%) | 14 (15%) | 4 (4%) | 2 | 3 |
| 42 | 1k | 112/129 (87%) | 99 (88%) | 10 (9%) | 3 (3%) | 5 | 7 |
| 42 | 2k | 112/129 (87%) | 100 (89%) | 10 (9%) | 2 (2%) | 8 | 14 |
| 43 | 1l | 119/132 (90%) | 111 (93%) | 8 (7%) | 0 | 100 | 100 |
| 43 | 2l | 119/132 (90%) | 110 (92%) | 8 (7%) | 1 (1%) | 19 | 35 |
| 44 | 1m | 121/126 (96%) | 109 (90%) | 10 (8%) | 2 (2%) | 9 | 16 |
| 44 | 2m | 120/126 (95%) | 97 (81%) | 21 (18%) | 2 (2%) | 9 | 16 |
| 45 | 1n | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 | 100 |
| 45 | 2n | 58/61 (95%) | 51 (88%) | 6 (10%) | 1 (2%) | 9 | 16 |
| 46 | 1o | 86/89 (97%) | 81 (94%) | 3 (4%) | 2 (2%) | 6 | 10 |
| 46 | 2o | 86/89 (97%) | 79 (92%) | 6 (7%) | 1 (1%) | 13 | 24 |
| 47 | 1p | 80/88 (91%) | 73 (91%) | 6 (8%) | 1 (1%) | 12 | 21 |
| 47 | 2p | 80/88 (91%) | 71 (89%) | 9 (11%) | 0 | 100 | 100 |
| 48 | 1q | 97/105 (92%) | 92 (95%) | 5 (5%) | 0 | 100 | 100 |
| 48 | 2q | 97/105 (92%) | 86 (89%) | 10 (10%) | 1 (1%) | 15 | 28 |
| 49 | 1r | 66/88 (75%) | 62 (94%) | 4 (6%) | 0 | 100 | 100 |
| 49 | 2r | 66/88 (75%) | 61 (92%) | 5 (8%) | 0 | 100 | 100 |
| 50 | 1s | 81/93 (87%) | 71 (88%) | 8 (10%) | 2 (2%) | 5 | 8 |
| 50 | 2s | 81/93 (87%) | 64 (79%) | 15 (18%) | 2 (2%) | 5 | 8 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 51 | 1t | 94/106 (89%) | 85 (90%) | 6 (6%) | 3 (3%) | 4 | 5 |
| 51 | 2t | 94/106 (89%) | 87 (93%) | 3 (3%) | 4 (4%) | 2 | 3 |
| 52 | 1u | 21/27 (78%) | 21 (100%) | 0 | 0 | 100 | 100 |
| 52 | 2u | 21/27 (78%) | 13 (62%) | 8 (38%) | 0 | 100 | 100 |
| All | All | 11370/12128 (94%) | 10356 (91%) | 891 (8%) | 123 (1%) | 14 | 26 |

5 of 123 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 1F | 130 | ALA |
| 11 | 1P | 38 | GLN |
| 21 | 1Z | 52 | SER |
| 21 | 1Z | 163 | LEU |
| 23 | 11 | 3 | LYS |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3 | 1D | 215/218 (99%) | 201 (94%) | 14 (6%) | 17 | 33 |
| 3 | 2D | 215/218 (99%) | 205 (95%) | 10 (5%) | 26 | 49 |
| 4 | 1E | 164/166 (99%) | 151 (92%) | 13 (8%) | 12 | 24 |
| 4 | 2E | 164/166 (99%) | 155 (94%) | 9 (6%) | 21 | 41 |
| 5 | 1F | 160/166 (96%) | 149 (93%) | 11 (7%) | 15 | 30 |
| 5 | 2F | 159/166 (96%) | 152 (96%) | 7 (4%) | 28 | 52 |
| 6 | 1G | 143/156 (92%) | 129 (90%) | 14 (10%) | 8 | 15 |
| 6 | 2G | 143/156 (92%) | 123 (86%) | 20 (14%) | 3 | 6 |
| 7 | 1H | 144/148 (97%) | 137 (95%) | 7 (5%) | 25 | 47 |
| 7 | 2H | 144/148 (97%) | 130 (90%) | 14 (10%) | 8 | 16 |
| 8 | 1I | 113/124 (91%) | 95 (84%) | 18 (16%) | 2 | 4 |
| 8 | 2I | 105/124 (85%) | 94 (90%) | 11 (10%) | 7 | 13 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 9 | 1N | 118/119 (99%) | 111 (94%) | 7 (6%) | 19 | 37 |
| 9 | 2N | 118/119 (99%) | 110 (93%) | 8 (7%) | 16 | 30 |
| 10 | 1O | 100/100 (100%) | 97 (97%) | 3 (3%) | 41 | 68 |
| 10 | 2O | 100/100 (100%) | 96 (96%) | 4 (4%) | 31 | 56 |
| 11 | 1P | 115/116 (99%) | 107 (93%) | 8 (7%) | 15 | 29 |
| 11 | 2P | 115/116 (99%) | 108 (94%) | 7 (6%) | 18 | 36 |
| 12 | 1Q | 111/111 (100%) | 105 (95%) | 6 (5%) | 22 | 42 |
| 12 | 2Q | 111/111 (100%) | 104 (94%) | 7 (6%) | 18 | 34 |
| 13 | 1R | 101/101 (100%) | 98 (97%) | 3 (3%) | 41 | 68 |
| 13 | 2R | 101/101 (100%) | 97 (96%) | 4 (4%) | 31 | 56 |
| 14 | 1S | 86/88 (98%) | 78 (91%) | 8 (9%) | 9 | 17 |
| 14 | 2S | 85/88 (97%) | 72 (85%) | 13 (15%) | 2 | 5 |
| 15 | 1T | 115/127 (91%) | 110 (96%) | 5 (4%) | 29 | 53 |
| 15 | 2T | 113/127 (89%) | 106 (94%) | 7 (6%) | 18 | 35 |
| 16 | 1U | 93/94 (99%) | 85 (91%) | 8 (9%) | 10 | 20 |
| 16 | 2U | 93/94 (99%) | 87 (94%) | 6 (6%) | 17 | 33 |
| 17 | 1V | 80/82 (98%) | 77 (96%) | 3 (4%) | 33 | 58 |
| 17 | 2V | 80/82 (98%) | 70 (88%) | 10 (12%) | 4 | 8 |
| 18 | 1W | 90/92 (98%) | 86 (96%) | 4 (4%) | 28 | 52 |
| 18 | 2W | 90/92 (98%) | 87 (97%) | 3 (3%) | 38 | 64 |
| 19 | 1X | 77/78 (99%) | 75 (97%) | 2 (3%) | 46 | 72 |
| 19 | 2X | 77/78 (99%) | 73 (95%) | 4 (5%) | 23 | 44 |
| 20 | 1Y | 85/91 (93%) | 81 (95%) | 4 (5%) | 26 | 49 |
| 20 | 2Y | 85/91 (93%) | 76 (89%) | 9 (11%) | 6 | 13 |
| 21 | 1Z | 135/179 (75%) | 125 (93%) | 10 (7%) | 13 | 27 |
| 21 | 2Z | 137/179 (76%) | 122 (89%) | 15 (11%) | 6 | 12 |
| 22 | 10 | 65/67 (97%) | 63 (97%) | 2 (3%) | 40 | 67 |
| 22 | 20 | 65/67 (97%) | 62 (95%) | 3 (5%) | 27 | 50 |
| 23 | 11 | 80/83 (96%) | 79 (99%) | 1 (1%) | 69 | 87 |
| 23 | 21 | 80/83 (96%) | 77 (96%) | 3 (4%) | 33 | 58 |
| 24 | 12 | 65/67 (97%) | 61 (94%) | 4 (6%) | 18 | 35 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 24 | 22 | 65/67 (97%) | 59 (91%) | 6 (9%) | 9 | 18 |
| 25 | 13 | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 24 |
| 25 | 23 | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 56 |
| 26 | 14 | 59/63 (94%) | 51 (86%) | 8 (14%) | 3 | 7 |
| 26 | 24 | 53/63 (84%) | 42 (79%) | 11 (21%) | 1 | 2 |
| 27 | 15 | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 56 |
| 27 | 25 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 37 |
| 28 | 16 | 51/52 (98%) | 47 (92%) | 4 (8%) | 12 | 24 |
| 28 | 26 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 37 |
| 29 | 17 | 41/42 (98%) | 36 (88%) | 5 (12%) | 5 | 9 |
| 29 | 27 | 41/42 (98%) | 37 (90%) | 4 (10%) | 8 | 15 |
| 30 | 18 | 54/55 (98%) | 50 (93%) | 4 (7%) | 13 | 27 |
| 30 | 28 | 54/55 (98%) | 49 (91%) | 5 (9%) | 9 | 17 |
| 31 | 19 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 69 |
| 31 | 29 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 69 |
| 33 | 1b | 192/220 (87%) | 166 (86%) | 26 (14%) | 4 | 7 |
| 33 | 2b | 187/220 (85%) | 162 (87%) | 25 (13%) | 4 | 7 |
| 34 | 1c | 142/188 (76%) | 128 (90%) | 14 (10%) | 8 | 15 |
| 34 | 2c | 140/188 (74%) | 124 (89%) | 16 (11%) | 5 | 11 |
| 35 | 1d | 169/181 (93%) | 153 (90%) | 16 (10%) | 8 | 17 |
| 35 | 2d | 173/181 (96%) | 159 (92%) | 14 (8%) | 11 | 23 |
| 36 | 1e | 113/123 (92%) | 103 (91%) | 10 (9%) | 10 | 19 |
| 36 | 2e | 114/123 (93%) | 102 (90%) | 12 (10%) | 7 | 13 |
| 37 | 1f | 84/90 (93%) | 80 (95%) | 4 (5%) | 25 | 48 |
| 37 | 2f | 85/90 (94%) | 79 (93%) | 6 (7%) | 14 | 28 |
| 38 | 1g | 119/127 (94%) | 110 (92%) | 9 (8%) | 13 | 25 |
| 38 | 2g | 120/127 (94%) | 104 (87%) | 16 (13%) | 4 | 7 |
| 39 | 1h | 114/119 (96%) | 108 (95%) | 6 (5%) | 22 | 43 |
| 39 | 2h | 114/119 (96%) | 102 (90%) | 12 (10%) | 7 | 13 |
| 40 | 1i | 90/99 (91%) | 79 (88%) | 11 (12%) | 5 | 9 |
| 40 | 2i | 89/99 (90%) | 78 (88%) | 11 (12%) | 4 | 9 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 41 | 1j | 66/92 (72%) | 60 (91%) | 6 (9%) | 9 | 18 |
| 41 | 2j | 69/92 (75%) | 61 (88%) | 8 (12%) | 5 | 10 |
| 42 | 1k | 82/99 (83%) | 75 (92%) | 7 (8%) | 10 | 21 |
| 42 | 2k | 83/99 (84%) | 74 (89%) | 9 (11%) | 6 | 12 |
| 43 | 1l | 96/108 (89%) | 92 (96%) | 4 (4%) | 30 | 54 |
| 43 | 2l | 96/108 (89%) | 88 (92%) | 8 (8%) | 11 | 22 |
| 44 | 1m | 93/101 (92%) | 84 (90%) | 9 (10%) | 8 | 16 |
| 44 | 2m | 92/101 (91%) | 82 (89%) | 10 (11%) | 6 | 12 |
| 45 | 1n | 49/50 (98%) | 47 (96%) | 2 (4%) | 30 | 55 |
| 45 | 2n | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 | 14 |
| 46 | 1o | 78/80 (98%) | 76 (97%) | 2 (3%) | 46 | 72 |
| 46 | 2o | 78/80 (98%) | 71 (91%) | 7 (9%) | 9 | 19 |
| 47 | 1p | 69/74 (93%) | 61 (88%) | 8 (12%) | 5 | 10 |
| 47 | 2p | 68/74 (92%) | 63 (93%) | 5 (7%) | 13 | 27 |
| 48 | 1q | 94/97 (97%) | 92 (98%) | 2 (2%) | 53 | 78 |
| 48 | 2q | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 27 |
| 49 | 1r | 59/77 (77%) | 57 (97%) | 2 (3%) | 37 | 63 |
| 49 | 2r | 59/77 (77%) | 55 (93%) | 4 (7%) | 16 | 30 |
| 50 | 1s | 69/80 (86%) | 66 (96%) | 3 (4%) | 29 | 53 |
| 50 | 2s | 67/80 (84%) | 58 (87%) | 9 (13%) | 4 | 7 |
| 51 | 1t | 70/82 (85%) | 66 (94%) | 4 (6%) | 20 | 39 |
| 51 | 2t | 70/82 (85%) | 66 (94%) | 4 (6%) | 20 | 39 |
| 52 | 1u | 18/22 (82%) | 18 (100%) | 0 | 100 | 100 |
| 52 | 2u | 18/22 (82%) | 16 (89%) | 2 (11%) | 6 | 11 |
| All | All | 9303/10064 (92%) | 8576 (92%) | 727 (8%) | 12 | 24 |

5 of 727 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | 2V | 98 | GLU |
| 34 | 2c | 132 | ARG |
| 20 | 2Y | 91 | GLU |
| 17 | 2V | 95 | LEU |
| 26 | 24 | 68 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 2F | 69 | HIS |
| 50 | 2s | 47 | HIS |
| 22 | 20 | 70 | GLN |
| 50 | 2s | 23 | ASN |
| 41 | 2j | 33 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 1A | 2863/2915 (98%) | 432 (15%) | 25 (0%) |
| 1 | 2A | 2790/2915 (95%) | 463 (16%) | 25 (0%) |
| 2 | 1B | 119/121 (98%) | 8 (6%) | 0 |
| 2 | 2B | 118/121 (97%) | 27 (22%) | 0 |
| 32 | 1a | 1494/1521 (98%) | 233 (15%) | 0 |
| 32 | 2a | 1498/1521 (98%) | 299 (19%) | 0 |
| 53 | 1v | 12/24 (50%) | 1 (8%) | 0 |
| 53 | 2v | 12/24 (50%) | 1 (8%) | 0 |
| 54 | 1w | 68/76 (89%) | 20 (29%) | 0 |
| 54 | 2w | 65/76 (85%) | 16 (24%) | 0 |
| 55 | 1x | 74/77 (96%) | 8 (10%) | 0 |
| 55 | 2x | 74/77 (96%) | 9 (12%) | 0 |
| 56 | 1y | 71/76 (93%) | 24 (33%) | 0 |
| 56 | 2y | 69/76 (90%) | 17 (24%) | 0 |
| All | All | 9327/9620 (96%) | 1558 (16%) | 50 (0%) |

5 of 1558 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1A | 10 | G |
| 1 | 1A | 12 | U |
| 1 | 1A | 34 | C |
| 1 | 1A | 36 | G |
| 1 | 1A | 45 | C |

5 of 50 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 2A | 271(M) | G |
| 1 | 2A | 900 | A |
| 1 | 2A | 2756 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2A | 277 | C |
| 1 | 2A | 774 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 32 | 5MC | 2a | 1407 | 32 | 15,22,23 | 1.36 | 1 (6%) | 19,32,35 | 1.38 | 3 (15%) |
| 32 | 5MC | 1a | 967 | 32 | 15,22,23 | 1.29 | 1 (6%) | 19,32,35 | 1.33 | 2 (10%) |
| 56 | PSU | 2y | 39 | 56 | 17,21,22 | 1.53 | 2 (11%) | 20,30,33 | 3.36 | 6 (30%) |
| 54 | 4SU | 1w | 8 | 54 | 14,21,22 | 1.32 | 1 (7%) | 15,30,33 | 1.49 | 2 (13%) |
| 32 | 4OC | 1a | 1402 | 32 | 16,23,24 | 0.63 | 0 | 17,32,35 | 0.95 | 0 |
| 1 | OMU | 1A | 2552 | 57,1 | 14,22,23 | 0.87 | 0 | 14,31,34 | 0.74 | 1 (7%) |
| 56 | 4SU | 1y | 8 | 56 | 14,21,22 | 1.36 | 2 (14%) | 15,30,33 | 1.43 | 2 (13%) |
| 32 | PSU | 2a | 516 | 32 | 17,21,22 | 1.52 | 3 (17%) | 20,30,33 | 3.17 | 7 (35%) |
| 1 | 2MA | 2A | 2503 | 57,1 | 17,25,26 | 1.28 | 2 (11%) | 19,37,40 | 1.89 | 3 (15%) |
| 54 | PSU | 1w | 39 | 54 | 17,21,22 | 1.45 | 2 (11%) | 20,30,33 | 2.94 | 6 (30%) |
| 32 | 2MG | 2a | 1207 | 32 | 19,26,27 | 1.27 | 2 (10%) | 21,38,41 | 2.08 | 6 (28%) |
| 56 | PSU | 1y | 55 | 56 | 17,21,22 | 1.49 | 3 (17%) | 20,30,33 | 3.06 | 5 (25%) |
| 32 | MA6 | 2a | 1519 | 32 | 19,26,27 | 0.79 | 0 | 18,38,41 | 1.48 | 2 (11%) |
| 32 | M2G | 2a | 966 | 32 | 20,27,28 | 1.44 | 3 (15%) | 22,40,43 | 2.14 | 6 (27%) |
| 32 | 5MC | 1a | 1407 | 32 | 15,22,23 | 1.31 | 1 (6%) | 19,32,35 | 1.29 | 3 (15%) |
| 32 | UR3 | 2a | 1498 | 32 | 14,22,23 | 0.85 | 1 (7%) | 15,32,35 | 0.85 | 1 (6%) |
| 55 | 5MU | 1x | 54 | 55 | 15,22,23 | 1.07 | 1 (6%) | 16,32,35 | 2.12 | 1 (6%) |
| 56 | 4SU | 2y | 8 | 56 | 14,21,22 | 1.25 | 1 (7%) | 15,30,33 | 1.51 | 2 (13%) |
| 54 | PSU | 1w | 55 | 54 | 17,21,22 | 1.42 | 2 (11%) | 20,30,33 | 3.35 | 6 (30%) |
| 54 | MIA | 1w | 37 | 54 | 24,31,32 | 2.16 | 3 (12%) | 26,44,47 | 2.58 | 9 (34%) |
| 32 | 5MC | 2a | 1404 | 32 | 15,22,23 | 1.33 | 1 (6%) | 19,32,35 | 1.37 | 3 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | PSU | 1A | 1917 | 1 | 17,21,22 | 1.45 | 3 (17%) | 20,30,33 | 3.08 | 6 (30%) |
| 32 | 5MC | 1a | 1400 | 32 | 15,22,23 | 1.35 | 1 (6%) | 19,32,35 | 1.30 | 3 (15%) |
| 56 | PSU | 1y | 32 | 56 | 17,21,22 | 1.42 | 2 (11%) | 20,30,33 | 3.16 | 6 (30%) |
| 54 | PSU | 1w | 32 | 57,54 | 17,21,22 | 1.48 | 2 (11%) | 20,30,33 | 3.20 | 6 (30%) |
| 32 | 7MG | 2a | 527 | 32,57 | 22,26,27 | 1.81 | 4 (18%) | 28,39,42 | 2.68 | 10 (35%) |
| 56 | 7MG | 2y | 46 | 56 | 22,26,27 | 1.88 | 4 (18%) | 28,39,42 | 2.98 | 10 (35%) |
| 32 | UR3 | 1a | 1498 | 32 | 14,22,23 | 0.75 | 0 | 15,32,35 | 0.71 | 0 |
| 32 | MA6 | 1a | 1519 | 32 | 19,26,27 | 0.84 | 0 | 18,38,41 | 1.57 | 2 (11%) |
| 54 | PSU | 2w | 32 | 54 | 17,21,22 | 1.51 | 2 (11%) | 20,30,33 | 3.16 | 6 (30%) |
| 32 | 5MC | 1a | 1404 | 32 | 15,22,23 | 1.38 | 1 (6%) | 19,32,35 | 1.24 | 3 (15%) |
| 1 | 5MC | 2A | 1962 | 1 | 15,22,23 | 1.31 | 1 (6%) | 19,32,35 | 1.31 | 3 (15%) |
| 32 | 5MC | 2a | 967 | 32 | 15,22,23 | 1.33 | 1 (6%) | 19,32,35 | 1.29 | 3 (15%) |
| 56 | MIA | 1y | 37 | 56 | 18,24,32 | 1.13 | 2 (11%) | 18,35,47 | 1.30 | 2 (11%) |
| 55 | 5MC | 2x | 32 | 55 | 15,22,23 | 1.28 | 1 (6%) | 19,32,35 | 1.40 | 2 (10%) |
| 1 | OMG | 1A | 2251 | 57,1,55 | 18,26,27 | 1.19 | 2 (11%) | 20,38,41 | 2.17 | 5 (25%) |
| 1 | 5MC | 1A | 1942 | 57,1 | 15,22,23 | 1.14 | 1 (6%) | 19,32,35 | 1.67 | 4 (21%) |
| 1 | 5MC | 1A | 1962 | 57,1 | 15,22,23 | 1.32 | 1 (6%) | 19,32,35 | 1.34 | 2 (10%) |
| 56 | MIA | 2y | 37 | 56 | 18,24,32 | 1.11 | 2 (11%) | 18,35,47 | 1.42 | 3 (16%) |
| 54 | 7MG | 1w | 46 | 54 | 22,26,27 | 1.83 | 4 (18%) | 28,39,42 | 2.72 | 8 (28%) |
| 1 | PSU | 1A | 2605 | 57,1 | 17,21,22 | 1.66 | 4 (23%) | 20,30,33 | 3.18 | 6 (30%) |
| 54 | PSU | 2w | 55 | 54 | 17,21,22 | 1.45 | 2 (11%) | 20,30,33 | 3.37 | 6 (30%) |
| 1 | OMC | 1A | 1920 | 1 | 15,22,23 | 0.71 | 0 | 17,31,34 | 1.49 | 2 (11%) |
| 54 | 7MG | 2w | 46 | 54 | 22,26,27 | 1.80 | 4 (18%) | 28,39,42 | 2.57 | 9 (32%) |
| 55 | 4SU | 2x | 8 | 55 | 14,21,22 | 1.28 | 2 (14%) | 15,30,33 | 2.39 | 2 (13%) |
| 1 | 5MC | 2A | 1942 | 1 | 15,22,23 | 1.33 | 1 (6%) | 19,32,35 | 1.48 | 3 (15%) |
| 1 | 5MU | 1A | 1915 | 1 | 15,22,23 | 1.05 | 1 (6%) | 16,32,35 | 1.69 | 2 (12%) |
| 1 | PSU | 1A | 1911 | 1 | 17,21,22 | 1.62 | 3 (17%) | 20,30,33 | 2.97 | 6 (30%) |
| 1 | 5MU | 2A | 1939 | 57,1 | 15,22,23 | 1.11 | 2 (13%) | 16,32,35 | 1.80 | 2 (12%) |
| 32 | PSU | 1a | 516 | 32 | 17,21,22 | 1.43 | 3 (17%) | 20,30,33 | 3.07 | 6 (30%) |
| 56 | PSU | 2y | 55 | 56 | 17,21,22 | 1.56 | 3 (17%) | 20,30,33 | 3.14 | 6 (30%) |
| 1 | 2MA | 1A | 2503 | 57,1 | 17,25,26 | 1.41 | 2 (11%) | 19,37,40 | 1.97 | 3 (15%) |
| 32 | 5MC | 2a | 1400 | 32 | 15,22,23 | 1.34 | 1 (6%) | 19,32,35 | 1.32 | 3 (15%) |
| 1 | PSU | 2A | 1917 | 1 | 17,21,22 | 1.59 | 2 (11%) | 20,30,33 | 3.15 | 6 (30%) |
| 1 | OMC | 2A | 1920 | 1 | 15,22,23 | 0.65 | 0 | 17,31,34 | 1.48 | 2 (11%) |
| 43 | 0TD | 1l | 92 | 43 | 4,9,10 | 3.13 | 1 (25%) | 3,11,13 | 7.23 | 1 (33%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | 5MU | 1A | 1939 | 1 | 15,22,23 | 1.21 | 2 (13%) | 16,32,35 | 2.00 | 2 (12%) |
| 54 | PSU | 2w | 39 | 54 | 17,21,22 | 1.49 | 3 (17%) | 20,30,33 | 3.17 | 5 (25%) |
| 55 | 5MU | 2x | 54 | 55 | 15,22,23 | 1.11 | 1 (6%) | 16,32,35 | 1.78 | 2 (12%) |
| 32 | 2MG | 1a | 1207 | 32 | 19,26,27 | 1.29 | 2 (10%) | 21,38,41 | 2.38 | 7 (33%) |
| 55 | 31H | 1x | 76 | 57,55 | 28,34,35 | 1.03 | 3 (10%) | 23,47,50 | 1.57 | 3 (13%) |
| 54 | 4SU | 2w | 8 | 54 | 14,21,22 | 1.24 | 1 (7%) | 15,30,33 | 1.44 | 2 (13%) |
| 32 | 7MG | 1a | 527 | 32,57 | 22,26,27 | 1.77 | 4 (18%) | 28,39,42 | 2.65 | 10 (35%) |
| 1 | PSU | 2A | 1911 | 1 | 17,21,22 | 1.54 | 4 (23%) | 20,30,33 | 3.17 | 6 (30%) |
| 1 | OMG | 2A | 2251 | 1,55 | 18,26,27 | 1.14 | 2 (11%) | 20,38,41 | 2.05 | 6 (30%) |
| 54 | MIA | 2w | 37 | 54 | 20,27,32 | 1.65 | 3 (15%) | 22,39,47 | 1.82 | 7 (31%) |
| 32 | MA6 | 2a | 1518 | 32 | 19,26,27 | 0.80 | 0 | 18,38,41 | 1.46 | 2 (11%) |
| 54 | 5MU | 2w | 54 | 54 | 15,22,23 | 1.10 | 1 (6%) | 16,32,35 | 2.23 | 1 (6%) |
| 55 | 31H | 2x | 76 | 57,55 | 28,34,35 | 1.04 | 3 (10%) | 23,47,50 | 1.57 | 4 (17%) |
| 56 | 7MG | 1y | 46 | 56 | 22,26,27 | 1.80 | 3 (13%) | 28,39,42 | 2.84 | 9 (32%) |
| 32 | M2G | 1a | 966 | 32 | 20,27,28 | 1.33 | 3 (15%) | 22,40,43 | 2.25 | 7 (31%) |
| 56 | PSU | 1y | 39 | 56 | 17,21,22 | 1.39 | 2 (11%) | 20,30,33 | 3.18 | 5 (25%) |
| 56 | 5MU | 1y | 54 | 56 | 15,22,23 | 1.03 | 1 (6%) | 16,32,35 | 2.42 | 1 (6%) |
| 56 | 5MU | 2y | 54 | 56 | 15,22,23 | 1.06 | 1 (6%) | 16,32,35 | 2.03 | 1 (6%) |
| 1 | 5MU | 2A | 1915 | 1 | 15,22,23 | 1.09 | 1 (6%) | 16,32,35 | 1.85 | 2 (12%) |
| 32 | 4OC | 2a | 1402 | 32,57 | 16,23,24 | 0.63 | 0 | 17,32,35 | 1.58 | 1 (5%) |
| 54 | 5MU | 1w | 54 | 54 | 15,22,23 | 1.08 | 1 (6%) | 16,32,35 | 1.92 | 2 (12%) |
| 55 | 5MC | 1x | 32 | 55 | 15,22,23 | 1.43 | 1 (6%) | 19,32,35 | 1.30 | 3 (15%) |
| 55 | 4SU | 1x | 8 | 55 | 14,21,22 | 1.36 | 2 (14%) | 15,30,33 | 2.72 | 2 (13%) |
| 43 | 0TD | 2l | 92 | 43 | 4,9,10 | 3.11 | 1 (25%) | 3,11,13 | 5.94 | 1 (33%) |
| 55 | PSU | 2x | 55 | 55 | 17,21,22 | 1.61 | 2 (11%) | 20,30,33 | 3.05 | 6 (30%) |
| 55 | PSU | 1x | 55 | 55 | 17,21,22 | 1.70 | 3 (17%) | 20,30,33 | 3.11 | 6 (30%) |
| 32 | MA6 | 1a | 1518 | 32 | 19,26,27 | 0.80 | 0 | 18,38,41 | 1.43 | 2 (11%) |
| 1 | PSU | 2A | 2605 | 1 | 17,21,22 | 1.49 | 3 (17%) | 20,30,33 | 3.10 | 6 (30%) |
| 56 | PSU | 2y | 32 | 56 | 17,21,22 | 1.39 | 2 (11%) | 20,30,33 | 3.05 | 5 (25%) |
| 1 | OMU | 2A | 2552 | 57,1 | 14,22,23 | 0.88 | 0 | 14,31,34 | 0.98 | 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 | 5MC | 2a | 1407 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 967 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 56 | PSU | 2y | 39 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 1w | 8 | 54 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 4OC | 1a | 1402 | 32 | - | 0/9/29/30 | 0/2/2/2 |
| 1 | OMU | 1A | 2552 | 57,1 | - | 0/7/27/28 | 0/2/2/2 |
| 56 | 4SU | 1y | 8 | 56 | - | 3/5/25/26 | 0/2/2/2 |
| 32 | PSU | 2a | 516 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 2A | 2503 | 57,1 | - | 1/3/25/26 | 0/3/3/3 |
| 54 | PSU | 1w | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 2a | 1207 | 32 | - | 4/5/27/28 | 0/3/3/3 |
| 56 | PSU | 1y | 55 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 2a | 1519 | 32 | - | 3/7/29/30 | 0/3/3/3 |
| 32 | M2G | 2a | 966 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 32 | 5MC | 1a | 1407 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | UR3 | 2a | 1498 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 55 | 5MU | 1x | 54 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 56 | 4SU | 2y | 8 | 56 | - | 0/5/25/26 | 0/2/2/2 |
| 54 | PSU | 1w | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | MIA | 1w | 37 | 54 | - | 4/11/33/34 | 0/3/3/3 |
| 32 | 5MC | 2a | 1404 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1400 | 32 | - | 2/5/25/26 | 0/2/2/2 |
| 56 | PSU | 1y | 32 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1w | 32 | 57,54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 7MG | 2a | 527 | 32,57 | - | 3/7/37/38 | 0/3/3/3 |
| 56 | 7MG | 2y | 46 | 56 | - | 3/7/37/38 | 0/3/3/3 |
| 32 | UR3 | 1a | 1498 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1519 | 32 | - | 3/7/29/30 | 0/3/3/3 |
| 54 | PSU | 2w | 32 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1404 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1962 | 1 | - | 2/5/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 967 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 56 | MIA | 1y | 37 | 56 | - | 0/3/25/34 | 0/3/3/3 |
| 55 | 5MC | 2x | 32 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | OMG | 1A | 2251 | 57,1,55 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | 1A | 1942 | 57,1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1962 | 57,1 | - | 2/5/25/26 | 0/2/2/2 |
| 56 | MIA | 2y | 37 | 56 | - | 0/3/25/34 | 0/3/3/3 |
| 54 | 7MG | 1w | 46 | 54 | - | 3/7/37/38 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|------------|---------|
| 1 | PSU | 1A | 2605 | 57,1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 2w | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | 1A | 1920 | 1 | - | 1/7/27/28 | 0/2/2/2 |
| 54 | 7MG | 2w | 46 | 54 | - | 1/7/37/38 | 0/3/3/3 |
| 55 | 4SU | 2x | 8 | 55 | - | 1/5/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1942 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1915 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1939 | 57,1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | PSU | 1a | 516 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | 2y | 55 | 56 | - | 3/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 57,1 | - | 2/3/25/26 | 0/3/3/3 |
| 32 | 5MC | 2a | 1400 | 32 | - | 2/5/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1917 | 1 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | OMC | 2A | 1920 | 1 | - | 0/7/27/28 | 0/2/2/2 |
| 43 | 0TD | 1l | 92 | 43 | - | 2/3/12/14 | - |
| 1 | 5MU | 1A | 1939 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 54 | PSU | 2w | 39 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MU | 2x | 54 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 2MG | 1a | 1207 | 32 | - | 0/5/27/28 | 0/3/3/3 |
| 55 | 31H | 1x | 76 | 57,55 | - | 4/18/40/41 | 0/3/3/3 |
| 54 | 4SU | 2w | 8 | 54 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 7MG | 1a | 527 | 32,57 | - | 3/7/37/38 | 0/3/3/3 |
| 1 | PSU | 2A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 2A | 2251 | 1,55 | - | 0/5/27/28 | 0/3/3/3 |
| 54 | MIA | 2w | 37 | 54 | - | 0/7/29/34 | 0/3/3/3 |
| 32 | MA6 | 2a | 1518 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 54 | 5MU | 2w | 54 | 54 | - | 0/5/25/26 | 0/2/2/2 |
| 55 | 31H | 2x | 76 | 57,55 | - | 3/18/40/41 | 0/3/3/3 |
| 56 | 7MG | 1y | 46 | 56 | - | 5/7/37/38 | 0/3/3/3 |
| 32 | M2G | 1a | 966 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 56 | PSU | 1y | 39 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | 5MU | 1y | 54 | 56 | - | 2/5/25/26 | 0/2/2/2 |
| 56 | 5MU | 2y | 54 | 56 | - | 3/5/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1915 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 4OC | 2a | 1402 | 32,57 | - | 4/9/29/30 | 0/2/2/2 |
| 54 | 5MU | 1w | 54 | 54 | - | 0/5/25/26 | 0/2/2/2 |
| 55 | 5MC | 1x | 32 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 55 | 4SU | 1x | 8 | 55 | - | 0/5/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 43 | 0TD | 2l | 92 | 43 | - | 3/3/12/14 | - |
| 55 | PSU | 2x | 55 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | PSU | 1x | 55 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1518 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | PSU | 2A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 56 | PSU | 2y | 32 | 56 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | 2A | 2552 | 57,1 | - | 0/7/27/28 | 0/2/2/2 |

