



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 08:36 PM UTC

PDB ID : 8FC1 / pdb_00008fc1
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, hygromycin A, and erythromycin at 2.50Å resolution
Authors : Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2022-12-01
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

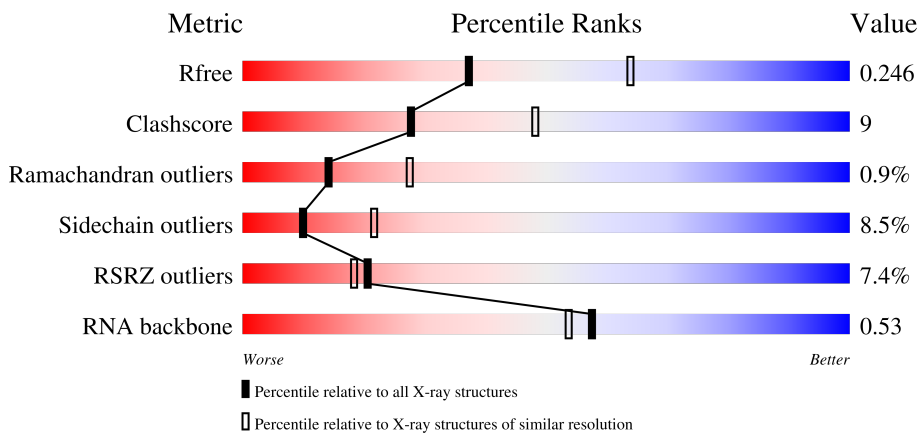
1 Overall quality at a glance i

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} | 180053 | 5829 (2.50-2.50) |
| Clashscore | 190562 | 6492 (2.50-2.50) |
| Ramachandran outliers | 187476 | 6378 (2.50-2.50) |
| Sidechain outliers | 187428 | 6380 (2.50-2.50) |
| RSRZ outliers | 180081 | 5833 (2.50-2.50) |
| RNA backbone | 3983 | 1003 (2.78-2.22) |

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 | |
| 1 | 2A | 2915 | |
| 2 | 1B | 121 | |
| 2 | 2B | 121 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------|
| 3 | 1D | 276 | 75% 21% . |
| 3 | 2D | 276 | 80% 17% . |
| 4 | 1E | 206 | 80% 17% .. |
| 4 | 2E | 206 | 74% 22% .. |
| 5 | 1F | 210 | 76% 18% . . |
| 5 | 2F | 210 | 62% 30% . . |
| 6 | 1G | 182 | 66% 29% . . |
| 6 | 2G | 182 | 62% 45% 49% 5% .. |
| 7 | 1H | 180 | 71% 23% . . |
| 7 | 2H | 180 | 19% 59% 34% . . |
| 8 | 1I | 148 | 74% 20% 5% . |
| 8 | 2I | 148 | 66% 30% .. |
| 9 | 1N | 140 | 75% 19% 6% |
| 9 | 2N | 140 | 79% 18% . |
| 10 | 1O | 122 | 84% 15% . |
| 10 | 2O | 122 | 79% 20% . |
| 11 | 1P | 150 | 78% 20% .. |
| 11 | 2P | 150 | 72% 26% .. |
| 12 | 1Q | 141 | 79% 18% .. |
| 12 | 2Q | 141 | 67% 28% . |
| 13 | 1R | 118 | 81% 17% . |
| 13 | 2R | 118 | 79% 19% . |
| 14 | 1S | 112 | 81% 13% . . . |
| 14 | 2S | 112 | 38% 54% 39% . . |
| 15 | 1T | 146 | 5% 71% 15% . 10% |




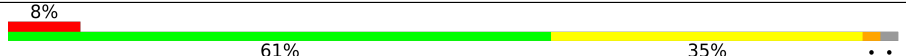
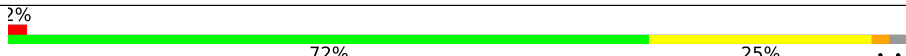
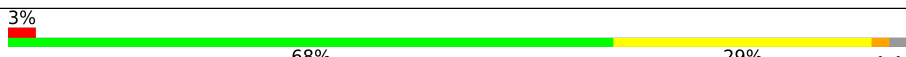
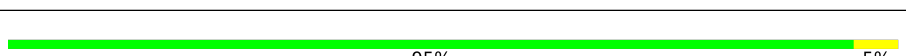
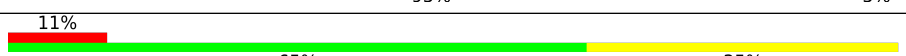
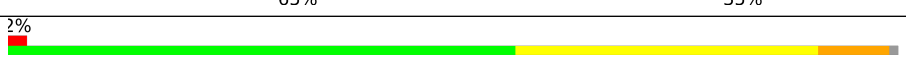


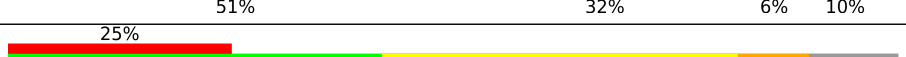

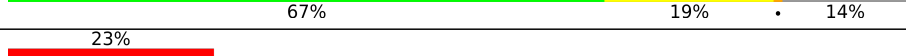





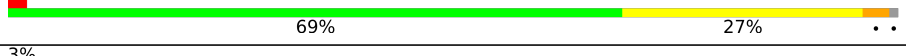

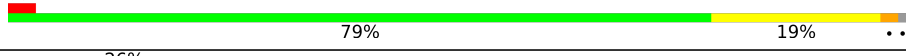



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------|
| 15 | 2T | 146 | 2% 71% 19% 10% |
| 16 | 1U | 118 | % 84% 14% .. |
| 16 | 2U | 118 | 69% 27% .. |
| 17 | 1V | 101 | % 77% 21% .. |
| 17 | 2V | 101 | 3% 77% 19% .. |
| 18 | 1W | 113 | 2% 81% 15% .. |
| 18 | 2W | 113 | 4% 78% 19% .. |
| 19 | 1X | 96 | 3% 74% 20% 5% . |
| 19 | 2X | 96 | 4% 77% 18% .. |
| 20 | 1Y | 110 | 3% 75% 22% .. |
| 20 | 2Y | 110 | 15% 68% 25% . . |
| 21 | 1Z | 206 | 4% 73% 23% .. |
| 21 | 2Z | 206 | 18% 62% 33% .. |
| 22 | 10 | 85 | 2% 80% 9% . 9% |
| 22 | 20 | 85 | 8% 79% 11% . 9% |
| 23 | 11 | 98 | % 76% 22% .. |
| 23 | 21 | 98 | 2% 76% 20% .. |
| 24 | 12 | 72 | 3% 78% 18% .. |
| 24 | 22 | 72 | % 67% 29% .. |
| 25 | 13 | 60 | 2% 75% 22% .. |
| 25 | 23 | 60 | 5% 62% 33% .. |
| 26 | 14 | 71 | 20% 63% 23% 10% .. |
| 26 | 24 | 71 | 65% 37% 51% 10% . |
| 27 | 15 | 60 | 72% 22% 5% . |
| 27 | 25 | 60 | 2% 77% 22% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 28 | 16 | 54 |  |
| 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 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------|
| 40 | 2i | 128 | 51% 46% 48% 5% |
| 41 | 1j | 105 | 27% 54% 33% 8% |
| 41 | 2j | 105 | 44% 53% 33% 5% 9% |
| 42 | 1k | 129 | 5% 70% 16% 12% |
| 42 | 2k | 129 | 12% 73% 14% 12% |
| 43 | 1l | 132 | 5% 78% 14% 8% |
| 43 | 2l | 132 | 7% 73% 15% 8% |
| 44 | 1m | 126 | 8% 60% 27% 5% 8% |
| 44 | 2m | 126 | 33% 44% 41% 5% 10% |
| 45 | 1n | 61 | 3% 59% 36% |
| 45 | 2n | 61 | 44% 67% 31% |
| 46 | 1o | 89 | 3% 66% 30% |
| 46 | 2o | 89 | 7% 65% 30% |
| 47 | 1p | 88 | 16% 50% 36% 7% 7% |
| 47 | 2p | 88 | 14% 60% 30% 7% |
| 48 | 1q | 105 | 5% 70% 23% 6% |
| 48 | 2q | 105 | 7% 70% 24% 6% |
| 49 | 1r | 88 | 63% 15% 23% |
| 49 | 2r | 88 | 3% 57% 20% 23% |
| 50 | 1s | 93 | 4% 56% 30% 11% |
| 50 | 2s | 93 | 48% 43% 41% 5% 11% |
| 51 | 1t | 106 | 14% 62% 25% 9% |
| 51 | 2t | 106 | 6% 67% 23% 8% |
| 52 | 1u | 27 | 19% 48% 37% 15% |
| 52 | 2u | 27 | 44% 56% 26% 15% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53 | 1y | 113 | |
| 53 | 2y | 113 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | MG | 1a | 1877 | - | - | - | X |
| 54 | MG | 2a | 3006 | - | - | - | X |
| 54 | MG | 2a | 3010 | - | - | - | X |
| 57 | MPD | 1a | 1880 | - | - | X | - |

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 296967 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 |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | 1A | 2872 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61869 | 27540 | 11574 | 19884 | 2871 | | | |
| 1 | 2A | 2867 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61758 | 27491 | 11552 | 19850 | 2865 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22 | 10 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 608 | 375 | 129 | 103 | 1 | | | |
| 22 | 20 | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 608 | 375 | 129 | 103 | 1 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|------|---------|---------|
| 54 | 1A | 1040 | Total | Mg | 0 | 0 |
| | | | 1040 | 1040 | | |
| 54 | 1B | 29 | Total | Mg | 0 | 0 |
| | | | 29 | 29 | | |
| 54 | 1D | 18 | Total | Mg | 0 | 0 |
| | | | 18 | 18 | | |
| 54 | 1E | 8 | Total | Mg | 0 | 0 |
| | | | 8 | 8 | | |
| 54 | 1F | 18 | Total | Mg | 0 | 0 |
| | | | 18 | 18 | | |
| 54 | 1G | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 54 | 1H | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 54 | 1N | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 54 | 1O | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | 1P | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 54 | 1Q | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 54 | 1R | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 54 | 1T | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 54 | 1U | 7 | Total | Mg | 0 | 0 |
| | | | 7 | 7 | | |
| 54 | 1V | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |
| 54 | 1W | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 54 | 1Y | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 54 | 1Z | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 54 | 10 | 8 | Total Mg 8 8 | 0 | 0 |
| 54 | 11 | 5 | Total Mg 5 5 | 0 | 0 |
| 54 | 13 | 3 | Total Mg 3 3 | 0 | 0 |
| 54 | 14 | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 15 | 8 | Total Mg 8 8 | 0 | 0 |
| 54 | 17 | 6 | Total Mg 6 6 | 0 | 0 |
| 54 | 18 | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 19 | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 1a | 279 | Total Mg 279 279 | 0 | 0 |
| 54 | 1b | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 1d | 5 | Total Mg 5 5 | 0 | 0 |
| 54 | 1e | 3 | Total Mg 3 3 | 0 | 0 |
| 54 | 1f | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 1g | 3 | Total Mg 3 3 | 0 | 0 |
| 54 | 1h | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 1i | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 1k | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 1l | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 1m | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 1n | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 1o | 1 | Total Mg 1 1 | 0 | 0 |

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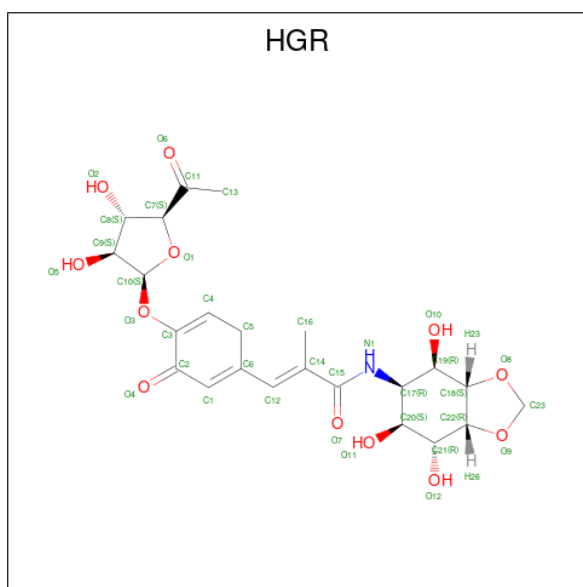
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|------------|--------------|-----------------|---------------------|----------------|----------------|
| 54 | 1t | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 1y | 3 | Total Mg 3 3 | 0 | 0 |
| 54 | 2A | 730 | Total Mg 730 730 | 0 | 0 |
| 54 | 2B | 18 | Total Mg 18 18 | 0 | 0 |
| 54 | 2D | 13 | Total Mg 13 13 | 0 | 0 |
| 54 | 2E | 6 | Total Mg 6 6 | 0 | 0 |
| 54 | 2F | 4 | Total Mg 4 4 | 0 | 0 |
| 54 | 2G | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 2I | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2O | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 2P | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2Q | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2R | 3 | Total Mg 3 3 | 0 | 0 |
| 54 | 2T | 3 | Total Mg 3 3 | 0 | 0 |
| 54 | 2U | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2V | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 2W | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 2X | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2Y | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 20 | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 21 | 2 | Total Mg 2 2 | 0 | 0 |

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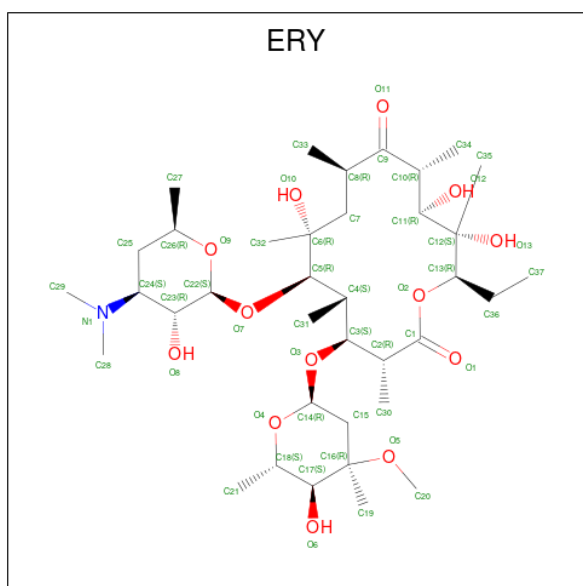
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 54 | 23 | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 25 | 3 | Total Mg 3 3 | 0 | 0 |
| 54 | 27 | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 28 | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 2a | 190 | Total Mg 190 190 | 0 | 0 |
| 54 | 2e | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 2f | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2j | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2k | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2n | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2r | 2 | Total Mg 2 2 | 0 | 0 |
| 54 | 2t | 1 | Total Mg 1 1 | 0 | 0 |
| 54 | 2y | 1 | Total Mg 1 1 | 0 | 0 |

- Molecule 55 is Hygromycin A (CCD ID: HGR) (formula: C₂₃H₂₉NO₁₂) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|---|---------|---------|---|
| | | | Total | C | N | | | O |
| 55 | 1A | 1 | 36 | 23 | 1 | 12 | 0 | 0 |
| 55 | 2A | 1 | 36 | 23 | 1 | 12 | 0 | 0 |

- Molecule 56 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



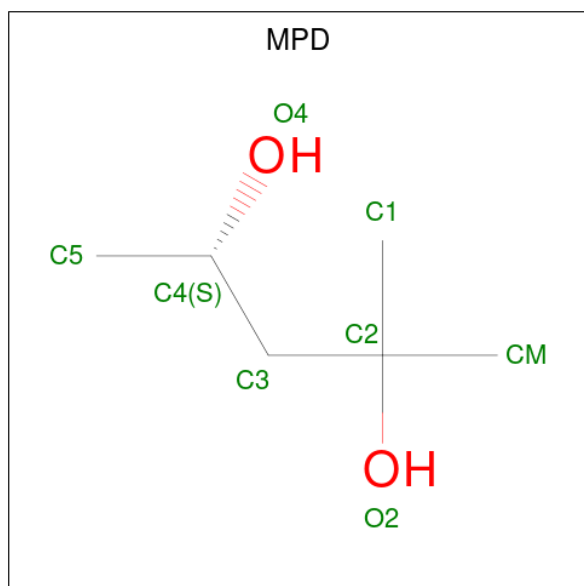
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------|----|---|---------|---------|---|
| | | | Total | C | N | | | O |
| 56 | 1A | 1 | 51 | 37 | 1 | 13 | 0 | 0 |

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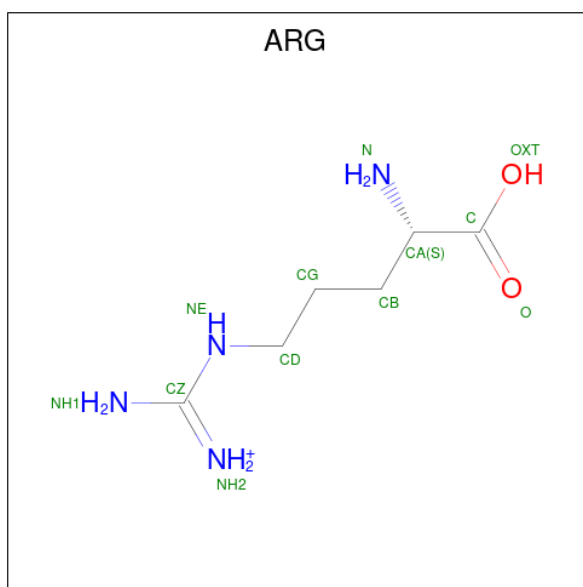
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| | | | Total | C | N | O | | |
| 56 | 2A | 1 | 51 | 37 | 1 | 13 | 0 | 0 |

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| | | | Total | C | O | | |
| 57 | 1A | 1 | 8 | 6 | 2 | 0 | 0 |
| 57 | 1T | 1 | 8 | 6 | 2 | 0 | 0 |
| 57 | 18 | 1 | 8 | 6 | 2 | 0 | 0 |
| 57 | 1a | 1 | 8 | 6 | 2 | 0 | 0 |
| 57 | 2A | 1 | 8 | 6 | 2 | 0 | 0 |
| 57 | 2A | 1 | 8 | 6 | 2 | 0 | 0 |
| 57 | 2B | 1 | 8 | 6 | 2 | 0 | 0 |

- Molecule 58 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 58 | 1B | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 6 | 4 | 2 | | |
| 58 | 1F | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 6 | 4 | 2 | | |

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

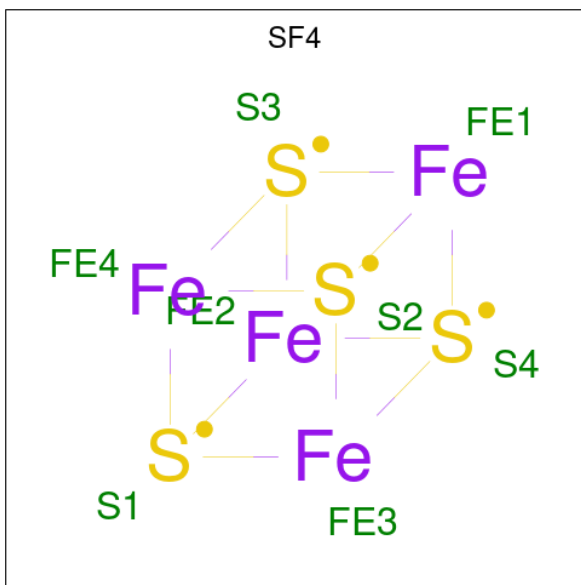
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59 | 1Y | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 14 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 15 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 16 | 1 | 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 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 59 | 29 | 1 | Total Zn 1 1 | 0 | 0 |
| 59 | 2n | 1 | Total Zn 1 1 | 0 | 0 |

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 61 | 1A | 3898 | Total O 3898 3898 | 0 | 0 |
| 61 | 1B | 94 | Total O 94 94 | 0 | 0 |
| 61 | 1D | 103 | Total O 103 103 | 0 | 0 |
| 61 | 1E | 68 | Total O 68 68 | 0 | 0 |
| 61 | 1F | 64 | Total O 64 64 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 61 | 1G | 16 | Total 16 | O 16 | 0 | 0 |
| 61 | 1H | 15 | Total 15 | O 15 | 0 | 0 |
| 61 | 1I | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | 1N | 45 | Total 45 | O 45 | 0 | 0 |
| 61 | 1O | 22 | Total 22 | O 22 | 0 | 0 |
| 61 | 1P | 56 | Total 56 | O 56 | 0 | 0 |
| 61 | 1Q | 37 | Total 37 | O 37 | 0 | 0 |
| 61 | 1R | 29 | Total 29 | O 29 | 0 | 0 |
| 61 | 1S | 12 | Total 12 | O 12 | 0 | 0 |
| 61 | 1T | 37 | Total 37 | O 37 | 0 | 0 |
| 61 | 1U | 41 | Total 41 | O 41 | 0 | 0 |
| 61 | 1V | 34 | Total 34 | O 34 | 0 | 0 |
| 61 | 1W | 27 | Total 27 | O 27 | 0 | 0 |
| 61 | 1X | 27 | Total 27 | O 27 | 0 | 0 |
| 61 | 1Y | 16 | Total 16 | O 16 | 0 | 0 |
| 61 | 1Z | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | 10 | 21 | Total 21 | O 21 | 0 | 0 |
| 61 | 11 | 28 | Total 28 | O 28 | 0 | 0 |
| 61 | 12 | 14 | Total 14 | O 14 | 0 | 0 |
| 61 | 13 | 22 | Total 22 | O 22 | 0 | 0 |
| 61 | 14 | 4 | Total 4 | O 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 61 | 15 | 25 | Total O 25 25 | 0 | 0 |
| 61 | 16 | 21 | Total O 21 21 | 0 | 0 |
| 61 | 17 | 13 | Total O 13 13 | 0 | 0 |
| 61 | 18 | 23 | Total O 23 23 | 0 | 0 |
| 61 | 19 | 2 | Total O 2 2 | 0 | 0 |
| 61 | 1a | 447 | Total O 447 447 | 0 | 0 |
| 61 | 1b | 1 | Total O 1 1 | 0 | 0 |
| 61 | 1c | 2 | Total O 2 2 | 0 | 0 |
| 61 | 1d | 9 | Total O 9 9 | 0 | 0 |
| 61 | 1e | 5 | Total O 5 5 | 0 | 0 |
| 61 | 1f | 1 | Total O 1 1 | 0 | 0 |
| 61 | 1h | 1 | Total O 1 1 | 0 | 0 |
| 61 | 1j | 1 | Total O 1 1 | 0 | 0 |
| 61 | 1l | 3 | Total O 3 3 | 0 | 0 |
| 61 | 1o | 2 | Total O 2 2 | 0 | 0 |
| 61 | 1p | 2 | Total O 2 2 | 0 | 0 |
| 61 | 1y | 1 | Total O 1 1 | 0 | 0 |
| 61 | 2A | 1941 | Total O 1941 1941 | 0 | 0 |
| 61 | 2B | 45 | Total O 45 45 | 0 | 0 |
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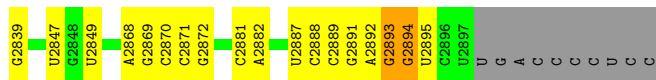
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|-----|-------|----------|-------------|---------|---------|---------|
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| 61 | 2H | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 2I | 1 | Total 1 | O 1 | 0 | 0 |
| 61 | 2N | 3 | Total 3 | O 3 | 0 | 0 |
| 61 | 2O | 10 | Total 10 | O 10 | 0 | 0 |
| 61 | 2P | 19 | Total 19 | O 19 | 0 | 0 |
| 61 | 2Q | 13 | Total 13 | O 13 | 0 | 0 |
| 61 | 2R | 17 | Total 17 | O 17 | 0 | 0 |
| 61 | 2T | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | 2U | 7 | Total 7 | O 7 | 0 | 0 |
| 61 | 2V | 4 | Total 4 | O 4 | 0 | 0 |
| 61 | 2W | 20 | Total 20 | O 20 | 0 | 0 |
| 61 | 2X | 7 | Total 7 | O 7 | 0 | 0 |
| 61 | 2Y | 2 | Total 2 | O 2 | 0 | 0 |
| 61 | 2Z | 7 | Total 7 | O 7 | 0 | 0 |
| 61 | 20 | 5 | Total 5 | O 5 | 0 | 0 |
| 61 | 21 | 15 | Total 15 | O 15 | 0 | 0 |
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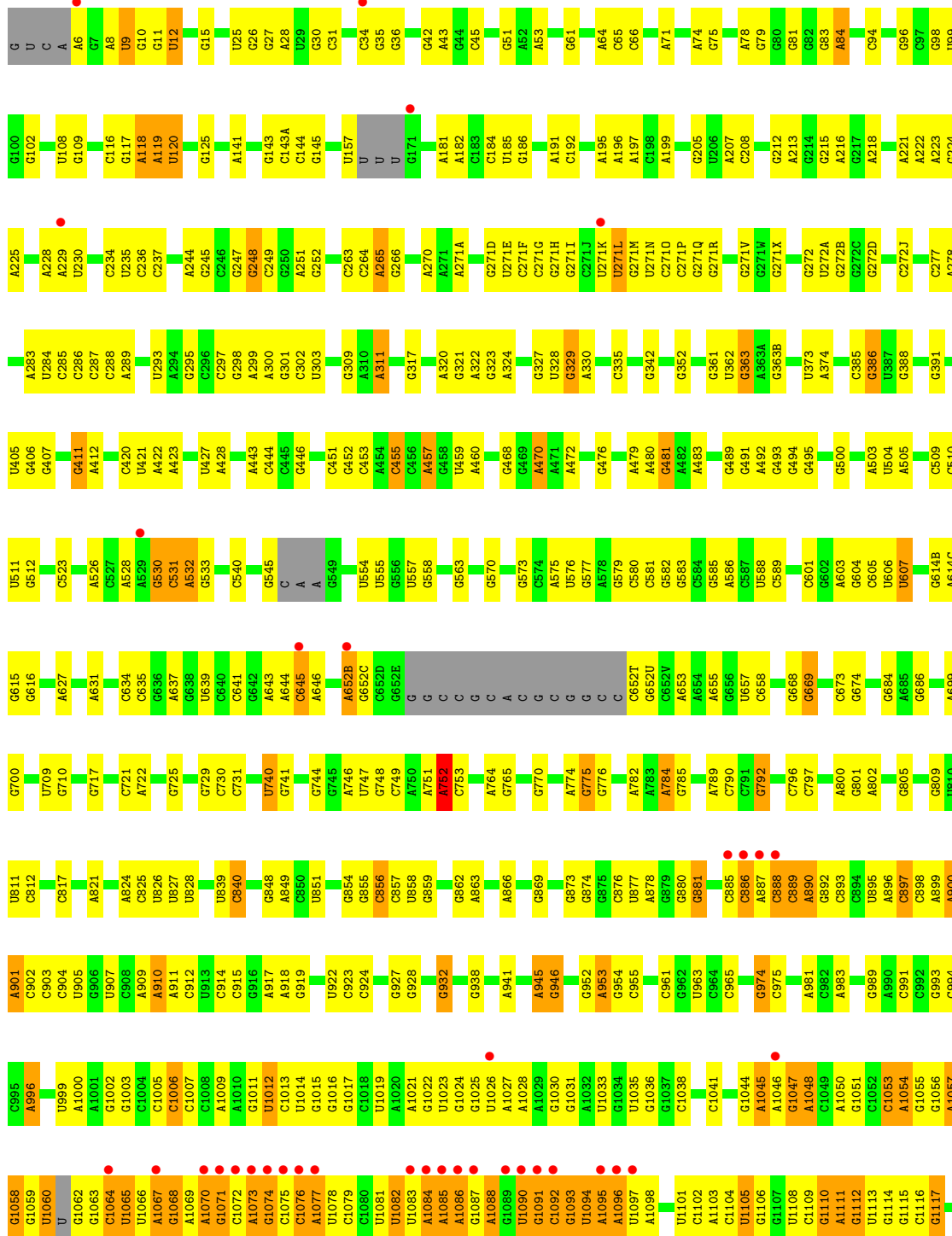
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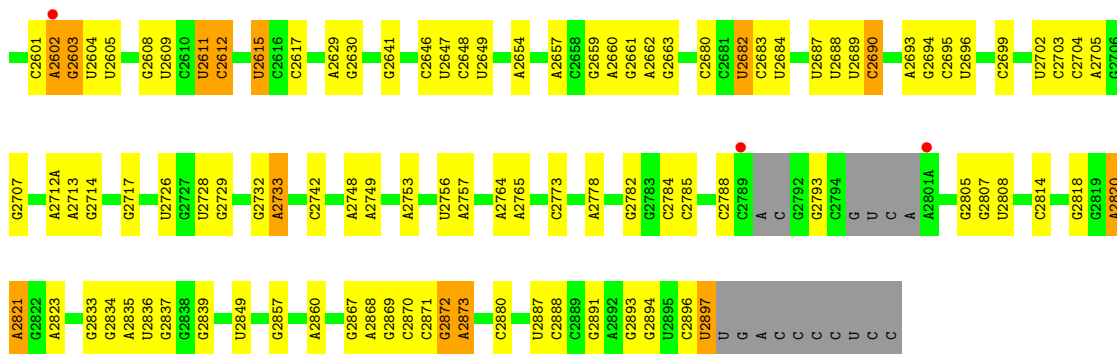
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| 61 | 28 | 9 | Total O 9 9 | 0 | 0 |
| 61 | 2a | 266 | Total O 266 266 | 0 | 0 |
| 61 | 2d | 4 | Total O 4 4 | 0 | 0 |
| 61 | 2e | 1 | Total O 1 1 | 0 | 0 |
| 61 | 2l | 1 | Total O 1 1 | 0 | 0 |
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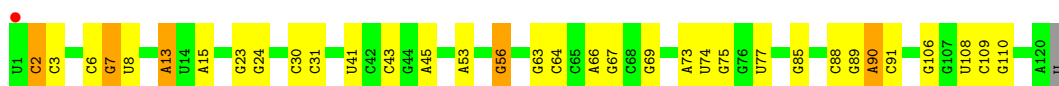
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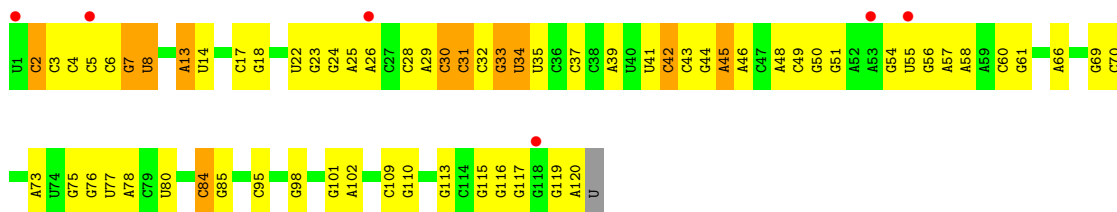
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| U2492 | G2290 | C2177 | A2117 | G2023 | A1912 | G1772 | G1630 | G1332 | A1226 | A1126 |
| G2493 | U2291 | C2178 | A2118 | G2023 | A1913 | A1773 | G1529 | G1332 | G1227 | A1127 |
| U2494 | C2292 | C2179 | A2119 | G2027 | C1631 | A1773 | G1530 | G1332 | A1128 | A1128 |
| A2497 | C2293 | U2180 | G2120 | G2027 | U1915 | U1778 | C1531 | G1336 | G1229 | A1129 |
| C2498 | C2294 | G2181 | G2121 | G2029 | A1916 | U1779 | C1532 | G1337 | G1229 | U1130 |
| C2499 | C2295 | C2183 | U2122 | A2030 | U1917 | A1780 | G1640 | G1340 | C1230 | C1135 |
| | U2296 | G2184 | G2123 | A2031 | C1920 | C1781 | A1642 | U1340 | G1231 | C1136 |
| | C2297 | C2185 | G2124 | G2032 | G1921 | U1782 | A1642 | U1341 | G1232 | G1137 |
| | A2298 | G2186 | A2125 | A2033 | G1921 | A1783 | G1647 | A1342 | G1236 | G1138 |
| | C2299 | G2187 | A2126 | G2037 | A1927 | A1784 | A1449 | A1354 | U1237 | G1153 |
| | A2305 | G2188 | G2127 | G2038 | A1928 | A1785 | G1538 | G1354 | A1237 | G1154 |
| | C2306 | U2189 | G2128 | G2038 | A1929 | A1786 | G1539 | G1355 | G1238 | A1155 |
| | C2307 | G2190 | G2129 | A2042 | G1930 | A1786 | U1540 | G1356 | G1239 | A1156 |
| | G2308 | G2191 | U2130 | U2043 | U1931 | A1791 | G1657 | U1357 | U1240 | |
| | A2311 | G2192 | U2131 | C2044 | U1932 | U1794 | C1658 | A1359 | U1241 | |
| | U2312 | G2198 | U2132 | C2047 | G1933 | C1795 | A1665 | A1360 | U1242 | |
| | C2313 | U2203 | U2133 | U2047 | A1937 | U1796 | G1667 | G1364 | G1250 | |
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| | C2316 | G2207 | C2137 | G2056 | U1940 | G1799 | A1669 | A1367 | U1159 | |
| | C2317 | A2208 | G2138 | U2074 | G1941 | C1800 | C1670 | A1367 | G1160 | |
| | G2318 | U2218 | C2139 | U2075 | G1942 | A1801 | G1674 | A1368 | G1256 | |
| | C2319 | G2219 | C2140 | A2059 | C1942 | A1802 | | G1369 | U1165 | |
| | A2320 | G2223 | G2141 | A2060 | U1952 | A1803 | U1688 | C1370 | C1166 | |
| | A2321 | G2224 | C2142 | G2061 | G1952 | U1804 | U1688 | G1371 | U1167 | |
| | A2322 | G2225 | C2143 | G2069 | U1955 | A1815 | G1696 | U1372 | G1171 | |
| | G2325 | A2225 | U2144 | G2069 | U1956 | A1816 | G1697 | A1378 | G | |
| | C2326 | C2226 | C2145 | U2074 | C1962 | G1817 | U1578 | A1379 | A | |
| | G2329 | G2239 | C2146 | U2075 | U1963 | G1817 | G1699 | G1380 | U | |
| | A2327 | U2243 | G2147 | U2079 | G1967 | U1818 | A1700 | U1405 | G | |
| | C2328 | U2243 | U2150 | U2086 | C1968 | G1826 | A1701 | U1406 | U | |
| | A2429 | U2244 | G2151 | U2086 | A1969 | G1827 | A1490 | G1410 | C1200 | |
| | A2430 | U2245 | G2152 | G2087 | A1970 | G1828 | C1582 | C1411 | C1201 | |
| | A2435 | U2245 | G2153 | G2087 | A1971 | U1833 | G1493 | C1412 | G1202 | |
| | G2436 | G2251 | G2154 | U2092 | A1972 | U1833 | A1496 | C1413 | A1204 | |
| | A2439 | G2255 | G2155 | G2093 | G1984 | G1839 | U1497 | G1414 | U1205 | |
| | C2440 | G2255 | G2156 | G2093 | U1984 | G1840 | U1497 | G1415 | G1209 | |
| | C2441 | U2262 | G2157 | G2096 | G1991 | G1840 | C1498 | C1416 | A1210 | |
| | A2448 | U2262 | A2158 | U2099 | U1991 | U1847 | U1503 | C1417 | U1211 | |
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| | G2454 | A2269 | C2161 | G2101 | C1996 | G1858 | C1506 | U1420 | G1221A | |
| | A2564 | A2269 | C2162 | U2102 | G1997 | G1858 | C1507 | C1421 | C1222 | |
| | A2565 | A2273 | C2163 | C2103 | G1997 | U1864 | A1508 | G1422 | | |
| | A2566 | A2274 | G2164 | G2104 | G2000 | A1877 | C1509 | G1416 | | |
| | G2567 | C2275 | G2165 | C2105 | A2001 | G1878 | A1509A | C1417 | | |
| | | G2280 | G2166 | G2106 | G2002 | G1878 | A1509B | G1418 | | |
| | | G2281 | C2168 | C2107 | G2002 | G1878 | G1510 | G1418 | | |
| | | G2282 | A2169 | C2108 | C2006 | G1889 | C1607 | U1419 | | |
| | | G2283 | A2170 | C2109 | C2006 | A1608 | U1514 | U1316 | | |
| | | A2286 | A2171 | G2111 | A2014 | A1609 | G1515 | G1421 | | |
| | | A2287 | U2172 | G2112 | A2014 | A1610 | U1518 | G1422 | | |
| | | A2288 | A2173 | U2113 | A2019 | A1614 | G1519 | G1428 | | |
| | | A2288 | C2174 | A2114 | A2020 | A1614 | G1519 | G1429 | | |
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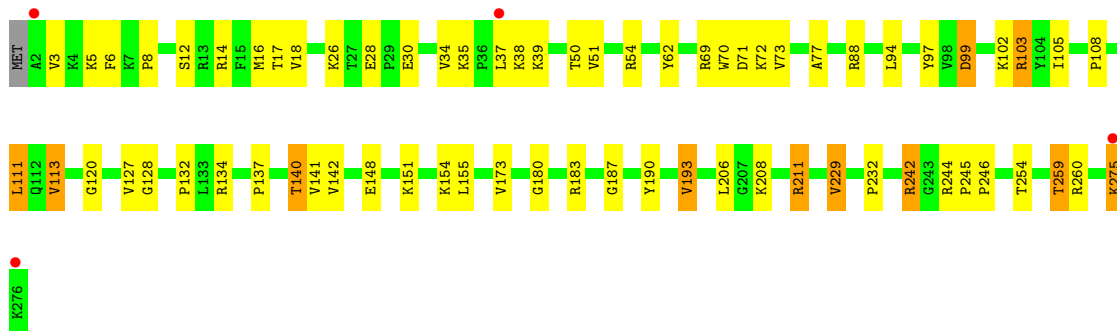
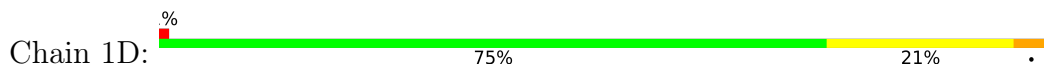
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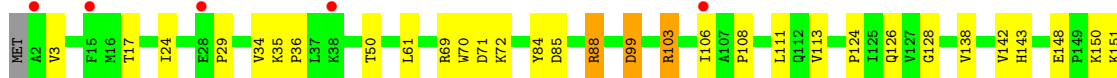
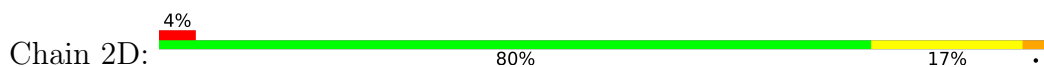
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

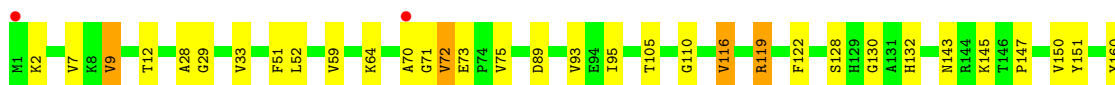
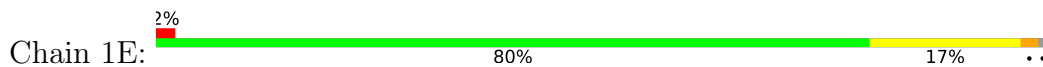


• Molecule 3: 50S ribosomal protein L2

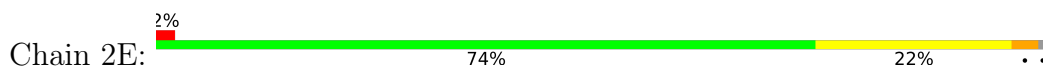




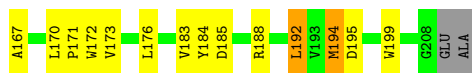
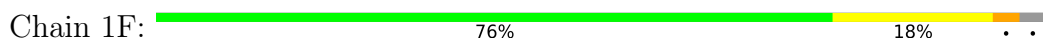
- Molecule 4: 50S ribosomal protein L3



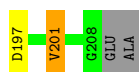
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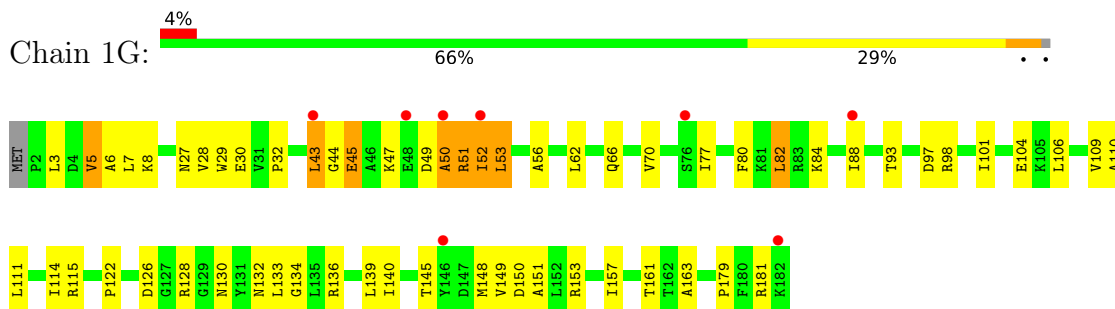
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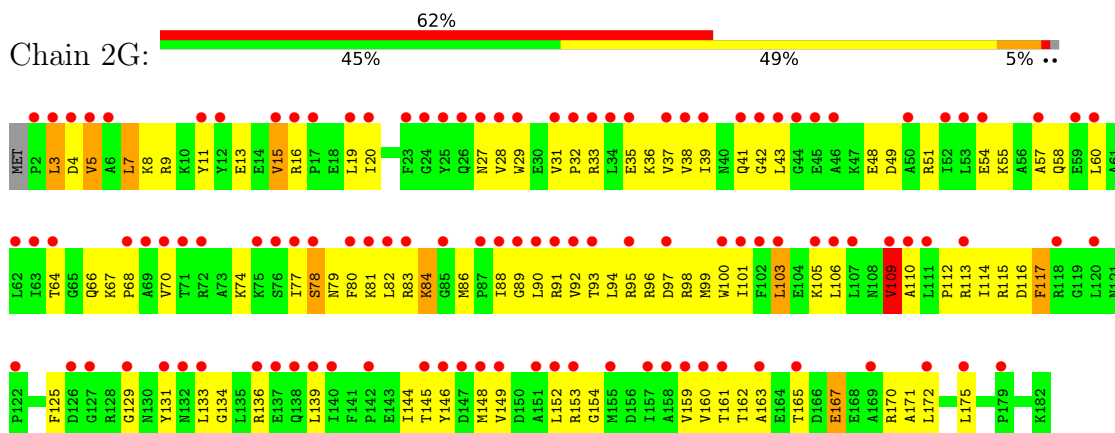
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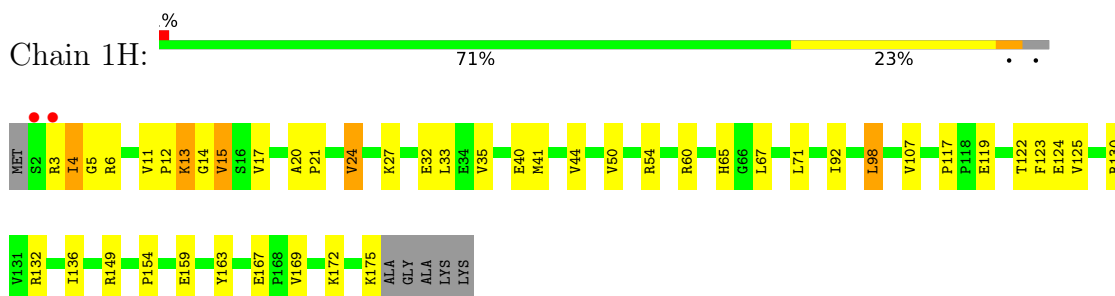
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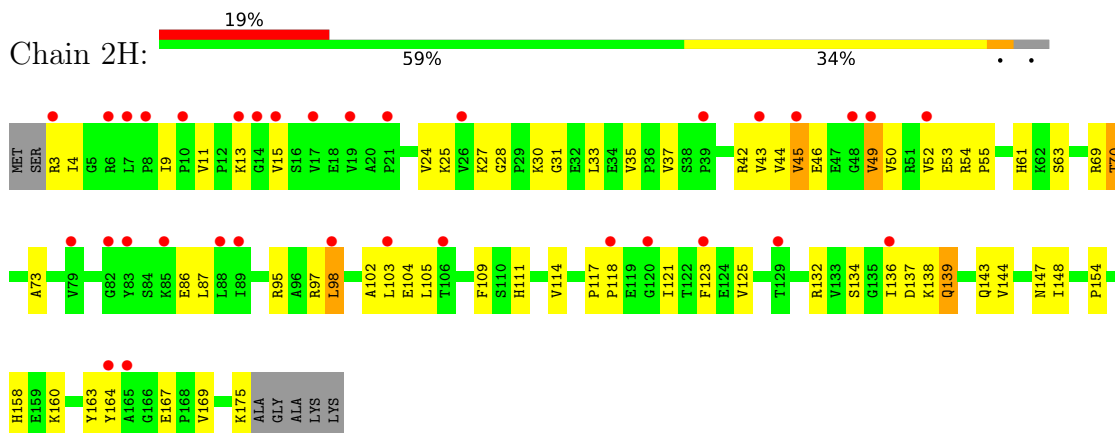
- Molecule 6: 50S ribosomal protein L5




- Molecule 7: 50S ribosomal protein L6

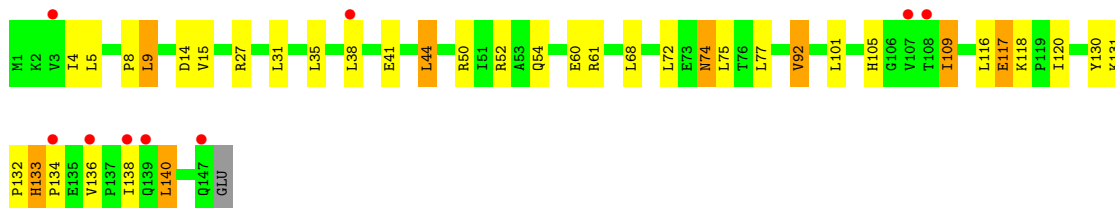


- Molecule 7: 50S ribosomal protein L6



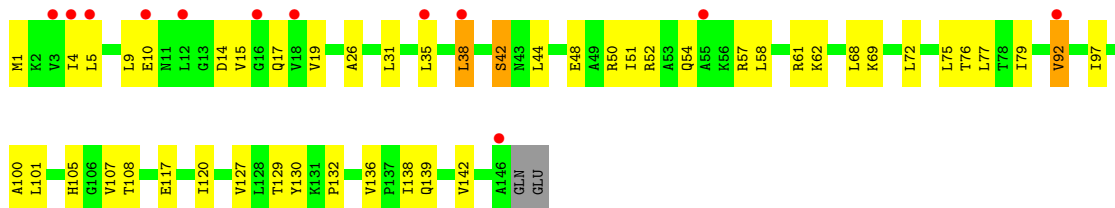
- Molecule 8: 50S ribosomal protein L9

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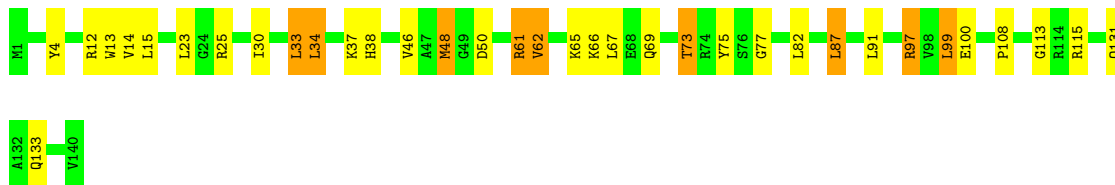
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Chain 2I: 




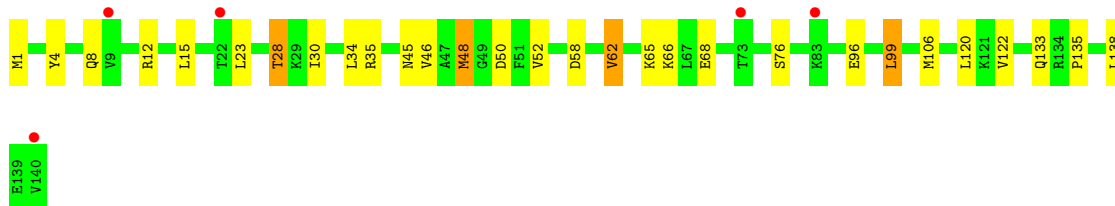
- Molecule 9: 50S ribosomal protein L13

Chain 1N: 




