# wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2026 – 10:36 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 6O97 / pdb_00006o97 |
| Title | : | Crystal structure of the Thermus thermophilus 70S ribosome in complex with propylamycin and bound to mRNA and A-, P-, and E-site tRNAs at 2.75A resolution |
| Authors | : | Matsushita, T.; Sati, G.C.; Kondasinghe, N.; Pirrone, M.G.; Kato, T.; Waduge, P.; Kumar, H.S.; Sanchon, A.C.; Dobosz-Bartoszek, M.; Shcherbakov, D.; Juhas, M.; Hobbie, S.N.; Schrepfer, T.; Chow, C.S.; Polikanov, Y.S.; Schacht, J.; Vasella, A.; Bottger, E.C.; Crich, D. |
| Deposited on | : | 2019-03-13 |
| Resolution | : | 2.75 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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The following versions of software and data (see references (1)) were used in the production of this report:

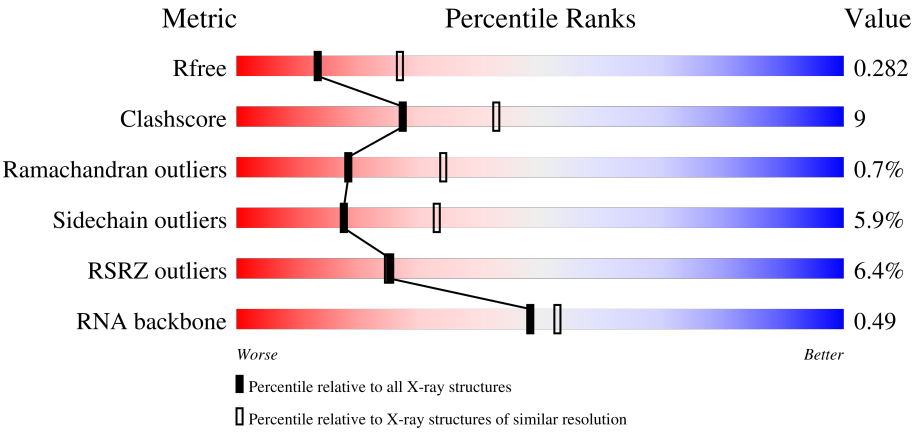
| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 2.0 |
| EDS | : | 3.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4 | : | 9.0.010 (Gargrove) |
| Density-Fitness | : | 1.0.12 |

# 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 2.75 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 | 1009 (2.76-2.76) |
| Clashscore | 190562 | 1044 (2.76-2.76) |
| Ramachandran outliers | 187476 | 1024 (2.76-2.76) |
| Sidechain outliers | 187428 | 1024 (2.76-2.76) |
| RSRZ outliers | 180081 | 1009 (2.76-2.76) |
| RNA backbone | 3983 | 1179 (3.00-2.52) |

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 <=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 | 3% 60% 32% 7% |

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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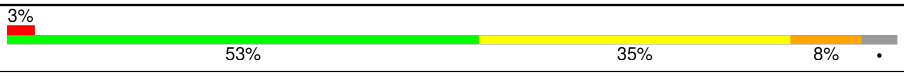
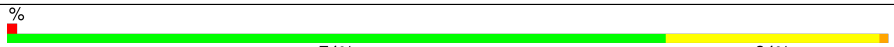
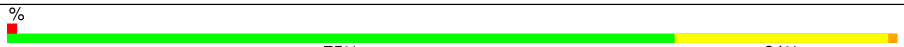
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 2A | 2915 |   |
| 2 | 1B | 121 | |
| 2 | 2B | 121 | |
| 3 | 1D | 276 |   |
| 3 | 2D | 276 |   |
| 4 | 1E | 206 | |
| 4 | 2E | 206 | |
| 5 | 1F | 210 | |
| 5 | 2F | 210 | |
| 6 | 1G | 182 | |
| 6 | 2G | 182 | |
| 7 | 1H | 180 | |
| 7 | 2H | 180 | |
| 8 | 1I | 148 | |
| 8 | 2I | 148 | |
| 9 | 1N | 140 | |
| 9 | 2N | 140 | |
| 10 | 1O | 122 | |
| 10 | 2O | 122 | |
| 11 | 1P | 150 | |
| 11 | 2P | 150 | |
| 12 | 1Q | 141 | |
| 12 | 2Q | 141 | |
| 13 | 1R | 118 | |
| 13 | 2R | 118 | |

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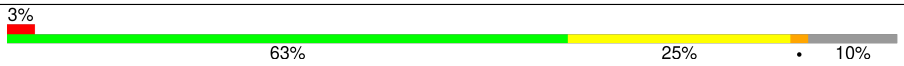
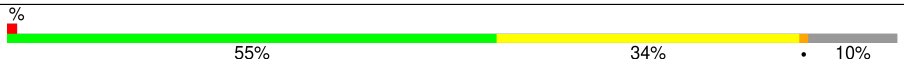
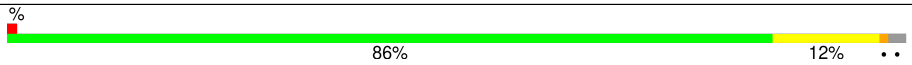
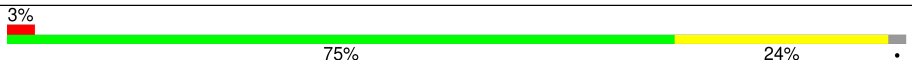
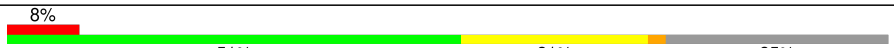
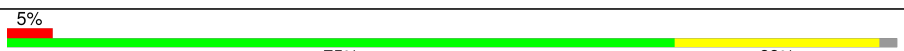
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 14 | 1S | 112 | |
| 14 | 2S | 112 | |
| 15 | 1T | 146 |   |
| 15 | 2T | 146 |   |
| 16 | 1U | 118 |   |
| 16 | 2U | 118 |   |
| 17 | 1V | 101 | |
| 17 | 2V | 101 | |
| 18 | 1W | 113 | |
| 18 | 2W | 113 | |
| 19 | 1X | 96 | |
| 19 | 2X | 96 | |
| 20 | 1Y | 110 | |
| 20 | 2Y | 110 | |
| 21 | 1Z | 206 |   |
| 21 | 2Z | 206 | |
| 22 | 10 | 85 | |
| 22 | 20 | 85 | |
| 23 | 11 | 98 | |
| 23 | 21 | 98 | |
| 24 | 12 | 72 | |
| 24 | 22 | 72 | |
| 25 | 13 | 60 | |
| 25 | 23 | 60 |   |
| 26 | 14 | 71 | |

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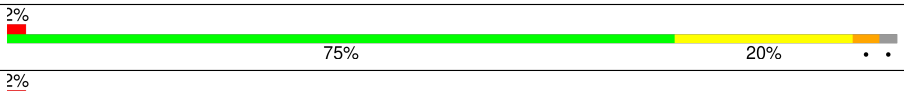
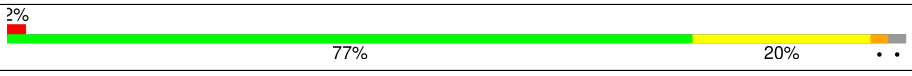
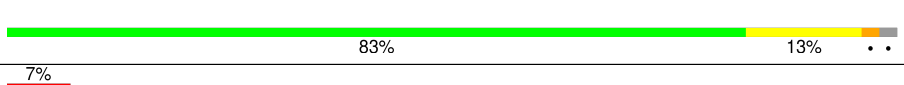
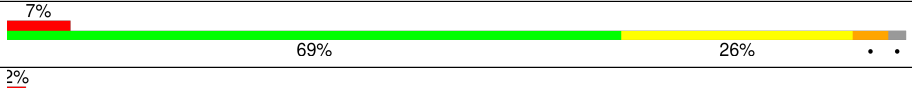
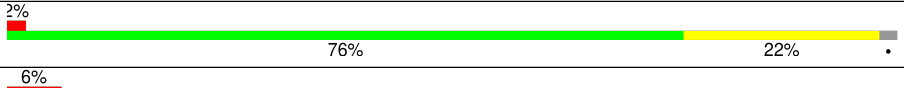
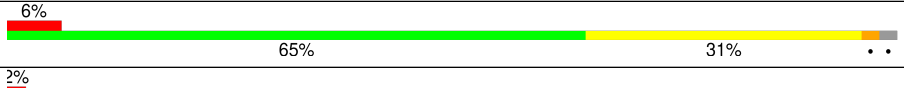
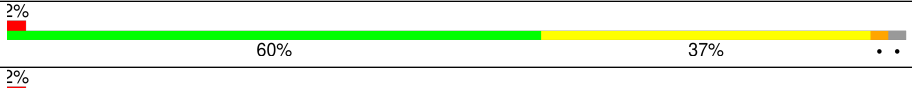
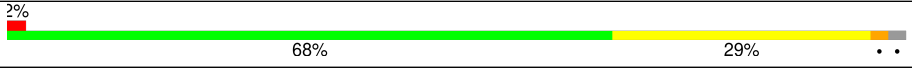
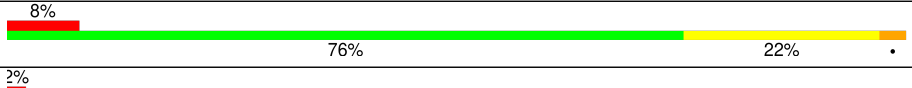
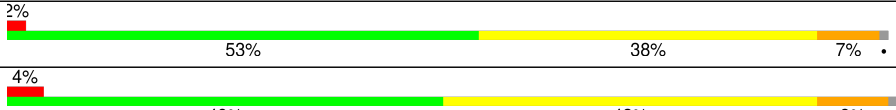
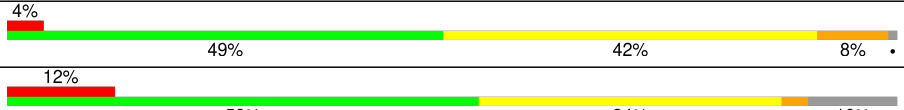
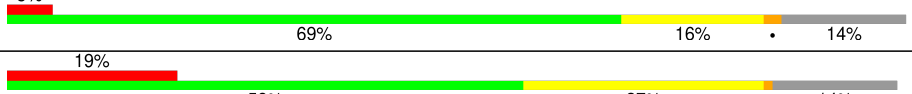
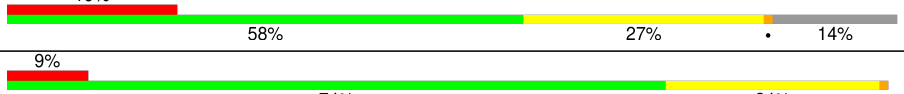
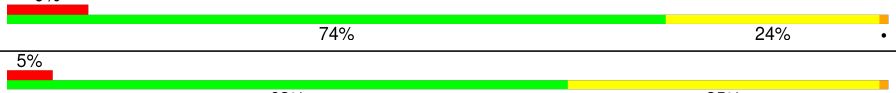
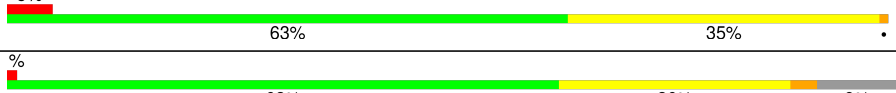
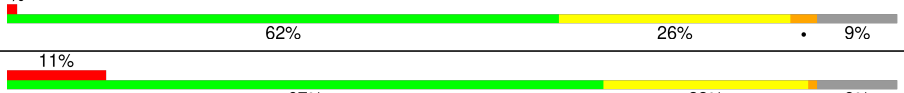
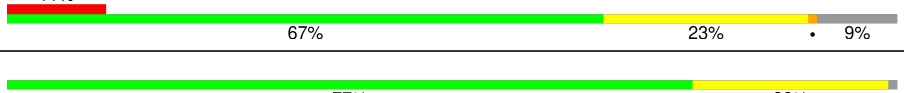
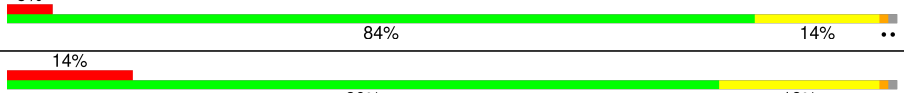
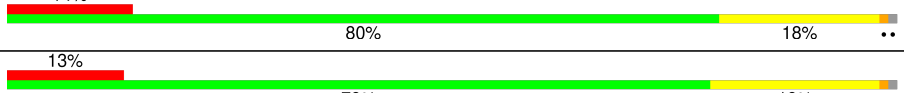
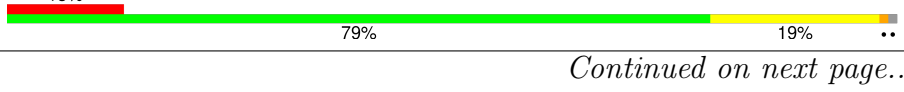
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 26 | 24 | 71 | |
| 27 | 15 | 60 |   |
| 27 | 25 | 60 |   |
| 28 | 16 | 54 |   |
| 28 | 26 | 54 |   |
| 29 | 17 | 49 |   |
| 29 | 27 | 49 |   |
| 30 | 18 | 65 |   |
| 30 | 28 | 65 |   |
| 31 | 19 | 37 | |
| 31 | 29 | 37 |   |
| 32 | 1a | 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 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 39 | 1h | 138 | 2% 75% 21% |
| 39 | 2h | 138 | 7% 68% 30% |
| 40 | 1i | 128 | 18% 74% 23% |
| 40 | 2i | 128 | 38% 64% 34% |
| 41 | 1j | 105 | 21% 70% 18% 8% |
| 41 | 2j | 105 | 43% 62% 29% 9% |
| 42 | 1k | 129 | 2% 71% 18% 12% |
| 42 | 2k | 129 | 8% 63% 24% 12% |
| 43 | 1l | 132 | 2% 72% 17% 8% |
| 43 | 2l | 132 | 8% 71% 20% 8% |
| 44 | 1m | 126 | 12% 68% 26% |
| 44 | 2m | 126 | 23% 66% 30% |
| 45 | 1n | 61 | 10% 62% 34% |
| 45 | 2n | 61 | 52% 69% 30% |
| 46 | 1o | 89 | 3% 80% 17% |
| 46 | 2o | 89 | 9% 75% 21% |
| 47 | 1p | 88 | 17% 60% 33% 7% |
| 47 | 2p | 88 | 8% 66% 23% 5% 7% |
| 48 | 1q | 105 | 5% 67% 27% 6% |
| 48 | 2q | 105 | 7% 65% 30% 6% |
| 49 | 1r | 88 | % 63% 14% 23% |
| 49 | 2r | 88 | 5% 56% 19% 23% |
| 50 | 1s | 93 | 9% 63% 26% 11% |
| 50 | 2s | 93 | 23% 55% 33% 11% |
| 51 | 1t | 106 | 12% 73% 16% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 51 | 2t | 106 | 13% 71% 15% 9% |
| 52 | 1u | 27 | 19% 52% 33% 15% |
| 52 | 2u | 27 | 37% 44% 41% 15% |
| 53 | 1v | 27 | 11% 33% 11% 52% |
| 53 | 2v | 27 | 19% 22% 19% 7% 52% |
| 54 | 1w | 76 | 22% 43% 30% 21% |
| 54 | 1y | 76 | 17% 34% 37% 21% |
| 54 | 2w | 76 | 29% 26% 49% 20% |
| 54 | 2y | 76 | 25% 36% 38% 21% |
| 55 | 1x | 77 | 5% 69% 21% 9% |
| 55 | 2x | 77 | 6% 48% 42% 9% |