The worst 5 of 152 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 54 | 1w | 37 | MIA | C13-C14 | 7.18 | 1.53 | 1.32 |
| 54 | 1w | 37 | MIA | C2-S10 | -6.20 | 1.70 | 1.75 |
| 43 | 2l | 92 | 0TD | CB-SB | -5.99 | 1.69 | 1.84 |
| 43 | 1l | 92 | 0TD | CB-SB | -5.90 | 1.69 | 1.84 |
| 54 | 2w | 37 | MIA | C2-S10 | -5.64 | 1.70 | 1.75 |

The worst 5 of 342 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 43 | 1l | 92 | 0TD | CSB-SB-CB | -12.44 | 77.39 | 101.85 |
| 43 | 2l | 92 | 0TD | CSB-SB-CB | -10.23 | 81.74 | 101.85 |
| 56 | 2y | 46 | 7MG | N3-C4-N9 | 9.70 | 139.37 | 126.91 |
| 56 | 1y | 46 | 7MG | N3-C4-N9 | 9.44 | 139.03 | 126.91 |
| 56 | 1y | 54 | 5MU | C4-N3-C2 | 9.28 | 122.98 | 115.14 |

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 43 | 1l | 92 | 0TD | CA-CB-SB-CSB |
| 43 | 1l | 92 | 0TD | CG-CB-SB-CSB |
| 56 | 1y | 46 | 7MG | C4'-C5'-O5'-P |
| 43 | 2l | 92 | 0TD | O-C-CA-CB |
| 43 | 2l | 92 | 0TD | CG-CB-SB-CSB |

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 2586 ligands modelled in this entry, 2582 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 60 | SF4 | 1d | 302 | 35 | 0,12,12 | - | - | - | | |
| 58 | 6IF | 1A | 4109 | - | 30,34,34 | 1.02 | 2 (6%) | 32,49,49 | 1.71 | 4 (12%) |
| 60 | SF4 | 2d | 302 | 35 | 0,12,12 | - | - | - | | |
| 58 | 6IF | 2A | 3731 | - | 30,34,34 | 0.80 | 1 (3%) | 32,49,49 | 1.59 | 4 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 60 | SF4 | 1d | 302 | 35 | - | - | 0/6/5/5 |
| 58 | 6IF | 1A | 4109 | - | - | 4/22/65/65 | 0/3/3/3 |
| 60 | SF4 | 2d | 302 | 35 | - | - | 0/6/5/5 |
| 58 | 6IF | 2A | 3731 | - | - | 2/22/65/65 | 0/3/3/3 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 58 | 1A | 4109 | 6IF | CG-CB | -2.37 | 1.49 | 1.53 |
| 58 | 2A | 3731 | 6IF | CAI-CLAJ | -2.23 | 1.77 | 1.81 |
| 58 | 1A | 4109 | 6IF | CAA-CAB | -2.02 | 1.49 | 1.53 |

The worst 5 of 8 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 58 | 1A | 4109 | 6IF | CBB-CBA-CAY | -6.20 | 110.73 | 116.03 |
| 58 | 2A | 3731 | 6IF | CBB-CBA-CAY | -5.45 | 111.37 | 116.03 |
| 58 | 2A | 3731 | 6IF | CD1-CG-CB | -4.84 | 97.81 | 103.80 |
| 58 | 1A | 4109 | 6IF | CD1-CG-CB | -4.73 | 97.95 | 103.80 |
| 58 | 1A | 4109 | 6IF | CAK-CAI-CAG | -3.09 | 110.28 | 114.26 |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

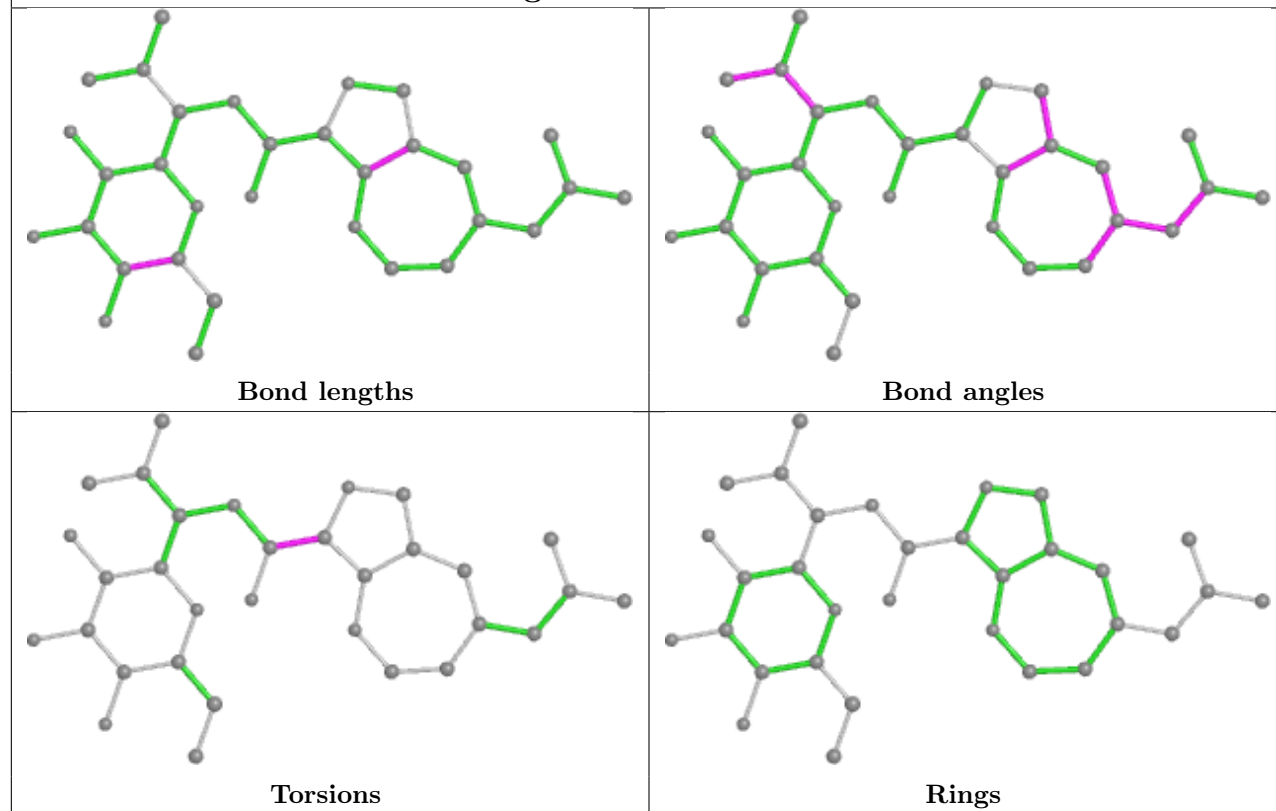
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 58 | 1A | 4109 | 6IF | O-C-CA-CB |
| 58 | 1A | 4109 | 6IF | NAH-C-CA-CB |
| 58 | 2A | 3731 | 6IF | NAH-C-CA-CB |
| 58 | 1A | 4109 | 6IF | NAH-C-CA-N |
| 58 | 2A | 3731 | 6IF | O-C-CA-CB |

There are no ring outliers.

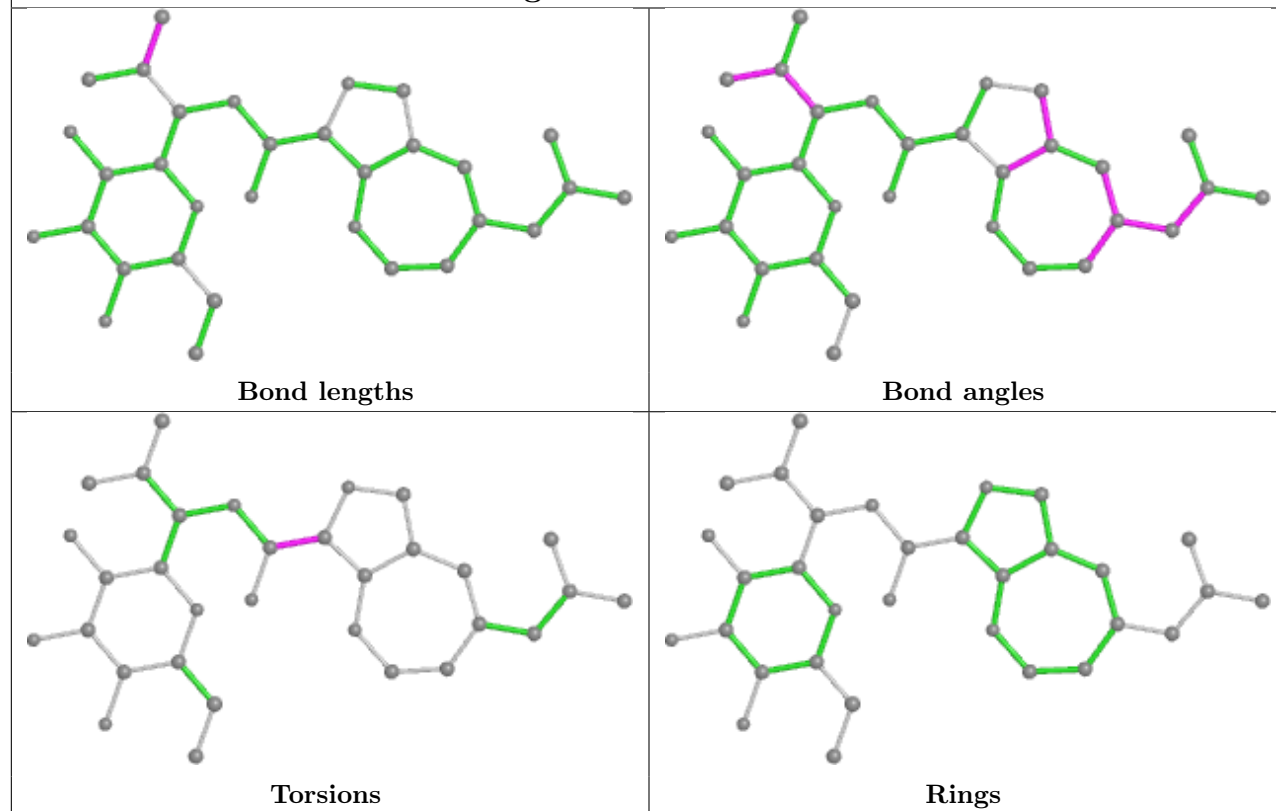
No monomer is involved in short contacts.

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.

Ligand 6IF 1A 4109



Ligand 6IF 2A 3731



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 | 2860/2915 (98%) | 0.42 | 68 (2%) 59 62 | 19, 36, 89, 102 | 0 |
| 1 | 2A | 2789/2915 (95%) | 0.17 | 80 (2%) 51 55 | 34, 57, 89, 99 | 0 |
| 2 | 1B | 120/121 (99%) | 0.20 | 0 100 100 | 29, 47, 62, 82 | 0 |
| 2 | 2B | 120/121 (99%) | 0.08 | 3 (2%) 57 61 | 62, 80, 88, 92 | 0 |
| 3 | 1D | 275/276 (99%) | 0.52 | 2 (0%) 87 89 | 21, 37, 51, 74 | 0 |
| 3 | 2D | 275/276 (99%) | 0.71 | 12 (4%) 34 37 | 33, 52, 64, 81 | 0 |
| 4 | 1E | 204/206 (99%) | 0.55 | 1 (0%) 91 91 | 18, 40, 58, 71 | 0 |
| 4 | 2E | 204/206 (99%) | 0.66 | 6 (2%) 51 55 | 33, 56, 68, 74 | 0 |
| 5 | 1F | 203/210 (96%) | 0.56 | 0 100 100 | 20, 41, 65, 79 | 0 |
| 5 | 2F | 203/210 (96%) | 0.42 | 4 (1%) 65 68 | 35, 66, 77, 83 | 0 |
| 6 | 1G | 181/182 (99%) | 0.31 | 4 (2%) 62 65 | 38, 56, 69, 83 | 0 |
| 6 | 2G | 181/182 (99%) | 1.09 | 36 (19%) 1 1 | 72, 79, 83, 88 | 0 |
| 7 | 1H | 174/180 (96%) | 0.36 | 0 100 100 | 36, 52, 63, 67 | 0 |
| 7 | 2H | 174/180 (96%) | 2.27 | 95 (54%) 0 0 | 66, 78, 85, 88 | 0 |
| 8 | 1I | 146/148 (98%) | 0.35 | 2 (1%) 75 77 | 45, 70, 79, 83 | 0 |
| 8 | 2I | 146/148 (98%) | 1.05 | 32 (21%) 0 0 | 53, 71, 79, 83 | 0 |
| 9 | 1N | 140/140 (100%) | 0.67 | 0 100 100 | 24, 39, 56, 71 | 0 |
| 9 | 2N | 140/140 (100%) | 0.75 | 13 (9%) 8 8 | 45, 63, 75, 79 | 0 |
| 10 | 1O | 122/122 (100%) | 0.49 | 1 (0%) 86 87 | 25, 40, 57, 62 | 0 |
| 10 | 2O | 122/122 (100%) | 0.81 | 9 (7%) 14 15 | 47, 57, 69, 73 | 0 |
| 11 | 1P | 149/150 (99%) | 0.55 | 2 (1%) 77 79 | 20, 44, 65, 71 | 0 |
| 11 | 2P | 149/150 (99%) | 0.83 | 12 (8%) 12 12 | 38, 65, 79, 83 | 0 |
| 12 | 1Q | 141/141 (100%) | 0.62 | 3 (2%) 63 66 | 28, 41, 56, 70 | 0 |
| 12 | 2Q | 141/141 (100%) | 1.34 | 32 (22%) 0 0 | 49, 66, 76, 83 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13 | 1R | 118/118 (100%) | 0.51 | 0 100 100 | 25, 33, 46, 54 | 0 |
| 13 | 2R | 118/118 (100%) | 0.53 | 3 (2%) 57 61 | 39, 50, 60, 64 | 0 |
| 14 | 1S | 110/112 (98%) | 0.46 | 1 (0%) 84 86 | 37, 48, 58, 64 | 0 |
| 14 | 2S | 110/112 (98%) | 0.93 | 19 (17%) 1 1 | 65, 74, 79, 81 | 0 |
| 15 | 1T | 131/146 (89%) | 0.34 | 4 (3%) 49 52 | 33, 44, 65, 70 | 0 |
| 15 | 2T | 131/146 (89%) | 0.62 | 6 (4%) 32 34 | 50, 59, 71, 78 | 0 |
| 16 | 1U | 116/118 (98%) | 0.68 | 1 (0%) 84 86 | 21, 29, 47, 62 | 0 |
| 16 | 2U | 116/118 (98%) | 0.63 | 3 (2%) 56 59 | 46, 61, 74, 83 | 0 |
| 17 | 1V | 101/101 (100%) | 0.61 | 0 100 100 | 22, 39, 56, 64 | 0 |
| 17 | 2V | 101/101 (100%) | 0.43 | 3 (2%) 50 53 | 42, 70, 75, 81 | 0 |
| 18 | 1W | 112/113 (99%) | 0.67 | 0 100 100 | 22, 31, 50, 73 | 0 |
| 18 | 2W | 112/113 (99%) | 0.62 | 2 (1%) 68 71 | 40, 50, 67, 85 | 0 |
| 19 | 1X | 95/96 (98%) | 0.58 | 2 (2%) 63 66 | 25, 37, 56, 76 | 0 |
| 19 | 2X | 95/96 (98%) | 0.66 | 4 (4%) 36 39 | 45, 59, 73, 83 | 0 |
| 20 | 1Y | 107/110 (97%) | 0.46 | 0 100 100 | 34, 47, 64, 71 | 0 |
| 20 | 2Y | 107/110 (97%) | 0.81 | 11 (10%) 6 6 | 56, 69, 79, 84 | 0 |
| 21 | 1Z | 154/206 (74%) | 0.47 | 7 (4%) 33 36 | 38, 61, 78, 84 | 0 |
| 21 | 2Z | 160/206 (77%) | 0.98 | 29 (18%) 1 1 | 65, 78, 87, 89 | 0 |
| 22 | 10 | 83/85 (97%) | 1.35 | 7 (8%) 11 11 | 27, 37, 66, 79 | 0 |
| 22 | 20 | 83/85 (97%) | 1.33 | 14 (16%) 1 1 | 46, 65, 76, 82 | 0 |
| 23 | 11 | 97/98 (98%) | 0.64 | 3 (3%) 49 52 | 27, 43, 66, 71 | 0 |
| 23 | 21 | 97/98 (98%) | 0.74 | 5 (5%) 27 29 | 40, 53, 71, 75 | 0 |
| 24 | 12 | 70/72 (97%) | 0.58 | 0 100 100 | 35, 47, 57, 70 | 0 |
| 24 | 22 | 70/72 (97%) | 0.40 | 1 (1%) 75 77 | 59, 69, 76, 78 | 0 |
| 25 | 13 | 59/60 (98%) | 0.52 | 0 100 100 | 24, 34, 57, 74 | 0 |
| 25 | 23 | 59/60 (98%) | 0.88 | 5 (8%) 10 10 | 54, 64, 74, 82 | 0 |
| 26 | 14 | 69/71 (97%) | 0.32 | 3 (4%) 35 38 | 48, 69, 83, 87 | 0 |
| 26 | 24 | 69/71 (97%) | 1.05 | 15 (21%) 0 0 | 75, 82, 88, 95 | 0 |
| 27 | 15 | 59/60 (98%) | 0.72 | 1 (1%) 70 72 | 20, 30, 52, 62 | 0 |
| 27 | 25 | 59/60 (98%) | 0.43 | 1 (1%) 70 72 | 35, 49, 61, 74 | 0 |
| 28 | 16 | 53/54 (98%) | 0.55 | 0 100 100 | 29, 42, 54, 61 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28 | 26 | 53/54 (98%) | 0.76 | 6 (11%) 5 4 | 54, 62, 68, 73 | 0 |
| 29 | 17 | 48/49 (97%) | 0.84 | 4 (8%) 11 11 | 21, 27, 55, 61 | 0 |
| 29 | 27 | 48/49 (97%) | 0.97 | 5 (10%) 6 6 | 32, 42, 64, 67 | 0 |
| 30 | 18 | 64/65 (98%) | 0.65 | 0 100 100 | 28, 34, 41, 55 | 0 |
| 30 | 28 | 64/65 (98%) | 1.07 | 6 (9%) 8 8 | 46, 56, 62, 68 | 0 |
| 31 | 19 | 37/37 (100%) | 0.58 | 0 100 100 | 29, 38, 54, 56 | 0 |
| 31 | 29 | 37/37 (100%) | 1.58 | 11 (29%) 0 0 | 59, 67, 75, 76 | 0 |
| 32 | 1a | 1488/1521 (97%) | 0.12 | 39 (2%) 56 59 | 35, 64, 87, 99 | 0 |
| 32 | 2a | 1491/1521 (98%) | 0.34 | 90 (6%) 21 22 | 52, 76, 92, 101 | 0 |
| 33 | 1b | 231/256 (90%) | 0.33 | 6 (2%) 56 59 | 62, 74, 82, 86 | 0 |
| 33 | 2b | 231/256 (90%) | 1.37 | 60 (25%) 0 0 | 71, 82, 87, 89 | 0 |
| 34 | 1c | 206/239 (86%) | 0.47 | 9 (4%) 34 37 | 56, 68, 76, 82 | 0 |
| 34 | 2c | 206/239 (86%) | 1.70 | 79 (38%) 0 0 | 72, 82, 88, 93 | 0 |
| 35 | 1d | 208/209 (99%) | 0.84 | 24 (11%) 4 4 | 52, 68, 75, 79 | 0 |
| 35 | 2d | 208/209 (99%) | 1.20 | 40 (19%) 1 1 | 61, 70, 77, 80 | 0 |
| 36 | 1e | 148/162 (91%) | 0.52 | 1 (0%) 87 89 | 49, 62, 70, 76 | 0 |
| 36 | 2e | 148/162 (91%) | 1.33 | 39 (26%) 0 0 | 68, 76, 81, 87 | 0 |
| 37 | 1f | 100/101 (99%) | 0.42 | 0 100 100 | 52, 64, 71, 74 | 0 |
| 37 | 2f | 100/101 (99%) | 0.30 | 2 (2%) 65 68 | 63, 70, 75, 79 | 0 |
| 38 | 1g | 155/156 (99%) | 0.65 | 12 (7%) 13 13 | 56, 67, 75, 81 | 0 |
| 38 | 2g | 155/156 (99%) | 0.96 | 23 (14%) 2 2 | 69, 77, 83, 86 | 0 |
| 39 | 1h | 137/138 (99%) | 0.56 | 5 (3%) 42 46 | 53, 64, 71, 79 | 0 |
| 39 | 2h | 137/138 (99%) | 1.25 | 32 (23%) 0 0 | 70, 77, 81, 82 | 0 |
| 40 | 1i | 127/128 (99%) | 0.92 | 14 (11%) 5 5 | 49, 72, 78, 83 | 0 |
| 40 | 2i | 127/128 (99%) | 2.53 | 75 (59%) 0 0 | 72, 81, 86, 87 | 0 |
| 41 | 1j | 97/105 (92%) | 0.65 | 8 (8%) 11 11 | 58, 74, 80, 83 | 0 |
| 41 | 2j | 96/105 (91%) | 2.39 | 51 (53%) 0 0 | 76, 83, 87, 90 | 0 |
| 42 | 1k | 114/129 (88%) | 0.40 | 1 (0%) 84 86 | 45, 63, 74, 77 | 0 |
| 42 | 2k | 114/129 (88%) | 0.64 | 10 (8%) 10 10 | 61, 73, 79, 82 | 0 |
| 43 | 1l | 121/132 (91%) | 0.59 | 8 (6%) 18 19 | 45, 54, 64, 75 | 0 |
| 43 | 2l | 121/132 (91%) | 1.86 | 45 (37%) 0 0 | 55, 70, 77, 80 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | 1m | 123/126 (97%) | 0.47 | 9 (7%) 15 15 | 54, 66, 74, 84 | 0 |
| 44 | 2m | 122/126 (96%) | 1.80 | 44 (36%) 0 0 | 72, 80, 85, 88 | 0 |
| 45 | 1n | 60/61 (98%) | 1.10 | 7 (11%) 4 4 | 55, 65, 70, 74 | 0 |
| 45 | 2n | 60/61 (98%) | 4.23 | 49 (81%) 0 0 | 76, 83, 87, 89 | 0 |
| 46 | 1o | 88/89 (98%) | 0.66 | 9 (10%) 6 6 | 50, 61, 71, 74 | 0 |
| 46 | 2o | 88/89 (98%) | 0.77 | 6 (6%) 17 17 | 63, 72, 80, 83 | 0 |
| 47 | 1p | 82/88 (93%) | 1.55 | 27 (32%) 0 0 | 56, 68, 74, 82 | 0 |
| 47 | 2p | 82/88 (93%) | 0.99 | 10 (12%) 4 3 | 57, 67, 74, 78 | 0 |
| 48 | 1q | 99/105 (94%) | 0.90 | 11 (11%) 5 5 | 52, 64, 72, 76 | 0 |
| 48 | 2q | 99/105 (94%) | 1.28 | 27 (27%) 0 0 | 61, 71, 78, 81 | 0 |
| 49 | 1r | 68/88 (77%) | 0.43 | 3 (4%) 34 37 | 54, 64, 75, 77 | 0 |
| 49 | 2r | 68/88 (77%) | 0.44 | 1 (1%) 73 75 | 65, 72, 78, 83 | 0 |
| 50 | 1s | 83/93 (89%) | 0.66 | 4 (4%) 30 32 | 61, 69, 78, 81 | 0 |
| 50 | 2s | 83/93 (89%) | 2.50 | 46 (55%) 0 0 | 76, 84, 88, 91 | 0 |
| 51 | 1t | 96/106 (90%) | 1.41 | 30 (31%) 0 0 | 58, 67, 74, 79 | 0 |
| 51 | 2t | 96/106 (90%) | 1.42 | 29 (30%) 0 0 | 58, 69, 76, 78 | 0 |
| 52 | 1u | 23/27 (85%) | 1.58 | 7 (30%) 0 0 | 57, 63, 67, 71 | 0 |
| 52 | 2u | 23/27 (85%) | 2.73 | 13 (56%) 0 0 | 76, 79, 83, 84 | 0 |
| 53 | 1v | 13/24 (54%) | 1.65 | 4 (30%) 0 0 | 49, 65, 82, 92 | 0 |
| 53 | 2v | 13/24 (54%) | 2.62 | 6 (46%) 0 0 | 75, 83, 93, 97 | 0 |
| 54 | 1w | 64/76 (84%) | 2.13 | 22 (34%) 0 0 | 64, 85, 97, 101 | 0 |
| 54 | 2w | 62/76 (81%) | 2.94 | 41 (66%) 0 0 | 84, 92, 98, 103 | 0 |
| 55 | 1x | 71/77 (92%) | 0.11 | 0 100 100 | 28, 60, 80, 86 | 0 |
| 55 | 2x | 71/77 (92%) | 0.01 | 0 100 100 | 46, 79, 89, 90 | 0 |
| 56 | 1y | 67/76 (88%) | 0.57 | 7 (10%) 6 6 | 38, 85, 93, 95 | 0 |
| 56 | 2y | 66/76 (86%) | 1.28 | 16 (24%) 0 0 | 54, 91, 94, 98 | 0 |
| All | All | 20867/21748 (95%) | 0.62 | 1700 (8%) 12 12 | 18, 63, 86, 103 | 0 |

The worst 5 of 1700 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 45 | 2n | 34 | TYR | 13.8 |
| 41 | 2j | 47 | PHE | 12.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 44 | 2m | 123 | ALA | 11.8 |
| 54 | 1w | 71 | G | 11.6 |
| 22 | 10 | 7 | LEU | 10.4 |