- Molecule 9: 50S ribosomal protein L13

Chain 2N: 

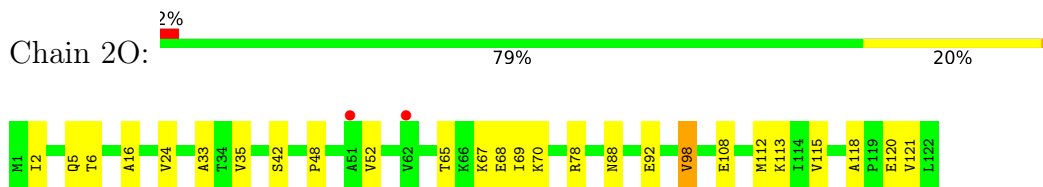


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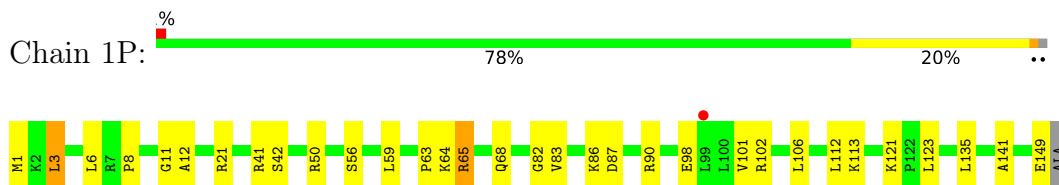
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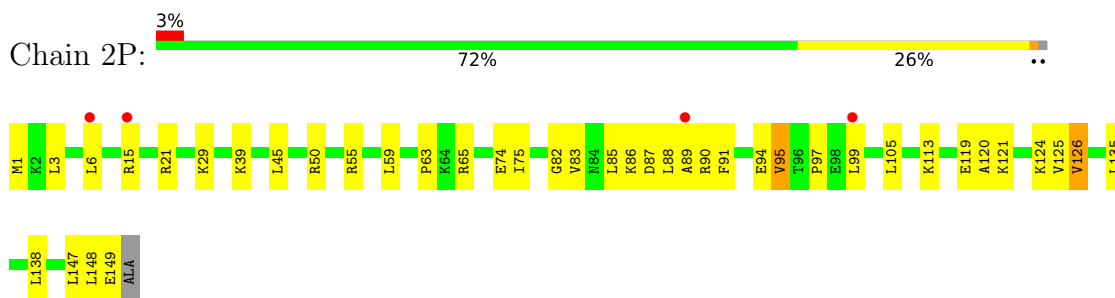
- Molecule 10: 50S ribosomal protein L14



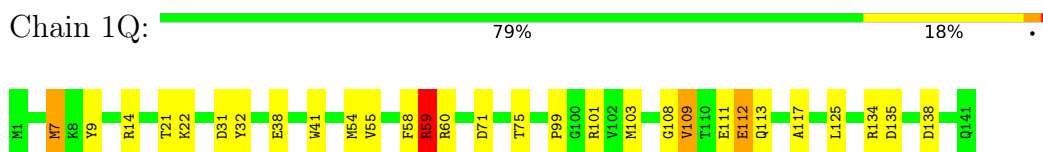
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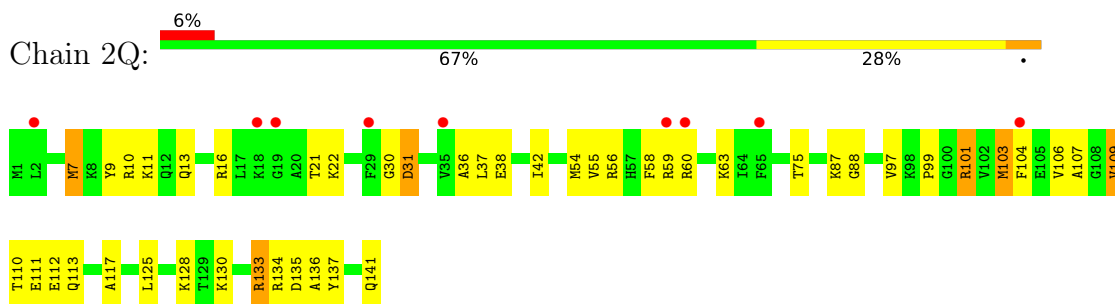
- Molecule 11: 50S ribosomal protein L15



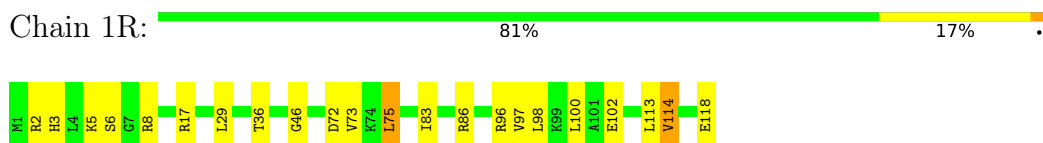
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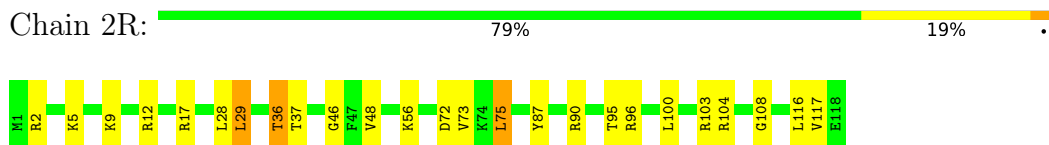
- Molecule 12: 50S ribosomal protein L16



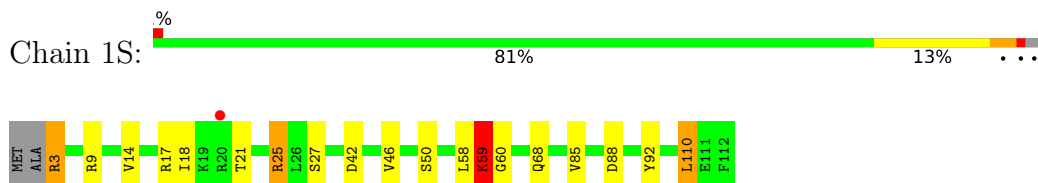
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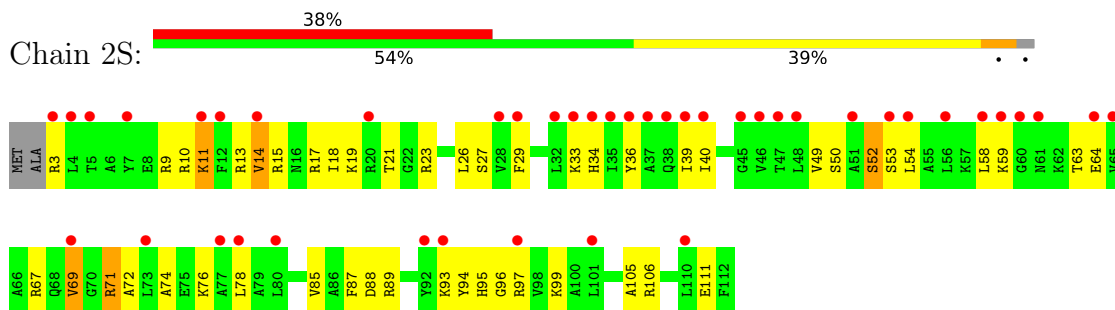
- Molecule 13: 50S ribosomal protein L17



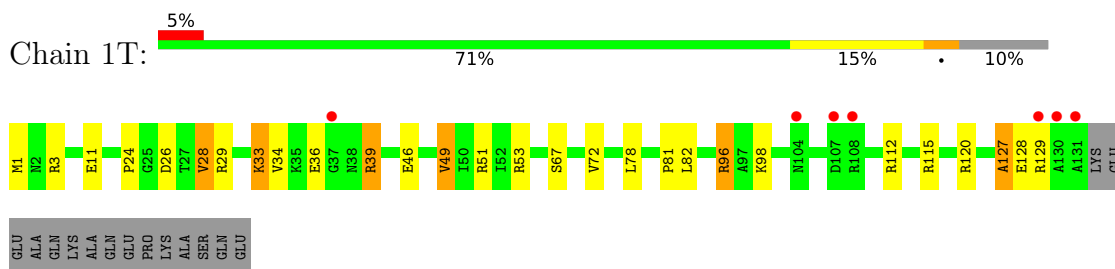
- Molecule 14: 50S ribosomal protein L18



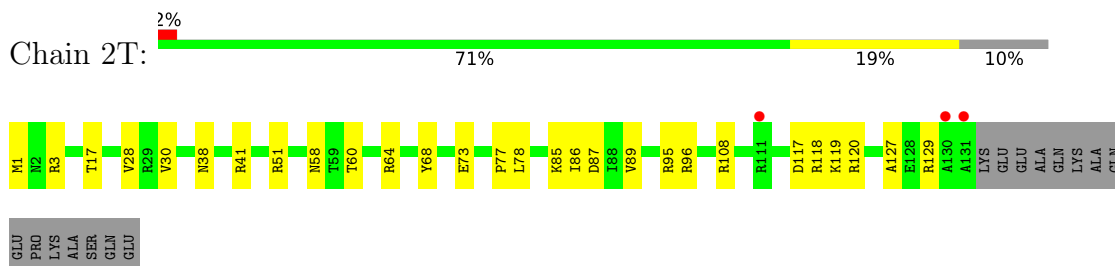
- Molecule 14: 50S ribosomal protein L18



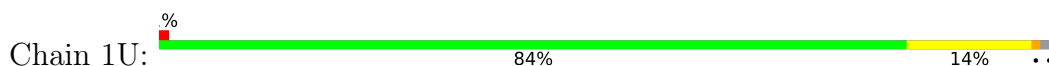
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

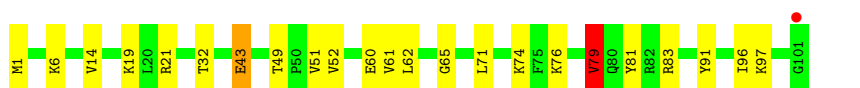
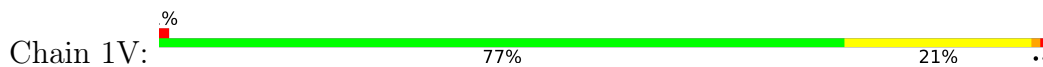




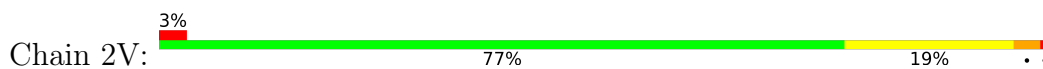
- Molecule 16: 50S ribosomal protein L20



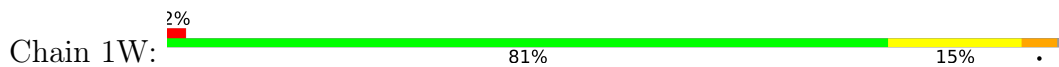
- Molecule 17: 50S ribosomal protein L21



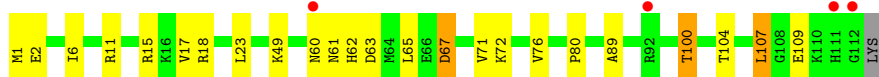
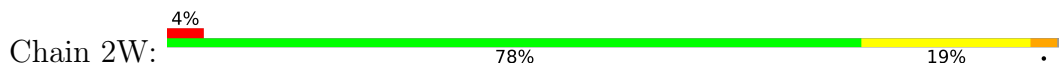
- Molecule 17: 50S ribosomal protein L21



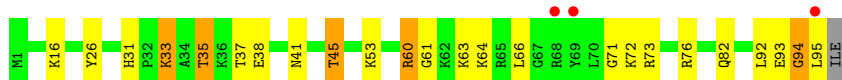
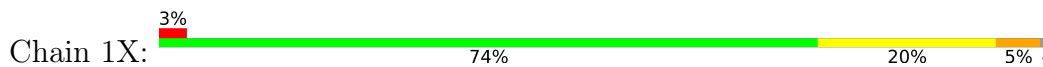
- Molecule 18: 50S ribosomal protein L22




- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23




- Molecule 19: 50S ribosomal protein L23

Chain 2X:  4% 77% 18% ..



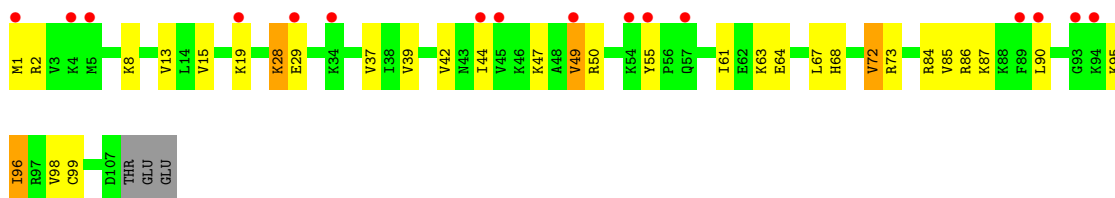
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:  3% 75% 22% ..




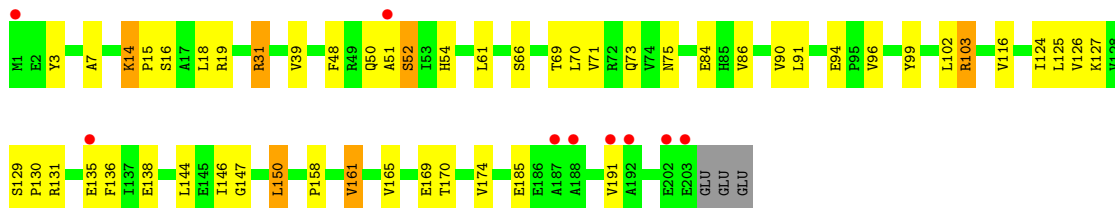
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:  15% 68% 25% ..



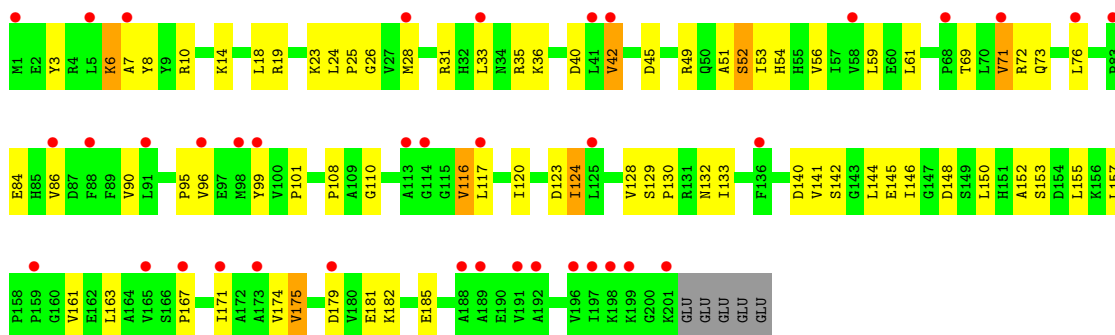
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:  4% 73% 23% ..

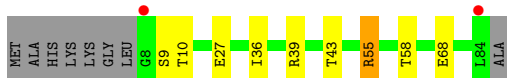
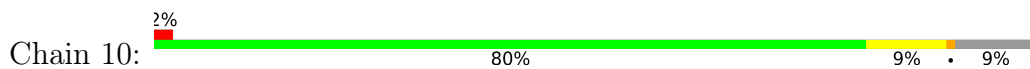


• Molecule 21: 50S ribosomal protein L25

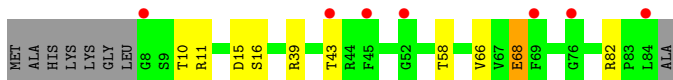
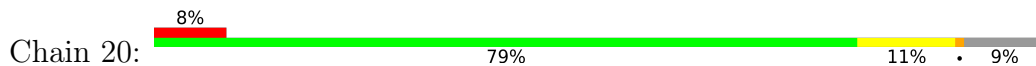
Chain 2Z:  18% 62% 33% ..



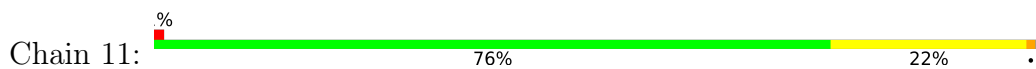
• Molecule 22: 50S ribosomal protein L27



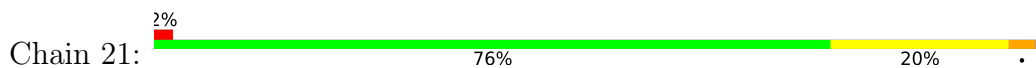
- Molecule 22: 50S ribosomal protein L27



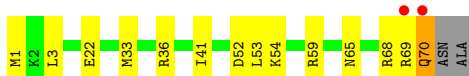
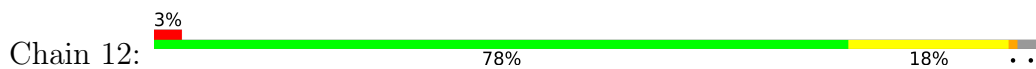
- Molecule 23: 50S ribosomal protein L28



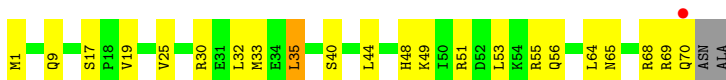
- Molecule 23: 50S ribosomal protein L28



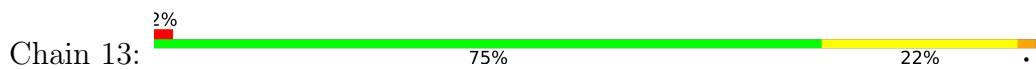
- Molecule 24: 50S ribosomal protein L29



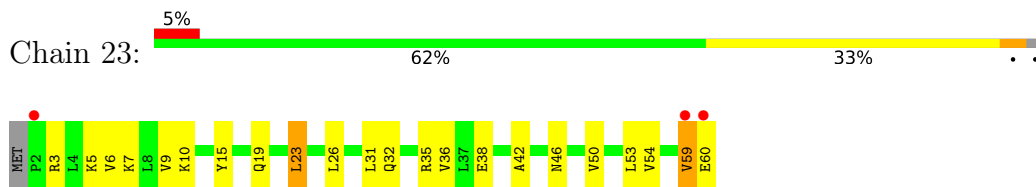
- Molecule 24: 50S ribosomal protein L29



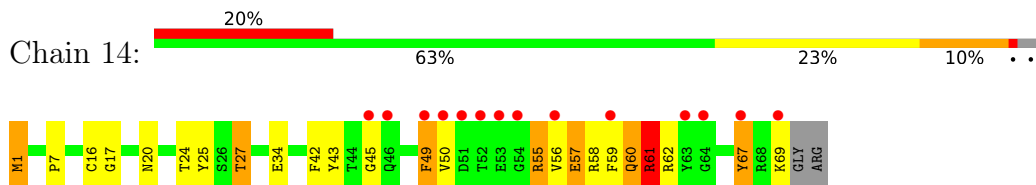
- Molecule 25: 50S ribosomal protein L30



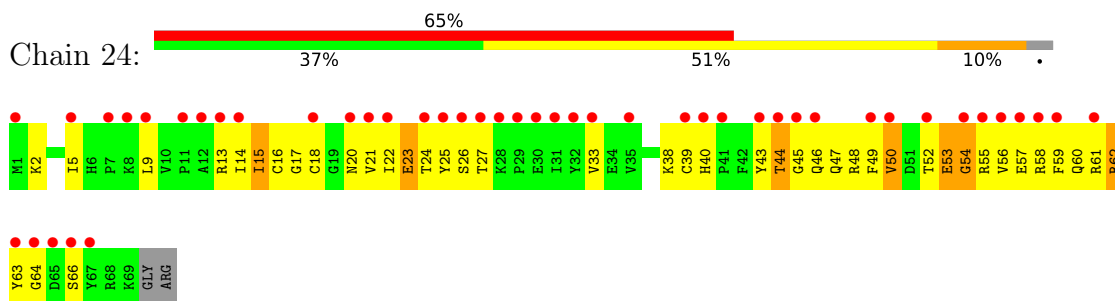
- Molecule 25: 50S ribosomal protein L30



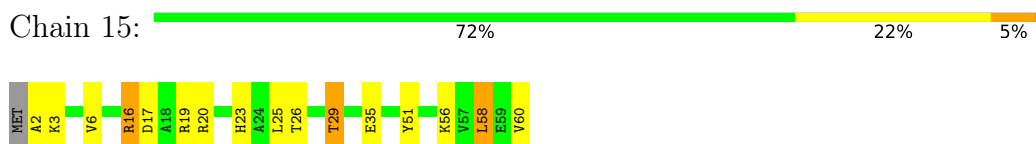
- Molecule 26: 50S ribosomal protein L31



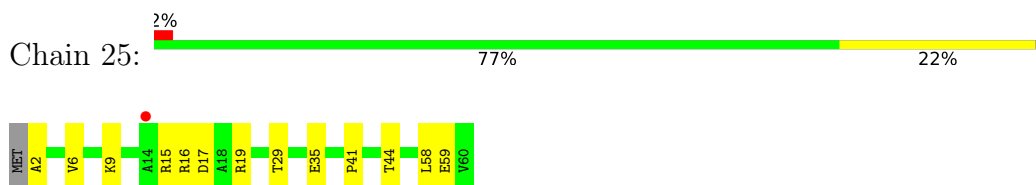
- Molecule 26: 50S ribosomal protein L31



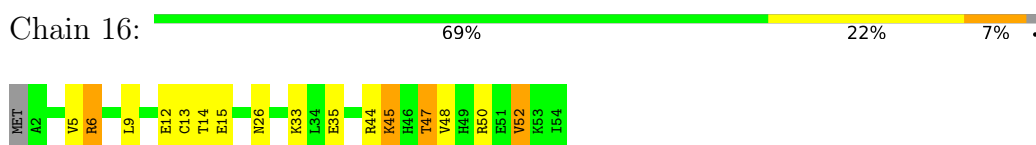
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

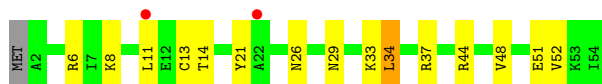


- Molecule 28: 50S ribosomal protein L33

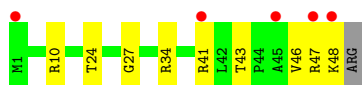
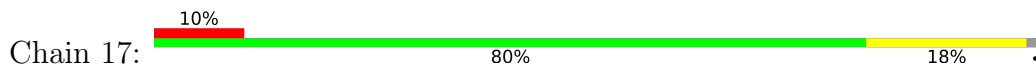


- Molecule 28: 50S ribosomal protein L33





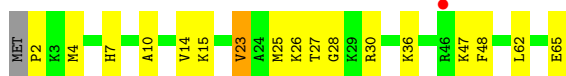
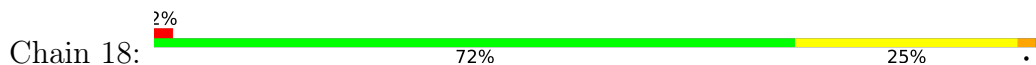
- Molecule 29: 50S ribosomal protein L34



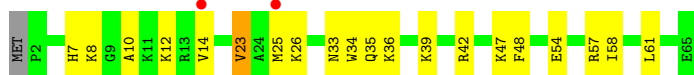
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



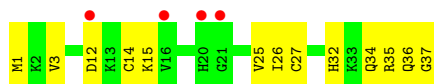
- Molecule 30: 50S ribosomal protein L35



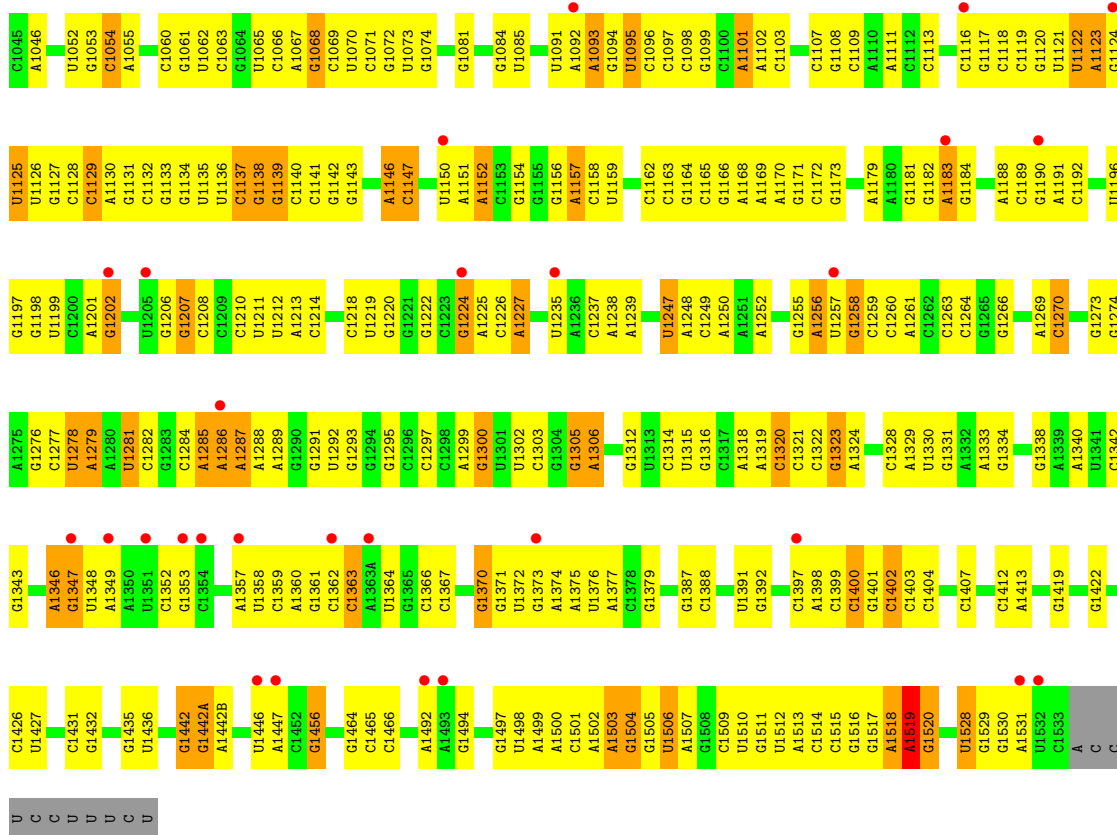
- Molecule 31: 50S ribosomal protein L36



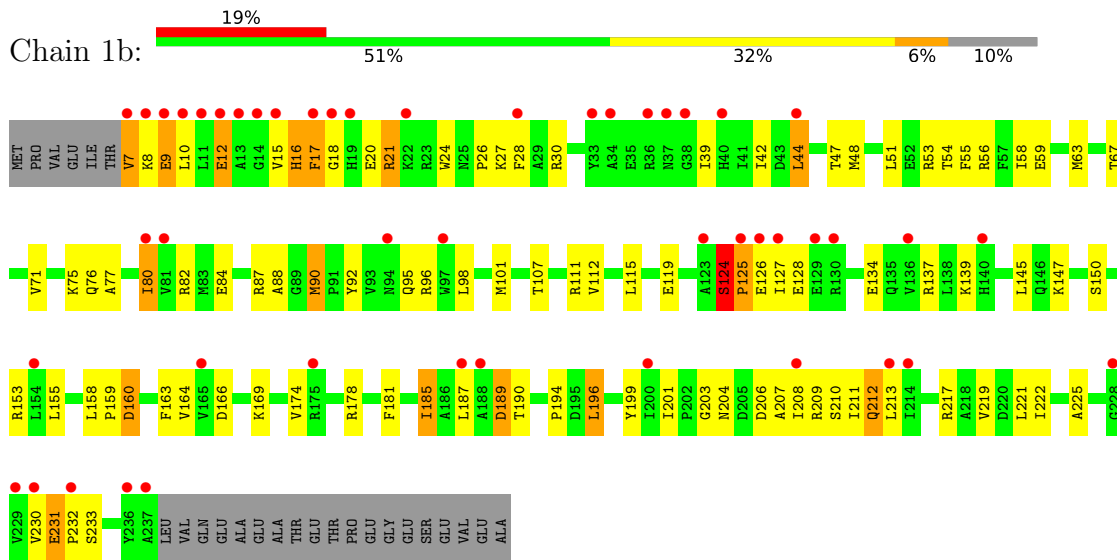
- Molecule 31: 50S ribosomal protein L36



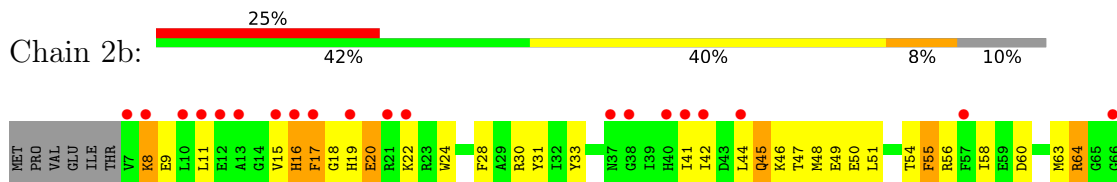
- Molecule 32: 16S Ribosomal RNA

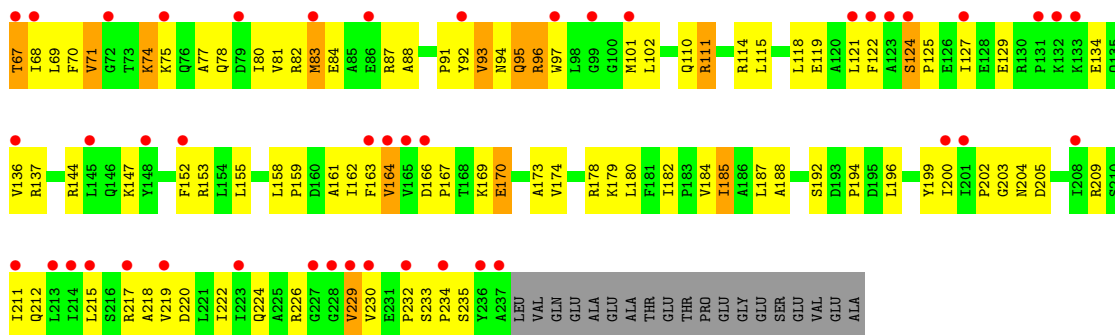


• Molecule 33: 30S ribosomal protein S2

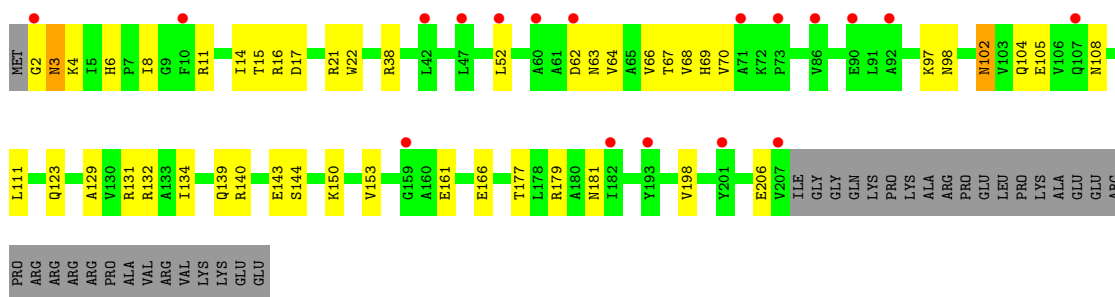


• Molecule 33: 30S ribosomal protein S2

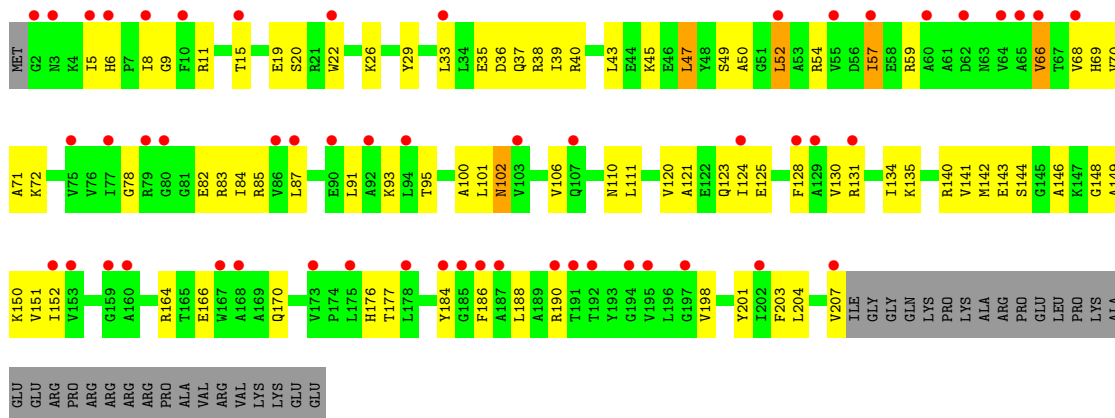




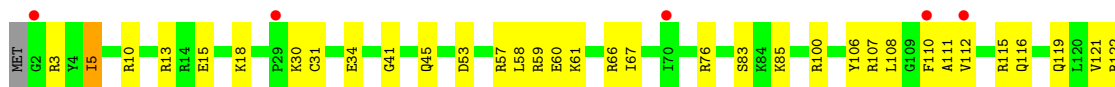
- Molecule 34: 30S ribosomal protein S3

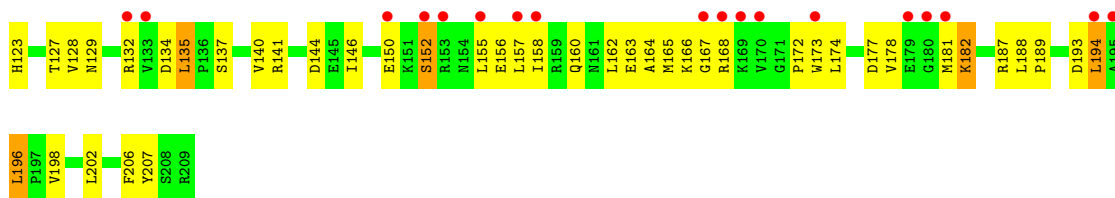


- Molecule 34: 30S ribosomal protein S3

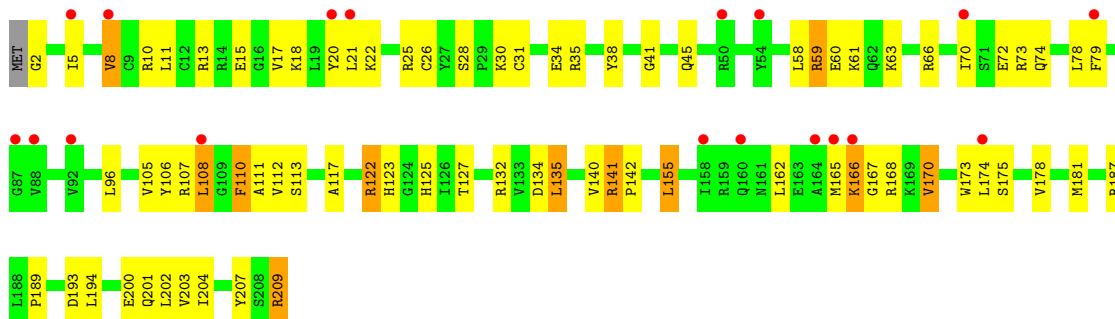


- Molecule 35: 30S ribosomal protein S4

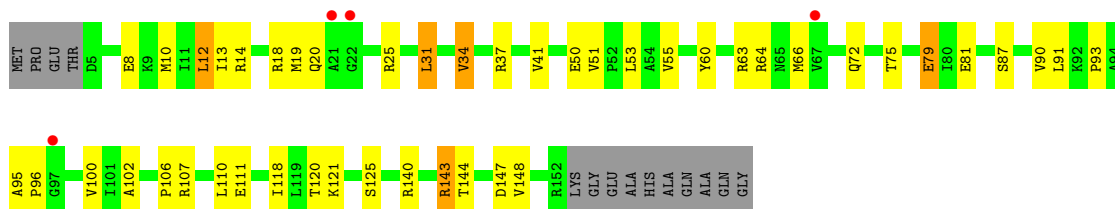




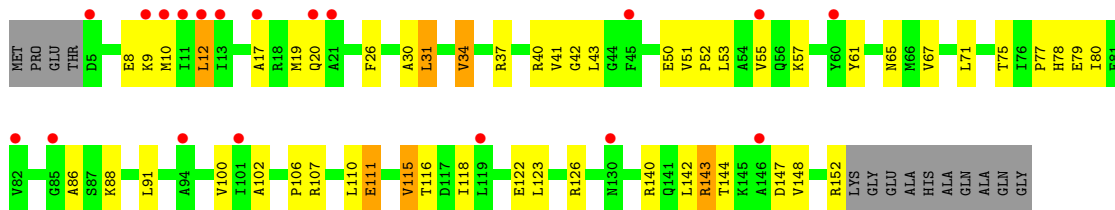
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5




• Molecule 36: 30S ribosomal protein S5

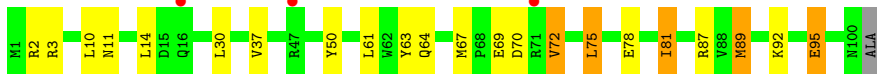


• Molecule 37: 30S ribosomal protein S6




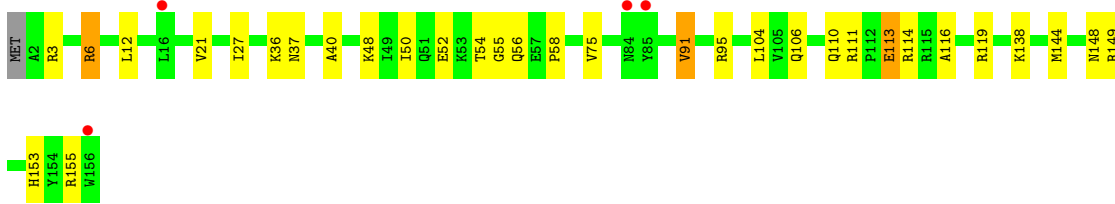
- Molecule 37: 30S ribosomal protein S6

Chain 2f: 



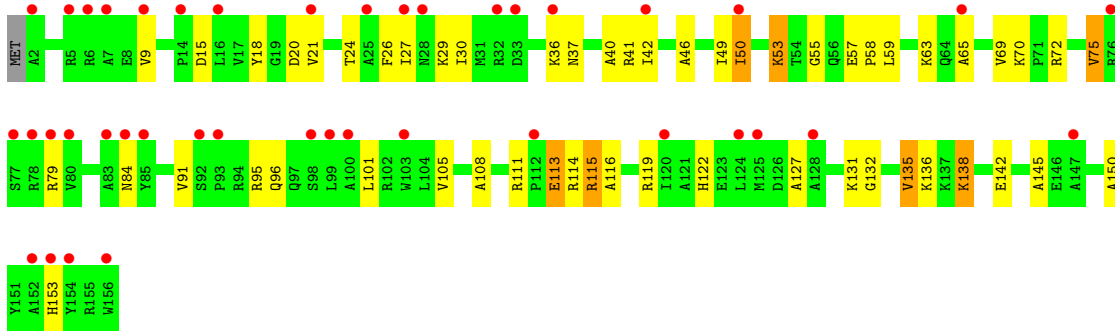
- Molecule 38: 30S ribosomal protein S7

Chain 1g: 



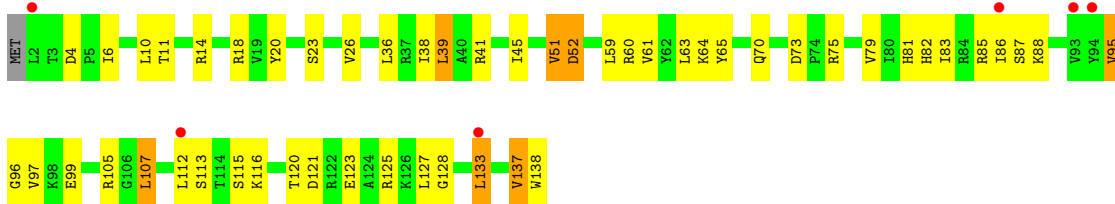
- Molecule 38: 30S ribosomal protein S7

Chain 2g: 




- Molecule 39: 30S ribosomal protein S8

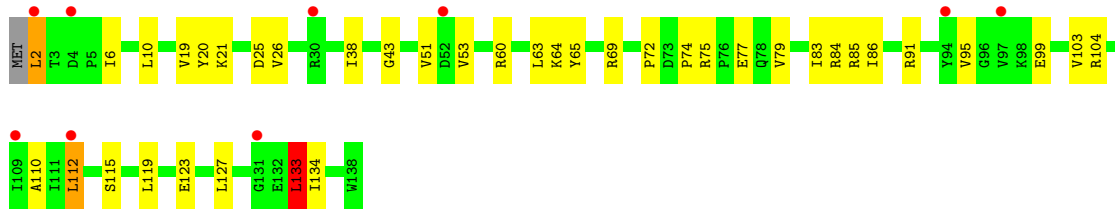
Chain 1h: 



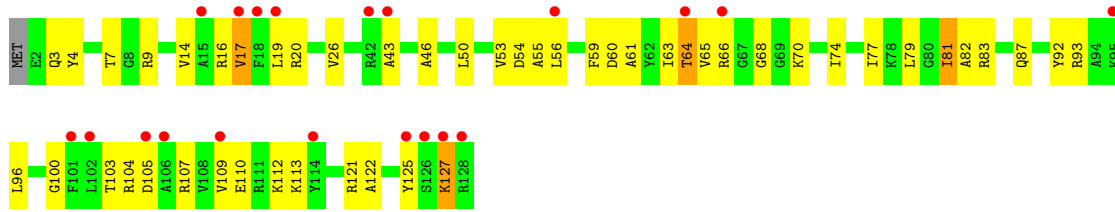
- Molecule 39: 30S ribosomal protein S8

Chain 2h: 

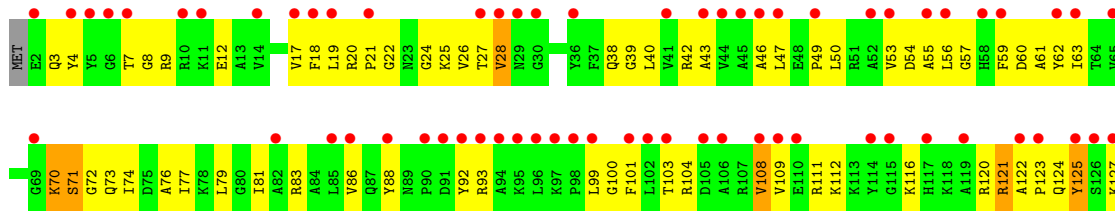




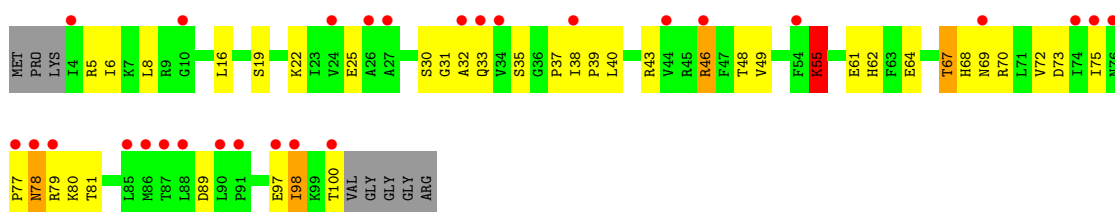
• Molecule 40: 30S ribosomal protein S9



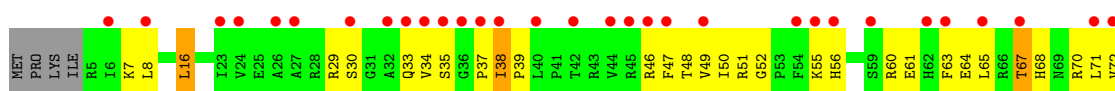
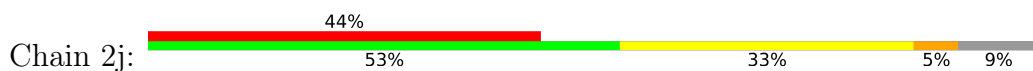
• Molecule 40: 30S ribosomal protein S9

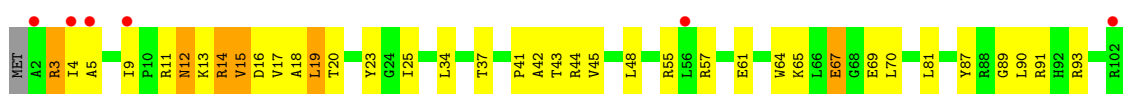
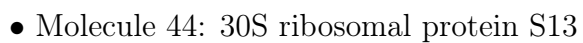
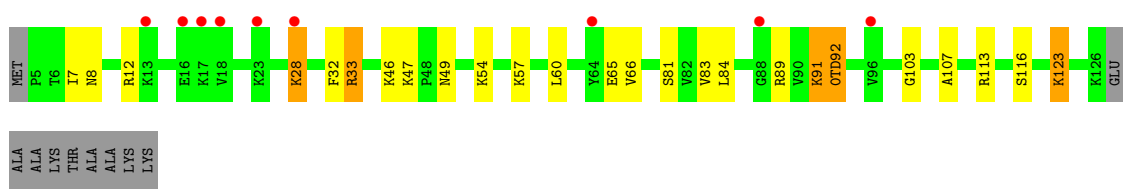
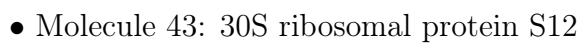
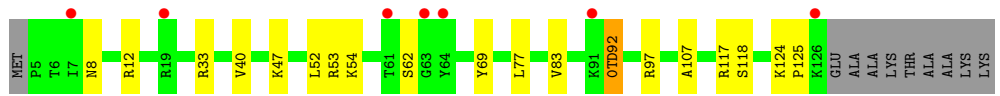
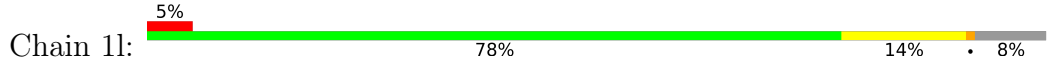
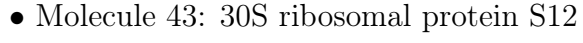
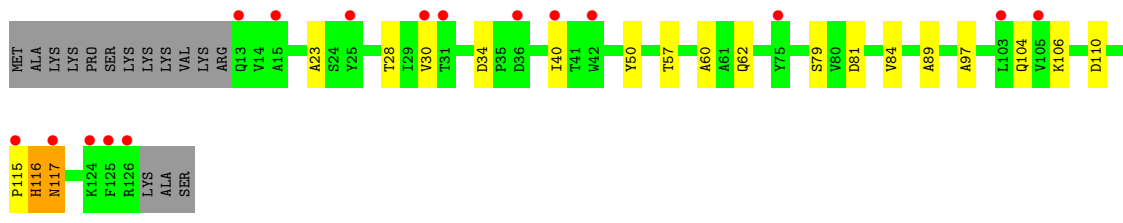
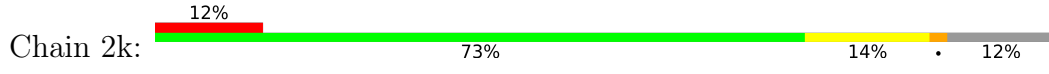
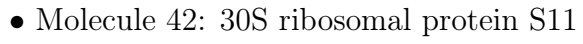
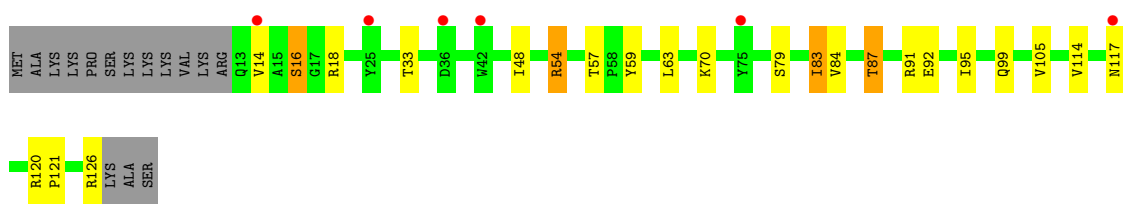
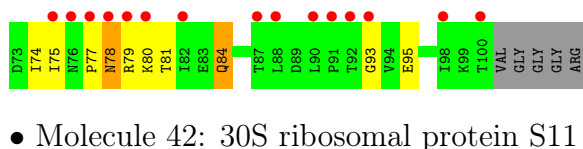