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 |
|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4053 | - | - | - | X |

## 2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 300702 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1A | 2871 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 61852 | 27531 | 11572 | 19878 | 2871 | | | |
| 1 | 2A | 2800 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 60322 | 26848 | 11284 | 19390 | 2800 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1B | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2577 | 1146 | 476 | 835 | 120 | | | |
| 2 | 2B | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2575 | 1146 | 476 | 833 | 120 | | | |

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | 1G | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1423 | 913 | 253 | 253 | 4 | | | |
| 6 | 2G | 181 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1428 | 913 | 258 | 253 | 4 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | 1S | 110 | Total<br>873 | C<br>550 | N<br>174 | O<br>149 | 0 | 0 | 0 |
| 14 | 2S | 110 | Total<br>870 | C<br>549 | N<br>173 | O<br>148 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | 1T | 131 | Total<br>1091 | C<br>680 | N<br>225 | O<br>185 | S<br>1 | 0 | 0 | 0 |
| 15 | 2T | 131 | Total<br>1083 | C<br>675 | N<br>224 | O<br>183 | S<br>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 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |
| 17 | 2V | 101 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 771 | 495 | 140 | 135 | 1 | | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | 1Y | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |
| 20 | 2Y | 107 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 806 | 517 | 152 | 131 | 6 | | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | 11 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |
| 23 | 21 | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 755 | 475 | 148 | 131 | 1 | | | |

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | 14 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 552 | 349 | 99 | 99 | 5 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | 24 | 69 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 532 | 339 | 97 | 91 | 5 | | | |

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | 1a | 1500 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32246 | 14358 | 5975 | 10413 | 1500 | | | |
| 32 | 2a | 1503 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32327 | 14396 | 5990 | 10438 | 1503 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | 1b | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1846 | 1179 | 331 | 331 | 5 | | | |
| 33 | 2b | 231 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1825 | 1167 | 326 | 327 | 5 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | 1c | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1548 | 973 | 301 | 273 | 1 | | | |
| 34 | 2c | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1542 | 968 | 300 | 273 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | 1d | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1655 | 1038 | 326 | 284 | 7 | | | |
| 35 | 2d | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1674 | 1050 | 333 | 284 | 7 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | 1e | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 213 | 198 | 4 | | | |
| 36 | 2e | 148 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1133 | 716 | 214 | 199 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | 1f | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 810 | 514 | 144 | 149 | 3 | | | |
| 37 | 2f | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 146 | 151 | 3 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 38 | 1g | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1231 | 766 | 243 | 216 | 6 | | | |
| 38 | 2g | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1235 | 769 | 244 | 216 | 6 | | | |

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

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

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | 1i | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 983 | 623 | 193 | 167 | | | |
| 40 | 2i | 127 | Total | C | N | O | 0 | 0 | 0 |
| | | | 978 | 619 | 190 | 169 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | 1j | 97 | Total | C | N | O | 0 | 0 | 0 |
| | | | 709 | 440 | 138 | 131 | | | |
| 41 | 2j | 96 | Total | C | N | O | 0 | 0 | 0 |
| | | | 714 | 445 | 138 | 131 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | 1k | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 829 | 516 | 155 | 155 | 3 | | | |

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | 1m | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 958 | 592 | 198 | 166 | 2 | | | |
| 44 | 2m | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 950 | 586 | 197 | 165 | 2 | | | |

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

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

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

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

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

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

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

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

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

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

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | 1s | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 652 | 417 | 120 | 113 | 2 | | | |
| 50 | 2s | 83 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 646 | 412 | 119 | 113 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 51 | 1t | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 728 | 446 | 156 | 124 | 2 | | | |
| 51 | 2t | 96 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 727 | 446 | 155 | 124 | 2 | | | |

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

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

- Molecule 53 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 53 | 1v | 13 | Total<br>276 | C<br>124 | N<br>48 | O<br>91 | P<br>13 | 0 | 0 | 0 |
| 53 | 2v | 13 | Total<br>276 | C<br>124 | N<br>48 | O<br>91 | P<br>13 | 0 | 0 | 0 |

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 54 | 1w | 73 | Total<br>1568 | C<br>700 | N<br>282 | O<br>512 | P<br>73 | S<br>1 | 0 | 0 | 0 |
| 54 | 1y | 73 | Total<br>1568 | C<br>700 | N<br>282 | O<br>512 | P<br>73 | S<br>1 | 0 | 0 | 0 |
| 54 | 2w | 73 | Total<br>1568 | C<br>700 | N<br>282 | O<br>512 | P<br>73 | S<br>1 | 0 | 0 | 0 |
| 54 | 2y | 73 | Total<br>1568 | C<br>700 | N<br>282 | O<br>512 | P<br>73 | S<br>1 | 0 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 55 | 1x | 76 | Total<br>1625 | C<br>725 | N<br>294 | O<br>529 | P<br>76 | S<br>1 | 0 | 0 | 0 |
| 55 | 2x | 76 | Total<br>1625 | C<br>725 | N<br>294 | O<br>529 | P<br>76 | S<br>1 | 0 | 0 | 0 |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 56 | 1A | 1134 | Total<br>1134 | Mg<br>1134 | 0 | 0 |
| 56 | 1B | 36 | Total<br>36 | Mg<br>36 | 0 | 0 |
| 56 | 1D | 13 | Total<br>13 | Mg<br>13 | 0 | 0 |
| 56 | 1E | 7 | Total<br>7 | Mg<br>7 | 0 | 0 |
| 56 | 1F | 10 | Total<br>10 | Mg<br>10 | 0 | 0 |
| 56 | 1G | 5 | Total<br>5 | Mg<br>5 | 0 | 0 |
| 56 | 1I | 1 | Total<br>1 | Mg<br>1 | 0 | 0 |
| 56 | 1N | 7 | Total<br>7 | Mg<br>7 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 1O | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 1P | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 1Q | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 1R | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 1S | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 1T | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1U | 7 | Total Mg<br>7 7 | 0 | 0 |
| 56 | 1V | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1W | 7 | Total Mg<br>7 7 | 0 | 0 |
| 56 | 1X | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 1Y | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 1Z | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 10 | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 11 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 12 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 13 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 14 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 15 | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 16 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 17 | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 18 | 4 | Total Mg<br>4 4 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 19 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1a | 233 | Total Mg<br>233 233 | 0 | 0 |
| 56 | 1b | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1e | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1f | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 1l | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 1n | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1q | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1t | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1v | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 1w | 8 | Total Mg<br>8 8 | 0 | 0 |
| 56 | 1x | 15 | Total Mg<br>15 15 | 0 | 0 |
| 56 | 1y | 6 | Total Mg<br>6 6 | 0 | 0 |
| 56 | 2A | 860 | Total Mg<br>860 860 | 0 | 0 |
| 56 | 2B | 18 | Total Mg<br>18 18 | 0 | 0 |
| 56 | 2D | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 2E | 8 | Total Mg<br>8 8 | 0 | 0 |
| 56 | 2F | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 2G | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2N | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2O | 2 | Total Mg<br>2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 2P | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 2Q | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 2R | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 2T | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 2U | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 2V | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 2W | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2X | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2Y | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 20 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 21 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 25 | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 27 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 28 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 29 | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2a | 231 | Total Mg<br>231 231 | 0 | 0 |
| 56 | 2d | 2 | Total Mg<br>2 2 | 0 | 0 |
| 56 | 2e | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2f | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2i | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2j | 2 | Total Mg<br>2 2 | 0 | 0 |

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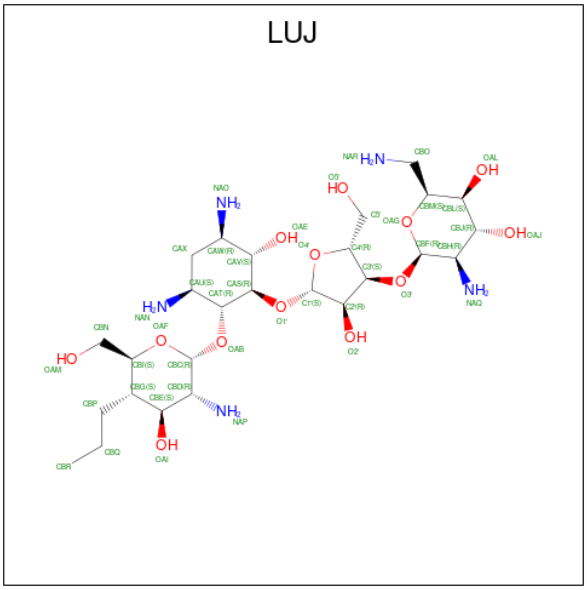
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 56 | 2k | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2l | 4 | Total Mg<br>4 4 | 0 | 0 |
| 56 | 2q | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 2r | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2t | 1 | Total Mg<br>1 1 | 0 | 0 |
| 56 | 2v | 3 | Total Mg<br>3 3 | 0 | 0 |
| 56 | 2x | 5 | Total Mg<br>5 5 | 0 | 0 |
| 56 | 2y | 6 | Total Mg<br>6 6 | 0 | 0 |

- Molecule 57 is (1R,2R,3S,4R,6S)-4,6-diamino-2-{[3-O-(2,6-diamino-2,6-dideoxy-beta-L-idopyranosyl)-beta-D-ribofuranosyl]oxy}-3-hydroxyc yclohexyl 2-amino-2,4-dideoxy-4-propyl-alpha-D-glucopyranoside (CCD ID: LUJ) (formula: $C_{26}H_{51}N_5O_{13}$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | 1A | 1 | Total C N O<br>42 24 5 13 | 0 | 0 |
| 57 | 1A | 1 | Total C N O<br>42 24 5 13 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 57 | 1a | 1 | Total C N O<br>44 26 5 13 | 0 | 0 |
| 57 | 2A | 1 | Total C N O<br>42 24 5 13 | 0 | 0 |
| 57 | 2A | 1 | Total C N O<br>42 24 5 13 | 0 | 0 |
| 57 | 2a | 1 | Total C N O<br>44 26 5 13 | 0 | 0 |

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 58 | 1A | 1 | Total K<br>1 1 | 0 | 0 |
| 58 | 2A | 1 | Total K<br>1 1 | 0 | 0 |

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

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

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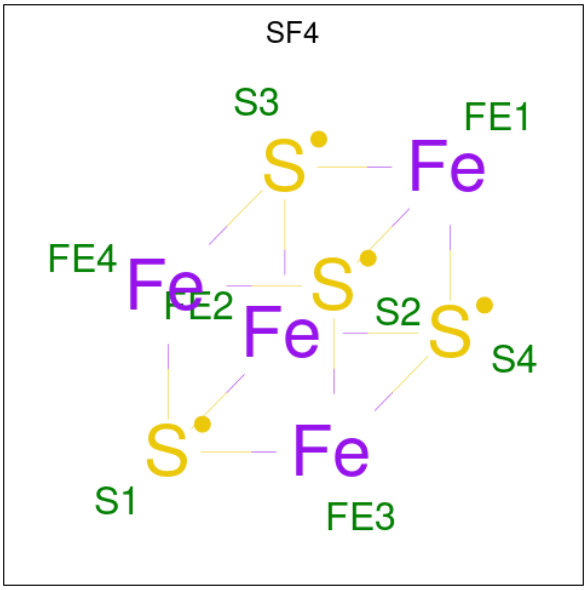
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 59 | 2n | 1 | Total Zn<br>1 1 | 0 | 0 |

- 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<br>8 4 4 | 0 | 0 |
| 60 | 2d | 1 | Total Fe S<br>8 4 4 | 0 | 0 |

- Molecule 61 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1A | 2225 | Total O<br>2225 2225 | 0 | 0 |
| 61 | 1B | 69 | Total O<br>69 69 | 0 | 0 |
| 61 | 1D | 28 | Total O<br>28 28 | 0 | 0 |
| 61 | 1E | 27 | Total O<br>27 27 | 0 | 0 |
| 61 | 1F | 17 | Total O<br>17 17 | 0 | 0 |
| 61 | 1G | 6 | Total O<br>6 6 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 1H | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1I | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1N | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1O | 7 | Total O<br>7 7 | 0 | 0 |
| 61 | 1P | 26 | Total O<br>26 26 | 0 | 0 |
| 61 | 1Q | 12 | Total O<br>12 12 | 0 | 0 |
| 61 | 1R | 14 | Total O<br>14 14 | 0 | 0 |
| 61 | 1S | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1T | 7 | Total O<br>7 7 | 0 | 0 |
| 61 | 1U | 13 | Total O<br>13 13 | 0 | 0 |
| 61 | 1V | 8 | Total O<br>8 8 | 0 | 0 |
| 61 | 1W | 9 | Total O<br>9 9 | 0 | 0 |
| 61 | 1X | 7 | Total O<br>7 7 | 0 | 0 |
| 61 | 1Y | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1Z | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 10 | 9 | Total O<br>9 9 | 0 | 0 |
| 61 | 11 | 12 | Total O<br>12 12 | 0 | 0 |
| 61 | 12 | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 13 | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 14 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 15 | 7 | Total O<br>7 7 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 16 | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 17 | 8 | Total O<br>8 8 | 0 | 0 |
| 61 | 18 | 13 | Total O<br>13 13 | 0 | 0 |
| 61 | 19 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1a | 438 | Total O<br>438 438 | 0 | 0 |
| 61 | 1b | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1d | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1e | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1g | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1j | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1l | 8 | Total O<br>8 8 | 0 | 0 |
| 61 | 1m | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 1n | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1p | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1q | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 1u | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 1v | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 1w | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 1x | 17 | Total O<br>17 17 | 0 | 0 |
| 61 | 1y | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2A | 1163 | Total O<br>1163 1163 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 2B | 20 | Total O<br>20 20 | 0 | 0 |
| 61 | 2D | 23 | Total O<br>23 23 | 0 | 0 |
| 61 | 2E | 10 | Total O<br>10 10 | 0 | 0 |
| 61 | 2F | 13 | Total O<br>13 13 | 0 | 0 |
| 61 | 2I | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2N | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2O | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2P | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2Q | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2R | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2T | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2U | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2V | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2W | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2X | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2Z | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 20 | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 21 | 9 | Total O<br>9 9 | 0 | 0 |
| 61 | 23 | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 25 | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 27 | 3 | Total O<br>3 3 | 0 | 0 |