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(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 56 | PSU | 2y | 55 | 20/21 | 0.71 | 0.34 | 87,95,102,109 | 0 |
| 56 | PSU | 1y | 55 | 20/21 | 0.74 | 0.28 | 83,88,100,106 | 0 |
| 56 | 7MG | 2y | 46 | 24/25 | 0.75 | 0.22 | 86,94,100,112 | 0 |
| 54 | 7MG | 1w | 46 | 24/25 | 0.76 | 0.20 | 77,86,96,115 | 0 |
| 54 | 7MG | 2w | 46 | 24/25 | 0.77 | 0.26 | 80,91,98,112 | 0 |
| 56 | 5MU | 2y | 54 | 21/22 | 0.78 | 0.36 | 88,92,99,117 | 0 |
| 56 | PSU | 2y | 32 | 20/21 | 0.79 | 0.24 | 71,82,95,95 | 0 |
| 56 | 5MU | 1y | 54 | 21/22 | 0.79 | 0.26 | 78,83,92,101 | 0 |
| 56 | 4SU | 2y | 8 | 20/21 | 0.80 | 0.15 | 88,92,98,104 | 0 |
| 54 | 4SU | 2w | 8 | 20/21 | 0.81 | 0.26 | 87,95,103,113 | 0 |
| 54 | PSU | 2w | 55 | 20/21 | 0.81 | 0.28 | 81,87,92,98 | 0 |
| 56 | 4SU | 1y | 8 | 20/21 | 0.84 | 0.16 | 83,87,95,95 | 0 |
| 56 | 7MG | 1y | 46 | 24/25 | 0.85 | 0.21 | 80,89,98,108 | 0 |
| 54 | PSU | 1w | 55 | 20/21 | 0.86 | 0.26 | 63,81,85,87 | 0 |
| 56 | MIA | 2y | 37 | 22/30 | 0.86 | 0.25 | 76,84,93,104 | 0 |
| 55 | 4SU | 2x | 8 | 20/21 | 0.86 | 0.15 | 74,79,83,91 | 0 |
| 54 | MIA | 2w | 37 | 25/30 | 0.87 | 0.30 | 78,85,89,102 | 0 |
| 32 | 2MG | 2a | 1207 | 24/25 | 0.87 | 0.18 | 79,87,95,98 | 0 |
| 54 | PSU | 2w | 32 | 20/21 | 0.87 | 0.38 | 82,88,94,98 | 0 |
| 54 | 5MU | 2w | 54 | 21/22 | 0.88 | 0.19 | 78,82,90,92 | 0 |
| 43 | 0TD | 1l | 92 | 10/11 | 0.88 | 0.19 | 44,53,57,69 | 0 |
| 32 | PSU | 2a | 516 | 20/21 | 0.88 | 0.19 | 79,81,87,89 | 0 |
| 32 | M2G | 2a | 966 | 25/26 | 0.88 | 0.24 | 60,70,84,89 | 0 |
| 43 | 0TD | 2l | 92 | 10/11 | 0.89 | 0.25 | 67,69,75,87 | 0 |
| 55 | 5MU | 2x | 54 | 21/22 | 0.89 | 0.20 | 77,81,89,99 | 0 |
| 56 | PSU | 1y | 39 | 20/21 | 0.90 | 0.17 | 70,76,82,83 | 0 |
| 56 | MIA | 1y | 37 | 22/30 | 0.90 | 0.17 | 65,74,81,86 | 0 |
| 32 | 5MC | 2a | 967 | 21/22 | 0.90 | 0.21 | 68,73,80,84 | 0 |
| 56 | PSU | 2y | 39 | 20/21 | 0.90 | 0.22 | 78,81,93,96 | 0 |
| 54 | 4SU | 1w | 8 | 20/21 | 0.90 | 0.20 | 78,82,90,94 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 55 | PSU | 2x | 55 | 20/21 | 0.90 | 0.17 | 75,81,83,89 | 0 |
| 54 | PSU | 2w | 39 | 20/21 | 0.91 | 0.45 | 79,84,88,89 | 0 |
| 54 | PSU | 1w | 32 | 20/21 | 0.92 | 0.32 | 68,73,86,90 | 0 |
| 1 | 5MU | 2A | 1915 | 21/22 | 0.92 | 0.13 | 71,75,81,92 | 0 |
| 32 | 5MC | 2a | 1404 | 21/22 | 0.92 | 0.23 | 59,64,67,71 | 0 |
| 56 | PSU | 1y | 32 | 20/21 | 0.93 | 0.21 | 73,76,81,82 | 0 |
| 54 | MIA | 1w | 37 | 29/30 | 0.93 | 0.28 | 55,64,74,79 | 0 |
| 54 | PSU | 1w | 39 | 20/21 | 0.94 | 0.27 | 63,74,77,81 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.94 | 0.16 | 54,63,72,74 | 0 |
| 32 | MA6 | 2a | 1519 | 24/25 | 0.94 | 0.26 | 51,66,71,73 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.94 | 0.16 | 62,70,76,83 | 0 |
| 55 | PSU | 1x | 55 | 20/21 | 0.94 | 0.17 | 46,61,70,71 | 0 |
| 32 | 4OC | 2a | 1402 | 22/23 | 0.94 | 0.15 | 58,66,73,76 | 0 |
| 32 | UR3 | 2a | 1498 | 21/22 | 0.95 | 0.21 | 60,63,70,74 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.95 | 0.16 | 40,55,60,62 | 0 |
| 1 | OMC | 2A | 1920 | 21/22 | 0.95 | 0.17 | 59,64,68,69 | 0 |
| 32 | PSU | 1a | 516 | 20/21 | 0.95 | 0.15 | 58,62,67,69 | 0 |
| 55 | 5MC | 2x | 32 | 21/22 | 0.95 | 0.18 | 68,74,78,81 | 0 |
| 55 | 5MU | 1x | 54 | 21/22 | 0.95 | 0.14 | 59,65,71,77 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.95 | 0.18 | 39,48,54,59 | 0 |
| 32 | 7MG | 2a | 527 | 24/25 | 0.95 | 0.18 | 60,67,73,83 | 0 |
| 54 | 5MU | 1w | 54 | 21/22 | 0.95 | 0.17 | 61,72,78,81 | 0 |
| 32 | MA6 | 2a | 1518 | 24/25 | 0.96 | 0.20 | 52,67,72,73 | 0 |
| 32 | 5MC | 1a | 967 | 21/22 | 0.96 | 0.21 | 50,56,63,64 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.96 | 0.18 | 42,50,58,66 | 0 |
| 32 | 2MG | 1a | 1207 | 24/25 | 0.96 | 0.15 | 56,65,68,72 | 0 |
| 32 | 7MG | 1a | 527 | 24/25 | 0.96 | 0.17 | 40,48,52,57 | 0 |
| 55 | 4SU | 1x | 8 | 20/21 | 0.96 | 0.15 | 55,61,65,65 | 0 |
| 32 | 5MC | 2a | 1400 | 21/22 | 0.96 | 0.26 | 71,74,78,82 | 0 |
| 32 | 4OC | 1a | 1402 | 22/23 | 0.96 | 0.18 | 39,48,54,54 | 0 |
| 1 | PSU | 2A | 2605 | 20/21 | 0.96 | 0.18 | 33,40,43,47 | 0 |
| 32 | M2G | 1a | 966 | 25/26 | 0.96 | 0.19 | 47,54,60,64 | 0 |
| 32 | 5MC | 2a | 1407 | 21/22 | 0.96 | 0.20 | 55,59,64,65 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.96 | 0.19 | 50,56,64,64 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.97 | 0.19 | 39,42,46,48 | 0 |
| 1 | OMU | 2A | 2552 | 21/22 | 0.97 | 0.22 | 39,44,49,59 | 0 |
| 32 | MA6 | 1a | 1519 | 24/25 | 0.97 | 0.20 | 35,41,45,52 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.97 | 0.17 | 33,40,46,48 | 0 |
| 55 | 5MC | 1x | 32 | 21/22 | 0.97 | 0.19 | 48,53,59,68 | 0 |
| 55 | 31H | 1x | 76 | 32/33 | 0.97 | 0.21 | 22,29,37,42 | 10 |
| 55 | 31H | 2x | 76 | 32/33 | 0.97 | 0.22 | 40,48,54,68 | 0 |
| 1 | OMC | 1A | 1920 | 21/22 | 0.98 | 0.19 | 38,45,50,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1 | 2MA | 1A | 2503 | 23/24 | 0.98 | 0.20 | 14,20,24,26 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.98 | 0.21 | 29,37,42,45 | 0 |
| 32 | 5MC | 1a | 1404 | 21/22 | 0.98 | 0.19 | 38,42,46,50 | 0 |
| 1 | OMU | 1A | 2552 | 21/22 | 0.98 | 0.22 | 23,30,35,38 | 0 |
| 32 | 5MC | 1a | 1407 | 21/22 | 0.98 | 0.18 | 33,40,45,49 | 0 |
| 1 | PSU | 1A | 1911 | 20/21 | 0.98 | 0.18 | 36,45,52,52 | 0 |
| 32 | UR3 | 1a | 1498 | 21/22 | 0.98 | 0.18 | 38,41,43,47 | 0 |
| 1 | 5MC | 1A | 1962 | 21/22 | 0.98 | 0.18 | 27,34,40,50 | 0 |
| 1 | 5MU | 2A | 1939 | 21/22 | 0.98 | 0.20 | 35,39,47,48 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.98 | 0.20 | 22,26,30,32 | 0 |
| 32 | 5MC | 1a | 1400 | 21/22 | 0.98 | 0.18 | 43,51,56,63 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.99 | 0.19 | 21,26,30,32 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.99 | 0.21 | 22,28,33,34 | 0 |
| 32 | MA6 | 1a | 1518 | 24/25 | 0.99 | 0.21 | 31,42,46,48 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3932 | 1/1 | 0.11 | 0.16 | 70,70,70,70 | 0 |
| 57 | MG | 1Y | 203 | 1/1 | 0.22 | 0.20 | 84,84,84,84 | 0 |
| 57 | MG | 1A | 3931 | 1/1 | 0.23 | 0.20 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3959 | 1/1 | 0.28 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | 1a | 1642 | 1/1 | 0.30 | 0.20 | 78,78,78,78 | 0 |
| 57 | MG | 2A | 3556 | 1/1 | 0.36 | 0.49 | 80,80,80,80 | 0 |
| 57 | MG | 1A | 3401 | 1/1 | 0.37 | 0.39 | 77,77,77,77 | 0 |
| 57 | MG | 2A | 3251 | 1/1 | 0.39 | 0.14 | 71,71,71,71 | 0 |
| 57 | MG | 2a | 1658 | 1/1 | 0.40 | 0.16 | 78,78,78,78 | 0 |
| 57 | MG | 1a | 1715 | 1/1 | 0.43 | 0.27 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 4014 | 1/1 | 0.44 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | 2a | 1753 | 1/1 | 0.45 | 0.24 | 71,71,71,71 | 0 |
| 57 | MG | 2a | 1616 | 1/1 | 0.46 | 0.43 | 80,80,80,80 | 0 |
| 57 | MG | 2A | 3341 | 1/1 | 0.48 | 0.30 | 63,63,63,63 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3953 | 1/1 | 0.49 | 0.09 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3754 | 1/1 | 0.50 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3576 | 1/1 | 0.52 | 0.08 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 3935 | 1/1 | 0.52 | 0.11 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3551 | 1/1 | 0.52 | 0.26 | 79,79,79,79 | 0 |
| 57 | MG | 1A | 4049 | 1/1 | 0.52 | 0.10 | 59,59,59,59 | 0 |
| 59 | ZN | 24 | 501 | 1/1 | 0.52 | 0.13 | 135,135,135,135 | 0 |
| 57 | MG | 1A | 4042 | 1/1 | 0.53 | 0.25 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3490 | 1/1 | 0.53 | 0.27 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3452 | 1/1 | 0.55 | 0.20 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 4006 | 1/1 | 0.55 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3853 | 1/1 | 0.57 | 0.11 | 55,55,55,55 | 0 |
| 57 | MG | 2a | 1663 | 1/1 | 0.57 | 0.27 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3579 | 1/1 | 0.58 | 0.16 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 3716 | 1/1 | 0.58 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3687 | 1/1 | 0.59 | 0.09 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3604 | 1/1 | 0.59 | 0.23 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 4033 | 1/1 | 0.59 | 0.12 | 80,80,80,80 | 0 |
| 57 | MG | 2A | 3560 | 1/1 | 0.59 | 0.20 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3486 | 1/1 | 0.59 | 0.17 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3533 | 1/1 | 0.59 | 0.15 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3722 | 1/1 | 0.60 | 0.19 | 78,78,78,78 | 0 |
| 57 | MG | 1A | 4003 | 1/1 | 0.60 | 0.19 | 74,74,74,74 | 0 |
| 57 | MG | 1A | 3972 | 1/1 | 0.61 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | 2a | 1646 | 1/1 | 0.61 | 0.17 | 76,76,76,76 | 0 |
| 57 | MG | 1a | 1784 | 1/1 | 0.61 | 0.19 | 69,69,69,69 | 0 |
| 57 | MG | 2A | 3544 | 1/1 | 0.62 | 0.60 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3930 | 1/1 | 0.62 | 0.13 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3555 | 1/1 | 0.62 | 0.31 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 4002 | 1/1 | 0.62 | 0.11 | 86,86,86,86 | 0 |
| 57 | MG | 1a | 1675 | 1/1 | 0.62 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3679 | 1/1 | 0.62 | 0.24 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3967 | 1/1 | 0.62 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3605 | 1/1 | 0.62 | 0.14 | 70,70,70,70 | 0 |
| 57 | MG | 2A | 3607 | 1/1 | 0.63 | 0.16 | 60,60,60,60 | 0 |
| 57 | MG | 2A | 3648 | 1/1 | 0.63 | 0.35 | 76,76,76,76 | 0 |
| 57 | MG | 1a | 1629 | 1/1 | 0.63 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3529 | 1/1 | 0.63 | 0.26 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3297 | 1/1 | 0.63 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | 1B | 212 | 1/1 | 0.64 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3553 | 1/1 | 0.64 | 0.42 | 62,62,62,62 | 0 |
| 57 | MG | 2a | 1626 | 1/1 | 0.65 | 0.13 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2a | 1640 | 1/1 | 0.65 | 0.29 | 76,76,76,76 | 0 |
| 57 | MG | 1A | 3973 | 1/1 | 0.65 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3656 | 1/1 | 0.65 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3259 | 1/1 | 0.65 | 0.26 | 71,71,71,71 | 0 |
| 57 | MG | 2A | 3168 | 1/1 | 0.65 | 0.20 | 67,67,67,67 | 0 |
| 57 | MG | 2v | 101 | 1/1 | 0.65 | 0.19 | 77,77,77,77 | 0 |
| 57 | MG | 2A | 3615 | 1/1 | 0.65 | 0.16 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3466 | 1/1 | 0.66 | 0.11 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3696 | 1/1 | 0.66 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3986 | 1/1 | 0.66 | 0.12 | 60,60,60,60 | 0 |
| 57 | MG | 1B | 234 | 1/1 | 0.66 | 0.14 | 67,67,67,67 | 0 |
| 57 | MG | 1b | 302 | 1/1 | 0.66 | 0.11 | 80,80,80,80 | 0 |
| 57 | MG | 1A | 3338 | 1/1 | 0.66 | 0.36 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3917 | 1/1 | 0.67 | 0.22 | 56,56,56,56 | 0 |
| 57 | MG | 2a | 1742 | 1/1 | 0.67 | 0.32 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3481 | 1/1 | 0.67 | 0.15 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3538 | 1/1 | 0.67 | 0.16 | 65,65,65,65 | 0 |
| 57 | MG | 1U | 209 | 1/1 | 0.67 | 0.20 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1621 | 1/1 | 0.68 | 0.14 | 78,78,78,78 | 0 |
| 57 | MG | 1a | 1788 | 1/1 | 0.68 | 0.31 | 85,85,85,85 | 0 |
| 57 | MG | 2a | 1629 | 1/1 | 0.68 | 0.18 | 74,74,74,74 | 0 |
| 57 | MG | 1a | 1678 | 1/1 | 0.68 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3355 | 1/1 | 0.68 | 0.21 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3100 | 1/1 | 0.68 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | 2A | 3719 | 1/1 | 0.68 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 1E | 314 | 1/1 | 0.68 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | 2B | 206 | 1/1 | 0.68 | 0.20 | 68,68,68,68 | 0 |
| 57 | MG | 28 | 103 | 1/1 | 0.68 | 0.17 | 75,75,75,75 | 0 |
| 57 | MG | 1A | 3692 | 1/1 | 0.68 | 0.24 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3409 | 1/1 | 0.69 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | 1w | 101 | 1/1 | 0.69 | 0.17 | 76,76,76,76 | 0 |
| 57 | MG | 2a | 1722 | 1/1 | 0.69 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3188 | 1/1 | 0.69 | 0.20 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 4031 | 1/1 | 0.69 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3552 | 1/1 | 0.69 | 0.20 | 79,79,79,79 | 0 |
| 57 | MG | 2A | 3684 | 1/1 | 0.69 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3404 | 1/1 | 0.70 | 0.10 | 67,67,67,67 | 0 |
| 57 | MG | 1f | 201 | 1/1 | 0.70 | 0.21 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3293 | 1/1 | 0.70 | 0.28 | 53,53,53,53 | 0 |
| 57 | MG | 1a | 1721 | 1/1 | 0.70 | 0.19 | 81,81,81,81 | 0 |
| 57 | MG | 1A | 4063 | 1/1 | 0.70 | 0.23 | 70,70,70,70 | 0 |
| 57 | MG | 2A | 3446 | 1/1 | 0.71 | 0.30 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3149 | 1/1 | 0.71 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3601 | 1/1 | 0.71 | 0.19 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3761 | 1/1 | 0.71 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | 18 | 3405 | 1/1 | 0.71 | 0.25 | 48,48,48,48 | 0 |
| 57 | MG | 1a | 1676 | 1/1 | 0.71 | 0.30 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3232 | 1/1 | 0.71 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 4101 | 1/1 | 0.72 | 0.20 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3952 | 1/1 | 0.72 | 0.11 | 51,51,51,51 | 0 |
| 57 | MG | 1a | 1615 | 1/1 | 0.72 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3265 | 1/1 | 0.72 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3575 | 1/1 | 0.72 | 0.12 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3005 | 1/1 | 0.72 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | 2a | 1687 | 1/1 | 0.72 | 0.14 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3459 | 1/1 | 0.72 | 0.16 | 70,70,70,70 | 0 |
| 57 | MG | 2A | 3496 | 1/1 | 0.72 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3778 | 1/1 | 0.72 | 0.19 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3370 | 1/1 | 0.72 | 0.26 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3811 | 1/1 | 0.72 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1760 | 1/1 | 0.73 | 0.09 | 80,80,80,80 | 0 |
| 57 | MG | 2A | 3039 | 1/1 | 0.73 | 0.24 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3075 | 1/1 | 0.73 | 0.23 | 65,65,65,65 | 0 |
| 57 | MG | 1a | 1781 | 1/1 | 0.73 | 0.13 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 3728 | 1/1 | 0.73 | 0.08 | 63,63,63,63 | 0 |
| 57 | MG | 2a | 1693 | 1/1 | 0.73 | 0.20 | 78,78,78,78 | 0 |
| 57 | MG | 2a | 1714 | 1/1 | 0.73 | 0.15 | 74,74,74,74 | 0 |
| 57 | MG | 1A | 3508 | 1/1 | 0.73 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | 1E | 301 | 1/1 | 0.73 | 0.21 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3232 | 1/1 | 0.73 | 0.17 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3057 | 1/1 | 0.73 | 0.22 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3722 | 1/1 | 0.73 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3640 | 1/1 | 0.74 | 0.14 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3243 | 1/1 | 0.74 | 0.23 | 52,52,52,52 | 0 |
| 57 | MG | 2a | 1644 | 1/1 | 0.74 | 0.21 | 61,61,61,61 | 0 |
| 57 | MG | 1a | 1717 | 1/1 | 0.74 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3415 | 1/1 | 0.74 | 0.15 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3442 | 1/1 | 0.74 | 0.17 | 69,69,69,69 | 0 |
| 57 | MG | 1E | 303 | 1/1 | 0.74 | 0.46 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3408 | 1/1 | 0.74 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3266 | 1/1 | 0.74 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3876 | 1/1 | 0.74 | 0.35 | 57,57,57,57 | 0 |
| 57 | MG | 1y | 101 | 1/1 | 0.74 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3934 | 1/1 | 0.74 | 0.10 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3028 | 1/1 | 0.74 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3378 | 1/1 | 0.74 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | 1a | 1693 | 1/1 | 0.75 | 0.15 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3703 | 1/1 | 0.75 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | 1B | 230 | 1/1 | 0.75 | 0.12 | 75,75,75,75 | 0 |
| 57 | MG | 1a | 1660 | 1/1 | 0.75 | 0.10 | 65,65,65,65 | 0 |
| 57 | MG | 1w | 105 | 1/1 | 0.75 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | 1x | 114 | 1/1 | 0.75 | 0.16 | 70,70,70,70 | 0 |
| 57 | MG | 2A | 3524 | 1/1 | 0.75 | 0.17 | 72,72,72,72 | 0 |
| 57 | MG | 1a | 1758 | 1/1 | 0.75 | 0.45 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3255 | 1/1 | 0.75 | 0.32 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3819 | 1/1 | 0.75 | 0.20 | 58,58,58,58 | 0 |
| 57 | MG | 2a | 1780 | 1/1 | 0.75 | 0.11 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3489 | 1/1 | 0.75 | 0.17 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3445 | 1/1 | 0.75 | 0.19 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 4046 | 1/1 | 0.76 | 0.33 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 4015 | 1/1 | 0.76 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3052 | 1/1 | 0.76 | 0.18 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3053 | 1/1 | 0.76 | 0.26 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3276 | 1/1 | 0.76 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 1a | 1734 | 1/1 | 0.76 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | 1l | 201 | 1/1 | 0.76 | 0.24 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3518 | 1/1 | 0.76 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1741 | 1/1 | 0.76 | 0.13 | 79,79,79,79 | 0 |
| 57 | MG | 2A | 3368 | 1/1 | 0.76 | 0.28 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3977 | 1/1 | 0.76 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3169 | 1/1 | 0.76 | 0.26 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3692 | 1/1 | 0.76 | 0.24 | 71,71,71,71 | 0 |
| 57 | MG | 2A | 3205 | 1/1 | 0.76 | 0.15 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3226 | 1/1 | 0.76 | 0.32 | 74,74,74,74 | 0 |
| 57 | MG | 2a | 1762 | 1/1 | 0.76 | 0.30 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3756 | 1/1 | 0.76 | 0.21 | 63,63,63,63 | 0 |
| 57 | MG | 1O | 201 | 1/1 | 0.76 | 0.43 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3569 | 1/1 | 0.76 | 0.14 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3016 | 1/1 | 0.77 | 0.29 | 56,56,56,56 | 0 |
| 57 | MG | 1a | 1786 | 1/1 | 0.77 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3768 | 1/1 | 0.77 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | 1a | 1669 | 1/1 | 0.77 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3047 | 1/1 | 0.77 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3399 | 1/1 | 0.77 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 4065 | 1/1 | 0.77 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3065 | 1/1 | 0.77 | 0.11 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2a | 1604 | 1/1 | 0.77 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3993 | 1/1 | 0.77 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3638 | 1/1 | 0.77 | 0.14 | 67,67,67,67 | 0 |
| 57 | MG | 1a | 1683 | 1/1 | 0.77 | 0.13 | 72,72,72,72 | 0 |
| 57 | MG | 1B | 204 | 1/1 | 0.77 | 0.35 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3158 | 1/1 | 0.77 | 0.12 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 4038 | 1/1 | 0.78 | 0.36 | 57,57,57,57 | 0 |
| 57 | MG | 2B | 203 | 1/1 | 0.78 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3093 | 1/1 | 0.78 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3170 | 1/1 | 0.78 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3175 | 1/1 | 0.78 | 0.18 | 71,71,71,71 | 0 |
| 57 | MG | 1a | 1779 | 1/1 | 0.78 | 0.15 | 55,55,55,55 | 0 |
| 57 | MG | 1y | 102 | 1/1 | 0.78 | 0.15 | 88,88,88,88 | 0 |
| 57 | MG | 2A | 3209 | 1/1 | 0.78 | 0.16 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3210 | 1/1 | 0.78 | 0.15 | 69,69,69,69 | 0 |
| 57 | MG | 2A | 3581 | 1/1 | 0.78 | 0.16 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3223 | 1/1 | 0.78 | 0.14 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3330 | 1/1 | 0.78 | 0.38 | 52,52,52,52 | 0 |
| 57 | MG | 1B | 224 | 1/1 | 0.78 | 0.24 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 3208 | 1/1 | 0.78 | 0.24 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 4050 | 1/1 | 0.78 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 1a | 1811 | 1/1 | 0.78 | 0.11 | 67,67,67,67 | 0 |
| 57 | MG | 1a | 1817 | 1/1 | 0.78 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 4056 | 1/1 | 0.78 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | 2a | 1727 | 1/1 | 0.78 | 0.17 | 71,71,71,71 | 0 |
| 57 | MG | 2A | 3663 | 1/1 | 0.78 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1651 | 1/1 | 0.78 | 0.15 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3519 | 1/1 | 0.78 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3313 | 1/1 | 0.78 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3550 | 1/1 | 0.78 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3365 | 1/1 | 0.78 | 0.30 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3966 | 1/1 | 0.79 | 0.15 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3703 | 1/1 | 0.79 | 0.21 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3711 | 1/1 | 0.79 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3537 | 1/1 | 0.79 | 0.13 | 60,60,60,60 | 0 |
| 57 | MG | 2A | 3309 | 1/1 | 0.79 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3102 | 1/1 | 0.79 | 0.11 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3476 | 1/1 | 0.79 | 0.26 | 70,70,70,70 | 0 |
| 57 | MG | 2B | 217 | 1/1 | 0.79 | 0.11 | 76,76,76,76 | 0 |
| 57 | MG | 2A | 3350 | 1/1 | 0.79 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3298 | 1/1 | 0.79 | 0.27 | 51,51,51,51 | 0 |
| 57 | MG | 1x | 108 | 1/1 | 0.79 | 0.17 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1x | 113 | 1/1 | 0.79 | 0.14 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3438 | 1/1 | 0.79 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3396 | 1/1 | 0.79 | 0.19 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 4061 | 1/1 | 0.79 | 0.13 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3268 | 1/1 | 0.79 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3001 | 1/1 | 0.79 | 0.29 | 57,57,57,57 | 0 |
| 57 | MG | 2a | 1650 | 1/1 | 0.79 | 0.12 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3434 | 1/1 | 0.79 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3509 | 1/1 | 0.79 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | 2a | 1680 | 1/1 | 0.79 | 0.11 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 4098 | 1/1 | 0.79 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | 2a | 1692 | 1/1 | 0.79 | 0.17 | 74,74,74,74 | 0 |
| 57 | MG | 1A | 3466 | 1/1 | 0.79 | 0.29 | 49,49,49,49 | 0 |
| 57 | MG | 1B | 203 | 1/1 | 0.79 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | 2a | 1717 | 1/1 | 0.79 | 0.15 | 75,75,75,75 | 0 |
| 57 | MG | 2A | 3048 | 1/1 | 0.79 | 0.15 | 63,63,63,63 | 0 |
| 57 | MG | 13 | 103 | 1/1 | 0.79 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 1a | 1698 | 1/1 | 0.79 | 0.30 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3658 | 1/1 | 0.79 | 0.05 | 75,75,75,75 | 0 |
| 57 | MG | 1A | 3525 | 1/1 | 0.79 | 0.18 | 49,49,49,49 | 0 |
| 57 | MG | 1a | 1610 | 1/1 | 0.79 | 0.25 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3095 | 1/1 | 0.79 | 0.23 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3532 | 1/1 | 0.79 | 0.12 | 78,78,78,78 | 0 |
| 57 | MG | 2A | 3562 | 1/1 | 0.80 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3422 | 1/1 | 0.80 | 0.11 | 62,62,62,62 | 0 |
| 57 | MG | 1m | 3001 | 1/1 | 0.80 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3957 | 1/1 | 0.80 | 0.09 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3342 | 1/1 | 0.80 | 0.36 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3961 | 1/1 | 0.80 | 0.06 | 52,52,52,52 | 0 |
| 57 | MG | 2a | 1622 | 1/1 | 0.80 | 0.19 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3582 | 1/1 | 0.80 | 0.14 | 75,75,75,75 | 0 |
| 57 | MG | 1A | 3183 | 1/1 | 0.80 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 3202 | 1/1 | 0.80 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 4030 | 1/1 | 0.80 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | 1F | 308 | 1/1 | 0.80 | 0.33 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3635 | 1/1 | 0.80 | 0.32 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 4095 | 1/1 | 0.80 | 0.29 | 66,66,66,66 | 0 |
| 57 | MG | 1O | 204 | 1/1 | 0.80 | 0.20 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3198 | 1/1 | 0.80 | 0.15 | 68,68,68,68 | 0 |
| 57 | MG | 2a | 1681 | 1/1 | 0.80 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3650 | 1/1 | 0.80 | 0.07 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3356 | 1/1 | 0.80 | 0.11 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3591 | 1/1 | 0.80 | 0.33 | 57,57,57,57 | 0 |
| 57 | MG | 2a | 1702 | 1/1 | 0.80 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | 2a | 1703 | 1/1 | 0.80 | 0.19 | 65,65,65,65 | 0 |
| 57 | MG | 1a | 1691 | 1/1 | 0.80 | 0.19 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3540 | 1/1 | 0.80 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3543 | 1/1 | 0.80 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3371 | 1/1 | 0.80 | 0.37 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3372 | 1/1 | 0.80 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1816 | 1/1 | 0.80 | 0.06 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3092 | 1/1 | 0.80 | 0.15 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3655 | 1/1 | 0.80 | 0.20 | 33,33,33,33 | 0 |
| 57 | MG | 2a | 1784 | 1/1 | 0.80 | 0.24 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 3869 | 1/1 | 0.80 | 0.13 | 48,48,48,48 | 0 |
| 59 | ZN | 14 | 102 | 1/1 | 0.80 | 0.05 | 97,97,97,97 | 0 |
| 57 | MG | 1A | 3295 | 1/1 | 0.80 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | 2a | 1620 | 1/1 | 0.81 | 0.11 | 79,79,79,79 | 0 |
| 57 | MG | 1A | 4019 | 1/1 | 0.81 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3583 | 1/1 | 0.81 | 0.22 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3160 | 1/1 | 0.81 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3484 | 1/1 | 0.81 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | 2a | 1636 | 1/1 | 0.81 | 0.07 | 81,81,81,81 | 0 |
| 57 | MG | 2A | 3004 | 1/1 | 0.81 | 0.28 | 68,68,68,68 | 0 |
| 57 | MG | 1B | 207 | 1/1 | 0.81 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3632 | 1/1 | 0.81 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 2a | 1649 | 1/1 | 0.81 | 0.19 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3506 | 1/1 | 0.81 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3191 | 1/1 | 0.81 | 0.24 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3496 | 1/1 | 0.81 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3040 | 1/1 | 0.81 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3203 | 1/1 | 0.81 | 0.21 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3673 | 1/1 | 0.81 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3235 | 1/1 | 0.81 | 0.15 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3050 | 1/1 | 0.81 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3481 | 1/1 | 0.81 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 4045 | 1/1 | 0.81 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | 1x | 102 | 1/1 | 0.81 | 0.17 | 33,33,33,33 | 0 |
| 57 | MG | 2A | 3407 | 1/1 | 0.81 | 0.13 | 69,69,69,69 | 0 |
| 57 | MG | 1a | 1692 | 1/1 | 0.81 | 0.13 | 74,74,74,74 | 0 |
| 57 | MG | 1A | 3562 | 1/1 | 0.81 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3460 | 1/1 | 0.81 | 0.69 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3260 | 1/1 | 0.81 | 0.12 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3563 | 1/1 | 0.81 | 0.11 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1a | 1791 | 1/1 | 0.81 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3121 | 1/1 | 0.81 | 0.28 | 67,67,67,67 | 0 |
| 57 | MG | 1a | 1650 | 1/1 | 0.81 | 0.42 | 64,64,64,64 | 0 |
| 57 | MG | 2x | 102 | 1/1 | 0.81 | 0.17 | 77,77,77,77 | 0 |
| 57 | MG | 2x | 103 | 1/1 | 0.81 | 0.17 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3449 | 1/1 | 0.81 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3286 | 1/1 | 0.81 | 0.26 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 4025 | 1/1 | 0.82 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3021 | 1/1 | 0.82 | 0.12 | 70,70,70,70 | 0 |
| 57 | MG | 1a | 1771 | 1/1 | 0.82 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3724 | 1/1 | 0.82 | 0.33 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3521 | 1/1 | 0.82 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | 1a | 1637 | 1/1 | 0.82 | 0.18 | 76,76,76,76 | 0 |
| 57 | MG | 2B | 201 | 1/1 | 0.82 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3061 | 1/1 | 0.82 | 0.26 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3269 | 1/1 | 0.82 | 0.13 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3535 | 1/1 | 0.82 | 0.09 | 59,59,59,59 | 0 |
| 57 | MG | 2F | 301 | 1/1 | 0.82 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | 28 | 102 | 1/1 | 0.82 | 0.27 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3420 | 1/1 | 0.82 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3284 | 1/1 | 0.82 | 0.26 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3542 | 1/1 | 0.82 | 0.22 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3924 | 1/1 | 0.82 | 0.21 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3548 | 1/1 | 0.82 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3304 | 1/1 | 0.82 | 0.34 | 70,70,70,70 | 0 |
| 57 | MG | 1a | 1809 | 1/1 | 0.82 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | 2a | 1627 | 1/1 | 0.82 | 0.19 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3064 | 1/1 | 0.82 | 0.12 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3090 | 1/1 | 0.82 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3074 | 1/1 | 0.82 | 0.17 | 55,55,55,55 | 0 |
| 57 | MG | 1a | 1813 | 1/1 | 0.82 | 0.08 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3555 | 1/1 | 0.82 | 0.28 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3212 | 1/1 | 0.82 | 0.31 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3997 | 1/1 | 0.82 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | 2a | 1657 | 1/1 | 0.82 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3103 | 1/1 | 0.82 | 0.13 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3163 | 1/1 | 0.82 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | 2a | 1672 | 1/1 | 0.82 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 4058 | 1/1 | 0.82 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3946 | 1/1 | 0.82 | 0.07 | 53,53,53,53 | 0 |
| 57 | MG | 1t | 201 | 1/1 | 0.82 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3719 | 1/1 | 0.82 | 0.16 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1w | 103 | 1/1 | 0.82 | 0.10 | 63,63,63,63 | 0 |
| 57 | MG | 1w | 104 | 1/1 | 0.82 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | 2A | 3187 | 1/1 | 0.82 | 0.16 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3426 | 1/1 | 0.82 | 0.10 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3628 | 1/1 | 0.82 | 0.13 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3837 | 1/1 | 0.82 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | 1a | 1708 | 1/1 | 0.82 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1713 | 1/1 | 0.82 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 4088 | 1/1 | 0.82 | 0.17 | 64,64,64,64 | 0 |
| 57 | MG | 1Z | 3702 | 1/1 | 0.82 | 0.17 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 3847 | 1/1 | 0.82 | 0.27 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3651 | 1/1 | 0.82 | 0.17 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3455 | 1/1 | 0.82 | 0.13 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3597 | 1/1 | 0.82 | 0.10 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3470 | 1/1 | 0.82 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 1a | 1605 | 1/1 | 0.82 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 4100 | 1/1 | 0.82 | 0.19 | 62,62,62,62 | 0 |
| 57 | MG | 25 | 101 | 1/1 | 0.83 | 0.15 | 59,59,59,59 | 0 |
| 57 | MG | 26 | 101 | 1/1 | 0.83 | 0.16 | 61,61,61,61 | 0 |
| 57 | MG | 1a | 1763 | 1/1 | 0.83 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | 1a | 1769 | 1/1 | 0.83 | 0.09 | 57,57,57,57 | 0 |
| 57 | MG | 2a | 1602 | 1/1 | 0.83 | 0.08 | 71,71,71,71 | 0 |
| 57 | MG | 2a | 1603 | 1/1 | 0.83 | 0.13 | 65,65,65,65 | 0 |
| 57 | MG | 1a | 1640 | 1/1 | 0.83 | 0.07 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3212 | 1/1 | 0.83 | 0.20 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3214 | 1/1 | 0.83 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 4044 | 1/1 | 0.83 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3062 | 1/1 | 0.83 | 0.25 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3731 | 1/1 | 0.83 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | 1a | 1659 | 1/1 | 0.83 | 0.11 | 74,74,74,74 | 0 |
| 57 | MG | 1A | 3277 | 1/1 | 0.83 | 0.35 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3254 | 1/1 | 0.83 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | 2a | 1637 | 1/1 | 0.83 | 0.12 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 3467 | 1/1 | 0.83 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | 1a | 1797 | 1/1 | 0.83 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3414 | 1/1 | 0.83 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 2a | 1648 | 1/1 | 0.83 | 0.24 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3666 | 1/1 | 0.83 | 0.17 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3777 | 1/1 | 0.83 | 0.24 | 31,31,31,31 | 0 |
| 57 | MG | 2a | 1654 | 1/1 | 0.83 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | 2a | 1655 | 1/1 | 0.83 | 0.09 | 73,73,73,73 | 0 |
| 57 | MG | 1a | 1681 | 1/1 | 0.83 | 0.49 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3942 | 1/1 | 0.83 | 0.15 | 49,49,49,49 | 0 |
| 57 | MG | 1b | 301 | 1/1 | 0.83 | 0.47 | 80,80,80,80 | 0 |
| 57 | MG | 1A | 3531 | 1/1 | 0.83 | 0.20 | 69,69,69,69 | 0 |
| 57 | MG | 2a | 1676 | 1/1 | 0.83 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 4074 | 1/1 | 0.83 | 0.29 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3653 | 1/1 | 0.83 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3343 | 1/1 | 0.83 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3525 | 1/1 | 0.83 | 0.21 | 84,84,84,84 | 0 |
| 57 | MG | 1A | 3542 | 1/1 | 0.83 | 0.22 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3547 | 1/1 | 0.83 | 0.28 | 52,52,52,52 | 0 |
| 57 | MG | 1a | 1709 | 1/1 | 0.83 | 0.16 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3351 | 1/1 | 0.83 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3436 | 1/1 | 0.83 | 0.14 | 77,77,77,77 | 0 |
| 57 | MG | 1A | 3437 | 1/1 | 0.83 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3308 | 1/1 | 0.83 | 0.16 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3264 | 1/1 | 0.83 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | 1a | 1623 | 1/1 | 0.83 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | 2a | 1754 | 1/1 | 0.83 | 0.29 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3730 | 1/1 | 0.83 | 0.33 | 66,66,66,66 | 0 |
| 57 | MG | 2a | 1765 | 1/1 | 0.83 | 0.32 | 68,68,68,68 | 0 |
| 57 | MG | 2a | 1778 | 1/1 | 0.83 | 0.11 | 72,72,72,72 | 0 |
| 57 | MG | 1a | 1736 | 1/1 | 0.83 | 0.27 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3895 | 1/1 | 0.83 | 0.19 | 35,35,35,35 | 0 |
| 57 | MG | 2l | 203 | 1/1 | 0.83 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | 2B | 204 | 1/1 | 0.83 | 0.29 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3395 | 1/1 | 0.83 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | 1B | 208 | 1/1 | 0.83 | 0.36 | 59,59,59,59 | 0 |
| 57 | MG | 1a | 1638 | 1/1 | 0.83 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | 20 | 101 | 1/1 | 0.83 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3561 | 1/1 | 0.84 | 0.12 | 73,73,73,73 | 0 |
| 57 | MG | 2A | 3178 | 1/1 | 0.84 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | 1a | 1804 | 1/1 | 0.84 | 0.10 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3844 | 1/1 | 0.84 | 0.12 | 33,33,33,33 | 0 |
| 57 | MG | 2a | 1612 | 1/1 | 0.84 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3845 | 1/1 | 0.84 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | 2a | 1617 | 1/1 | 0.84 | 0.19 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3758 | 1/1 | 0.84 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3589 | 1/1 | 0.84 | 0.27 | 58,58,58,58 | 0 |
| 57 | MG | 1S | 203 | 1/1 | 0.84 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | 1a | 1824 | 1/1 | 0.84 | 0.08 | 79,79,79,79 | 0 |
| 57 | MG | 1A | 3428 | 1/1 | 0.84 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3600 | 1/1 | 0.84 | 0.14 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3049 | 1/1 | 0.84 | 0.20 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3676 | 1/1 | 0.84 | 0.22 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3437 | 1/1 | 0.84 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3440 | 1/1 | 0.84 | 0.13 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3617 | 1/1 | 0.84 | 0.20 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3051 | 1/1 | 0.84 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | 1Z | 3701 | 1/1 | 0.84 | 0.22 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3454 | 1/1 | 0.84 | 0.17 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3055 | 1/1 | 0.84 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3253 | 1/1 | 0.84 | 0.24 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3906 | 1/1 | 0.84 | 0.28 | 46,46,46,46 | 0 |
| 57 | MG | 15 | 108 | 1/1 | 0.84 | 0.27 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3066 | 1/1 | 0.84 | 0.27 | 51,51,51,51 | 0 |
| 57 | MG | 2a | 1665 | 1/1 | 0.84 | 0.21 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3261 | 1/1 | 0.84 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3787 | 1/1 | 0.84 | 0.09 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3375 | 1/1 | 0.84 | 0.31 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3085 | 1/1 | 0.84 | 0.11 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3667 | 1/1 | 0.84 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3088 | 1/1 | 0.84 | 0.10 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3094 | 1/1 | 0.84 | 0.07 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3648 | 1/1 | 0.84 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3287 | 1/1 | 0.84 | 0.30 | 48,48,48,48 | 0 |
| 57 | MG | 2a | 1707 | 1/1 | 0.84 | 0.09 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 3970 | 1/1 | 0.84 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | 1a | 1618 | 1/1 | 0.84 | 0.10 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3307 | 1/1 | 0.84 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | 1x | 103 | 1/1 | 0.84 | 0.12 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3114 | 1/1 | 0.84 | 0.13 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3319 | 1/1 | 0.84 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | 1x | 105 | 1/1 | 0.84 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3820 | 1/1 | 0.84 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | 1a | 1696 | 1/1 | 0.84 | 0.21 | 72,72,72,72 | 0 |
| 57 | MG | 1a | 1787 | 1/1 | 0.84 | 0.08 | 57,57,57,57 | 0 |
| 57 | MG | 2a | 1779 | 1/1 | 0.84 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3166 | 1/1 | 0.84 | 0.45 | 59,59,59,59 | 0 |
| 57 | MG | 2Q | 201 | 1/1 | 0.84 | 0.15 | 53,53,53,53 | 0 |
| 57 | MG | 2X | 101 | 1/1 | 0.84 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | 2Z | 301 | 1/1 | 0.84 | 0.15 | 76,76,76,76 | 0 |
| 57 | MG | 2x | 101 | 1/1 | 0.84 | 0.16 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3366 | 1/1 | 0.84 | 0.28 | 68,68,68,68 | 0 |
| 57 | MG | 1a | 1697 | 1/1 | 0.84 | 0.14 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3332 | 1/1 | 0.84 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | 1a | 1702 | 1/1 | 0.84 | 0.21 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 4013 | 1/1 | 0.85 | 0.15 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3107 | 1/1 | 0.85 | 0.08 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3891 | 1/1 | 0.85 | 0.12 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3343 | 1/1 | 0.85 | 0.25 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3349 | 1/1 | 0.85 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3116 | 1/1 | 0.85 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3469 | 1/1 | 0.85 | 0.25 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3354 | 1/1 | 0.85 | 0.12 | 71,71,71,71 | 0 |
| 57 | MG | 2a | 1610 | 1/1 | 0.85 | 0.07 | 73,73,73,73 | 0 |
| 57 | MG | 2A | 3133 | 1/1 | 0.85 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3138 | 1/1 | 0.85 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3565 | 1/1 | 0.85 | 0.12 | 75,75,75,75 | 0 |
| 57 | MG | 2A | 3567 | 1/1 | 0.85 | 0.09 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3145 | 1/1 | 0.85 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3263 | 1/1 | 0.85 | 0.30 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 4023 | 1/1 | 0.85 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3416 | 1/1 | 0.85 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3559 | 1/1 | 0.85 | 0.26 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3089 | 1/1 | 0.85 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | 1U | 202 | 1/1 | 0.85 | 0.27 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3586 | 1/1 | 0.85 | 0.15 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3589 | 1/1 | 0.85 | 0.26 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3590 | 1/1 | 0.85 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3422 | 1/1 | 0.85 | 0.15 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 4037 | 1/1 | 0.85 | 0.51 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3344 | 1/1 | 0.85 | 0.38 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3595 | 1/1 | 0.85 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | 10 | 106 | 1/1 | 0.85 | 0.06 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3355 | 1/1 | 0.85 | 0.22 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3164 | 1/1 | 0.85 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3431 | 1/1 | 0.85 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3625 | 1/1 | 0.85 | 0.14 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3435 | 1/1 | 0.85 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3950 | 1/1 | 0.85 | 0.19 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3635 | 1/1 | 0.85 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3638 | 1/1 | 0.85 | 0.11 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3216 | 1/1 | 0.85 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3641 | 1/1 | 0.85 | 0.17 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3374 | 1/1 | 0.85 | 0.43 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3448 | 1/1 | 0.85 | 0.44 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3238 | 1/1 | 0.85 | 0.19 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 4071 | 1/1 | 0.85 | 0.10 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3827 | 1/1 | 0.85 | 0.20 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3476 | 1/1 | 0.85 | 0.22 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3689 | 1/1 | 0.85 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3378 | 1/1 | 0.85 | 0.22 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3535 | 1/1 | 0.85 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3289 | 1/1 | 0.85 | 0.24 | 48,48,48,48 | 0 |
| 57 | MG | 1a | 1808 | 1/1 | 0.85 | 0.07 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3165 | 1/1 | 0.85 | 0.22 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3849 | 1/1 | 0.85 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3989 | 1/1 | 0.85 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3696 | 1/1 | 0.85 | 0.25 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3082 | 1/1 | 0.85 | 0.24 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3994 | 1/1 | 0.85 | 0.26 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 3861 | 1/1 | 0.85 | 0.26 | 35,35,35,35 | 0 |
| 57 | MG | 2B | 212 | 1/1 | 0.85 | 0.08 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3341 | 1/1 | 0.85 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3706 | 1/1 | 0.85 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3306 | 1/1 | 0.85 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 1a | 1684 | 1/1 | 0.85 | 0.11 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3880 | 1/1 | 0.85 | 0.30 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3514 | 1/1 | 0.86 | 0.42 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3492 | 1/1 | 0.86 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3596 | 1/1 | 0.86 | 0.23 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3690 | 1/1 | 0.86 | 0.10 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3273 | 1/1 | 0.86 | 0.18 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1602 | 1/1 | 0.86 | 0.09 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 4028 | 1/1 | 0.86 | 0.08 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3863 | 1/1 | 0.86 | 0.10 | 50,50,50,50 | 0 |
| 57 | MG | 1r | 101 | 1/1 | 0.86 | 0.14 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3962 | 1/1 | 0.86 | 0.21 | 80,80,80,80 | 0 |
| 57 | MG | 2A | 3299 | 1/1 | 0.86 | 0.32 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3302 | 1/1 | 0.86 | 0.29 | 64,64,64,64 | 0 |
| 57 | MG | 1v | 101 | 1/1 | 0.86 | 0.20 | 71,71,71,71 | 0 |
| 57 | MG | 2A | 3305 | 1/1 | 0.86 | 0.45 | 67,67,67,67 | 0 |
| 57 | MG | 1a | 1616 | 1/1 | 0.86 | 0.11 | 63,63,63,63 | 0 |
| 57 | MG | 1a | 1720 | 1/1 | 0.86 | 0.13 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3964 | 1/1 | 0.86 | 0.23 | 43,43,43,43 | 0 |
| 57 | MG | 1a | 1728 | 1/1 | 0.86 | 0.19 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3128 | 1/1 | 0.86 | 0.22 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3337 | 1/1 | 0.86 | 0.18 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3307 | 1/1 | 0.86 | 0.26 | 63,63,63,63 | 0 |
| 57 | MG | 1a | 1624 | 1/1 | 0.86 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3765 | 1/1 | 0.86 | 0.07 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3230 | 1/1 | 0.86 | 0.19 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3151 | 1/1 | 0.86 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3570 | 1/1 | 0.86 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 1x | 110 | 1/1 | 0.86 | 0.13 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3775 | 1/1 | 0.86 | 0.18 | 34,34,34,34 | 0 |
| 57 | MG | 1B | 236 | 1/1 | 0.86 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3699 | 1/1 | 0.86 | 0.19 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3258 | 1/1 | 0.86 | 0.23 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3174 | 1/1 | 0.86 | 0.13 | 60,60,60,60 | 0 |