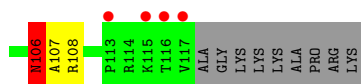
• Molecule 41: 30S ribosomal protein S10



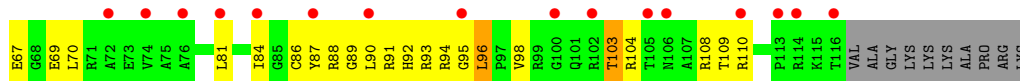
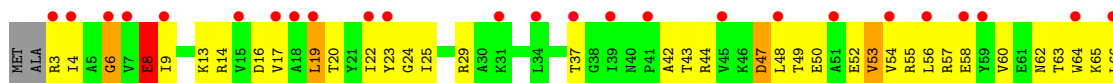
• Molecule 41: 30S ribosomal protein S10



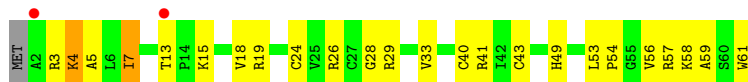




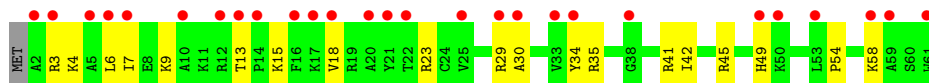
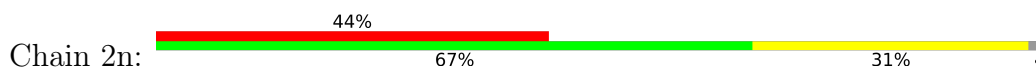
- Molecule 44: 30S ribosomal protein S13



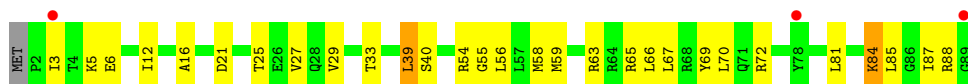
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

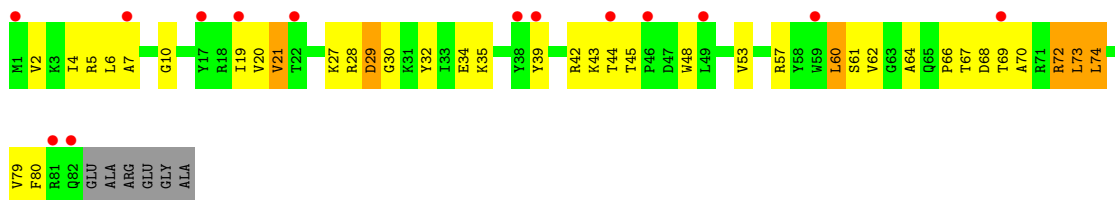


- Molecule 46: 30S ribosomal protein S15

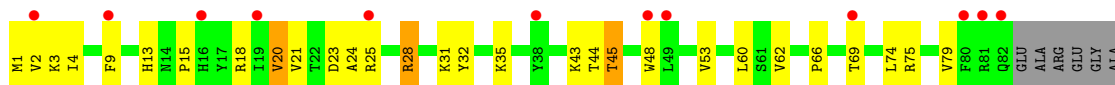


- Molecule 47: 30S ribosomal protein S16

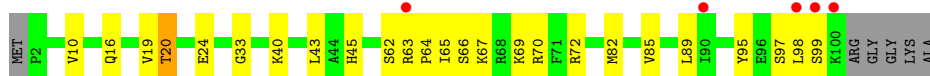




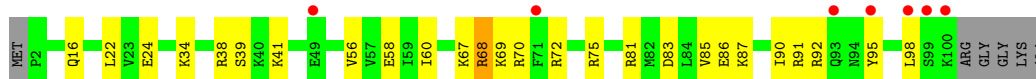
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

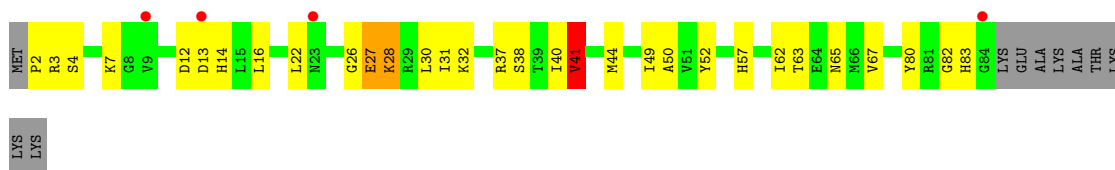


- Molecule 49: 30S ribosomal protein S18

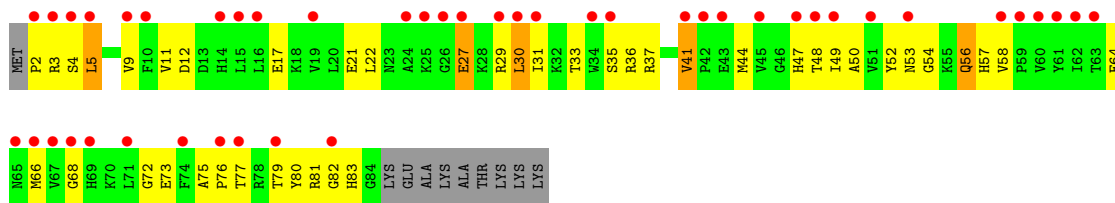
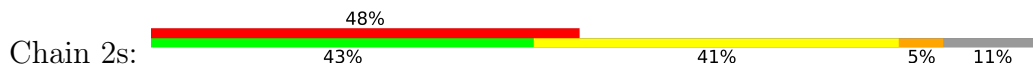


- Molecule 50: 30S ribosomal protein S19

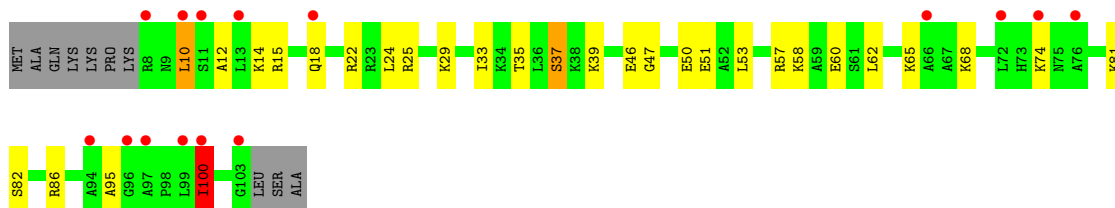




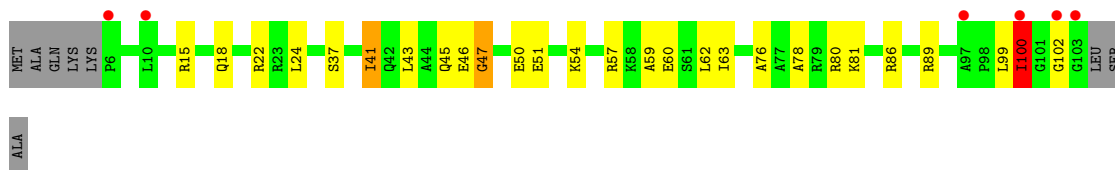
• Molecule 50: 30S ribosomal protein S19



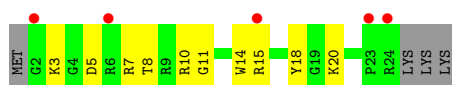
• Molecule 51: 30S ribosomal protein S20



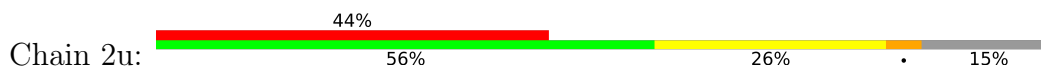
• Molecule 51: 30S ribosomal protein S20

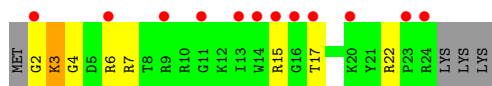


• Molecule 52: 30S ribosomal protein Thx

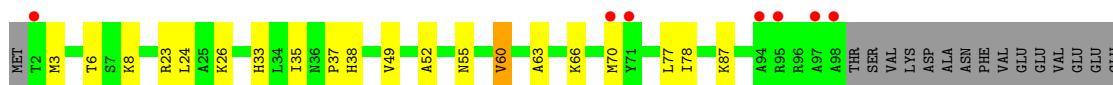


• Molecule 52: 30S ribosomal protein Thx

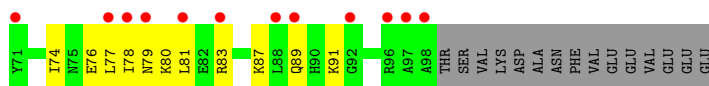
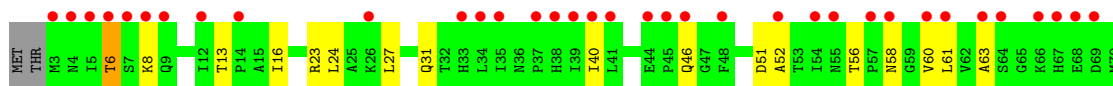
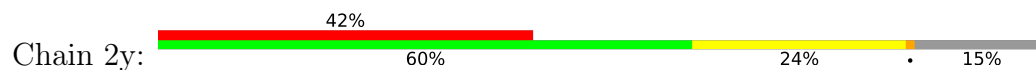




• Molecule 53: Ribosome-associated inhibitor A



• Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 208.57Å 448.58Å 617.47Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 151.65 – 2.50 151.65 – 2.50 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (151.65-2.50) 99.9 (151.65-2.50) | Depositor EDS |
| R_{merge} | 0.17 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.22 (at 2.52Å) | Xtrriage |
| Refinement program | PHENIX 1.8.2 | Depositor |
| R, R_{free} | 0.206 , 0.246 0.206 , 0.246 | Depositor DCC |
| R_{free} test set | 98630 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 57.6 | Xtrriage |
| Anisotropy | 0.189 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 64.5 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 296967 | wwPDB-VP |
| Average B, all atoms (Å ²) | 65.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, SF4, G7M, MA6, 2MA, 5MU, OMG, 0TD, MG, UR3, MPD, PSU, HGR, 2MU, 4OC, M2G, ZN, 2MG, 5MC, ERY

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 | 0.31 | 0/69030 | 0.49 | 5/107750 (0.0%) |
| 1 | 2A | 0.24 | 0/68902 | 0.43 | 2/107548 (0.0%) |
| 2 | 1B | 0.25 | 0/2876 | 0.44 | 0/4486 |
| 2 | 2B | 0.21 | 0/2878 | 0.40 | 0/4490 |
| 3 | 1D | 0.30 | 0/2181 | 0.55 | 0/2940 |
| 3 | 2D | 0.24 | 0/2186 | 0.48 | 0/2944 |
| 4 | 1E | 0.27 | 0/1592 | 0.51 | 0/2149 |
| 4 | 2E | 0.21 | 0/1592 | 0.45 | 0/2149 |
| 5 | 1F | 0.26 | 0/1619 | 0.50 | 0/2193 |
| 5 | 2F | 0.22 | 0/1615 | 0.48 | 0/2188 |
| 6 | 1G | 0.21 | 0/1451 | 0.41 | 0/1961 |
| 6 | 2G | 0.23 | 0/1449 | 0.44 | 0/1957 |
| 7 | 1H | 0.23 | 0/1356 | 0.44 | 0/1834 |
| 7 | 2H | 0.19 | 0/1350 | 0.40 | 0/1826 |
| 8 | 1I | 0.20 | 0/1109 | 0.42 | 0/1512 |
| 8 | 2I | 0.17 | 0/1091 | 0.40 | 0/1490 |
| 9 | 1N | 0.27 | 0/1148 | 0.48 | 0/1547 |
| 9 | 2N | 0.19 | 0/1144 | 0.38 | 0/1543 |
| 10 | 1O | 0.28 | 0/943 | 0.47 | 0/1269 |
| 10 | 2O | 0.23 | 0/943 | 0.47 | 0/1269 |
| 11 | 1P | 0.28 | 0/1152 | 0.52 | 0/1533 |
| 11 | 2P | 0.22 | 0/1152 | 0.45 | 0/1533 |
| 12 | 1Q | 0.28 | 0/1143 | 0.49 | 0/1527 |
| 12 | 2Q | 0.19 | 0/1143 | 0.43 | 0/1527 |
| 13 | 1R | 0.29 | 0/982 | 0.53 | 0/1312 |
| 13 | 2R | 0.25 | 0/982 | 0.46 | 0/1312 |
| 14 | 1S | 0.23 | 0/887 | 0.46 | 0/1180 |
| 14 | 2S | 0.20 | 0/880 | 0.45 | 0/1172 |
| 15 | 1T | 0.26 | 0/1105 | 0.50 | 0/1477 |
| 15 | 2T | 0.21 | 0/1097 | 0.45 | 0/1468 |
| 16 | 1U | 0.30 | 0/977 | 0.53 | 0/1301 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | 2U | 0.19 | 0/977 | 0.40 | 0/1301 |
| 17 | 1V | 0.27 | 0/786 | 0.47 | 0/1053 |
| 17 | 2V | 0.20 | 0/782 | 0.40 | 0/1049 |
| 18 | 1W | 0.29 | 0/897 | 0.46 | 0/1205 |
| 18 | 2W | 0.23 | 0/897 | 0.43 | 0/1205 |
| 19 | 1X | 0.28 | 0/764 | 0.52 | 0/1025 |
| 19 | 2X | 0.21 | 0/764 | 0.44 | 0/1025 |
| 20 | 1Y | 0.26 | 0/823 | 0.52 | 0/1099 |
| 20 | 2Y | 0.20 | 0/823 | 0.46 | 0/1100 |
| 21 | 1Z | 0.23 | 0/1620 | 0.46 | 0/2200 |
| 21 | 2Z | 0.20 | 0/1590 | 0.45 | 0/2162 |
| 22 | 10 | 0.29 | 0/616 | 0.54 | 0/821 |
| 22 | 20 | 0.20 | 0/616 | 0.45 | 0/821 |
| 23 | 11 | 0.27 | 0/761 | 0.46 | 0/1013 |
| 23 | 21 | 0.23 | 0/766 | 0.41 | 0/1018 |
| 24 | 12 | 0.23 | 0/590 | 0.45 | 0/781 |
| 24 | 22 | 0.21 | 0/594 | 0.43 | 0/785 |
| 25 | 13 | 0.28 | 0/474 | 0.52 | 0/635 |
| 25 | 23 | 0.19 | 0/469 | 0.40 | 0/630 |
| 26 | 14 | 0.26 | 0/559 | 0.59 | 0/754 |
| 26 | 24 | 0.30 | 0/549 | 0.70 | 0/741 |
| 27 | 15 | 0.32 | 0/473 | 0.60 | 0/639 |
| 27 | 25 | 0.26 | 0/469 | 0.45 | 0/635 |
| 28 | 16 | 0.26 | 0/460 | 0.50 | 0/613 |
| 28 | 26 | 0.21 | 0/456 | 0.45 | 0/608 |
| 29 | 17 | 0.33 | 0/426 | 0.50 | 0/561 |
| 29 | 27 | 0.25 | 0/426 | 0.50 | 0/561 |
| 30 | 18 | 0.27 | 0/525 | 0.51 | 0/691 |
| 30 | 28 | 0.21 | 0/525 | 0.41 | 0/691 |
| 31 | 19 | 0.31 | 0/310 | 0.50 | 0/407 |
| 31 | 29 | 0.20 | 0/310 | 0.42 | 0/407 |
| 32 | 1a | 0.21 | 0/35795 | 0.40 | 0/55864 |
| 32 | 2a | 0.20 | 1/35890 (0.0%) | 0.39 | 2/56012 (0.0%) |
| 33 | 1b | 0.22 | 0/1876 | 0.48 | 0/2533 |
| 33 | 2b | 0.25 | 0/1860 | 0.51 | 2/2518 (0.1%) |
| 34 | 1c | 0.19 | 0/1582 | 0.42 | 0/2137 |
| 34 | 2c | 0.22 | 0/1566 | 0.41 | 0/2119 |
| 35 | 1d | 0.20 | 0/1695 | 0.44 | 0/2274 |
| 35 | 2d | 0.19 | 0/1698 | 0.42 | 0/2277 |
| 36 | 1e | 0.21 | 0/1149 | 0.44 | 0/1548 |
| 36 | 2e | 0.20 | 0/1149 | 0.41 | 0/1548 |
| 37 | 1f | 0.21 | 0/827 | 0.40 | 0/1120 |
| 37 | 2f | 0.20 | 0/829 | 0.41 | 0/1123 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | 1g | 0.19 | 0/1254 | 0.40 | 0/1683 |
| 38 | 2g | 0.20 | 0/1248 | 0.40 | 0/1676 |
| 39 | 1h | 0.19 | 0/1118 | 0.42 | 0/1506 |
| 39 | 2h | 0.17 | 0/1108 | 0.40 | 0/1494 |
| 40 | 1i | 0.20 | 0/1005 | 0.46 | 0/1351 |
| 40 | 2i | 0.23 | 0/985 | 0.47 | 0/1329 |
| 41 | 1j | 0.24 | 0/732 | 0.40 | 0/993 |
| 41 | 2j | 0.23 | 0/723 | 0.41 | 0/984 |
| 42 | 1k | 0.20 | 0/849 | 0.45 | 0/1150 |
| 42 | 2k | 0.20 | 0/848 | 0.44 | 0/1149 |
| 43 | 1l | 0.20 | 0/937 | 0.43 | 0/1260 |
| 43 | 2l | 0.18 | 0/937 | 0.40 | 0/1260 |
| 44 | 1m | 0.19 | 0/924 | 0.46 | 0/1242 |
| 44 | 2m | 0.23 | 0/905 | 0.46 | 0/1217 |
| 45 | 1n | 0.20 | 0/501 | 0.48 | 0/664 |
| 45 | 2n | 0.21 | 0/501 | 0.43 | 0/664 |
| 46 | 1o | 0.20 | 0/739 | 0.40 | 0/985 |
| 46 | 2o | 0.21 | 0/739 | 0.40 | 0/985 |
| 47 | 1p | 0.20 | 0/697 | 0.49 | 0/939 |
| 47 | 2p | 0.20 | 0/693 | 0.45 | 0/935 |
| 48 | 1q | 0.21 | 0/836 | 0.42 | 0/1117 |
| 48 | 2q | 0.21 | 0/836 | 0.41 | 0/1117 |
| 49 | 1r | 0.21 | 0/560 | 0.52 | 0/746 |
| 49 | 2r | 0.20 | 0/560 | 0.38 | 0/746 |
| 50 | 1s | 0.19 | 0/663 | 0.51 | 1/895 (0.1%) |
| 50 | 2s | 0.22 | 0/660 | 0.44 | 0/893 |
| 51 | 1t | 0.21 | 0/734 | 0.50 | 0/969 |
| 51 | 2t | 0.19 | 0/736 | 0.42 | 0/976 |
| 52 | 1u | 0.21 | 0/203 | 0.48 | 0/266 |
| 52 | 2u | 0.23 | 0/203 | 0.48 | 0/266 |
| 53 | 1y | 0.20 | 0/776 | 0.40 | 0/1048 |
| 53 | 2y | 0.20 | 0/761 | 0.37 | 0/1030 |
| All | All | 0.25 | 1/309939 (0.0%) | 0.44 | 12/463231 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 26 | 14 | 0 | 1 |
| 26 | 24 | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 33 | 1b | 0 | 1 |
| All | All | 0 | 3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 32 | 2a | 1498 | UR3 | O3'-P | 5.25 | 1.61 | 1.56 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | 1A | 1042 | G | OP1-P-O3' | -8.93 | 81.21 | 108.00 |
| 1 | 1A | 1042 | G | OP2-P-O3' | -6.96 | 87.13 | 108.00 |
| 50 | 1s | 41 | VAL | CB-CA-C | 6.42 | 115.62 | 109.33 |
| 33 | 2b | 232 | PRO | CA-C-N | 6.00 | 138.01 | 120.97 |
| 33 | 2b | 232 | PRO | C-N-CA | 6.00 | 138.01 | 120.97 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 26 | 14 | 67 | TYR | Peptide |
| 33 | 1b | 231 | GLU | Peptide |
| 26 | 24 | 18 | CYS | Peptide |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 1A | 61869 | 0 | 31205 | 610 | 0 |
| 1 | 2A | 61758 | 0 | 31152 | 750 | 0 |
| 2 | 1B | 2572 | 0 | 1305 | 24 | 0 |
| 2 | 2B | 2573 | 0 | 1306 | 60 | 0 |
| 3 | 1D | 2131 | 0 | 2207 | 54 | 0 |
| 3 | 2D | 2136 | 0 | 2218 | 36 | 0 |
| 4 | 1E | 1559 | 0 | 1618 | 27 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 2E | 1559 | 0 | 1618 | 36 | 0 |
| 5 | 1F | 1584 | 0 | 1625 | 26 | 0 |
| 5 | 2F | 1580 | 0 | 1619 | 52 | 0 |
| 6 | 1G | 1426 | 0 | 1445 | 42 | 0 |
| 6 | 2G | 1424 | 0 | 1441 | 89 | 0 |
| 7 | 1H | 1330 | 0 | 1407 | 26 | 0 |
| 7 | 2H | 1324 | 0 | 1402 | 41 | 0 |
| 8 | 1I | 1094 | 0 | 1127 | 25 | 0 |
| 8 | 2I | 1076 | 0 | 1094 | 29 | 0 |
| 9 | 1N | 1121 | 0 | 1195 | 25 | 0 |
| 9 | 2N | 1117 | 0 | 1184 | 20 | 0 |
| 10 | 1O | 933 | 0 | 996 | 13 | 0 |
| 10 | 2O | 933 | 0 | 996 | 18 | 0 |
| 11 | 1P | 1135 | 0 | 1212 | 25 | 0 |
| 11 | 2P | 1135 | 0 | 1212 | 28 | 0 |
| 12 | 1Q | 1122 | 0 | 1179 | 19 | 0 |
| 12 | 2Q | 1122 | 0 | 1179 | 28 | 0 |
| 13 | 1R | 968 | 0 | 1033 | 16 | 0 |
| 13 | 2R | 968 | 0 | 1033 | 16 | 0 |
| 14 | 1S | 877 | 0 | 938 | 17 | 0 |
| 14 | 2S | 870 | 0 | 923 | 30 | 0 |
| 15 | 1T | 1091 | 0 | 1151 | 21 | 0 |
| 15 | 2T | 1083 | 0 | 1136 | 25 | 0 |
| 16 | 1U | 959 | 0 | 1019 | 15 | 0 |
| 16 | 2U | 959 | 0 | 1019 | 26 | 0 |
| 17 | 1V | 775 | 0 | 841 | 16 | 0 |
| 17 | 2V | 771 | 0 | 830 | 16 | 0 |
| 18 | 1W | 886 | 0 | 940 | 14 | 0 |
| 18 | 2W | 886 | 0 | 940 | 11 | 0 |
| 19 | 1X | 750 | 0 | 814 | 18 | 0 |
| 19 | 2X | 750 | 0 | 814 | 15 | 0 |
| 20 | 1Y | 810 | 0 | 892 | 16 | 0 |
| 20 | 2Y | 810 | 0 | 887 | 21 | 0 |
| 21 | 1Z | 1587 | 0 | 1598 | 31 | 0 |
| 21 | 2Z | 1557 | 0 | 1564 | 49 | 0 |
| 22 | 10 | 608 | 0 | 622 | 9 | 0 |
| 22 | 20 | 608 | 0 | 622 | 4 | 0 |
| 23 | 11 | 754 | 0 | 823 | 13 | 0 |
| 23 | 21 | 759 | 0 | 837 | 18 | 0 |
| 24 | 12 | 588 | 0 | 643 | 11 | 0 |
| 24 | 22 | 592 | 0 | 654 | 10 | 0 |
| 25 | 13 | 469 | 0 | 518 | 8 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 25 | 23 | 464 | 0 | 514 | 14 | 0 |
| 26 | 14 | 546 | 0 | 522 | 21 | 0 |
| 26 | 24 | 536 | 0 | 514 | 36 | 0 |
| 27 | 15 | 459 | 0 | 476 | 11 | 0 |
| 27 | 25 | 455 | 0 | 465 | 7 | 0 |
| 28 | 16 | 453 | 0 | 473 | 7 | 0 |
| 28 | 26 | 449 | 0 | 469 | 8 | 0 |
| 29 | 17 | 418 | 0 | 467 | 5 | 0 |
| 29 | 27 | 418 | 0 | 467 | 10 | 0 |
| 30 | 18 | 517 | 0 | 582 | 15 | 0 |
| 30 | 28 | 517 | 0 | 582 | 16 | 0 |
| 31 | 19 | 307 | 0 | 335 | 1 | 0 |
| 31 | 29 | 307 | 0 | 335 | 10 | 0 |
| 32 | 1a | 32246 | 0 | 16295 | 415 | 0 |
| 32 | 2a | 32331 | 0 | 16338 | 532 | 0 |
| 33 | 1b | 1842 | 0 | 1862 | 65 | 0 |
| 33 | 2b | 1825 | 0 | 1828 | 86 | 0 |
| 34 | 1c | 1558 | 0 | 1557 | 33 | 0 |
| 34 | 2c | 1542 | 0 | 1517 | 62 | 0 |
| 35 | 1d | 1665 | 0 | 1687 | 56 | 0 |
| 35 | 2d | 1668 | 0 | 1703 | 58 | 0 |
| 36 | 1e | 1133 | 0 | 1191 | 29 | 0 |
| 36 | 2e | 1133 | 0 | 1191 | 36 | 0 |
| 37 | 1f | 814 | 0 | 808 | 17 | 0 |
| 37 | 2f | 816 | 0 | 808 | 16 | 0 |
| 38 | 1g | 1235 | 0 | 1249 | 20 | 0 |
| 38 | 2g | 1229 | 0 | 1238 | 30 | 0 |
| 39 | 1h | 1098 | 0 | 1143 | 39 | 0 |
| 39 | 2h | 1088 | 0 | 1126 | 22 | 0 |
| 40 | 1i | 986 | 0 | 990 | 34 | 0 |
| 40 | 2i | 966 | 0 | 953 | 51 | 0 |
| 41 | 1j | 719 | 0 | 672 | 26 | 0 |
| 41 | 2j | 710 | 0 | 661 | 30 | 0 |
| 42 | 1k | 834 | 0 | 838 | 20 | 0 |
| 42 | 2k | 833 | 0 | 836 | 11 | 0 |
| 43 | 1l | 932 | 0 | 981 | 14 | 0 |
| 43 | 2l | 932 | 0 | 981 | 18 | 0 |
| 44 | 1m | 914 | 0 | 954 | 33 | 0 |
| 44 | 2m | 895 | 0 | 920 | 45 | 0 |
| 45 | 1n | 492 | 0 | 529 | 19 | 0 |
| 45 | 2n | 492 | 0 | 529 | 17 | 0 |
| 46 | 1o | 728 | 0 | 760 | 18 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 46 | 2o | 728 | 0 | 760 | 20 | 0 |
| 47 | 1p | 681 | 0 | 697 | 28 | 0 |
| 47 | 2p | 677 | 0 | 686 | 21 | 0 |
| 48 | 1q | 823 | 0 | 891 | 18 | 0 |
| 48 | 2q | 823 | 0 | 891 | 18 | 0 |
| 49 | 1r | 555 | 0 | 618 | 9 | 0 |
| 49 | 2r | 555 | 0 | 618 | 12 | 0 |
| 50 | 1s | 648 | 0 | 658 | 20 | 0 |
| 50 | 2s | 645 | 0 | 635 | 39 | 0 |
| 51 | 1t | 732 | 0 | 809 | 24 | 0 |
| 51 | 2t | 733 | 0 | 795 | 17 | 0 |
| 52 | 1u | 199 | 0 | 208 | 7 | 0 |
| 52 | 2u | 199 | 0 | 208 | 7 | 0 |
| 53 | 1y | 764 | 0 | 786 | 17 | 0 |
| 53 | 2y | 749 | 0 | 757 | 18 | 0 |
| 54 | 10 | 8 | 0 | 0 | 0 | 0 |
| 54 | 11 | 5 | 0 | 0 | 0 | 0 |
| 54 | 13 | 3 | 0 | 0 | 0 | 0 |
| 54 | 14 | 1 | 0 | 0 | 0 | 0 |
| 54 | 15 | 8 | 0 | 0 | 0 | 0 |
| 54 | 17 | 6 | 0 | 0 | 0 | 0 |
| 54 | 18 | 2 | 0 | 0 | 0 | 0 |
| 54 | 19 | 2 | 0 | 0 | 0 | 0 |
| 54 | 1A | 1040 | 0 | 0 | 0 | 0 |
| 54 | 1B | 29 | 0 | 0 | 0 | 0 |
| 54 | 1D | 18 | 0 | 0 | 0 | 0 |
| 54 | 1E | 8 | 0 | 0 | 0 | 0 |
| 54 | 1F | 18 | 0 | 0 | 0 | 0 |
| 54 | 1G | 4 | 0 | 0 | 0 | 0 |
| 54 | 1H | 2 | 0 | 0 | 0 | 0 |
| 54 | 1N | 4 | 0 | 0 | 0 | 0 |
| 54 | 1O | 1 | 0 | 0 | 0 | 0 |
| 54 | 1P | 5 | 0 | 0 | 0 | 0 |
| 54 | 1Q | 5 | 0 | 0 | 0 | 0 |
| 54 | 1R | 5 | 0 | 0 | 0 | 0 |
| 54 | 1T | 5 | 0 | 0 | 0 | 0 |
| 54 | 1U | 7 | 0 | 0 | 0 | 0 |
| 54 | 1V | 6 | 0 | 0 | 0 | 0 |
| 54 | 1W | 3 | 0 | 0 | 0 | 0 |
| 54 | 1Y | 1 | 0 | 0 | 0 | 0 |
| 54 | 1Z | 1 | 0 | 0 | 0 | 0 |
| 54 | 1a | 279 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 54 | 1b | 1 | 0 | 0 | 0 | 0 |
| 54 | 1d | 5 | 0 | 0 | 0 | 0 |
| 54 | 1e | 3 | 0 | 0 | 0 | 0 |
| 54 | 1f | 2 | 0 | 0 | 0 | 0 |
| 54 | 1g | 3 | 0 | 0 | 0 | 0 |
| 54 | 1h | 2 | 0 | 0 | 0 | 0 |
| 54 | 1i | 1 | 0 | 0 | 0 | 0 |
| 54 | 1k | 1 | 0 | 0 | 0 | 0 |
| 54 | 1l | 2 | 0 | 0 | 0 | 0 |
| 54 | 1m | 2 | 0 | 0 | 0 | 0 |
| 54 | 1n | 2 | 0 | 0 | 0 | 0 |
| 54 | 1o | 1 | 0 | 0 | 0 | 0 |
| 54 | 1t | 1 | 0 | 0 | 0 | 0 |
| 54 | 1y | 3 | 0 | 0 | 0 | 0 |
| 54 | 20 | 1 | 0 | 0 | 0 | 0 |
| 54 | 21 | 2 | 0 | 0 | 0 | 0 |
| 54 | 23 | 1 | 0 | 0 | 0 | 0 |
| 54 | 25 | 3 | 0 | 0 | 0 | 0 |
| 54 | 27 | 2 | 0 | 0 | 0 | 0 |
| 54 | 28 | 2 | 0 | 0 | 0 | 0 |
| 54 | 2A | 730 | 0 | 0 | 0 | 0 |
| 54 | 2B | 18 | 0 | 0 | 0 | 0 |
| 54 | 2D | 13 | 0 | 0 | 0 | 0 |
| 54 | 2E | 6 | 0 | 0 | 0 | 0 |
| 54 | 2F | 4 | 0 | 0 | 0 | 0 |
| 54 | 2G | 2 | 0 | 0 | 0 | 0 |
| 54 | 2I | 1 | 0 | 0 | 0 | 0 |
| 54 | 2O | 2 | 0 | 0 | 0 | 0 |
| 54 | 2P | 1 | 0 | 0 | 0 | 0 |
| 54 | 2Q | 1 | 0 | 0 | 0 | 0 |
| 54 | 2R | 3 | 0 | 0 | 0 | 0 |
| 54 | 2T | 3 | 0 | 0 | 0 | 0 |
| 54 | 2U | 1 | 0 | 0 | 0 | 0 |
| 54 | 2V | 2 | 0 | 0 | 0 | 0 |
| 54 | 2W | 2 | 0 | 0 | 0 | 0 |
| 54 | 2X | 1 | 0 | 0 | 0 | 0 |
| 54 | 2Y | 1 | 0 | 0 | 0 | 0 |
| 54 | 2a | 190 | 0 | 0 | 0 | 0 |
| 54 | 2e | 2 | 0 | 0 | 0 | 0 |
| 54 | 2f | 1 | 0 | 0 | 0 | 0 |
| 54 | 2j | 1 | 0 | 0 | 0 | 0 |
| 54 | 2k | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 54 | 2n | 1 | 0 | 0 | 0 | 0 |
| 54 | 2r | 2 | 0 | 0 | 0 | 0 |
| 54 | 2t | 1 | 0 | 0 | 0 | 0 |
| 54 | 2y | 1 | 0 | 0 | 0 | 0 |
| 55 | 1A | 36 | 0 | 29 | 1 | 0 |
| 55 | 2A | 36 | 0 | 29 | 1 | 0 |
| 56 | 1A | 51 | 0 | 67 | 0 | 0 |
| 56 | 2A | 51 | 0 | 67 | 1 | 0 |
| 57 | 18 | 8 | 0 | 14 | 3 | 0 |
| 57 | 1A | 8 | 0 | 14 | 1 | 0 |
| 57 | 1T | 8 | 0 | 14 | 0 | 0 |
| 57 | 1a | 8 | 0 | 13 | 6 | 0 |
| 57 | 2A | 16 | 0 | 28 | 0 | 0 |
| 57 | 2B | 8 | 0 | 14 | 0 | 0 |
| 58 | 1B | 12 | 0 | 12 | 0 | 0 |
| 58 | 1F | 12 | 0 | 12 | 1 | 0 |
| 59 | 14 | 1 | 0 | 0 | 0 | 0 |
| 59 | 15 | 1 | 0 | 0 | 0 | 0 |
| 59 | 16 | 1 | 0 | 0 | 0 | 0 |
| 59 | 19 | 1 | 0 | 0 | 0 | 0 |
| 59 | 1Y | 1 | 0 | 0 | 0 | 0 |
| 59 | 1n | 1 | 0 | 0 | 0 | 0 |
| 59 | 24 | 1 | 0 | 0 | 0 | 0 |
| 59 | 25 | 1 | 0 | 0 | 0 | 0 |
| 59 | 26 | 1 | 0 | 0 | 0 | 0 |
| 59 | 29 | 1 | 0 | 0 | 0 | 0 |
| 59 | 2Y | 1 | 0 | 0 | 0 | 0 |
| 59 | 2n | 1 | 0 | 0 | 0 | 0 |
| 60 | 1d | 8 | 0 | 0 | 0 | 0 |
| 60 | 2d | 8 | 0 | 0 | 1 | 0 |
| 61 | 10 | 21 | 0 | 0 | 1 | 0 |
| 61 | 11 | 28 | 0 | 0 | 1 | 0 |
| 61 | 12 | 14 | 0 | 0 | 2 | 0 |
| 61 | 13 | 22 | 0 | 0 | 1 | 0 |
| 61 | 14 | 4 | 0 | 0 | 0 | 0 |
| 61 | 15 | 25 | 0 | 0 | 0 | 0 |
| 61 | 16 | 21 | 0 | 0 | 0 | 0 |
| 61 | 17 | 13 | 0 | 0 | 0 | 0 |
| 61 | 18 | 23 | 0 | 0 | 1 | 0 |
| 61 | 19 | 2 | 0 | 0 | 0 | 0 |
| 61 | 1A | 3898 | 0 | 0 | 87 | 0 |
| 61 | 1B | 94 | 0 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61 | 1D | 103 | 0 | 0 | 2 | 0 |
| 61 | 1E | 68 | 0 | 0 | 1 | 0 |
| 61 | 1F | 64 | 0 | 0 | 0 | 0 |
| 61 | 1G | 16 | 0 | 0 | 0 | 0 |
| 61 | 1H | 15 | 0 | 0 | 0 | 0 |
| 61 | 1I | 5 | 0 | 0 | 0 | 0 |
| 61 | 1N | 45 | 0 | 0 | 1 | 0 |
| 61 | 1O | 22 | 0 | 0 | 1 | 0 |
| 61 | 1P | 56 | 0 | 0 | 3 | 0 |
| 61 | 1Q | 37 | 0 | 0 | 1 | 0 |
| 61 | 1R | 29 | 0 | 0 | 0 | 0 |
| 61 | 1S | 12 | 0 | 0 | 2 | 0 |
| 61 | 1T | 37 | 0 | 0 | 3 | 0 |
| 61 | 1U | 41 | 0 | 0 | 4 | 0 |
| 61 | 1V | 34 | 0 | 0 | 1 | 0 |
| 61 | 1W | 27 | 0 | 0 | 1 | 0 |
| 61 | 1X | 27 | 0 | 0 | 1 | 0 |
| 61 | 1Y | 16 | 0 | 0 | 1 | 0 |
| 61 | 1Z | 5 | 0 | 0 | 0 | 0 |
| 61 | 1a | 447 | 0 | 0 | 18 | 0 |
| 61 | 1b | 1 | 0 | 0 | 0 | 0 |
| 61 | 1c | 2 | 0 | 0 | 0 | 0 |
| 61 | 1d | 9 | 0 | 0 | 2 | 0 |
| 61 | 1e | 5 | 0 | 0 | 1 | 0 |
| 61 | 1f | 1 | 0 | 0 | 0 | 0 |
| 61 | 1h | 1 | 0 | 0 | 0 | 0 |
| 61 | 1j | 1 | 0 | 0 | 0 | 0 |
| 61 | 1l | 3 | 0 | 0 | 1 | 0 |
| 61 | 1o | 2 | 0 | 0 | 0 | 0 |
| 61 | 1p | 2 | 0 | 0 | 0 | 0 |
| 61 | 1y | 1 | 0 | 0 | 0 | 0 |
| 61 | 20 | 5 | 0 | 0 | 0 | 0 |
| 61 | 21 | 15 | 0 | 0 | 0 | 0 |
| 61 | 22 | 1 | 0 | 0 | 1 | 0 |
| 61 | 23 | 2 | 0 | 0 | 0 | 0 |
| 61 | 25 | 7 | 0 | 0 | 1 | 0 |
| 61 | 26 | 2 | 0 | 0 | 0 | 0 |
| 61 | 27 | 8 | 0 | 0 | 0 | 0 |
| 61 | 28 | 9 | 0 | 0 | 1 | 0 |
| 61 | 2A | 1941 | 0 | 0 | 97 | 0 |
| 61 | 2B | 45 | 0 | 0 | 13 | 0 |
| 61 | 2D | 45 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 61 | 2E | 25 | 0 | 0 | 1 | 0 |
| 61 | 2F | 15 | 0 | 0 | 0 | 0 |
| 61 | 2G | 2 | 0 | 0 | 0 | 0 |
| 61 | 2H | 1 | 0 | 0 | 0 | 0 |
| 61 | 2I | 1 | 0 | 0 | 0 | 0 |
| 61 | 2N | 3 | 0 | 0 | 1 | 0 |
| 61 | 2O | 10 | 0 | 0 | 0 | 0 |
| 61 | 2P | 19 | 0 | 0 | 1 | 0 |
| 61 | 2Q | 13 | 0 | 0 | 0 | 0 |
| 61 | 2R | 17 | 0 | 0 | 2 | 0 |
| 61 | 2T | 6 | 0 | 0 | 0 | 0 |
| 61 | 2U | 7 | 0 | 0 | 0 | 0 |
| 61 | 2V | 4 | 0 | 0 | 1 | 0 |
| 61 | 2W | 20 | 0 | 0 | 0 | 0 |
| 61 | 2X | 7 | 0 | 0 | 0 | 0 |
| 61 | 2Y | 2 | 0 | 0 | 0 | 0 |
| 61 | 2Z | 7 | 0 | 0 | 0 | 0 |
| 61 | 2a | 266 | 0 | 0 | 18 | 0 |
| 61 | 2d | 4 | 0 | 0 | 0 | 0 |
| 61 | 2e | 1 | 0 | 0 | 0 | 0 |
| 61 | 2l | 1 | 0 | 0 | 0 | 0 |
| 61 | 2o | 2 | 0 | 0 | 0 | 0 |
| 61 | 2q | 1 | 0 | 0 | 0 | 0 |
| 61 | 2r | 3 | 0 | 0 | 0 | 0 |
| 61 | 2u | 1 | 0 | 0 | 0 | 0 |
| All | All | 296967 | 0 | 194709 | 4218 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 4218 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1A:1082:U:H3 | 1:1A:1086:A:N6 | 1.38 | 1.21 |
| 1:1A:1082:U:O4 | 1:1A:1086:A:N1 | 1.98 | 0.95 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:HG22 | 1.48 | 0.95 |
| 10:2O:48:PRO:HB3 | 32:2a:1422:G:H5'' | 1.49 | 0.94 |
| 1:2A:2100:G:H1 | 1:2A:2189:U:H3 | 1.11 | 0.94 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3 | 1D | 273/276 (99%) | 258 (94%) | 14 (5%) | 1 (0%) | 30 | 49 |
| 3 | 2D | 273/276 (99%) | 257 (94%) | 15 (6%) | 1 (0%) | 30 | 49 |
| 4 | 1E | 202/206 (98%) | 191 (95%) | 9 (4%) | 2 (1%) | 12 | 24 |
| 4 | 2E | 202/206 (98%) | 192 (95%) | 8 (4%) | 2 (1%) | 12 | 24 |
| 5 | 1F | 201/210 (96%) | 197 (98%) | 3 (2%) | 1 (0%) | 24 | 43 |
| 5 | 2F | 201/210 (96%) | 190 (94%) | 10 (5%) | 1 (0%) | 24 | 43 |
| 6 | 1G | 179/182 (98%) | 163 (91%) | 12 (7%) | 4 (2%) | 5 | 9 |
| 6 | 2G | 179/182 (98%) | 149 (83%) | 26 (14%) | 4 (2%) | 5 | 9 |
| 7 | 1H | 172/180 (96%) | 161 (94%) | 10 (6%) | 1 (1%) | 21 | 38 |
| 7 | 2H | 171/180 (95%) | 148 (86%) | 23 (14%) | 0 | 100 | 100 |
| 8 | 1I | 145/148 (98%) | 128 (88%) | 16 (11%) | 1 (1%) | 18 | 34 |
| 8 | 2I | 144/148 (97%) | 130 (90%) | 13 (9%) | 1 (1%) | 18 | 34 |
| 9 | 1N | 138/140 (99%) | 133 (96%) | 5 (4%) | 0 | 100 | 100 |
| 9 | 2N | 138/140 (99%) | 134 (97%) | 4 (3%) | 0 | 100 | 100 |
| 10 | 1O | 120/122 (98%) | 113 (94%) | 6 (5%) | 1 (1%) | 16 | 31 |
| 10 | 2O | 120/122 (98%) | 112 (93%) | 7 (6%) | 1 (1%) | 16 | 31 |
| 11 | 1P | 147/150 (98%) | 141 (96%) | 6 (4%) | 0 | 100 | 100 |
| 11 | 2P | 147/150 (98%) | 140 (95%) | 6 (4%) | 1 (1%) | 18 | 34 |
| 12 | 1Q | 139/141 (99%) | 134 (96%) | 4 (3%) | 1 (1%) | 18 | 34 |
| 12 | 2Q | 139/141 (99%) | 130 (94%) | 9 (6%) | 0 | 100 | 100 |
| 13 | 1R | 116/118 (98%) | 114 (98%) | 2 (2%) | 0 | 100 | 100 |
| 13 | 2R | 116/118 (98%) | 113 (97%) | 3 (3%) | 0 | 100 | 100 |
| 14 | 1S | 108/112 (96%) | 102 (94%) | 5 (5%) | 1 (1%) | 14 | 27 |
| 14 | 2S | 108/112 (96%) | 96 (89%) | 11 (10%) | 1 (1%) | 14 | 27 |
| 15 | 1T | 129/146 (88%) | 120 (93%) | 8 (6%) | 1 (1%) | 16 | 31 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 15 | 2T | 129/146 (88%) | 122 (95%) | 7 (5%) | 0 | 100 | 100 |
| 16 | 1U | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 16 | 2U | 114/118 (97%) | 114 (100%) | 0 | 0 | 100 | 100 |
| 17 | 1V | 99/101 (98%) | 95 (96%) | 2 (2%) | 2 (2%) | 6 | 10 |
| 17 | 2V | 99/101 (98%) | 95 (96%) | 3 (3%) | 1 (1%) | 12 | 24 |
| 18 | 1W | 110/113 (97%) | 110 (100%) | 0 | 0 | 100 | 100 |
| 18 | 2W | 110/113 (97%) | 108 (98%) | 2 (2%) | 0 | 100 | 100 |
| 19 | 1X | 93/96 (97%) | 90 (97%) | 2 (2%) | 1 (1%) | 11 | 22 |
| 19 | 2X | 93/96 (97%) | 87 (94%) | 5 (5%) | 1 (1%) | 11 | 22 |
| 20 | 1Y | 105/110 (96%) | 95 (90%) | 10 (10%) | 0 | 100 | 100 |
| 20 | 2Y | 105/110 (96%) | 99 (94%) | 6 (6%) | 0 | 100 | 100 |
| 21 | 1Z | 201/206 (98%) | 186 (92%) | 14 (7%) | 1 (0%) | 24 | 43 |
| 21 | 2Z | 199/206 (97%) | 177 (89%) | 20 (10%) | 2 (1%) | 12 | 24 |
| 22 | 10 | 75/85 (88%) | 71 (95%) | 4 (5%) | 0 | 100 | 100 |
| 22 | 20 | 75/85 (88%) | 71 (95%) | 4 (5%) | 0 | 100 | 100 |
| 23 | 11 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 11 | 22 |
| 23 | 21 | 95/98 (97%) | 93 (98%) | 1 (1%) | 1 (1%) | 11 | 22 |
| 24 | 12 | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 24 | 22 | 68/72 (94%) | 64 (94%) | 4 (6%) | 0 | 100 | 100 |
| 25 | 13 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | 23 | 57/60 (95%) | 54 (95%) | 3 (5%) | 0 | 100 | 100 |
| 26 | 14 | 67/71 (94%) | 53 (79%) | 10 (15%) | 4 (6%) | 1 | 1 |
| 26 | 24 | 67/71 (94%) | 45 (67%) | 15 (22%) | 7 (10%) | 0 | 0 |
| 27 | 15 | 57/60 (95%) | 57 (100%) | 0 | 0 | 100 | 100 |
| 27 | 25 | 57/60 (95%) | 54 (95%) | 2 (4%) | 1 (2%) | 6 | 12 |
| 28 | 16 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 28 | 26 | 51/54 (94%) | 46 (90%) | 5 (10%) | 0 | 100 | 100 |
| 29 | 17 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 29 | 27 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 30 | 18 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 30 | 28 | 62/65 (95%) | 61 (98%) | 1 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 31 | 19 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 31 | 29 | 35/37 (95%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 33 | 1b | 229/256 (90%) | 193 (84%) | 28 (12%) | 8 (4%) | 3 | 4 |
| 33 | 2b | 229/256 (90%) | 191 (83%) | 32 (14%) | 6 (3%) | 4 | 7 |
| 34 | 1c | 204/239 (85%) | 188 (92%) | 15 (7%) | 1 (0%) | 24 | 43 |
| 34 | 2c | 204/239 (85%) | 176 (86%) | 26 (13%) | 2 (1%) | 12 | 24 |
| 35 | 1d | 206/209 (99%) | 188 (91%) | 17 (8%) | 1 (0%) | 24 | 43 |
| 35 | 2d | 206/209 (99%) | 197 (96%) | 9 (4%) | 0 | 100 | 100 |
| 36 | 1e | 146/162 (90%) | 137 (94%) | 9 (6%) | 0 | 100 | 100 |
| 36 | 2e | 146/162 (90%) | 138 (94%) | 8 (6%) | 0 | 100 | 100 |
| 37 | 1f | 98/101 (97%) | 93 (95%) | 4 (4%) | 1 (1%) | 12 | 24 |
| 37 | 2f | 98/101 (97%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 38 | 1g | 153/156 (98%) | 148 (97%) | 4 (3%) | 1 (1%) | 18 | 34 |
| 38 | 2g | 153/156 (98%) | 142 (93%) | 9 (6%) | 2 (1%) | 9 | 18 |
| 39 | 1h | 135/138 (98%) | 129 (96%) | 6 (4%) | 0 | 100 | 100 |
| 39 | 2h | 135/138 (98%) | 124 (92%) | 10 (7%) | 1 (1%) | 18 | 34 |
| 40 | 1i | 125/128 (98%) | 113 (90%) | 11 (9%) | 1 (1%) | 16 | 31 |
| 40 | 2i | 124/128 (97%) | 107 (86%) | 14 (11%) | 3 (2%) | 4 | 8 |
| 41 | 1j | 95/105 (90%) | 78 (82%) | 13 (14%) | 4 (4%) | 2 | 2 |
| 41 | 2j | 94/105 (90%) | 80 (85%) | 10 (11%) | 4 (4%) | 2 | 2 |
| 42 | 1k | 112/129 (87%) | 104 (93%) | 8 (7%) | 0 | 100 | 100 |
| 42 | 2k | 112/129 (87%) | 100 (89%) | 11 (10%) | 1 (1%) | 14 | 27 |
| 43 | 1l | 119/132 (90%) | 115 (97%) | 4 (3%) | 0 | 100 | 100 |
| 43 | 2l | 119/132 (90%) | 112 (94%) | 7 (6%) | 0 | 100 | 100 |
| 44 | 1m | 114/126 (90%) | 103 (90%) | 7 (6%) | 4 (4%) | 3 | 4 |
| 44 | 2m | 112/126 (89%) | 100 (89%) | 8 (7%) | 4 (4%) | 2 | 3 |
| 45 | 1n | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 | 100 |
| 45 | 2n | 58/61 (95%) | 56 (97%) | 2 (3%) | 0 | 100 | 100 |
| 46 | 1o | 86/89 (97%) | 83 (96%) | 3 (4%) | 0 | 100 | 100 |
| 46 | 2o | 86/89 (97%) | 79 (92%) | 6 (7%) | 1 (1%) | 10 | 20 |
| 47 | 1p | 80/88 (91%) | 70 (88%) | 9 (11%) | 1 (1%) | 9 | 18 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 47 | 2p | 80/88 (91%) | 69 (86%) | 10 (12%) | 1 (1%) | 9 | 18 |
| 48 | 1q | 97/105 (92%) | 87 (90%) | 9 (9%) | 1 (1%) | 12 | 24 |
| 48 | 2q | 97/105 (92%) | 89 (92%) | 7 (7%) | 1 (1%) | 12 | 24 |
| 49 | 1r | 66/88 (75%) | 63 (96%) | 3 (4%) | 0 | 100 | 100 |
| 49 | 2r | 66/88 (75%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 50 | 1s | 81/93 (87%) | 69 (85%) | 10 (12%) | 2 (2%) | 4 | 7 |
| 50 | 2s | 81/93 (87%) | 68 (84%) | 11 (14%) | 2 (2%) | 4 | 7 |
| 51 | 1t | 94/106 (89%) | 87 (93%) | 4 (4%) | 3 (3%) | 3 | 4 |
| 51 | 2t | 96/106 (91%) | 88 (92%) | 5 (5%) | 3 (3%) | 3 | 5 |
| 52 | 1u | 21/27 (78%) | 21 (100%) | 0 | 0 | 100 | 100 |
| 52 | 2u | 21/27 (78%) | 16 (76%) | 4 (19%) | 1 (5%) | 2 | 2 |
| 53 | 1y | 95/113 (84%) | 95 (100%) | 0 | 0 | 100 | 100 |
| 53 | 2y | 94/113 (83%) | 90 (96%) | 4 (4%) | 0 | 100 | 100 |
| All | All | 11629/12354 (94%) | 10793 (93%) | 728 (6%) | 108 (1%) | 14 | 27 |