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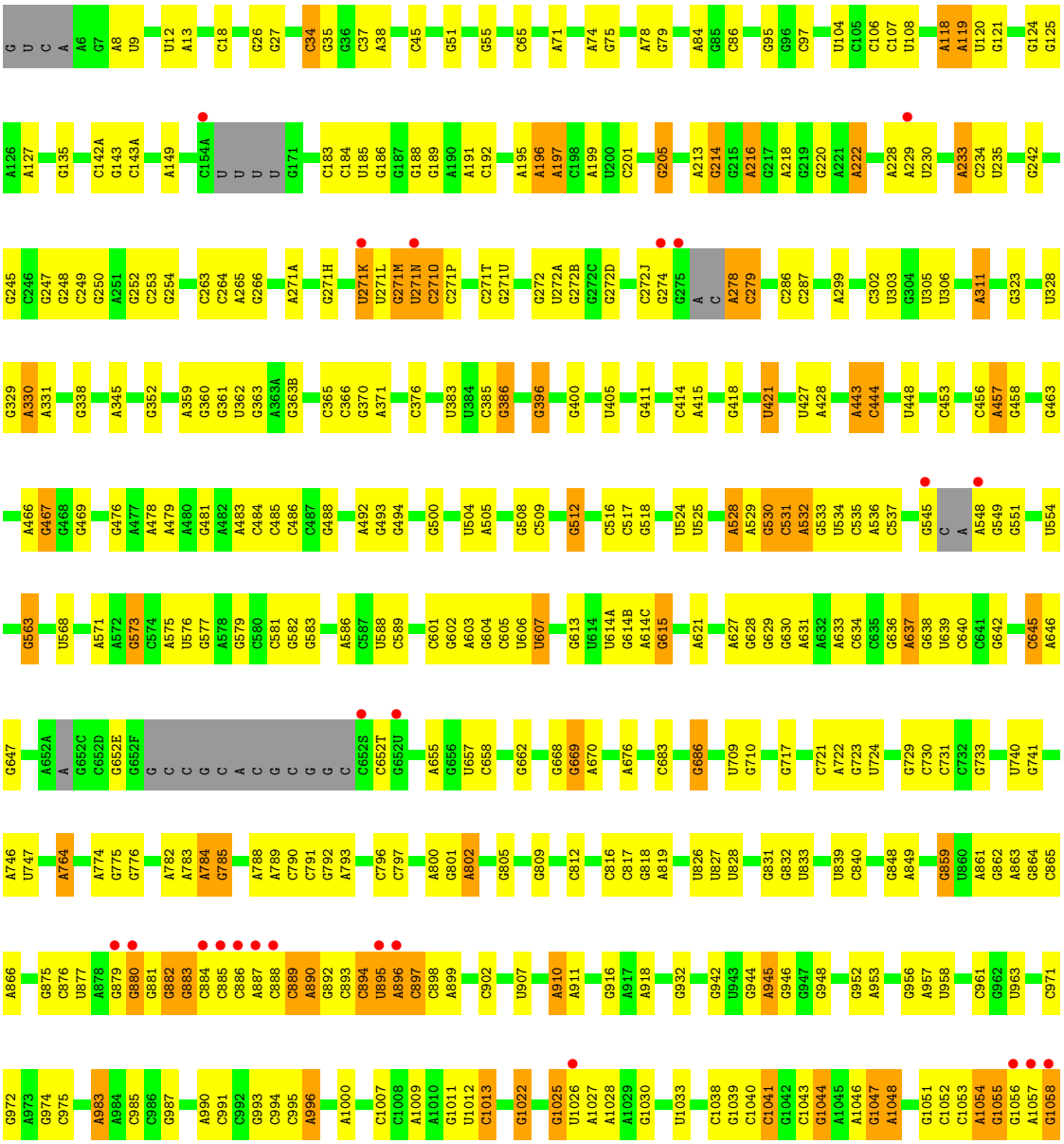
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 61 | 28 | 6 | Total O<br>6 6 | 0 | 0 |
| 61 | 2a | 322 | Total O<br>322 322 | 0 | 0 |
| 61 | 2e | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2f | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2g | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2j | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2l | 5 | Total O<br>5 5 | 0 | 0 |
| 61 | 2o | 2 | Total O<br>2 2 | 0 | 0 |
| 61 | 2p | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2q | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2r | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2t | 4 | Total O<br>4 4 | 0 | 0 |
| 61 | 2u | 1 | Total O<br>1 1 | 0 | 0 |
| 61 | 2v | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2w | 3 | Total O<br>3 3 | 0 | 0 |
| 61 | 2x | 7 | Total O<br>7 7 | 0 | 0 |
| 61 | 2y | 9 | Total O<br>9 9 | 0 | 0 |

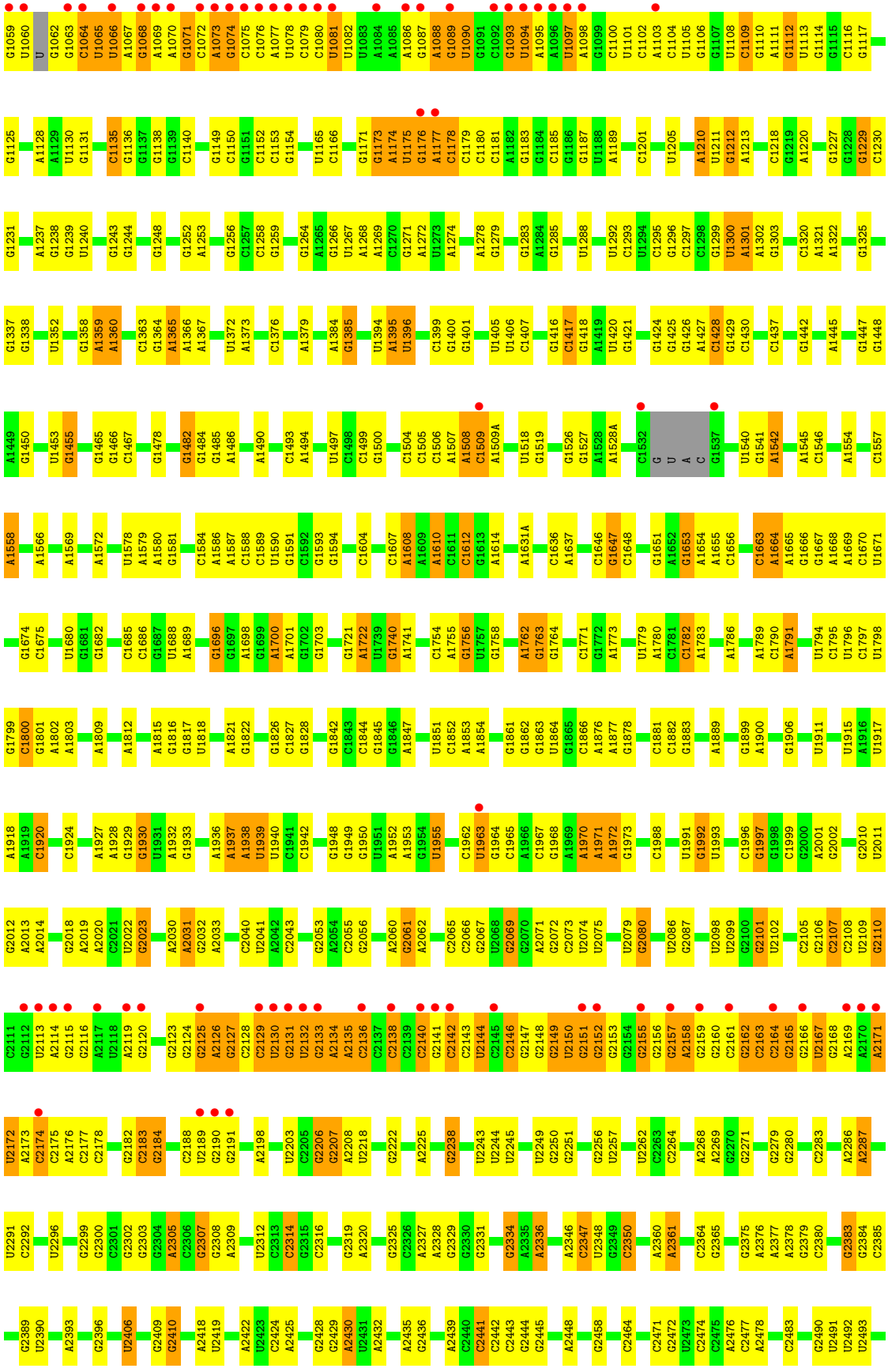
# 3 Residue-property plots (i)

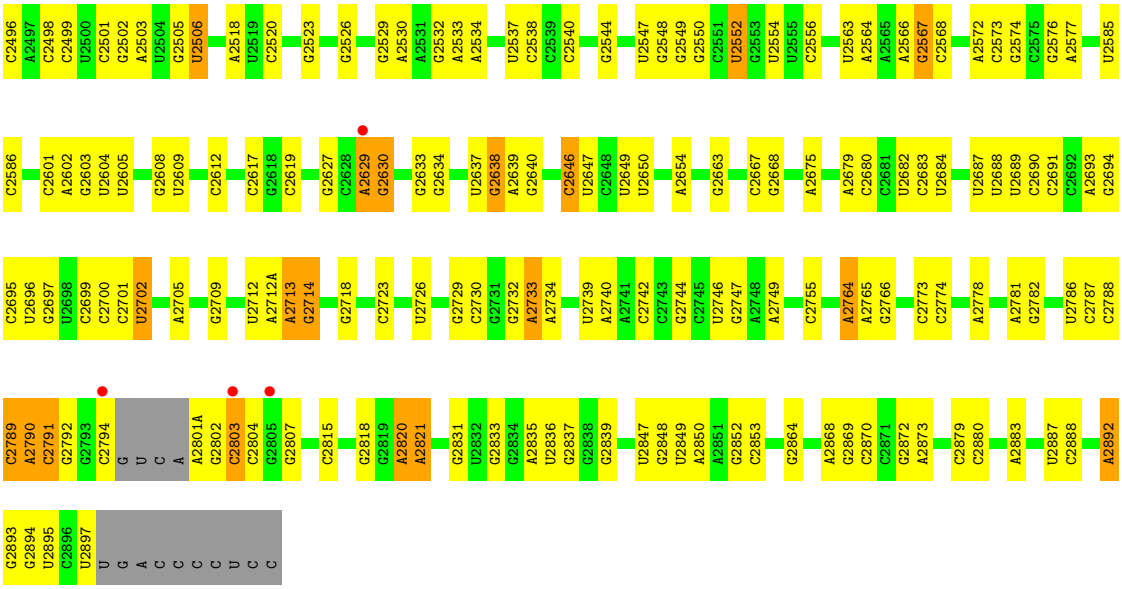
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain 1A:

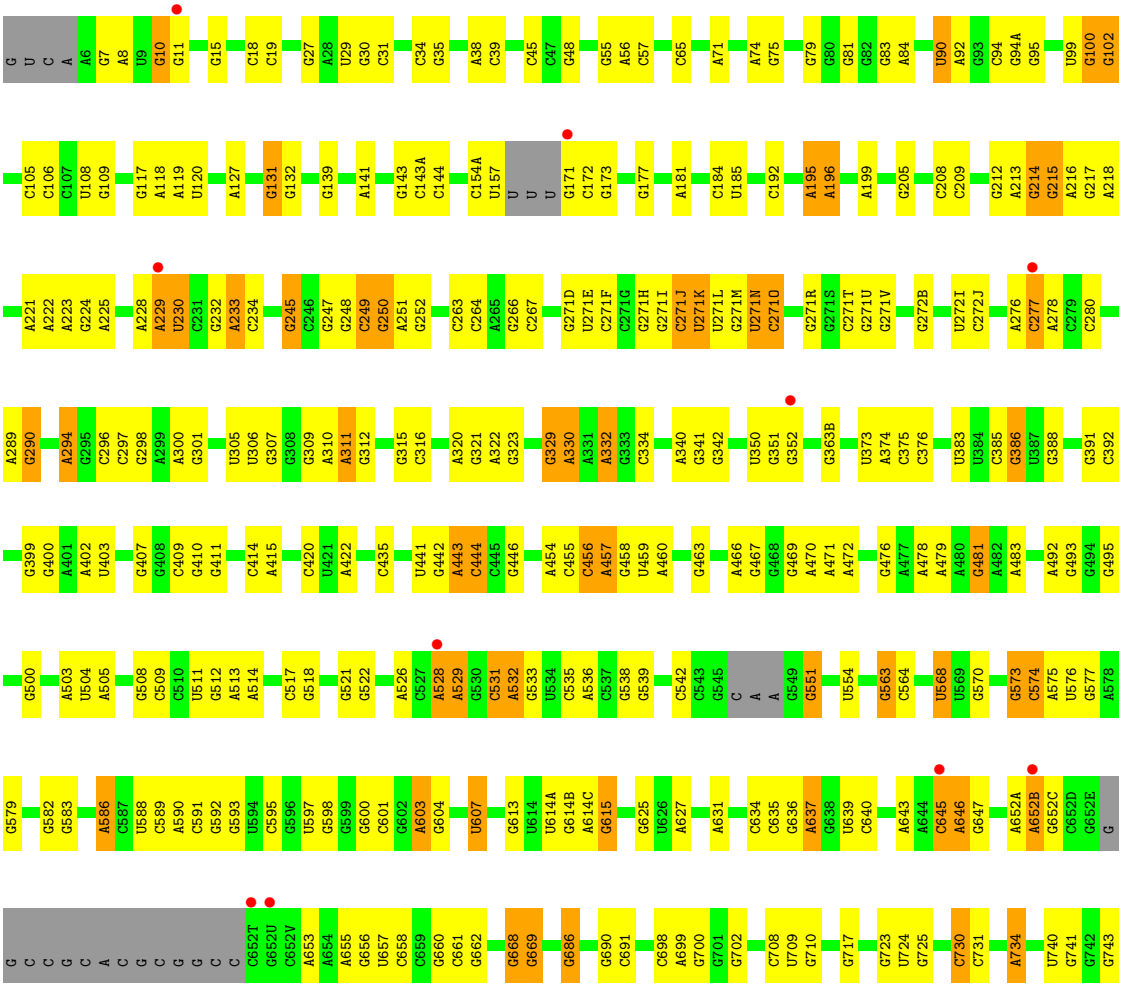


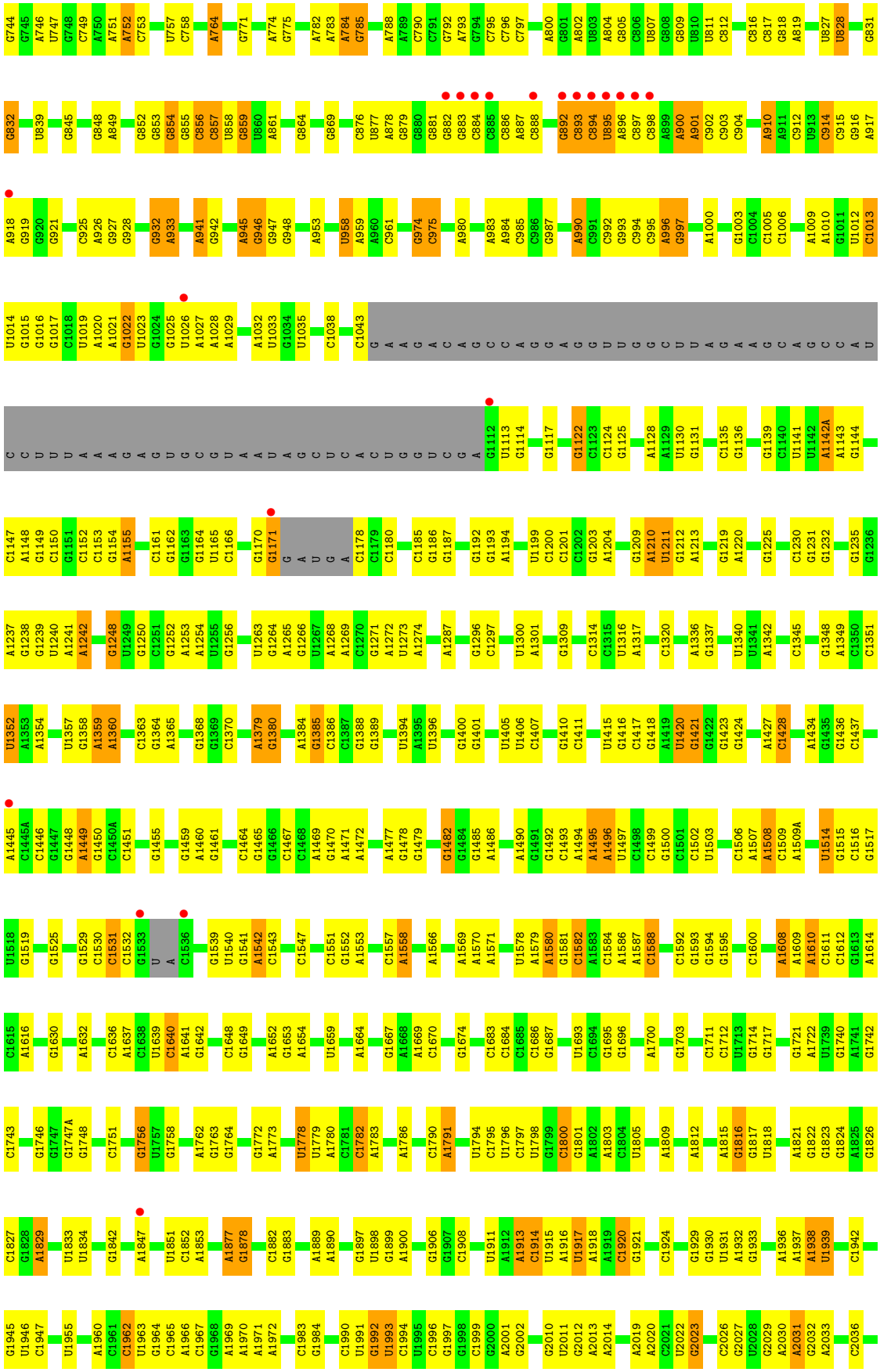


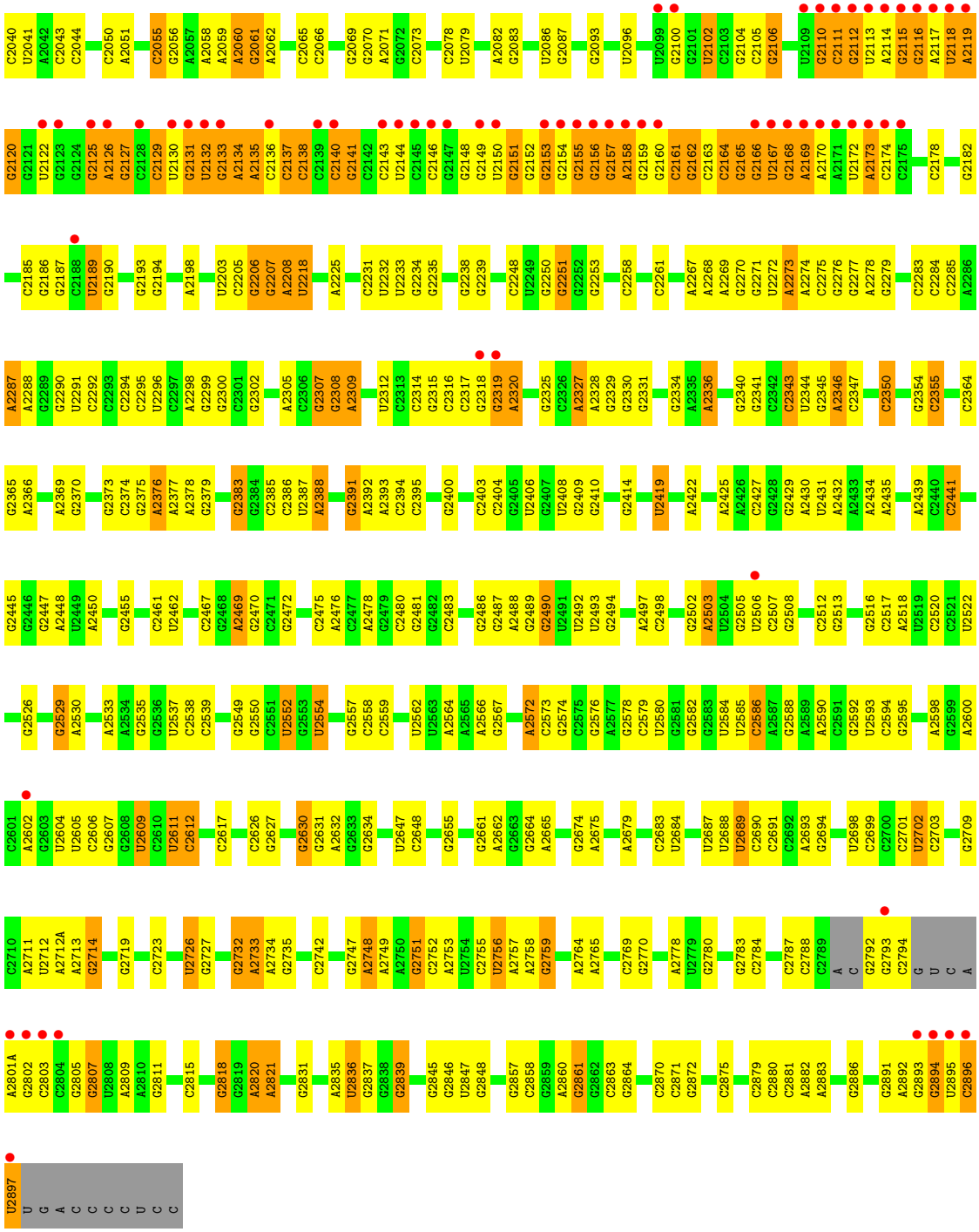


• Molecule 1: 23S Ribosomal RNA

Chain 2A:





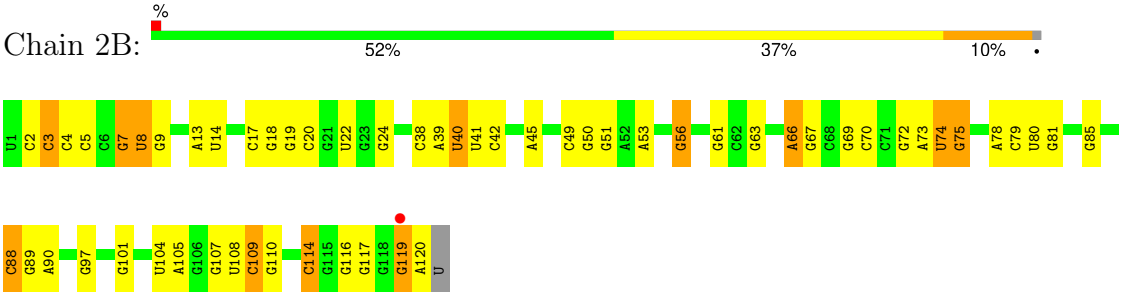


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

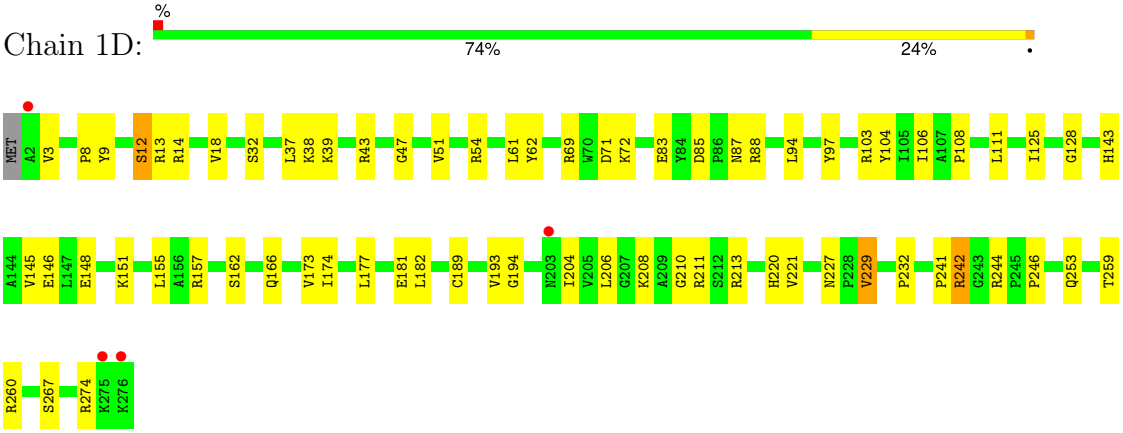
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



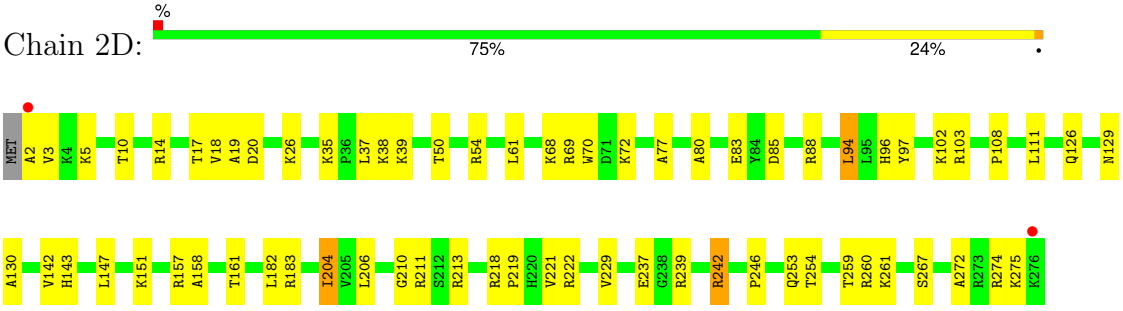

• Molecule 3: 50S ribosomal protein L2

Chain 1D:



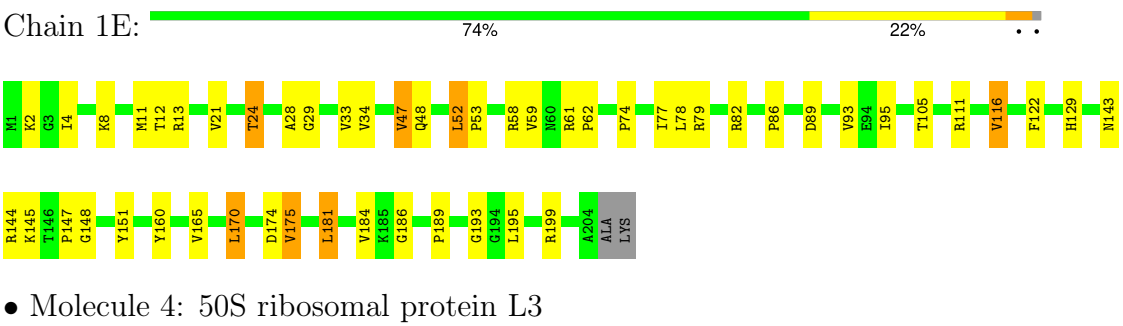

• Molecule 3: 50S ribosomal protein L2

Chain 2D:



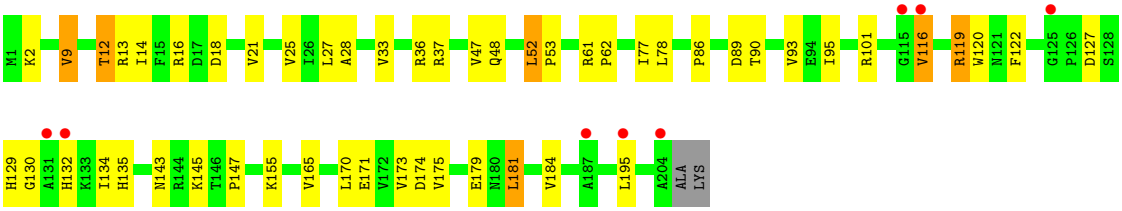

• Molecule 4: 50S ribosomal protein L3

Chain 1E:




• Molecule 4: 50S ribosomal protein L3

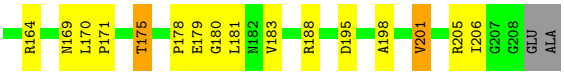
Chain 2E:





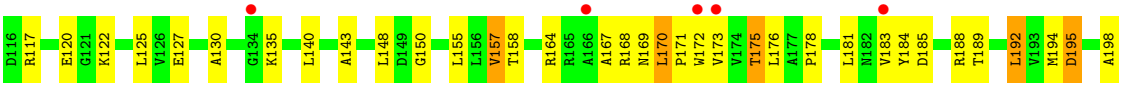
• Molecule 5: 50S ribosomal protein L4

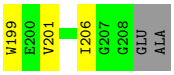
Chain 1F:



• Molecule 5: 50S ribosomal protein L4

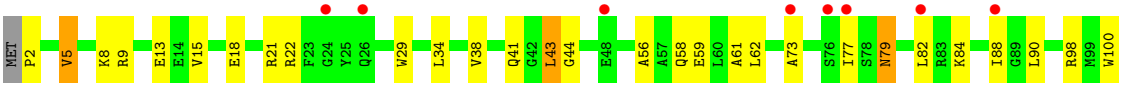
Chain 2F:

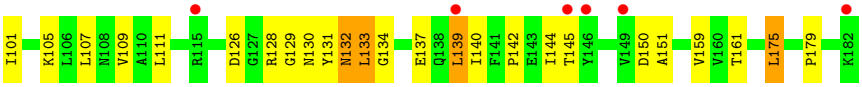




• Molecule 6: 50S ribosomal protein L5

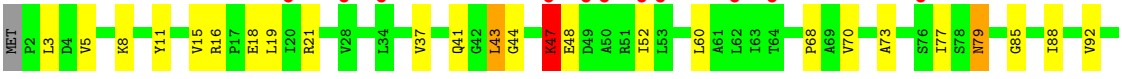
Chain 1G:

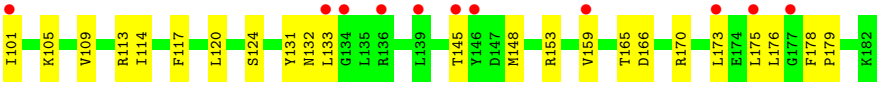




• Molecule 6: 50S ribosomal protein L5

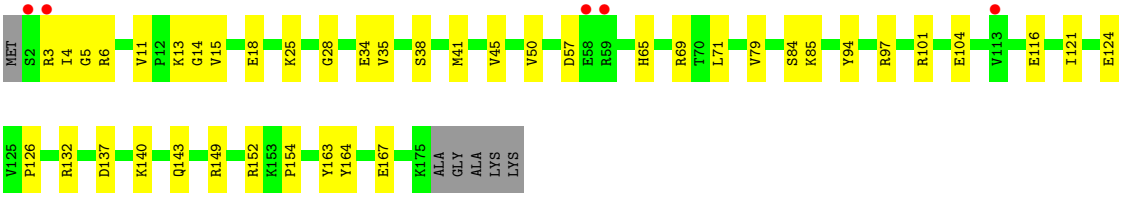
Chain 2G:





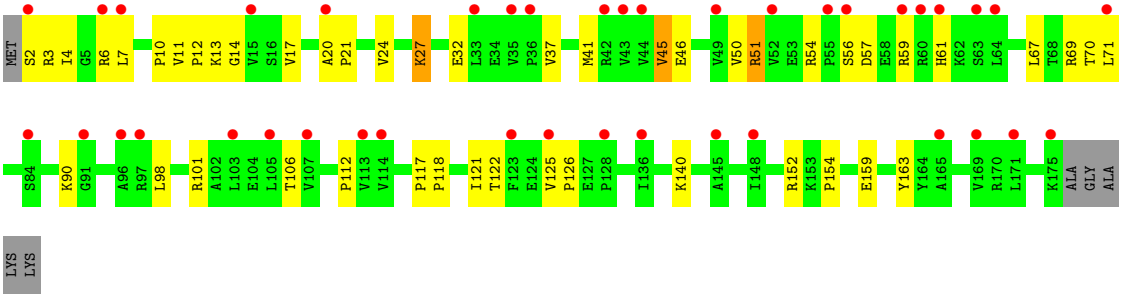

• Molecule 7: 50S ribosomal protein L6

Chain 1H:



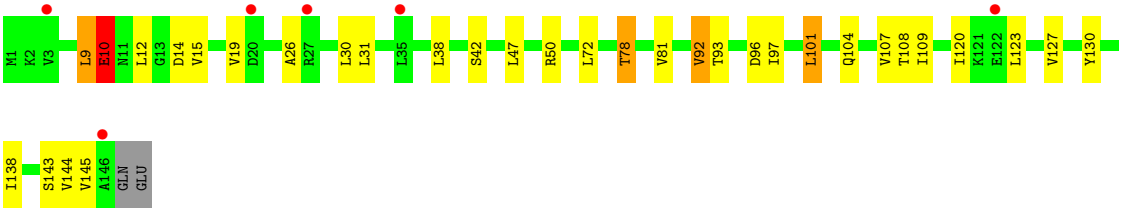

• Molecule 7: 50S ribosomal protein L6

Chain 2H:



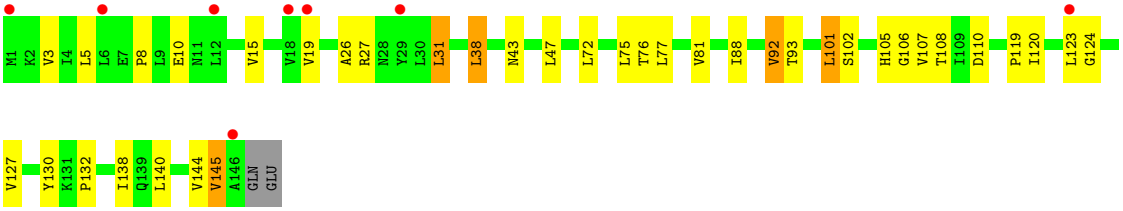

• Molecule 8: 50S ribosomal protein L9

Chain 1I:



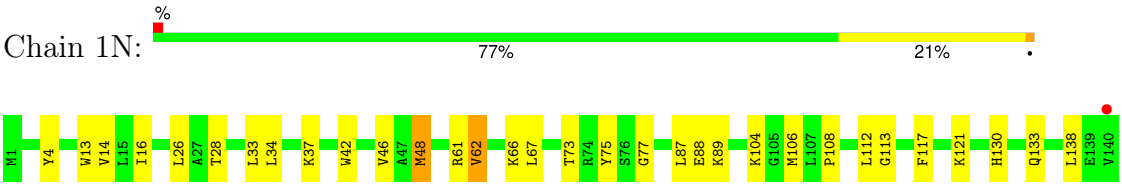

• Molecule 8: 50S ribosomal protein L9

Chain 2I:



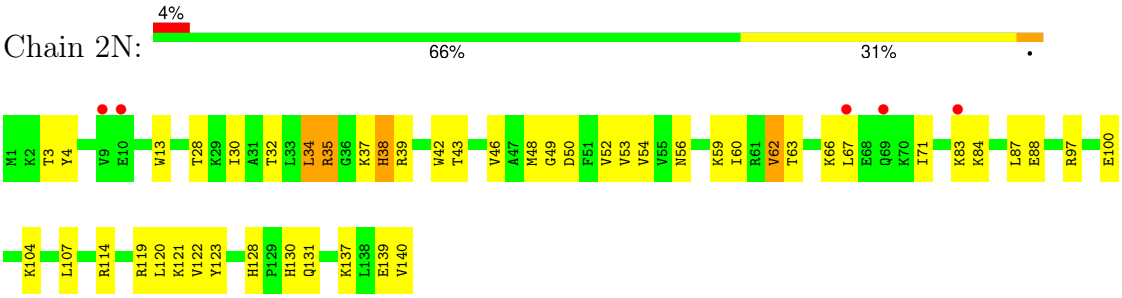

• Molecule 9: 50S ribosomal protein L13

Chain 1N:



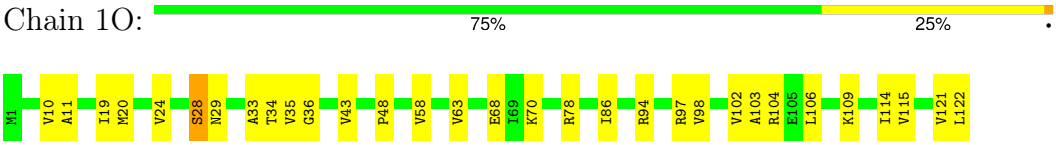

• Molecule 9: 50S ribosomal protein L13

Chain 2N:



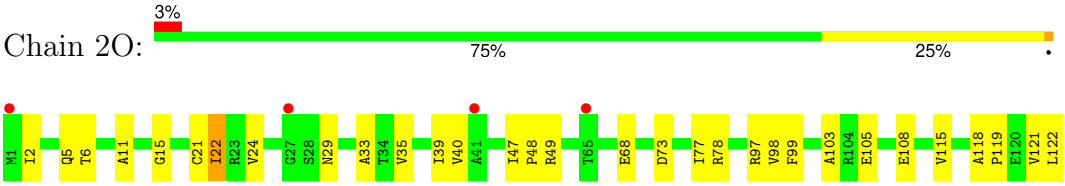

• Molecule 10: 50S ribosomal protein L14

Chain 1O:



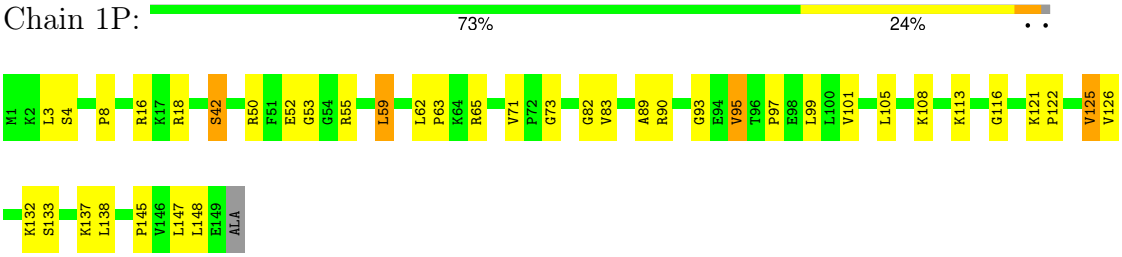

• Molecule 10: 50S ribosomal protein L14

Chain 2O:



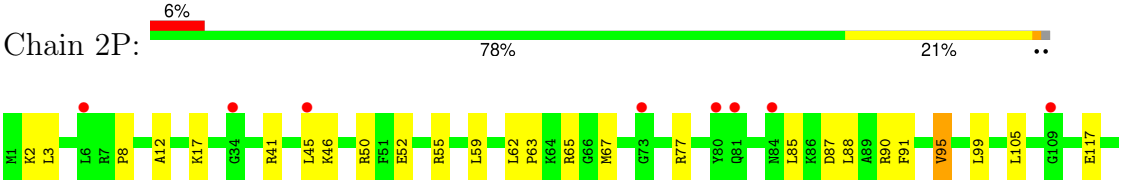

• Molecule 11: 50S ribosomal protein L15

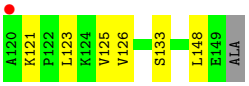
Chain 1P:




• Molecule 11: 50S ribosomal protein L15

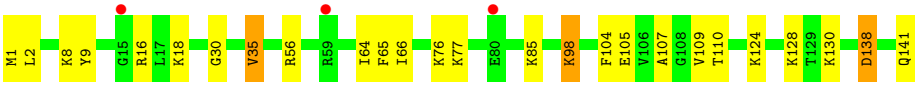
Chain 2P:





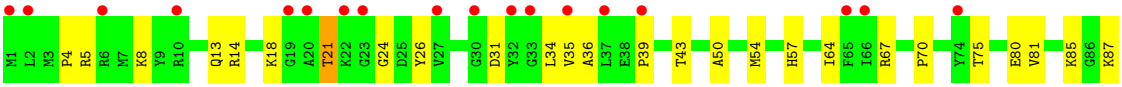

• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



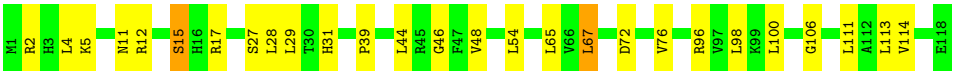

• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



• Molecule 13: 50S ribosomal protein L17

Chain 1R:




• Molecule 13: 50S ribosomal protein L17

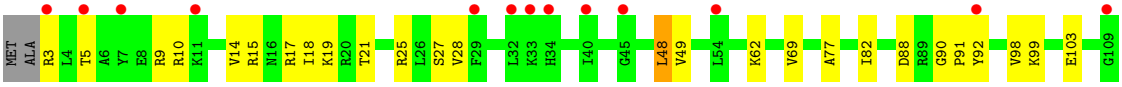
Chain 2R:

• Molecule 14: 50S ribosomal protein L18

Chain 1S:

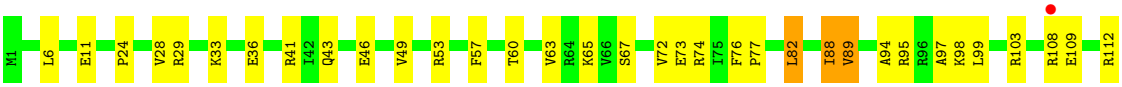
• Molecule 14: 50S ribosomal protein L18

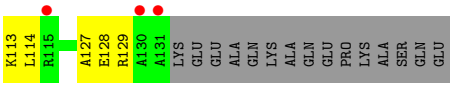
Chain 2S:



• Molecule 15: 50S ribosomal protein L19

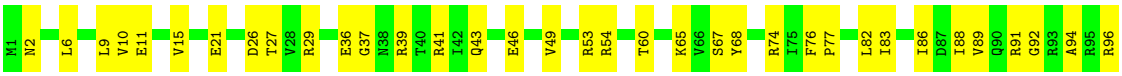
Chain 1T:

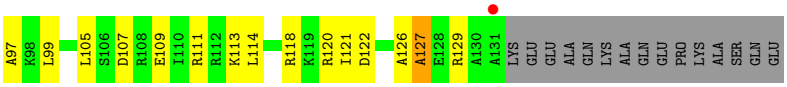



• Molecule 15: 50S ribosomal protein L19

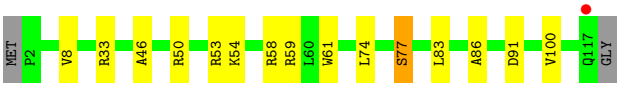
Chain 2T:



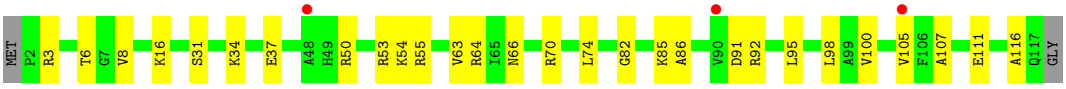

• Molecule 16: 50S ribosomal protein L20

Chain 1U:



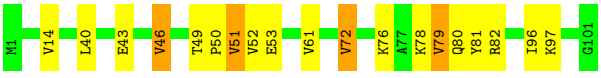

• Molecule 16: 50S ribosomal protein L20

Chain 2U:



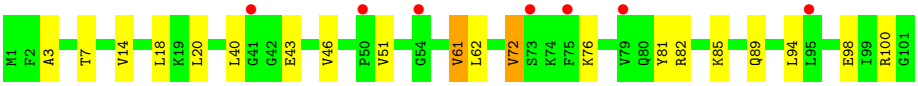

• Molecule 17: 50S ribosomal protein L21

Chain 1V:



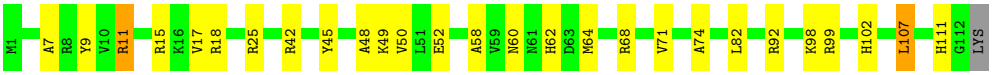

• Molecule 17: 50S ribosomal protein L21

Chain 2V:




• Molecule 18: 50S ribosomal protein L22

Chain 1W:




• Molecule 18: 50S ribosomal protein L22

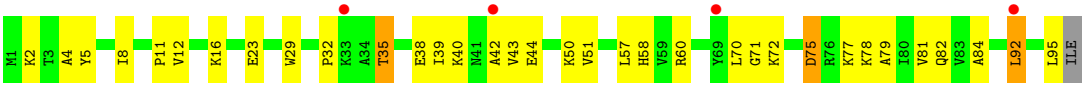
Chain 2W:

• Molecule 19: 50S ribosomal protein L23

Chain 1X:

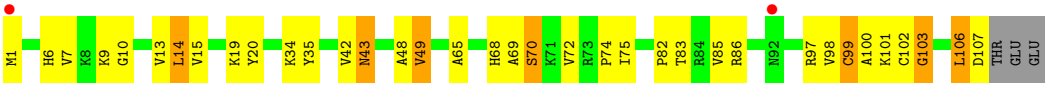
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