| 57 | MG | 1y | 104 | 1/1 | 0.86 | 0.19 | 87,87,87,87 | 0 |
| 57 | MG | 1A | 3471 | 1/1 | 0.86 | 0.13 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3179 | 1/1 | 0.86 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3596 | 1/1 | 0.86 | 0.14 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3184 | 1/1 | 0.86 | 0.31 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3792 | 1/1 | 0.86 | 0.21 | 53,53,53,53 | 0 |
| 57 | MG | 1F | 312 | 1/1 | 0.86 | 0.19 | 56,56,56,56 | 0 |
| 57 | MG | 2a | 1659 | 1/1 | 0.86 | 0.12 | 62,62,62,62 | 0 |
| 57 | MG | 2a | 1660 | 1/1 | 0.86 | 0.09 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3194 | 1/1 | 0.86 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3197 | 1/1 | 0.86 | 0.18 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3407 | 1/1 | 0.86 | 0.15 | 45,45,45,45 | 0 |
| 57 | MG | 2a | 1673 | 1/1 | 0.86 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3619 | 1/1 | 0.86 | 0.13 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3202 | 1/1 | 0.86 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3022 | 1/1 | 0.86 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3527 | 1/1 | 0.86 | 0.17 | 47,47,47,47 | 0 |
| 57 | MG | 1R | 201 | 1/1 | 0.86 | 0.34 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3560 | 1/1 | 0.86 | 0.25 | 63,63,63,63 | 0 |
| 57 | MG | 2a | 1696 | 1/1 | 0.86 | 0.33 | 66,66,66,66 | 0 |
| 57 | MG | 1a | 1793 | 1/1 | 0.86 | 0.06 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3348 | 1/1 | 0.86 | 0.21 | 58,58,58,58 | 0 |
| 57 | MG | 2a | 1704 | 1/1 | 0.86 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | 1a | 1803 | 1/1 | 0.86 | 0.19 | 68,68,68,68 | 0 |
| 57 | MG | 2a | 1711 | 1/1 | 0.86 | 0.14 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 3410 | 1/1 | 0.86 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3224 | 1/1 | 0.86 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | 1W | 201 | 1/1 | 0.86 | 0.36 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3659 | 1/1 | 0.86 | 0.07 | 77,77,77,77 | 0 |
| 57 | MG | 2A | 3662 | 1/1 | 0.86 | 0.17 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3230 | 1/1 | 0.86 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | 1a | 1690 | 1/1 | 0.86 | 0.20 | 74,74,74,74 | 0 |
| 57 | MG | 2a | 1757 | 1/1 | 0.86 | 0.08 | 59,59,59,59 | 0 |
| 57 | MG | 2a | 1759 | 1/1 | 0.86 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3680 | 1/1 | 0.86 | 0.07 | 69,69,69,69 | 0 |
| 57 | MG | 2A | 3460 | 1/1 | 0.86 | 0.12 | 73,73,73,73 | 0 |
| 57 | MG | 2a | 1767 | 1/1 | 0.86 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 2a | 1770 | 1/1 | 0.86 | 0.20 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3842 | 1/1 | 0.86 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3469 | 1/1 | 0.86 | 0.22 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3461 | 1/1 | 0.86 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3693 | 1/1 | 0.86 | 0.04 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3058 | 1/1 | 0.86 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | 1a | 1814 | 1/1 | 0.86 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3255 | 1/1 | 0.86 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3743 | 1/1 | 0.86 | 0.08 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3752 | 1/1 | 0.86 | 0.23 | 21,21,21,21 | 0 |
| 57 | MG | 1a | 1818 | 1/1 | 0.86 | 0.05 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3512 | 1/1 | 0.86 | 0.23 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 4078 | 1/1 | 0.87 | 0.16 | 28,28,28,28 | 0 |
| 57 | MG | 2a | 1601 | 1/1 | 0.87 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3180 | 1/1 | 0.87 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3182 | 1/1 | 0.87 | 0.19 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3888 | 1/1 | 0.87 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | 2a | 1609 | 1/1 | 0.87 | 0.12 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 4090 | 1/1 | 0.87 | 0.24 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3017 | 1/1 | 0.87 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3189 | 1/1 | 0.87 | 0.28 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3193 | 1/1 | 0.87 | 0.08 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 4093 | 1/1 | 0.87 | 0.19 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3196 | 1/1 | 0.87 | 0.28 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3988 | 1/1 | 0.87 | 0.13 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3319 | 1/1 | 0.87 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3674 | 1/1 | 0.87 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3250 | 1/1 | 0.87 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | 2a | 1631 | 1/1 | 0.87 | 0.08 | 64,64,64,64 | 0 |
| 57 | MG | 2a | 1633 | 1/1 | 0.87 | 0.19 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3593 | 1/1 | 0.87 | 0.07 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3043 | 1/1 | 0.87 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3913 | 1/1 | 0.87 | 0.21 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3417 | 1/1 | 0.87 | 0.16 | 35,35,35,35 | 0 |
| 57 | MG | 1a | 1789 | 1/1 | 0.87 | 0.06 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 4000 | 1/1 | 0.87 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | 2A | 3613 | 1/1 | 0.87 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | 1a | 1643 | 1/1 | 0.87 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | 2A | 3433 | 1/1 | 0.87 | 0.09 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3051 | 1/1 | 0.87 | 0.24 | 42,42,42,42 | 0 |
| 57 | MG | 1a | 1802 | 1/1 | 0.87 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3689 | 1/1 | 0.87 | 0.28 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3292 | 1/1 | 0.87 | 0.17 | 60,60,60,60 | 0 |
| 57 | MG | 2A | 3637 | 1/1 | 0.87 | 0.09 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3227 | 1/1 | 0.87 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3781 | 1/1 | 0.87 | 0.18 | 16,16,16,16 | 0 |
| 57 | MG | 2a | 1669 | 1/1 | 0.87 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3231 | 1/1 | 0.87 | 0.10 | 65,65,65,65 | 0 |
| 57 | MG | 1a | 1664 | 1/1 | 0.87 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | 1B | 229 | 1/1 | 0.87 | 0.14 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3500 | 1/1 | 0.87 | 0.50 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3572 | 1/1 | 0.87 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | 2a | 1684 | 1/1 | 0.87 | 0.09 | 76,76,76,76 | 0 |
| 57 | MG | 1A | 3502 | 1/1 | 0.87 | 0.33 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3207 | 1/1 | 0.87 | 0.22 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3945 | 1/1 | 0.87 | 0.16 | 60,60,60,60 | 0 |
| 57 | MG | 1a | 1819 | 1/1 | 0.87 | 0.12 | 56,56,56,56 | 0 |
| 57 | MG | 1E | 313 | 1/1 | 0.87 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3064 | 1/1 | 0.87 | 0.17 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3107 | 1/1 | 0.87 | 0.53 | 34,34,34,34 | 0 |
| 57 | MG | 2a | 1705 | 1/1 | 0.87 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3718 | 1/1 | 0.87 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | 1I | 201 | 1/1 | 0.87 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3305 | 1/1 | 0.87 | 0.18 | 29,29,29,29 | 0 |
| 57 | MG | 2A | 3279 | 1/1 | 0.87 | 0.21 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 4035 | 1/1 | 0.87 | 0.13 | 80,80,80,80 | 0 |
| 57 | MG | 1A | 3955 | 1/1 | 0.87 | 0.15 | 25,25,25,25 | 0 |
| 57 | MG | 2a | 1728 | 1/1 | 0.87 | 0.20 | 64,64,64,64 | 0 |
| 57 | MG | 2a | 1730 | 1/1 | 0.87 | 0.33 | 72,72,72,72 | 0 |
| 57 | MG | 2a | 1739 | 1/1 | 0.87 | 0.32 | 75,75,75,75 | 0 |
| 57 | MG | 2A | 3120 | 1/1 | 0.87 | 0.23 | 70,70,70,70 | 0 |
| 57 | MG | 2a | 1743 | 1/1 | 0.87 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | 2a | 1747 | 1/1 | 0.87 | 0.33 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3245 | 1/1 | 0.87 | 0.34 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3958 | 1/1 | 0.87 | 0.15 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3269 | 1/1 | 0.87 | 0.33 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3310 | 1/1 | 0.87 | 0.38 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3366 | 1/1 | 0.87 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3373 | 1/1 | 0.87 | 0.21 | 60,60,60,60 | 0 |
| 57 | MG | 1a | 1719 | 1/1 | 0.87 | 0.08 | 60,60,60,60 | 0 |
| 57 | MG | 2a | 1769 | 1/1 | 0.87 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3965 | 1/1 | 0.87 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3747 | 1/1 | 0.87 | 0.21 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3480 | 1/1 | 0.87 | 0.24 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3320 | 1/1 | 0.87 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | 2T | 202 | 1/1 | 0.87 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3969 | 1/1 | 0.87 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3435 | 1/1 | 0.87 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3482 | 1/1 | 0.87 | 0.23 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3346 | 1/1 | 0.87 | 0.27 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3878 | 1/1 | 0.87 | 0.17 | 41,41,41,41 | 0 |
| 57 | MG | 2x | 104 | 1/1 | 0.87 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | 27 | 101 | 1/1 | 0.87 | 0.24 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3670 | 1/1 | 0.87 | 0.18 | 24,24,24,24 | 0 |
| 57 | MG | 1B | 233 | 1/1 | 0.88 | 0.16 | 73,73,73,73 | 0 |
| 57 | MG | 2G | 201 | 1/1 | 0.88 | 0.10 | 76,76,76,76 | 0 |
| 57 | MG | 1A | 3312 | 1/1 | 0.88 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3251 | 1/1 | 0.88 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3900 | 1/1 | 0.88 | 0.14 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 4007 | 1/1 | 0.88 | 0.11 | 39,39,39,39 | 0 |
| 57 | MG | 1y | 103 | 1/1 | 0.88 | 0.37 | 77,77,77,77 | 0 |
| 57 | MG | 1A | 3904 | 1/1 | 0.88 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | 1a | 1712 | 1/1 | 0.88 | 0.07 | 79,79,79,79 | 0 |
| 57 | MG | 2A | 3003 | 1/1 | 0.88 | 0.28 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3320 | 1/1 | 0.88 | 0.21 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3517 | 1/1 | 0.88 | 0.28 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3114 | 1/1 | 0.88 | 0.38 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 4017 | 1/1 | 0.88 | 0.19 | 23,23,23,23 | 0 |
| 57 | MG | 1A | 3457 | 1/1 | 0.88 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3558 | 1/1 | 0.88 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3238 | 1/1 | 0.88 | 0.33 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3926 | 1/1 | 0.88 | 0.23 | 41,41,41,41 | 0 |
| 57 | MG | 1Q | 204 | 1/1 | 0.88 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1729 | 1/1 | 0.88 | 0.35 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 4026 | 1/1 | 0.88 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3271 | 1/1 | 0.88 | 0.27 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3256 | 1/1 | 0.88 | 0.39 | 75,75,75,75 | 0 |
| 57 | MG | 2A | 3258 | 1/1 | 0.88 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1625 | 1/1 | 0.88 | 0.28 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1a | 1738 | 1/1 | 0.88 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3767 | 1/1 | 0.88 | 0.28 | 50,50,50,50 | 0 |
| 57 | MG | 1a | 1744 | 1/1 | 0.88 | 0.15 | 67,67,67,67 | 0 |
| 57 | MG | 1a | 1751 | 1/1 | 0.88 | 0.08 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1754 | 1/1 | 0.88 | 0.17 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3131 | 1/1 | 0.88 | 0.28 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3561 | 1/1 | 0.88 | 0.15 | 55,55,55,55 | 0 |
| 57 | MG | 2a | 1638 | 1/1 | 0.88 | 0.22 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3340 | 1/1 | 0.88 | 0.33 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3059 | 1/1 | 0.88 | 0.20 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3062 | 1/1 | 0.88 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3938 | 1/1 | 0.88 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3004 | 1/1 | 0.88 | 0.12 | 26,26,26,26 | 0 |
| 57 | MG | 1a | 1778 | 1/1 | 0.88 | 0.13 | 64,64,64,64 | 0 |
| 57 | MG | 10 | 105 | 1/1 | 0.88 | 0.28 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3574 | 1/1 | 0.88 | 0.34 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3079 | 1/1 | 0.88 | 0.38 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 4043 | 1/1 | 0.88 | 0.11 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3785 | 1/1 | 0.88 | 0.06 | 36,36,36,36 | 0 |
| 57 | MG | 18 | 3403 | 1/1 | 0.88 | 0.25 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3091 | 1/1 | 0.88 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3092 | 1/1 | 0.88 | 0.22 | 47,47,47,47 | 0 |
| 57 | MG | 2a | 1666 | 1/1 | 0.88 | 0.08 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3314 | 1/1 | 0.88 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3691 | 1/1 | 0.88 | 0.12 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3579 | 1/1 | 0.88 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3598 | 1/1 | 0.88 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | 1a | 1603 | 1/1 | 0.88 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 4048 | 1/1 | 0.88 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3694 | 1/1 | 0.88 | 0.13 | 36,36,36,36 | 0 |
| 57 | MG | 1a | 1612 | 1/1 | 0.88 | 0.14 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3111 | 1/1 | 0.88 | 0.18 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3813 | 1/1 | 0.88 | 0.11 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1694 | 1/1 | 0.88 | 0.07 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 4054 | 1/1 | 0.88 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3119 | 1/1 | 0.88 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3583 | 1/1 | 0.88 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3427 | 1/1 | 0.88 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3365 | 1/1 | 0.88 | 0.24 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3700 | 1/1 | 0.88 | 0.21 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3522 | 1/1 | 0.88 | 0.34 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3840 | 1/1 | 0.88 | 0.15 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 4069 | 1/1 | 0.88 | 0.14 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 3290 | 1/1 | 0.88 | 0.17 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3708 | 1/1 | 0.88 | 0.21 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3155 | 1/1 | 0.88 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3470 | 1/1 | 0.88 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | 2a | 1732 | 1/1 | 0.88 | 0.28 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 4080 | 1/1 | 0.88 | 0.15 | 52,52,52,52 | 0 |
| 57 | MG | 1a | 1827 | 1/1 | 0.88 | 0.33 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 3429 | 1/1 | 0.88 | 0.21 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3434 | 1/1 | 0.88 | 0.75 | 52,52,52,52 | 0 |
| 57 | MG | 1e | 202 | 1/1 | 0.88 | 0.25 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3609 | 1/1 | 0.88 | 0.43 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3681 | 1/1 | 0.88 | 0.24 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3177 | 1/1 | 0.88 | 0.21 | 60,60,60,60 | 0 |
| 57 | MG | 2a | 1760 | 1/1 | 0.88 | 0.22 | 54,54,54,54 | 0 |
| 57 | MG | 2a | 1761 | 1/1 | 0.88 | 0.22 | 59,59,59,59 | 0 |
| 57 | MG | 1a | 1663 | 1/1 | 0.88 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3613 | 1/1 | 0.88 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3615 | 1/1 | 0.88 | 0.19 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3389 | 1/1 | 0.88 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3870 | 1/1 | 0.88 | 0.07 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3735 | 1/1 | 0.88 | 0.19 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3182 | 1/1 | 0.88 | 0.20 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3990 | 1/1 | 0.88 | 0.16 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3992 | 1/1 | 0.88 | 0.05 | 68,68,68,68 | 0 |
| 57 | MG | 2l | 201 | 1/1 | 0.88 | 0.10 | 70,70,70,70 | 0 |
| 57 | MG | 2A | 3729 | 1/1 | 0.88 | 0.22 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3879 | 1/1 | 0.88 | 0.21 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3451 | 1/1 | 0.88 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3745 | 1/1 | 0.88 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | 1x | 104 | 1/1 | 0.88 | 0.27 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3746 | 1/1 | 0.88 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3462 | 1/1 | 0.88 | 0.07 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3889 | 1/1 | 0.88 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3077 | 1/1 | 0.89 | 0.15 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3556 | 1/1 | 0.89 | 0.31 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3327 | 1/1 | 0.89 | 0.27 | 45,45,45,45 | 0 |
| 57 | MG | 1a | 1662 | 1/1 | 0.89 | 0.15 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3770 | 1/1 | 0.89 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3531 | 1/1 | 0.89 | 0.08 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3002 | 1/1 | 0.89 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | 1a | 1666 | 1/1 | 0.89 | 0.14 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3272 | 1/1 | 0.89 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3405 | 1/1 | 0.89 | 0.60 | 46,46,46,46 | 0 |
| 57 | MG | 1a | 1673 | 1/1 | 0.89 | 0.10 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3920 | 1/1 | 0.89 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | 2a | 1608 | 1/1 | 0.89 | 0.10 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3493 | 1/1 | 0.89 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3451 | 1/1 | 0.89 | 0.33 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3106 | 1/1 | 0.89 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | 1a | 1829 | 1/1 | 0.89 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3929 | 1/1 | 0.89 | 0.15 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3452 | 1/1 | 0.89 | 0.37 | 36,36,36,36 | 0 |
| 57 | MG | 1d | 301 | 1/1 | 0.89 | 0.20 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3361 | 1/1 | 0.89 | 0.22 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3507 | 1/1 | 0.89 | 0.20 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3933 | 1/1 | 0.89 | 0.14 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3799 | 1/1 | 0.89 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3809 | 1/1 | 0.89 | 0.13 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3810 | 1/1 | 0.89 | 0.09 | 36,36,36,36 | 0 |
| 57 | MG | 1G | 203 | 1/1 | 0.89 | 0.15 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3455 | 1/1 | 0.89 | 0.13 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3362 | 1/1 | 0.89 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | 1a | 1703 | 1/1 | 0.89 | 0.20 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3342 | 1/1 | 0.89 | 0.45 | 60,60,60,60 | 0 |
| 57 | MG | 1a | 1706 | 1/1 | 0.89 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | 1O | 203 | 1/1 | 0.89 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3514 | 1/1 | 0.89 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3948 | 1/1 | 0.89 | 0.12 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3275 | 1/1 | 0.89 | 0.30 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 4039 | 1/1 | 0.89 | 0.07 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3520 | 1/1 | 0.89 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3133 | 1/1 | 0.89 | 0.31 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3360 | 1/1 | 0.89 | 0.32 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3367 | 1/1 | 0.89 | 0.21 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3419 | 1/1 | 0.89 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | 1a | 1725 | 1/1 | 0.89 | 0.08 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3369 | 1/1 | 0.89 | 0.42 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3143 | 1/1 | 0.89 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3621 | 1/1 | 0.89 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3730 | 1/1 | 0.89 | 0.08 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3384 | 1/1 | 0.89 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | 2a | 1674 | 1/1 | 0.89 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3622 | 1/1 | 0.89 | 0.11 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2a | 1679 | 1/1 | 0.89 | 0.11 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3534 | 1/1 | 0.89 | 0.14 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3190 | 1/1 | 0.89 | 0.31 | 40,40,40,40 | 0 |
| 57 | MG | 2a | 1683 | 1/1 | 0.89 | 0.28 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3397 | 1/1 | 0.89 | 0.11 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3636 | 1/1 | 0.89 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3170 | 1/1 | 0.89 | 0.18 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3015 | 1/1 | 0.89 | 0.27 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3195 | 1/1 | 0.89 | 0.17 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3414 | 1/1 | 0.89 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 2a | 1698 | 1/1 | 0.89 | 0.07 | 62,62,62,62 | 0 |
| 57 | MG | 2a | 1699 | 1/1 | 0.89 | 0.13 | 73,73,73,73 | 0 |
| 57 | MG | 2A | 3649 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3179 | 1/1 | 0.89 | 0.18 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3416 | 1/1 | 0.89 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3867 | 1/1 | 0.89 | 0.22 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3246 | 1/1 | 0.89 | 0.39 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3642 | 1/1 | 0.89 | 0.16 | 23,23,23,23 | 0 |
| 57 | MG | 1a | 1604 | 1/1 | 0.89 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3660 | 1/1 | 0.89 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3543 | 1/1 | 0.89 | 0.25 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3748 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3975 | 1/1 | 0.89 | 0.24 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3668 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3673 | 1/1 | 0.89 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | 2a | 1736 | 1/1 | 0.89 | 0.24 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3211 | 1/1 | 0.89 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | 2a | 1740 | 1/1 | 0.89 | 0.33 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3652 | 1/1 | 0.89 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | 2A | 3682 | 1/1 | 0.89 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3478 | 1/1 | 0.89 | 0.28 | 60,60,60,60 | 0 |
| 57 | MG | 2a | 1751 | 1/1 | 0.89 | 0.31 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 4081 | 1/1 | 0.89 | 0.16 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3218 | 1/1 | 0.89 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1755 | 1/1 | 0.89 | 0.23 | 60,60,60,60 | 0 |
| 57 | MG | 1a | 1782 | 1/1 | 0.89 | 0.09 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 4082 | 1/1 | 0.89 | 0.21 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3225 | 1/1 | 0.89 | 0.13 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3987 | 1/1 | 0.89 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3706 | 1/1 | 0.89 | 0.28 | 56,56,56,56 | 0 |
| 57 | MG | 2a | 1764 | 1/1 | 0.89 | 0.30 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3661 | 1/1 | 0.89 | 0.14 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3056 | 1/1 | 0.89 | 0.12 | 47,47,47,47 | 0 |
| 57 | MG | 1a | 1630 | 1/1 | 0.89 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3130 | 1/1 | 0.89 | 0.16 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3237 | 1/1 | 0.89 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3472 | 1/1 | 0.89 | 0.18 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3390 | 1/1 | 0.89 | 0.26 | 45,45,45,45 | 0 |
| 57 | MG | 2a | 1781 | 1/1 | 0.89 | 0.14 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3477 | 1/1 | 0.89 | 0.21 | 65,65,65,65 | 0 |
| 57 | MG | 2B | 205 | 1/1 | 0.89 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3893 | 1/1 | 0.89 | 0.22 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3244 | 1/1 | 0.89 | 0.18 | 65,65,65,65 | 0 |
| 57 | MG | 2B | 216 | 1/1 | 0.89 | 0.22 | 75,75,75,75 | 0 |
| 57 | MG | 1A | 3396 | 1/1 | 0.89 | 0.42 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3896 | 1/1 | 0.89 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3067 | 1/1 | 0.89 | 0.11 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 4103 | 1/1 | 0.89 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3995 | 1/1 | 0.89 | 0.08 | 44,44,44,44 | 0 |
| 57 | MG | 1B | 228 | 1/1 | 0.90 | 0.36 | 73,73,73,73 | 0 |
| 57 | MG | 2A | 3071 | 1/1 | 0.90 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3843 | 1/1 | 0.90 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3482 | 1/1 | 0.90 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3483 | 1/1 | 0.90 | 0.19 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3325 | 1/1 | 0.90 | 0.27 | 52,52,52,52 | 0 |
| 57 | MG | 1a | 1810 | 1/1 | 0.90 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3491 | 1/1 | 0.90 | 0.08 | 70,70,70,70 | 0 |
| 57 | MG | 2A | 3493 | 1/1 | 0.90 | 0.15 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 4027 | 1/1 | 0.90 | 0.41 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3500 | 1/1 | 0.90 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | 20 | 102 | 1/1 | 0.90 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3479 | 1/1 | 0.90 | 0.16 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3083 | 1/1 | 0.90 | 0.20 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3622 | 1/1 | 0.90 | 0.20 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3537 | 1/1 | 0.90 | 0.17 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3055 | 1/1 | 0.90 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3520 | 1/1 | 0.90 | 0.21 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3026 | 1/1 | 0.90 | 0.27 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3121 | 1/1 | 0.90 | 0.25 | 38,38,38,38 | 0 |
| 57 | MG | 1a | 1823 | 1/1 | 0.90 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3544 | 1/1 | 0.90 | 0.28 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3275 | 1/1 | 0.90 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | 1F | 309 | 1/1 | 0.90 | 0.26 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3749 | 1/1 | 0.90 | 0.15 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3960 | 1/1 | 0.90 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3539 | 1/1 | 0.90 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | 2a | 1619 | 1/1 | 0.90 | 0.22 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3247 | 1/1 | 0.90 | 0.36 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3874 | 1/1 | 0.90 | 0.23 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3288 | 1/1 | 0.90 | 0.31 | 60,60,60,60 | 0 |
| 57 | MG | 2a | 1623 | 1/1 | 0.90 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3113 | 1/1 | 0.90 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3545 | 1/1 | 0.90 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3963 | 1/1 | 0.90 | 0.11 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3010 | 1/1 | 0.90 | 0.16 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 3549 | 1/1 | 0.90 | 0.26 | 65,65,65,65 | 0 |
| 57 | MG | 1l | 202 | 1/1 | 0.90 | 0.09 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3094 | 1/1 | 0.90 | 0.28 | 34,34,34,34 | 0 |
| 57 | MG | 1S | 202 | 1/1 | 0.90 | 0.19 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3132 | 1/1 | 0.90 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3398 | 1/1 | 0.90 | 0.16 | 67,67,67,67 | 0 |
| 57 | MG | 2a | 1641 | 1/1 | 0.90 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3881 | 1/1 | 0.90 | 0.14 | 29,29,29,29 | 0 |
| 57 | MG | 2A | 3316 | 1/1 | 0.90 | 0.27 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3318 | 1/1 | 0.90 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3886 | 1/1 | 0.90 | 0.26 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3147 | 1/1 | 0.90 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3321 | 1/1 | 0.90 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3324 | 1/1 | 0.90 | 0.28 | 61,61,61,61 | 0 |
| 57 | MG | 2a | 1656 | 1/1 | 0.90 | 0.15 | 84,84,84,84 | 0 |
| 57 | MG | 2A | 3329 | 1/1 | 0.90 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3216 | 1/1 | 0.90 | 0.50 | 40,40,40,40 | 0 |
| 57 | MG | 1Y | 202 | 1/1 | 0.90 | 0.28 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3557 | 1/1 | 0.90 | 0.26 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3157 | 1/1 | 0.90 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3219 | 1/1 | 0.90 | 0.18 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3301 | 1/1 | 0.90 | 0.45 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3591 | 1/1 | 0.90 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | 2a | 1670 | 1/1 | 0.90 | 0.08 | 63,63,63,63 | 0 |
| 57 | MG | 2a | 1671 | 1/1 | 0.90 | 0.19 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3164 | 1/1 | 0.90 | 0.21 | 61,61,61,61 | 0 |
| 57 | MG | 1Z | 3703 | 1/1 | 0.90 | 0.25 | 52,52,52,52 | 0 |
| 57 | MG | 1a | 1718 | 1/1 | 0.90 | 0.13 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 4067 | 1/1 | 0.90 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3505 | 1/1 | 0.90 | 0.23 | 34,34,34,34 | 0 |
| 57 | MG | 1x | 111 | 1/1 | 0.90 | 0.09 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 10 | 107 | 1/1 | 0.90 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3608 | 1/1 | 0.90 | 0.08 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 4070 | 1/1 | 0.90 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3345 | 1/1 | 0.90 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | 2a | 1688 | 1/1 | 0.90 | 0.09 | 62,62,62,62 | 0 |
| 57 | MG | 17 | 103 | 1/1 | 0.90 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3259 | 1/1 | 0.90 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3779 | 1/1 | 0.90 | 0.26 | 26,26,26,26 | 0 |
| 57 | MG | 2A | 3624 | 1/1 | 0.90 | 0.15 | 76,76,76,76 | 0 |
| 57 | MG | 2A | 3625 | 1/1 | 0.90 | 0.17 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3627 | 1/1 | 0.90 | 0.14 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3373 | 1/1 | 0.90 | 0.18 | 62,62,62,62 | 0 |
| 57 | MG | 18 | 3406 | 1/1 | 0.90 | 0.37 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3224 | 1/1 | 0.90 | 0.22 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3386 | 1/1 | 0.90 | 0.18 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3573 | 1/1 | 0.90 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | 2a | 1709 | 1/1 | 0.90 | 0.11 | 78,78,78,78 | 0 |
| 57 | MG | 2a | 1710 | 1/1 | 0.90 | 0.16 | 59,59,59,59 | 0 |
| 57 | MG | 1a | 1746 | 1/1 | 0.90 | 0.22 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3192 | 1/1 | 0.90 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3643 | 1/1 | 0.90 | 0.08 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3399 | 1/1 | 0.90 | 0.11 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3358 | 1/1 | 0.90 | 0.33 | 82,82,82,82 | 0 |
| 57 | MG | 1A | 4086 | 1/1 | 0.90 | 0.31 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3408 | 1/1 | 0.90 | 0.16 | 48,48,48,48 | 0 |
| 57 | MG | 1a | 1757 | 1/1 | 0.90 | 0.26 | 73,73,73,73 | 0 |
| 57 | MG | 2A | 3410 | 1/1 | 0.90 | 0.14 | 63,63,63,63 | 0 |
| 57 | MG | 2a | 1737 | 1/1 | 0.90 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3518 | 1/1 | 0.90 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3026 | 1/1 | 0.90 | 0.23 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3463 | 1/1 | 0.90 | 0.18 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3037 | 1/1 | 0.90 | 0.27 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3097 | 1/1 | 0.90 | 0.19 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3424 | 1/1 | 0.90 | 0.17 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 4094 | 1/1 | 0.90 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3429 | 1/1 | 0.90 | 0.09 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3677 | 1/1 | 0.90 | 0.07 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3679 | 1/1 | 0.90 | 0.11 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3042 | 1/1 | 0.90 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3102 | 1/1 | 0.90 | 0.29 | 42,42,42,42 | 0 |
| 57 | MG | 1a | 1777 | 1/1 | 0.90 | 0.08 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 4096 | 1/1 | 0.90 | 0.28 | 54,54,54,54 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3593 | 1/1 | 0.90 | 0.19 | 34,34,34,34 | 0 |
| 57 | MG | 1a | 1627 | 1/1 | 0.90 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3233 | 1/1 | 0.90 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | 2a | 1768 | 1/1 | 0.90 | 0.12 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3147 | 1/1 | 0.90 | 0.16 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3274 | 1/1 | 0.90 | 0.22 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3697 | 1/1 | 0.90 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3601 | 1/1 | 0.90 | 0.42 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3530 | 1/1 | 0.90 | 0.23 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3707 | 1/1 | 0.90 | 0.22 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3708 | 1/1 | 0.90 | 0.11 | 56,56,56,56 | 0 |
| 57 | MG | 2a | 1785 | 1/1 | 0.90 | 0.11 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3936 | 1/1 | 0.90 | 0.23 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3937 | 1/1 | 0.90 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | 2q | 202 | 1/1 | 0.90 | 0.13 | 75,75,75,75 | 0 |
| 57 | MG | 2A | 3061 | 1/1 | 0.90 | 0.13 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3461 | 1/1 | 0.90 | 0.09 | 65,65,65,65 | 0 |
| 57 | MG | 1a | 1645 | 1/1 | 0.90 | 0.13 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3236 | 1/1 | 0.90 | 0.15 | 63,63,63,63 | 0 |
| 57 | MG | 1a | 1647 | 1/1 | 0.90 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3322 | 1/1 | 0.90 | 0.15 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3533 | 1/1 | 0.90 | 0.12 | 81,81,81,81 | 0 |
| 57 | MG | 1A | 3771 | 1/1 | 0.91 | 0.22 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3720 | 1/1 | 0.91 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3152 | 1/1 | 0.91 | 0.23 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3158 | 1/1 | 0.91 | 0.11 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3620 | 1/1 | 0.91 | 0.16 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3450 | 1/1 | 0.91 | 0.11 | 44,44,44,44 | 0 |
| 57 | MG | 1a | 1665 | 1/1 | 0.91 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3199 | 1/1 | 0.91 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3201 | 1/1 | 0.91 | 0.18 | 77,77,77,77 | 0 |
| 57 | MG | 1A | 3511 | 1/1 | 0.91 | 0.11 | 64,64,64,64 | 0 |
| 57 | MG | 2B | 211 | 1/1 | 0.91 | 0.29 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3956 | 1/1 | 0.91 | 0.24 | 26,26,26,26 | 0 |
| 57 | MG | 2B | 213 | 1/1 | 0.91 | 0.23 | 64,64,64,64 | 0 |
| 57 | MG | 2B | 214 | 1/1 | 0.91 | 0.23 | 70,70,70,70 | 0 |
| 57 | MG | 1a | 1672 | 1/1 | 0.91 | 0.21 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3425 | 1/1 | 0.91 | 0.11 | 40,40,40,40 | 0 |
| 57 | MG | 2B | 218 | 1/1 | 0.91 | 0.22 | 64,64,64,64 | 0 |
| 57 | MG | 2E | 303 | 1/1 | 0.91 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3006 | 1/1 | 0.91 | 0.21 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3786 | 1/1 | 0.91 | 0.15 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3634 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3284 | 1/1 | 0.91 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | 2W | 201 | 1/1 | 0.91 | 0.27 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3794 | 1/1 | 0.91 | 0.17 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3072 | 1/1 | 0.91 | 0.30 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3433 | 1/1 | 0.91 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | 1B | 206 | 1/1 | 0.91 | 0.27 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3008 | 1/1 | 0.91 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3485 | 1/1 | 0.91 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3010 | 1/1 | 0.91 | 0.22 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3086 | 1/1 | 0.91 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3234 | 1/1 | 0.91 | 0.43 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3495 | 1/1 | 0.91 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3649 | 1/1 | 0.91 | 0.21 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3115 | 1/1 | 0.91 | 0.22 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3235 | 1/1 | 0.91 | 0.23 | 60,60,60,60 | 0 |
| 57 | MG | 2a | 1606 | 1/1 | 0.91 | 0.12 | 71,71,71,71 | 0 |
| 57 | MG | 1B | 226 | 1/1 | 0.91 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3513 | 1/1 | 0.91 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3653 | 1/1 | 0.91 | 0.12 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3825 | 1/1 | 0.91 | 0.20 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3241 | 1/1 | 0.91 | 0.17 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3038 | 1/1 | 0.91 | 0.21 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3116 | 1/1 | 0.91 | 0.19 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3246 | 1/1 | 0.91 | 0.15 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3247 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3529 | 1/1 | 0.91 | 0.25 | 73,73,73,73 | 0 |
| 57 | MG | 2A | 3248 | 1/1 | 0.91 | 0.49 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3172 | 1/1 | 0.91 | 0.13 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3664 | 1/1 | 0.91 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3981 | 1/1 | 0.91 | 0.11 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3532 | 1/1 | 0.91 | 0.11 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 3439 | 1/1 | 0.91 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3444 | 1/1 | 0.91 | 0.25 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3118 | 1/1 | 0.91 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3846 | 1/1 | 0.91 | 0.23 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3364 | 1/1 | 0.91 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3018 | 1/1 | 0.91 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3687 | 1/1 | 0.91 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 3856 | 1/1 | 0.91 | 0.11 | 55,55,55,55 | 0 |
| 57 | MG | 1N | 205 | 1/1 | 0.91 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3554 | 1/1 | 0.91 | 0.17 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3539 | 1/1 | 0.91 | 0.17 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3128 | 1/1 | 0.91 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3557 | 1/1 | 0.91 | 0.06 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3187 | 1/1 | 0.91 | 0.09 | 44,44,44,44 | 0 |
| 57 | MG | 1P | 205 | 1/1 | 0.91 | 0.40 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3280 | 1/1 | 0.91 | 0.08 | 58,58,58,58 | 0 |
| 57 | MG | 1Q | 203 | 1/1 | 0.91 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3368 | 1/1 | 0.91 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 4004 | 1/1 | 0.91 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | 2a | 1661 | 1/1 | 0.91 | 0.17 | 71,71,71,71 | 0 |
| 57 | MG | 2A | 3068 | 1/1 | 0.91 | 0.18 | 29,29,29,29 | 0 |
| 57 | MG | 2A | 3069 | 1/1 | 0.91 | 0.14 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3571 | 1/1 | 0.91 | 0.09 | 66,66,66,66 | 0 |
| 57 | MG | 2a | 1667 | 1/1 | 0.91 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | 1a | 1753 | 1/1 | 0.91 | 0.11 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3005 | 1/1 | 0.91 | 0.17 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3872 | 1/1 | 0.91 | 0.19 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3076 | 1/1 | 0.91 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 4012 | 1/1 | 0.91 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3371 | 1/1 | 0.91 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | 1a | 1762 | 1/1 | 0.91 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3588 | 1/1 | 0.91 | 0.25 | 71,71,71,71 | 0 |
| 57 | MG | 1V | 202 | 1/1 | 0.91 | 0.25 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3257 | 1/1 | 0.91 | 0.19 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3087 | 1/1 | 0.91 | 0.12 | 70,70,70,70 | 0 |
| 57 | MG | 2A | 3592 | 1/1 | 0.91 | 0.08 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3550 | 1/1 | 0.91 | 0.32 | 47,47,47,47 | 0 |
| 57 | MG | 1a | 1776 | 1/1 | 0.91 | 0.18 | 70,70,70,70 | 0 |
| 57 | MG | 2a | 1689 | 1/1 | 0.91 | 0.19 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3701 | 1/1 | 0.91 | 0.20 | 23,23,23,23 | 0 |
| 57 | MG | 1A | 3313 | 1/1 | 0.91 | 0.29 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3554 | 1/1 | 0.91 | 0.30 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3882 | 1/1 | 0.91 | 0.16 | 34,34,34,34 | 0 |
| 57 | MG | 10 | 103 | 1/1 | 0.91 | 0.12 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3338 | 1/1 | 0.91 | 0.51 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3340 | 1/1 | 0.91 | 0.31 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3707 | 1/1 | 0.91 | 0.18 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3316 | 1/1 | 0.91 | 0.27 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3058 | 1/1 | 0.91 | 0.30 | 54,54,54,54 | 0 |
| 57 | MG | 13 | 102 | 1/1 | 0.91 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3384 | 1/1 | 0.91 | 0.21 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3388 | 1/1 | 0.91 | 0.24 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3060 | 1/1 | 0.91 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3321 | 1/1 | 0.91 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3899 | 1/1 | 0.91 | 0.21 | 25,25,25,25 | 0 |
| 57 | MG | 2A | 3633 | 1/1 | 0.91 | 0.09 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3395 | 1/1 | 0.91 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3126 | 1/1 | 0.91 | 0.18 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3903 | 1/1 | 0.91 | 0.15 | 23,23,23,23 | 0 |
| 57 | MG | 1A | 3034 | 1/1 | 0.91 | 0.12 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3209 | 1/1 | 0.91 | 0.18 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3733 | 1/1 | 0.91 | 0.13 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3645 | 1/1 | 0.91 | 0.06 | 47,47,47,47 | 0 |
| 57 | MG | 1a | 1607 | 1/1 | 0.91 | 0.27 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3915 | 1/1 | 0.91 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3734 | 1/1 | 0.91 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3326 | 1/1 | 0.91 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3152 | 1/1 | 0.91 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3049 | 1/1 | 0.91 | 0.29 | 32,32,32,32 | 0 |
| 57 | MG | 1a | 1617 | 1/1 | 0.91 | 0.10 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3483 | 1/1 | 0.91 | 0.27 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 4053 | 1/1 | 0.91 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3487 | 1/1 | 0.91 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | 1a | 1625 | 1/1 | 0.91 | 0.26 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3666 | 1/1 | 0.91 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3402 | 1/1 | 0.91 | 0.30 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3149 | 1/1 | 0.91 | 0.44 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3331 | 1/1 | 0.91 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1633 | 1/1 | 0.91 | 0.24 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3176 | 1/1 | 0.91 | 0.36 | 42,42,42,42 | 0 |
| 57 | MG | 1a | 1634 | 1/1 | 0.91 | 0.16 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3218 | 1/1 | 0.91 | 0.39 | 39,39,39,39 | 0 |
| 57 | MG | 2a | 1776 | 1/1 | 0.91 | 0.13 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3333 | 1/1 | 0.91 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3420 | 1/1 | 0.91 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3411 | 1/1 | 0.91 | 0.24 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3599 | 1/1 | 0.91 | 0.15 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3690 | 1/1 | 0.91 | 0.10 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3334 | 1/1 | 0.91 | 0.11 | 51,51,51,51 | 0 |
| 57 | MG | 2d | 301 | 1/1 | 0.91 | 0.25 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3428 | 1/1 | 0.91 | 0.21 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3185 | 1/1 | 0.91 | 0.13 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3336 | 1/1 | 0.91 | 0.25 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3941 | 1/1 | 0.91 | 0.06 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3273 | 1/1 | 0.91 | 0.22 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3610 | 1/1 | 0.91 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 1a | 1653 | 1/1 | 0.91 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3710 | 1/1 | 0.91 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3611 | 1/1 | 0.91 | 0.31 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3715 | 1/1 | 0.91 | 0.11 | 68,68,68,68 | 0 |
| 59 | ZN | 2n | 501 | 1/1 | 0.91 | 0.07 | 95,95,95,95 | 0 |
| 61 | K | 2A | 3330 | 1/1 | 0.91 | 0.23 | 75,75,75,75 | 0 |
| 57 | MG | 2A | 3292 | 1/1 | 0.92 | 0.33 | 49,49,49,49 | 0 |
| 57 | MG | 2R | 201 | 1/1 | 0.92 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3423 | 1/1 | 0.92 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3295 | 1/1 | 0.92 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3125 | 1/1 | 0.92 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3300 | 1/1 | 0.92 | 0.34 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3536 | 1/1 | 0.92 | 0.10 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3506 | 1/1 | 0.92 | 0.13 | 41,41,41,41 | 0 |
| 57 | MG | 20 | 103 | 1/1 | 0.92 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | 23 | 102 | 1/1 | 0.92 | 0.13 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3127 | 1/1 | 0.92 | 0.24 | 66,66,66,66 | 0 |
| 57 | MG | 13 | 104 | 1/1 | 0.92 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | 1w | 102 | 1/1 | 0.92 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | 1a | 1710 | 1/1 | 0.92 | 0.17 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3308 | 1/1 | 0.92 | 0.09 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3919 | 1/1 | 0.92 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3143 | 1/1 | 0.92 | 0.14 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3714 | 1/1 | 0.92 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3552 | 1/1 | 0.92 | 0.39 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3349 | 1/1 | 0.92 | 0.33 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3150 | 1/1 | 0.92 | 0.23 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3148 | 1/1 | 0.92 | 0.48 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3720 | 1/1 | 0.92 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | 2a | 1611 | 1/1 | 0.92 | 0.11 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3154 | 1/1 | 0.92 | 0.13 | 41,41,41,41 | 0 |