5 of 108 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 1E | 71 | GLY |
| 5 | 1F | 130 | ALA |
| 6 | 1G | 47 | LYS |
| 6 | 1G | 50 | ALA |
| 26 | 14 | 49 | PHE |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3 | 1D | 214/218 (98%) | 195 (91%) | 19 (9%) | 9 | 20 |
| 3 | 2D | 215/218 (99%) | 199 (93%) | 16 (7%) | 13 | 27 |
| 4 | 1E | 164/166 (99%) | 154 (94%) | 10 (6%) | 17 | 35 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 4 | 2E | 164/166 (99%) | 153 (93%) | 11 (7%) | 15 | 31 |
| 5 | 1F | 160/166 (96%) | 144 (90%) | 16 (10%) | 7 | 15 |
| 5 | 2F | 159/166 (96%) | 140 (88%) | 19 (12%) | 5 | 11 |
| 6 | 1G | 144/156 (92%) | 132 (92%) | 12 (8%) | 10 | 22 |
| 6 | 2G | 142/156 (91%) | 126 (89%) | 16 (11%) | 5 | 12 |
| 7 | 1H | 144/148 (97%) | 131 (91%) | 13 (9%) | 9 | 19 |
| 7 | 2H | 143/148 (97%) | 129 (90%) | 14 (10%) | 7 | 16 |
| 8 | 1I | 111/124 (90%) | 98 (88%) | 13 (12%) | 5 | 11 |
| 8 | 2I | 108/124 (87%) | 98 (91%) | 10 (9%) | 8 | 18 |
| 9 | 1N | 119/119 (100%) | 107 (90%) | 12 (10%) | 7 | 15 |
| 9 | 2N | 118/119 (99%) | 107 (91%) | 11 (9%) | 8 | 18 |
| 10 | 1O | 100/100 (100%) | 96 (96%) | 4 (4%) | 28 | 54 |
| 10 | 2O | 100/100 (100%) | 97 (97%) | 3 (3%) | 36 | 64 |
| 11 | 1P | 115/116 (99%) | 108 (94%) | 7 (6%) | 17 | 35 |
| 11 | 2P | 115/116 (99%) | 106 (92%) | 9 (8%) | 11 | 24 |
| 12 | 1Q | 111/111 (100%) | 105 (95%) | 6 (5%) | 20 | 41 |
| 12 | 2Q | 111/111 (100%) | 98 (88%) | 13 (12%) | 5 | 11 |
| 13 | 1R | 101/101 (100%) | 92 (91%) | 9 (9%) | 9 | 20 |
| 13 | 2R | 101/101 (100%) | 95 (94%) | 6 (6%) | 18 | 37 |
| 14 | 1S | 87/88 (99%) | 79 (91%) | 8 (9%) | 8 | 19 |
| 14 | 2S | 85/88 (97%) | 75 (88%) | 10 (12%) | 5 | 11 |
| 15 | 1T | 115/127 (91%) | 106 (92%) | 9 (8%) | 11 | 24 |
| 15 | 2T | 113/127 (89%) | 106 (94%) | 7 (6%) | 16 | 34 |
| 16 | 1U | 93/94 (99%) | 89 (96%) | 4 (4%) | 26 | 51 |
| 16 | 2U | 93/94 (99%) | 87 (94%) | 6 (6%) | 15 | 32 |
| 17 | 1V | 81/82 (99%) | 75 (93%) | 6 (7%) | 13 | 27 |
| 17 | 2V | 80/82 (98%) | 73 (91%) | 7 (9%) | 9 | 20 |
| 18 | 1W | 90/92 (98%) | 83 (92%) | 7 (8%) | 11 | 24 |
| 18 | 2W | 90/92 (98%) | 80 (89%) | 10 (11%) | 6 | 12 |
| 19 | 1X | 77/78 (99%) | 72 (94%) | 5 (6%) | 15 | 32 |
| 19 | 2X | 77/78 (99%) | 74 (96%) | 3 (4%) | 28 | 55 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 20 | 1Y | 86/91 (94%) | 80 (93%) | 6 (7%) | 14 | 29 |
| 20 | 2Y | 86/91 (94%) | 75 (87%) | 11 (13%) | 4 | 9 |
| 21 | 1Z | 169/179 (94%) | 151 (89%) | 18 (11%) | 6 | 13 |
| 21 | 2Z | 165/179 (92%) | 152 (92%) | 13 (8%) | 11 | 24 |
| 22 | 10 | 61/67 (91%) | 59 (97%) | 2 (3%) | 33 | 61 |
| 22 | 20 | 61/67 (91%) | 57 (93%) | 4 (7%) | 15 | 32 |
| 23 | 11 | 79/83 (95%) | 73 (92%) | 6 (8%) | 12 | 26 |
| 23 | 21 | 81/83 (98%) | 75 (93%) | 6 (7%) | 13 | 27 |
| 24 | 12 | 65/67 (97%) | 63 (97%) | 2 (3%) | 35 | 62 |
| 24 | 22 | 66/67 (98%) | 56 (85%) | 10 (15%) | 3 | 5 |
| 25 | 13 | 51/52 (98%) | 46 (90%) | 5 (10%) | 7 | 16 |
| 25 | 23 | 50/52 (96%) | 45 (90%) | 5 (10%) | 7 | 15 |
| 26 | 14 | 58/63 (92%) | 52 (90%) | 6 (10%) | 7 | 14 |
| 26 | 24 | 54/63 (86%) | 45 (83%) | 9 (17%) | 2 | 4 |
| 27 | 15 | 51/52 (98%) | 45 (88%) | 6 (12%) | 5 | 11 |
| 27 | 25 | 50/52 (96%) | 47 (94%) | 3 (6%) | 17 | 36 |
| 28 | 16 | 51/52 (98%) | 43 (84%) | 8 (16%) | 2 | 5 |
| 28 | 26 | 50/52 (96%) | 44 (88%) | 6 (12%) | 5 | 10 |
| 29 | 17 | 41/42 (98%) | 38 (93%) | 3 (7%) | 13 | 27 |
| 29 | 27 | 41/42 (98%) | 37 (90%) | 4 (10%) | 7 | 16 |
| 30 | 18 | 54/55 (98%) | 52 (96%) | 2 (4%) | 30 | 57 |
| 30 | 28 | 54/55 (98%) | 52 (96%) | 2 (4%) | 30 | 57 |
| 31 | 19 | 34/34 (100%) | 33 (97%) | 1 (3%) | 37 | 65 |
| 31 | 29 | 34/34 (100%) | 32 (94%) | 2 (6%) | 18 | 37 |
| 33 | 1b | 191/220 (87%) | 169 (88%) | 22 (12%) | 5 | 11 |
| 33 | 2b | 187/220 (85%) | 162 (87%) | 25 (13%) | 4 | 8 |
| 34 | 1c | 144/188 (77%) | 137 (95%) | 7 (5%) | 22 | 45 |
| 34 | 2c | 140/188 (74%) | 126 (90%) | 14 (10%) | 7 | 15 |
| 35 | 1d | 171/181 (94%) | 157 (92%) | 14 (8%) | 10 | 23 |
| 35 | 2d | 172/181 (95%) | 151 (88%) | 21 (12%) | 5 | 10 |
| 36 | 1e | 114/123 (93%) | 108 (95%) | 6 (5%) | 20 | 42 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 36 | 2e | 114/123 (93%) | 103 (90%) | 11 (10%) | 8 | 17 |
| 37 | 1f | 85/90 (94%) | 77 (91%) | 8 (9%) | 8 | 18 |
| 37 | 2f | 85/90 (94%) | 77 (91%) | 8 (9%) | 8 | 18 |
| 38 | 1g | 120/127 (94%) | 115 (96%) | 5 (4%) | 26 | 52 |
| 38 | 2g | 119/127 (94%) | 107 (90%) | 12 (10%) | 7 | 15 |
| 39 | 1h | 116/119 (98%) | 106 (91%) | 10 (9%) | 10 | 21 |
| 39 | 2h | 114/119 (96%) | 102 (90%) | 12 (10%) | 6 | 14 |
| 40 | 1i | 91/99 (92%) | 85 (93%) | 6 (7%) | 15 | 32 |
| 40 | 2i | 88/99 (89%) | 78 (89%) | 10 (11%) | 5 | 12 |
| 41 | 1j | 68/92 (74%) | 59 (87%) | 9 (13%) | 4 | 8 |
| 41 | 2j | 68/92 (74%) | 56 (82%) | 12 (18%) | 2 | 3 |
| 42 | 1k | 83/99 (84%) | 77 (93%) | 6 (7%) | 13 | 28 |
| 42 | 2k | 83/99 (84%) | 77 (93%) | 6 (7%) | 13 | 28 |
| 43 | 1l | 96/108 (89%) | 95 (99%) | 1 (1%) | 68 | 86 |
| 43 | 2l | 96/108 (89%) | 89 (93%) | 7 (7%) | 13 | 27 |
| 44 | 1m | 90/101 (89%) | 84 (93%) | 6 (7%) | 15 | 31 |
| 44 | 2m | 87/101 (86%) | 77 (88%) | 10 (12%) | 5 | 11 |
| 45 | 1n | 49/50 (98%) | 44 (90%) | 5 (10%) | 7 | 15 |
| 45 | 2n | 49/50 (98%) | 43 (88%) | 6 (12%) | 5 | 10 |
| 46 | 1o | 78/80 (98%) | 73 (94%) | 5 (6%) | 16 | 33 |
| 46 | 2o | 78/80 (98%) | 74 (95%) | 4 (5%) | 21 | 43 |
| 47 | 1p | 69/74 (93%) | 57 (83%) | 12 (17%) | 2 | 3 |
| 47 | 2p | 68/74 (92%) | 60 (88%) | 8 (12%) | 5 | 11 |
| 48 | 1q | 94/97 (97%) | 90 (96%) | 4 (4%) | 26 | 51 |
| 48 | 2q | 94/97 (97%) | 87 (93%) | 7 (7%) | 13 | 27 |
| 49 | 1r | 59/77 (77%) | 57 (97%) | 2 (3%) | 32 | 60 |
| 49 | 2r | 59/77 (77%) | 55 (93%) | 4 (7%) | 14 | 31 |
| 50 | 1s | 68/80 (85%) | 63 (93%) | 5 (7%) | 13 | 27 |
| 50 | 2s | 67/80 (84%) | 58 (87%) | 9 (13%) | 4 | 8 |
| 51 | 1t | 71/82 (87%) | 65 (92%) | 6 (8%) | 10 | 22 |
| 51 | 2t | 70/82 (85%) | 62 (89%) | 8 (11%) | 5 | 12 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 52 | 1u | 18/22 (82%) | 17 (94%) | 1 (6%) | 19 | 39 |
| 52 | 2u | 18/22 (82%) | 18 (100%) | 0 | 100 | 100 |
| 53 | 1y | 82/98 (84%) | 81 (99%) | 1 (1%) | 63 | 83 |
| 53 | 2y | 79/98 (81%) | 73 (92%) | 6 (8%) | 12 | 26 |
| All | All | 9524/10260 (93%) | 8712 (92%) | 812 (8%) | 10 | 22 |

5 of 812 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | 2O | 69 | ILE |
| 24 | 22 | 25 | VAL |
| 51 | 2t | 41 | ILE |
| 12 | 2Q | 16 | ARG |
| 9 | 2N | 138 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37 | 2f | 94 | GLN |
| 38 | 2g | 86 | GLN |
| 47 | 2p | 13 | HIS |
| 38 | 1g | 148 | ASN |
| 38 | 1g | 64 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 1A | 2865/2915 (98%) | 403 (14%) | 35 (1%) |
| 1 | 2A | 2858/2915 (98%) | 463 (16%) | 37 (1%) |
| 2 | 1B | 119/121 (98%) | 13 (10%) | 0 |
| 2 | 2B | 119/121 (98%) | 17 (14%) | 0 |
| 32 | 1a | 1497/1521 (98%) | 246 (16%) | 0 |
| 32 | 2a | 1501/1521 (98%) | 259 (17%) | 0 |
| All | All | 8959/9114 (98%) | 1401 (15%) | 72 (0%) |

5 of 1401 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1A | 12 | U |
| 1 | 1A | 13 | A |
| 1 | 1A | 15 | G |
| 1 | 1A | 33 | U |
| 1 | 1A | 34 | C |

5 of 72 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 1491 | G |
| 1 | 2A | 2756 | U |
| 1 | 2A | 1992 | G |
| 1 | 2A | 2406 | U |
| 1 | 1A | 1762 | A |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 32 | MA6 | 1a | 1519 | 32 | 23,26,27 | 0.42 | 0 | 33,38,41 | 1.98 | 9 (27%) |
| 1 | 5MU | 1A | 1915 | 1,54 | 19,22,23 | 1.49 | 5 (26%) | 27,32,35 | 2.25 | 9 (33%) |
| 1 | PSU | 2A | 1911 | 1 | 18,21,22 | 1.38 | 2 (11%) | 21,30,33 | 2.07 | 4 (19%) |
| 1 | PSU | 2A | 1917 | 1 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 2.07 | 3 (14%) |
| 1 | 5MU | 1A | 1939 | 1,54 | 19,22,23 | 1.36 | 4 (21%) | 27,32,35 | 2.27 | 6 (22%) |
| 32 | UR3 | 1a | 1498 | 32 | 19,22,23 | 0.92 | 0 | 26,32,35 | 1.82 | 3 (11%) |
| 1 | 5MC | 2A | 1962 | 1 | 19,22,23 | 1.61 | 3 (15%) | 26,32,35 | 1.12 | 2 (7%) |
| 32 | 4OC | 2a | 1402 | 32 | 20,23,24 | 0.76 | 0 | 25,32,35 | 0.93 | 1 (4%) |
| 32 | G7M | 2a | 527 | 32,54 | 23,26,27 | 2.36 | 5 (21%) | 34,39,42 | 3.04 | 10 (29%) |
| 32 | UR3 | 2a | 1498 | 32 | 19,22,23 | 1.04 | 2 (10%) | 26,32,35 | 1.70 | 3 (11%) |
| 1 | 5MU | 2A | 1915 | 1 | 19,22,23 | 1.49 | 4 (21%) | 27,32,35 | 2.24 | 9 (33%) |
| 1 | PSU | 1A | 2605 | 1 | 18,21,22 | 1.46 | 3 (16%) | 21,30,33 | 2.16 | 5 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 32 | 2MG | 2a | 1207 | 32 | 23,26,27 | 1.28 | 4 (17%) | 33,38,41 | 2.06 | 5 (15%) |
| 1 | PSU | 2A | 2605 | 1 | 18,21,22 | 1.42 | 3 (16%) | 21,30,33 | 2.14 | 5 (23%) |
| 1 | 2MA | 1A | 2503 | 1,54 | 22,25,26 | 1.48 | 6 (27%) | 32,37,40 | 2.42 | 9 (28%) |
| 1 | 5MC | 1A | 1942 | 1,54 | 19,22,23 | 1.41 | 3 (15%) | 26,32,35 | 1.10 | 2 (7%) |
| 1 | 2MU | 1A | 2552 | 1,54 | 19,22,24 | 1.26 | 3 (15%) | 25,31,36 | 1.75 | 6 (24%) |
| 43 | 0TD | 1l | 92 | 43 | 8,9,10 | 4.65 | 1 (12%) | 6,11,13 | 2.13 | 3 (50%) |
| 32 | M2G | 2a | 966 | 32 | 24,27,28 | 1.33 | 4 (16%) | 33,40,43 | 1.84 | 5 (15%) |
| 1 | OMC | 1A | 1920 | 1,54 | 19,22,23 | 0.80 | 0 | 25,31,34 | 0.87 | 1 (4%) |
| 32 | 5MC | 2a | 1400 | 32 | 19,22,23 | 1.64 | 3 (15%) | 26,32,35 | 1.20 | 2 (7%) |
| 32 | 5MC | 1a | 1404 | 32 | 19,22,23 | 1.54 | 2 (10%) | 26,32,35 | 1.04 | 2 (7%) |
| 1 | OMC | 2A | 1920 | 1 | 19,22,23 | 0.78 | 0 | 25,31,34 | 0.95 | 1 (4%) |
| 32 | PSU | 2a | 516 | 32,54 | 18,21,22 | 1.36 | 3 (16%) | 21,30,33 | 2.01 | 5 (23%) |
| 43 | 0TD | 2l | 92 | 43 | 8,9,10 | 4.34 | 1 (12%) | 6,11,13 | 1.92 | 3 (50%) |
| 1 | 2MA | 2A | 2503 | 1,54 | 22,25,26 | 1.45 | 4 (18%) | 32,37,40 | 2.35 | 8 (25%) |
| 32 | M2G | 1a | 966 | 32 | 24,27,28 | 1.29 | 5 (20%) | 33,40,43 | 1.81 | 6 (18%) |
| 1 | 2MU | 2A | 2552 | 1,54 | 19,22,24 | 1.26 | 3 (15%) | 25,31,36 | 1.88 | 6 (24%) |
| 1 | PSU | 1A | 1917 | 1,54 | 18,21,22 | 1.40 | 2 (11%) | 21,30,33 | 2.02 | 3 (14%) |
| 1 | OMG | 2A | 2251 | 1,54 | 23,26,27 | 1.20 | 3 (13%) | 32,38,41 | 2.03 | 6 (18%) |
| 32 | MA6 | 1a | 1518 | 32 | 23,26,27 | 0.39 | 0 | 33,38,41 | 1.89 | 8 (24%) |
| 32 | 5MC | 1a | 1400 | 32 | 19,22,23 | 1.73 | 3 (15%) | 26,32,35 | 1.22 | 2 (7%) |
| 32 | G7M | 1a | 527 | 32,54 | 23,26,27 | 2.32 | 5 (21%) | 34,39,42 | 2.95 | 10 (29%) |
| 1 | 5MC | 1A | 1962 | 1,54 | 19,22,23 | 1.74 | 3 (15%) | 26,32,35 | 1.19 | 4 (15%) |
| 32 | 5MC | 2a | 1407 | 32 | 19,22,23 | 1.64 | 3 (15%) | 26,32,35 | 1.19 | 3 (11%) |
| 1 | 5MC | 2A | 1942 | 1 | 19,22,23 | 1.80 | 3 (15%) | 26,32,35 | 1.25 | 3 (11%) |
| 32 | 2MG | 1a | 1207 | 32 | 23,26,27 | 1.22 | 2 (8%) | 33,38,41 | 2.23 | 8 (24%) |
| 32 | 5MC | 2a | 967 | 32 | 19,22,23 | 1.87 | 2 (10%) | 26,32,35 | 1.10 | 2 (7%) |
| 32 | 5MC | 2a | 1404 | 32 | 19,22,23 | 1.72 | 3 (15%) | 26,32,35 | 1.17 | 3 (11%) |
| 1 | 5MU | 2A | 1939 | 1 | 19,22,23 | 1.50 | 6 (31%) | 27,32,35 | 2.28 | 8 (29%) |
| 32 | 5MC | 1a | 1407 | 32 | 19,22,23 | 1.52 | 3 (15%) | 26,32,35 | 1.20 | 3 (11%) |
| 32 | PSU | 1a | 516 | 32,54 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 2.00 | 4 (19%) |
| 1 | OMG | 1A | 2251 | 1,54 | 23,26,27 | 1.23 | 3 (13%) | 32,38,41 | 2.05 | 7 (21%) |
| 32 | MA6 | 2a | 1519 | 32 | 23,26,27 | 0.43 | 0 | 33,38,41 | 2.15 | 9 (27%) |
| 32 | 4OC | 1a | 1402 | 32 | 20,23,24 | 0.72 | 0 | 25,32,35 | 0.96 | 1 (4%) |
| 32 | 5MC | 1a | 967 | 32 | 19,22,23 | 1.52 | 3 (15%) | 26,32,35 | 1.03 | 2 (7%) |
| 1 | PSU | 1A | 1911 | 1 | 18,21,22 | 1.36 | 2 (11%) | 21,30,33 | 2.03 | 4 (19%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 32 | MA6 | 2a | 1518 | 32 | 23,26,27 | 0.40 | 0 | 33,38,41 | 2.02 | 9 (27%) |

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 | MA6 | 1a | 1519 | 32 | - | 2/11/29/30 | 0/3/3/3 |
| 1 | 5MU | 1A | 1915 | 1,54 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1939 | 1,54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | UR3 | 1a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1962 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 32 | 4OC | 2a | 1402 | 32 | - | 2/9/29/30 | 0/2/2/2 |
| 32 | G7M | 2a | 527 | 32,54 | - | 2/7/25/26 | 0/3/3/3 |
| 32 | UR3 | 2a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1915 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 2a | 1207 | 32 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | PSU | 2A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 1,54 | - | 1/7/25/26 | 0/3/3/3 |
| 1 | 5MC | 1A | 1942 | 1,54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MU | 1A | 2552 | 1,54 | - | 0/9/27/28 | 0/2/2/2 |
| 43 | 0TD | 1l | 92 | 43 | - | 3/7/12/14 | - |
| 32 | M2G | 2a | 966 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 1 | OMC | 1A | 1920 | 1,54 | - | 1/9/27/28 | 0/2/2/2 |
| 32 | 5MC | 2a | 1400 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1404 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | 2A | 1920 | 1 | - | 2/9/27/28 | 0/2/2/2 |
| 32 | PSU | 2a | 516 | 32,54 | - | 1/7/25/26 | 0/2/2/2 |
| 43 | 0TD | 2l | 92 | 43 | - | 1/7/12/14 | - |
| 1 | 2MA | 2A | 2503 | 1,54 | - | 0/7/25/26 | 0/3/3/3 |
| 32 | M2G | 1a | 966 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 1 | 2MU | 2A | 2552 | 1,54 | - | 2/9/27/28 | 0/2/2/2 |
| 1 | PSU | 1A | 1917 | 1,54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 2A | 2251 | 1,54 | - | 0/9/27/28 | 0/3/3/3 |
| 32 | MA6 | 1a | 1518 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 32 | 5MC | 1a | 1400 | 32 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|------------|---------|
| 32 | G7M | 1a | 527 | 32,54 | - | 1/7/25/26 | 0/3/3/3 |
| 1 | 5MC | 1A | 1962 | 1,54 | - | 2/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 1a | 1207 | 32 | - | 0/9/27/28 | 0/3/3/3 |
| 32 | 5MC | 2a | 967 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1404 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1939 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | PSU | 1a | 516 | 32,54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 1A | 2251 | 1,54 | - | 0/9/27/28 | 0/3/3/3 |
| 32 | MA6 | 2a | 1519 | 32 | - | 2/11/29/30 | 0/3/3/3 |
| 32 | 4OC | 1a | 1402 | 32 | - | 0/9/29/30 | 0/2/2/2 |
| 32 | 5MC | 1a | 967 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 2a | 1518 | 32 | - | 0/11/29/30 | 0/3/3/3 |

The worst 5 of 123 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 43 | 1l | 92 | 0TD | CB-SB | -12.75 | 1.69 | 1.82 |
| 43 | 2l | 92 | 0TD | CB-SB | -11.92 | 1.70 | 1.82 |
| 32 | 2a | 527 | G7M | C8-N7 | 7.55 | 1.45 | 1.33 |
| 32 | 1a | 527 | G7M | C8-N7 | 7.38 | 1.45 | 1.33 |
| 32 | 2a | 967 | 5MC | C5-C4 | 7.00 | 1.49 | 1.44 |

The worst 5 of 232 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 32 | 2a | 527 | G7M | CN7-N7-C8 | -8.36 | 112.13 | 124.79 |
| 1 | 1A | 2503 | 2MA | C5-C4-N3 | -8.28 | 118.46 | 127.18 |
| 1 | 2A | 2503 | 2MA | C5-C4-N3 | -8.12 | 118.63 | 127.18 |
| 32 | 1a | 527 | G7M | CN7-N7-C8 | -8.08 | 112.55 | 124.79 |
| 32 | 1a | 1498 | UR3 | C4-N3-C2 | -7.34 | 118.67 | 124.58 |

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 1 | 1A | 1915 | 5MU | O4'-C1'-N1-C2 |
| 1 | 1A | 1915 | 5MU | O4'-C1'-N1-C6 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|---------------|
| 43 | 1l | 92 | 0TD | O-C-CA-CB |
| 43 | 1l | 92 | 0TD | CG-CB-SB-CSB |
| 1 | 2A | 1915 | 5MU | O4'-C1'-N1-C2 |

There are no ring outliers.

19 monomers are involved in 25 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 32 | 1a | 1519 | MA6 | 2 | 0 |
| 1 | 2A | 1917 | PSU | 1 | 0 |
| 1 | 1A | 1939 | 5MU | 2 | 0 |
| 32 | 2a | 1402 | 4OC | 1 | 0 |
| 32 | 2a | 1207 | 2MG | 2 | 0 |
| 1 | 1A | 2552 | 2MU | 1 | 0 |
| 43 | 1l | 92 | 0TD | 1 | 0 |
| 32 | 2a | 966 | M2G | 1 | 0 |
| 1 | 1A | 1920 | OMC | 1 | 0 |
| 32 | 2a | 1400 | 5MC | 1 | 0 |
| 1 | 2A | 1920 | OMC | 1 | 0 |
| 43 | 2l | 92 | 0TD | 3 | 0 |
| 1 | 2A | 2251 | OMG | 1 | 0 |
| 32 | 1a | 1518 | MA6 | 2 | 0 |
| 32 | 1a | 1400 | 5MC | 2 | 0 |
| 32 | 2a | 967 | 5MC | 1 | 0 |
| 1 | 2A | 1939 | 5MU | 1 | 0 |
| 32 | 2a | 1519 | MA6 | 3 | 0 |
| 32 | 2a | 1518 | MA6 | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2534 ligands modelled in this entry, 2519 are monoatomic - leaving 15 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 | 2d | 501 | 35 | 0,12,12 | - | - | - | - | - |
| 56 | ERY | 1A | 4042 | - | 53,53,53 | 0.94 | 2 (3%) | 82,82,82 | 1.31 | 10 (12%) |
| 57 | MPD | 1a | 1880 | 32 | 7,7,7 | 0.45 | 0 | 9,10,10 | 0.58 | 0 |
| 58 | ARG | 1B | 230 | 54 | 10,11,11 | 0.79 | 1 (10%) | 9,13,13 | 0.96 | 1 (11%) |
| 57 | MPD | 2B | 219 | - | 7,7,7 | 0.33 | 0 | 9,10,10 | 0.19 | 0 |
| 57 | MPD | 2A | 3734 | - | 7,7,7 | 0.32 | 0 | 9,10,10 | 0.19 | 0 |
| 55 | HGR | 1A | 4041 | - | 39,39,39 | 2.39 | 8 (20%) | 48,58,58 | 1.82 | 13 (27%) |
| 57 | MPD | 2A | 3733 | - | 7,7,7 | 0.39 | 0 | 9,10,10 | 0.49 | 0 |
| 57 | MPD | 1A | 4043 | - | 7,7,7 | 0.34 | 0 | 9,10,10 | 0.22 | 0 |
| 57 | MPD | 1T | 206 | - | 7,7,7 | 0.37 | 0 | 9,10,10 | 0.23 | 0 |
| 58 | ARG | 1F | 319 | - | 10,11,11 | 0.73 | 1 (10%) | 9,13,13 | 0.88 | 1 (11%) |
| 56 | ERY | 2A | 3732 | - | 53,53,53 | 0.96 | 2 (3%) | 82,82,82 | 1.39 | 11 (13%) |
| 60 | SF4 | 1d | 306 | 35 | 0,12,12 | - | - | - | - | - |
| 55 | HGR | 2A | 3731 | - | 39,39,39 | 2.42 | 9 (23%) | 48,58,58 | 1.68 | 13 (27%) |
| 57 | MPD | 18 | 103 | - | 7,7,7 | 0.32 | 0 | 9,10,10 | 0.40 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|--------------|---------|
| 60 | SF4 | 2d | 501 | 35 | - | - | 0/6/5/5 |
| 56 | ERY | 1A | 4042 | - | - | 0/72/107/107 | 0/3/3/3 |
| 57 | MPD | 1a | 1880 | 32 | - | 5/5/5/5 | - |
| 58 | ARG | 1B | 230 | 54 | - | 0/11/11/11 | - |
| 57 | MPD | 2B | 219 | - | - | 1/5/5/5 | - |
| 57 | MPD | 2A | 3734 | - | - | 1/5/5/5 | - |
| 55 | HGR | 1A | 4041 | - | - | 5/20/79/79 | 0/4/4/4 |
| 57 | MPD | 2A | 3733 | - | - | 0/5/5/5 | - |
| 57 | MPD | 1A | 4043 | - | - | 2/5/5/5 | - |
| 57 | MPD | 1T | 206 | - | - | 0/5/5/5 | - |
| 58 | ARG | 1F | 319 | - | - | 3/11/11/11 | - |
| 56 | ERY | 2A | 3732 | - | - | 4/72/107/107 | 0/3/3/3 |
| 60 | SF4 | 1d | 306 | 35 | - | - | 0/6/5/5 |
| 55 | HGR | 2A | 3731 | - | - | 5/20/79/79 | 0/4/4/4 |
| 57 | MPD | 18 | 103 | - | - | 2/5/5/5 | - |

The worst 5 of 23 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55 | 2A | 3731 | HGR | C12-C14 | 9.37 | 1.55 | 1.33 |
| 55 | 1A | 4041 | HGR | C12-C14 | 8.86 | 1.54 | 1.33 |
| 55 | 1A | 4041 | HGR | C5-C4 | -5.62 | 1.39 | 1.49 |
| 55 | 2A | 3731 | HGR | C5-C4 | -5.47 | 1.39 | 1.49 |
| 55 | 1A | 4041 | HGR | C5-C6 | -5.24 | 1.39 | 1.50 |

The worst 5 of 49 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 55 | 2A | 3731 | HGR | C4-C5-C6 | 4.72 | 122.42 | 112.35 |
| 55 | 1A | 4041 | HGR | C4-C5-C6 | 4.56 | 122.08 | 112.35 |
| 56 | 2A | 3732 | ERY | O5-C16-C17 | 3.90 | 109.51 | 103.86 |
| 56 | 2A | 3732 | ERY | C13-O2-C1 | -3.73 | 111.68 | 118.20 |
| 55 | 1A | 4041 | HGR | O9-C22-C18 | -3.70 | 98.20 | 106.03 |

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|----------------|
| 56 | 2A | 3732 | ERY | C15-C16-O5-C20 |
| 56 | 2A | 3732 | ERY | C19-C16-O5-C20 |
| 57 | 18 | 103 | MPD | C2-C3-C4-O4 |
| 57 | 18 | 103 | MPD | C2-C3-C4-C5 |
| 57 | 2B | 219 | MPD | C2-C3-C4-O4 |

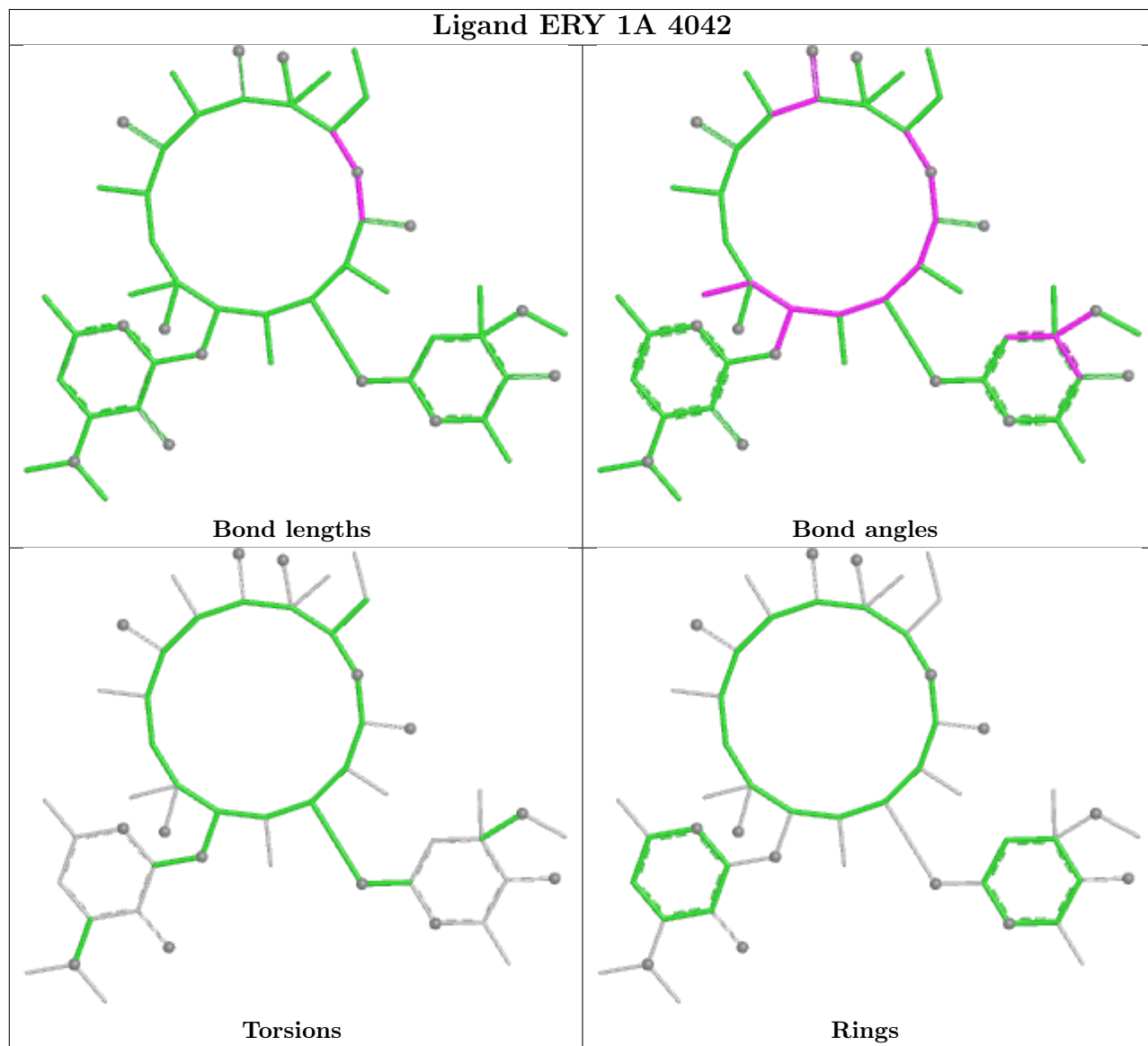
There are no ring outliers.

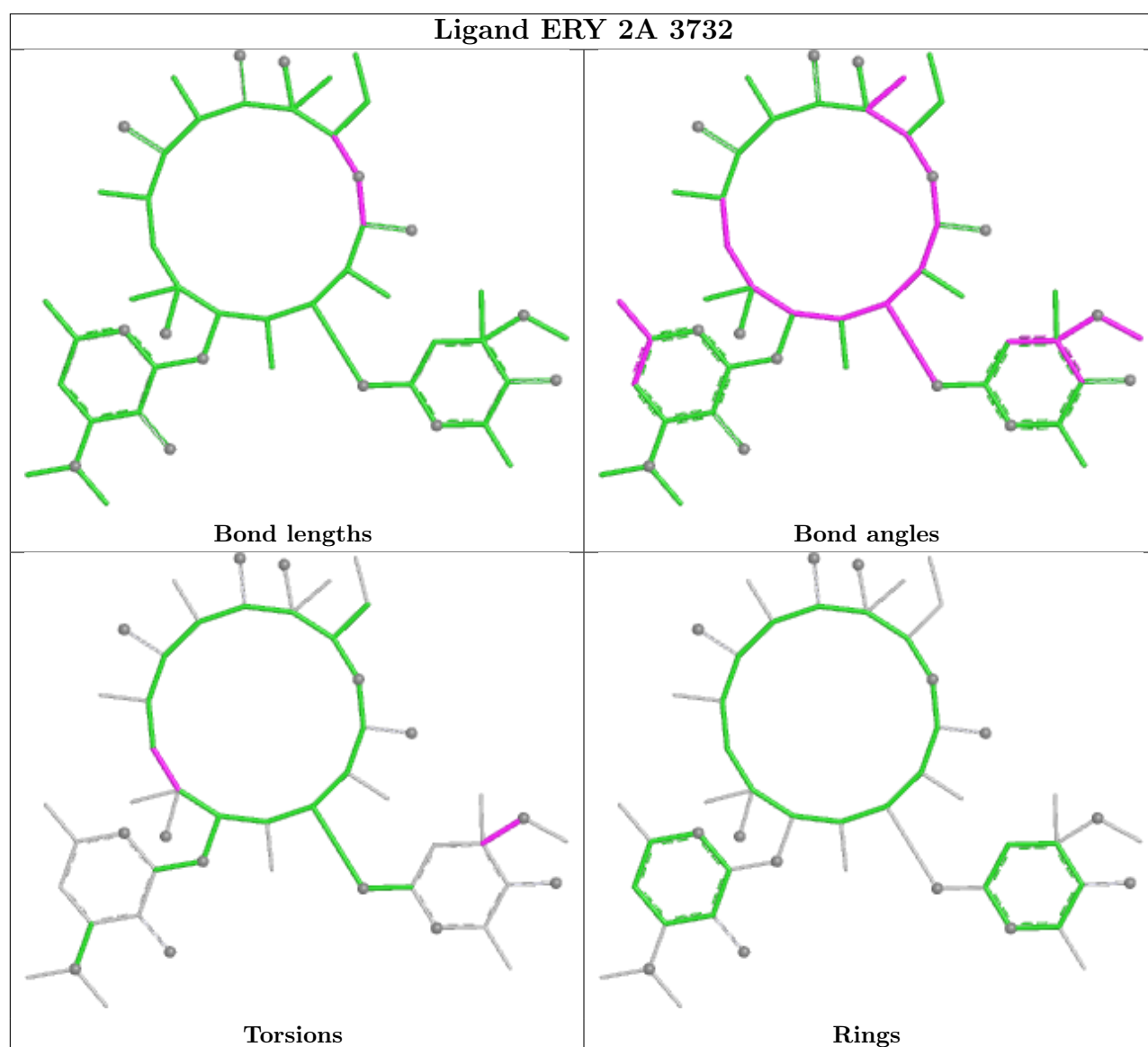
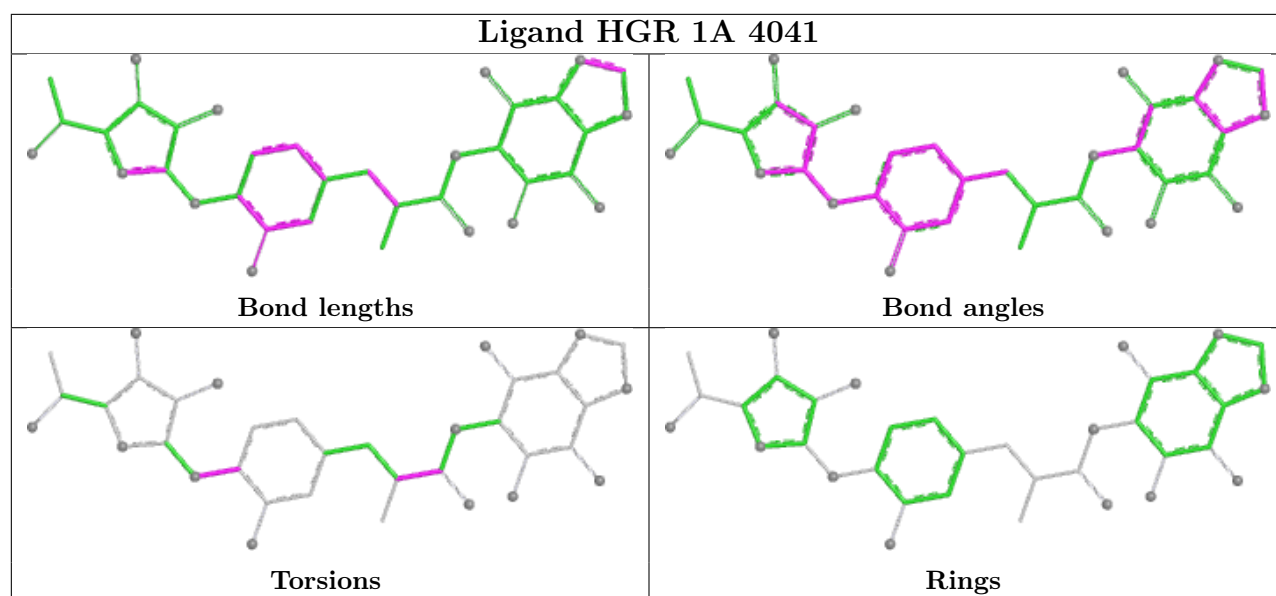
8 monomers are involved in 15 short contacts:

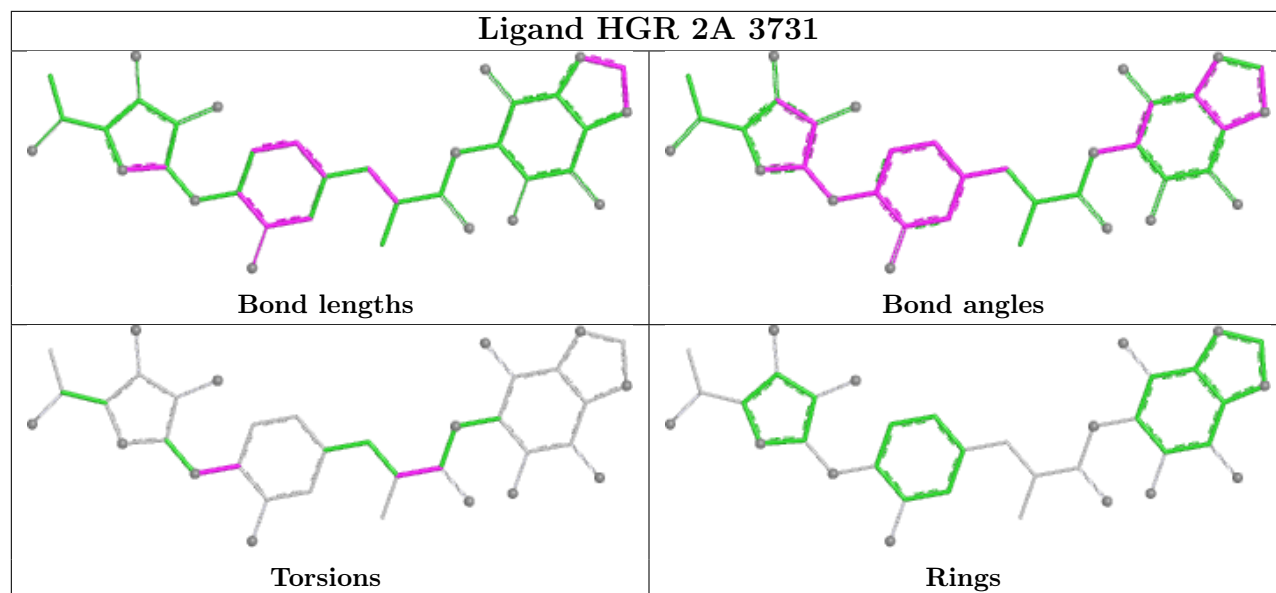
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 60 | 2d | 501 | SF4 | 1 | 0 |
| 57 | 1a | 1880 | MPD | 6 | 0 |
| 55 | 1A | 4041 | HGR | 1 | 0 |
| 57 | 1A | 4043 | MPD | 1 | 0 |
| 58 | 1F | 319 | ARG | 1 | 0 |
| 56 | 2A | 3732 | ERY | 1 | 0 |
| 55 | 2A | 3731 | HGR | 1 | 0 |
| 57 | 18 | 103 | MPD | 3 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | 1A | 2861/2915 (98%) | -0.51 | 90 (3%) 51 47 | 26, 43, 97, 110 | 0 |
| 1 | 2A | 2856/2915 (97%) | -0.04 | 117 (4%) 41 37 | 39, 63, 100, 111 | 0 |
| 2 | 1B | 120/121 (99%) | -0.36 | 1 (0%) 82 80 | 37, 55, 69, 84 | 0 |
| 2 | 2B | 120/121 (99%) | 0.98 | 6 (5%) 34 30 | 68, 88, 96, 98 | 0 |
| 3 | 1D | 275/276 (99%) | -0.03 | 4 (1%) 72 68 | 27, 43, 56, 79 | 0 |
| 3 | 2D | 275/276 (99%) | 0.40 | 10 (3%) 46 41 | 36, 56, 68, 82 | 0 |
| 4 | 1E | 204/206 (99%) | 0.11 | 4 (1%) 65 61 | 26, 46, 64, 79 | 0 |
| 4 | 2E | 204/206 (99%) | 0.42 | 5 (2%) 58 54 | 38, 62, 75, 85 | 0 |
| 5 | 1F | 203/210 (96%) | 0.02 | 1 (0%) 87 85 | 24, 48, 72, 87 | 0 |
| 5 | 2F | 203/210 (96%) | 0.65 | 4 (1%) 65 61 | 41, 73, 83, 92 | 0 |
| 6 | 1G | 181/182 (99%) | 0.69 | 8 (4%) 39 34 | 52, 68, 81, 90 | 0 |
| 6 | 2G | 181/182 (99%) | 2.34 | 112 (61%) 0 0 | 81, 89, 94, 97 | 0 |
| 7 | 1H | 174/180 (96%) | 0.37 | 2 (1%) 78 75 | 43, 58, 70, 79 | 0 |
| 7 | 2H | 173/180 (96%) | 1.43 | 34 (19%) 3 2 | 74, 84, 90, 94 | 0 |
| 8 | 1I | 147/148 (99%) | 0.91 | 9 (6%) 27 23 | 48, 76, 85, 87 | 0 |
| 8 | 2I | 146/148 (98%) | 1.04 | 12 (8%) 17 15 | 58, 78, 87, 91 | 0 |
| 9 | 1N | 140/140 (100%) | 0.01 | 0 100 100 | 33, 44, 65, 80 | 0 |
| 9 | 2N | 140/140 (100%) | 0.80 | 5 (3%) 46 41 | 50, 69, 81, 84 | 0 |
| 10 | 1O | 122/122 (100%) | 0.14 | 1 (0%) 82 80 | 37, 45, 65, 68 | 0 |
| 10 | 2O | 122/122 (100%) | 0.44 | 2 (1%) 70 67 | 50, 60, 72, 78 | 0 |
| 11 | 1P | 149/150 (99%) | 0.05 | 1 (0%) 84 81 | 26, 50, 71, 83 | 0 |
| 11 | 2P | 149/150 (99%) | 0.53 | 4 (2%) 56 51 | 43, 71, 86, 90 | 0 |
| 12 | 1Q | 141/141 (100%) | -0.06 | 0 100 100 | 33, 45, 59, 72 | 0 |
| 12 | 2Q | 141/141 (100%) | 0.95 | 9 (6%) 25 22 | 52, 71, 79, 87 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 13 | 1R | 118/118 (100%) | -0.10 | 0 100 100 | 33, 42, 58, 65 | 0 |
| 13 | 2R | 118/118 (100%) | 0.23 | 0 100 100 | 45, 57, 67, 74 | 0 |
| 14 | 1S | 110/112 (98%) | 0.26 | 1 (0%) 81 78 | 45, 55, 66, 70 | 0 |
| 14 | 2S | 110/112 (98%) | 1.74 | 43 (39%) 1 0 | 72, 82, 86, 90 | 0 |
| 15 | 1T | 131/146 (89%) | 0.38 | 7 (5%) 32 28 | 40, 50, 72, 83 | 0 |
| 15 | 2T | 131/146 (89%) | 0.49 | 3 (2%) 61 57 | 52, 63, 79, 86 | 0 |
| 16 | 1U | 116/118 (98%) | -0.17 | 1 (0%) 81 78 | 28, 38, 50, 69 | 0 |
| 16 | 2U | 116/118 (98%) | 0.53 | 0 100 100 | 47, 66, 78, 86 | 0 |
| 17 | 1V | 101/101 (100%) | -0.06 | 1 (0%) 79 76 | 29, 46, 62, 72 | 0 |
| 17 | 2V | 101/101 (100%) | 0.82 | 3 (2%) 52 48 | 49, 76, 82, 89 | 0 |
| 18 | 1W | 112/113 (99%) | -0.10 | 2 (1%) 67 64 | 31, 38, 58, 86 | 0 |
| 18 | 2W | 112/113 (99%) | 0.41 | 4 (3%) 46 41 | 46, 56, 74, 87 | 0 |
| 19 | 1X | 95/96 (98%) | 0.15 | 3 (3%) 50 46 | 32, 43, 64, 79 | 0 |
| 19 | 2X | 95/96 (98%) | 0.81 | 4 (4%) 40 36 | 55, 66, 79, 86 | 0 |
| 20 | 1Y | 107/110 (97%) | 0.42 | 3 (2%) 55 50 | 40, 54, 72, 82 | 0 |
| 20 | 2Y | 107/110 (97%) | 1.28 | 16 (14%) 5 4 | 65, 75, 83, 89 | 0 |
| 21 | 1Z | 203/206 (98%) | 0.50 | 9 (4%) 39 34 | 45, 62, 77, 87 | 0 |
| 21 | 2Z | 201/206 (97%) | 1.50 | 38 (18%) 3 2 | 73, 82, 88, 90 | 0 |
| 22 | 10 | 77/85 (90%) | 0.05 | 2 (2%) 57 52 | 35, 43, 60, 68 | 0 |
| 22 | 20 | 77/85 (90%) | 1.07 | 7 (9%) 15 13 | 59, 69, 78, 83 | 0 |
| 23 | 11 | 97/98 (98%) | 0.27 | 1 (1%) 79 76 | 34, 49, 71, 84 | 0 |
| 23 | 21 | 97/98 (98%) | 0.68 | 2 (2%) 63 59 | 47, 61, 79, 86 | 0 |
| 24 | 12 | 70/72 (97%) | 0.31 | 2 (2%) 53 49 | 42, 55, 65, 84 | 0 |
| 24 | 22 | 70/72 (97%) | 0.67 | 1 (1%) 73 70 | 67, 75, 82, 83 | 0 |
| 25 | 13 | 59/60 (98%) | -0.12 | 1 (1%) 69 65 | 30, 42, 63, 76 | 0 |
| 25 | 23 | 59/60 (98%) | 0.60 | 3 (5%) 33 29 | 57, 67, 82, 93 | 0 |
| 26 | 14 | 69/71 (97%) | 1.14 | 14 (20%) 3 2 | 61, 77, 92, 96 | 0 |
| 26 | 24 | 69/71 (97%) | 2.35 | 46 (66%) 0 0 | 83, 93, 99, 100 | 0 |
| 27 | 15 | 59/60 (98%) | -0.21 | 0 100 100 | 28, 40, 58, 64 | 0 |
| 27 | 25 | 59/60 (98%) | 0.25 | 1 (1%) 69 65 | 41, 56, 70, 75 | 0 |
| 28 | 16 | 53/54 (98%) | -0.09 | 0 100 100 | 39, 47, 61, 67 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 28 | 26 | 53/54 (98%) | 0.67 | 2 (3%) 44 39 | 60, 67, 74, 79 | 0 |
| 29 | 17 | 48/49 (97%) | 0.07 | 5 (10%) 11 10 | 28, 35, 59, 71 | 0 |
| 29 | 27 | 48/49 (97%) | 0.38 | 4 (8%) 17 15 | 39, 48, 70, 78 | 0 |
| 30 | 18 | 64/65 (98%) | -0.16 | 1 (1%) 70 67 | 35, 40, 47, 59 | 0 |
| 30 | 28 | 64/65 (98%) | 0.55 | 2 (3%) 51 47 | 54, 62, 68, 71 | 0 |
| 31 | 19 | 37/37 (100%) | 0.05 | 0 100 100 | 37, 46, 61, 67 | 0 |
| 31 | 29 | 37/37 (100%) | 1.08 | 4 (10%) 11 9 | 61, 72, 80, 82 | 0 |
| 32 | 1a | 1488/1521 (97%) | 0.13 | 29 (1%) 66 62 | 41, 73, 96, 110 | 0 |
| 32 | 2a | 1492/1521 (98%) | 0.49 | 56 (3%) 44 39 | 53, 81, 100, 110 | 0 |
| 33 | 1b | 231/256 (90%) | 1.34 | 48 (20%) 2 2 | 68, 82, 90, 94 | 0 |
| 33 | 2b | 231/256 (90%) | 1.65 | 65 (28%) 1 1 | 80, 88, 94, 97 | 0 |
| 34 | 1c | 206/239 (86%) | 0.98 | 18 (8%) 16 14 | 64, 76, 87, 91 | 0 |
| 34 | 2c | 206/239 (86%) | 1.59 | 54 (26%) 1 1 | 79, 88, 93, 95 | 0 |
| 35 | 1d | 208/209 (99%) | 1.07 | 23 (11%) 10 8 | 62, 76, 85, 88 | 0 |
| 35 | 2d | 208/209 (99%) | 1.19 | 18 (8%) 16 14 | 66, 76, 84, 87 | 0 |
| 36 | 1e | 148/162 (91%) | 0.58 | 4 (2%) 56 51 | 52, 70, 78, 91 | 0 |
| 36 | 2e | 148/162 (91%) | 1.17 | 19 (12%) 7 6 | 66, 78, 86, 93 | 0 |
| 37 | 1f | 100/101 (99%) | 0.70 | 2 (2%) 65 61 | 59, 70, 78, 82 | 0 |
| 37 | 2f | 100/101 (99%) | 0.79 | 3 (3%) 52 48 | 63, 74, 83, 86 | 0 |
| 38 | 1g | 155/156 (99%) | 0.61 | 4 (2%) 57 52 | 68, 76, 83, 89 | 0 |
| 38 | 2g | 155/156 (99%) | 1.56 | 41 (26%) 1 1 | 81, 86, 91, 95 | 0 |
| 39 | 1h | 137/138 (99%) | 0.80 | 6 (4%) 39 34 | 63, 71, 78, 83 | 0 |
| 39 | 2h | 137/138 (99%) | 1.07 | 9 (6%) 24 21 | 69, 79, 84, 88 | 0 |
| 40 | 1i | 127/128 (99%) | 1.32 | 20 (15%) 5 4 | 65, 82, 89, 91 | 0 |
| 40 | 2i | 126/128 (98%) | 2.12 | 65 (51%) 0 0 | 81, 90, 95, 96 | 0 |
| 41 | 1j | 97/105 (92%) | 1.60 | 28 (28%) 1 1 | 64, 83, 91, 93 | 0 |
| 41 | 2j | 96/105 (91%) | 1.96 | 46 (47%) 0 0 | 83, 90, 94, 98 | 0 |
| 42 | 1k | 114/129 (88%) | 0.68 | 6 (5%) 32 28 | 48, 68, 78, 83 | 0 |
| 42 | 2k | 114/129 (88%) | 1.24 | 16 (14%) 6 5 | 66, 78, 85, 87 | 0 |
| 43 | 1l | 121/132 (91%) | 0.74 | 7 (5%) 29 25 | 53, 64, 75, 81 | 0 |
| 43 | 2l | 121/132 (91%) | 0.85 | 9 (7%) 20 18 | 64, 73, 78, 85 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 44 | 1m | 116/126 (92%) | 0.93 | 10 (8%) 16 14 | 64, 78, 83, 88 | 0 |
| 44 | 2m | 114/126 (90%) | 1.83 | 41 (35%) 1 1 | 84, 89, 93, 95 | 0 |
| 45 | 1n | 60/61 (98%) | 0.85 | 2 (3%) 49 45 | 68, 75, 81, 83 | 0 |
| 45 | 2n | 60/61 (98%) | 2.05 | 27 (45%) 0 0 | 83, 88, 93, 95 | 0 |
| 46 | 1o | 88/89 (98%) | 0.72 | 3 (3%) 48 43 | 51, 69, 79, 84 | 0 |
| 46 | 2o | 88/89 (98%) | 0.92 | 6 (6%) 23 20 | 64, 77, 83, 89 | 0 |
| 47 | 1p | 82/88 (93%) | 1.33 | 14 (17%) 4 3 | 69, 77, 85, 89 | 0 |
| 47 | 2p | 82/88 (93%) | 1.25 | 12 (14%) 6 4 | 66, 75, 83, 91 | 0 |
| 48 | 1q | 99/105 (94%) | 0.95 | 5 (5%) 33 29 | 59, 72, 82, 84 | 0 |
| 48 | 2q | 99/105 (94%) | 0.96 | 7 (7%) 22 19 | 63, 75, 82, 85 | 0 |
| 49 | 1r | 68/88 (77%) | 0.60 | 0 100 100 | 59, 68, 80, 85 | 0 |
| 49 | 2r | 68/88 (77%) | 0.97 | 3 (4%) 39 34 | 70, 77, 84, 89 | 0 |
| 50 | 1s | 83/93 (89%) | 0.97 | 4 (4%) 35 31 | 70, 80, 86, 93 | 0 |
| 50 | 2s | 83/93 (89%) | 2.05 | 45 (54%) 0 0 | 82, 91, 95, 98 | 0 |
| 51 | 1t | 96/106 (90%) | 1.19 | 15 (15%) 5 4 | 68, 76, 85, 86 | 0 |
| 51 | 2t | 98/106 (92%) | 0.88 | 6 (6%) 27 23 | 65, 75, 85, 88 | 0 |
| 52 | 1u | 23/27 (85%) | 1.22 | 5 (21%) 2 2 | 70, 74, 79, 79 | 0 |
| 52 | 2u | 23/27 (85%) | 2.29 | 12 (52%) 0 0 | 84, 89, 91, 93 | 0 |
| 53 | 1y | 97/113 (85%) | 0.93 | 7 (7%) 21 19 | 57, 67, 79, 82 | 0 |
| 53 | 2y | 96/113 (84%) | 2.01 | 47 (48%) 0 0 | 76, 84, 90, 93 | 0 |
| All | All | 20766/21468 (96%) | 0.43 | 1544 (7%) 20 18 | 24, 69, 93, 111 | 0 |

The worst 5 of 1544 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | 1H | 2 | SER | 6.7 |
| 45 | 2n | 2 | ALA | 6.4 |
| 53 | 2y | 98 | ALA | 6.1 |
| 1 | 1A | 1087 | G | 6.0 |
| 1 | 2A | 2602 | A | 5.7 |

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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 1 | 5MU | 2A | 1915 | 21/22 | 0.83 | 0.12 | 85,90,94,108 | 0 |
| 32 | 2MG | 2a | 1207 | 24/25 | 0.84 | 0.13 | 87,93,99,103 | 0 |
| 32 | 5MC | 2a | 967 | 21/22 | 0.86 | 0.14 | 75,80,86,92 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.86 | 0.13 | 75,82,90,93 | 0 |
| 32 | M2G | 2a | 966 | 25/26 | 0.88 | 0.14 | 70,75,90,97 | 0 |
| 32 | G7M | 2a | 527 | 24/25 | 0.89 | 0.13 | 75,77,79,84 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.89 | 0.09 | 80,85,95,100 | 0 |
| 43 | 0TD | 1l | 92 | 10/11 | 0.91 | 0.12 | 59,62,66,79 | 0 |
| 43 | 0TD | 2l | 92 | 10/11 | 0.91 | 0.11 | 68,72,75,85 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.92 | 0.09 | 66,75,86,86 | 0 |
| 1 | PSU | 1A | 1911 | 20/21 | 0.92 | 0.10 | 64,73,76,86 | 0 |
| 32 | PSU | 2a | 516 | 20/21 | 0.92 | 0.09 | 77,81,88,88 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.92 | 0.10 | 72,75,83,91 | 0 |
| 32 | 2MG | 1a | 1207 | 24/25 | 0.93 | 0.09 | 73,78,81,83 | 0 |
| 32 | 4OC | 2a | 1402 | 22/23 | 0.93 | 0.11 | 68,72,77,81 | 0 |
| 1 | OMC | 2A | 1920 | 21/22 | 0.93 | 0.11 | 70,74,81,84 | 0 |
| 32 | 5MC | 1a | 967 | 21/22 | 0.94 | 0.12 | 63,69,77,82 | 0 |
| 32 | 5MC | 2a | 1404 | 21/22 | 0.94 | 0.09 | 65,72,77,79 | 0 |
| 32 | UR3 | 2a | 1498 | 21/22 | 0.94 | 0.10 | 64,70,75,78 | 0 |
| 32 | MA6 | 2a | 1519 | 24/25 | 0.94 | 0.13 | 64,74,78,79 | 0 |
| 32 | 5MC | 2a | 1400 | 21/22 | 0.94 | 0.13 | 73,80,82,85 | 0 |
| 32 | 5MC | 2a | 1407 | 21/22 | 0.95 | 0.09 | 63,72,76,82 | 0 |
| 32 | G7M | 1a | 527 | 24/25 | 0.95 | 0.09 | 51,57,62,65 | 0 |
| 32 | MA6 | 2a | 1518 | 24/25 | 0.95 | 0.11 | 66,73,78,78 | 0 |
| 32 | 5MC | 1a | 1407 | 21/22 | 0.95 | 0.11 | 56,61,66,72 | 0 |
| 32 | PSU | 1a | 516 | 20/21 | 0.95 | 0.08 | 65,69,73,75 | 0 |
| 32 | 4OC | 1a | 1402 | 22/23 | 0.96 | 0.10 | 51,60,65,67 | 0 |
| 32 | M2G | 1a | 966 | 25/26 | 0.96 | 0.09 | 49,62,70,80 | 0 |
| 32 | UR3 | 1a | 1498 | 21/22 | 0.96 | 0.10 | 52,57,60,70 | 0 |
| 32 | MA6 | 1a | 1518 | 24/25 | 0.96 | 0.10 | 47,53,57,58 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.96 | 0.09 | 53,59,62,75 | 0 |
| 32 | 5MC | 1a | 1400 | 21/22 | 0.96 | 0.09 | 49,57,63,63 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.97 | 0.07 | 45,52,59,65 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.97 | 0.09 | 43,47,50,51 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.97 | 0.08 | 35,43,47,49 | 0 |
| 32 | 5MC | 1a | 1404 | 21/22 | 0.97 | 0.08 | 50,54,57,61 | 0 |
| 32 | MA6 | 1a | 1519 | 24/25 | 0.97 | 0.09 | 49,54,59,61 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.97 | 0.08 | 29,34,37,38 | 0 |
| 1 | 5MU | 2A | 1939 | 21/22 | 0.97 | 0.07 | 38,45,49,51 | 0 |
| 1 | OMC | 1A | 1920 | 21/22 | 0.97 | 0.08 | 56,64,67,69 | 0 |
| 1 | 2MA | 1A | 2503 | 23/24 | 0.98 | 0.05 | 24,28,32,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1 | 2MU | 2A | 2552 | 21/23 | 0.98 | 0.07 | 41,45,50,54 | 0 |
| 1 | PSU | 2A | 2605 | 20/21 | 0.98 | 0.06 | 37,45,51,51 | 0 |
| 1 | 2MU | 1A | 2552 | 21/23 | 0.98 | 0.08 | 29,36,38,45 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.98 | 0.06 | 30,35,38,41 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.98 | 0.07 | 39,43,47,49 | 0 |
| 1 | 5MC | 1A | 1962 | 21/22 | 0.98 | 0.06 | 34,42,47,51 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.98 | 0.07 | 26,32,35,37 | 0 |