| 57 | MG | 2a | 1614 | 1/1 | 0.92 | 0.07 | 56,56,56,56 | 0 |
| 57 | MG | 1x | 106 | 1/1 | 0.92 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3019 | 1/1 | 0.92 | 0.21 | 43,43,43,43 | 0 |
| 57 | MG | 2a | 1618 | 1/1 | 0.92 | 0.15 | 73,73,73,73 | 0 |
| 57 | MG | 1B | 202 | 1/1 | 0.92 | 0.35 | 61,61,61,61 | 0 |
| 57 | MG | 1a | 1723 | 1/1 | 0.92 | 0.13 | 38,38,38,38 | 0 |
| 57 | MG | 1x | 112 | 1/1 | 0.92 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3210 | 1/1 | 0.92 | 0.11 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3167 | 1/1 | 0.92 | 0.08 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3176 | 1/1 | 0.92 | 0.19 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3572 | 1/1 | 0.92 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3639 | 1/1 | 0.92 | 0.11 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3172 | 1/1 | 0.92 | 0.16 | 51,51,51,51 | 0 |
| 57 | MG | 1a | 1731 | 1/1 | 0.92 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3214 | 1/1 | 0.92 | 0.14 | 47,47,47,47 | 0 |
| 57 | MG | 1a | 1735 | 1/1 | 0.92 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3078 | 1/1 | 0.92 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3358 | 1/1 | 0.92 | 0.21 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3359 | 1/1 | 0.92 | 0.09 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3024 | 1/1 | 0.92 | 0.24 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3362 | 1/1 | 0.92 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3363 | 1/1 | 0.92 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | 1a | 1739 | 1/1 | 0.92 | 0.12 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 4020 | 1/1 | 0.92 | 0.17 | 21,21,21,21 | 0 |
| 57 | MG | 2A | 3595 | 1/1 | 0.92 | 0.16 | 40,40,40,40 | 0 |
| 57 | MG | 1a | 1743 | 1/1 | 0.92 | 0.31 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3335 | 1/1 | 0.92 | 0.25 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1745 | 1/1 | 0.92 | 0.25 | 68,68,68,68 | 0 |
| 57 | MG | 1a | 1622 | 1/1 | 0.92 | 0.32 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3602 | 1/1 | 0.92 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3018 | 1/1 | 0.92 | 0.22 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3374 | 1/1 | 0.92 | 0.31 | 40,40,40,40 | 0 |
| 57 | MG | 1a | 1747 | 1/1 | 0.92 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3736 | 1/1 | 0.92 | 0.20 | 60,60,60,60 | 0 |
| 57 | MG | 2A | 3023 | 1/1 | 0.92 | 0.38 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3650 | 1/1 | 0.92 | 0.17 | 26,26,26,26 | 0 |
| 57 | MG | 2A | 3027 | 1/1 | 0.92 | 0.09 | 46,46,46,46 | 0 |
| 57 | MG | 2a | 1668 | 1/1 | 0.92 | 0.12 | 71,71,71,71 | 0 |
| 57 | MG | 2A | 3621 | 1/1 | 0.92 | 0.27 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3852 | 1/1 | 0.92 | 0.07 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 3045 | 1/1 | 0.92 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3400 | 1/1 | 0.92 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3855 | 1/1 | 0.92 | 0.10 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3315 | 1/1 | 0.92 | 0.24 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3630 | 1/1 | 0.92 | 0.20 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3857 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3441 | 1/1 | 0.92 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | 1E | 306 | 1/1 | 0.92 | 0.10 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3657 | 1/1 | 0.92 | 0.12 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 3864 | 1/1 | 0.92 | 0.14 | 21,21,21,21 | 0 |
| 57 | MG | 1A | 3658 | 1/1 | 0.92 | 0.15 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3252 | 1/1 | 0.92 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3642 | 1/1 | 0.92 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | 2a | 1690 | 1/1 | 0.92 | 0.20 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3663 | 1/1 | 0.92 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | 1a | 1780 | 1/1 | 0.92 | 0.12 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3445 | 1/1 | 0.92 | 0.24 | 57,57,57,57 | 0 |
| 57 | MG | 1a | 1649 | 1/1 | 0.92 | 0.16 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3217 | 1/1 | 0.92 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | 1G | 204 | 1/1 | 0.92 | 0.18 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3220 | 1/1 | 0.92 | 0.19 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3757 | 1/1 | 0.92 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3484 | 1/1 | 0.92 | 0.29 | 43,43,43,43 | 0 |
| 57 | MG | 1a | 1655 | 1/1 | 0.92 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1657 | 1/1 | 0.92 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3438 | 1/1 | 0.92 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3760 | 1/1 | 0.92 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | 1a | 1792 | 1/1 | 0.92 | 0.20 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3588 | 1/1 | 0.92 | 0.27 | 40,40,40,40 | 0 |
| 57 | MG | 2a | 1715 | 1/1 | 0.92 | 0.43 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3486 | 1/1 | 0.92 | 0.32 | 41,41,41,41 | 0 |
| 57 | MG | 2a | 1719 | 1/1 | 0.92 | 0.16 | 67,67,67,67 | 0 |
| 57 | MG | 2a | 1720 | 1/1 | 0.92 | 0.14 | 65,65,65,65 | 0 |
| 57 | MG | 1a | 1801 | 1/1 | 0.92 | 0.10 | 51,51,51,51 | 0 |
| 57 | MG | 2a | 1723 | 1/1 | 0.92 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | 2a | 1724 | 1/1 | 0.92 | 0.27 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3590 | 1/1 | 0.92 | 0.16 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3447 | 1/1 | 0.92 | 0.21 | 38,38,38,38 | 0 |
| 57 | MG | 2a | 1729 | 1/1 | 0.92 | 0.27 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3073 | 1/1 | 0.92 | 0.07 | 47,47,47,47 | 0 |
| 57 | MG | 2a | 1731 | 1/1 | 0.92 | 0.31 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3454 | 1/1 | 0.92 | 0.17 | 59,59,59,59 | 0 |
| 57 | MG | 2a | 1733 | 1/1 | 0.92 | 0.28 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3318 | 1/1 | 0.92 | 0.17 | 50,50,50,50 | 0 |
| 57 | MG | 1Q | 206 | 1/1 | 0.92 | 0.23 | 34,34,34,34 | 0 |
| 57 | MG | 1a | 1667 | 1/1 | 0.92 | 0.50 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 4057 | 1/1 | 0.92 | 0.19 | 31,31,31,31 | 0 |
| 57 | MG | 1a | 1670 | 1/1 | 0.92 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3412 | 1/1 | 0.92 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3221 | 1/1 | 0.92 | 0.11 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3695 | 1/1 | 0.92 | 0.21 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3252 | 1/1 | 0.92 | 0.09 | 71,71,71,71 | 0 |
| 57 | MG | 1a | 1815 | 1/1 | 0.92 | 0.07 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3698 | 1/1 | 0.92 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3701 | 1/1 | 0.92 | 0.23 | 61,61,61,61 | 0 |
| 57 | MG | 2a | 1758 | 1/1 | 0.92 | 0.24 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3122 | 1/1 | 0.92 | 0.24 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3540 | 1/1 | 0.92 | 0.22 | 34,34,34,34 | 0 |
| 57 | MG | 1a | 1677 | 1/1 | 0.92 | 0.17 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3257 | 1/1 | 0.92 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3495 | 1/1 | 0.92 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3144 | 1/1 | 0.92 | 0.22 | 46,46,46,46 | 0 |
| 57 | MG | 2a | 1766 | 1/1 | 0.92 | 0.29 | 62,62,62,62 | 0 |
| 57 | MG | 1W | 206 | 1/1 | 0.92 | 0.15 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3098 | 1/1 | 0.92 | 0.10 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3982 | 1/1 | 0.92 | 0.21 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3985 | 1/1 | 0.92 | 0.06 | 62,62,62,62 | 0 |
| 57 | MG | 2a | 1775 | 1/1 | 0.92 | 0.23 | 76,76,76,76 | 0 |
| 57 | MG | 2A | 3723 | 1/1 | 0.92 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | 2A | 3268 | 1/1 | 0.92 | 0.24 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3498 | 1/1 | 0.92 | 0.13 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3167 | 1/1 | 0.92 | 0.23 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3503 | 1/1 | 0.92 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | 2a | 1782 | 1/1 | 0.92 | 0.20 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3504 | 1/1 | 0.92 | 0.18 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3546 | 1/1 | 0.92 | 0.34 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3508 | 1/1 | 0.92 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | 2f | 201 | 1/1 | 0.92 | 0.16 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3901 | 1/1 | 0.92 | 0.14 | 29,29,29,29 | 0 |
| 57 | MG | 2A | 3108 | 1/1 | 0.92 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3110 | 1/1 | 0.92 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | 2q | 203 | 1/1 | 0.92 | 0.09 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3516 | 1/1 | 0.92 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | 1a | 1694 | 1/1 | 0.92 | 0.19 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3501 | 1/1 | 0.92 | 0.12 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3612 | 1/1 | 0.92 | 0.19 | 24,24,24,24 | 0 |
| 57 | MG | 2D | 304 | 1/1 | 0.92 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3126 | 1/1 | 0.92 | 0.27 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3614 | 1/1 | 0.92 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | 2F | 302 | 1/1 | 0.92 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | 1l | 103 | 1/1 | 0.92 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | 1a | 1606 | 1/1 | 0.93 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | 1a | 1756 | 1/1 | 0.93 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3276 | 1/1 | 0.93 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3902 | 1/1 | 0.93 | 0.20 | 27,27,27,27 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2E | 305 | 1/1 | 0.93 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | 1a | 1759 | 1/1 | 0.93 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3063 | 1/1 | 0.93 | 0.22 | 52,52,52,52 | 0 |
| 57 | MG | 2F | 306 | 1/1 | 0.93 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3181 | 1/1 | 0.93 | 0.17 | 47,47,47,47 | 0 |
| 57 | MG | 2O | 201 | 1/1 | 0.93 | 0.16 | 70,70,70,70 | 0 |
| 57 | MG | 1A | 3059 | 1/1 | 0.93 | 0.12 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3491 | 1/1 | 0.93 | 0.24 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3511 | 1/1 | 0.93 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | 1a | 1766 | 1/1 | 0.93 | 0.12 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3253 | 1/1 | 0.93 | 0.26 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 4106 | 1/1 | 0.93 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3515 | 1/1 | 0.93 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 4107 | 1/1 | 0.93 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3999 | 1/1 | 0.93 | 0.15 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3914 | 1/1 | 0.93 | 0.16 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3519 | 1/1 | 0.93 | 0.16 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3618 | 1/1 | 0.93 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | 1a | 1626 | 1/1 | 0.93 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3153 | 1/1 | 0.93 | 0.12 | 37,37,37,37 | 0 |
| 57 | MG | 1a | 1628 | 1/1 | 0.93 | 0.17 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3324 | 1/1 | 0.93 | 0.10 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 4005 | 1/1 | 0.93 | 0.09 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3821 | 1/1 | 0.93 | 0.17 | 28,28,28,28 | 0 |
| 57 | MG | 1B | 217 | 1/1 | 0.93 | 0.22 | 34,34,34,34 | 0 |
| 57 | MG | 1a | 1635 | 1/1 | 0.93 | 0.14 | 59,59,59,59 | 0 |
| 57 | MG | 1B | 223 | 1/1 | 0.93 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3281 | 1/1 | 0.93 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3923 | 1/1 | 0.93 | 0.17 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3400 | 1/1 | 0.93 | 0.20 | 64,64,64,64 | 0 |
| 57 | MG | 1a | 1641 | 1/1 | 0.93 | 0.23 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3096 | 1/1 | 0.93 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3097 | 1/1 | 0.93 | 0.09 | 62,62,62,62 | 0 |
| 57 | MG | 1a | 1800 | 1/1 | 0.93 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3356 | 1/1 | 0.93 | 0.20 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3101 | 1/1 | 0.93 | 0.10 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3829 | 1/1 | 0.93 | 0.10 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3553 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | 1a | 1644 | 1/1 | 0.93 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3303 | 1/1 | 0.93 | 0.25 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3104 | 1/1 | 0.93 | 0.25 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3835 | 1/1 | 0.93 | 0.15 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1B | 231 | 1/1 | 0.93 | 0.19 | 54,54,54,54 | 0 |
| 57 | MG | 1B | 232 | 1/1 | 0.93 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3256 | 1/1 | 0.93 | 0.19 | 66,66,66,66 | 0 |
| 57 | MG | 2a | 1632 | 1/1 | 0.93 | 0.28 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3111 | 1/1 | 0.93 | 0.24 | 33,33,33,33 | 0 |
| 57 | MG | 2A | 3564 | 1/1 | 0.93 | 0.15 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3311 | 1/1 | 0.93 | 0.23 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3406 | 1/1 | 0.93 | 0.36 | 51,51,51,51 | 0 |
| 57 | MG | 2a | 1639 | 1/1 | 0.93 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | 1D | 312 | 1/1 | 0.93 | 0.20 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3296 | 1/1 | 0.93 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1643 | 1/1 | 0.93 | 0.32 | 73,73,73,73 | 0 |
| 57 | MG | 2A | 3118 | 1/1 | 0.93 | 0.16 | 39,39,39,39 | 0 |
| 57 | MG | 1a | 1658 | 1/1 | 0.93 | 0.28 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3456 | 1/1 | 0.93 | 0.16 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3188 | 1/1 | 0.93 | 0.47 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3643 | 1/1 | 0.93 | 0.18 | 59,59,59,59 | 0 |
| 57 | MG | 2a | 1651 | 1/1 | 0.93 | 0.38 | 58,58,58,58 | 0 |
| 57 | MG | 2a | 1653 | 1/1 | 0.93 | 0.17 | 69,69,69,69 | 0 |
| 57 | MG | 1a | 1821 | 1/1 | 0.93 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3332 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3644 | 1/1 | 0.93 | 0.18 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3939 | 1/1 | 0.93 | 0.14 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3130 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1826 | 1/1 | 0.93 | 0.14 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3848 | 1/1 | 0.93 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3134 | 1/1 | 0.93 | 0.28 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3136 | 1/1 | 0.93 | 0.25 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3458 | 1/1 | 0.93 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3139 | 1/1 | 0.93 | 0.15 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3850 | 1/1 | 0.93 | 0.25 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3353 | 1/1 | 0.93 | 0.28 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3052 | 1/1 | 0.93 | 0.08 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3261 | 1/1 | 0.93 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | 1e | 201 | 1/1 | 0.93 | 0.17 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3603 | 1/1 | 0.93 | 0.07 | 60,60,60,60 | 0 |
| 57 | MG | 1a | 1671 | 1/1 | 0.93 | 0.31 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3070 | 1/1 | 0.93 | 0.40 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3136 | 1/1 | 0.93 | 0.17 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3465 | 1/1 | 0.93 | 0.20 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3575 | 1/1 | 0.93 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | 1n | 102 | 1/1 | 0.93 | 0.12 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1O | 206 | 1/1 | 0.93 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3620 | 1/1 | 0.93 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | 1P | 203 | 1/1 | 0.93 | 0.16 | 33,33,33,33 | 0 |
| 57 | MG | 2A | 3162 | 1/1 | 0.93 | 0.22 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3623 | 1/1 | 0.93 | 0.10 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3137 | 1/1 | 0.93 | 0.25 | 40,40,40,40 | 0 |
| 57 | MG | 2a | 1691 | 1/1 | 0.93 | 0.18 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1682 | 1/1 | 0.93 | 0.88 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3660 | 1/1 | 0.93 | 0.17 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3582 | 1/1 | 0.93 | 0.53 | 39,39,39,39 | 0 |
| 57 | MG | 2a | 1695 | 1/1 | 0.93 | 0.23 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3375 | 1/1 | 0.93 | 0.32 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3169 | 1/1 | 0.93 | 0.13 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3382 | 1/1 | 0.93 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3383 | 1/1 | 0.93 | 0.16 | 55,55,55,55 | 0 |
| 57 | MG | 1a | 1686 | 1/1 | 0.93 | 0.06 | 51,51,51,51 | 0 |
| 57 | MG | 1a | 1687 | 1/1 | 0.93 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3394 | 1/1 | 0.93 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3095 | 1/1 | 0.93 | 0.10 | 32,32,32,32 | 0 |
| 57 | MG | 2a | 1708 | 1/1 | 0.93 | 0.10 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3584 | 1/1 | 0.93 | 0.21 | 44,44,44,44 | 0 |
| 57 | MG | 1S | 201 | 1/1 | 0.93 | 0.96 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3398 | 1/1 | 0.93 | 0.08 | 44,44,44,44 | 0 |
| 57 | MG | 2a | 1712 | 1/1 | 0.93 | 0.10 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 4052 | 1/1 | 0.93 | 0.28 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3372 | 1/1 | 0.93 | 0.17 | 32,32,32,32 | 0 |
| 57 | MG | 2a | 1716 | 1/1 | 0.93 | 0.25 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3667 | 1/1 | 0.93 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3421 | 1/1 | 0.93 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3652 | 1/1 | 0.93 | 0.08 | 80,80,80,80 | 0 |
| 57 | MG | 2A | 3181 | 1/1 | 0.93 | 0.24 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3654 | 1/1 | 0.93 | 0.22 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3877 | 1/1 | 0.93 | 0.09 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3657 | 1/1 | 0.93 | 0.09 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3337 | 1/1 | 0.93 | 0.26 | 43,43,43,43 | 0 |
| 57 | MG | 1W | 205 | 1/1 | 0.93 | 0.13 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 4059 | 1/1 | 0.93 | 0.27 | 70,70,70,70 | 0 |
| 57 | MG | 1a | 1707 | 1/1 | 0.93 | 0.19 | 57,57,57,57 | 0 |
| 57 | MG | 1X | 103 | 1/1 | 0.93 | 0.13 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3474 | 1/1 | 0.93 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | 2a | 1735 | 1/1 | 0.93 | 0.17 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3044 | 1/1 | 0.93 | 0.18 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 4064 | 1/1 | 0.93 | 0.14 | 68,68,68,68 | 0 |
| 57 | MG | 2a | 1738 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3594 | 1/1 | 0.93 | 0.29 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3774 | 1/1 | 0.93 | 0.19 | 28,28,28,28 | 0 |
| 57 | MG | 1a | 1716 | 1/1 | 0.93 | 0.15 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3007 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3885 | 1/1 | 0.93 | 0.28 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 3339 | 1/1 | 0.93 | 0.18 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3014 | 1/1 | 0.93 | 0.30 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3685 | 1/1 | 0.93 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3376 | 1/1 | 0.93 | 0.39 | 58,58,58,58 | 0 |
| 57 | MG | 2a | 1756 | 1/1 | 0.93 | 0.28 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 3976 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3204 | 1/1 | 0.93 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | 11 | 101 | 1/1 | 0.93 | 0.56 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3443 | 1/1 | 0.93 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3444 | 1/1 | 0.93 | 0.18 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 4076 | 1/1 | 0.93 | 0.23 | 41,41,41,41 | 0 |
| 57 | MG | 1a | 1724 | 1/1 | 0.93 | 0.14 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3447 | 1/1 | 0.93 | 0.10 | 39,39,39,39 | 0 |
| 57 | MG | 12 | 102 | 1/1 | 0.93 | 0.22 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 4077 | 1/1 | 0.93 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3098 | 1/1 | 0.93 | 0.28 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3890 | 1/1 | 0.93 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3033 | 1/1 | 0.93 | 0.27 | 56,56,56,56 | 0 |
| 57 | MG | 2a | 1771 | 1/1 | 0.93 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | 2a | 1773 | 1/1 | 0.93 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3034 | 1/1 | 0.93 | 0.13 | 40,40,40,40 | 0 |
| 57 | MG | 15 | 105 | 1/1 | 0.93 | 0.21 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3712 | 1/1 | 0.93 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | 15 | 107 | 1/1 | 0.93 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3716 | 1/1 | 0.93 | 0.17 | 60,60,60,60 | 0 |
| 57 | MG | 2A | 3717 | 1/1 | 0.93 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3379 | 1/1 | 0.93 | 0.17 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3983 | 1/1 | 0.93 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3467 | 1/1 | 0.93 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3041 | 1/1 | 0.93 | 0.10 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3728 | 1/1 | 0.93 | 0.22 | 51,51,51,51 | 0 |
| 57 | MG | 18 | 3401 | 1/1 | 0.93 | 0.40 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3100 | 1/1 | 0.93 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | 1a | 1742 | 1/1 | 0.93 | 0.22 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3603 | 1/1 | 0.93 | 0.22 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3234 | 1/1 | 0.93 | 0.09 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 4089 | 1/1 | 0.93 | 0.18 | 53,53,53,53 | 0 |
| 57 | MG | 1a | 1601 | 1/1 | 0.93 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | 2B | 208 | 1/1 | 0.93 | 0.23 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3386 | 1/1 | 0.93 | 0.13 | 24,24,24,24 | 0 |
| 57 | MG | 2y | 101 | 1/1 | 0.93 | 0.23 | 56,56,56,56 | 0 |
| 57 | MG | 2y | 103 | 1/1 | 0.93 | 0.28 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 4092 | 1/1 | 0.93 | 0.12 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3387 | 1/1 | 0.93 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3091 | 1/1 | 0.93 | 0.20 | 25,25,25,25 | 0 |
| 57 | MG | 2A | 3492 | 1/1 | 0.93 | 0.10 | 56,56,56,56 | 0 |
| 57 | MG | 2B | 215 | 1/1 | 0.94 | 0.22 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3490 | 1/1 | 0.94 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | 1a | 1772 | 1/1 | 0.94 | 0.14 | 68,68,68,68 | 0 |
| 57 | MG | 1B | 227 | 1/1 | 0.94 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | 2D | 301 | 1/1 | 0.94 | 0.19 | 55,55,55,55 | 0 |
| 57 | MG | 2D | 303 | 1/1 | 0.94 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3139 | 1/1 | 0.94 | 0.12 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 3905 | 1/1 | 0.94 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | 2E | 304 | 1/1 | 0.94 | 0.10 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3796 | 1/1 | 0.94 | 0.11 | 29,29,29,29 | 0 |
| 57 | MG | 2A | 3497 | 1/1 | 0.94 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1631 | 1/1 | 0.94 | 0.12 | 62,62,62,62 | 0 |
| 57 | MG | 2F | 305 | 1/1 | 0.94 | 0.52 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3499 | 1/1 | 0.94 | 0.22 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3909 | 1/1 | 0.94 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | 2N | 201 | 1/1 | 0.94 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3697 | 1/1 | 0.94 | 0.20 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3803 | 1/1 | 0.94 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3078 | 1/1 | 0.94 | 0.29 | 41,41,41,41 | 0 |
| 57 | MG | 1a | 1785 | 1/1 | 0.94 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3509 | 1/1 | 0.94 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3510 | 1/1 | 0.94 | 0.16 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3080 | 1/1 | 0.94 | 0.20 | 45,45,45,45 | 0 |
| 57 | MG | 1a | 1636 | 1/1 | 0.94 | 0.24 | 76,76,76,76 | 0 |
| 57 | MG | 2A | 3262 | 1/1 | 0.94 | 0.21 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3263 | 1/1 | 0.94 | 0.27 | 72,72,72,72 | 0 |
| 57 | MG | 2A | 3264 | 1/1 | 0.94 | 0.16 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3805 | 1/1 | 0.94 | 0.16 | 19,19,19,19 | 0 |
| 57 | MG | 25 | 103 | 1/1 | 0.94 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3808 | 1/1 | 0.94 | 0.23 | 20,20,20,20 | 0 |
| 57 | MG | 2A | 3086 | 1/1 | 0.94 | 0.12 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 27 | 103 | 1/1 | 0.94 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | 28 | 101 | 1/1 | 0.94 | 0.13 | 46,46,46,46 | 0 |
| 57 | MG | 1a | 1639 | 1/1 | 0.94 | 0.17 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3270 | 1/1 | 0.94 | 0.22 | 49,49,49,49 | 0 |
| 57 | MG | 1D | 305 | 1/1 | 0.94 | 0.22 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3523 | 1/1 | 0.94 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | 1D | 309 | 1/1 | 0.94 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3415 | 1/1 | 0.94 | 0.26 | 63,63,63,63 | 0 |
| 57 | MG | 1a | 1794 | 1/1 | 0.94 | 0.09 | 56,56,56,56 | 0 |
| 57 | MG | 2a | 1607 | 1/1 | 0.94 | 0.22 | 69,69,69,69 | 0 |
| 57 | MG | 2A | 3278 | 1/1 | 0.94 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3142 | 1/1 | 0.94 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3921 | 1/1 | 0.94 | 0.25 | 36,36,36,36 | 0 |
| 57 | MG | 1E | 304 | 1/1 | 0.94 | 0.18 | 34,34,34,34 | 0 |
| 57 | MG | 1a | 1646 | 1/1 | 0.94 | 0.09 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3417 | 1/1 | 0.94 | 0.15 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3538 | 1/1 | 0.94 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1648 | 1/1 | 0.94 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | 1E | 310 | 1/1 | 0.94 | 0.12 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3039 | 1/1 | 0.94 | 0.30 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3704 | 1/1 | 0.94 | 0.24 | 21,21,21,21 | 0 |
| 57 | MG | 2A | 3294 | 1/1 | 0.94 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | 1a | 1652 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3547 | 1/1 | 0.94 | 0.17 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3296 | 1/1 | 0.94 | 0.17 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3297 | 1/1 | 0.94 | 0.36 | 56,56,56,56 | 0 |
| 57 | MG | 1a | 1812 | 1/1 | 0.94 | 0.12 | 62,62,62,62 | 0 |
| 57 | MG | 1E | 315 | 1/1 | 0.94 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3109 | 1/1 | 0.94 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | 1F | 304 | 1/1 | 0.94 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3928 | 1/1 | 0.94 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3329 | 1/1 | 0.94 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | 1F | 311 | 1/1 | 0.94 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3007 | 1/1 | 0.94 | 0.17 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3117 | 1/1 | 0.94 | 0.29 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3822 | 1/1 | 0.94 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3310 | 1/1 | 0.94 | 0.24 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1642 | 1/1 | 0.94 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3823 | 1/1 | 0.94 | 0.09 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3312 | 1/1 | 0.94 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3184 | 1/1 | 0.94 | 0.21 | 36,36,36,36 | 0 |
| 57 | MG | 1N | 201 | 1/1 | 0.94 | 0.39 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3124 | 1/1 | 0.94 | 0.15 | 62,62,62,62 | 0 |
| 57 | MG | 1N | 202 | 1/1 | 0.94 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | 1N | 204 | 1/1 | 0.94 | 0.28 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3288 | 1/1 | 0.94 | 0.25 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3578 | 1/1 | 0.94 | 0.15 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3074 | 1/1 | 0.94 | 0.15 | 28,28,28,28 | 0 |
| 57 | MG | 2A | 3129 | 1/1 | 0.94 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3325 | 1/1 | 0.94 | 0.24 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3328 | 1/1 | 0.94 | 0.22 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3830 | 1/1 | 0.94 | 0.08 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3331 | 1/1 | 0.94 | 0.17 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3833 | 1/1 | 0.94 | 0.10 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3334 | 1/1 | 0.94 | 0.23 | 55,55,55,55 | 0 |
| 57 | MG | 1O | 205 | 1/1 | 0.94 | 0.11 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3426 | 1/1 | 0.94 | 0.12 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 4047 | 1/1 | 0.94 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3594 | 1/1 | 0.94 | 0.09 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3137 | 1/1 | 0.94 | 0.27 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3027 | 1/1 | 0.94 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3838 | 1/1 | 0.94 | 0.21 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3140 | 1/1 | 0.94 | 0.28 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3377 | 1/1 | 0.94 | 0.40 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3190 | 1/1 | 0.94 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | 2a | 1675 | 1/1 | 0.94 | 0.23 | 63,63,63,63 | 0 |
| 57 | MG | 2A | 3146 | 1/1 | 0.94 | 0.22 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3352 | 1/1 | 0.94 | 0.09 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3606 | 1/1 | 0.94 | 0.11 | 74,74,74,74 | 0 |
| 57 | MG | 1A | 3431 | 1/1 | 0.94 | 0.11 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3294 | 1/1 | 0.94 | 0.13 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3610 | 1/1 | 0.94 | 0.08 | 62,62,62,62 | 0 |
| 57 | MG | 2a | 1685 | 1/1 | 0.94 | 0.17 | 67,67,67,67 | 0 |
| 57 | MG | 2a | 1686 | 1/1 | 0.94 | 0.08 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3383 | 1/1 | 0.94 | 0.11 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3119 | 1/1 | 0.94 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | 1T | 201 | 1/1 | 0.94 | 0.10 | 56,56,56,56 | 0 |
| 57 | MG | 1T | 202 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3385 | 1/1 | 0.94 | 0.22 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3361 | 1/1 | 0.94 | 0.11 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3083 | 1/1 | 0.94 | 0.26 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3494 | 1/1 | 0.94 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3159 | 1/1 | 0.94 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | 1V | 205 | 1/1 | 0.94 | 0.28 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3626 | 1/1 | 0.94 | 0.07 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3646 | 1/1 | 0.94 | 0.07 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3163 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | 1W | 204 | 1/1 | 0.94 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3739 | 1/1 | 0.94 | 0.18 | 50,50,50,50 | 0 |
| 57 | MG | 1x | 107 | 1/1 | 0.94 | 0.18 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3647 | 1/1 | 0.94 | 0.13 | 35,35,35,35 | 0 |
| 57 | MG | 1a | 1704 | 1/1 | 0.94 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | 1X | 102 | 1/1 | 0.94 | 0.23 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3379 | 1/1 | 0.94 | 0.18 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3639 | 1/1 | 0.94 | 0.10 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 4066 | 1/1 | 0.94 | 0.17 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3641 | 1/1 | 0.94 | 0.12 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3205 | 1/1 | 0.94 | 0.08 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3206 | 1/1 | 0.94 | 0.21 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3497 | 1/1 | 0.94 | 0.12 | 35,35,35,35 | 0 |
| 57 | MG | 2a | 1718 | 1/1 | 0.94 | 0.15 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3048 | 1/1 | 0.94 | 0.15 | 16,16,16,16 | 0 |
| 57 | MG | 1A | 3157 | 1/1 | 0.94 | 0.21 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3750 | 1/1 | 0.94 | 0.15 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3751 | 1/1 | 0.94 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3087 | 1/1 | 0.94 | 0.23 | 48,48,48,48 | 0 |
| 57 | MG | 2a | 1726 | 1/1 | 0.94 | 0.15 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3101 | 1/1 | 0.94 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3871 | 1/1 | 0.94 | 0.10 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3397 | 1/1 | 0.94 | 0.31 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3873 | 1/1 | 0.94 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3009 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 57 | MG | 1a | 1722 | 1/1 | 0.94 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3449 | 1/1 | 0.94 | 0.19 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3412 | 1/1 | 0.94 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3191 | 1/1 | 0.94 | 0.20 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3664 | 1/1 | 0.94 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3581 | 1/1 | 0.94 | 0.23 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3129 | 1/1 | 0.94 | 0.23 | 31,31,31,31 | 0 |
| 57 | MG | 1a | 1726 | 1/1 | 0.94 | 0.09 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1741 | 1/1 | 0.94 | 0.22 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3020 | 1/1 | 0.94 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3674 | 1/1 | 0.94 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | 2a | 1745 | 1/1 | 0.94 | 0.13 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3675 | 1/1 | 0.94 | 0.13 | 37,37,37,37 | 0 |
| 57 | MG | 2a | 1749 | 1/1 | 0.94 | 0.23 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2a | 1750 | 1/1 | 0.94 | 0.21 | 55,55,55,55 | 0 |
| 57 | MG | 14 | 101 | 1/1 | 0.94 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3979 | 1/1 | 0.94 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3425 | 1/1 | 0.94 | 0.22 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3347 | 1/1 | 0.94 | 0.08 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3762 | 1/1 | 0.94 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3025 | 1/1 | 0.94 | 0.14 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3104 | 1/1 | 0.94 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3262 | 1/1 | 0.94 | 0.11 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3688 | 1/1 | 0.94 | 0.07 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3065 | 1/1 | 0.94 | 0.20 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3036 | 1/1 | 0.94 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | 2a | 1763 | 1/1 | 0.94 | 0.12 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3206 | 1/1 | 0.94 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | 1a | 1740 | 1/1 | 0.94 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3439 | 1/1 | 0.94 | 0.14 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3135 | 1/1 | 0.94 | 0.15 | 49,49,49,49 | 0 |
| 57 | MG | 19 | 101 | 1/1 | 0.94 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3773 | 1/1 | 0.94 | 0.17 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3213 | 1/1 | 0.94 | 0.17 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3702 | 1/1 | 0.94 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | 2a | 1772 | 1/1 | 0.94 | 0.13 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3220 | 1/1 | 0.94 | 0.21 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3215 | 1/1 | 0.94 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3067 | 1/1 | 0.94 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 4108 | 1/1 | 0.94 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3044 | 1/1 | 0.94 | 0.07 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3685 | 1/1 | 0.94 | 0.21 | 21,21,21,21 | 0 |
| 57 | MG | 1A | 3892 | 1/1 | 0.94 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3270 | 1/1 | 0.94 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | 1B | 205 | 1/1 | 0.94 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3462 | 1/1 | 0.94 | 0.15 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3780 | 1/1 | 0.94 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | 2e | 201 | 1/1 | 0.94 | 0.10 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3898 | 1/1 | 0.94 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3112 | 1/1 | 0.94 | 0.20 | 33,33,33,33 | 0 |
| 57 | MG | 1B | 216 | 1/1 | 0.94 | 0.27 | 38,38,38,38 | 0 |
| 57 | MG | 2q | 201 | 1/1 | 0.94 | 0.12 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3468 | 1/1 | 0.94 | 0.21 | 67,67,67,67 | 0 |
| 57 | MG | 2A | 3233 | 1/1 | 0.94 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3464 | 1/1 | 0.94 | 0.21 | 48,48,48,48 | 0 |
| 57 | MG | 1B | 221 | 1/1 | 0.94 | 0.22 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3474 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3060 | 1/1 | 0.94 | 0.20 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1764 | 1/1 | 0.94 | 0.14 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1765 | 1/1 | 0.94 | 0.05 | 61,61,61,61 | 0 |
| 57 | MG | 2y | 102 | 1/1 | 0.94 | 0.07 | 81,81,81,81 | 0 |
| 57 | MG | 1A | 3226 | 1/1 | 0.94 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3242 | 1/1 | 0.94 | 0.51 | 67,67,67,67 | 0 |
| 57 | MG | 1a | 1767 | 1/1 | 0.94 | 0.11 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3693 | 1/1 | 0.94 | 0.19 | 22,22,22,22 | 0 |
| 57 | MG | 1A | 3413 | 1/1 | 0.94 | 0.22 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3571 | 1/1 | 0.95 | 0.22 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3359 | 1/1 | 0.95 | 0.26 | 62,62,62,62 | 0 |
| 57 | MG | 1B | 210 | 1/1 | 0.95 | 0.49 | 55,55,55,55 | 0 |
| 57 | MG | 1B | 211 | 1/1 | 0.95 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3159 | 1/1 | 0.95 | 0.23 | 29,29,29,29 | 0 |
| 57 | MG | 1B | 213 | 1/1 | 0.95 | 0.22 | 42,42,42,42 | 0 |
| 57 | MG | 1B | 214 | 1/1 | 0.95 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | 2T | 201 | 1/1 | 0.95 | 0.24 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3081 | 1/1 | 0.95 | 0.16 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3227 | 1/1 | 0.95 | 0.21 | 36,36,36,36 | 0 |
| 57 | MG | 1a | 1619 | 1/1 | 0.95 | 0.09 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3510 | 1/1 | 0.95 | 0.18 | 69,69,69,69 | 0 |
| 57 | MG | 1B | 219 | 1/1 | 0.95 | 0.24 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3363 | 1/1 | 0.95 | 0.32 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3763 | 1/1 | 0.95 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3089 | 1/1 | 0.95 | 0.18 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3282 | 1/1 | 0.95 | 0.21 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3884 | 1/1 | 0.95 | 0.18 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3530 | 1/1 | 0.95 | 0.10 | 67,67,67,67 | 0 |
| 57 | MG | 1B | 225 | 1/1 | 0.95 | 0.20 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3093 | 1/1 | 0.95 | 0.25 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3996 | 1/1 | 0.95 | 0.23 | 26,26,26,26 | 0 |
| 57 | MG | 2A | 3291 | 1/1 | 0.95 | 0.31 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3580 | 1/1 | 0.95 | 0.37 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3512 | 1/1 | 0.95 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3668 | 1/1 | 0.95 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | 1a | 1790 | 1/1 | 0.95 | 0.11 | 73,73,73,73 | 0 |
| 57 | MG | 2A | 3099 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | 2a | 1605 | 1/1 | 0.95 | 0.11 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 4001 | 1/1 | 0.95 | 0.17 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3769 | 1/1 | 0.95 | 0.17 | 16,16,16,16 | 0 |
| 57 | MG | 1A | 3513 | 1/1 | 0.95 | 0.20 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3301 | 1/1 | 0.95 | 0.15 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3671 | 1/1 | 0.95 | 0.20 | 24,24,24,24 | 0 |
| 57 | MG | 1a | 1795 | 1/1 | 0.95 | 0.33 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3105 | 1/1 | 0.95 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | 1a | 1796 | 1/1 | 0.95 | 0.21 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3672 | 1/1 | 0.95 | 0.23 | 23,23,23,23 | 0 |
| 57 | MG | 1a | 1799 | 1/1 | 0.95 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3017 | 1/1 | 0.95 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | 1D | 302 | 1/1 | 0.95 | 0.34 | 43,43,43,43 | 0 |
| 57 | MG | 1D | 303 | 1/1 | 0.95 | 0.13 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3112 | 1/1 | 0.95 | 0.26 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3894 | 1/1 | 0.95 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | 1D | 308 | 1/1 | 0.95 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | 1a | 1807 | 1/1 | 0.95 | 0.09 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3516 | 1/1 | 0.95 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | 1D | 311 | 1/1 | 0.95 | 0.14 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3776 | 1/1 | 0.95 | 0.19 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3517 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3678 | 1/1 | 0.95 | 0.14 | 22,22,22,22 | 0 |
| 57 | MG | 1A | 3103 | 1/1 | 0.95 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3680 | 1/1 | 0.95 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3573 | 1/1 | 0.95 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | 1E | 307 | 1/1 | 0.95 | 0.34 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3193 | 1/1 | 0.95 | 0.35 | 37,37,37,37 | 0 |
| 57 | MG | 1E | 312 | 1/1 | 0.95 | 0.17 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3194 | 1/1 | 0.95 | 0.37 | 36,36,36,36 | 0 |
| 57 | MG | 1a | 1654 | 1/1 | 0.95 | 0.11 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3336 | 1/1 | 0.95 | 0.67 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3198 | 1/1 | 0.95 | 0.14 | 40,40,40,40 | 0 |
| 57 | MG | 1a | 1656 | 1/1 | 0.95 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3339 | 1/1 | 0.95 | 0.06 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3523 | 1/1 | 0.95 | 0.20 | 34,34,34,34 | 0 |
| 57 | MG | 1a | 1825 | 1/1 | 0.95 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3789 | 1/1 | 0.95 | 0.15 | 25,25,25,25 | 0 |
| 57 | MG | 2a | 1652 | 1/1 | 0.95 | 0.09 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3120 | 1/1 | 0.95 | 0.36 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3344 | 1/1 | 0.95 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | 1a | 1828 | 1/1 | 0.95 | 0.21 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3793 | 1/1 | 0.95 | 0.20 | 25,25,25,25 | 0 |
| 57 | MG | 2A | 3141 | 1/1 | 0.95 | 0.28 | 54,54,54,54 | 0 |
| 57 | MG | 1a | 1661 | 1/1 | 0.95 | 0.21 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3599 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3370 | 1/1 | 0.95 | 0.34 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3243 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | 1G | 201 | 1/1 | 0.95 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | 2a | 1664 | 1/1 | 0.95 | 0.08 | 55,55,55,55 | 0 |
| 57 | MG | 1G | 202 | 1/1 | 0.95 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 4034 | 1/1 | 0.95 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3244 | 1/1 | 0.95 | 0.09 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 4036 | 1/1 | 0.95 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3153 | 1/1 | 0.95 | 0.22 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3053 | 1/1 | 0.95 | 0.11 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3804 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3105 | 1/1 | 0.95 | 0.20 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3616 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3125 | 1/1 | 0.95 | 0.32 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3291 | 1/1 | 0.95 | 0.28 | 53,53,53,53 | 0 |
| 57 | MG | 1O | 202 | 1/1 | 0.95 | 0.42 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1678 | 1/1 | 0.95 | 0.11 | 76,76,76,76 | 0 |
| 57 | MG | 2A | 3161 | 1/1 | 0.95 | 0.29 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3248 | 1/1 | 0.95 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3702 | 1/1 | 0.95 | 0.15 | 26,26,26,26 | 0 |
| 57 | MG | 1a | 1679 | 1/1 | 0.95 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | 1a | 1680 | 1/1 | 0.95 | 0.06 | 70,70,70,70 | 0 |
| 57 | MG | 1x | 101 | 1/1 | 0.95 | 0.09 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3812 | 1/1 | 0.95 | 0.09 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3536 | 1/1 | 0.95 | 0.14 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3629 | 1/1 | 0.95 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3380 | 1/1 | 0.95 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3816 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3171 | 1/1 | 0.95 | 0.26 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3817 | 1/1 | 0.95 | 0.14 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3171 | 1/1 | 0.95 | 0.41 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3387 | 1/1 | 0.95 | 0.11 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3388 | 1/1 | 0.95 | 0.19 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3392 | 1/1 | 0.95 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | 2a | 1697 | 1/1 | 0.95 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3145 | 1/1 | 0.95 | 0.21 | 29,29,29,29 | 0 |
| 57 | MG | 1a | 1689 | 1/1 | 0.95 | 0.16 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3073 | 1/1 | 0.95 | 0.23 | 21,21,21,21 | 0 |
| 57 | MG | 1A | 3177 | 1/1 | 0.95 | 0.23 | 19,19,19,19 | 0 |
| 57 | MG | 2A | 3644 | 1/1 | 0.95 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | 1R | 203 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 57 | MG | 2a | 1706 | 1/1 | 0.95 | 0.09 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1R | 204 | 1/1 | 0.95 | 0.23 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3710 | 1/1 | 0.95 | 0.16 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3402 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 57 | MG | 1a | 1695 | 1/1 | 0.95 | 0.09 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3711 | 1/1 | 0.95 | 0.21 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3713 | 1/1 | 0.95 | 0.14 | 14,14,14,14 | 0 |
| 57 | MG | 1A | 3940 | 1/1 | 0.95 | 0.14 | 35,35,35,35 | 0 |
| 57 | MG | 1a | 1701 | 1/1 | 0.95 | 0.29 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3002 | 1/1 | 0.95 | 0.30 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 4060 | 1/1 | 0.95 | 0.14 | 17,17,17,17 | 0 |
| 57 | MG | 1A | 3616 | 1/1 | 0.95 | 0.11 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3715 | 1/1 | 0.95 | 0.14 | 25,25,25,25 | 0 |
| 57 | MG | 1a | 1705 | 1/1 | 0.95 | 0.19 | 49,49,49,49 | 0 |
| 57 | MG | 2a | 1721 | 1/1 | 0.95 | 0.25 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3028 | 1/1 | 0.95 | 0.24 | 39,39,39,39 | 0 |
| 57 | MG | 1V | 204 | 1/1 | 0.95 | 0.15 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3075 | 1/1 | 0.95 | 0.19 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3303 | 1/1 | 0.95 | 0.31 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3217 | 1/1 | 0.95 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3670 | 1/1 | 0.95 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3671 | 1/1 | 0.95 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | 1a | 1711 | 1/1 | 0.95 | 0.25 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3306 | 1/1 | 0.95 | 0.25 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3430 | 1/1 | 0.95 | 0.17 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3723 | 1/1 | 0.95 | 0.07 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3628 | 1/1 | 0.95 | 0.25 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3726 | 1/1 | 0.95 | 0.27 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3630 | 1/1 | 0.95 | 0.20 | 23,23,23,23 | 0 |
| 57 | MG | 2A | 3024 | 1/1 | 0.95 | 0.14 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3683 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3207 | 1/1 | 0.95 | 0.17 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3729 | 1/1 | 0.95 | 0.23 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3099 | 1/1 | 0.95 | 0.14 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3392 | 1/1 | 0.95 | 0.29 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3029 | 1/1 | 0.95 | 0.11 | 54,54,54,54 | 0 |
| 57 | MG | 2a | 1746 | 1/1 | 0.95 | 0.22 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3030 | 1/1 | 0.95 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3031 | 1/1 | 0.95 | 0.11 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3032 | 1/1 | 0.95 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | 2A | 3694 | 1/1 | 0.95 | 0.11 | 41,41,41,41 | 0 |
| 57 | MG | 2a | 1752 | 1/1 | 0.95 | 0.35 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3636 | 1/1 | 0.95 | 0.23 | 24,24,24,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 10 | 101 | 1/1 | 0.95 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3393 | 1/1 | 0.95 | 0.35 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3551 | 1/1 | 0.95 | 0.22 | 17,17,17,17 | 0 |
| 57 | MG | 2A | 3222 | 1/1 | 0.95 | 0.11 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3442 | 1/1 | 0.95 | 0.24 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3854 | 1/1 | 0.95 | 0.14 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3705 | 1/1 | 0.95 | 0.29 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3457 | 1/1 | 0.95 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3459 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3737 | 1/1 | 0.95 | 0.06 | 52,52,52,52 | 0 |
| 57 | MG | 11 | 102 | 1/1 | 0.95 | 0.12 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3015 | 1/1 | 0.95 | 0.18 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3465 | 1/1 | 0.95 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3229 | 1/1 | 0.95 | 0.08 | 60,60,60,60 | 0 |
| 57 | MG | 11 | 105 | 1/1 | 0.95 | 0.21 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3742 | 1/1 | 0.95 | 0.19 | 23,23,23,23 | 0 |
| 57 | MG | 13 | 101 | 1/1 | 0.95 | 0.21 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3260 | 1/1 | 0.95 | 0.15 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3971 | 1/1 | 0.95 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3080 | 1/1 | 0.95 | 0.20 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3475 | 1/1 | 0.95 | 0.24 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 4097 | 1/1 | 0.95 | 0.15 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3185 | 1/1 | 0.95 | 0.21 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 4099 | 1/1 | 0.95 | 0.29 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3054 | 1/1 | 0.95 | 0.20 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3974 | 1/1 | 0.95 | 0.10 | 24,24,24,24 | 0 |
| 57 | MG | 16 | 101 | 1/1 | 0.95 | 0.13 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3057 | 1/1 | 0.95 | 0.13 | 61,61,61,61 | 0 |
| 57 | MG | 2B | 207 | 1/1 | 0.95 | 0.18 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 3866 | 1/1 | 0.95 | 0.20 | 34,34,34,34 | 0 |
| 57 | MG | 2B | 209 | 1/1 | 0.95 | 0.25 | 65,65,65,65 | 0 |
| 57 | MG | 2A | 3489 | 1/1 | 0.95 | 0.11 | 43,43,43,43 | 0 |
| 57 | MG | 2f | 202 | 1/1 | 0.95 | 0.16 | 73,73,73,73 | 0 |
| 57 | MG | 17 | 105 | 1/1 | 0.95 | 0.10 | 54,54,54,54 | 0 |
| 57 | MG | 17 | 106 | 1/1 | 0.95 | 0.16 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3498 | 1/1 | 0.95 | 0.41 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 4105 | 1/1 | 0.95 | 0.16 | 47,47,47,47 | 0 |
| 57 | MG | 1a | 1755 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | 2r | 101 | 1/1 | 0.95 | 0.12 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3352 | 1/1 | 0.95 | 0.20 | 49,49,49,49 | 0 |
| 57 | MG | 2w | 101 | 1/1 | 0.95 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3353 | 1/1 | 0.95 | 0.17 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3223 | 1/1 | 0.95 | 0.12 | 47,47,47,47 | 0 |
| 57 | MG | 2D | 302 | 1/1 | 0.95 | 0.37 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3117 | 1/1 | 0.95 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3317 | 1/1 | 0.95 | 0.18 | 42,42,42,42 | 0 |
| 57 | MG | 2E | 302 | 1/1 | 0.95 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3984 | 1/1 | 0.95 | 0.13 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3070 | 1/1 | 0.95 | 0.10 | 46,46,46,46 | 0 |
| 57 | MG | 2A | 3505 | 1/1 | 0.95 | 0.17 | 35,35,35,35 | 0 |
| 59 | ZN | 26 | 102 | 1/1 | 0.95 | 0.21 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3568 | 1/1 | 0.95 | 0.17 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3875 | 1/1 | 0.95 | 0.14 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3141 | 1/1 | 0.96 | 0.20 | 20,20,20,20 | 0 |
| 57 | MG | 1A | 3293 | 1/1 | 0.96 | 0.25 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3443 | 1/1 | 0.96 | 0.24 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3522 | 1/1 | 0.96 | 0.25 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3042 | 1/1 | 0.96 | 0.33 | 30,30,30,30 | 0 |
| 57 | MG | 1P | 201 | 1/1 | 0.96 | 0.15 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3504 | 1/1 | 0.96 | 0.12 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3054 | 1/1 | 0.96 | 0.25 | 35,35,35,35 | 0 |
| 57 | MG | 1P | 206 | 1/1 | 0.96 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3951 | 1/1 | 0.96 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3741 | 1/1 | 0.96 | 0.20 | 26,26,26,26 | 0 |
| 57 | MG | 1Q | 205 | 1/1 | 0.96 | 0.14 | 40,40,40,40 | 0 |
| 57 | MG | 2Y | 201 | 1/1 | 0.96 | 0.24 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3534 | 1/1 | 0.96 | 0.22 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3564 | 1/1 | 0.96 | 0.11 | 23,23,23,23 | 0 |
| 57 | MG | 1I | 203 | 1/1 | 0.96 | 0.12 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3954 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 57 | MG | 23 | 101 | 1/1 | 0.96 | 0.18 | 52,52,52,52 | 0 |
| 57 | MG | 1R | 202 | 1/1 | 0.96 | 0.24 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3567 | 1/1 | 0.96 | 0.25 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 4068 | 1/1 | 0.96 | 0.14 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3744 | 1/1 | 0.96 | 0.14 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3394 | 1/1 | 0.96 | 0.19 | 24,24,24,24 | 0 |
| 57 | MG | 27 | 102 | 1/1 | 0.96 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3043 | 1/1 | 0.96 | 0.14 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3142 | 1/1 | 0.96 | 0.07 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3656 | 1/1 | 0.96 | 0.20 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3548 | 1/1 | 0.96 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3549 | 1/1 | 0.96 | 0.09 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3249 | 1/1 | 0.96 | 0.26 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3326 | 1/1 | 0.96 | 0.20 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1a | 1688 | 1/1 | 0.96 | 0.10 | 64,64,64,64 | 0 |
| 57 | MG | 1U | 201 | 1/1 | 0.96 | 0.16 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3148 | 1/1 | 0.96 | 0.22 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3346 | 1/1 | 0.96 | 0.27 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3333 | 1/1 | 0.96 | 0.08 | 62,62,62,62 | 0 |
| 57 | MG | 1U | 208 | 1/1 | 0.96 | 0.21 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3173 | 1/1 | 0.96 | 0.19 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 4079 | 1/1 | 0.96 | 0.21 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3299 | 1/1 | 0.96 | 0.13 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3123 | 1/1 | 0.96 | 0.14 | 31,31,31,31 | 0 |
| 57 | MG | 2a | 1615 | 1/1 | 0.96 | 0.13 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3858 | 1/1 | 0.96 | 0.09 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3156 | 1/1 | 0.96 | 0.38 | 61,61,61,61 | 0 |
| 57 | MG | 1W | 202 | 1/1 | 0.96 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 4085 | 1/1 | 0.96 | 0.15 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3753 | 1/1 | 0.96 | 0.21 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3011 | 1/1 | 0.96 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3348 | 1/1 | 0.96 | 0.19 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3968 | 1/1 | 0.96 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | 1x | 115 | 1/1 | 0.96 | 0.23 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3755 | 1/1 | 0.96 | 0.14 | 17,17,17,17 | 0 |
| 57 | MG | 2A | 3577 | 1/1 | 0.96 | 0.14 | 55,55,55,55 | 0 |
| 57 | MG | 1Y | 201 | 1/1 | 0.96 | 0.22 | 47,47,47,47 | 0 |
| 57 | MG | 2a | 1630 | 1/1 | 0.96 | 0.29 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3165 | 1/1 | 0.96 | 0.13 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3031 | 1/1 | 0.96 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3515 | 1/1 | 0.96 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | 2a | 1635 | 1/1 | 0.96 | 0.27 | 67,67,67,67 | 0 |
| 57 | MG | 1A | 3868 | 1/1 | 0.96 | 0.23 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3585 | 1/1 | 0.96 | 0.13 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3254 | 1/1 | 0.96 | 0.13 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3587 | 1/1 | 0.96 | 0.11 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3180 | 1/1 | 0.96 | 0.21 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3587 | 1/1 | 0.96 | 0.11 | 37,37,37,37 | 0 |
| 57 | MG | 10 | 102 | 1/1 | 0.96 | 0.37 | 47,47,47,47 | 0 |
| 57 | MG | 2A | 3173 | 1/1 | 0.96 | 0.21 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3110 | 1/1 | 0.96 | 0.32 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3151 | 1/1 | 0.96 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3032 | 1/1 | 0.96 | 0.22 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3980 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3011 | 1/1 | 0.96 | 0.10 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3597 | 1/1 | 0.96 | 0.09 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3675 | 1/1 | 0.96 | 0.20 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3521 | 1/1 | 0.96 | 0.19 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3016 | 1/1 | 0.96 | 0.07 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 3677 | 1/1 | 0.96 | 0.20 | 25,25,25,25 | 0 |
| 57 | MG | 11 | 104 | 1/1 | 0.96 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3019 | 1/1 | 0.96 | 0.15 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3020 | 1/1 | 0.96 | 0.14 | 44,44,44,44 | 0 |
| 57 | MG | 12 | 101 | 1/1 | 0.96 | 0.20 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 3050 | 1/1 | 0.96 | 0.21 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3772 | 1/1 | 0.96 | 0.21 | 20,20,20,20 | 0 |
| 57 | MG | 1A | 3524 | 1/1 | 0.96 | 0.28 | 33,33,33,33 | 0 |
| 57 | MG | 2A | 3612 | 1/1 | 0.96 | 0.13 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3025 | 1/1 | 0.96 | 0.50 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3186 | 1/1 | 0.96 | 0.23 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3079 | 1/1 | 0.96 | 0.26 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3390 | 1/1 | 0.96 | 0.18 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3225 | 1/1 | 0.96 | 0.16 | 49,49,49,49 | 0 |
| 57 | MG | 1a | 1733 | 1/1 | 0.96 | 0.30 | 50,50,50,50 | 0 |
| 57 | MG | 15 | 102 | 1/1 | 0.96 | 0.18 | 35,35,35,35 | 0 |
| 57 | MG | 15 | 103 | 1/1 | 0.96 | 0.15 | 29,29,29,29 | 0 |
| 57 | MG | 15 | 104 | 1/1 | 0.96 | 0.23 | 28,28,28,28 | 0 |
| 57 | MG | 2A | 3200 | 1/1 | 0.96 | 0.13 | 52,52,52,52 | 0 |
| 57 | MG | 1a | 1737 | 1/1 | 0.96 | 0.20 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3991 | 1/1 | 0.96 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3012 | 1/1 | 0.96 | 0.09 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3403 | 1/1 | 0.96 | 0.18 | 60,60,60,60 | 0 |
| 57 | MG | 1B | 209 | 1/1 | 0.96 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3887 | 1/1 | 0.96 | 0.14 | 30,30,30,30 | 0 |
| 57 | MG | 17 | 102 | 1/1 | 0.96 | 0.13 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3265 | 1/1 | 0.96 | 0.18 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3634 | 1/1 | 0.96 | 0.15 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 3418 | 1/1 | 0.96 | 0.13 | 33,33,33,33 | 0 |
| 57 | MG | 2A | 3411 | 1/1 | 0.96 | 0.09 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3606 | 1/1 | 0.96 | 0.30 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3413 | 1/1 | 0.96 | 0.18 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3607 | 1/1 | 0.96 | 0.21 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3998 | 1/1 | 0.96 | 0.18 | 36,36,36,36 | 0 |
| 57 | MG | 1a | 1748 | 1/1 | 0.96 | 0.14 | 60,60,60,60 | 0 |
| 57 | MG | 18 | 3404 | 1/1 | 0.96 | 0.16 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3418 | 1/1 | 0.96 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3419 | 1/1 | 0.96 | 0.15 | 51,51,51,51 | 0 |
| 57 | MG | 1a | 1752 | 1/1 | 0.96 | 0.10 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3421 | 1/1 | 0.96 | 0.17 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3608 | 1/1 | 0.96 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | 1B | 218 | 1/1 | 0.96 | 0.21 | 60,60,60,60 | 0 |
| 57 | MG | 2a | 1700 | 1/1 | 0.96 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | 2a | 1701 | 1/1 | 0.96 | 0.15 | 75,75,75,75 | 0 |
| 57 | MG | 1A | 3472 | 1/1 | 0.96 | 0.25 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3267 | 1/1 | 0.96 | 0.16 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3221 | 1/1 | 0.96 | 0.19 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3189 | 1/1 | 0.96 | 0.12 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3655 | 1/1 | 0.96 | 0.28 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3162 | 1/1 | 0.96 | 0.35 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3231 | 1/1 | 0.96 | 0.19 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3063 | 1/1 | 0.96 | 0.20 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3424 | 1/1 | 0.96 | 0.22 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3797 | 1/1 | 0.96 | 0.11 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3228 | 1/1 | 0.96 | 0.33 | 59,59,59,59 | 0 |
| 57 | MG | 1a | 1608 | 1/1 | 0.96 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 4008 | 1/1 | 0.96 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | 2A | 3665 | 1/1 | 0.96 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | 1a | 1611 | 1/1 | 0.96 | 0.17 | 28,28,28,28 | 0 |
| 57 | MG | 2A | 3441 | 1/1 | 0.96 | 0.25 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 4009 | 1/1 | 0.96 | 0.15 | 16,16,16,16 | 0 |
| 57 | MG | 1A | 4010 | 1/1 | 0.96 | 0.20 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 4011 | 1/1 | 0.96 | 0.20 | 19,19,19,19 | 0 |
| 57 | MG | 2A | 3672 | 1/1 | 0.96 | 0.12 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3272 | 1/1 | 0.96 | 0.16 | 38,38,38,38 | 0 |
| 57 | MG | 1a | 1775 | 1/1 | 0.96 | 0.11 | 51,51,51,51 | 0 |
| 57 | MG | 2a | 1725 | 1/1 | 0.96 | 0.29 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3801 | 1/1 | 0.96 | 0.27 | 74,74,74,74 | 0 |
| 57 | MG | 2A | 3448 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3678 | 1/1 | 0.96 | 0.14 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3802 | 1/1 | 0.96 | 0.12 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3239 | 1/1 | 0.96 | 0.27 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3240 | 1/1 | 0.96 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 1a | 1620 | 1/1 | 0.96 | 0.12 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3084 | 1/1 | 0.96 | 0.26 | 27,27,27,27 | 0 |
| 57 | MG | 2a | 1734 | 1/1 | 0.96 | 0.28 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3072 | 1/1 | 0.96 | 0.22 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3456 | 1/1 | 0.96 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3040 | 1/1 | 0.96 | 0.12 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3458 | 1/1 | 0.96 | 0.10 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 4018 | 1/1 | 0.96 | 0.06 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3166 | 1/1 | 0.96 | 0.28 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3691 | 1/1 | 0.96 | 0.15 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3910 | 1/1 | 0.96 | 0.19 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3911 | 1/1 | 0.96 | 0.14 | 46,46,46,46 | 0 |
| 57 | MG | 2a | 1744 | 1/1 | 0.96 | 0.24 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3463 | 1/1 | 0.96 | 0.23 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3912 | 1/1 | 0.96 | 0.13 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3806 | 1/1 | 0.96 | 0.23 | 21,21,21,21 | 0 |
| 57 | MG | 1E | 302 | 1/1 | 0.96 | 0.31 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3236 | 1/1 | 0.96 | 0.24 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3699 | 1/1 | 0.96 | 0.20 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3712 | 1/1 | 0.96 | 0.18 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 4029 | 1/1 | 0.96 | 0.31 | 77,77,77,77 | 0 |
| 57 | MG | 2A | 3084 | 1/1 | 0.96 | 0.21 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3916 | 1/1 | 0.96 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | 1E | 309 | 1/1 | 0.96 | 0.30 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3623 | 1/1 | 0.96 | 0.11 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3624 | 1/1 | 0.96 | 0.15 | 21,21,21,21 | 0 |
| 57 | MG | 2A | 3709 | 1/1 | 0.96 | 0.13 | 64,64,64,64 | 0 |
| 57 | MG | 2A | 3479 | 1/1 | 0.96 | 0.07 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3480 | 1/1 | 0.96 | 0.13 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3488 | 1/1 | 0.96 | 0.25 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3714 | 1/1 | 0.96 | 0.06 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 3237 | 1/1 | 0.96 | 0.23 | 30,30,30,30 | 0 |
| 57 | MG | 1a | 1798 | 1/1 | 0.96 | 0.07 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3629 | 1/1 | 0.96 | 0.15 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3718 | 1/1 | 0.96 | 0.18 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3267 | 1/1 | 0.96 | 0.18 | 38,38,38,38 | 0 |
| 57 | MG | 1F | 301 | 1/1 | 0.96 | 0.35 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3487 | 1/1 | 0.96 | 0.11 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3488 | 1/1 | 0.96 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3724 | 1/1 | 0.96 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | 2A | 3727 | 1/1 | 0.96 | 0.09 | 58,58,58,58 | 0 |
| 57 | MG | 2a | 1774 | 1/1 | 0.96 | 0.10 | 61,61,61,61 | 0 |
| 57 | MG | 1F | 302 | 1/1 | 0.96 | 0.17 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3432 | 1/1 | 0.96 | 0.12 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3271 | 1/1 | 0.96 | 0.28 | 62,62,62,62 | 0 |
| 57 | MG | 1F | 305 | 1/1 | 0.96 | 0.23 | 34,34,34,34 | 0 |
| 57 | MG | 2B | 202 | 1/1 | 0.96 | 0.34 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3382 | 1/1 | 0.96 | 0.16 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3494 | 1/1 | 0.96 | 0.10 | 39,39,39,39 | 0 |
| 57 | MG | 2a | 1783 | 1/1 | 0.96 | 0.23 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3274 | 1/1 | 0.96 | 0.45 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3280 | 1/1 | 0.96 | 0.38 | 38,38,38,38 | 0 |
| 57 | MG | 1F | 310 | 1/1 | 0.96 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 4040 | 1/1 | 0.96 | 0.18 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3201 | 1/1 | 0.96 | 0.14 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3637 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3725 | 1/1 | 0.96 | 0.13 | 16,16,16,16 | 0 |
| 57 | MG | 1A | 3824 | 1/1 | 0.96 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3240 | 1/1 | 0.96 | 0.17 | 31,31,31,31 | 0 |
| 57 | MG | 1G | 205 | 1/1 | 0.96 | 0.10 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3507 | 1/1 | 0.96 | 0.11 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3826 | 1/1 | 0.96 | 0.12 | 31,31,31,31 | 0 |
| 57 | MG | 2t | 201 | 1/1 | 0.96 | 0.13 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3241 | 1/1 | 0.96 | 0.25 | 29,29,29,29 | 0 |
| 57 | MG | 2A | 3290 | 1/1 | 0.96 | 0.23 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3640 | 1/1 | 0.96 | 0.10 | 19,19,19,19 | 0 |
| 57 | MG | 1N | 203 | 1/1 | 0.96 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3140 | 1/1 | 0.96 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | 2D | 306 | 1/1 | 0.96 | 0.72 | 42,42,42,42 | 0 |
| 57 | MG | 2E | 301 | 1/1 | 0.96 | 0.25 | 59,59,59,59 | 0 |
| 57 | MG | 1a | 1822 | 1/1 | 0.96 | 0.10 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3203 | 1/1 | 0.96 | 0.19 | 22,22,22,22 | 0 |
| 58 | 6IF | 2A | 3731 | 32/32 | 0.96 | 0.24 | 28,36,41,45 | 0 |
| 57 | MG | 1A | 3834 | 1/1 | 0.96 | 0.14 | 40,40,40,40 | 0 |
| 59 | ZN | 2Y | 202 | 1/1 | 0.96 | 0.12 | 95,95,95,95 | 0 |
| 57 | MG | 1A | 3732 | 1/1 | 0.96 | 0.19 | 25,25,25,25 | 0 |
| 57 | MG | 2E | 306 | 1/1 | 0.96 | 0.22 | 57,57,57,57 | 0 |
| 57 | MG | 2E | 307 | 1/1 | 0.96 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3298 | 1/1 | 0.96 | 0.33 | 58,58,58,58 | 0 |
| 57 | MG | 1P | 202 | 1/1 | 0.97 | 0.14 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3302 | 1/1 | 0.97 | 0.34 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3160 | 1/1 | 0.97 | 0.20 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3609 | 1/1 | 0.97 | 0.16 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3430 | 1/1 | 0.97 | 0.31 | 36,36,36,36 | 0 |
| 57 | MG | 1Q | 202 | 1/1 | 0.97 | 0.17 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3266 | 1/1 | 0.97 | 0.23 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3113 | 1/1 | 0.97 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 4084 | 1/1 | 0.97 | 0.10 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3541 | 1/1 | 0.97 | 0.22 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3695 | 1/1 | 0.97 | 0.17 | 23,23,23,23 | 0 |
| 57 | MG | 1A | 4087 | 1/1 | 0.97 | 0.29 | 55,55,55,55 | 0 |
| 57 | MG | 2A | 3245 | 1/1 | 0.97 | 0.17 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1a | 1806 | 1/1 | 0.97 | 0.10 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3485 | 1/1 | 0.97 | 0.16 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3090 | 1/1 | 0.97 | 0.17 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3250 | 1/1 | 0.97 | 0.06 | 59,59,59,59 | 0 |
| 57 | MG | 2a | 1634 | 1/1 | 0.97 | 0.12 | 72,72,72,72 | 0 |
| 57 | MG | 1A | 3038 | 1/1 | 0.97 | 0.30 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3698 | 1/1 | 0.97 | 0.16 | 22,22,22,22 | 0 |
| 57 | MG | 1A | 4091 | 1/1 | 0.97 | 0.14 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3127 | 1/1 | 0.97 | 0.22 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3617 | 1/1 | 0.97 | 0.16 | 22,22,22,22 | 0 |
| 57 | MG | 2A | 3631 | 1/1 | 0.97 | 0.16 | 56,56,56,56 | 0 |
| 57 | MG | 1A | 3782 | 1/1 | 0.97 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3309 | 1/1 | 0.97 | 0.18 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3883 | 1/1 | 0.97 | 0.16 | 34,34,34,34 | 0 |
| 57 | MG | 1U | 203 | 1/1 | 0.97 | 0.19 | 28,28,28,28 | 0 |
| 57 | MG | 2a | 1645 | 1/1 | 0.97 | 0.08 | 54,54,54,54 | 0 |
| 57 | MG | 1U | 204 | 1/1 | 0.97 | 0.24 | 32,32,32,32 | 0 |
| 57 | MG | 2a | 1647 | 1/1 | 0.97 | 0.36 | 76,76,76,76 | 0 |
| 57 | MG | 1U | 205 | 1/1 | 0.97 | 0.20 | 30,30,30,30 | 0 |
| 57 | MG | 1U | 207 | 1/1 | 0.97 | 0.28 | 32,32,32,32 | 0 |
| 57 | MG | 1a | 1820 | 1/1 | 0.97 | 0.24 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3619 | 1/1 | 0.97 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | 1a | 1674 | 1/1 | 0.97 | 0.12 | 66,66,66,66 | 0 |
| 57 | MG | 1A | 3391 | 1/1 | 0.97 | 0.26 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3788 | 1/1 | 0.97 | 0.10 | 21,21,21,21 | 0 |
| 57 | MG | 1A | 3211 | 1/1 | 0.97 | 0.26 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3791 | 1/1 | 0.97 | 0.09 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 4102 | 1/1 | 0.97 | 0.16 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3082 | 1/1 | 0.97 | 0.28 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3351 | 1/1 | 0.97 | 0.22 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3440 | 1/1 | 0.97 | 0.24 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3709 | 1/1 | 0.97 | 0.24 | 23,23,23,23 | 0 |
| 57 | MG | 2a | 1662 | 1/1 | 0.97 | 0.12 | 55,55,55,55 | 0 |
| 57 | MG | 1X | 101 | 1/1 | 0.97 | 0.40 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3213 | 1/1 | 0.97 | 0.13 | 38,38,38,38 | 0 |
| 57 | MG | 1B | 201 | 1/1 | 0.97 | 0.23 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3626 | 1/1 | 0.97 | 0.19 | 10,10,10,10 | 0 |
| 57 | MG | 1A | 3800 | 1/1 | 0.97 | 0.22 | 20,20,20,20 | 0 |
| 57 | MG | 1A | 3314 | 1/1 | 0.97 | 0.18 | 59,59,59,59 | 0 |
| 57 | MG | 2A | 3122 | 1/1 | 0.97 | 0.33 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3283 | 1/1 | 0.97 | 0.30 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3123 | 1/1 | 0.97 | 0.10 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3285 | 1/1 | 0.97 | 0.28 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3046 | 1/1 | 0.97 | 0.21 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3473 | 1/1 | 0.97 | 0.16 | 68,68,68,68 | 0 |
| 57 | MG | 1A | 3215 | 1/1 | 0.97 | 0.26 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3633 | 1/1 | 0.97 | 0.21 | 42,42,42,42 | 0 |
| 57 | MG | 2a | 1677 | 1/1 | 0.97 | 0.23 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 3357 | 1/1 | 0.97 | 0.25 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3499 | 1/1 | 0.97 | 0.12 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3807 | 1/1 | 0.97 | 0.22 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3446 | 1/1 | 0.97 | 0.19 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3146 | 1/1 | 0.97 | 0.18 | 29,29,29,29 | 0 |
| 57 | MG | 1a | 1699 | 1/1 | 0.97 | 0.24 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3721 | 1/1 | 0.97 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3907 | 1/1 | 0.97 | 0.13 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3047 | 1/1 | 0.97 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3503 | 1/1 | 0.97 | 0.26 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3085 | 1/1 | 0.97 | 0.27 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3815 | 1/1 | 0.97 | 0.15 | 24,24,24,24 | 0 |
| 57 | MG | 1B | 220 | 1/1 | 0.97 | 0.20 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3450 | 1/1 | 0.97 | 0.15 | 32,32,32,32 | 0 |
| 57 | MG | 1B | 222 | 1/1 | 0.97 | 0.12 | 51,51,51,51 | 0 |
| 57 | MG | 2A | 3144 | 1/1 | 0.97 | 0.04 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3404 | 1/1 | 0.97 | 0.28 | 29,29,29,29 | 0 |
| 57 | MG | 1x | 109 | 1/1 | 0.97 | 0.10 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3727 | 1/1 | 0.97 | 0.10 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 3279 | 1/1 | 0.97 | 0.17 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3570 | 1/1 | 0.97 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | 1a | 1714 | 1/1 | 0.97 | 0.12 | 46,46,46,46 | 0 |
| 57 | MG | 15 | 101 | 1/1 | 0.97 | 0.21 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3132 | 1/1 | 0.97 | 0.18 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3501 | 1/1 | 0.97 | 0.15 | 54,54,54,54 | 0 |
| 57 | MG | 2A | 3502 | 1/1 | 0.97 | 0.15 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3283 | 1/1 | 0.97 | 0.61 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3323 | 1/1 | 0.97 | 0.18 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3317 | 1/1 | 0.97 | 0.15 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 4021 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 4022 | 1/1 | 0.97 | 0.16 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3409 | 1/1 | 0.97 | 0.22 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3704 | 1/1 | 0.97 | 0.06 | 53,53,53,53 | 0 |
| 57 | MG | 15 | 109 | 1/1 | 0.97 | 0.13 | 57,57,57,57 | 0 |
| 57 | MG | 2a | 1713 | 1/1 | 0.97 | 0.13 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3322 | 1/1 | 0.97 | 0.25 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 4024 | 1/1 | 0.97 | 0.20 | 33,33,33,33 | 0 |
| 57 | MG | 17 | 101 | 1/1 | 0.97 | 0.14 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3066 | 1/1 | 0.97 | 0.15 | 25,25,25,25 | 0 |
| 57 | MG | 2A | 3327 | 1/1 | 0.97 | 0.21 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3006 | 1/1 | 0.97 | 0.27 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3925 | 1/1 | 0.97 | 0.19 | 35,35,35,35 | 0 |
| 57 | MG | 17 | 104 | 1/1 | 0.97 | 0.15 | 31,31,31,31 | 0 |
| 57 | MG | 1D | 301 | 1/1 | 0.97 | 0.21 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3576 | 1/1 | 0.97 | 0.23 | 24,24,24,24 | 0 |
| 57 | MG | 1a | 1732 | 1/1 | 0.97 | 0.13 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3335 | 1/1 | 0.97 | 0.07 | 62,62,62,62 | 0 |
| 57 | MG | 1A | 3927 | 1/1 | 0.97 | 0.23 | 33,33,33,33 | 0 |
| 57 | MG | 18 | 3402 | 1/1 | 0.97 | 0.16 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3721 | 1/1 | 0.97 | 0.14 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3828 | 1/1 | 0.97 | 0.41 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3578 | 1/1 | 0.97 | 0.18 | 24,24,24,24 | 0 |
| 57 | MG | 2A | 3526 | 1/1 | 0.97 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | 2A | 3527 | 1/1 | 0.97 | 0.19 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3654 | 1/1 | 0.97 | 0.32 | 24,24,24,24 | 0 |
| 57 | MG | 1D | 310 | 1/1 | 0.97 | 0.20 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 4032 | 1/1 | 0.97 | 0.11 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3832 | 1/1 | 0.97 | 0.13 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 3286 | 1/1 | 0.97 | 0.23 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3109 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3347 | 1/1 | 0.97 | 0.29 | 39,39,39,39 | 0 |
| 57 | MG | 1A | 3222 | 1/1 | 0.97 | 0.22 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3836 | 1/1 | 0.97 | 0.11 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3195 | 1/1 | 0.97 | 0.29 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3659 | 1/1 | 0.97 | 0.14 | 69,69,69,69 | 0 |
| 57 | MG | 1A | 3839 | 1/1 | 0.97 | 0.16 | 36,36,36,36 | 0 |
| 57 | MG | 2B | 210 | 1/1 | 0.97 | 0.32 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3541 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | 1a | 1609 | 1/1 | 0.97 | 0.18 | 48,48,48,48 | 0 |
| 57 | MG | 2a | 1748 | 1/1 | 0.97 | 0.31 | 62,62,62,62 | 0 |
| 57 | MG | 1a | 1749 | 1/1 | 0.97 | 0.16 | 59,59,59,59 | 0 |
| 57 | MG | 1a | 1750 | 1/1 | 0.97 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3196 | 1/1 | 0.97 | 0.20 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3357 | 1/1 | 0.97 | 0.14 | 64,64,64,64 | 0 |
| 57 | MG | 1A | 3175 | 1/1 | 0.97 | 0.16 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3199 | 1/1 | 0.97 | 0.23 | 24,24,24,24 | 0 |
| 57 | MG | 2A | 3035 | 1/1 | 0.97 | 0.18 | 31,31,31,31 | 0 |
| 57 | MG | 1a | 1613 | 1/1 | 0.97 | 0.06 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1a | 1614 | 1/1 | 0.97 | 0.22 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3200 | 1/1 | 0.97 | 0.22 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3943 | 1/1 | 0.97 | 0.10 | 51,51,51,51 | 0 |
| 57 | MG | 1E | 316 | 1/1 | 0.97 | 0.08 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3944 | 1/1 | 0.97 | 0.14 | 12,12,12,12 | 0 |
| 57 | MG | 2A | 3369 | 1/1 | 0.97 | 0.20 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3559 | 1/1 | 0.97 | 0.08 | 61,61,61,61 | 0 |
| 57 | MG | 1A | 3076 | 1/1 | 0.97 | 0.11 | 33,33,33,33 | 0 |
| 57 | MG | 1a | 1761 | 1/1 | 0.97 | 0.14 | 42,42,42,42 | 0 |
| 57 | MG | 1F | 303 | 1/1 | 0.97 | 0.19 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3046 | 1/1 | 0.97 | 0.35 | 46,46,46,46 | 0 |
| 57 | MG | 1a | 1621 | 1/1 | 0.97 | 0.17 | 45,45,45,45 | 0 |
| 57 | MG | 2F | 304 | 1/1 | 0.97 | 0.49 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3468 | 1/1 | 0.97 | 0.19 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3377 | 1/1 | 0.97 | 0.33 | 56,56,56,56 | 0 |
| 57 | MG | 2A | 3568 | 1/1 | 0.97 | 0.15 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3947 | 1/1 | 0.97 | 0.15 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3155 | 1/1 | 0.97 | 0.15 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3949 | 1/1 | 0.97 | 0.18 | 30,30,30,30 | 0 |
| 57 | MG | 1a | 1768 | 1/1 | 0.97 | 0.15 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3208 | 1/1 | 0.97 | 0.32 | 58,58,58,58 | 0 |
| 57 | MG | 2A | 3574 | 1/1 | 0.97 | 0.35 | 77,77,77,77 | 0 |
| 57 | MG | 2T | 203 | 1/1 | 0.97 | 0.13 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3669 | 1/1 | 0.97 | 0.19 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3385 | 1/1 | 0.97 | 0.24 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 4055 | 1/1 | 0.97 | 0.09 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3056 | 1/1 | 0.97 | 0.18 | 28,28,28,28 | 0 |
| 57 | MG | 1a | 1773 | 1/1 | 0.97 | 0.09 | 57,57,57,57 | 0 |
| 57 | MG | 2a | 1786 | 1/1 | 0.97 | 0.12 | 53,53,53,53 | 0 |
| 57 | MG | 2A | 3580 | 1/1 | 0.97 | 0.10 | 49,49,49,49 | 0 |
| 57 | MG | 1a | 1774 | 1/1 | 0.97 | 0.08 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 3204 | 1/1 | 0.97 | 0.12 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3393 | 1/1 | 0.97 | 0.12 | 48,48,48,48 | 0 |
| 57 | MG | 2A | 3584 | 1/1 | 0.97 | 0.15 | 32,32,32,32 | 0 |
| 57 | MG | 2l | 202 | 1/1 | 0.97 | 0.22 | 65,65,65,65 | 0 |
| 57 | MG | 1A | 3851 | 1/1 | 0.97 | 0.21 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3009 | 1/1 | 0.97 | 0.12 | 22,22,22,22 | 0 |
| 57 | MG | 1A | 3528 | 1/1 | 0.97 | 0.25 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3473 | 1/1 | 0.97 | 0.11 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 4062 | 1/1 | 0.97 | 0.19 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3598 | 1/1 | 0.97 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3380 | 1/1 | 0.97 | 0.42 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3401 | 1/1 | 0.97 | 0.12 | 44,44,44,44 | 0 |
| 57 | MG | 1a | 1783 | 1/1 | 0.97 | 0.08 | 71,71,71,71 | 0 |
| 57 | MG | 1A | 3475 | 1/1 | 0.97 | 0.11 | 47,47,47,47 | 0 |
| 57 | MG | 1A | 3602 | 1/1 | 0.97 | 0.24 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3406 | 1/1 | 0.97 | 0.18 | 66,66,66,66 | 0 |
| 57 | MG | 2x | 105 | 1/1 | 0.97 | 0.13 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3859 | 1/1 | 0.97 | 0.15 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3381 | 1/1 | 0.97 | 0.18 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3862 | 1/1 | 0.97 | 0.17 | 56,56,56,56 | 0 |
| 58 | 6IF | 1A | 4109 | 32/32 | 0.97 | 0.21 | 18,25,31,31 | 0 |
| 57 | MG | 1A | 3764 | 1/1 | 0.97 | 0.11 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3477 | 1/1 | 0.97 | 0.20 | 51,51,51,51 | 0 |
| 57 | MG | 1A | 3684 | 1/1 | 0.97 | 0.16 | 20,20,20,20 | 0 |
| 57 | MG | 1A | 3300 | 1/1 | 0.97 | 0.29 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3604 | 1/1 | 0.97 | 0.13 | 53,53,53,53 | 0 |
| 59 | ZN | 29 | 501 | 1/1 | 0.97 | 0.10 | 66,66,66,66 | 0 |
| 57 | MG | 2a | 1613 | 1/1 | 0.97 | 0.09 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3124 | 1/1 | 0.97 | 0.20 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3033 | 1/1 | 0.98 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | 2a | 1682 | 1/1 | 0.98 | 0.17 | 66,66,66,66 | 0 |
| 57 | MG | 2A | 3367 | 1/1 | 0.98 | 0.29 | 39,39,39,39 | 0 |
| 57 | MG | 1a | 1730 | 1/1 | 0.98 | 0.19 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3287 | 1/1 | 0.98 | 0.15 | 39,39,39,39 | 0 |
| 57 | MG | 2A | 3611 | 1/1 | 0.98 | 0.18 | 55,55,55,55 | 0 |
| 57 | MG | 1A | 3350 | 1/1 | 0.98 | 0.47 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3013 | 1/1 | 0.98 | 0.27 | 30,30,30,30 | 0 |
| 57 | MG | 1X | 104 | 1/1 | 0.98 | 0.25 | 33,33,33,33 | 0 |
| 57 | MG | 1X | 105 | 1/1 | 0.98 | 0.09 | 42,42,42,42 | 0 |
| 57 | MG | 1A | 3192 | 1/1 | 0.98 | 0.27 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3618 | 1/1 | 0.98 | 0.09 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 4083 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 57 | MG | 2A | 3376 | 1/1 | 0.98 | 0.24 | 47,47,47,47 | 0 |
| 57 | MG | 2D | 305 | 1/1 | 0.98 | 0.13 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3108 | 1/1 | 0.98 | 0.23 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3154 | 1/1 | 0.98 | 0.20 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3239 | 1/1 | 0.98 | 0.27 | 30,30,30,30 | 0 |
| 57 | MG | 1E | 311 | 1/1 | 0.98 | 0.18 | 38,38,38,38 | 0 |
| 57 | MG | 2A | 3381 | 1/1 | 0.98 | 0.15 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3453 | 1/1 | 0.98 | 0.18 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3138 | 1/1 | 0.98 | 0.29 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 4016 | 1/1 | 0.98 | 0.14 | 21,21,21,21 | 0 |
| 57 | MG | 1n | 101 | 1/1 | 0.98 | 0.29 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 10 | 104 | 1/1 | 0.98 | 0.34 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3645 | 1/1 | 0.98 | 0.15 | 24,24,24,24 | 0 |
| 57 | MG | 2A | 3277 | 1/1 | 0.98 | 0.17 | 61,61,61,61 | 0 |
| 57 | MG | 2A | 3389 | 1/1 | 0.98 | 0.10 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3156 | 1/1 | 0.98 | 0.34 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3391 | 1/1 | 0.98 | 0.14 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3600 | 1/1 | 0.98 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3242 | 1/1 | 0.98 | 0.43 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3197 | 1/1 | 0.98 | 0.15 | 32,32,32,32 | 0 |
| 57 | MG | 1A | 3069 | 1/1 | 0.98 | 0.22 | 21,21,21,21 | 0 |
| 57 | MG | 1A | 3705 | 1/1 | 0.98 | 0.13 | 38,38,38,38 | 0 |
| 57 | MG | 1F | 307 | 1/1 | 0.98 | 0.22 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 3178 | 1/1 | 0.98 | 0.19 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3605 | 1/1 | 0.98 | 0.11 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3766 | 1/1 | 0.98 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3526 | 1/1 | 0.98 | 0.15 | 25,25,25,25 | 0 |
| 57 | MG | 2A | 3647 | 1/1 | 0.98 | 0.06 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3081 | 1/1 | 0.98 | 0.32 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3831 | 1/1 | 0.98 | 0.14 | 24,24,24,24 | 0 |
| 57 | MG | 2I | 101 | 1/1 | 0.98 | 0.50 | 52,52,52,52 | 0 |
| 57 | MG | 1A | 3563 | 1/1 | 0.98 | 0.19 | 34,34,34,34 | 0 |
| 57 | MG | 1A | 4104 | 1/1 | 0.98 | 0.23 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3036 | 1/1 | 0.98 | 0.17 | 23,23,23,23 | 0 |
| 57 | MG | 25 | 102 | 1/1 | 0.98 | 0.48 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3897 | 1/1 | 0.98 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3528 | 1/1 | 0.98 | 0.15 | 63,63,63,63 | 0 |
| 57 | MG | 1A | 3565 | 1/1 | 0.98 | 0.21 | 49,49,49,49 | 0 |
| 57 | MG | 1A | 3566 | 1/1 | 0.98 | 0.16 | 32,32,32,32 | 0 |
| 57 | MG | 15 | 106 | 1/1 | 0.98 | 0.14 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3071 | 1/1 | 0.98 | 0.18 | 16,16,16,16 | 0 |
| 57 | MG | 1A | 3037 | 1/1 | 0.98 | 0.21 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3662 | 1/1 | 0.98 | 0.10 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3661 | 1/1 | 0.98 | 0.10 | 62,62,62,62 | 0 |
| 57 | MG | 1a | 1770 | 1/1 | 0.98 | 0.21 | 60,60,60,60 | 0 |
| 57 | MG | 1A | 3569 | 1/1 | 0.98 | 0.23 | 44,44,44,44 | 0 |
| 57 | MG | 1N | 206 | 1/1 | 0.98 | 0.25 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3030 | 1/1 | 0.98 | 0.17 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3841 | 1/1 | 0.98 | 0.22 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 4041 | 1/1 | 0.98 | 0.11 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3665 | 1/1 | 0.98 | 0.20 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3669 | 1/1 | 0.98 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3022 | 1/1 | 0.98 | 0.14 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 2A | 3423 | 1/1 | 0.98 | 0.19 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3001 | 1/1 | 0.98 | 0.21 | 34,34,34,34 | 0 |
| 57 | MG | 1a | 1685 | 1/1 | 0.98 | 0.10 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3229 | 1/1 | 0.98 | 0.32 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3427 | 1/1 | 0.98 | 0.12 | 37,37,37,37 | 0 |
| 57 | MG | 2A | 3676 | 1/1 | 0.98 | 0.12 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3403 | 1/1 | 0.98 | 0.21 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 3783 | 1/1 | 0.98 | 0.15 | 17,17,17,17 | 0 |
| 57 | MG | 2A | 3315 | 1/1 | 0.98 | 0.22 | 59,59,59,59 | 0 |
| 57 | MG | 1P | 204 | 1/1 | 0.98 | 0.31 | 31,31,31,31 | 0 |
| 57 | MG | 2A | 3432 | 1/1 | 0.98 | 0.17 | 68,68,68,68 | 0 |
| 57 | MG | 2A | 3012 | 1/1 | 0.98 | 0.10 | 42,42,42,42 | 0 |
| 57 | MG | 2A | 3013 | 1/1 | 0.98 | 0.17 | 53,53,53,53 | 0 |
| 57 | MG | 2a | 1624 | 1/1 | 0.98 | 0.11 | 59,59,59,59 | 0 |
| 57 | MG | 1A | 3278 | 1/1 | 0.98 | 0.17 | 25,25,25,25 | 0 |
| 57 | MG | 1A | 3088 | 1/1 | 0.98 | 0.39 | 34,34,34,34 | 0 |
| 57 | MG | 2A | 3558 | 1/1 | 0.98 | 0.13 | 62,62,62,62 | 0 |
| 57 | MG | 2a | 1628 | 1/1 | 0.98 | 0.11 | 83,83,83,83 | 0 |
| 57 | MG | 1Q | 201 | 1/1 | 0.98 | 0.21 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3577 | 1/1 | 0.98 | 0.24 | 21,21,21,21 | 0 |
| 57 | MG | 2A | 3323 | 1/1 | 0.98 | 0.39 | 52,52,52,52 | 0 |
| 57 | MG | 2A | 3219 | 1/1 | 0.98 | 0.22 | 50,50,50,50 | 0 |
| 57 | MG | 1A | 4051 | 1/1 | 0.98 | 0.24 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3041 | 1/1 | 0.98 | 0.19 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 3311 | 1/1 | 0.98 | 0.29 | 50,50,50,50 | 0 |
| 57 | MG | 2A | 3566 | 1/1 | 0.98 | 0.19 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3918 | 1/1 | 0.98 | 0.14 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3790 | 1/1 | 0.98 | 0.10 | 29,29,29,29 | 0 |
| 57 | MG | 1A | 3281 | 1/1 | 0.98 | 0.22 | 28,28,28,28 | 0 |
| 57 | MG | 1a | 1700 | 1/1 | 0.98 | 0.25 | 45,45,45,45 | 0 |
| 57 | MG | 2A | 3700 | 1/1 | 0.98 | 0.06 | 58,58,58,58 | 0 |
| 57 | MG | 1A | 3282 | 1/1 | 0.98 | 0.45 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3922 | 1/1 | 0.98 | 0.15 | 20,20,20,20 | 0 |
| 57 | MG | 1A | 3168 | 1/1 | 0.98 | 0.32 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3077 | 1/1 | 0.98 | 0.24 | 24,24,24,24 | 0 |
| 57 | MG | 2A | 3453 | 1/1 | 0.98 | 0.14 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3795 | 1/1 | 0.98 | 0.20 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3285 | 1/1 | 0.98 | 0.18 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3860 | 1/1 | 0.98 | 0.21 | 15,15,15,15 | 0 |
| 57 | MG | 2A | 3131 | 1/1 | 0.98 | 0.34 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3631 | 1/1 | 0.98 | 0.23 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 3798 | 1/1 | 0.98 | 0.07 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3681 | 1/1 | 0.98 | 0.14 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3713 | 1/1 | 0.98 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3682 | 1/1 | 0.98 | 0.15 | 19,19,19,19 | 0 |
| 57 | MG | 2A | 3345 | 1/1 | 0.98 | 0.18 | 54,54,54,54 | 0 |
| 57 | MG | 1A | 3865 | 1/1 | 0.98 | 0.26 | 17,17,17,17 | 0 |
| 57 | MG | 2A | 3464 | 1/1 | 0.98 | 0.14 | 38,38,38,38 | 0 |
| 57 | MG | 1A | 3683 | 1/1 | 0.98 | 0.23 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3632 | 1/1 | 0.98 | 0.19 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3585 | 1/1 | 0.98 | 0.32 | 33,33,33,33 | 0 |
| 57 | MG | 1V | 201 | 1/1 | 0.98 | 0.25 | 24,24,24,24 | 0 |
| 57 | MG | 1D | 304 | 1/1 | 0.98 | 0.11 | 21,21,21,21 | 0 |
| 57 | MG | 1V | 203 | 1/1 | 0.98 | 0.23 | 30,30,30,30 | 0 |
| 57 | MG | 2A | 3471 | 1/1 | 0.98 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | 2A | 3725 | 1/1 | 0.98 | 0.14 | 62,62,62,62 | 0 |
| 57 | MG | 2A | 3726 | 1/1 | 0.98 | 0.13 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 4072 | 1/1 | 0.98 | 0.20 | 15,15,15,15 | 0 |
| 57 | MG | 1D | 307 | 1/1 | 0.98 | 0.23 | 36,36,36,36 | 0 |
| 57 | MG | 2A | 3045 | 1/1 | 0.98 | 0.16 | 26,26,26,26 | 0 |
| 57 | MG | 2A | 3249 | 1/1 | 0.98 | 0.11 | 49,49,49,49 | 0 |
| 57 | MG | 1V | 206 | 1/1 | 0.98 | 0.23 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3686 | 1/1 | 0.98 | 0.12 | 26,26,26,26 | 0 |
| 59 | ZN | 1Y | 205 | 1/1 | 0.98 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 4075 | 1/1 | 0.98 | 0.19 | 23,23,23,23 | 0 |
| 59 | ZN | 19 | 102 | 1/1 | 0.98 | 0.30 | 67,67,67,67 | 0 |
| 57 | MG | 1a | 1632 | 1/1 | 0.98 | 0.20 | 59,59,59,59 | 0 |
| 57 | MG | 1W | 203 | 1/1 | 0.98 | 0.27 | 35,35,35,35 | 0 |
| 59 | ZN | 25 | 104 | 1/1 | 0.98 | 0.20 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3545 | 1/1 | 0.98 | 0.22 | 59,59,59,59 | 0 |
| 57 | MG | 1a | 1727 | 1/1 | 0.98 | 0.24 | 40,40,40,40 | 0 |
| 57 | MG | 2A | 3364 | 1/1 | 0.98 | 0.12 | 47,47,47,47 | 0 |
| 60 | SF4 | 2d | 302 | 8/8 | 0.98 | 0.12 | 62,75,82,85 | 0 |
| 57 | MG | 1A | 3688 | 1/1 | 0.98 | 0.13 | 27,27,27,27 | 0 |
| 57 | MG | 1Y | 204 | 1/1 | 0.99 | 0.24 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3328 | 1/1 | 0.99 | 0.29 | 41,41,41,41 | 0 |
| 57 | MG | 2A | 3289 | 1/1 | 0.99 | 0.27 | 43,43,43,43 | 0 |
| 57 | MG | 1A | 3014 | 1/1 | 0.99 | 0.18 | 23,23,23,23 | 0 |
| 57 | MG | 1F | 306 | 1/1 | 0.99 | 0.25 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3021 | 1/1 | 0.99 | 0.20 | 22,22,22,22 | 0 |
| 57 | MG | 2A | 3436 | 1/1 | 0.99 | 0.15 | 36,36,36,36 | 0 |
| 57 | MG | 1A | 3068 | 1/1 | 0.99 | 0.21 | 26,26,26,26 | 0 |
| 57 | MG | 1B | 235 | 1/1 | 0.99 | 0.09 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3008 | 1/1 | 0.99 | 0.18 | 24,24,24,24 | 0 |