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3769 | 1/1 | 0.42 | 0.24 | 73,73,73,73 | 0 |
| 54 | MG | 2a | 3049 | 1/1 | 0.43 | 0.25 | 86,86,86,86 | 0 |
| 54 | MG | 2O | 202 | 1/1 | 0.46 | 0.23 | 87,87,87,87 | 0 |
| 54 | MG | 1a | 1772 | 1/1 | 0.46 | 0.18 | 92,92,92,92 | 0 |
| 54 | MG | 2a | 3010 | 1/1 | 0.49 | 0.40 | 92,92,92,92 | 0 |
| 54 | MG | 1A | 3719 | 1/1 | 0.51 | 0.24 | 82,82,82,82 | 0 |
| 54 | MG | 1a | 1680 | 1/1 | 0.53 | 0.32 | 87,87,87,87 | 0 |
| 54 | MG | 1A | 3458 | 1/1 | 0.54 | 0.22 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3270 | 1/1 | 0.58 | 0.34 | 88,88,88,88 | 0 |
| 54 | MG | 2A | 3724 | 1/1 | 0.59 | 0.16 | 88,88,88,88 | 0 |
| 54 | MG | 1a | 1797 | 1/1 | 0.59 | 0.22 | 95,95,95,95 | 0 |
| 54 | MG | 2B | 211 | 1/1 | 0.60 | 0.21 | 86,86,86,86 | 0 |
| 54 | MG | 1A | 3384 | 1/1 | 0.60 | 0.26 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3478 | 1/1 | 0.60 | 0.23 | 77,77,77,77 | 0 |
| 54 | MG | 1a | 1867 | 1/1 | 0.60 | 0.26 | 89,89,89,89 | 0 |
| 54 | MG | 2A | 3521 | 1/1 | 0.61 | 0.23 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3723 | 1/1 | 0.61 | 0.32 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 4001 | 1/1 | 0.61 | 0.17 | 85,85,85,85 | 0 |
| 54 | MG | 1a | 1869 | 1/1 | 0.62 | 0.14 | 85,85,85,85 | 0 |
| 54 | MG | 1a | 1774 | 1/1 | 0.62 | 0.18 | 87,87,87,87 | 0 |
| 54 | MG | 2B | 213 | 1/1 | 0.62 | 0.14 | 84,84,84,84 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 1a | 1704 | 1/1 | 0.63 | 0.24 | 81,81,81,81 | 0 |
| 54 | MG | 2a | 3175 | 1/1 | 0.63 | 0.27 | 91,91,91,91 | 0 |
| 54 | MG | 1a | 1665 | 1/1 | 0.64 | 0.21 | 86,86,86,86 | 0 |
| 54 | MG | 1A | 3661 | 1/1 | 0.65 | 0.33 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3635 | 1/1 | 0.67 | 0.37 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3805 | 1/1 | 0.67 | 0.25 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3697 | 1/1 | 0.68 | 0.20 | 68,68,68,68 | 0 |
| 54 | MG | 1B | 206 | 1/1 | 0.68 | 0.39 | 81,81,81,81 | 0 |
| 54 | MG | 1a | 1635 | 1/1 | 0.68 | 0.24 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3844 | 1/1 | 0.68 | 0.31 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3477 | 1/1 | 0.68 | 0.26 | 83,83,83,83 | 0 |
| 54 | MG | 1a | 1874 | 1/1 | 0.69 | 0.20 | 86,86,86,86 | 0 |
| 54 | MG | 1a | 1611 | 1/1 | 0.69 | 0.27 | 88,88,88,88 | 0 |
| 54 | MG | 1a | 1821 | 1/1 | 0.69 | 0.27 | 86,86,86,86 | 0 |
| 54 | MG | 2a | 3106 | 1/1 | 0.69 | 0.40 | 86,86,86,86 | 0 |
| 54 | MG | 2a | 3118 | 1/1 | 0.69 | 0.23 | 82,82,82,82 | 0 |
| 54 | MG | 2B | 214 | 1/1 | 0.69 | 0.12 | 95,95,95,95 | 0 |
| 54 | MG | 2A | 3321 | 1/1 | 0.70 | 0.29 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3441 | 1/1 | 0.70 | 0.14 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3294 | 1/1 | 0.70 | 0.22 | 83,83,83,83 | 0 |
| 54 | MG | 2G | 201 | 1/1 | 0.70 | 0.22 | 86,86,86,86 | 0 |
| 54 | MG | 1A | 3668 | 1/1 | 0.70 | 0.17 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3500 | 1/1 | 0.70 | 0.21 | 85,85,85,85 | 0 |
| 54 | MG | 2A | 3090 | 1/1 | 0.70 | 0.16 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3094 | 1/1 | 0.70 | 0.39 | 89,89,89,89 | 0 |
| 54 | MG | 1a | 1696 | 1/1 | 0.70 | 0.24 | 86,86,86,86 | 0 |
| 54 | MG | 2a | 3139 | 1/1 | 0.70 | 0.24 | 84,84,84,84 | 0 |
| 54 | MG | 2B | 204 | 1/1 | 0.70 | 0.16 | 84,84,84,84 | 0 |
| 54 | MG | 2r | 102 | 1/1 | 0.70 | 0.21 | 78,78,78,78 | 0 |
| 54 | MG | 1a | 1604 | 1/1 | 0.71 | 0.24 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3542 | 1/1 | 0.71 | 0.20 | 83,83,83,83 | 0 |
| 54 | MG | 1A | 3541 | 1/1 | 0.71 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1878 | 1/1 | 0.71 | 0.12 | 93,93,93,93 | 0 |
| 54 | MG | 2A | 3468 | 1/1 | 0.71 | 0.20 | 82,82,82,82 | 0 |
| 54 | MG | 1g | 202 | 1/1 | 0.71 | 0.21 | 83,83,83,83 | 0 |
| 54 | MG | 1a | 1841 | 1/1 | 0.71 | 0.15 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3670 | 1/1 | 0.71 | 0.17 | 67,67,67,67 | 0 |
| 54 | MG | 2D | 309 | 1/1 | 0.71 | 0.29 | 88,88,88,88 | 0 |
| 54 | MG | 1H | 201 | 1/1 | 0.72 | 0.27 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3634 | 1/1 | 0.72 | 0.15 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1803 | 1/1 | 0.72 | 0.25 | 77,77,77,77 | 0 |
| 54 | MG | 1b | 301 | 1/1 | 0.72 | 0.27 | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 2A | 3095 | 1/1 | 0.72 | 0.31 | 81,81,81,81 | 0 |
| 54 | MG | 2j | 201 | 1/1 | 0.72 | 0.19 | 84,84,84,84 | 0 |
| 54 | MG | 2A | 3522 | 1/1 | 0.72 | 0.24 | 85,85,85,85 | 0 |
| 54 | MG | 10 | 106 | 1/1 | 0.73 | 0.22 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3976 | 1/1 | 0.73 | 0.20 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3038 | 1/1 | 0.73 | 0.20 | 94,94,94,94 | 0 |
| 54 | MG | 1a | 1824 | 1/1 | 0.73 | 0.17 | 84,84,84,84 | 0 |
| 54 | MG | 1B | 220 | 1/1 | 0.73 | 0.20 | 53,53,53,53 | 0 |
| 54 | MG | 1a | 1850 | 1/1 | 0.73 | 0.22 | 72,72,72,72 | 0 |
| 54 | MG | 1B | 226 | 1/1 | 0.73 | 0.15 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3907 | 1/1 | 0.73 | 0.18 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1666 | 1/1 | 0.73 | 0.35 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3543 | 1/1 | 0.73 | 0.14 | 74,74,74,74 | 0 |
| 54 | MG | 1T | 204 | 1/1 | 0.74 | 0.22 | 78,78,78,78 | 0 |
| 54 | MG | 2G | 202 | 1/1 | 0.74 | 0.20 | 91,91,91,91 | 0 |
| 54 | MG | 1a | 1629 | 1/1 | 0.74 | 0.35 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3461 | 1/1 | 0.74 | 0.16 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3853 | 1/1 | 0.74 | 0.20 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3601 | 1/1 | 0.74 | 0.21 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3059 | 1/1 | 0.74 | 0.32 | 91,91,91,91 | 0 |
| 54 | MG | 2a | 3061 | 1/1 | 0.74 | 0.34 | 84,84,84,84 | 0 |
| 54 | MG | 2a | 3099 | 1/1 | 0.74 | 0.30 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3261 | 1/1 | 0.74 | 0.25 | 81,81,81,81 | 0 |
| 54 | MG | 2B | 209 | 1/1 | 0.74 | 0.32 | 80,80,80,80 | 0 |
| 54 | MG | 1a | 1852 | 1/1 | 0.74 | 0.23 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3506 | 1/1 | 0.74 | 0.24 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3298 | 1/1 | 0.74 | 0.21 | 90,90,90,90 | 0 |
| 54 | MG | 2A | 3320 | 1/1 | 0.74 | 0.17 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3630 | 1/1 | 0.75 | 0.11 | 100,100,100,100 | 0 |
| 54 | MG | 1a | 1610 | 1/1 | 0.75 | 0.29 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3674 | 1/1 | 0.75 | 0.20 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3366 | 1/1 | 0.75 | 0.22 | 83,83,83,83 | 0 |
| 54 | MG | 2I | 201 | 1/1 | 0.75 | 0.15 | 78,78,78,78 | 0 |
| 54 | MG | 2a | 3137 | 1/1 | 0.75 | 0.16 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3776 | 1/1 | 0.75 | 0.25 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 4032 | 1/1 | 0.75 | 0.18 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3864 | 1/1 | 0.75 | 0.19 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3455 | 1/1 | 0.75 | 0.22 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3585 | 1/1 | 0.76 | 0.17 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3604 | 1/1 | 0.76 | 0.25 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3713 | 1/1 | 0.76 | 0.26 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3275 | 1/1 | 0.76 | 0.39 | 72,72,72,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3721 | 1/1 | 0.76 | 0.19 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3295 | 1/1 | 0.76 | 0.24 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1693 | 1/1 | 0.76 | 0.19 | 88,88,88,88 | 0 |
| 54 | MG | 1A | 3887 | 1/1 | 0.76 | 0.16 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3895 | 1/1 | 0.76 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1771 | 1/1 | 0.76 | 0.13 | 94,94,94,94 | 0 |
| 54 | MG | 2A | 3430 | 1/1 | 0.76 | 0.34 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3131 | 1/1 | 0.76 | 0.34 | 81,81,81,81 | 0 |
| 54 | MG | 2E | 306 | 1/1 | 0.76 | 0.25 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3567 | 1/1 | 0.76 | 0.28 | 87,87,87,87 | 0 |
| 54 | MG | 2A | 3568 | 1/1 | 0.76 | 0.19 | 82,82,82,82 | 0 |
| 57 | MPD | 2B | 219 | 8/8 | 0.76 | 0.25 | 72,74,84,90 | 0 |
| 54 | MG | 1A | 3666 | 1/1 | 0.77 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3492 | 1/1 | 0.77 | 0.16 | 64,64,64,64 | 0 |
| 54 | MG | 1P | 204 | 1/1 | 0.77 | 0.26 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 4015 | 1/1 | 0.77 | 0.27 | 36,36,36,36 | 0 |
| 54 | MG | 2a | 3037 | 1/1 | 0.77 | 0.13 | 85,85,85,85 | 0 |
| 54 | MG | 1e | 203 | 1/1 | 0.77 | 0.12 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3452 | 1/1 | 0.77 | 0.17 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 4030 | 1/1 | 0.77 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1681 | 1/1 | 0.77 | 0.14 | 90,90,90,90 | 0 |
| 54 | MG | 2a | 3085 | 1/1 | 0.77 | 0.27 | 89,89,89,89 | 0 |
| 54 | MG | 2A | 3725 | 1/1 | 0.77 | 0.21 | 87,87,87,87 | 0 |
| 54 | MG | 1a | 1692 | 1/1 | 0.77 | 0.25 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1829 | 1/1 | 0.77 | 0.19 | 83,83,83,83 | 0 |
| 54 | MG | 1A | 3477 | 1/1 | 0.77 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3828 | 1/1 | 0.77 | 0.17 | 79,79,79,79 | 0 |
| 54 | MG | 2a | 3148 | 1/1 | 0.77 | 0.15 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3561 | 1/1 | 0.77 | 0.23 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1863 | 1/1 | 0.77 | 0.21 | 78,78,78,78 | 0 |
| 54 | MG | 1a | 1769 | 1/1 | 0.77 | 0.25 | 85,85,85,85 | 0 |
| 54 | MG | 1a | 1868 | 1/1 | 0.77 | 0.16 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3445 | 1/1 | 0.78 | 0.19 | 80,80,80,80 | 0 |
| 54 | MG | 1a | 1877 | 1/1 | 0.78 | 0.41 | 73,73,73,73 | 0 |
| 54 | MG | 18 | 102 | 1/1 | 0.78 | 0.31 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3014 | 1/1 | 0.78 | 0.35 | 70,70,70,70 | 0 |
| 54 | MG | 1d | 303 | 1/1 | 0.78 | 0.21 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3024 | 1/1 | 0.78 | 0.33 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3323 | 1/1 | 0.78 | 0.18 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3829 | 1/1 | 0.78 | 0.24 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3378 | 1/1 | 0.78 | 0.28 | 84,84,84,84 | 0 |
| 54 | MG | 1a | 1703 | 1/1 | 0.78 | 0.30 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 2A | 3689 | 1/1 | 0.78 | 0.14 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3437 | 1/1 | 0.78 | 0.12 | 87,87,87,87 | 0 |
| 54 | MG | 2a | 3087 | 1/1 | 0.78 | 0.25 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3022 | 1/1 | 0.78 | 0.40 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3052 | 1/1 | 0.78 | 0.21 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3728 | 1/1 | 0.78 | 0.24 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3058 | 1/1 | 0.78 | 0.20 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3906 | 1/1 | 0.78 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3197 | 1/1 | 0.78 | 0.30 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3969 | 1/1 | 0.78 | 0.22 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3848 | 1/1 | 0.78 | 0.23 | 70,70,70,70 | 0 |
| 54 | MG | 2n | 101 | 1/1 | 0.78 | 0.34 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3987 | 1/1 | 0.78 | 0.24 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3391 | 1/1 | 0.78 | 0.15 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3162 | 1/1 | 0.79 | 0.25 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3180 | 1/1 | 0.79 | 0.16 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3181 | 1/1 | 0.79 | 0.25 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3216 | 1/1 | 0.79 | 0.22 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1777 | 1/1 | 0.79 | 0.16 | 82,82,82,82 | 0 |
| 54 | MG | 2a | 3006 | 1/1 | 0.79 | 0.42 | 87,87,87,87 | 0 |
| 54 | MG | 15 | 107 | 1/1 | 0.79 | 0.21 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3480 | 1/1 | 0.79 | 0.17 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3730 | 1/1 | 0.79 | 0.20 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3488 | 1/1 | 0.79 | 0.16 | 55,55,55,55 | 0 |
| 54 | MG | 2a | 3044 | 1/1 | 0.79 | 0.17 | 91,91,91,91 | 0 |
| 54 | MG | 1B | 222 | 1/1 | 0.79 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3200 | 1/1 | 0.79 | 0.18 | 86,86,86,86 | 0 |
| 54 | MG | 1y | 202 | 1/1 | 0.79 | 0.22 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1712 | 1/1 | 0.79 | 0.20 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3697 | 1/1 | 0.79 | 0.17 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3024 | 1/1 | 0.79 | 0.17 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3386 | 1/1 | 0.79 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 2a | 3110 | 1/1 | 0.79 | 0.19 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3047 | 1/1 | 0.79 | 0.20 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1738 | 1/1 | 0.79 | 0.22 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1861 | 1/1 | 0.79 | 0.16 | 84,84,84,84 | 0 |
| 54 | MG | 2A | 3074 | 1/1 | 0.79 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3703 | 1/1 | 0.79 | 0.15 | 71,71,71,71 | 0 |
| 54 | MG | 2e | 201 | 1/1 | 0.79 | 0.29 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3312 | 1/1 | 0.79 | 0.21 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 4017 | 1/1 | 0.79 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 2B | 216 | 1/1 | 0.79 | 0.15 | 86,86,86,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3335 | 1/1 | 0.79 | 0.21 | 78,78,78,78 | 0 |
| 58 | ARG | 1F | 319 | 12/12 | 0.79 | 0.18 | 61,72,79,80 | 0 |
| 54 | MG | 1A | 4011 | 1/1 | 0.80 | 0.16 | 84,84,84,84 | 0 |
| 54 | MG | 2A | 3362 | 1/1 | 0.80 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1745 | 1/1 | 0.80 | 0.25 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3578 | 1/1 | 0.80 | 0.18 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3374 | 1/1 | 0.80 | 0.21 | 82,82,82,82 | 0 |
| 54 | MG | 2a | 3021 | 1/1 | 0.80 | 0.32 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3618 | 1/1 | 0.80 | 0.13 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3027 | 1/1 | 0.80 | 0.21 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3623 | 1/1 | 0.80 | 0.19 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3296 | 1/1 | 0.80 | 0.16 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3631 | 1/1 | 0.80 | 0.28 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3164 | 1/1 | 0.80 | 0.27 | 88,88,88,88 | 0 |
| 54 | MG | 1A | 3810 | 1/1 | 0.80 | 0.20 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3060 | 1/1 | 0.80 | 0.25 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3943 | 1/1 | 0.80 | 0.16 | 75,75,75,75 | 0 |
| 54 | MG | 2a | 3064 | 1/1 | 0.80 | 0.28 | 89,89,89,89 | 0 |
| 54 | MG | 2a | 3066 | 1/1 | 0.80 | 0.21 | 82,82,82,82 | 0 |
| 54 | MG | 2a | 3067 | 1/1 | 0.80 | 0.08 | 95,95,95,95 | 0 |
| 54 | MG | 2a | 3073 | 1/1 | 0.80 | 0.38 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3192 | 1/1 | 0.80 | 0.39 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3706 | 1/1 | 0.80 | 0.11 | 88,88,88,88 | 0 |
| 54 | MG | 2a | 3098 | 1/1 | 0.80 | 0.30 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3211 | 1/1 | 0.80 | 0.28 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3811 | 1/1 | 0.80 | 0.19 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3974 | 1/1 | 0.80 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3814 | 1/1 | 0.80 | 0.24 | 69,69,69,69 | 0 |
| 54 | MG | 2B | 202 | 1/1 | 0.80 | 0.29 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3273 | 1/1 | 0.80 | 0.31 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3986 | 1/1 | 0.80 | 0.23 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3556 | 1/1 | 0.80 | 0.17 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3185 | 1/1 | 0.80 | 0.16 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3089 | 1/1 | 0.80 | 0.24 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3149 | 1/1 | 0.80 | 0.29 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3526 | 1/1 | 0.80 | 0.18 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3535 | 1/1 | 0.80 | 0.18 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3539 | 1/1 | 0.80 | 0.19 | 90,90,90,90 | 0 |
| 54 | MG | 1a | 1717 | 1/1 | 0.80 | 0.26 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3620 | 1/1 | 0.81 | 0.26 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1864 | 1/1 | 0.81 | 0.12 | 95,95,95,95 | 0 |
| 54 | MG | 1A | 3581 | 1/1 | 0.81 | 0.16 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 1a | 1749 | 1/1 | 0.81 | 0.25 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3140 | 1/1 | 0.81 | 0.24 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3473 | 1/1 | 0.81 | 0.18 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1669 | 1/1 | 0.81 | 0.22 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3691 | 1/1 | 0.81 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3165 | 1/1 | 0.81 | 0.18 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3705 | 1/1 | 0.81 | 0.17 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3459 | 1/1 | 0.81 | 0.21 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3460 | 1/1 | 0.81 | 0.14 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3174 | 1/1 | 0.81 | 0.10 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3522 | 1/1 | 0.81 | 0.10 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3079 | 1/1 | 0.81 | 0.22 | 83,83,83,83 | 0 |
| 54 | MG | 1A | 3607 | 1/1 | 0.81 | 0.14 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3729 | 1/1 | 0.81 | 0.34 | 74,74,74,74 | 0 |
| 54 | MG | 2a | 3088 | 1/1 | 0.81 | 0.26 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3923 | 1/1 | 0.81 | 0.11 | 30,30,30,30 | 0 |
| 54 | MG | 1a | 1794 | 1/1 | 0.81 | 0.17 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3089 | 1/1 | 0.81 | 0.21 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3953 | 1/1 | 0.81 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3543 | 1/1 | 0.81 | 0.16 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3555 | 1/1 | 0.81 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3138 | 1/1 | 0.81 | 0.22 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3154 | 1/1 | 0.81 | 0.21 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3284 | 1/1 | 0.81 | 0.32 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3171 | 1/1 | 0.81 | 0.20 | 84,84,84,84 | 0 |
| 54 | MG | 2A | 3043 | 1/1 | 0.81 | 0.29 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1713 | 1/1 | 0.81 | 0.29 | 77,77,77,77 | 0 |
| 54 | MG | 1a | 1842 | 1/1 | 0.81 | 0.21 | 87,87,87,87 | 0 |
| 54 | MG | 1A | 3395 | 1/1 | 0.81 | 0.16 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1722 | 1/1 | 0.81 | 0.26 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3005 | 1/1 | 0.81 | 0.19 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1737 | 1/1 | 0.81 | 0.16 | 82,82,82,82 | 0 |
| 54 | MG | 1a | 1641 | 1/1 | 0.81 | 0.13 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3539 | 1/1 | 0.82 | 0.15 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3182 | 1/1 | 0.82 | 0.14 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3514 | 1/1 | 0.82 | 0.15 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3184 | 1/1 | 0.82 | 0.27 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3188 | 1/1 | 0.82 | 0.27 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3605 | 1/1 | 0.82 | 0.32 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3208 | 1/1 | 0.82 | 0.13 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3168 | 1/1 | 0.82 | 0.27 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3724 | 1/1 | 0.82 | 0.17 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2a | 3032 | 1/1 | 0.82 | 0.14 | 91,91,91,91 | 0 |
| 54 | MG | 2A | 3248 | 1/1 | 0.82 | 0.21 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3656 | 1/1 | 0.82 | 0.22 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3266 | 1/1 | 0.82 | 0.31 | 82,82,82,82 | 0 |
| 54 | MG | 1a | 1786 | 1/1 | 0.82 | 0.14 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3742 | 1/1 | 0.82 | 0.13 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 4036 | 1/1 | 0.82 | 0.20 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1799 | 1/1 | 0.82 | 0.20 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3286 | 1/1 | 0.82 | 0.21 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3626 | 1/1 | 0.82 | 0.15 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3034 | 1/1 | 0.82 | 0.33 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3328 | 1/1 | 0.82 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1820 | 1/1 | 0.82 | 0.18 | 84,84,84,84 | 0 |
| 54 | MG | 1A | 3330 | 1/1 | 0.82 | 0.16 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3053 | 1/1 | 0.82 | 0.27 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3356 | 1/1 | 0.82 | 0.14 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3801 | 1/1 | 0.82 | 0.15 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3667 | 1/1 | 0.82 | 0.24 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3262 | 1/1 | 0.82 | 0.26 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3362 | 1/1 | 0.82 | 0.16 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3385 | 1/1 | 0.82 | 0.13 | 70,70,70,70 | 0 |
| 54 | MG | 2a | 3129 | 1/1 | 0.82 | 0.21 | 70,70,70,70 | 0 |
| 54 | MG | 2a | 3131 | 1/1 | 0.82 | 0.12 | 83,83,83,83 | 0 |
| 54 | MG | 1A | 3504 | 1/1 | 0.82 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 1Z | 301 | 1/1 | 0.82 | 0.17 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3104 | 1/1 | 0.82 | 0.23 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3118 | 1/1 | 0.82 | 0.29 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3442 | 1/1 | 0.82 | 0.18 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3446 | 1/1 | 0.82 | 0.17 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3826 | 1/1 | 0.82 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3981 | 1/1 | 0.82 | 0.17 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3589 | 1/1 | 0.82 | 0.16 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3376 | 1/1 | 0.82 | 0.13 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3990 | 1/1 | 0.82 | 0.16 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3999 | 1/1 | 0.82 | 0.11 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1760 | 1/1 | 0.82 | 0.10 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1679 | 1/1 | 0.83 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1781 | 1/1 | 0.83 | 0.18 | 89,89,89,89 | 0 |
| 54 | MG | 1a | 1785 | 1/1 | 0.83 | 0.15 | 73,73,73,73 | 0 |
| 54 | MG | 1m | 202 | 1/1 | 0.83 | 0.23 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3501 | 1/1 | 0.83 | 0.12 | 75,75,75,75 | 0 |
| 54 | MG | 1O | 201 | 1/1 | 0.83 | 0.17 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3511 | 1/1 | 0.83 | 0.20 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3213 | 1/1 | 0.83 | 0.18 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3546 | 1/1 | 0.83 | 0.20 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3016 | 1/1 | 0.83 | 0.16 | 79,79,79,79 | 0 |
| 54 | MG | 2a | 3019 | 1/1 | 0.83 | 0.23 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3219 | 1/1 | 0.83 | 0.11 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3230 | 1/1 | 0.83 | 0.26 | 72,72,72,72 | 0 |
| 54 | MG | 1R | 205 | 1/1 | 0.83 | 0.23 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3893 | 1/1 | 0.83 | 0.20 | 39,39,39,39 | 0 |
| 54 | MG | 2a | 3036 | 1/1 | 0.83 | 0.22 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3262 | 1/1 | 0.83 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3037 | 1/1 | 0.83 | 0.30 | 74,74,74,74 | 0 |
| 54 | MG | 2a | 3041 | 1/1 | 0.83 | 0.27 | 80,80,80,80 | 0 |
| 54 | MG | 1W | 201 | 1/1 | 0.83 | 0.25 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3456 | 1/1 | 0.83 | 0.14 | 41,41,41,41 | 0 |
| 54 | MG | 2a | 3050 | 1/1 | 0.83 | 0.36 | 87,87,87,87 | 0 |
| 54 | MG | 2A | 3048 | 1/1 | 0.83 | 0.17 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3639 | 1/1 | 0.83 | 0.21 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3167 | 1/1 | 0.83 | 0.27 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3464 | 1/1 | 0.83 | 0.23 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1835 | 1/1 | 0.83 | 0.23 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3087 | 1/1 | 0.83 | 0.23 | 90,90,90,90 | 0 |
| 54 | MG | 2a | 3071 | 1/1 | 0.83 | 0.26 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1716 | 1/1 | 0.83 | 0.27 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3472 | 1/1 | 0.83 | 0.22 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3335 | 1/1 | 0.83 | 0.23 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1718 | 1/1 | 0.83 | 0.17 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3673 | 1/1 | 0.83 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3685 | 1/1 | 0.83 | 0.19 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3583 | 1/1 | 0.83 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3102 | 1/1 | 0.83 | 0.35 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3368 | 1/1 | 0.83 | 0.15 | 78,78,78,78 | 0 |
| 54 | MG | 1a | 1860 | 1/1 | 0.83 | 0.12 | 90,90,90,90 | 0 |
| 54 | MG | 1A | 3437 | 1/1 | 0.83 | 0.18 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3707 | 1/1 | 0.83 | 0.18 | 75,75,75,75 | 0 |
| 54 | MG | 2a | 3136 | 1/1 | 0.83 | 0.23 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3669 | 1/1 | 0.83 | 0.30 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3722 | 1/1 | 0.83 | 0.25 | 76,76,76,76 | 0 |
| 54 | MG | 1B | 216 | 1/1 | 0.83 | 0.17 | 51,51,51,51 | 0 |
| 54 | MG | 2a | 3143 | 1/1 | 0.83 | 0.21 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3142 | 1/1 | 0.83 | 0.16 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3170 | 1/1 | 0.83 | 0.24 | 68,68,68,68 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1638 | 1/1 | 0.83 | 0.20 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3163 | 1/1 | 0.83 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3179 | 1/1 | 0.83 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 1a | 1758 | 1/1 | 0.83 | 0.19 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3278 | 1/1 | 0.83 | 0.34 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1642 | 1/1 | 0.83 | 0.15 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3861 | 1/1 | 0.83 | 0.22 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3225 | 1/1 | 0.83 | 0.12 | 77,77,77,77 | 0 |
| 54 | MG | 2y | 3200 | 1/1 | 0.83 | 0.13 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3871 | 1/1 | 0.83 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3466 | 1/1 | 0.83 | 0.34 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1646 | 1/1 | 0.84 | 0.22 | 76,76,76,76 | 0 |
| 54 | MG | 1e | 201 | 1/1 | 0.84 | 0.29 | 71,71,71,71 | 0 |
| 54 | MG | 2a | 3026 | 1/1 | 0.84 | 0.23 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3607 | 1/1 | 0.84 | 0.12 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1656 | 1/1 | 0.84 | 0.16 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1805 | 1/1 | 0.84 | 0.31 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3622 | 1/1 | 0.84 | 0.23 | 85,85,85,85 | 0 |
| 54 | MG | 1a | 1813 | 1/1 | 0.84 | 0.31 | 78,78,78,78 | 0 |
| 54 | MG | 1a | 1817 | 1/1 | 0.84 | 0.12 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3937 | 1/1 | 0.84 | 0.14 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3736 | 1/1 | 0.84 | 0.17 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3031 | 1/1 | 0.84 | 0.27 | 84,84,84,84 | 0 |
| 54 | MG | 1A | 3662 | 1/1 | 0.84 | 0.19 | 66,66,66,66 | 0 |
| 54 | MG | 1B | 221 | 1/1 | 0.84 | 0.19 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1751 | 1/1 | 0.84 | 0.18 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1756 | 1/1 | 0.84 | 0.25 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3210 | 1/1 | 0.84 | 0.17 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3325 | 1/1 | 0.84 | 0.19 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3606 | 1/1 | 0.84 | 0.35 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1761 | 1/1 | 0.84 | 0.20 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3054 | 1/1 | 0.84 | 0.19 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1690 | 1/1 | 0.84 | 0.33 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3086 | 1/1 | 0.84 | 0.15 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3231 | 1/1 | 0.84 | 0.43 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3474 | 1/1 | 0.84 | 0.11 | 84,84,84,84 | 0 |
| 54 | MG | 2A | 3069 | 1/1 | 0.84 | 0.28 | 72,72,72,72 | 0 |
| 54 | MG | 1F | 314 | 1/1 | 0.84 | 0.15 | 52,52,52,52 | 0 |
| 54 | MG | 2a | 3100 | 1/1 | 0.84 | 0.24 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3491 | 1/1 | 0.84 | 0.14 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1862 | 1/1 | 0.84 | 0.14 | 82,82,82,82 | 0 |
| 54 | MG | 2a | 3116 | 1/1 | 0.84 | 0.35 | 87,87,87,87 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3261 | 1/1 | 0.84 | 0.22 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3503 | 1/1 | 0.84 | 0.16 | 76,76,76,76 | 0 |
| 54 | MG | 1N | 202 | 1/1 | 0.84 | 0.21 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1617 | 1/1 | 0.84 | 0.11 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3193 | 1/1 | 0.84 | 0.24 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3276 | 1/1 | 0.84 | 0.33 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3277 | 1/1 | 0.84 | 0.36 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3096 | 1/1 | 0.84 | 0.18 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1782 | 1/1 | 0.84 | 0.19 | 79,79,79,79 | 0 |
| 54 | MG | 2a | 3149 | 1/1 | 0.84 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3536 | 1/1 | 0.84 | 0.15 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3538 | 1/1 | 0.84 | 0.13 | 75,75,75,75 | 0 |
| 54 | MG | 1P | 203 | 1/1 | 0.84 | 0.25 | 74,74,74,74 | 0 |
| 54 | MG | 2U | 201 | 1/1 | 0.84 | 0.22 | 79,79,79,79 | 0 |
| 54 | MG | 2a | 3002 | 1/1 | 0.84 | 0.17 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3109 | 1/1 | 0.84 | 0.23 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3310 | 1/1 | 0.84 | 0.17 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3008 | 1/1 | 0.84 | 0.20 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3555 | 1/1 | 0.84 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 2a | 3013 | 1/1 | 0.84 | 0.34 | 79,79,79,79 | 0 |
| 57 | MPD | 1a | 1880 | 8/8 | 0.84 | 0.16 | 60,72,78,78 | 0 |
| 57 | MPD | 2A | 3733 | 8/8 | 0.84 | 0.27 | 54,60,66,66 | 0 |
| 54 | MG | 1A | 3172 | 1/1 | 0.84 | 0.15 | 50,50,50,50 | 0 |
| 54 | MG | 1T | 201 | 1/1 | 0.84 | 0.26 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1798 | 1/1 | 0.85 | 0.10 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3530 | 1/1 | 0.85 | 0.19 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1697 | 1/1 | 0.85 | 0.29 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3036 | 1/1 | 0.85 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3748 | 1/1 | 0.85 | 0.11 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 4025 | 1/1 | 0.85 | 0.29 | 44,44,44,44 | 0 |
| 54 | MG | 1a | 1811 | 1/1 | 0.85 | 0.18 | 85,85,85,85 | 0 |
| 54 | MG | 2A | 3271 | 1/1 | 0.85 | 0.20 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1709 | 1/1 | 0.85 | 0.20 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 4028 | 1/1 | 0.85 | 0.19 | 66,66,66,66 | 0 |
| 54 | MG | 18 | 101 | 1/1 | 0.85 | 0.21 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3573 | 1/1 | 0.85 | 0.10 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3574 | 1/1 | 0.85 | 0.18 | 60,60,60,60 | 0 |
| 54 | MG | 2a | 3040 | 1/1 | 0.85 | 0.15 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1715 | 1/1 | 0.85 | 0.25 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3767 | 1/1 | 0.85 | 0.13 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3596 | 1/1 | 0.85 | 0.11 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3947 | 1/1 | 0.85 | 0.12 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3612 | 1/1 | 0.85 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1831 | 1/1 | 0.85 | 0.19 | 86,86,86,86 | 0 |
| 54 | MG | 1A | 4034 | 1/1 | 0.85 | 0.17 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3299 | 1/1 | 0.85 | 0.14 | 43,43,43,43 | 0 |
| 54 | MG | 1a | 1840 | 1/1 | 0.85 | 0.13 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3702 | 1/1 | 0.85 | 0.24 | 85,85,85,85 | 0 |
| 54 | MG | 1A | 4037 | 1/1 | 0.85 | 0.18 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1623 | 1/1 | 0.85 | 0.40 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1744 | 1/1 | 0.85 | 0.27 | 78,78,78,78 | 0 |
| 54 | MG | 1a | 1853 | 1/1 | 0.85 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 1B | 205 | 1/1 | 0.85 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3954 | 1/1 | 0.85 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3112 | 1/1 | 0.85 | 0.16 | 78,78,78,78 | 0 |
| 54 | MG | 2a | 3096 | 1/1 | 0.85 | 0.17 | 73,73,73,73 | 0 |
| 54 | MG | 2a | 3097 | 1/1 | 0.85 | 0.30 | 84,84,84,84 | 0 |
| 54 | MG | 2A | 3113 | 1/1 | 0.85 | 0.14 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3321 | 1/1 | 0.85 | 0.34 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3703 | 1/1 | 0.85 | 0.13 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3125 | 1/1 | 0.85 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3389 | 1/1 | 0.85 | 0.18 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3784 | 1/1 | 0.85 | 0.17 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3609 | 1/1 | 0.85 | 0.19 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3804 | 1/1 | 0.85 | 0.15 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3875 | 1/1 | 0.85 | 0.13 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3557 | 1/1 | 0.85 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1870 | 1/1 | 0.85 | 0.26 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3640 | 1/1 | 0.85 | 0.24 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3993 | 1/1 | 0.85 | 0.22 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3462 | 1/1 | 0.85 | 0.23 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3526 | 1/1 | 0.85 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 4006 | 1/1 | 0.85 | 0.23 | 54,54,54,54 | 0 |
| 54 | MG | 2a | 3167 | 1/1 | 0.85 | 0.13 | 75,75,75,75 | 0 |
| 54 | MG | 2a | 3169 | 1/1 | 0.85 | 0.23 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1686 | 1/1 | 0.85 | 0.27 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3689 | 1/1 | 0.85 | 0.21 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 4012 | 1/1 | 0.85 | 0.25 | 88,88,88,88 | 0 |
| 54 | MG | 2B | 217 | 1/1 | 0.85 | 0.10 | 79,79,79,79 | 0 |
| 54 | MG | 2a | 3181 | 1/1 | 0.85 | 0.17 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3485 | 1/1 | 0.85 | 0.20 | 82,82,82,82 | 0 |
| 54 | MG | 2a | 3188 | 1/1 | 0.85 | 0.18 | 88,88,88,88 | 0 |
| 54 | MG | 2A | 3205 | 1/1 | 0.85 | 0.36 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3207 | 1/1 | 0.85 | 0.15 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1h | 202 | 1/1 | 0.85 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 1a | 1788 | 1/1 | 0.85 | 0.15 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1793 | 1/1 | 0.85 | 0.19 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3002 | 1/1 | 0.85 | 0.23 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3010 | 1/1 | 0.85 | 0.33 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 4013 | 1/1 | 0.85 | 0.19 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3283 | 1/1 | 0.85 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3813 | 1/1 | 0.86 | 0.11 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1667 | 1/1 | 0.86 | 0.43 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3403 | 1/1 | 0.86 | 0.18 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3406 | 1/1 | 0.86 | 0.17 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3421 | 1/1 | 0.86 | 0.20 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3185 | 1/1 | 0.86 | 0.14 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3552 | 1/1 | 0.86 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3034 | 1/1 | 0.86 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3051 | 1/1 | 0.86 | 0.35 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3053 | 1/1 | 0.86 | 0.32 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3636 | 1/1 | 0.86 | 0.14 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3653 | 1/1 | 0.86 | 0.10 | 94,94,94,94 | 0 |
| 54 | MG | 1A | 3379 | 1/1 | 0.86 | 0.08 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3273 | 1/1 | 0.86 | 0.27 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3450 | 1/1 | 0.86 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1682 | 1/1 | 0.86 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3833 | 1/1 | 0.86 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3635 | 1/1 | 0.86 | 0.24 | 42,42,42,42 | 0 |
| 54 | MG | 1a | 1775 | 1/1 | 0.86 | 0.20 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3082 | 1/1 | 0.86 | 0.41 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3959 | 1/1 | 0.86 | 0.13 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1780 | 1/1 | 0.86 | 0.12 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3714 | 1/1 | 0.86 | 0.11 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3083 | 1/1 | 0.86 | 0.21 | 72,72,72,72 | 0 |
| 54 | MG | 2a | 3092 | 1/1 | 0.86 | 0.40 | 86,86,86,86 | 0 |
| 54 | MG | 10 | 107 | 1/1 | 0.86 | 0.15 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3233 | 1/1 | 0.86 | 0.12 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3847 | 1/1 | 0.86 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3490 | 1/1 | 0.86 | 0.17 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3035 | 1/1 | 0.86 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 2a | 3105 | 1/1 | 0.86 | 0.54 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3093 | 1/1 | 0.86 | 0.20 | 82,82,82,82 | 0 |
| 54 | MG | 2a | 3108 | 1/1 | 0.86 | 0.37 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3691 | 1/1 | 0.86 | 0.12 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3269 | 1/1 | 0.86 | 0.23 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3471 | 1/1 | 0.86 | 0.21 | 71,71,71,71 | 0 |
| 54 | MG | 2a | 3121 | 1/1 | 0.86 | 0.11 | 81,81,81,81 | 0 |
| 54 | MG | 2a | 3122 | 1/1 | 0.86 | 0.19 | 67,67,67,67 | 0 |
| 54 | MG | 1a | 1789 | 1/1 | 0.86 | 0.20 | 64,64,64,64 | 0 |
| 54 | MG | 1B | 210 | 1/1 | 0.86 | 0.23 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3652 | 1/1 | 0.86 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3038 | 1/1 | 0.86 | 0.27 | 69,69,69,69 | 0 |
| 54 | MG | 1d | 301 | 1/1 | 0.86 | 0.28 | 74,74,74,74 | 0 |
| 54 | MG | 2D | 311 | 1/1 | 0.86 | 0.11 | 36,36,36,36 | 0 |
| 54 | MG | 2a | 3140 | 1/1 | 0.86 | 0.22 | 72,72,72,72 | 0 |
| 54 | MG | 2E | 303 | 1/1 | 0.86 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3704 | 1/1 | 0.86 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3877 | 1/1 | 0.86 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3153 | 1/1 | 0.86 | 0.13 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3033 | 1/1 | 0.86 | 0.15 | 55,55,55,55 | 0 |
| 54 | MG | 1B | 229 | 1/1 | 0.86 | 0.08 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3809 | 1/1 | 0.86 | 0.10 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3312 | 1/1 | 0.86 | 0.17 | 70,70,70,70 | 0 |
| 54 | MG | 28 | 102 | 1/1 | 0.86 | 0.20 | 66,66,66,66 | 0 |
| 54 | MG | 1F | 316 | 1/1 | 0.86 | 0.20 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3546 | 1/1 | 0.86 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3143 | 1/1 | 0.86 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 1a | 1814 | 1/1 | 0.86 | 0.18 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3238 | 1/1 | 0.86 | 0.23 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3355 | 1/1 | 0.86 | 0.20 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1743 | 1/1 | 0.86 | 0.23 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3019 | 1/1 | 0.86 | 0.52 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3170 | 1/1 | 0.86 | 0.23 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1651 | 1/1 | 0.86 | 0.13 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3179 | 1/1 | 0.86 | 0.25 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3901 | 1/1 | 0.86 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3134 | 1/1 | 0.86 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3775 | 1/1 | 0.87 | 0.13 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3890 | 1/1 | 0.87 | 0.17 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3410 | 1/1 | 0.87 | 0.31 | 78,78,78,78 | 0 |
| 54 | MG | 2B | 210 | 1/1 | 0.87 | 0.24 | 77,77,77,77 | 0 |
| 54 | MG | 11 | 104 | 1/1 | 0.87 | 0.16 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3422 | 1/1 | 0.87 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3427 | 1/1 | 0.87 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3228 | 1/1 | 0.87 | 0.24 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3436 | 1/1 | 0.87 | 0.15 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3112 | 1/1 | 0.87 | 0.10 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3439 | 1/1 | 0.87 | 0.11 | 41,41,41,41 | 0 |
| 54 | MG | 2D | 313 | 1/1 | 0.87 | 0.35 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3899 | 1/1 | 0.87 | 0.19 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1601 | 1/1 | 0.87 | 0.38 | 78,78,78,78 | 0 |
| 54 | MG | 1a | 1730 | 1/1 | 0.87 | 0.21 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3156 | 1/1 | 0.87 | 0.18 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1733 | 1/1 | 0.87 | 0.12 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3259 | 1/1 | 0.87 | 0.16 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3127 | 1/1 | 0.87 | 0.22 | 58,58,58,58 | 0 |
| 54 | MG | 2I | 102 | 1/1 | 0.87 | 0.15 | 84,84,84,84 | 0 |
| 54 | MG | 1A | 3679 | 1/1 | 0.87 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3462 | 1/1 | 0.87 | 0.16 | 72,72,72,72 | 0 |
| 54 | MG | 2a | 3004 | 1/1 | 0.87 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3465 | 1/1 | 0.87 | 0.16 | 67,67,67,67 | 0 |
| 54 | MG | 1a | 1614 | 1/1 | 0.87 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3007 | 1/1 | 0.87 | 0.10 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 4035 | 1/1 | 0.87 | 0.21 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3204 | 1/1 | 0.87 | 0.15 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1750 | 1/1 | 0.87 | 0.17 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3015 | 1/1 | 0.87 | 0.18 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3690 | 1/1 | 0.87 | 0.21 | 41,41,41,41 | 0 |
| 54 | MG | 2a | 3018 | 1/1 | 0.87 | 0.25 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3479 | 1/1 | 0.87 | 0.17 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3481 | 1/1 | 0.87 | 0.16 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3483 | 1/1 | 0.87 | 0.10 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3401 | 1/1 | 0.87 | 0.13 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3486 | 1/1 | 0.87 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1757 | 1/1 | 0.87 | 0.16 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3693 | 1/1 | 0.87 | 0.10 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3610 | 1/1 | 0.87 | 0.14 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3612 | 1/1 | 0.87 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 2a | 3039 | 1/1 | 0.87 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3197 | 1/1 | 0.87 | 0.26 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1765 | 1/1 | 0.87 | 0.20 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3206 | 1/1 | 0.87 | 0.16 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3046 | 1/1 | 0.87 | 0.17 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3048 | 1/1 | 0.87 | 0.21 | 84,84,84,84 | 0 |
| 54 | MG | 1a | 1645 | 1/1 | 0.87 | 0.24 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3958 | 1/1 | 0.87 | 0.09 | 34,34,34,34 | 0 |
| 54 | MG | 1I | 202 | 1/1 | 0.87 | 0.18 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3524 | 1/1 | 0.87 | 0.21 | 69,69,69,69 | 0 |
| 54 | MG | 2a | 3056 | 1/1 | 0.87 | 0.16 | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3613 | 1/1 | 0.87 | 0.21 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3527 | 1/1 | 0.87 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1773 | 1/1 | 0.87 | 0.18 | 83,83,83,83 | 0 |
| 54 | MG | 1a | 1655 | 1/1 | 0.87 | 0.26 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3621 | 1/1 | 0.87 | 0.13 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3537 | 1/1 | 0.87 | 0.13 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1662 | 1/1 | 0.87 | 0.15 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3623 | 1/1 | 0.87 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3429 | 1/1 | 0.87 | 0.20 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3238 | 1/1 | 0.87 | 0.38 | 51,51,51,51 | 0 |
| 54 | MG | 1D | 317 | 1/1 | 0.87 | 0.15 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1668 | 1/1 | 0.87 | 0.20 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3977 | 1/1 | 0.87 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3264 | 1/1 | 0.87 | 0.10 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3570 | 1/1 | 0.87 | 0.18 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3571 | 1/1 | 0.87 | 0.16 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1673 | 1/1 | 0.87 | 0.33 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1676 | 1/1 | 0.87 | 0.19 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1790 | 1/1 | 0.87 | 0.14 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1678 | 1/1 | 0.87 | 0.20 | 55,55,55,55 | 0 |
| 54 | MG | 1F | 315 | 1/1 | 0.87 | 0.23 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3602 | 1/1 | 0.87 | 0.15 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3435 | 1/1 | 0.87 | 0.27 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3355 | 1/1 | 0.87 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 2a | 3112 | 1/1 | 0.87 | 0.10 | 84,84,84,84 | 0 |
| 54 | MG | 2A | 3055 | 1/1 | 0.87 | 0.35 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3280 | 1/1 | 0.87 | 0.23 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3283 | 1/1 | 0.87 | 0.31 | 73,73,73,73 | 0 |
| 54 | MG | 1H | 202 | 1/1 | 0.87 | 0.15 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3124 | 1/1 | 0.87 | 0.14 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3060 | 1/1 | 0.87 | 0.18 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3294 | 1/1 | 0.87 | 0.17 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3134 | 1/1 | 0.87 | 0.12 | 92,92,92,92 | 0 |
| 54 | MG | 2A | 3068 | 1/1 | 0.87 | 0.21 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3852 | 1/1 | 0.87 | 0.10 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1804 | 1/1 | 0.87 | 0.28 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3077 | 1/1 | 0.87 | 0.20 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3081 | 1/1 | 0.87 | 0.23 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3661 | 1/1 | 0.87 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3047 | 1/1 | 0.87 | 0.24 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3680 | 1/1 | 0.87 | 0.13 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3449 | 1/1 | 0.87 | 0.17 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3373 | 1/1 | 0.87 | 0.14 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1694 | 1/1 | 0.87 | 0.24 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3866 | 1/1 | 0.87 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3699 | 1/1 | 0.87 | 0.15 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3702 | 1/1 | 0.87 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 4004 | 1/1 | 0.87 | 0.23 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1700 | 1/1 | 0.87 | 0.28 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3510 | 1/1 | 0.87 | 0.10 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3097 | 1/1 | 0.87 | 0.18 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3520 | 1/1 | 0.87 | 0.20 | 60,60,60,60 | 0 |
| 54 | MG | 2e | 202 | 1/1 | 0.87 | 0.17 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3718 | 1/1 | 0.87 | 0.22 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3590 | 1/1 | 0.87 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1710 | 1/1 | 0.87 | 0.12 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3723 | 1/1 | 0.87 | 0.16 | 85,85,85,85 | 0 |
| 57 | MPD | 1T | 206 | 8/8 | 0.87 | 0.24 | 71,73,77,78 | 0 |
| 54 | MG | 2A | 3387 | 1/1 | 0.87 | 0.16 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3111 | 1/1 | 0.87 | 0.20 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3391 | 1/1 | 0.87 | 0.17 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3395 | 1/1 | 0.87 | 0.18 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1729 | 1/1 | 0.88 | 0.16 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3952 | 1/1 | 0.88 | 0.12 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3161 | 1/1 | 0.88 | 0.15 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1732 | 1/1 | 0.88 | 0.12 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3201 | 1/1 | 0.88 | 0.25 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1632 | 1/1 | 0.88 | 0.16 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3722 | 1/1 | 0.88 | 0.23 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3133 | 1/1 | 0.88 | 0.19 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3173 | 1/1 | 0.88 | 0.30 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3588 | 1/1 | 0.88 | 0.16 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3470 | 1/1 | 0.88 | 0.13 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3177 | 1/1 | 0.88 | 0.13 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1872 | 1/1 | 0.88 | 0.11 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3349 | 1/1 | 0.88 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1876 | 1/1 | 0.88 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1746 | 1/1 | 0.88 | 0.21 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1643 | 1/1 | 0.88 | 0.16 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3518 | 1/1 | 0.88 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3737 | 1/1 | 0.88 | 0.19 | 35,35,35,35 | 0 |
| 54 | MG | 1a | 1753 | 1/1 | 0.88 | 0.15 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3194 | 1/1 | 0.88 | 0.48 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3494 | 1/1 | 0.88 | 0.13 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1650 | 1/1 | 0.88 | 0.28 | 65,65,65,65 | 0 |
| 54 | MG | 1D | 301 | 1/1 | 0.88 | 0.18 | 50,50,50,50 | 0 |
| 54 | MG | 1f | 201 | 1/1 | 0.88 | 0.21 | 78,78,78,78 | 0 |
| 54 | MG | 1a | 1652 | 1/1 | 0.88 | 0.29 | 74,74,74,74 | 0 |
| 54 | MG | 1D | 311 | 1/1 | 0.88 | 0.38 | 57,57,57,57 | 0 |
| 54 | MG | 1D | 313 | 1/1 | 0.88 | 0.18 | 53,53,53,53 | 0 |
| 54 | MG | 1a | 1764 | 1/1 | 0.88 | 0.14 | 72,72,72,72 | 0 |
| 54 | MG | 1n | 101 | 1/1 | 0.88 | 0.38 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3850 | 1/1 | 0.88 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1663 | 1/1 | 0.88 | 0.20 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1664 | 1/1 | 0.88 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3528 | 1/1 | 0.88 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3042 | 1/1 | 0.88 | 0.22 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3043 | 1/1 | 0.88 | 0.12 | 85,85,85,85 | 0 |
| 54 | MG | 2A | 3017 | 1/1 | 0.88 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3045 | 1/1 | 0.88 | 0.24 | 73,73,73,73 | 0 |
| 54 | MG | 1F | 311 | 1/1 | 0.88 | 0.23 | 61,61,61,61 | 0 |
| 54 | MG | 1F | 312 | 1/1 | 0.88 | 0.17 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3247 | 1/1 | 0.88 | 0.45 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3739 | 1/1 | 0.88 | 0.20 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3250 | 1/1 | 0.88 | 0.14 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3251 | 1/1 | 0.88 | 0.18 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3982 | 1/1 | 0.88 | 0.15 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3207 | 1/1 | 0.88 | 0.24 | 67,67,67,67 | 0 |
| 54 | MG | 1a | 1779 | 1/1 | 0.88 | 0.15 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3293 | 1/1 | 0.88 | 0.10 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3267 | 1/1 | 0.88 | 0.30 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3039 | 1/1 | 0.88 | 0.27 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3040 | 1/1 | 0.88 | 0.16 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3068 | 1/1 | 0.88 | 0.20 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3760 | 1/1 | 0.88 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3524 | 1/1 | 0.88 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3575 | 1/1 | 0.88 | 0.16 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3274 | 1/1 | 0.88 | 0.20 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1784 | 1/1 | 0.88 | 0.09 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3049 | 1/1 | 0.88 | 0.38 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3051 | 1/1 | 0.88 | 0.15 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3604 | 1/1 | 0.88 | 0.13 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3869 | 1/1 | 0.88 | 0.15 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3282 | 1/1 | 0.88 | 0.39 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3616 | 1/1 | 0.88 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3022 | 1/1 | 0.88 | 0.12 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3872 | 1/1 | 0.88 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3285 | 1/1 | 0.88 | 0.20 | 61,61,61,61 | 0 |
| 54 | MG | 2a | 3103 | 1/1 | 0.88 | 0.22 | 65,65,65,65 | 0 |
| 54 | MG | 1P | 205 | 1/1 | 0.88 | 0.28 | 61,61,61,61 | 0 |
| 54 | MG | 1a | 1684 | 1/1 | 0.88 | 0.26 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1685 | 1/1 | 0.88 | 0.37 | 78,78,78,78 | 0 |
| 54 | MG | 2a | 3109 | 1/1 | 0.88 | 0.33 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3536 | 1/1 | 0.88 | 0.09 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3633 | 1/1 | 0.88 | 0.18 | 70,70,70,70 | 0 |
| 54 | MG | 2a | 3113 | 1/1 | 0.88 | 0.28 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3114 | 1/1 | 0.88 | 0.37 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1688 | 1/1 | 0.88 | 0.10 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3188 | 1/1 | 0.88 | 0.16 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3780 | 1/1 | 0.88 | 0.18 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3115 | 1/1 | 0.88 | 0.11 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3322 | 1/1 | 0.88 | 0.14 | 78,78,78,78 | 0 |
| 54 | MG | 2a | 3127 | 1/1 | 0.88 | 0.23 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3792 | 1/1 | 0.88 | 0.09 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3797 | 1/1 | 0.88 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3350 | 1/1 | 0.88 | 0.11 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 4018 | 1/1 | 0.88 | 0.15 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1699 | 1/1 | 0.88 | 0.24 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3027 | 1/1 | 0.88 | 0.26 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3388 | 1/1 | 0.88 | 0.11 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3905 | 1/1 | 0.88 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 2a | 3141 | 1/1 | 0.88 | 0.21 | 70,70,70,70 | 0 |
| 54 | MG | 1a | 1706 | 1/1 | 0.88 | 0.35 | 71,71,71,71 | 0 |
| 54 | MG | 2a | 3144 | 1/1 | 0.88 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 4031 | 1/1 | 0.88 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3098 | 1/1 | 0.88 | 0.12 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1826 | 1/1 | 0.88 | 0.11 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3166 | 1/1 | 0.88 | 0.14 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3617 | 1/1 | 0.88 | 0.13 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3716 | 1/1 | 0.88 | 0.17 | 81,81,81,81 | 0 |
| 54 | MG | 1a | 1602 | 1/1 | 0.88 | 0.21 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3315 | 1/1 | 0.88 | 0.19 | 38,38,38,38 | 0 |
| 54 | MG | 1a | 1609 | 1/1 | 0.88 | 0.32 | 62,62,62,62 | 0 |
| 54 | MG | 2a | 3177 | 1/1 | 0.88 | 0.18 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3199 | 1/1 | 0.88 | 0.11 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3116 | 1/1 | 0.88 | 0.22 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3408 | 1/1 | 0.88 | 0.14 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3186 | 1/1 | 0.88 | 0.16 | 75,75,75,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3128 | 1/1 | 0.88 | 0.31 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3121 | 1/1 | 0.88 | 0.15 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3124 | 1/1 | 0.88 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3426 | 1/1 | 0.88 | 0.14 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3407 | 1/1 | 0.88 | 0.17 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3126 | 1/1 | 0.88 | 0.14 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3432 | 1/1 | 0.88 | 0.23 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3129 | 1/1 | 0.88 | 0.13 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3266 | 1/1 | 0.88 | 0.10 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3138 | 1/1 | 0.88 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1723 | 1/1 | 0.88 | 0.14 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1727 | 1/1 | 0.88 | 0.11 | 64,64,64,64 | 0 |
| 54 | MG | 1B | 225 | 1/1 | 0.89 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3512 | 1/1 | 0.89 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3513 | 1/1 | 0.89 | 0.15 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1639 | 1/1 | 0.89 | 0.24 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3576 | 1/1 | 0.89 | 0.10 | 44,44,44,44 | 0 |
| 54 | MG | 1B | 228 | 1/1 | 0.89 | 0.11 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3523 | 1/1 | 0.89 | 0.19 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3301 | 1/1 | 0.89 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3651 | 1/1 | 0.89 | 0.17 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3390 | 1/1 | 0.89 | 0.22 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3344 | 1/1 | 0.89 | 0.15 | 59,59,59,59 | 0 |
| 54 | MG | 1D | 316 | 1/1 | 0.89 | 0.16 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3533 | 1/1 | 0.89 | 0.10 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1747 | 1/1 | 0.89 | 0.31 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1748 | 1/1 | 0.89 | 0.19 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3657 | 1/1 | 0.89 | 0.11 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3248 | 1/1 | 0.89 | 0.11 | 73,73,73,73 | 0 |
| 54 | MG | 2a | 3031 | 1/1 | 0.89 | 0.17 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3115 | 1/1 | 0.89 | 0.24 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3352 | 1/1 | 0.89 | 0.14 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1657 | 1/1 | 0.89 | 0.13 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3663 | 1/1 | 0.89 | 0.21 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3551 | 1/1 | 0.89 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3854 | 1/1 | 0.89 | 0.11 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3744 | 1/1 | 0.89 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3309 | 1/1 | 0.89 | 0.13 | 70,70,70,70 | 0 |
| 54 | MG | 1F | 317 | 1/1 | 0.89 | 0.15 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3596 | 1/1 | 0.89 | 0.23 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1762 | 1/1 | 0.89 | 0.22 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1763 | 1/1 | 0.89 | 0.30 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 2a | 3047 | 1/1 | 0.89 | 0.34 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3527 | 1/1 | 0.89 | 0.11 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3141 | 1/1 | 0.89 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3580 | 1/1 | 0.89 | 0.13 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3583 | 1/1 | 0.89 | 0.13 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3339 | 1/1 | 0.89 | 0.10 | 52,52,52,52 | 0 |
| 54 | MG | 2a | 3055 | 1/1 | 0.89 | 0.13 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3867 | 1/1 | 0.89 | 0.11 | 41,41,41,41 | 0 |
| 54 | MG | 2a | 3058 | 1/1 | 0.89 | 0.23 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3351 | 1/1 | 0.89 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 1e | 202 | 1/1 | 0.89 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3144 | 1/1 | 0.89 | 0.16 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3154 | 1/1 | 0.89 | 0.28 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3155 | 1/1 | 0.89 | 0.17 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3762 | 1/1 | 0.89 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3373 | 1/1 | 0.89 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 4005 | 1/1 | 0.89 | 0.15 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3250 | 1/1 | 0.89 | 0.33 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3280 | 1/1 | 0.89 | 0.24 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3430 | 1/1 | 0.89 | 0.15 | 61,61,61,61 | 0 |
| 54 | MG | 2a | 3083 | 1/1 | 0.89 | 0.33 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3673 | 1/1 | 0.89 | 0.14 | 62,62,62,62 | 0 |
| 54 | MG | 1T | 203 | 1/1 | 0.89 | 0.20 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3171 | 1/1 | 0.89 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 4014 | 1/1 | 0.89 | 0.10 | 93,93,93,93 | 0 |
| 54 | MG | 2a | 3090 | 1/1 | 0.89 | 0.17 | 70,70,70,70 | 0 |
| 54 | MG | 1V | 205 | 1/1 | 0.89 | 0.17 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3638 | 1/1 | 0.89 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3882 | 1/1 | 0.89 | 0.27 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3407 | 1/1 | 0.89 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3016 | 1/1 | 0.89 | 0.30 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3678 | 1/1 | 0.89 | 0.13 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3192 | 1/1 | 0.89 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 2a | 3104 | 1/1 | 0.89 | 0.32 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3683 | 1/1 | 0.89 | 0.11 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3544 | 1/1 | 0.89 | 0.07 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3790 | 1/1 | 0.89 | 0.27 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3690 | 1/1 | 0.89 | 0.09 | 57,57,57,57 | 0 |
| 54 | MG | 11 | 102 | 1/1 | 0.89 | 0.13 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3486 | 1/1 | 0.89 | 0.21 | 73,73,73,73 | 0 |
| 54 | MG | 14 | 101 | 1/1 | 0.89 | 0.08 | 82,82,82,82 | 0 |
| 54 | MG | 2A | 3190 | 1/1 | 0.89 | 0.20 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3191 | 1/1 | 0.89 | 0.31 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3375 | 1/1 | 0.89 | 0.15 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3198 | 1/1 | 0.89 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3904 | 1/1 | 0.89 | 0.10 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3709 | 1/1 | 0.89 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3198 | 1/1 | 0.89 | 0.41 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3200 | 1/1 | 0.89 | 0.26 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3130 | 1/1 | 0.89 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3448 | 1/1 | 0.89 | 0.20 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3720 | 1/1 | 0.89 | 0.14 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3616 | 1/1 | 0.89 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3696 | 1/1 | 0.89 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3458 | 1/1 | 0.89 | 0.11 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1603 | 1/1 | 0.89 | 0.15 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3499 | 1/1 | 0.89 | 0.09 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3699 | 1/1 | 0.89 | 0.10 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3067 | 1/1 | 0.89 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 2B | 201 | 1/1 | 0.89 | 0.10 | 86,86,86,86 | 0 |
| 54 | MG | 1A | 3206 | 1/1 | 0.89 | 0.08 | 50,50,50,50 | 0 |
| 54 | MG | 2B | 203 | 1/1 | 0.89 | 0.21 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1812 | 1/1 | 0.89 | 0.08 | 78,78,78,78 | 0 |
| 54 | MG | 2a | 3165 | 1/1 | 0.89 | 0.27 | 79,79,79,79 | 0 |
| 54 | MG | 1B | 207 | 1/1 | 0.89 | 0.43 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3226 | 1/1 | 0.89 | 0.26 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3229 | 1/1 | 0.89 | 0.11 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3476 | 1/1 | 0.89 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1714 | 1/1 | 0.89 | 0.16 | 68,68,68,68 | 0 |
| 54 | MG | 2a | 3172 | 1/1 | 0.89 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3624 | 1/1 | 0.89 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3821 | 1/1 | 0.89 | 0.12 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3066 | 1/1 | 0.89 | 0.07 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1625 | 1/1 | 0.89 | 0.12 | 64,64,64,64 | 0 |
| 54 | MG | 2D | 312 | 1/1 | 0.89 | 0.14 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1628 | 1/1 | 0.89 | 0.33 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3822 | 1/1 | 0.89 | 0.13 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3190 | 1/1 | 0.89 | 0.16 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1828 | 1/1 | 0.89 | 0.18 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3563 | 1/1 | 0.89 | 0.36 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3955 | 1/1 | 0.89 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3263 | 1/1 | 0.89 | 0.40 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1636 | 1/1 | 0.89 | 0.31 | 66,66,66,66 | 0 |
| 54 | MG | 2P | 201 | 1/1 | 0.89 | 0.12 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3265 | 1/1 | 0.89 | 0.14 | 74,74,74,74 | 0 |
| 54 | MG | 2V | 202 | 1/1 | 0.89 | 0.24 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1837 | 1/1 | 0.89 | 0.23 | 72,72,72,72 | 0 |
| 54 | MG | 25 | 101 | 1/1 | 0.89 | 0.50 | 57,57,57,57 | 0 |
| 54 | MG | 25 | 103 | 1/1 | 0.89 | 0.14 | 74,74,74,74 | 0 |
| 54 | MG | 1h | 201 | 1/1 | 0.90 | 0.18 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3449 | 1/1 | 0.90 | 0.28 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3525 | 1/1 | 0.90 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 1l | 201 | 1/1 | 0.90 | 0.30 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3187 | 1/1 | 0.90 | 0.22 | 78,78,78,78 | 0 |
| 54 | MG | 1B | 224 | 1/1 | 0.90 | 0.19 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3302 | 1/1 | 0.90 | 0.17 | 50,50,50,50 | 0 |
| 54 | MG | 1a | 1644 | 1/1 | 0.90 | 0.25 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3685 | 1/1 | 0.90 | 0.08 | 24,24,24,24 | 0 |
| 54 | MG | 2A | 3193 | 1/1 | 0.90 | 0.20 | 67,67,67,67 | 0 |
| 54 | MG | 1y | 203 | 1/1 | 0.90 | 0.13 | 90,90,90,90 | 0 |
| 54 | MG | 1B | 227 | 1/1 | 0.90 | 0.19 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3808 | 1/1 | 0.90 | 0.10 | 64,64,64,64 | 0 |
| 54 | MG | 2T | 203 | 1/1 | 0.90 | 0.18 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3105 | 1/1 | 0.90 | 0.11 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3533 | 1/1 | 0.90 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 20 | 101 | 1/1 | 0.90 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3110 | 1/1 | 0.90 | 0.15 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3211 | 1/1 | 0.90 | 0.27 | 70,70,70,70 | 0 |
| 54 | MG | 1D | 315 | 1/1 | 0.90 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1659 | 1/1 | 0.90 | 0.33 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3032 | 1/1 | 0.90 | 0.31 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3212 | 1/1 | 0.90 | 0.13 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3316 | 1/1 | 0.90 | 0.15 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3968 | 1/1 | 0.90 | 0.09 | 61,61,61,61 | 0 |
| 54 | MG | 1E | 301 | 1/1 | 0.90 | 0.34 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3224 | 1/1 | 0.90 | 0.21 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3225 | 1/1 | 0.90 | 0.47 | 57,57,57,57 | 0 |
| 54 | MG | 1E | 303 | 1/1 | 0.90 | 0.30 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3277 | 1/1 | 0.90 | 0.14 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3505 | 1/1 | 0.90 | 0.10 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3041 | 1/1 | 0.90 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3620 | 1/1 | 0.90 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3823 | 1/1 | 0.90 | 0.26 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3234 | 1/1 | 0.90 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3235 | 1/1 | 0.90 | 0.15 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3518 | 1/1 | 0.90 | 0.14 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2a | 3029 | 1/1 | 0.90 | 0.20 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3030 | 1/1 | 0.90 | 0.19 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3519 | 1/1 | 0.90 | 0.11 | 85,85,85,85 | 0 |
| 54 | MG | 1A | 3322 | 1/1 | 0.90 | 0.31 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3033 | 1/1 | 0.90 | 0.28 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3239 | 1/1 | 0.90 | 0.35 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3980 | 1/1 | 0.90 | 0.17 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3031 | 1/1 | 0.90 | 0.08 | 25,25,25,25 | 0 |
| 54 | MG | 1a | 1677 | 1/1 | 0.90 | 0.16 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3327 | 1/1 | 0.90 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3984 | 1/1 | 0.90 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3630 | 1/1 | 0.90 | 0.09 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3056 | 1/1 | 0.90 | 0.22 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3534 | 1/1 | 0.90 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3843 | 1/1 | 0.90 | 0.09 | 20,20,20,20 | 0 |
| 54 | MG | 1A | 3152 | 1/1 | 0.90 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3061 | 1/1 | 0.90 | 0.17 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3063 | 1/1 | 0.90 | 0.23 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3065 | 1/1 | 0.90 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3720 | 1/1 | 0.90 | 0.13 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3998 | 1/1 | 0.90 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3721 | 1/1 | 0.90 | 0.35 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3637 | 1/1 | 0.90 | 0.21 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3483 | 1/1 | 0.90 | 0.14 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3061 | 1/1 | 0.90 | 0.14 | 56,56,56,56 | 0 |
| 54 | MG | 1V | 204 | 1/1 | 0.90 | 0.13 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3085 | 1/1 | 0.90 | 0.46 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3644 | 1/1 | 0.90 | 0.11 | 29,29,29,29 | 0 |
| 54 | MG | 2a | 3062 | 1/1 | 0.90 | 0.15 | 81,81,81,81 | 0 |
| 54 | MG | 2a | 3063 | 1/1 | 0.90 | 0.24 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3732 | 1/1 | 0.90 | 0.13 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3647 | 1/1 | 0.90 | 0.12 | 39,39,39,39 | 0 |
| 54 | MG | 10 | 102 | 1/1 | 0.90 | 0.22 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3577 | 1/1 | 0.90 | 0.13 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3648 | 1/1 | 0.90 | 0.14 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3405 | 1/1 | 0.90 | 0.17 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3077 | 1/1 | 0.90 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1825 | 1/1 | 0.90 | 0.12 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3489 | 1/1 | 0.90 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3590 | 1/1 | 0.90 | 0.15 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3592 | 1/1 | 0.90 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1705 | 1/1 | 0.90 | 0.26 | 62,62,62,62 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3599 | 1/1 | 0.90 | 0.12 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3300 | 1/1 | 0.90 | 0.18 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3290 | 1/1 | 0.90 | 0.33 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3103 | 1/1 | 0.90 | 0.23 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3095 | 1/1 | 0.90 | 0.27 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3610 | 1/1 | 0.90 | 0.16 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3319 | 1/1 | 0.90 | 0.09 | 44,44,44,44 | 0 |
| 54 | MG | 11 | 105 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3340 | 1/1 | 0.90 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1711 | 1/1 | 0.90 | 0.20 | 69,69,69,69 | 0 |
| 54 | MG | 15 | 103 | 1/1 | 0.90 | 0.26 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3326 | 1/1 | 0.90 | 0.26 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3624 | 1/1 | 0.90 | 0.15 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3328 | 1/1 | 0.90 | 0.25 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3332 | 1/1 | 0.90 | 0.15 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3658 | 1/1 | 0.90 | 0.18 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3114 | 1/1 | 0.90 | 0.31 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3341 | 1/1 | 0.90 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3349 | 1/1 | 0.90 | 0.15 | 67,67,67,67 | 0 |
| 54 | MG | 17 | 106 | 1/1 | 0.90 | 0.16 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1843 | 1/1 | 0.90 | 0.08 | 77,77,77,77 | 0 |
| 54 | MG | 1a | 1849 | 1/1 | 0.90 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3656 | 1/1 | 0.90 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3502 | 1/1 | 0.90 | 0.11 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3666 | 1/1 | 0.90 | 0.16 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3126 | 1/1 | 0.90 | 0.27 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3671 | 1/1 | 0.90 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 2a | 3128 | 1/1 | 0.90 | 0.21 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 4029 | 1/1 | 0.90 | 0.23 | 59,59,59,59 | 0 |
| 54 | MG | 19 | 102 | 1/1 | 0.90 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3679 | 1/1 | 0.90 | 0.16 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3160 | 1/1 | 0.90 | 0.69 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3886 | 1/1 | 0.90 | 0.14 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3768 | 1/1 | 0.90 | 0.23 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3375 | 1/1 | 0.90 | 0.30 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3376 | 1/1 | 0.90 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3889 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3694 | 1/1 | 0.90 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3696 | 1/1 | 0.90 | 0.08 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1607 | 1/1 | 0.90 | 0.18 | 69,69,69,69 | 0 |
| 54 | MG | 2a | 3145 | 1/1 | 0.90 | 0.20 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3506 | 1/1 | 0.90 | 0.12 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3664 | 1/1 | 0.90 | 0.15 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3036 | 1/1 | 0.90 | 0.10 | 41,41,41,41 | 0 |
| 54 | MG | 2a | 3156 | 1/1 | 0.90 | 0.23 | 72,72,72,72 | 0 |
| 54 | MG | 2a | 3160 | 1/1 | 0.90 | 0.19 | 79,79,79,79 | 0 |
| 54 | MG | 1a | 1735 | 1/1 | 0.90 | 0.13 | 70,70,70,70 | 0 |
| 54 | MG | 1B | 201 | 1/1 | 0.90 | 0.20 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3399 | 1/1 | 0.90 | 0.12 | 45,45,45,45 | 0 |
| 54 | MG | 2a | 3168 | 1/1 | 0.90 | 0.20 | 75,75,75,75 | 0 |
| 54 | MG | 1B | 203 | 1/1 | 0.90 | 0.38 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3404 | 1/1 | 0.90 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3405 | 1/1 | 0.90 | 0.12 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1620 | 1/1 | 0.90 | 0.19 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3595 | 1/1 | 0.90 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3176 | 1/1 | 0.90 | 0.14 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3783 | 1/1 | 0.90 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 1a | 1879 | 1/1 | 0.90 | 0.20 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3414 | 1/1 | 0.90 | 0.23 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3350 | 1/1 | 0.90 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 1B | 209 | 1/1 | 0.90 | 0.11 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3727 | 1/1 | 0.90 | 0.13 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3167 | 1/1 | 0.90 | 0.24 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3169 | 1/1 | 0.90 | 0.15 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3428 | 1/1 | 0.90 | 0.23 | 67,67,67,67 | 0 |
| 54 | MG | 1d | 302 | 1/1 | 0.90 | 0.36 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3785 | 1/1 | 0.90 | 0.17 | 52,52,52,52 | 0 |
| 54 | MG | 2r | 101 | 1/1 | 0.90 | 0.22 | 80,80,80,80 | 0 |
| 54 | MG | 1B | 211 | 1/1 | 0.90 | 0.29 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3032 | 1/1 | 0.90 | 0.15 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3130 | 1/1 | 0.90 | 0.16 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3450 | 1/1 | 0.90 | 0.09 | 27,27,27,27 | 0 |
| 54 | MG | 2B | 212 | 1/1 | 0.90 | 0.09 | 95,95,95,95 | 0 |
| 54 | MG | 1f | 202 | 1/1 | 0.90 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1754 | 1/1 | 0.90 | 0.16 | 77,77,77,77 | 0 |
| 59 | ZN | 24 | 501 | 1/1 | 0.90 | 0.09 | 140,140,140,140 | 0 |
| 54 | MG | 2A | 3520 | 1/1 | 0.91 | 0.16 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3110 | 1/1 | 0.91 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3222 | 1/1 | 0.91 | 0.20 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3945 | 1/1 | 0.91 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3571 | 1/1 | 0.91 | 0.12 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1739 | 1/1 | 0.91 | 0.16 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1740 | 1/1 | 0.91 | 0.21 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1871 | 1/1 | 0.91 | 0.27 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3289 | 1/1 | 0.91 | 0.20 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3531 | 1/1 | 0.91 | 0.34 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3532 | 1/1 | 0.91 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3385 | 1/1 | 0.91 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3120 | 1/1 | 0.91 | 0.20 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3706 | 1/1 | 0.91 | 0.10 | 80,80,80,80 | 0 |
| 54 | MG | 1a | 1875 | 1/1 | 0.91 | 0.32 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3709 | 1/1 | 0.91 | 0.09 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3308 | 1/1 | 0.91 | 0.19 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3819 | 1/1 | 0.91 | 0.10 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3540 | 1/1 | 0.91 | 0.26 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1640 | 1/1 | 0.91 | 0.21 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3712 | 1/1 | 0.91 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 2a | 3025 | 1/1 | 0.91 | 0.27 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3544 | 1/1 | 0.91 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3132 | 1/1 | 0.91 | 0.14 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3550 | 1/1 | 0.91 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3133 | 1/1 | 0.91 | 0.37 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3515 | 1/1 | 0.91 | 0.08 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3557 | 1/1 | 0.91 | 0.26 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3559 | 1/1 | 0.91 | 0.09 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3966 | 1/1 | 0.91 | 0.23 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3141 | 1/1 | 0.91 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3587 | 1/1 | 0.91 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 1d | 304 | 1/1 | 0.91 | 0.28 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3827 | 1/1 | 0.91 | 0.27 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3049 | 1/1 | 0.91 | 0.28 | 57,57,57,57 | 0 |
| 54 | MG | 1E | 305 | 1/1 | 0.91 | 0.12 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3650 | 1/1 | 0.91 | 0.11 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3461 | 1/1 | 0.91 | 0.08 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3836 | 1/1 | 0.91 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3581 | 1/1 | 0.91 | 0.12 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3837 | 1/1 | 0.91 | 0.11 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3584 | 1/1 | 0.91 | 0.09 | 54,54,54,54 | 0 |
| 54 | MG | 1a | 1658 | 1/1 | 0.91 | 0.21 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3587 | 1/1 | 0.91 | 0.16 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3838 | 1/1 | 0.91 | 0.07 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3363 | 1/1 | 0.91 | 0.15 | 84,84,84,84 | 0 |
| 54 | MG | 1A | 3343 | 1/1 | 0.91 | 0.23 | 65,65,65,65 | 0 |
| 54 | MG | 1G | 203 | 1/1 | 0.91 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3369 | 1/1 | 0.91 | 0.13 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3591 | 1/1 | 0.91 | 0.15 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1t | 201 | 1/1 | 0.91 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3172 | 1/1 | 0.91 | 0.15 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3593 | 1/1 | 0.91 | 0.16 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3311 | 1/1 | 0.91 | 0.27 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3995 | 1/1 | 0.91 | 0.11 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3065 | 1/1 | 0.91 | 0.30 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3178 | 1/1 | 0.91 | 0.11 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3005 | 1/1 | 0.91 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3470 | 1/1 | 0.91 | 0.21 | 77,77,77,77 | 0 |
| 54 | MG | 2a | 3070 | 1/1 | 0.91 | 0.08 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1776 | 1/1 | 0.91 | 0.16 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3625 | 1/1 | 0.91 | 0.10 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3738 | 1/1 | 0.91 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3627 | 1/1 | 0.91 | 0.14 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3628 | 1/1 | 0.91 | 0.09 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3396 | 1/1 | 0.91 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 1a | 1670 | 1/1 | 0.91 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3632 | 1/1 | 0.91 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3400 | 1/1 | 0.91 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3598 | 1/1 | 0.91 | 0.17 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3186 | 1/1 | 0.91 | 0.20 | 70,70,70,70 | 0 |
| 54 | MG | 2a | 3091 | 1/1 | 0.91 | 0.15 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3023 | 1/1 | 0.91 | 0.20 | 74,74,74,74 | 0 |
| 54 | MG | 1R | 202 | 1/1 | 0.91 | 0.15 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3639 | 1/1 | 0.91 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3231 | 1/1 | 0.91 | 0.22 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3529 | 1/1 | 0.91 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3657 | 1/1 | 0.91 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3531 | 1/1 | 0.91 | 0.17 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3759 | 1/1 | 0.91 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3314 | 1/1 | 0.91 | 0.17 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3004 | 1/1 | 0.91 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3766 | 1/1 | 0.91 | 0.15 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3107 | 1/1 | 0.91 | 0.41 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3537 | 1/1 | 0.91 | 0.07 | 23,23,23,23 | 0 |
| 54 | MG | 1A | 3208 | 1/1 | 0.91 | 0.08 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3044 | 1/1 | 0.91 | 0.11 | 62,62,62,62 | 0 |
| 54 | MG | 2a | 3111 | 1/1 | 0.91 | 0.43 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3611 | 1/1 | 0.91 | 0.11 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3433 | 1/1 | 0.91 | 0.12 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 4019 | 1/1 | 0.91 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3209 | 1/1 | 0.91 | 0.33 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2a | 3117 | 1/1 | 0.91 | 0.14 | 76,76,76,76 | 0 |
| 54 | MG | 10 | 108 | 1/1 | 0.91 | 0.14 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3695 | 1/1 | 0.91 | 0.16 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3879 | 1/1 | 0.91 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3249 | 1/1 | 0.91 | 0.23 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3885 | 1/1 | 0.91 | 0.09 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3676 | 1/1 | 0.91 | 0.14 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3218 | 1/1 | 0.91 | 0.22 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3432 | 1/1 | 0.91 | 0.13 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3221 | 1/1 | 0.91 | 0.20 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3454 | 1/1 | 0.91 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3457 | 1/1 | 0.91 | 0.16 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3710 | 1/1 | 0.91 | 0.08 | 70,70,70,70 | 0 |
| 54 | MG | 15 | 105 | 1/1 | 0.91 | 0.22 | 72,72,72,72 | 0 |
| 54 | MG | 15 | 106 | 1/1 | 0.91 | 0.23 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3717 | 1/1 | 0.91 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3059 | 1/1 | 0.91 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3719 | 1/1 | 0.91 | 0.10 | 79,79,79,79 | 0 |
| 54 | MG | 2a | 3142 | 1/1 | 0.91 | 0.11 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3888 | 1/1 | 0.91 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3093 | 1/1 | 0.91 | 0.12 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3687 | 1/1 | 0.91 | 0.12 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3254 | 1/1 | 0.91 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3786 | 1/1 | 0.91 | 0.09 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 4039 | 1/1 | 0.91 | 0.15 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3726 | 1/1 | 0.91 | 0.23 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3473 | 1/1 | 0.91 | 0.09 | 79,79,79,79 | 0 |
| 54 | MG | 2a | 3161 | 1/1 | 0.91 | 0.16 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3619 | 1/1 | 0.91 | 0.11 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3443 | 1/1 | 0.91 | 0.11 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3240 | 1/1 | 0.91 | 0.21 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3243 | 1/1 | 0.91 | 0.19 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3245 | 1/1 | 0.91 | 0.08 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3214 | 1/1 | 0.91 | 0.21 | 56,56,56,56 | 0 |
| 54 | MG | 2B | 205 | 1/1 | 0.91 | 0.34 | 71,71,71,71 | 0 |
| 54 | MG | 2B | 207 | 1/1 | 0.91 | 0.24 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3078 | 1/1 | 0.91 | 0.09 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3799 | 1/1 | 0.91 | 0.14 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3447 | 1/1 | 0.91 | 0.11 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3487 | 1/1 | 0.91 | 0.17 | 87,87,87,87 | 0 |
| 54 | MG | 2A | 3489 | 1/1 | 0.91 | 0.22 | 72,72,72,72 | 0 |
| 54 | MG | 2a | 3183 | 1/1 | 0.91 | 0.11 | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3448 | 1/1 | 0.91 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3909 | 1/1 | 0.91 | 0.17 | 43,43,43,43 | 0 |
| 54 | MG | 1a | 1613 | 1/1 | 0.91 | 0.23 | 75,75,75,75 | 0 |
| 54 | MG | 2B | 218 | 1/1 | 0.91 | 0.13 | 79,79,79,79 | 0 |
| 54 | MG | 2D | 302 | 1/1 | 0.91 | 0.16 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3915 | 1/1 | 0.91 | 0.08 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1725 | 1/1 | 0.91 | 0.20 | 53,53,53,53 | 0 |
| 54 | MG | 1a | 1726 | 1/1 | 0.91 | 0.14 | 86,86,86,86 | 0 |
| 54 | MG | 1A | 3698 | 1/1 | 0.91 | 0.18 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3924 | 1/1 | 0.91 | 0.15 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3508 | 1/1 | 0.91 | 0.16 | 72,72,72,72 | 0 |
| 57 | MPD | 1A | 4043 | 8/8 | 0.91 | 0.18 | 56,63,69,69 | 0 |
| 54 | MG | 1a | 1854 | 1/1 | 0.91 | 0.17 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1858 | 1/1 | 0.91 | 0.14 | 86,86,86,86 | 0 |
| 54 | MG | 1A | 3931 | 1/1 | 0.91 | 0.12 | 31,31,31,31 | 0 |
| 57 | MPD | 2A | 3734 | 8/8 | 0.91 | 0.23 | 72,77,82,83 | 0 |
| 54 | MG | 1a | 1731 | 1/1 | 0.91 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3220 | 1/1 | 0.91 | 0.38 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1627 | 1/1 | 0.91 | 0.40 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3174 | 1/1 | 0.92 | 0.16 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3076 | 1/1 | 0.92 | 0.08 | 44,44,44,44 | 0 |
| 54 | MG | 27 | 101 | 1/1 | 0.92 | 0.34 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3134 | 1/1 | 0.92 | 0.32 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3314 | 1/1 | 0.92 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 2a | 3003 | 1/1 | 0.92 | 0.10 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3281 | 1/1 | 0.92 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3324 | 1/1 | 0.92 | 0.23 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1661 | 1/1 | 0.92 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3868 | 1/1 | 0.92 | 0.11 | 43,43,43,43 | 0 |
| 54 | MG | 1N | 204 | 1/1 | 0.92 | 0.13 | 60,60,60,60 | 0 |
| 54 | MG | 1g | 201 | 1/1 | 0.92 | 0.28 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3151 | 1/1 | 0.92 | 0.17 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3282 | 1/1 | 0.92 | 0.09 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1766 | 1/1 | 0.92 | 0.27 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3556 | 1/1 | 0.92 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3338 | 1/1 | 0.92 | 0.10 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3465 | 1/1 | 0.92 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3563 | 1/1 | 0.92 | 0.28 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3566 | 1/1 | 0.92 | 0.10 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3160 | 1/1 | 0.92 | 0.29 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3344 | 1/1 | 0.92 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1i | 201 | 1/1 | 0.92 | 0.21 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 1A | 3469 | 1/1 | 0.92 | 0.14 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3011 | 1/1 | 0.92 | 0.22 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3683 | 1/1 | 0.92 | 0.07 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3119 | 1/1 | 0.92 | 0.32 | 47,47,47,47 | 0 |
| 54 | MG | 1n | 102 | 1/1 | 0.92 | 0.10 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 4007 | 1/1 | 0.92 | 0.13 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1671 | 1/1 | 0.92 | 0.30 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1672 | 1/1 | 0.92 | 0.30 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1778 | 1/1 | 0.92 | 0.09 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3370 | 1/1 | 0.92 | 0.12 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3686 | 1/1 | 0.92 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3006 | 1/1 | 0.92 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3176 | 1/1 | 0.92 | 0.19 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3399 | 1/1 | 0.92 | 0.10 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3012 | 1/1 | 0.92 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3384 | 1/1 | 0.92 | 0.12 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3012 | 1/1 | 0.92 | 0.13 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3603 | 1/1 | 0.92 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3404 | 1/1 | 0.92 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3018 | 1/1 | 0.92 | 0.41 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3255 | 1/1 | 0.92 | 0.24 | 53,53,53,53 | 0 |
| 54 | MG | 2a | 3054 | 1/1 | 0.92 | 0.34 | 72,72,72,72 | 0 |
| 54 | MG | 1W | 202 | 1/1 | 0.92 | 0.20 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3339 | 1/1 | 0.92 | 0.16 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3622 | 1/1 | 0.92 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3398 | 1/1 | 0.92 | 0.08 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3026 | 1/1 | 0.92 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1683 | 1/1 | 0.92 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3402 | 1/1 | 0.92 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3189 | 1/1 | 0.92 | 0.13 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3484 | 1/1 | 0.92 | 0.08 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3033 | 1/1 | 0.92 | 0.27 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1792 | 1/1 | 0.92 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3802 | 1/1 | 0.92 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3411 | 1/1 | 0.92 | 0.11 | 29,29,29,29 | 0 |
| 54 | MG | 1a | 1796 | 1/1 | 0.92 | 0.12 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3627 | 1/1 | 0.92 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3418 | 1/1 | 0.92 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3075 | 1/1 | 0.92 | 0.26 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3419 | 1/1 | 0.92 | 0.19 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3903 | 1/1 | 0.92 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3201 | 1/1 | 0.92 | 0.11 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 2A | 3203 | 1/1 | 0.92 | 0.31 | 76,76,76,76 | 0 |
| 54 | MG | 2a | 3084 | 1/1 | 0.92 | 0.34 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3807 | 1/1 | 0.92 | 0.14 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1802 | 1/1 | 0.92 | 0.12 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3701 | 1/1 | 0.92 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3658 | 1/1 | 0.92 | 0.07 | 86,86,86,86 | 0 |
| 54 | MG | 2a | 3089 | 1/1 | 0.92 | 0.28 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3660 | 1/1 | 0.92 | 0.15 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 4033 | 1/1 | 0.92 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3629 | 1/1 | 0.92 | 0.35 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3667 | 1/1 | 0.92 | 0.10 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3418 | 1/1 | 0.92 | 0.11 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3632 | 1/1 | 0.92 | 0.23 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3438 | 1/1 | 0.92 | 0.11 | 64,64,64,64 | 0 |
| 54 | MG | 17 | 105 | 1/1 | 0.92 | 0.18 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3910 | 1/1 | 0.92 | 0.23 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3634 | 1/1 | 0.92 | 0.28 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3443 | 1/1 | 0.92 | 0.27 | 75,75,75,75 | 0 |
| 54 | MG | 2A | 3445 | 1/1 | 0.92 | 0.14 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3217 | 1/1 | 0.92 | 0.13 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3918 | 1/1 | 0.92 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3692 | 1/1 | 0.92 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3922 | 1/1 | 0.92 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1823 | 1/1 | 0.92 | 0.13 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3295 | 1/1 | 0.92 | 0.11 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3257 | 1/1 | 0.92 | 0.31 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3455 | 1/1 | 0.92 | 0.14 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3701 | 1/1 | 0.92 | 0.11 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3930 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3575 | 1/1 | 0.92 | 0.27 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3297 | 1/1 | 0.92 | 0.12 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3300 | 1/1 | 0.92 | 0.20 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1832 | 1/1 | 0.92 | 0.13 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1834 | 1/1 | 0.92 | 0.16 | 69,69,69,69 | 0 |
| 54 | MG | 2a | 3125 | 1/1 | 0.92 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | 1B | 215 | 1/1 | 0.92 | 0.08 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3712 | 1/1 | 0.92 | 0.09 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3582 | 1/1 | 0.92 | 0.15 | 65,65,65,65 | 0 |
| 54 | MG | 1a | 1838 | 1/1 | 0.92 | 0.13 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1612 | 1/1 | 0.92 | 0.11 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3241 | 1/1 | 0.92 | 0.26 | 51,51,51,51 | 0 |
| 54 | MG | 1B | 218 | 1/1 | 0.92 | 0.08 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3215 | 1/1 | 0.92 | 0.20 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3949 | 1/1 | 0.92 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3950 | 1/1 | 0.92 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3092 | 1/1 | 0.92 | 0.18 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3480 | 1/1 | 0.92 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3951 | 1/1 | 0.92 | 0.08 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3482 | 1/1 | 0.92 | 0.10 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3253 | 1/1 | 0.92 | 0.20 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3256 | 1/1 | 0.92 | 0.16 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3258 | 1/1 | 0.92 | 0.27 | 50,50,50,50 | 0 |
| 54 | MG | 2a | 3147 | 1/1 | 0.92 | 0.19 | 81,81,81,81 | 0 |
| 54 | MG | 1A | 3441 | 1/1 | 0.92 | 0.11 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3488 | 1/1 | 0.92 | 0.14 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3507 | 1/1 | 0.92 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3351 | 1/1 | 0.92 | 0.14 | 38,38,38,38 | 0 |
| 54 | MG | 2a | 3158 | 1/1 | 0.92 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3511 | 1/1 | 0.92 | 0.14 | 71,71,71,71 | 0 |
| 54 | MG | 2B | 206 | 1/1 | 0.92 | 0.25 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1631 | 1/1 | 0.92 | 0.27 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3155 | 1/1 | 0.92 | 0.16 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1634 | 1/1 | 0.92 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3099 | 1/1 | 0.92 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3839 | 1/1 | 0.92 | 0.18 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3967 | 1/1 | 0.92 | 0.08 | 34,34,34,34 | 0 |
| 54 | MG | 1D | 314 | 1/1 | 0.92 | 0.26 | 49,49,49,49 | 0 |
| 54 | MG | 2B | 215 | 1/1 | 0.92 | 0.17 | 77,77,77,77 | 0 |
| 54 | MG | 2a | 3173 | 1/1 | 0.92 | 0.18 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3659 | 1/1 | 0.92 | 0.15 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3263 | 1/1 | 0.92 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3970 | 1/1 | 0.92 | 0.18 | 60,60,60,60 | 0 |
| 54 | MG | 2D | 301 | 1/1 | 0.92 | 0.23 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3971 | 1/1 | 0.92 | 0.12 | 73,73,73,73 | 0 |
| 54 | MG | 2D | 307 | 1/1 | 0.92 | 0.28 | 60,60,60,60 | 0 |
| 54 | MG | 2D | 308 | 1/1 | 0.92 | 0.24 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3278 | 1/1 | 0.92 | 0.19 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3279 | 1/1 | 0.92 | 0.30 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3189 | 1/1 | 0.92 | 0.30 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3002 | 1/1 | 0.92 | 0.09 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3117 | 1/1 | 0.92 | 0.18 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3597 | 1/1 | 0.92 | 0.09 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3849 | 1/1 | 0.92 | 0.10 | 64,64,64,64 | 0 |
| 54 | MG | 2F | 302 | 1/1 | 0.92 | 0.10 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1647 | 1/1 | 0.92 | 0.23 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3106 | 1/1 | 0.92 | 0.21 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3751 | 1/1 | 0.92 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3291 | 1/1 | 0.92 | 0.30 | 78,78,78,78 | 0 |
| 54 | MG | 2A | 3529 | 1/1 | 0.92 | 0.08 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3756 | 1/1 | 0.92 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3128 | 1/1 | 0.92 | 0.24 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1755 | 1/1 | 0.92 | 0.18 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3130 | 1/1 | 0.92 | 0.25 | 61,61,61,61 | 0 |
| 54 | MG | 2I | 101 | 1/1 | 0.92 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3039 | 1/1 | 0.92 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3270 | 1/1 | 0.93 | 0.22 | 49,49,49,49 | 0 |
| 54 | MG | 2F | 301 | 1/1 | 0.93 | 0.34 | 48,48,48,48 | 0 |
| 54 | MG | 1I | 101 | 1/1 | 0.93 | 0.24 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3272 | 1/1 | 0.93 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3272 | 1/1 | 0.93 | 0.34 | 72,72,72,72 | 0 |
| 54 | MG | 1I | 103 | 1/1 | 0.93 | 0.11 | 58,58,58,58 | 0 |
| 54 | MG | 2O | 201 | 1/1 | 0.93 | 0.14 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3517 | 1/1 | 0.93 | 0.07 | 81,81,81,81 | 0 |
| 54 | MG | 1a | 1708 | 1/1 | 0.93 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 2R | 203 | 1/1 | 0.93 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3066 | 1/1 | 0.93 | 0.15 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 4009 | 1/1 | 0.93 | 0.12 | 84,84,84,84 | 0 |
| 54 | MG | 2V | 201 | 1/1 | 0.93 | 0.22 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3860 | 1/1 | 0.93 | 0.24 | 60,60,60,60 | 0 |
| 54 | MG | 2W | 201 | 1/1 | 0.93 | 0.23 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3105 | 1/1 | 0.93 | 0.08 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3106 | 1/1 | 0.93 | 0.20 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3010 | 1/1 | 0.93 | 0.15 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3158 | 1/1 | 0.93 | 0.07 | 53,53,53,53 | 0 |
| 54 | MG | 25 | 102 | 1/1 | 0.93 | 0.20 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3628 | 1/1 | 0.93 | 0.13 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3213 | 1/1 | 0.93 | 0.21 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3345 | 1/1 | 0.93 | 0.28 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1856 | 1/1 | 0.93 | 0.10 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3348 | 1/1 | 0.93 | 0.17 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3290 | 1/1 | 0.93 | 0.27 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3068 | 1/1 | 0.93 | 0.25 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1720 | 1/1 | 0.93 | 0.21 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3020 | 1/1 | 0.93 | 0.33 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3297 | 1/1 | 0.93 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3009 | 1/1 | 0.93 | 0.13 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 19 | 101 | 1/1 | 0.93 | 0.21 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3011 | 1/1 | 0.93 | 0.12 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3740 | 1/1 | 0.93 | 0.32 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3125 | 1/1 | 0.93 | 0.09 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3305 | 1/1 | 0.93 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3084 | 1/1 | 0.93 | 0.17 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3553 | 1/1 | 0.93 | 0.17 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3311 | 1/1 | 0.93 | 0.22 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3086 | 1/1 | 0.93 | 0.30 | 50,50,50,50 | 0 |
| 54 | MG | 1a | 1605 | 1/1 | 0.93 | 0.24 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3318 | 1/1 | 0.93 | 0.09 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3554 | 1/1 | 0.93 | 0.08 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3754 | 1/1 | 0.93 | 0.08 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1873 | 1/1 | 0.93 | 0.22 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3645 | 1/1 | 0.93 | 0.08 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3757 | 1/1 | 0.93 | 0.09 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3561 | 1/1 | 0.93 | 0.09 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3358 | 1/1 | 0.93 | 0.05 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3565 | 1/1 | 0.93 | 0.08 | 83,83,83,83 | 0 |
| 54 | MG | 1A | 3227 | 1/1 | 0.93 | 0.13 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3139 | 1/1 | 0.93 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3331 | 1/1 | 0.93 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3761 | 1/1 | 0.93 | 0.09 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3649 | 1/1 | 0.93 | 0.14 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1741 | 1/1 | 0.93 | 0.13 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1615 | 1/1 | 0.93 | 0.17 | 76,76,76,76 | 0 |
| 54 | MG | 1a | 1616 | 1/1 | 0.93 | 0.11 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3342 | 1/1 | 0.93 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3148 | 1/1 | 0.93 | 0.14 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3346 | 1/1 | 0.93 | 0.11 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3897 | 1/1 | 0.93 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3764 | 1/1 | 0.93 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3558 | 1/1 | 0.93 | 0.08 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3353 | 1/1 | 0.93 | 0.09 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3560 | 1/1 | 0.93 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3157 | 1/1 | 0.93 | 0.15 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3364 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3595 | 1/1 | 0.93 | 0.09 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3466 | 1/1 | 0.93 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3364 | 1/1 | 0.93 | 0.14 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3774 | 1/1 | 0.93 | 0.20 | 49,49,49,49 | 0 |
| 54 | MG | 1B | 212 | 1/1 | 0.93 | 0.07 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3565 | 1/1 | 0.93 | 0.07 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3569 | 1/1 | 0.93 | 0.09 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3609 | 1/1 | 0.93 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3166 | 1/1 | 0.93 | 0.17 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3777 | 1/1 | 0.93 | 0.12 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3168 | 1/1 | 0.93 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3617 | 1/1 | 0.93 | 0.07 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3467 | 1/1 | 0.93 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3619 | 1/1 | 0.93 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3574 | 1/1 | 0.93 | 0.23 | 73,73,73,73 | 0 |
| 54 | MG | 2a | 3076 | 1/1 | 0.93 | 0.13 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3621 | 1/1 | 0.93 | 0.12 | 68,68,68,68 | 0 |
| 54 | MG | 1a | 1759 | 1/1 | 0.93 | 0.16 | 70,70,70,70 | 0 |
| 54 | MG | 2a | 3080 | 1/1 | 0.93 | 0.18 | 61,61,61,61 | 0 |
| 54 | MG | 2a | 3081 | 1/1 | 0.93 | 0.26 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3919 | 1/1 | 0.93 | 0.09 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3369 | 1/1 | 0.93 | 0.13 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3372 | 1/1 | 0.93 | 0.08 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3580 | 1/1 | 0.93 | 0.09 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3927 | 1/1 | 0.93 | 0.09 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3665 | 1/1 | 0.93 | 0.30 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3629 | 1/1 | 0.93 | 0.14 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3001 | 1/1 | 0.93 | 0.37 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3177 | 1/1 | 0.93 | 0.23 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3003 | 1/1 | 0.93 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3004 | 1/1 | 0.93 | 0.09 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3401 | 1/1 | 0.93 | 0.11 | 82,82,82,82 | 0 |
| 54 | MG | 1a | 1768 | 1/1 | 0.93 | 0.09 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3087 | 1/1 | 0.93 | 0.26 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1770 | 1/1 | 0.93 | 0.10 | 75,75,75,75 | 0 |
| 54 | MG | 1D | 305 | 1/1 | 0.93 | 0.22 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3652 | 1/1 | 0.93 | 0.07 | 71,71,71,71 | 0 |
| 54 | MG | 2a | 3102 | 1/1 | 0.93 | 0.33 | 62,62,62,62 | 0 |
| 54 | MG | 1D | 309 | 1/1 | 0.93 | 0.13 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3232 | 1/1 | 0.93 | 0.11 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3586 | 1/1 | 0.93 | 0.07 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3377 | 1/1 | 0.93 | 0.07 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3233 | 1/1 | 0.93 | 0.28 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3416 | 1/1 | 0.93 | 0.17 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3662 | 1/1 | 0.93 | 0.08 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3417 | 1/1 | 0.93 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3190 | 1/1 | 0.93 | 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3239 | 1/1 | 0.93 | 0.21 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3195 | 1/1 | 0.93 | 0.07 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3025 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 2a | 3115 | 1/1 | 0.93 | 0.33 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3423 | 1/1 | 0.93 | 0.07 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3424 | 1/1 | 0.93 | 0.07 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3677 | 1/1 | 0.93 | 0.24 | 65,65,65,65 | 0 |
| 54 | MG | 2a | 3120 | 1/1 | 0.93 | 0.15 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3684 | 1/1 | 0.93 | 0.09 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3305 | 1/1 | 0.93 | 0.11 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3132 | 1/1 | 0.93 | 0.07 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3202 | 1/1 | 0.93 | 0.23 | 53,53,53,53 | 0 |
| 54 | MG | 1E | 307 | 1/1 | 0.93 | 0.14 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3204 | 1/1 | 0.93 | 0.34 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3435 | 1/1 | 0.93 | 0.09 | 58,58,58,58 | 0 |
| 54 | MG | 1a | 1783 | 1/1 | 0.93 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3684 | 1/1 | 0.93 | 0.09 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3058 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3392 | 1/1 | 0.93 | 0.09 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3962 | 1/1 | 0.93 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3816 | 1/1 | 0.93 | 0.17 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3498 | 1/1 | 0.93 | 0.13 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3194 | 1/1 | 0.93 | 0.27 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3045 | 1/1 | 0.93 | 0.18 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3599 | 1/1 | 0.93 | 0.09 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3501 | 1/1 | 0.93 | 0.07 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3196 | 1/1 | 0.93 | 0.28 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3711 | 1/1 | 0.93 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3451 | 1/1 | 0.93 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1675 | 1/1 | 0.93 | 0.32 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3972 | 1/1 | 0.93 | 0.08 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3222 | 1/1 | 0.93 | 0.16 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3456 | 1/1 | 0.93 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 2a | 3154 | 1/1 | 0.93 | 0.09 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3695 | 1/1 | 0.93 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3060 | 1/1 | 0.93 | 0.08 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3135 | 1/1 | 0.93 | 0.23 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3831 | 1/1 | 0.93 | 0.10 | 39,39,39,39 | 0 |
| 54 | MG | 2a | 3162 | 1/1 | 0.93 | 0.10 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3320 | 1/1 | 0.93 | 0.18 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1809 | 1/1 | 0.93 | 0.10 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3463 | 1/1 | 0.93 | 0.13 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1810 | 1/1 | 0.93 | 0.07 | 76,76,76,76 | 0 |
| 54 | MG | 1R | 203 | 1/1 | 0.93 | 0.12 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3467 | 1/1 | 0.93 | 0.08 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3062 | 1/1 | 0.93 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3138 | 1/1 | 0.93 | 0.07 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3064 | 1/1 | 0.93 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3260 | 1/1 | 0.93 | 0.11 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3475 | 1/1 | 0.93 | 0.14 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3041 | 1/1 | 0.93 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3242 | 1/1 | 0.93 | 0.11 | 69,69,69,69 | 0 |
| 54 | MG | 1a | 1816 | 1/1 | 0.93 | 0.15 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3424 | 1/1 | 0.93 | 0.05 | 30,30,30,30 | 0 |
| 54 | MG | 2a | 3184 | 1/1 | 0.93 | 0.12 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3425 | 1/1 | 0.93 | 0.10 | 32,32,32,32 | 0 |
| 54 | MG | 1a | 1689 | 1/1 | 0.93 | 0.13 | 68,68,68,68 | 0 |
| 54 | MG | 2a | 3187 | 1/1 | 0.93 | 0.11 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3614 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3080 | 1/1 | 0.93 | 0.13 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3252 | 1/1 | 0.93 | 0.12 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3845 | 1/1 | 0.93 | 0.08 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3255 | 1/1 | 0.93 | 0.41 | 48,48,48,48 | 0 |
| 54 | MG | 2f | 201 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3082 | 1/1 | 0.93 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3257 | 1/1 | 0.93 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3143 | 1/1 | 0.93 | 0.34 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3062 | 1/1 | 0.93 | 0.22 | 50,50,50,50 | 0 |
| 54 | MG | 2t | 201 | 1/1 | 0.93 | 0.16 | 53,53,53,53 | 0 |
| 54 | MG | 2D | 303 | 1/1 | 0.93 | 0.33 | 50,50,50,50 | 0 |
| 54 | MG | 2D | 304 | 1/1 | 0.93 | 0.28 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3065 | 1/1 | 0.93 | 0.08 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3499 | 1/1 | 0.93 | 0.11 | 69,69,69,69 | 0 |
| 54 | MG | 10 | 103 | 1/1 | 0.93 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1830 | 1/1 | 0.93 | 0.11 | 79,79,79,79 | 0 |
| 54 | MG | 2A | 3091 | 1/1 | 0.93 | 0.15 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 4002 | 1/1 | 0.93 | 0.07 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3434 | 1/1 | 0.93 | 0.09 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3008 | 1/1 | 0.94 | 0.06 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3478 | 1/1 | 0.94 | 0.08 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3560 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 54 | MG | 1B | 202 | 1/1 | 0.94 | 0.25 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3169 | 1/1 | 0.94 | 0.06 | 36,36,36,36 | 0 |
| 54 | MG | 1a | 1752 | 1/1 | 0.94 | 0.07 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1k | 201 | 1/1 | 0.94 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3579 | 1/1 | 0.94 | 0.14 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3170 | 1/1 | 0.94 | 0.16 | 54,54,54,54 | 0 |
| 54 | MG | 1m | 201 | 1/1 | 0.94 | 0.07 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3365 | 1/1 | 0.94 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3210 | 1/1 | 0.94 | 0.18 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3778 | 1/1 | 0.94 | 0.06 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3397 | 1/1 | 0.94 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 2a | 3017 | 1/1 | 0.94 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3025 | 1/1 | 0.94 | 0.45 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3265 | 1/1 | 0.94 | 0.09 | 53,53,53,53 | 0 |
| 54 | MG | 2a | 3020 | 1/1 | 0.94 | 0.08 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3107 | 1/1 | 0.94 | 0.45 | 42,42,42,42 | 0 |
| 54 | MG | 2a | 3023 | 1/1 | 0.94 | 0.41 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3175 | 1/1 | 0.94 | 0.06 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3497 | 1/1 | 0.94 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3787 | 1/1 | 0.94 | 0.09 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3920 | 1/1 | 0.94 | 0.07 | 64,64,64,64 | 0 |
| 54 | MG | 2a | 3028 | 1/1 | 0.94 | 0.10 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3921 | 1/1 | 0.94 | 0.07 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3326 | 1/1 | 0.94 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3671 | 1/1 | 0.94 | 0.15 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3388 | 1/1 | 0.94 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3796 | 1/1 | 0.94 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3034 | 1/1 | 0.94 | 0.21 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3390 | 1/1 | 0.94 | 0.14 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3268 | 1/1 | 0.94 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3015 | 1/1 | 0.94 | 0.21 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3409 | 1/1 | 0.94 | 0.07 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3605 | 1/1 | 0.94 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3592 | 1/1 | 0.94 | 0.09 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3410 | 1/1 | 0.94 | 0.09 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3175 | 1/1 | 0.94 | 0.23 | 60,60,60,60 | 0 |
| 54 | MG | 1D | 303 | 1/1 | 0.94 | 0.13 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3271 | 1/1 | 0.94 | 0.16 | 36,36,36,36 | 0 |
| 54 | MG | 1D | 307 | 1/1 | 0.94 | 0.09 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3419 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3333 | 1/1 | 0.94 | 0.13 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3030 | 1/1 | 0.94 | 0.20 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3334 | 1/1 | 0.94 | 0.08 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3600 | 1/1 | 0.94 | 0.11 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3109 | 1/1 | 0.94 | 0.14 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3411 | 1/1 | 0.94 | 0.18 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3217 | 1/1 | 0.94 | 0.13 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3035 | 1/1 | 0.94 | 0.21 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3218 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3521 | 1/1 | 0.94 | 0.10 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3038 | 1/1 | 0.94 | 0.13 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3341 | 1/1 | 0.94 | 0.12 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3219 | 1/1 | 0.94 | 0.33 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1787 | 1/1 | 0.94 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3279 | 1/1 | 0.94 | 0.23 | 55,55,55,55 | 0 |
| 54 | MG | 1E | 308 | 1/1 | 0.94 | 0.19 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3964 | 1/1 | 0.94 | 0.09 | 24,24,24,24 | 0 |
| 54 | MG | 2A | 3046 | 1/1 | 0.94 | 0.21 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3178 | 1/1 | 0.94 | 0.12 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3431 | 1/1 | 0.94 | 0.12 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3646 | 1/1 | 0.94 | 0.09 | 67,67,67,67 | 0 |
| 54 | MG | 1F | 313 | 1/1 | 0.94 | 0.27 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3074 | 1/1 | 0.94 | 0.28 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3442 | 1/1 | 0.94 | 0.13 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3434 | 1/1 | 0.94 | 0.21 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1795 | 1/1 | 0.94 | 0.10 | 78,78,78,78 | 0 |
| 54 | MG | 1A | 3528 | 1/1 | 0.94 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 2A | 3220 | 1/1 | 0.94 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3221 | 1/1 | 0.94 | 0.44 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3615 | 1/1 | 0.94 | 0.09 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3665 | 1/1 | 0.94 | 0.07 | 81,81,81,81 | 0 |
| 54 | MG | 1G | 202 | 1/1 | 0.94 | 0.25 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1800 | 1/1 | 0.94 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3668 | 1/1 | 0.94 | 0.08 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3057 | 1/1 | 0.94 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3672 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3444 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3677 | 1/1 | 0.94 | 0.17 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3530 | 1/1 | 0.94 | 0.08 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3705 | 1/1 | 0.94 | 0.06 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3973 | 1/1 | 0.94 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3682 | 1/1 | 0.94 | 0.08 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3184 | 1/1 | 0.94 | 0.41 | 46,46,46,46 | 0 |
| 54 | MG | 1N | 203 | 1/1 | 0.94 | 0.14 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3045 | 1/1 | 0.94 | 0.17 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3236 | 1/1 | 0.94 | 0.07 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3453 | 1/1 | 0.94 | 0.07 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3286 | 1/1 | 0.94 | 0.19 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3226 | 1/1 | 0.94 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3716 | 1/1 | 0.94 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3067 | 1/1 | 0.94 | 0.16 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3353 | 1/1 | 0.94 | 0.10 | 33,33,33,33 | 0 |
| 54 | MG | 1a | 1815 | 1/1 | 0.94 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 1Q | 203 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3075 | 1/1 | 0.94 | 0.39 | 60,60,60,60 | 0 |
| 54 | MG | 1Q | 204 | 1/1 | 0.94 | 0.13 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1819 | 1/1 | 0.94 | 0.07 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3079 | 1/1 | 0.94 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3453 | 1/1 | 0.94 | 0.07 | 21,21,21,21 | 0 |
| 54 | MG | 1a | 1687 | 1/1 | 0.94 | 0.15 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3291 | 1/1 | 0.94 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 1R | 204 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3472 | 1/1 | 0.94 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3625 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1691 | 1/1 | 0.94 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3715 | 1/1 | 0.94 | 0.13 | 71,71,71,71 | 0 |