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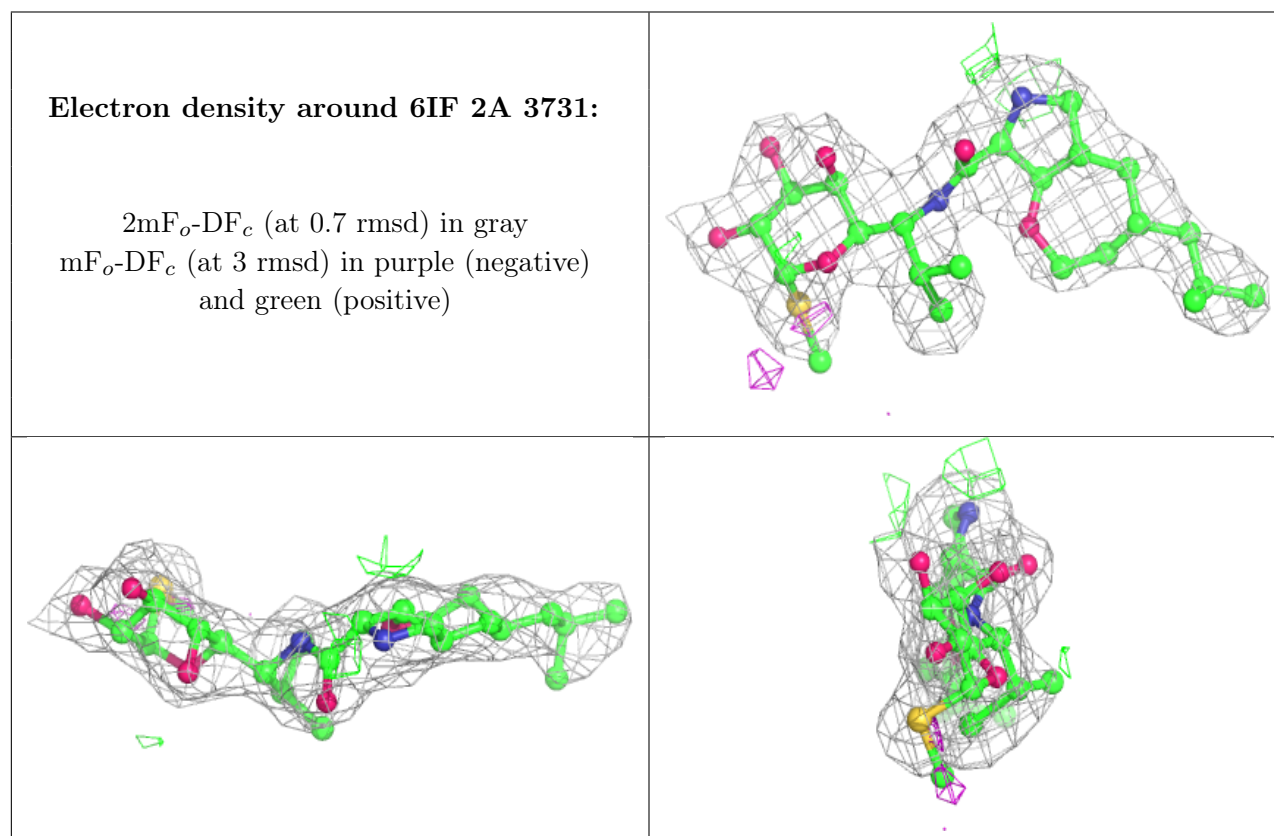
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3023 | 1/1 | 0.99 | 0.15 | 18,18,18,18 | 0 |
| 57 | MG | 2a | 1777 | 1/1 | 0.99 | 0.24 | 73,73,73,73 | 0 |
| 57 | MG | 1A | 3134 | 1/1 | 0.99 | 0.18 | 25,25,25,25 | 0 |
| 57 | MG | 2A | 3115 | 1/1 | 0.99 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | 2A | 3646 | 1/1 | 0.99 | 0.09 | 48,48,48,48 | 0 |
| 57 | MG | 1A | 3035 | 1/1 | 0.99 | 0.11 | 32,32,32,32 | 0 |
| 57 | MG | 10 | 108 | 1/1 | 0.99 | 0.15 | 46,46,46,46 | 0 |
| 57 | MG | 1A | 3228 | 1/1 | 0.99 | 0.31 | 24,24,24,24 | 0 |
| 57 | MG | 2A | 3546 | 1/1 | 0.99 | 0.18 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3784 | 1/1 | 0.99 | 0.19 | 22,22,22,22 | 0 |
| 57 | MG | 1D | 306 | 1/1 | 0.99 | 0.22 | 26,26,26,26 | 0 |
| 57 | MG | 1A | 3354 | 1/1 | 0.99 | 0.15 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3759 | 1/1 | 0.99 | 0.14 | 33,33,33,33 | 0 |
| 57 | MG | 1U | 206 | 1/1 | 0.99 | 0.33 | 33,33,33,33 | 0 |
| 57 | MG | 2F | 303 | 1/1 | 0.99 | 0.25 | 53,53,53,53 | 0 |
| 57 | MG | 1A | 3814 | 1/1 | 0.99 | 0.13 | 22,22,22,22 | 0 |
| 57 | MG | 1A | 3304 | 1/1 | 0.99 | 0.22 | 23,23,23,23 | 0 |
| 57 | MG | 1A | 3096 | 1/1 | 0.99 | 0.24 | 22,22,22,22 | 0 |
| 57 | MG | 2A | 3405 | 1/1 | 0.99 | 0.16 | 24,24,24,24 | 0 |
| 57 | MG | 1A | 3106 | 1/1 | 0.99 | 0.22 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3818 | 1/1 | 0.99 | 0.31 | 26,26,26,26 | 0 |
| 57 | MG | 1B | 215 | 1/1 | 0.99 | 0.17 | 35,35,35,35 | 0 |
| 57 | MG | 1A | 3627 | 1/1 | 0.99 | 0.22 | 37,37,37,37 | 0 |
| 57 | MG | 1A | 3738 | 1/1 | 0.99 | 0.10 | 52,52,52,52 | 0 |
| 57 | MG | 1E | 305 | 1/1 | 0.99 | 0.21 | 28,28,28,28 | 0 |
| 57 | MG | 1A | 3908 | 1/1 | 0.99 | 0.15 | 28,28,28,28 | 0 |
| 57 | MG | 2A | 3614 | 1/1 | 0.99 | 0.34 | 45,45,45,45 | 0 |
| 57 | MG | 1A | 3586 | 1/1 | 0.99 | 0.10 | 32,32,32,32 | 0 |
| 57 | MG | 2A | 3135 | 1/1 | 0.99 | 0.19 | 54,54,54,54 | 0 |
| 57 | MG | 1E | 308 | 1/1 | 0.99 | 0.10 | 30,30,30,30 | 0 |
| 57 | MG | 1A | 3740 | 1/1 | 0.99 | 0.16 | 44,44,44,44 | 0 |
| 57 | MG | 1A | 3174 | 1/1 | 0.99 | 0.21 | 25,25,25,25 | 0 |
| 57 | MG | 2A | 3183 | 1/1 | 0.99 | 0.06 | 58,58,58,58 | 0 |
| 57 | MG | 1a | 1668 | 1/1 | 0.99 | 0.12 | 57,57,57,57 | 0 |
| 57 | MG | 1A | 3717 | 1/1 | 0.99 | 0.20 | 27,27,27,27 | 0 |
| 57 | MG | 2A | 3186 | 1/1 | 0.99 | 0.27 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3651 | 1/1 | 0.99 | 0.17 | 15,15,15,15 | 0 |
| 59 | ZN | 16 | 102 | 1/1 | 0.99 | 0.21 | 41,41,41,41 | 0 |
| 57 | MG | 1A | 3161 | 1/1 | 0.99 | 0.17 | 27,27,27,27 | 0 |
| 57 | MG | 1A | 3360 | 1/1 | 0.99 | 0.14 | 33,33,33,33 | 0 |
| 57 | MG | 1A | 3029 | 1/1 | 0.99 | 0.22 | 31,31,31,31 | 0 |
| 57 | MG | 1A | 3150 | 1/1 | 0.99 | 0.28 | 32,32,32,32 | 0 |