| 54 | MG | 1a | 1827 | 1/1 | 0.94 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3003 | 1/1 | 0.94 | 0.07 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3991 | 1/1 | 0.94 | 0.10 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3545 | 1/1 | 0.94 | 0.19 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1695 | 1/1 | 0.94 | 0.16 | 52,52,52,52 | 0 |
| 54 | MG | 1U | 206 | 1/1 | 0.94 | 0.28 | 44,44,44,44 | 0 |
| 54 | MG | 1V | 203 | 1/1 | 0.94 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3994 | 1/1 | 0.94 | 0.09 | 71,71,71,71 | 0 |
| 54 | MG | 2a | 3132 | 1/1 | 0.94 | 0.11 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3191 | 1/1 | 0.94 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3997 | 1/1 | 0.94 | 0.08 | 32,32,32,32 | 0 |
| 54 | MG | 1a | 1839 | 1/1 | 0.94 | 0.08 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3019 | 1/1 | 0.94 | 0.37 | 34,34,34,34 | 0 |
| 54 | MG | 1Y | 201 | 1/1 | 0.94 | 0.12 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3631 | 1/1 | 0.94 | 0.11 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3730 | 1/1 | 0.94 | 0.08 | 68,68,68,68 | 0 |
| 54 | MG | 10 | 101 | 1/1 | 0.94 | 0.17 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 4000 | 1/1 | 0.94 | 0.11 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3855 | 1/1 | 0.94 | 0.06 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3495 | 1/1 | 0.94 | 0.19 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3497 | 1/1 | 0.94 | 0.19 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3116 | 1/1 | 0.94 | 0.18 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3633 | 1/1 | 0.94 | 0.30 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 2a | 3151 | 1/1 | 0.94 | 0.16 | 80,80,80,80 | 0 |
| 54 | MG | 2B | 208 | 1/1 | 0.94 | 0.24 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3281 | 1/1 | 0.94 | 0.34 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3091 | 1/1 | 0.94 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3865 | 1/1 | 0.94 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3153 | 1/1 | 0.94 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 4008 | 1/1 | 0.94 | 0.20 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3510 | 1/1 | 0.94 | 0.11 | 66,66,66,66 | 0 |
| 54 | MG | 2a | 3164 | 1/1 | 0.94 | 0.14 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3741 | 1/1 | 0.94 | 0.17 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3287 | 1/1 | 0.94 | 0.11 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3092 | 1/1 | 0.94 | 0.16 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3119 | 1/1 | 0.94 | 0.09 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1719 | 1/1 | 0.94 | 0.20 | 63,63,63,63 | 0 |
| 54 | MG | 13 | 102 | 1/1 | 0.94 | 0.15 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3122 | 1/1 | 0.94 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3123 | 1/1 | 0.94 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 2D | 305 | 1/1 | 0.94 | 0.44 | 49,49,49,49 | 0 |
| 54 | MG | 1a | 1721 | 1/1 | 0.94 | 0.11 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3126 | 1/1 | 0.94 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | 15 | 102 | 1/1 | 0.94 | 0.26 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3054 | 1/1 | 0.94 | 0.20 | 34,34,34,34 | 0 |
| 54 | MG | 2a | 3180 | 1/1 | 0.94 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 2A | 3307 | 1/1 | 0.94 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3749 | 1/1 | 0.94 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3874 | 1/1 | 0.94 | 0.15 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3643 | 1/1 | 0.94 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3001 | 1/1 | 0.94 | 0.06 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3878 | 1/1 | 0.94 | 0.06 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3317 | 1/1 | 0.94 | 0.07 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 4022 | 1/1 | 0.94 | 0.14 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3562 | 1/1 | 0.94 | 0.14 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 4026 | 1/1 | 0.94 | 0.08 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3164 | 1/1 | 0.94 | 0.30 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3883 | 1/1 | 0.94 | 0.08 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3758 | 1/1 | 0.94 | 0.18 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3101 | 1/1 | 0.94 | 0.11 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3566 | 1/1 | 0.94 | 0.08 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3541 | 1/1 | 0.94 | 0.16 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3146 | 1/1 | 0.94 | 0.27 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1742 | 1/1 | 0.94 | 0.12 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3567 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3152 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3205 | 1/1 | 0.94 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3474 | 1/1 | 0.94 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3572 | 1/1 | 0.94 | 0.19 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3573 | 1/1 | 0.94 | 0.10 | 57,57,57,57 | 0 |
| 58 | ARG | 1B | 230 | 12/12 | 0.94 | 0.09 | 32,44,59,61 | 0 |
| 54 | MG | 2A | 3158 | 1/1 | 0.94 | 0.15 | 76,76,76,76 | 0 |
| 54 | MG | 28 | 101 | 1/1 | 0.94 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3415 | 1/1 | 0.95 | 0.09 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3798 | 1/1 | 0.95 | 0.11 | 30,30,30,30 | 0 |
| 54 | MG | 2A | 3586 | 1/1 | 0.95 | 0.09 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3397 | 1/1 | 0.95 | 0.08 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3589 | 1/1 | 0.95 | 0.08 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3416 | 1/1 | 0.95 | 0.07 | 35,35,35,35 | 0 |
| 54 | MG | 2a | 3014 | 1/1 | 0.95 | 0.19 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3591 | 1/1 | 0.95 | 0.07 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1818 | 1/1 | 0.95 | 0.11 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3593 | 1/1 | 0.95 | 0.06 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3108 | 1/1 | 0.95 | 0.19 | 40,40,40,40 | 0 |
| 54 | MG | 10 | 105 | 1/1 | 0.95 | 0.07 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3908 | 1/1 | 0.95 | 0.10 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3485 | 1/1 | 0.95 | 0.16 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1698 | 1/1 | 0.95 | 0.30 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3803 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3214 | 1/1 | 0.95 | 0.24 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3215 | 1/1 | 0.95 | 0.13 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3304 | 1/1 | 0.95 | 0.06 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3409 | 1/1 | 0.95 | 0.12 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1702 | 1/1 | 0.95 | 0.20 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3613 | 1/1 | 0.95 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3615 | 1/1 | 0.95 | 0.05 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3223 | 1/1 | 0.95 | 0.15 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3564 | 1/1 | 0.95 | 0.07 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3057 | 1/1 | 0.95 | 0.15 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3490 | 1/1 | 0.95 | 0.10 | 57,57,57,57 | 0 |
| 54 | MG | 1a | 1707 | 1/1 | 0.95 | 0.29 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3223 | 1/1 | 0.95 | 0.11 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 4040 | 1/1 | 0.95 | 0.08 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3017 | 1/1 | 0.95 | 0.19 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3495 | 1/1 | 0.95 | 0.05 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3228 | 1/1 | 0.95 | 0.21 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3812 | 1/1 | 0.95 | 0.06 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 15 | 104 | 1/1 | 0.95 | 0.10 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3496 | 1/1 | 0.95 | 0.09 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3232 | 1/1 | 0.95 | 0.10 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3202 | 1/1 | 0.95 | 0.15 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3636 | 1/1 | 0.95 | 0.14 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3086 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 54 | MG | 15 | 108 | 1/1 | 0.95 | 0.07 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1847 | 1/1 | 0.95 | 0.11 | 73,73,73,73 | 0 |
| 54 | MG | 2a | 3052 | 1/1 | 0.95 | 0.14 | 55,55,55,55 | 0 |
| 54 | MG | 17 | 101 | 1/1 | 0.95 | 0.08 | 38,38,38,38 | 0 |
| 54 | MG | 17 | 102 | 1/1 | 0.95 | 0.10 | 48,48,48,48 | 0 |
| 54 | MG | 17 | 104 | 1/1 | 0.95 | 0.17 | 43,43,43,43 | 0 |
| 54 | MG | 1B | 208 | 1/1 | 0.95 | 0.06 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3640 | 1/1 | 0.95 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3714 | 1/1 | 0.95 | 0.11 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3649 | 1/1 | 0.95 | 0.06 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3820 | 1/1 | 0.95 | 0.13 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3015 | 1/1 | 0.95 | 0.18 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3040 | 1/1 | 0.95 | 0.14 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3249 | 1/1 | 0.95 | 0.13 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3948 | 1/1 | 0.95 | 0.11 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3366 | 1/1 | 0.95 | 0.12 | 37,37,37,37 | 0 |
| 54 | MG | 1B | 217 | 1/1 | 0.95 | 0.09 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3825 | 1/1 | 0.95 | 0.09 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3069 | 1/1 | 0.95 | 0.19 | 74,74,74,74 | 0 |
| 54 | MG | 1a | 1866 | 1/1 | 0.95 | 0.15 | 67,67,67,67 | 0 |
| 54 | MG | 1B | 219 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3108 | 1/1 | 0.95 | 0.09 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3642 | 1/1 | 0.95 | 0.13 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3259 | 1/1 | 0.95 | 0.05 | 70,70,70,70 | 0 |
| 54 | MG | 2A | 3260 | 1/1 | 0.95 | 0.29 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3080 | 1/1 | 0.95 | 0.23 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3675 | 1/1 | 0.95 | 0.07 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3676 | 1/1 | 0.95 | 0.06 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3439 | 1/1 | 0.95 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3505 | 1/1 | 0.95 | 0.09 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3727 | 1/1 | 0.95 | 0.15 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3957 | 1/1 | 0.95 | 0.06 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3681 | 1/1 | 0.95 | 0.05 | 76,76,76,76 | 0 |
| 54 | MG | 1A | 3440 | 1/1 | 0.95 | 0.08 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3319 | 1/1 | 0.95 | 0.21 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3464 | 1/1 | 0.95 | 0.09 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3733 | 1/1 | 0.95 | 0.08 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3686 | 1/1 | 0.95 | 0.09 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3734 | 1/1 | 0.95 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3965 | 1/1 | 0.95 | 0.05 | 32,32,32,32 | 0 |
| 54 | MG | 2a | 3094 | 1/1 | 0.95 | 0.27 | 59,59,59,59 | 0 |
| 54 | MG | 1a | 1619 | 1/1 | 0.95 | 0.11 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3144 | 1/1 | 0.95 | 0.14 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3585 | 1/1 | 0.95 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3236 | 1/1 | 0.95 | 0.15 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3444 | 1/1 | 0.95 | 0.08 | 35,35,35,35 | 0 |
| 54 | MG | 1D | 312 | 1/1 | 0.95 | 0.17 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3655 | 1/1 | 0.95 | 0.07 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3148 | 1/1 | 0.95 | 0.14 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3323 | 1/1 | 0.95 | 0.16 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1633 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3209 | 1/1 | 0.95 | 0.29 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3241 | 1/1 | 0.95 | 0.30 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3975 | 1/1 | 0.95 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3660 | 1/1 | 0.95 | 0.16 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3484 | 1/1 | 0.95 | 0.08 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3136 | 1/1 | 0.95 | 0.12 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3137 | 1/1 | 0.95 | 0.22 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3713 | 1/1 | 0.95 | 0.25 | 71,71,71,71 | 0 |
| 54 | MG | 2A | 3288 | 1/1 | 0.95 | 0.14 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3243 | 1/1 | 0.95 | 0.29 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3752 | 1/1 | 0.95 | 0.07 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3452 | 1/1 | 0.95 | 0.06 | 32,32,32,32 | 0 |
| 54 | MG | 1F | 306 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3387 | 1/1 | 0.95 | 0.06 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3863 | 1/1 | 0.95 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3496 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3100 | 1/1 | 0.95 | 0.06 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3284 | 1/1 | 0.95 | 0.39 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3147 | 1/1 | 0.95 | 0.13 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3120 | 1/1 | 0.95 | 0.14 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3150 | 1/1 | 0.95 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3289 | 1/1 | 0.95 | 0.16 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3992 | 1/1 | 0.95 | 0.07 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3153 | 1/1 | 0.95 | 0.13 | 63,63,63,63 | 0 |
| 54 | MG | 1F | 318 | 1/1 | 0.95 | 0.06 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1653 | 1/1 | 0.95 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3135 | 1/1 | 0.95 | 0.17 | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3316 | 1/1 | 0.95 | 0.06 | 41,41,41,41 | 0 |
| 54 | MG | 1a | 1654 | 1/1 | 0.95 | 0.21 | 66,66,66,66 | 0 |
| 54 | MG | 1G | 201 | 1/1 | 0.95 | 0.16 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3515 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3052 | 1/1 | 0.95 | 0.23 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3396 | 1/1 | 0.95 | 0.06 | 58,58,58,58 | 0 |
| 54 | MG | 1G | 204 | 1/1 | 0.95 | 0.11 | 51,51,51,51 | 0 |
| 54 | MG | 2A | 3008 | 1/1 | 0.95 | 0.09 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3870 | 1/1 | 0.95 | 0.08 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3324 | 1/1 | 0.95 | 0.07 | 47,47,47,47 | 0 |
| 54 | MG | 2a | 3146 | 1/1 | 0.95 | 0.13 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3011 | 1/1 | 0.95 | 0.07 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1660 | 1/1 | 0.95 | 0.10 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3329 | 1/1 | 0.95 | 0.15 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3996 | 1/1 | 0.95 | 0.06 | 65,65,65,65 | 0 |
| 54 | MG | 1N | 201 | 1/1 | 0.95 | 0.13 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3333 | 1/1 | 0.95 | 0.19 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3102 | 1/1 | 0.95 | 0.12 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3292 | 1/1 | 0.95 | 0.13 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3538 | 1/1 | 0.95 | 0.06 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3103 | 1/1 | 0.95 | 0.26 | 50,50,50,50 | 0 |
| 54 | MG | 1P | 202 | 1/1 | 0.95 | 0.22 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3675 | 1/1 | 0.95 | 0.10 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3064 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3542 | 1/1 | 0.95 | 0.05 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3028 | 1/1 | 0.95 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 2A | 3029 | 1/1 | 0.95 | 0.08 | 52,52,52,52 | 0 |
| 54 | MG | 1Q | 201 | 1/1 | 0.95 | 0.12 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3258 | 1/1 | 0.95 | 0.17 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3681 | 1/1 | 0.95 | 0.10 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3357 | 1/1 | 0.95 | 0.12 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3360 | 1/1 | 0.95 | 0.23 | 72,72,72,72 | 0 |
| 54 | MG | 1a | 1674 | 1/1 | 0.95 | 0.18 | 75,75,75,75 | 0 |
| 54 | MG | 2F | 303 | 1/1 | 0.95 | 0.14 | 66,66,66,66 | 0 |
| 54 | MG | 2A | 3547 | 1/1 | 0.95 | 0.07 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3178 | 1/1 | 0.95 | 0.10 | 82,82,82,82 | 0 |
| 54 | MG | 1A | 3682 | 1/1 | 0.95 | 0.06 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3779 | 1/1 | 0.95 | 0.06 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3553 | 1/1 | 0.95 | 0.07 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3129 | 1/1 | 0.95 | 0.11 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3162 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 54 | MG | 2R | 202 | 1/1 | 0.95 | 0.09 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3367 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 54 | MG | 2T | 201 | 1/1 | 0.95 | 0.22 | 71,71,71,71 | 0 |
| 54 | MG | 2T | 202 | 1/1 | 0.95 | 0.19 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3030 | 1/1 | 0.95 | 0.06 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3548 | 1/1 | 0.95 | 0.07 | 53,53,53,53 | 0 |
| 54 | MG | 1a | 1801 | 1/1 | 0.95 | 0.05 | 76,76,76,76 | 0 |
| 54 | MG | 2A | 3371 | 1/1 | 0.95 | 0.06 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3891 | 1/1 | 0.95 | 0.05 | 30,30,30,30 | 0 |
| 54 | MG | 1U | 201 | 1/1 | 0.95 | 0.17 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3551 | 1/1 | 0.95 | 0.39 | 37,37,37,37 | 0 |
| 54 | MG | 1U | 207 | 1/1 | 0.95 | 0.17 | 40,40,40,40 | 0 |
| 54 | MG | 1a | 1806 | 1/1 | 0.95 | 0.11 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3383 | 1/1 | 0.95 | 0.26 | 60,60,60,60 | 0 |
| 54 | MG | 1a | 1808 | 1/1 | 0.95 | 0.07 | 61,61,61,61 | 0 |
| 55 | HGR | 2A | 3731 | 36/36 | 0.95 | 0.11 | 36,44,52,57 | 0 |
| 54 | MG | 1A | 4016 | 1/1 | 0.95 | 0.09 | 19,19,19,19 | 0 |
| 54 | MG | 27 | 102 | 1/1 | 0.95 | 0.23 | 47,47,47,47 | 0 |
| 57 | MPD | 18 | 103 | 8/8 | 0.95 | 0.12 | 36,41,45,49 | 0 |
| 54 | MG | 1A | 3088 | 1/1 | 0.95 | 0.41 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3199 | 1/1 | 0.95 | 0.10 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3412 | 1/1 | 0.95 | 0.06 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3791 | 1/1 | 0.95 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3413 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3479 | 1/1 | 0.95 | 0.09 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3393 | 1/1 | 0.95 | 0.13 | 71,71,71,71 | 0 |
| 54 | MG | 1D | 308 | 1/1 | 0.96 | 0.19 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3694 | 1/1 | 0.96 | 0.12 | 52,52,52,52 | 0 |
| 54 | MG | 1D | 310 | 1/1 | 0.96 | 0.10 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3572 | 1/1 | 0.96 | 0.08 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3298 | 1/1 | 0.96 | 0.10 | 31,31,31,31 | 0 |
| 54 | MG | 1a | 1637 | 1/1 | 0.96 | 0.06 | 45,45,45,45 | 0 |
| 54 | MG | 2a | 3001 | 1/1 | 0.96 | 0.07 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3361 | 1/1 | 0.96 | 0.16 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3171 | 1/1 | 0.96 | 0.04 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3382 | 1/1 | 0.96 | 0.07 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3094 | 1/1 | 0.96 | 0.28 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3532 | 1/1 | 0.96 | 0.07 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3700 | 1/1 | 0.96 | 0.08 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3173 | 1/1 | 0.96 | 0.30 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3303 | 1/1 | 0.96 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3142 | 1/1 | 0.96 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3095 | 1/1 | 0.96 | 0.18 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2a | 3012 | 1/1 | 0.96 | 0.07 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3588 | 1/1 | 0.96 | 0.07 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3817 | 1/1 | 0.96 | 0.11 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1648 | 1/1 | 0.96 | 0.12 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3818 | 1/1 | 0.96 | 0.06 | 81,81,81,81 | 0 |
| 54 | MG | 2A | 3394 | 1/1 | 0.96 | 0.06 | 72,72,72,72 | 0 |
| 54 | MG | 1F | 304 | 1/1 | 0.96 | 0.21 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3176 | 1/1 | 0.96 | 0.06 | 41,41,41,41 | 0 |
| 54 | MG | 1F | 307 | 1/1 | 0.96 | 0.27 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3597 | 1/1 | 0.96 | 0.10 | 72,72,72,72 | 0 |
| 54 | MG | 2A | 3598 | 1/1 | 0.96 | 0.09 | 71,71,71,71 | 0 |
| 54 | MG | 1F | 309 | 1/1 | 0.96 | 0.24 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3960 | 1/1 | 0.96 | 0.15 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3059 | 1/1 | 0.96 | 0.13 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3708 | 1/1 | 0.96 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3457 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3606 | 1/1 | 0.96 | 0.09 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3146 | 1/1 | 0.96 | 0.15 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3824 | 1/1 | 0.96 | 0.10 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3459 | 1/1 | 0.96 | 0.09 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3460 | 1/1 | 0.96 | 0.17 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3313 | 1/1 | 0.96 | 0.34 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3614 | 1/1 | 0.96 | 0.07 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3717 | 1/1 | 0.96 | 0.06 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3718 | 1/1 | 0.96 | 0.17 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3830 | 1/1 | 0.96 | 0.09 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3383 | 1/1 | 0.96 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3413 | 1/1 | 0.96 | 0.07 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3179 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3834 | 1/1 | 0.96 | 0.09 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3267 | 1/1 | 0.96 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3181 | 1/1 | 0.96 | 0.15 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3317 | 1/1 | 0.96 | 0.05 | 21,21,21,21 | 0 |
| 54 | MG | 2A | 3420 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3389 | 1/1 | 0.96 | 0.06 | 22,22,22,22 | 0 |
| 54 | MG | 1A | 3841 | 1/1 | 0.96 | 0.22 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3842 | 1/1 | 0.96 | 0.10 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3725 | 1/1 | 0.96 | 0.17 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3425 | 1/1 | 0.96 | 0.10 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3269 | 1/1 | 0.96 | 0.29 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3729 | 1/1 | 0.96 | 0.09 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3071 | 1/1 | 0.96 | 0.12 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3072 | 1/1 | 0.96 | 0.06 | 34,34,34,34 | 0 |
| 54 | MG | 1Q | 202 | 1/1 | 0.96 | 0.06 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3846 | 1/1 | 0.96 | 0.05 | 25,25,25,25 | 0 |
| 54 | MG | 1A | 3183 | 1/1 | 0.96 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 1Q | 205 | 1/1 | 0.96 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3028 | 1/1 | 0.96 | 0.24 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3641 | 1/1 | 0.96 | 0.05 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3645 | 1/1 | 0.96 | 0.06 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3393 | 1/1 | 0.96 | 0.05 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3081 | 1/1 | 0.96 | 0.31 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3651 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3150 | 1/1 | 0.96 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3274 | 1/1 | 0.96 | 0.13 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3655 | 1/1 | 0.96 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3440 | 1/1 | 0.96 | 0.08 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3072 | 1/1 | 0.96 | 0.06 | 63,63,63,63 | 0 |
| 54 | MG | 2A | 3084 | 1/1 | 0.96 | 0.13 | 51,51,51,51 | 0 |
| 54 | MG | 1T | 202 | 1/1 | 0.96 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3246 | 1/1 | 0.96 | 0.10 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3276 | 1/1 | 0.96 | 0.18 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3151 | 1/1 | 0.96 | 0.29 | 41,41,41,41 | 0 |
| 54 | MG | 2A | 3664 | 1/1 | 0.96 | 0.06 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3856 | 1/1 | 0.96 | 0.15 | 50,50,50,50 | 0 |
| 54 | MG | 1a | 1833 | 1/1 | 0.96 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 1U | 202 | 1/1 | 0.96 | 0.16 | 40,40,40,40 | 0 |
| 54 | MG | 1U | 204 | 1/1 | 0.96 | 0.27 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3669 | 1/1 | 0.96 | 0.13 | 78,78,78,78 | 0 |
| 54 | MG | 1U | 205 | 1/1 | 0.96 | 0.30 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3402 | 1/1 | 0.96 | 0.08 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 4003 | 1/1 | 0.96 | 0.06 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3051 | 1/1 | 0.96 | 0.31 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3570 | 1/1 | 0.96 | 0.06 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3085 | 1/1 | 0.96 | 0.37 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3099 | 1/1 | 0.96 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3101 | 1/1 | 0.96 | 0.14 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3093 | 1/1 | 0.96 | 0.30 | 63,63,63,63 | 0 |
| 54 | MG | 1V | 206 | 1/1 | 0.96 | 0.07 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3745 | 1/1 | 0.96 | 0.06 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3406 | 1/1 | 0.96 | 0.15 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3487 | 1/1 | 0.96 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3750 | 1/1 | 0.96 | 0.13 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3107 | 1/1 | 0.96 | 0.05 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3268 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3688 | 1/1 | 0.96 | 0.09 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3654 | 1/1 | 0.96 | 0.06 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3329 | 1/1 | 0.96 | 0.05 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3753 | 1/1 | 0.96 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 10 | 104 | 1/1 | 0.96 | 0.08 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3026 | 1/1 | 0.96 | 0.25 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3873 | 1/1 | 0.96 | 0.14 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3755 | 1/1 | 0.96 | 0.08 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3332 | 1/1 | 0.96 | 0.10 | 29,29,29,29 | 0 |
| 54 | MG | 2A | 3698 | 1/1 | 0.96 | 0.05 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3577 | 1/1 | 0.96 | 0.07 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3063 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3157 | 1/1 | 0.96 | 0.15 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3069 | 1/1 | 0.96 | 0.10 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3414 | 1/1 | 0.96 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3337 | 1/1 | 0.96 | 0.05 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3584 | 1/1 | 0.96 | 0.10 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3708 | 1/1 | 0.96 | 0.07 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3159 | 1/1 | 0.96 | 0.28 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3285 | 1/1 | 0.96 | 0.07 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3131 | 1/1 | 0.96 | 0.09 | 64,64,64,64 | 0 |
| 54 | MG | 1a | 1724 | 1/1 | 0.96 | 0.06 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3420 | 1/1 | 0.96 | 0.06 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3770 | 1/1 | 0.96 | 0.14 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3892 | 1/1 | 0.96 | 0.04 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1728 | 1/1 | 0.96 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3292 | 1/1 | 0.96 | 0.18 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3287 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 4038 | 1/1 | 0.96 | 0.14 | 57,57,57,57 | 0 |
| 54 | MG | 2a | 3133 | 1/1 | 0.96 | 0.10 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3070 | 1/1 | 0.96 | 0.23 | 45,45,45,45 | 0 |
| 54 | MG | 17 | 103 | 1/1 | 0.96 | 0.24 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3072 | 1/1 | 0.96 | 0.27 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3508 | 1/1 | 0.96 | 0.13 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3301 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3502 | 1/1 | 0.96 | 0.07 | 47,47,47,47 | 0 |
| 54 | MG | 2A | 3302 | 1/1 | 0.96 | 0.07 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3303 | 1/1 | 0.96 | 0.10 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3346 | 1/1 | 0.96 | 0.07 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3347 | 1/1 | 0.96 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 1B | 204 | 1/1 | 0.96 | 0.07 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3513 | 1/1 | 0.96 | 0.08 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3781 | 1/1 | 0.96 | 0.08 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3433 | 1/1 | 0.96 | 0.06 | 26,26,26,26 | 0 |
| 54 | MG | 2A | 3145 | 1/1 | 0.96 | 0.08 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3165 | 1/1 | 0.96 | 0.17 | 42,42,42,42 | 0 |
| 54 | MG | 2a | 3150 | 1/1 | 0.96 | 0.11 | 73,73,73,73 | 0 |
| 54 | MG | 2A | 3516 | 1/1 | 0.96 | 0.09 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3680 | 1/1 | 0.96 | 0.20 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3519 | 1/1 | 0.96 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 2a | 3155 | 1/1 | 0.96 | 0.09 | 81,81,81,81 | 0 |
| 54 | MG | 2A | 3149 | 1/1 | 0.96 | 0.12 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3073 | 1/1 | 0.96 | 0.06 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1606 | 1/1 | 0.96 | 0.10 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3911 | 1/1 | 0.96 | 0.09 | 63,63,63,63 | 0 |
| 54 | MG | 1a | 1608 | 1/1 | 0.96 | 0.07 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3913 | 1/1 | 0.96 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3325 | 1/1 | 0.96 | 0.06 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3788 | 1/1 | 0.96 | 0.06 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3327 | 1/1 | 0.96 | 0.16 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 3111 | 1/1 | 0.96 | 0.14 | 49,49,49,49 | 0 |
| 54 | MG | 1o | 101 | 1/1 | 0.96 | 0.14 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3603 | 1/1 | 0.96 | 0.11 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3159 | 1/1 | 0.96 | 0.33 | 55,55,55,55 | 0 |
| 54 | MG | 1y | 201 | 1/1 | 0.96 | 0.07 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3253 | 1/1 | 0.96 | 0.28 | 40,40,40,40 | 0 |
| 54 | MG | 2D | 306 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3336 | 1/1 | 0.96 | 0.06 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3795 | 1/1 | 0.96 | 0.06 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3523 | 1/1 | 0.96 | 0.08 | 46,46,46,46 | 0 |
| 54 | MG | 2D | 310 | 1/1 | 0.96 | 0.09 | 61,61,61,61 | 0 |
| 54 | MG | 2A | 3340 | 1/1 | 0.96 | 0.10 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3136 | 1/1 | 0.96 | 0.20 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3074 | 1/1 | 0.96 | 0.12 | 32,32,32,32 | 0 |
| 54 | MG | 2A | 3343 | 1/1 | 0.96 | 0.08 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3925 | 1/1 | 0.96 | 0.07 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3608 | 1/1 | 0.96 | 0.10 | 44,44,44,44 | 0 |
| 54 | MG | 1a | 1622 | 1/1 | 0.96 | 0.09 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3007 | 1/1 | 0.96 | 0.08 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3929 | 1/1 | 0.96 | 0.08 | 27,27,27,27 | 0 |
| 54 | MG | 2A | 3548 | 1/1 | 0.96 | 0.08 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3549 | 1/1 | 0.96 | 0.14 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3352 | 1/1 | 0.96 | 0.09 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3009 | 1/1 | 0.96 | 0.07 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3552 | 1/1 | 0.96 | 0.06 | 88,88,88,88 | 0 |
| 54 | MG | 2k | 201 | 1/1 | 0.96 | 0.12 | 69,69,69,69 | 0 |
| 54 | MG | 2R | 201 | 1/1 | 0.96 | 0.24 | 55,55,55,55 | 0 |
| 54 | MG | 1a | 1624 | 1/1 | 0.96 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3354 | 1/1 | 0.96 | 0.10 | 26,26,26,26 | 0 |
| 54 | MG | 1A | 3692 | 1/1 | 0.96 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3013 | 1/1 | 0.96 | 0.07 | 28,28,28,28 | 0 |
| 55 | HGR | 1A | 4041 | 36/36 | 0.96 | 0.08 | 21,29,35,39 | 0 |
| 54 | MG | 2A | 3014 | 1/1 | 0.96 | 0.09 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3558 | 1/1 | 0.96 | 0.07 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3256 | 1/1 | 0.96 | 0.19 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3938 | 1/1 | 0.96 | 0.08 | 46,46,46,46 | 0 |
| 54 | MG | 1a | 1630 | 1/1 | 0.96 | 0.11 | 50,50,50,50 | 0 |
| 54 | MG | 2Y | 201 | 1/1 | 0.96 | 0.14 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3939 | 1/1 | 0.96 | 0.07 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3942 | 1/1 | 0.96 | 0.05 | 60,60,60,60 | 0 |
| 54 | MG | 2A | 3021 | 1/1 | 0.96 | 0.06 | 52,52,52,52 | 0 |
| 54 | MG | 23 | 101 | 1/1 | 0.96 | 0.12 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3183 | 1/1 | 0.96 | 0.08 | 55,55,55,55 | 0 |
| 59 | ZN | 2n | 102 | 1/1 | 0.96 | 0.07 | 108,108,108,108 | 0 |
| 54 | MG | 1A | 3638 | 1/1 | 0.97 | 0.09 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3840 | 1/1 | 0.97 | 0.29 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3212 | 1/1 | 0.97 | 0.30 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3113 | 1/1 | 0.97 | 0.26 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3659 | 1/1 | 0.97 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 2a | 3035 | 1/1 | 0.97 | 0.06 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3114 | 1/1 | 0.97 | 0.28 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3313 | 1/1 | 0.97 | 0.06 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1649 | 1/1 | 0.97 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3663 | 1/1 | 0.97 | 0.06 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3020 | 1/1 | 0.97 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3023 | 1/1 | 0.97 | 0.16 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3559 | 1/1 | 0.97 | 0.06 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3216 | 1/1 | 0.97 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3077 | 1/1 | 0.97 | 0.25 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3979 | 1/1 | 0.97 | 0.08 | 81,81,81,81 | 0 |
| 54 | MG | 2A | 3670 | 1/1 | 0.97 | 0.06 | 72,72,72,72 | 0 |
| 54 | MG | 1A | 3147 | 1/1 | 0.97 | 0.05 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3027 | 1/1 | 0.97 | 0.06 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3117 | 1/1 | 0.97 | 0.18 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3096 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 2A | 3493 | 1/1 | 0.97 | 0.06 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3983 | 1/1 | 0.97 | 0.10 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3182 | 1/1 | 0.97 | 0.16 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3985 | 1/1 | 0.97 | 0.12 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3394 | 1/1 | 0.97 | 0.09 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3653 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | 1P | 201 | 1/1 | 0.97 | 0.34 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3988 | 1/1 | 0.97 | 0.04 | 28,28,28,28 | 0 |
| 54 | MG | 2A | 3334 | 1/1 | 0.97 | 0.08 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3098 | 1/1 | 0.97 | 0.03 | 22,22,22,22 | 0 |
| 54 | MG | 2A | 3504 | 1/1 | 0.97 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3122 | 1/1 | 0.97 | 0.33 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3337 | 1/1 | 0.97 | 0.06 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3858 | 1/1 | 0.97 | 0.06 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3859 | 1/1 | 0.97 | 0.06 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3185 | 1/1 | 0.97 | 0.17 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3187 | 1/1 | 0.97 | 0.27 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3481 | 1/1 | 0.97 | 0.06 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3400 | 1/1 | 0.97 | 0.06 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3124 | 1/1 | 0.97 | 0.09 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3331 | 1/1 | 0.97 | 0.07 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3403 | 1/1 | 0.97 | 0.06 | 55,55,55,55 | 0 |
| 54 | MG | 2A | 3700 | 1/1 | 0.97 | 0.06 | 64,64,64,64 | 0 |
| 54 | MG | 1A | 3189 | 1/1 | 0.97 | 0.28 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3050 | 1/1 | 0.97 | 0.15 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3578 | 1/1 | 0.97 | 0.11 | 55,55,55,55 | 0 |
| 54 | MG | 2a | 3078 | 1/1 | 0.97 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 2A | 3704 | 1/1 | 0.97 | 0.05 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3229 | 1/1 | 0.97 | 0.16 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3354 | 1/1 | 0.97 | 0.06 | 40,40,40,40 | 0 |
| 54 | MG | 2A | 3196 | 1/1 | 0.97 | 0.07 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3763 | 1/1 | 0.97 | 0.05 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3079 | 1/1 | 0.97 | 0.17 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3359 | 1/1 | 0.97 | 0.09 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3765 | 1/1 | 0.97 | 0.08 | 50,50,50,50 | 0 |
| 54 | MG | 2A | 3361 | 1/1 | 0.97 | 0.08 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3053 | 1/1 | 0.97 | 0.11 | 37,37,37,37 | 0 |
| 54 | MG | 1U | 203 | 1/1 | 0.97 | 0.31 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3491 | 1/1 | 0.97 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3408 | 1/1 | 0.97 | 0.08 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3024 | 1/1 | 0.97 | 0.06 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3338 | 1/1 | 0.97 | 0.12 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3880 | 1/1 | 0.97 | 0.05 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3881 | 1/1 | 0.97 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3771 | 1/1 | 0.97 | 0.05 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3773 | 1/1 | 0.97 | 0.10 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3884 | 1/1 | 0.97 | 0.06 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3235 | 1/1 | 0.97 | 0.23 | 42,42,42,42 | 0 |
| 54 | MG | 1W | 203 | 1/1 | 0.97 | 0.06 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3101 | 1/1 | 0.97 | 0.31 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3156 | 1/1 | 0.97 | 0.21 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3070 | 1/1 | 0.97 | 0.24 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3545 | 1/1 | 0.97 | 0.09 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3237 | 1/1 | 0.97 | 0.32 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3342 | 1/1 | 0.97 | 0.05 | 29,29,29,29 | 0 |
| 54 | MG | 2A | 3073 | 1/1 | 0.97 | 0.11 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3288 | 1/1 | 0.97 | 0.09 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 4027 | 1/1 | 0.97 | 0.06 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3076 | 1/1 | 0.97 | 0.09 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3678 | 1/1 | 0.97 | 0.07 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1701 | 1/1 | 0.97 | 0.10 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3083 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3417 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3392 | 1/1 | 0.97 | 0.12 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3782 | 1/1 | 0.97 | 0.14 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3055 | 1/1 | 0.97 | 0.23 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3227 | 1/1 | 0.97 | 0.12 | 56,56,56,56 | 0 |
| 54 | MG | 2a | 3119 | 1/1 | 0.97 | 0.05 | 74,74,74,74 | 0 |
| 54 | MG | 1A | 3594 | 1/1 | 0.97 | 0.06 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3898 | 1/1 | 0.97 | 0.06 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3104 | 1/1 | 0.97 | 0.20 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3242 | 1/1 | 0.97 | 0.27 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3422 | 1/1 | 0.97 | 0.07 | 23,23,23,23 | 0 |
| 54 | MG | 2A | 3088 | 1/1 | 0.97 | 0.07 | 47,47,47,47 | 0 |
| 54 | MG | 13 | 101 | 1/1 | 0.97 | 0.11 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3569 | 1/1 | 0.97 | 0.11 | 73,73,73,73 | 0 |
| 54 | MG | 1A | 3056 | 1/1 | 0.97 | 0.10 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3244 | 1/1 | 0.97 | 0.21 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3237 | 1/1 | 0.97 | 0.29 | 44,44,44,44 | 0 |
| 54 | MG | 15 | 101 | 1/1 | 0.97 | 0.11 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1859 | 1/1 | 0.97 | 0.13 | 60,60,60,60 | 0 |
| 54 | MG | 1A | 3514 | 1/1 | 0.97 | 0.05 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3576 | 1/1 | 0.97 | 0.08 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3426 | 1/1 | 0.97 | 0.05 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3516 | 1/1 | 0.97 | 0.06 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3427 | 1/1 | 0.97 | 0.08 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3412 | 1/1 | 0.97 | 0.07 | 45,45,45,45 | 0 |
| 54 | MG | 2E | 301 | 1/1 | 0.97 | 0.22 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3246 | 1/1 | 0.97 | 0.28 | 38,38,38,38 | 0 |
| 54 | MG | 2E | 305 | 1/1 | 0.97 | 0.07 | 43,43,43,43 | 0 |
| 54 | MG | 1a | 1865 | 1/1 | 0.97 | 0.05 | 71,71,71,71 | 0 |
| 54 | MG | 1A | 3161 | 1/1 | 0.97 | 0.15 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3018 | 1/1 | 0.97 | 0.19 | 31,31,31,31 | 0 |
| 54 | MG | 1A | 3800 | 1/1 | 0.97 | 0.06 | 42,42,42,42 | 0 |
| 54 | MG | 2F | 304 | 1/1 | 0.97 | 0.22 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3006 | 1/1 | 0.97 | 0.05 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3251 | 1/1 | 0.97 | 0.29 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3016 | 1/1 | 0.97 | 0.30 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3356 | 1/1 | 0.97 | 0.11 | 28,28,28,28 | 0 |
| 54 | MG | 2a | 3152 | 1/1 | 0.97 | 0.06 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3357 | 1/1 | 0.97 | 0.06 | 30,30,30,30 | 0 |
| 54 | MG | 1B | 213 | 1/1 | 0.97 | 0.07 | 52,52,52,52 | 0 |
| 54 | MG | 2Q | 201 | 1/1 | 0.97 | 0.04 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3203 | 1/1 | 0.97 | 0.16 | 51,51,51,51 | 0 |
| 54 | MG | 2a | 3157 | 1/1 | 0.97 | 0.09 | 75,75,75,75 | 0 |
| 54 | MG | 1A | 3359 | 1/1 | 0.97 | 0.06 | 15,15,15,15 | 0 |
| 54 | MG | 1A | 3166 | 1/1 | 0.97 | 0.18 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3071 | 1/1 | 0.97 | 0.34 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3928 | 1/1 | 0.97 | 0.04 | 35,35,35,35 | 0 |
| 54 | MG | 2a | 3163 | 1/1 | 0.97 | 0.16 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3600 | 1/1 | 0.97 | 0.04 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3363 | 1/1 | 0.97 | 0.10 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3618 | 1/1 | 0.97 | 0.06 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3707 | 1/1 | 0.97 | 0.07 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3934 | 1/1 | 0.97 | 0.18 | 48,48,48,48 | 0 |
| 54 | MG | 2W | 202 | 1/1 | 0.97 | 0.07 | 68,68,68,68 | 0 |
| 54 | MG | 2X | 101 | 1/1 | 0.97 | 0.09 | 67,67,67,67 | 0 |
| 54 | MG | 1A | 3048 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3815 | 1/1 | 0.97 | 0.07 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3446 | 1/1 | 0.97 | 0.11 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3940 | 1/1 | 0.97 | 0.08 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3941 | 1/1 | 0.97 | 0.07 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3307 | 1/1 | 0.97 | 0.11 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3367 | 1/1 | 0.97 | 0.09 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3368 | 1/1 | 0.97 | 0.08 | 48,48,48,48 | 0 |
| 54 | MG | 1g | 203 | 1/1 | 0.97 | 0.07 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3946 | 1/1 | 0.97 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3715 | 1/1 | 0.97 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3308 | 1/1 | 0.97 | 0.27 | 48,48,48,48 | 0 |
| 54 | MG | 1a | 1618 | 1/1 | 0.97 | 0.05 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3451 | 1/1 | 0.97 | 0.10 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3626 | 1/1 | 0.97 | 0.06 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3370 | 1/1 | 0.97 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3309 | 1/1 | 0.97 | 0.14 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3137 | 1/1 | 0.97 | 0.19 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3021 | 1/1 | 0.97 | 0.23 | 45,45,45,45 | 0 |
| 54 | MG | 1a | 1626 | 1/1 | 0.97 | 0.05 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3139 | 1/1 | 0.97 | 0.19 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3547 | 1/1 | 0.97 | 0.06 | 24,24,24,24 | 0 |
| 54 | MG | 1D | 318 | 1/1 | 0.97 | 0.11 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3140 | 1/1 | 0.97 | 0.25 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3726 | 1/1 | 0.97 | 0.09 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3832 | 1/1 | 0.97 | 0.12 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3005 | 1/1 | 0.97 | 0.09 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3963 | 1/1 | 0.97 | 0.06 | 70,70,70,70 | 0 |
| 54 | MG | 1F | 301 | 1/1 | 0.97 | 0.11 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3380 | 1/1 | 0.97 | 0.08 | 30,30,30,30 | 0 |
| 56 | ERY | 1A | 4042 | 51/51 | 0.97 | 0.08 | 20,37,45,53 | 0 |
| 56 | ERY | 2A | 3732 | 51/51 | 0.97 | 0.09 | 38,48,57,63 | 0 |
| 54 | MG | 1F | 305 | 1/1 | 0.97 | 0.12 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3835 | 1/1 | 0.97 | 0.09 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3381 | 1/1 | 0.97 | 0.12 | 41,41,41,41 | 0 |
| 54 | MG | 2a | 3022 | 1/1 | 0.97 | 0.04 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3469 | 1/1 | 0.97 | 0.09 | 42,42,42,42 | 0 |
| 54 | MG | 1F | 308 | 1/1 | 0.97 | 0.13 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3471 | 1/1 | 0.97 | 0.05 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3731 | 1/1 | 0.97 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | 1F | 310 | 1/1 | 0.97 | 0.10 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3554 | 1/1 | 0.97 | 0.07 | 34,34,34,34 | 0 |
| 59 | ZN | 29 | 501 | 1/1 | 0.97 | 0.04 | 77,77,77,77 | 0 |
| 54 | MG | 2A | 3654 | 1/1 | 0.97 | 0.06 | 52,52,52,52 | 0 |
| 60 | SF4 | 1d | 306 | 8/8 | 0.97 | 0.07 | 68,77,83,90 | 0 |
| 60 | SF4 | 2d | 501 | 8/8 | 0.97 | 0.06 | 74,89,98,98 | 0 |
| 54 | MG | 1V | 202 | 1/1 | 0.98 | 0.20 | 38,38,38,38 | 0 |
| 54 | MG | 2E | 302 | 1/1 | 0.98 | 0.08 | 53,53,53,53 | 0 |
| 54 | MG | 1A | 3118 | 1/1 | 0.98 | 0.09 | 46,46,46,46 | 0 |
| 54 | MG | 1D | 302 | 1/1 | 0.98 | 0.07 | 57,57,57,57 | 0 |
| 54 | MG | 2A | 3637 | 1/1 | 0.98 | 0.04 | 83,83,83,83 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3378 | 1/1 | 0.98 | 0.04 | 28,28,28,28 | 0 |
| 54 | MG | 1D | 304 | 1/1 | 0.98 | 0.04 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3746 | 1/1 | 0.98 | 0.04 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3747 | 1/1 | 0.98 | 0.05 | 80,80,80,80 | 0 |
| 54 | MG | 2A | 3643 | 1/1 | 0.98 | 0.07 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3641 | 1/1 | 0.98 | 0.14 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3932 | 1/1 | 0.98 | 0.05 | 21,21,21,21 | 0 |
| 54 | MG | 2A | 3647 | 1/1 | 0.98 | 0.06 | 89,89,89,89 | 0 |
| 54 | MG | 2A | 3648 | 1/1 | 0.98 | 0.06 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3293 | 1/1 | 0.98 | 0.06 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3650 | 1/1 | 0.98 | 0.13 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3100 | 1/1 | 0.98 | 0.09 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3933 | 1/1 | 0.98 | 0.07 | 53,53,53,53 | 0 |
| 54 | MG | 2A | 3296 | 1/1 | 0.98 | 0.08 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3525 | 1/1 | 0.98 | 0.06 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3264 | 1/1 | 0.98 | 0.23 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3935 | 1/1 | 0.98 | 0.04 | 52,52,52,52 | 0 |
| 54 | MG | 1a | 1734 | 1/1 | 0.98 | 0.06 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3936 | 1/1 | 0.98 | 0.06 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 3240 | 1/1 | 0.98 | 0.17 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3415 | 1/1 | 0.98 | 0.04 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 3318 | 1/1 | 0.98 | 0.16 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3503 | 1/1 | 0.98 | 0.05 | 29,29,29,29 | 0 |
| 54 | MG | 1A | 3382 | 1/1 | 0.98 | 0.05 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3306 | 1/1 | 0.98 | 0.05 | 43,43,43,43 | 0 |
| 54 | MG | 1A | 4010 | 1/1 | 0.98 | 0.06 | 57,57,57,57 | 0 |
| 54 | MG | 1A | 3186 | 1/1 | 0.98 | 0.10 | 38,38,38,38 | 0 |
| 54 | MG | 1E | 302 | 1/1 | 0.98 | 0.13 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3078 | 1/1 | 0.98 | 0.26 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3145 | 1/1 | 0.98 | 0.12 | 27,27,27,27 | 0 |
| 54 | MG | 2a | 3123 | 1/1 | 0.98 | 0.06 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3602 | 1/1 | 0.98 | 0.06 | 24,24,24,24 | 0 |
| 54 | MG | 1A | 3421 | 1/1 | 0.98 | 0.07 | 46,46,46,46 | 0 |
| 54 | MG | 2A | 3315 | 1/1 | 0.98 | 0.05 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3876 | 1/1 | 0.98 | 0.04 | 39,39,39,39 | 0 |
| 54 | MG | 2A | 3429 | 1/1 | 0.98 | 0.04 | 55,55,55,55 | 0 |
| 54 | MG | 13 | 103 | 1/1 | 0.98 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 1F | 302 | 1/1 | 0.98 | 0.11 | 39,39,39,39 | 0 |
| 54 | MG | 1F | 303 | 1/1 | 0.98 | 0.14 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3509 | 1/1 | 0.98 | 0.05 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3463 | 1/1 | 0.98 | 0.05 | 18,18,18,18 | 0 |
| 54 | MG | 1A | 3042 | 1/1 | 0.98 | 0.04 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1a | 1845 | 1/1 | 0.98 | 0.06 | 70,70,70,70 | 0 |
| 54 | MG | 1A | 4020 | 1/1 | 0.98 | 0.04 | 42,42,42,42 | 0 |
| 54 | MG | 1a | 1848 | 1/1 | 0.98 | 0.06 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3127 | 1/1 | 0.98 | 0.22 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 4021 | 1/1 | 0.98 | 0.04 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3687 | 1/1 | 0.98 | 0.05 | 52,52,52,52 | 0 |
| 54 | MG | 1A | 3512 | 1/1 | 0.98 | 0.12 | 28,28,28,28 | 0 |
| 54 | MG | 1a | 1851 | 1/1 | 0.98 | 0.09 | 65,65,65,65 | 0 |
| 54 | MG | 2A | 3330 | 1/1 | 0.98 | 0.11 | 63,63,63,63 | 0 |
| 54 | MG | 1A | 4023 | 1/1 | 0.98 | 0.10 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3423 | 1/1 | 0.98 | 0.11 | 29,29,29,29 | 0 |
| 54 | MG | 2A | 3693 | 1/1 | 0.98 | 0.08 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3562 | 1/1 | 0.98 | 0.05 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3245 | 1/1 | 0.98 | 0.12 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3564 | 1/1 | 0.98 | 0.06 | 64,64,64,64 | 0 |
| 54 | MG | 2A | 3447 | 1/1 | 0.98 | 0.06 | 47,47,47,47 | 0 |
| 54 | MG | 1a | 1855 | 1/1 | 0.98 | 0.08 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3224 | 1/1 | 0.98 | 0.14 | 29,29,29,29 | 0 |
| 54 | MG | 1a | 1857 | 1/1 | 0.98 | 0.05 | 58,58,58,58 | 0 |
| 54 | MG | 2A | 3042 | 1/1 | 0.98 | 0.09 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3710 | 1/1 | 0.98 | 0.05 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3956 | 1/1 | 0.98 | 0.04 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3468 | 1/1 | 0.98 | 0.04 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3517 | 1/1 | 0.98 | 0.07 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3050 | 1/1 | 0.98 | 0.18 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1767 | 1/1 | 0.98 | 0.05 | 80,80,80,80 | 0 |
| 54 | MG | 1A | 3123 | 1/1 | 0.98 | 0.04 | 22,22,22,22 | 0 |
| 54 | MG | 2A | 3345 | 1/1 | 0.98 | 0.07 | 58,58,58,58 | 0 |
| 54 | MG | 1A | 3961 | 1/1 | 0.98 | 0.05 | 48,48,48,48 | 0 |
| 54 | MG | 2A | 3347 | 1/1 | 0.98 | 0.06 | 35,35,35,35 | 0 |
| 54 | MG | 2A | 3348 | 1/1 | 0.98 | 0.09 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3568 | 1/1 | 0.98 | 0.06 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3299 | 1/1 | 0.98 | 0.09 | 22,22,22,22 | 0 |
| 54 | MG | 2A | 3244 | 1/1 | 0.98 | 0.13 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3090 | 1/1 | 0.98 | 0.10 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3431 | 1/1 | 0.98 | 0.06 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3275 | 1/1 | 0.98 | 0.22 | 41,41,41,41 | 0 |
| 54 | MG | 1A | 3163 | 1/1 | 0.98 | 0.10 | 39,39,39,39 | 0 |
| 54 | MG | 2a | 3174 | 1/1 | 0.98 | 0.10 | 68,68,68,68 | 0 |
| 54 | MG | 1A | 3252 | 1/1 | 0.98 | 0.16 | 32,32,32,32 | 0 |
| 54 | MG | 1A | 3043 | 1/1 | 0.98 | 0.10 | 22,22,22,22 | 0 |
| 54 | MG | 2A | 3358 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 54 | MG | 1A | 3672 | 1/1 | 0.98 | 0.11 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3398 | 1/1 | 0.98 | 0.04 | 30,30,30,30 | 0 |
| 54 | MG | 1A | 3902 | 1/1 | 0.98 | 0.05 | 67,67,67,67 | 0 |
| 54 | MG | 2A | 3254 | 1/1 | 0.98 | 0.11 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3230 | 1/1 | 0.98 | 0.05 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3306 | 1/1 | 0.98 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3365 | 1/1 | 0.98 | 0.05 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3195 | 1/1 | 0.98 | 0.14 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3336 | 1/1 | 0.98 | 0.10 | 38,38,38,38 | 0 |
| 54 | MG | 2a | 3057 | 1/1 | 0.98 | 0.13 | 66,66,66,66 | 0 |
| 54 | MG | 1A | 3978 | 1/1 | 0.98 | 0.08 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 3082 | 1/1 | 0.98 | 0.07 | 48,48,48,48 | 0 |
| 54 | MG | 1A | 3534 | 1/1 | 0.98 | 0.04 | 31,31,31,31 | 0 |
| 54 | MG | 1d | 305 | 1/1 | 0.98 | 0.04 | 74,74,74,74 | 0 |
| 54 | MG | 2A | 3608 | 1/1 | 0.98 | 0.06 | 54,54,54,54 | 0 |
| 54 | MG | 2A | 3372 | 1/1 | 0.98 | 0.09 | 35,35,35,35 | 0 |
| 54 | MG | 1R | 201 | 1/1 | 0.98 | 0.10 | 44,44,44,44 | 0 |
| 54 | MG | 2A | 3611 | 1/1 | 0.98 | 0.04 | 73,73,73,73 | 0 |
| 54 | MG | 1a | 1621 | 1/1 | 0.98 | 0.04 | 55,55,55,55 | 0 |
| 54 | MG | 1B | 214 | 1/1 | 0.98 | 0.05 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3180 | 1/1 | 0.98 | 0.20 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3735 | 1/1 | 0.98 | 0.04 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3379 | 1/1 | 0.98 | 0.05 | 59,59,59,59 | 0 |
| 54 | MG | 1A | 3912 | 1/1 | 0.98 | 0.03 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3234 | 1/1 | 0.98 | 0.20 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3793 | 1/1 | 0.98 | 0.04 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3371 | 1/1 | 0.98 | 0.08 | 31,31,31,31 | 0 |
| 54 | MG | 2A | 3498 | 1/1 | 0.98 | 0.04 | 65,65,65,65 | 0 |
| 54 | MG | 1A | 3044 | 1/1 | 0.98 | 0.15 | 40,40,40,40 | 0 |
| 54 | MG | 1T | 205 | 1/1 | 0.98 | 0.10 | 54,54,54,54 | 0 |
| 54 | MG | 1A | 3540 | 1/1 | 0.98 | 0.05 | 27,27,27,27 | 0 |
| 54 | MG | 1A | 3007 | 1/1 | 0.98 | 0.08 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3037 | 1/1 | 0.98 | 0.09 | 47,47,47,47 | 0 |
| 54 | MG | 1A | 3857 | 1/1 | 0.98 | 0.05 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3029 | 1/1 | 0.98 | 0.10 | 48,48,48,48 | 0 |
| 59 | ZN | 15 | 109 | 1/1 | 0.98 | 0.03 | 46,46,46,46 | 0 |
| 59 | ZN | 2Y | 202 | 1/1 | 0.98 | 0.05 | 94,94,94,94 | 0 |
| 54 | MG | 1A | 3743 | 1/1 | 0.98 | 0.04 | 35,35,35,35 | 0 |
| 59 | ZN | 26 | 501 | 1/1 | 0.98 | 0.05 | 75,75,75,75 | 0 |
| 54 | MG | 1a | 1807 | 1/1 | 0.98 | 0.04 | 83,83,83,83 | 0 |
| 54 | MG | 2A | 3509 | 1/1 | 0.98 | 0.07 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3926 | 1/1 | 0.98 | 0.04 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1V | 201 | 1/1 | 0.98 | 0.20 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3989 | 1/1 | 0.99 | 0.07 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3013 | 1/1 | 0.99 | 0.03 | 23,23,23,23 | 0 |
| 54 | MG | 2A | 3579 | 1/1 | 0.99 | 0.04 | 59,59,59,59 | 0 |
| 54 | MG | 2a | 3159 | 1/1 | 0.99 | 0.06 | 51,51,51,51 | 0 |
| 54 | MG | 1a | 1844 | 1/1 | 0.99 | 0.04 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3097 | 1/1 | 0.99 | 0.19 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3644 | 1/1 | 0.99 | 0.06 | 49,49,49,49 | 0 |
| 54 | MG | 2A | 3582 | 1/1 | 0.99 | 0.05 | 56,56,56,56 | 0 |
| 54 | MG | 1a | 1846 | 1/1 | 0.99 | 0.03 | 61,61,61,61 | 0 |
| 54 | MG | 1D | 306 | 1/1 | 0.99 | 0.04 | 20,20,20,20 | 0 |
| 54 | MG | 1A | 3549 | 1/1 | 0.99 | 0.03 | 49,49,49,49 | 0 |
| 54 | MG | 1A | 3914 | 1/1 | 0.99 | 0.08 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3550 | 1/1 | 0.99 | 0.06 | 37,37,37,37 | 0 |
| 54 | MG | 2A | 3304 | 1/1 | 0.99 | 0.05 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3916 | 1/1 | 0.99 | 0.03 | 51,51,51,51 | 0 |
| 54 | MG | 1A | 3917 | 1/1 | 0.99 | 0.07 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3046 | 1/1 | 0.99 | 0.05 | 14,14,14,14 | 0 |
| 54 | MG | 1A | 3789 | 1/1 | 0.99 | 0.03 | 36,36,36,36 | 0 |
| 54 | MG | 1A | 3009 | 1/1 | 0.99 | 0.10 | 33,33,33,33 | 0 |
| 54 | MG | 2A | 3594 | 1/1 | 0.99 | 0.05 | 43,43,43,43 | 0 |
| 54 | MG | 2A | 3310 | 1/1 | 0.99 | 0.10 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3851 | 1/1 | 0.99 | 0.05 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3711 | 1/1 | 0.99 | 0.03 | 37,37,37,37 | 0 |
| 54 | MG | 1A | 3475 | 1/1 | 0.99 | 0.04 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3688 | 1/1 | 0.99 | 0.03 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3794 | 1/1 | 0.99 | 0.06 | 47,47,47,47 | 0 |
| 54 | MG | 2a | 3182 | 1/1 | 0.99 | 0.03 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3601 | 1/1 | 0.99 | 0.04 | 42,42,42,42 | 0 |
| 54 | MG | 1A | 3493 | 1/1 | 0.99 | 0.02 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3494 | 1/1 | 0.99 | 0.04 | 35,35,35,35 | 0 |
| 54 | MG | 1E | 304 | 1/1 | 0.99 | 0.14 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3476 | 1/1 | 0.99 | 0.04 | 35,35,35,35 | 0 |
| 54 | MG | 1E | 306 | 1/1 | 0.99 | 0.07 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3535 | 1/1 | 0.99 | 0.07 | 28,28,28,28 | 0 |
| 54 | MG | 1A | 3646 | 1/1 | 0.99 | 0.10 | 38,38,38,38 | 0 |
| 54 | MG | 2A | 3377 | 1/1 | 0.99 | 0.06 | 46,46,46,46 | 0 |
| 54 | MG | 1A | 3374 | 1/1 | 0.99 | 0.08 | 34,34,34,34 | 0 |
| 54 | MG | 2A | 3674 | 1/1 | 0.99 | 0.07 | 62,62,62,62 | 0 |
| 54 | MG | 1A | 3894 | 1/1 | 0.99 | 0.04 | 36,36,36,36 | 0 |
| 54 | MG | 2A | 3381 | 1/1 | 0.99 | 0.06 | 45,45,45,45 | 0 |
| 54 | MG | 1A | 3862 | 1/1 | 0.99 | 0.03 | 27,27,27,27 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | MG | 1A | 3896 | 1/1 | 0.99 | 0.06 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3772 | 1/1 | 0.99 | 0.10 | 39,39,39,39 | 0 |
| 54 | MG | 1a | 1822 | 1/1 | 0.99 | 0.04 | 61,61,61,61 | 0 |
| 54 | MG | 1A | 3075 | 1/1 | 0.99 | 0.04 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3436 | 1/1 | 0.99 | 0.04 | 34,34,34,34 | 0 |
| 54 | MG | 1A | 3900 | 1/1 | 0.99 | 0.06 | 50,50,50,50 | 0 |
| 54 | MG | 1A | 3247 | 1/1 | 0.99 | 0.20 | 33,33,33,33 | 0 |
| 54 | MG | 1A | 3438 | 1/1 | 0.99 | 0.05 | 35,35,35,35 | 0 |
| 54 | MG | 1A | 3806 | 1/1 | 0.99 | 0.05 | 44,44,44,44 | 0 |
| 54 | MG | 1A | 3482 | 1/1 | 0.99 | 0.03 | 62,62,62,62 | 0 |
| 54 | MG | 1a | 1736 | 1/1 | 0.99 | 0.06 | 45,45,45,45 | 0 |
| 54 | MG | 2A | 3507 | 1/1 | 0.99 | 0.06 | 40,40,40,40 | 0 |
| 54 | MG | 1B | 223 | 1/1 | 0.99 | 0.03 | 55,55,55,55 | 0 |
| 54 | MG | 1A | 3386 | 1/1 | 0.99 | 0.02 | 19,19,19,19 | 0 |
| 54 | MG | 1A | 3944 | 1/1 | 0.99 | 0.05 | 56,56,56,56 | 0 |
| 54 | MG | 1A | 4024 | 1/1 | 0.99 | 0.03 | 69,69,69,69 | 0 |
| 54 | MG | 1A | 3360 | 1/1 | 0.99 | 0.05 | 43,43,43,43 | 0 |
| 59 | ZN | 1Y | 202 | 1/1 | 0.99 | 0.06 | 61,61,61,61 | 0 |
| 59 | ZN | 14 | 102 | 1/1 | 0.99 | 0.04 | 94,94,94,94 | 0 |
| 54 | MG | 1a | 1836 | 1/1 | 0.99 | 0.09 | 67,67,67,67 | 0 |
| 59 | ZN | 16 | 501 | 1/1 | 0.99 | 0.05 | 49,49,49,49 | 0 |
| 59 | ZN | 19 | 103 | 1/1 | 0.99 | 0.04 | 45,45,45,45 | 0 |
| 59 | ZN | 1n | 103 | 1/1 | 0.99 | 0.03 | 79,79,79,79 | 0 |
| 54 | MG | 1A | 3454 | 1/1 | 0.99 | 0.04 | 39,39,39,39 | 0 |
| 54 | MG | 1A | 3728 | 1/1 | 0.99 | 0.03 | 48,48,48,48 | 0 |
| 59 | ZN | 25 | 104 | 1/1 | 0.99 | 0.06 | 68,68,68,68 | 0 |
| 54 | MG | 2A | 3135 | 1/1 | 0.99 | 0.06 | 38,38,38,38 | 0 |
| 54 | MG | 1A | 3428 | 1/1 | 0.99 | 0.04 | 28,28,28,28 | 0 |
| 54 | MG | 1a | 1791 | 1/1 | 0.99 | 0.04 | 77,77,77,77 | 0 |
| 54 | MG | 1A | 3121 | 1/1 | 0.99 | 0.19 | 38,38,38,38 | 0 |
| 54 | MG | 2E | 304 | 1/1 | 0.99 | 0.05 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3642 | 1/1 | 1.00 | 0.03 | 62,62,62,62 | 0 |
| 54 | MG | 2A | 3492 | 1/1 | 1.00 | 0.06 | 42,42,42,42 | 0 |
| 54 | MG | 2A | 3380 | 1/1 | 1.00 | 0.04 | 40,40,40,40 | 0 |
| 54 | MG | 1A | 3500 | 1/1 | 1.00 | 0.09 | 51,51,51,51 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.