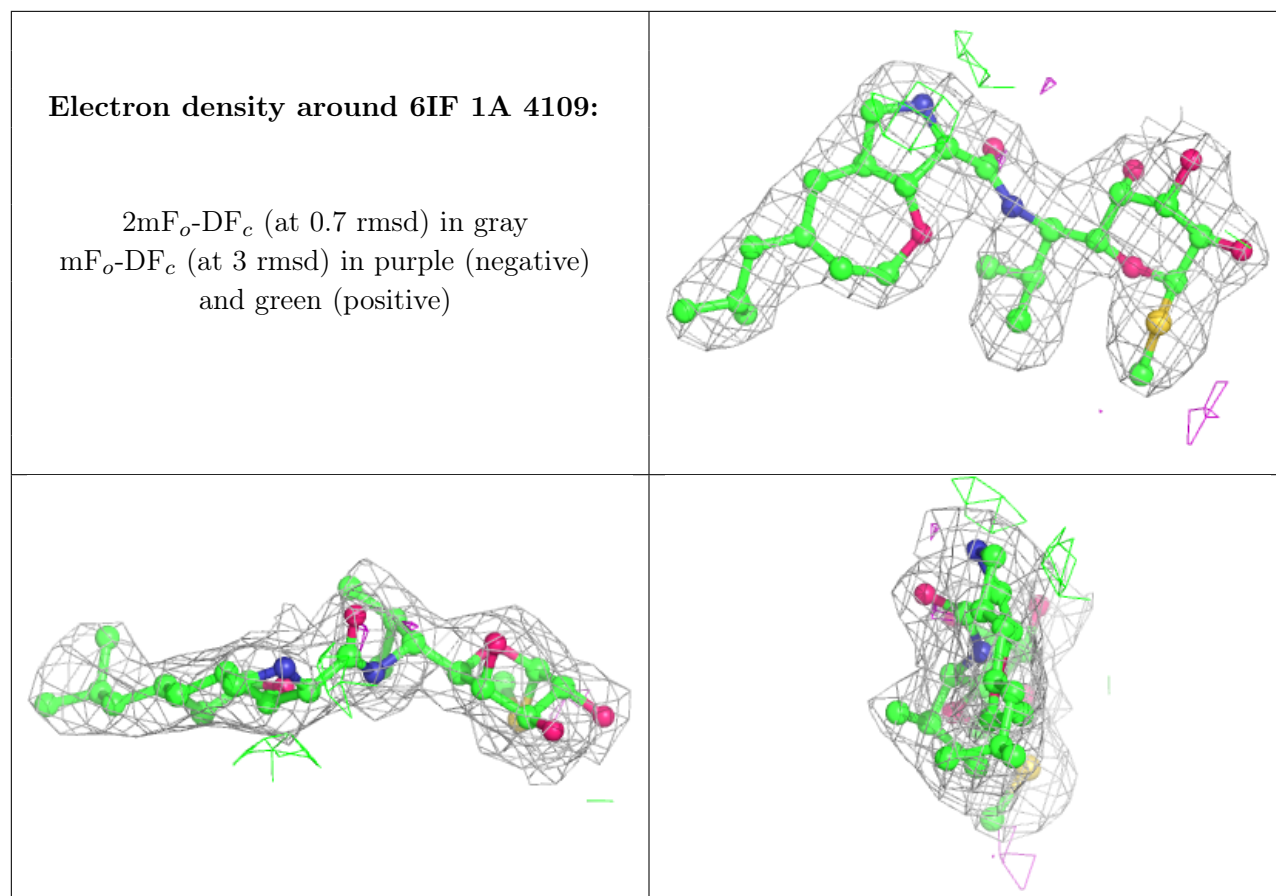
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 57 | MG | 1A | 3978 | 1/1 | 0.99 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3003 | 1/1 | 0.99 | 0.15 | 28,28,28,28 | 0 |
| 57 | MG | 2A | 3478 | 1/1 | 0.99 | 0.23 | 64,64,64,64 | 0 |
| 60 | SF4 | 1d | 302 | 8/8 | 0.99 | 0.16 | 57,60,69,76 | 0 |
| 57 | MG | 1A | 4073 | 1/1 | 0.99 | 0.20 | 28,28,28,28 | 0 |
| 57 | MG | 2A | 3686 | 1/1 | 0.99 | 0.17 | 30,30,30,30 | 0 |
| 57 | MG | 1a | 1805 | 1/1 | 1.00 | 0.10 | 40,40,40,40 | 0 |
| 57 | MG | 1A | 3592 | 1/1 | 1.00 | 0.15 | 37,37,37,37 | 0 |
| 59 | ZN | 1n | 103 | 1/1 | 1.00 | 0.15 | 63,63,63,63 | 0 |
| 59 | ZN | 15 | 110 | 1/1 | 1.00 | 0.27 | 47,47,47,47 | 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 ⓘ

There are no such residues in this entry.