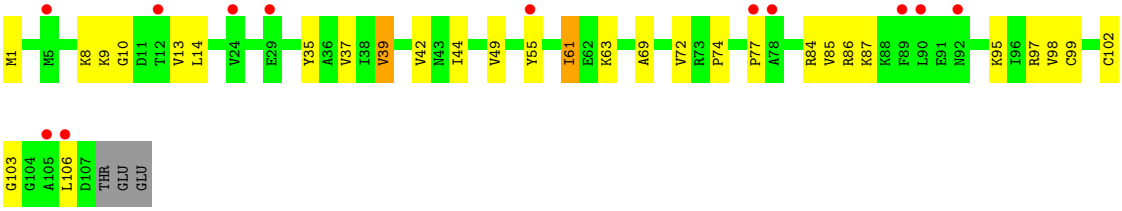

• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



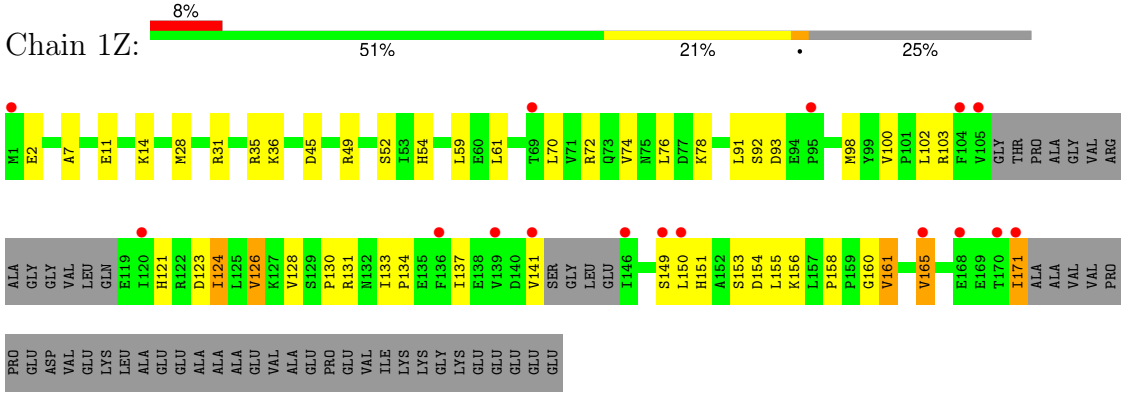

• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



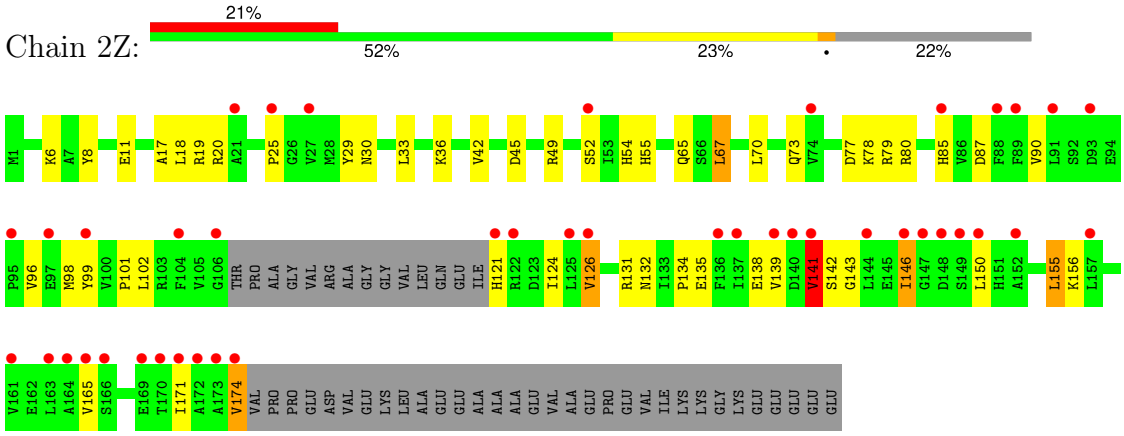
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



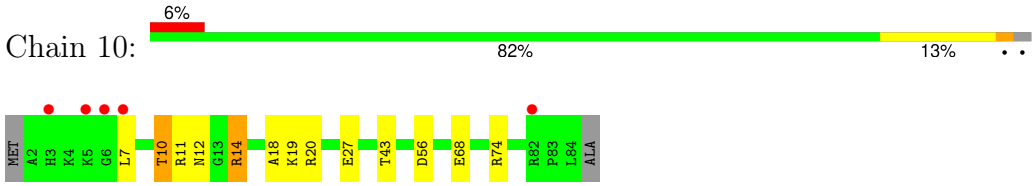

• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



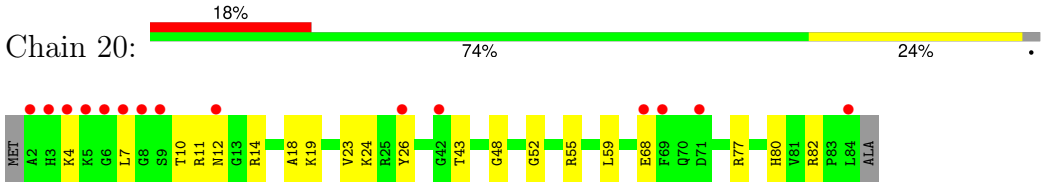

• Molecule 22: 50S ribosomal protein L27

Chain 10:



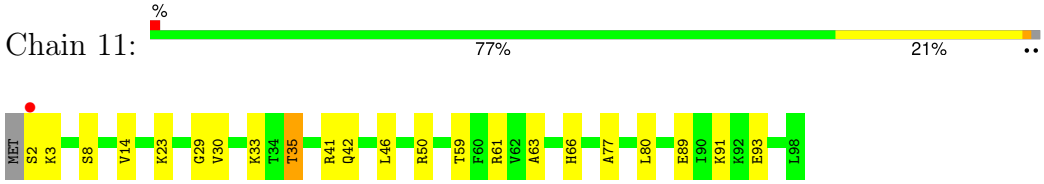

• Molecule 22: 50S ribosomal protein L27

Chain 20:



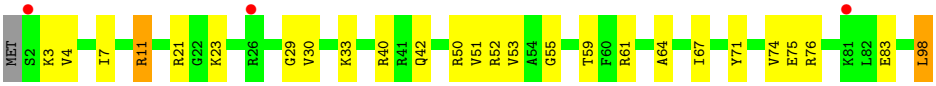

• Molecule 23: 50S ribosomal protein L28

Chain 11:



• Molecule 23: 50S ribosomal protein L28

Chain 21:

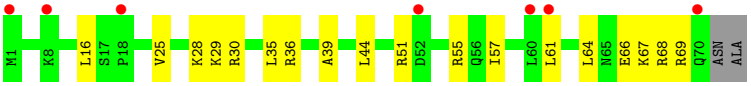



• Molecule 24: 50S ribosomal protein L29

Chain 12:

• Molecule 24: 50S ribosomal protein L29

Chain 22:

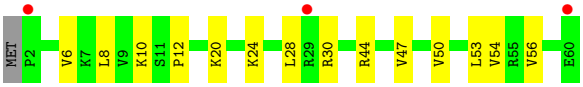



• Molecule 25: 50S ribosomal protein L30

Chain 13:

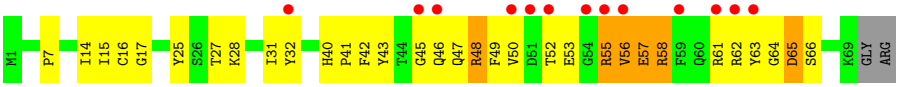
• Molecule 25: 50S ribosomal protein L30

Chain 23:



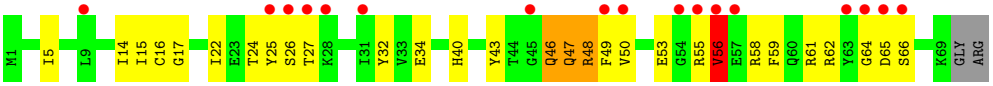

• Molecule 26: 50S ribosomal protein L31

Chain 14:




• Molecule 26: 50S ribosomal protein L31

Chain 24:

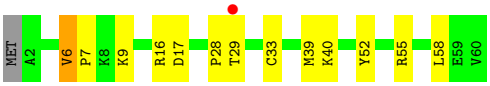



• Molecule 27: 50S ribosomal protein L32

Chain 15:

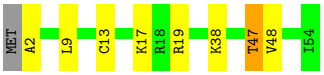
• Molecule 27: 50S ribosomal protein L32

Chain 25:



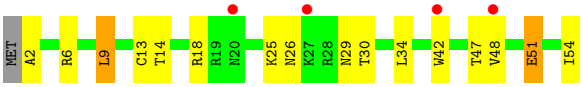

• Molecule 28: 50S ribosomal protein L33

Chain 16:



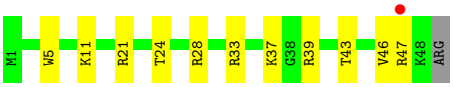

• Molecule 28: 50S ribosomal protein L33

Chain 26:



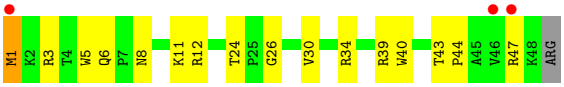

• Molecule 29: 50S ribosomal protein L34

Chain 17:



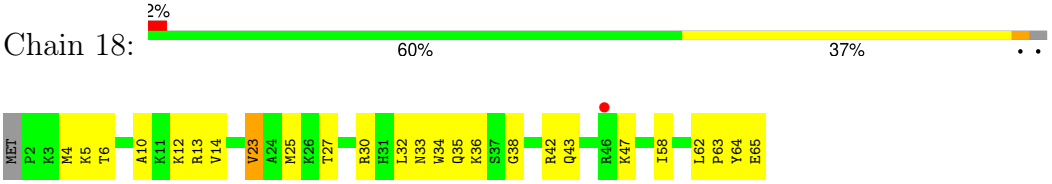

• Molecule 29: 50S ribosomal protein L34

Chain 27:



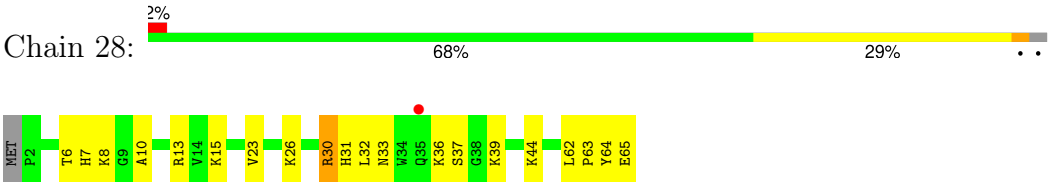

• Molecule 30: 50S ribosomal protein L35

Chain 18:



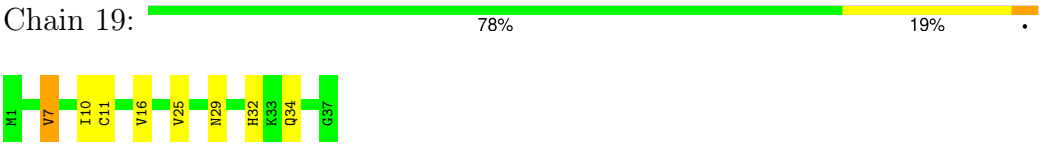

• Molecule 30: 50S ribosomal protein L35

Chain 28:



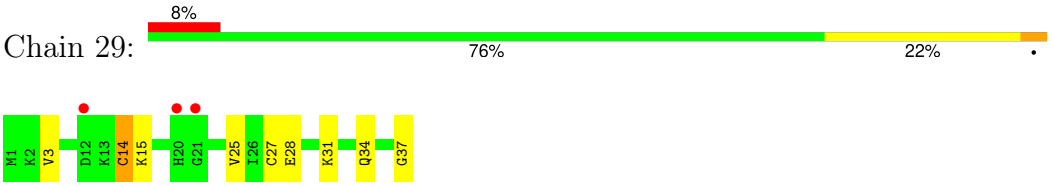

• Molecule 31: 50S ribosomal protein L36

Chain 19:



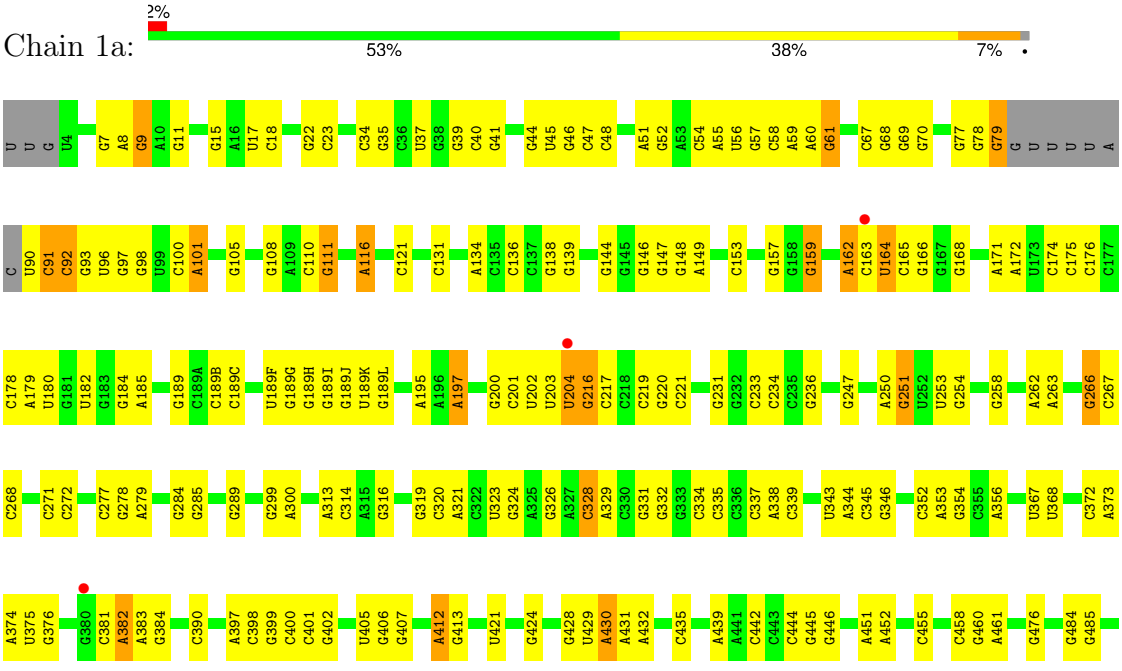

• Molecule 31: 50S ribosomal protein L36

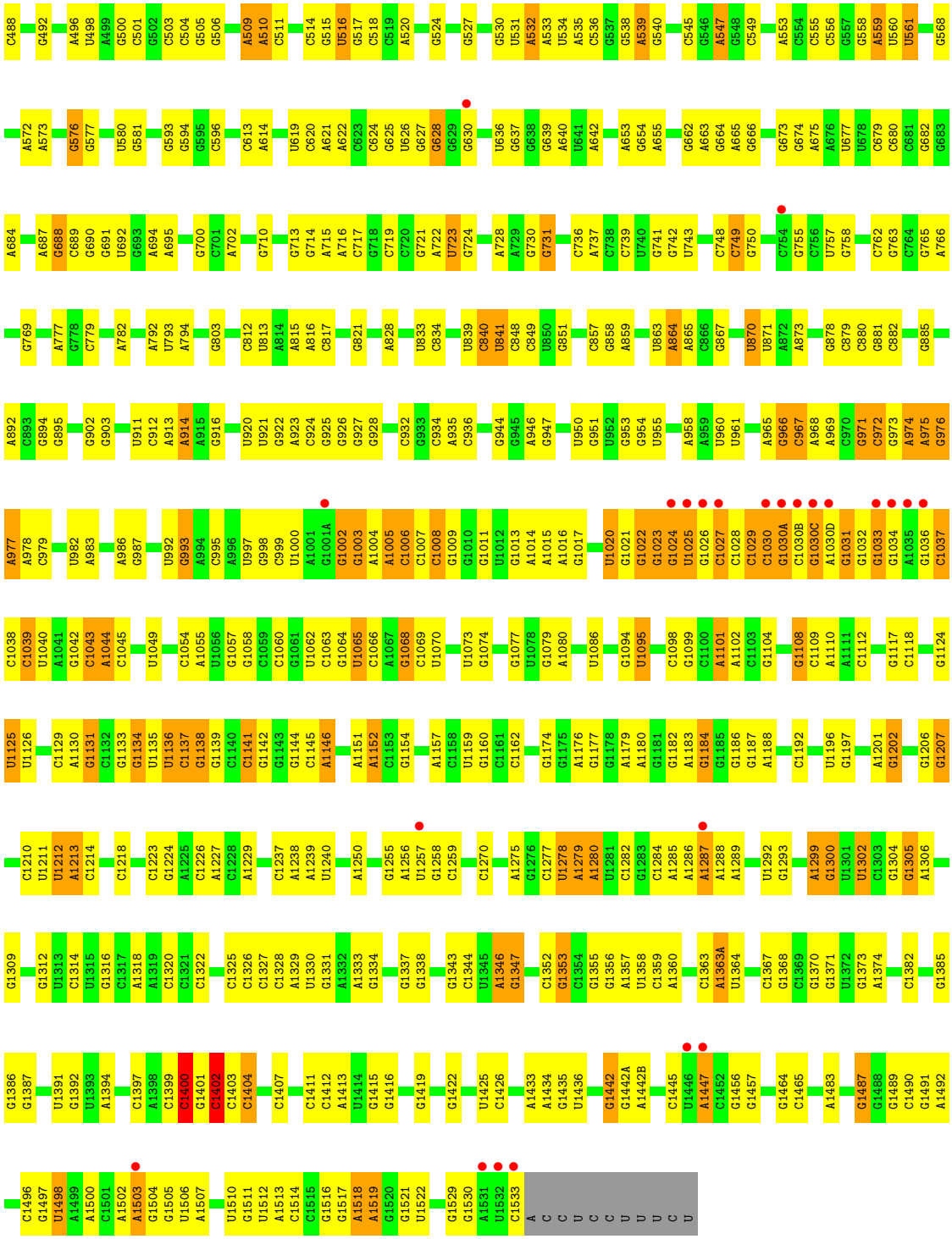
Chain 29:




• Molecule 32: 16S Ribosomal RNA

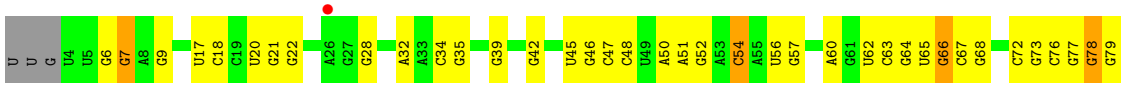
Chain 1a:

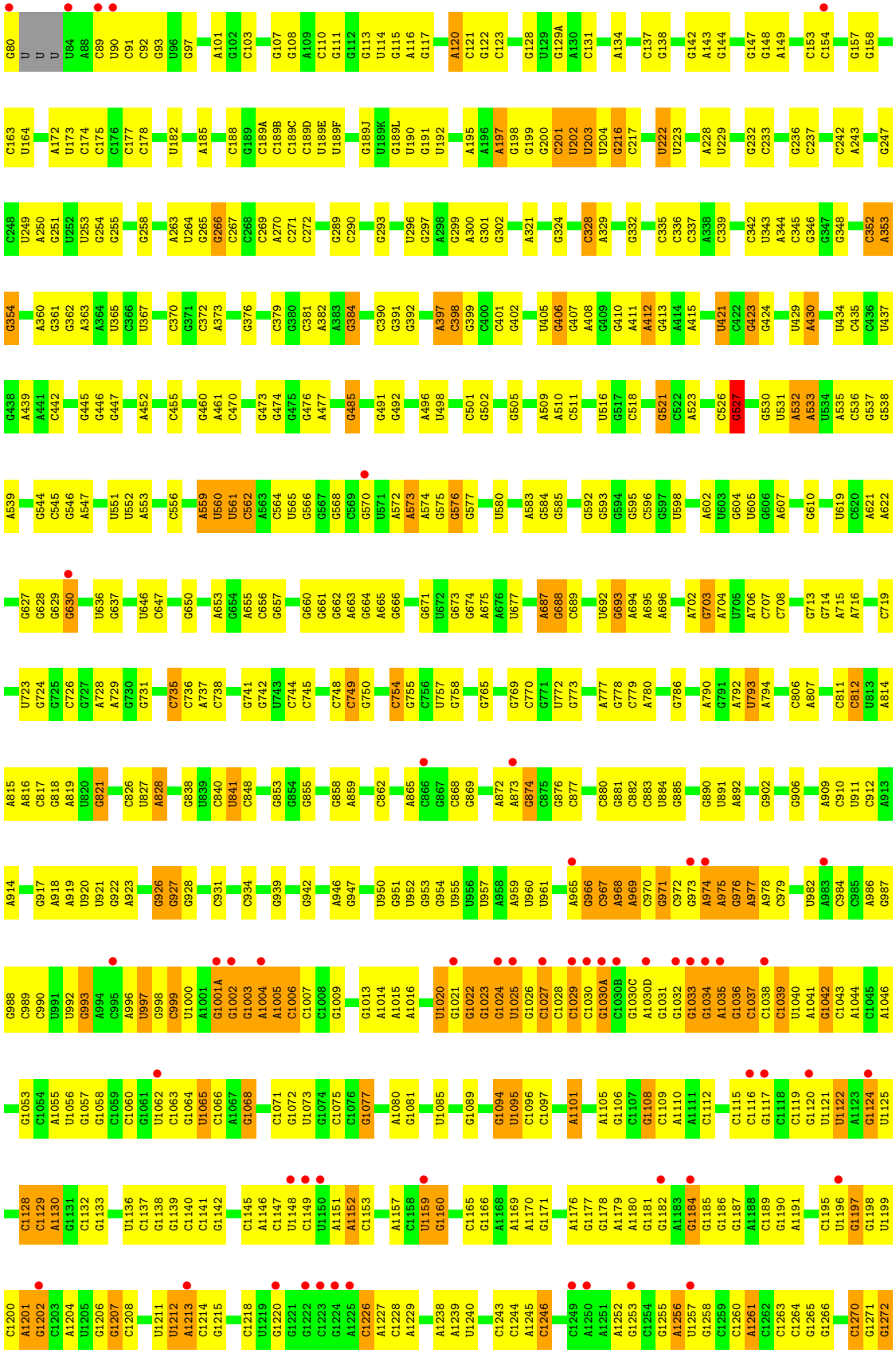




• Molecule 32: 16S Ribosomal RNA

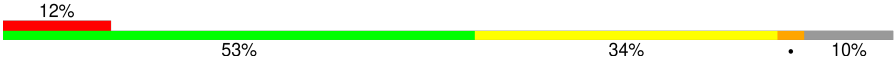
Chain 2a:

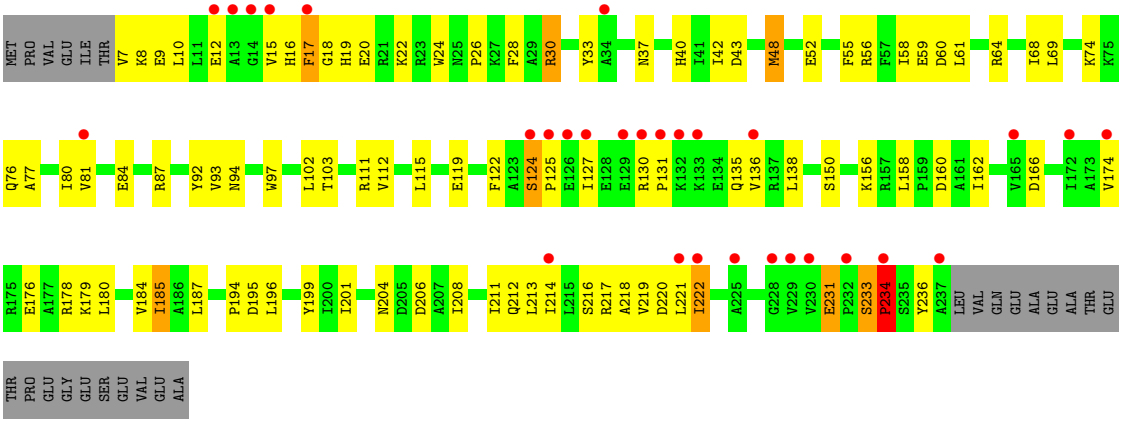




• Molecule 33: 30S ribosomal protein S2

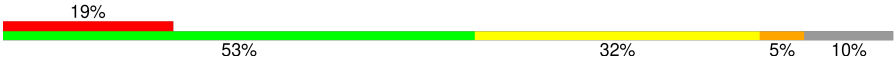
Chain 1b:

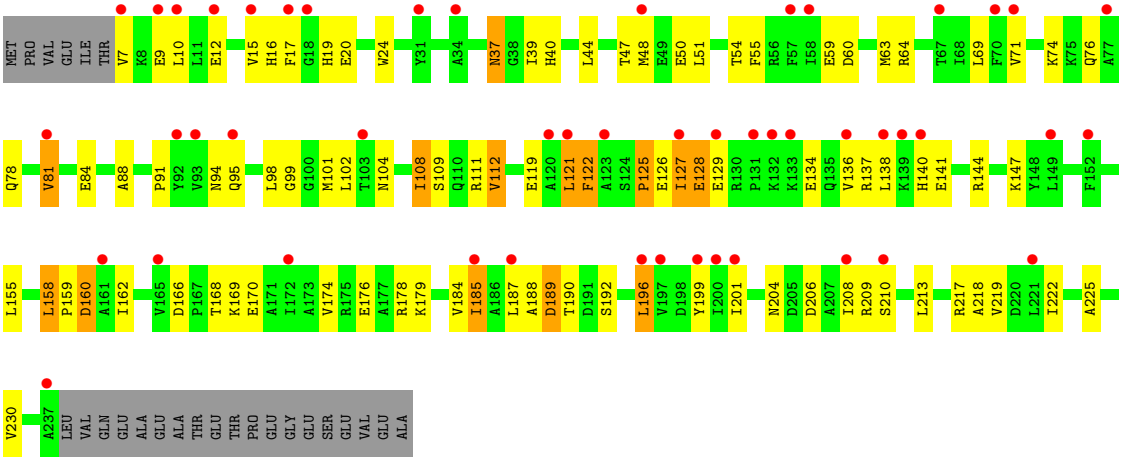


• Molecule 33: 30S ribosomal protein S2

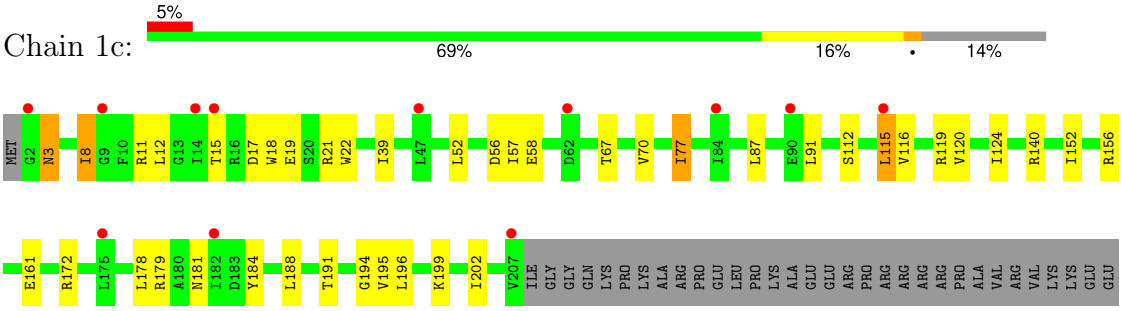
Chain 2b:



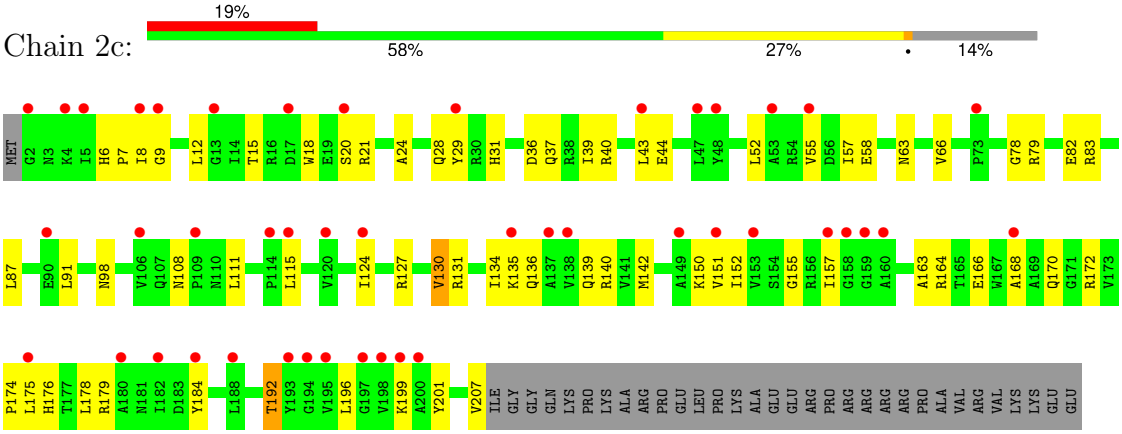
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



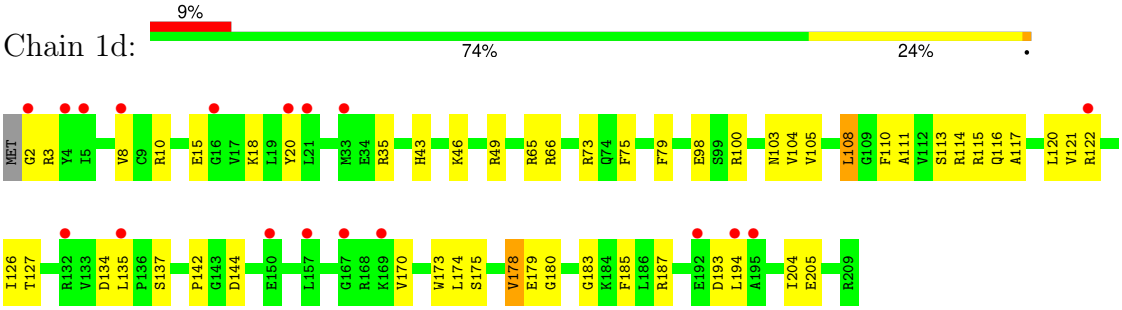

• Molecule 34: 30S ribosomal protein S3

Chain 2c:



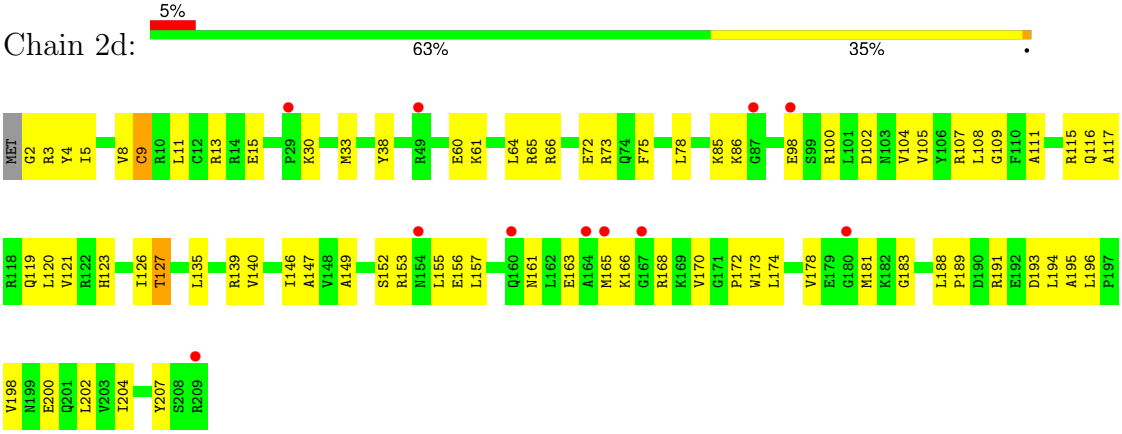

• Molecule 35: 30S ribosomal protein S4

Chain 1d:



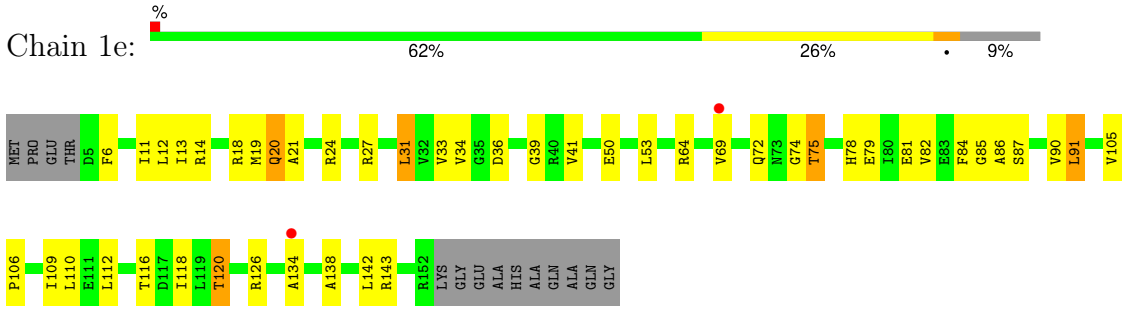

• Molecule 35: 30S ribosomal protein S4

Chain 2d:



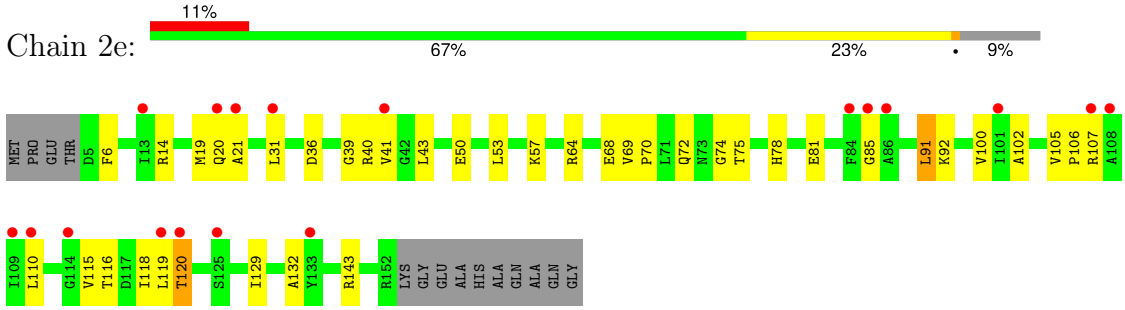
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



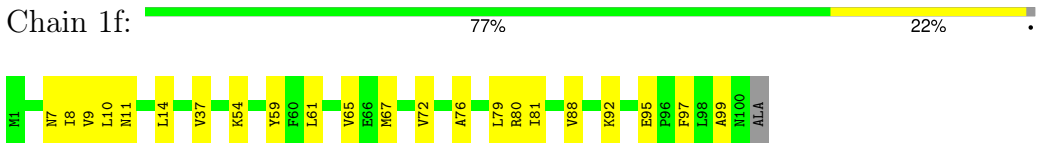

• Molecule 36: 30S ribosomal protein S5

Chain 2e:



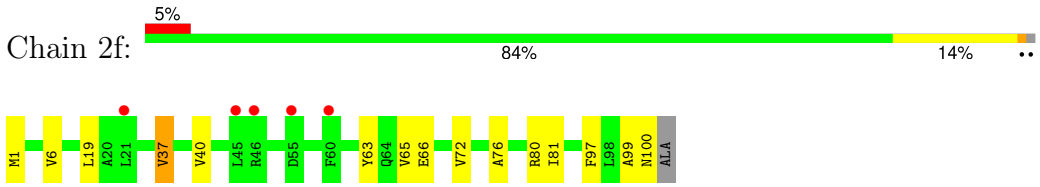

• Molecule 37: 30S ribosomal protein S6

Chain 1f:



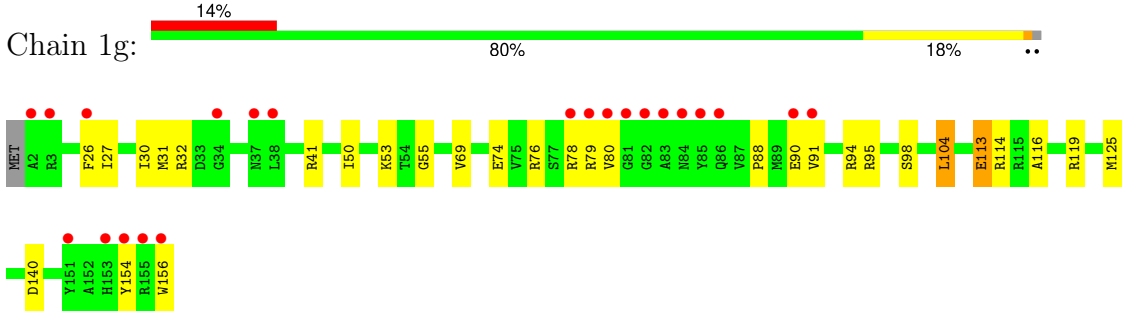

• Molecule 37: 30S ribosomal protein S6

Chain 2f:



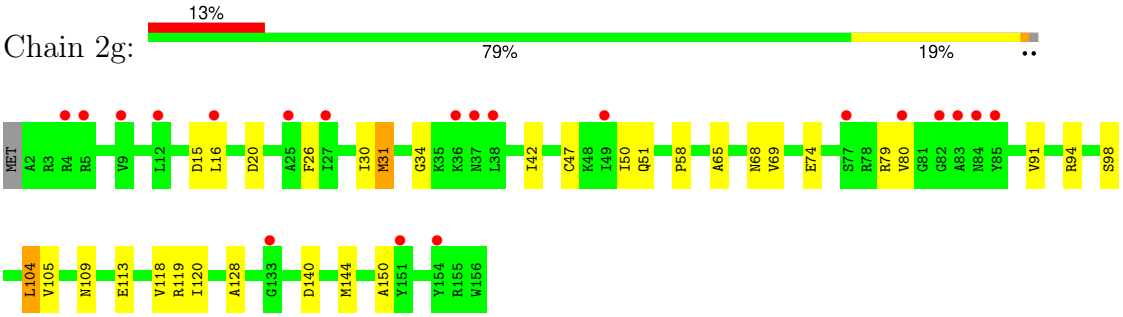

• Molecule 38: 30S ribosomal protein S7

Chain 1g:



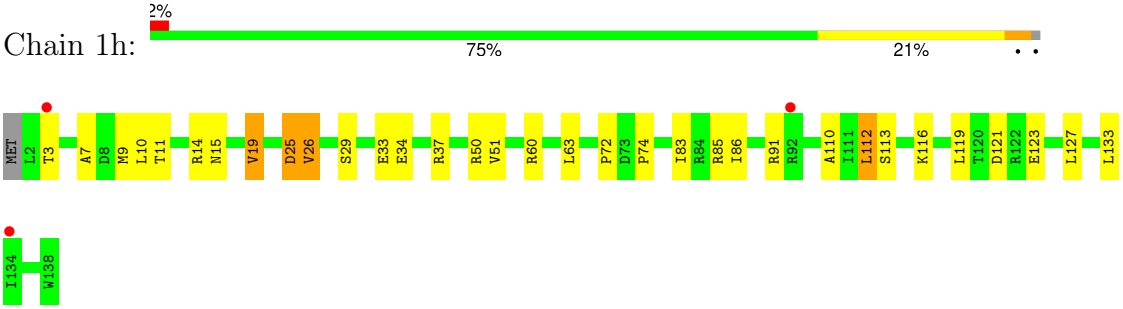

• Molecule 38: 30S ribosomal protein S7

Chain 2g:



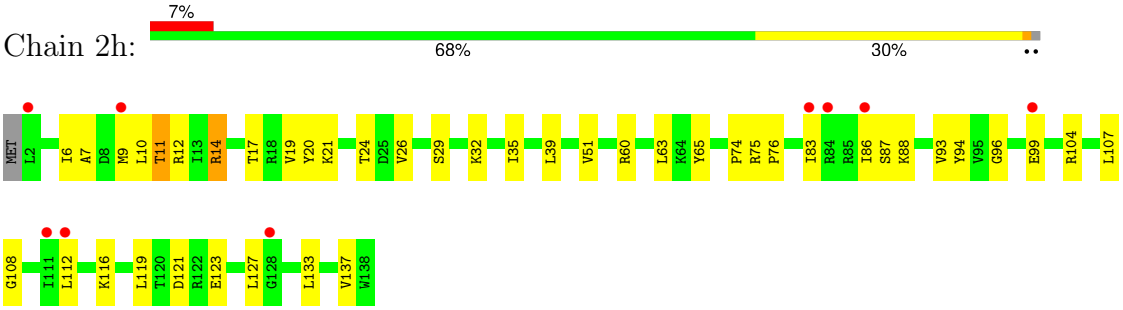

• Molecule 39: 30S ribosomal protein S8

Chain 1h:



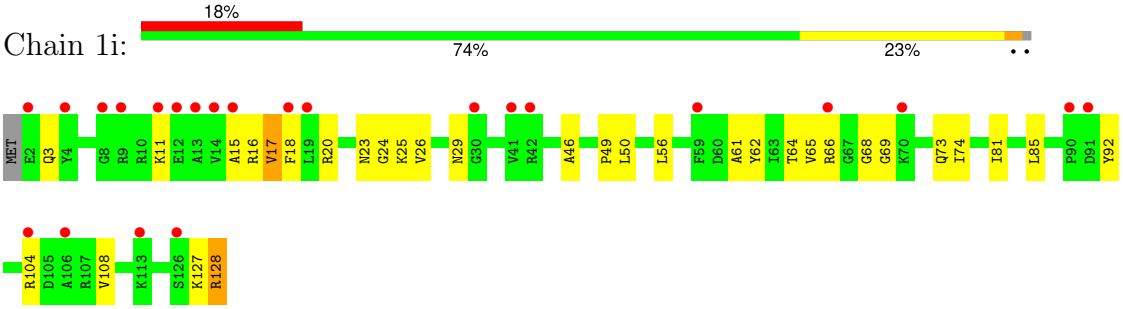

• Molecule 39: 30S ribosomal protein S8

Chain 2h:



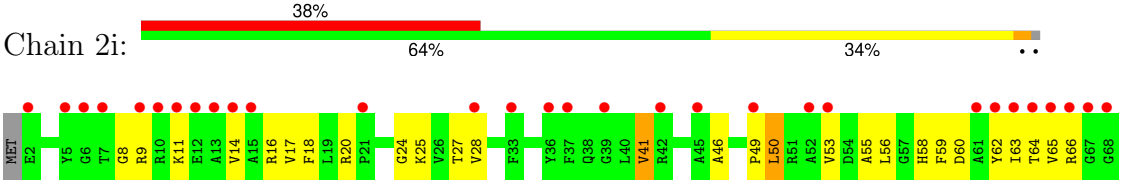

• Molecule 40: 30S ribosomal protein S9

Chain 1i:



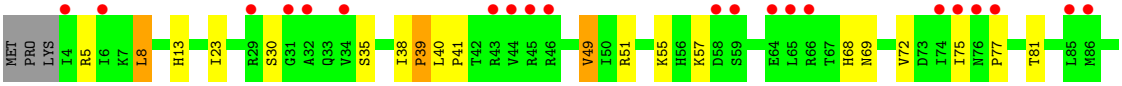

• Molecule 40: 30S ribosomal protein S9

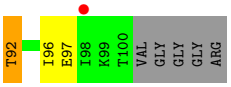
Chain 2i:



• Molecule 41: 30S ribosomal protein S10

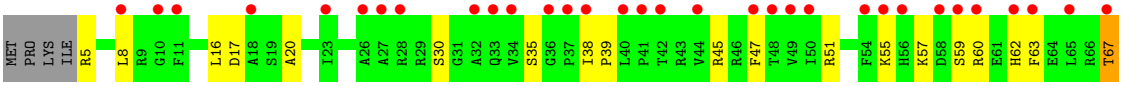
Chain 1j:

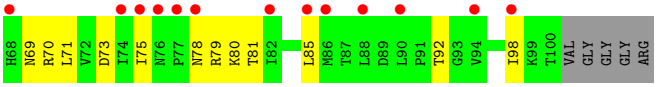



• Molecule 41: 30S ribosomal protein S10

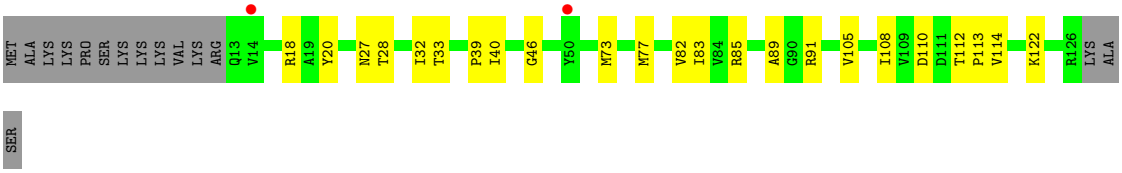
Chain 2j:



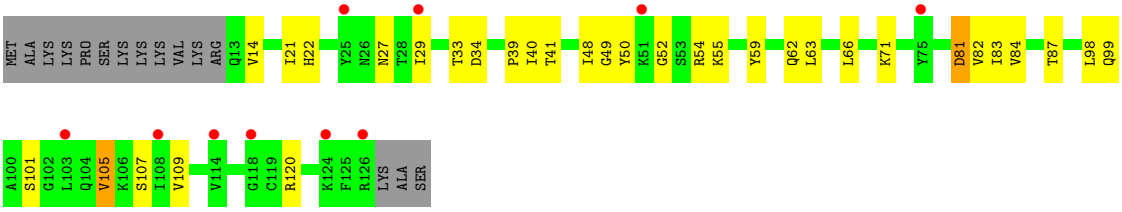

• Molecule 42: 30S ribosomal protein S11

Chain 1k:




• Molecule 42: 30S ribosomal protein S11

Chain 2k:

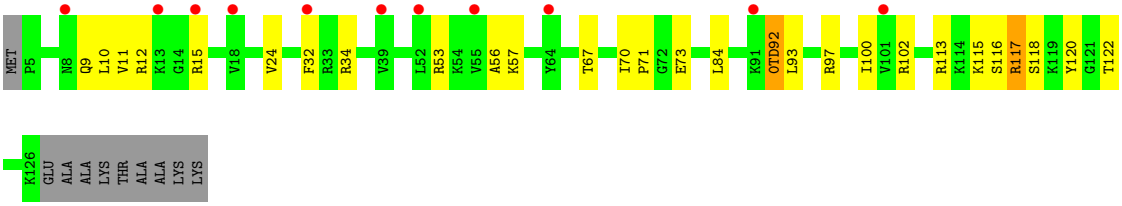



• Molecule 43: 30S ribosomal protein S12

Chain 1l:

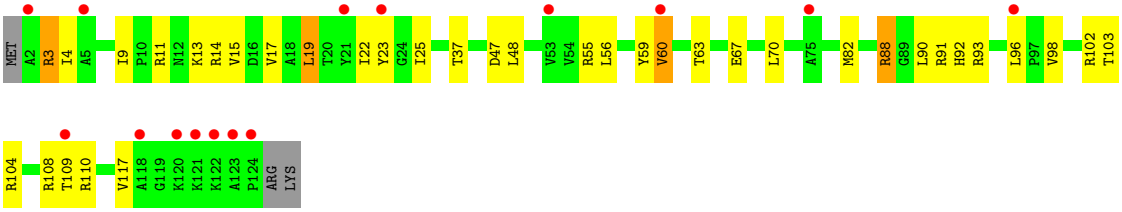
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



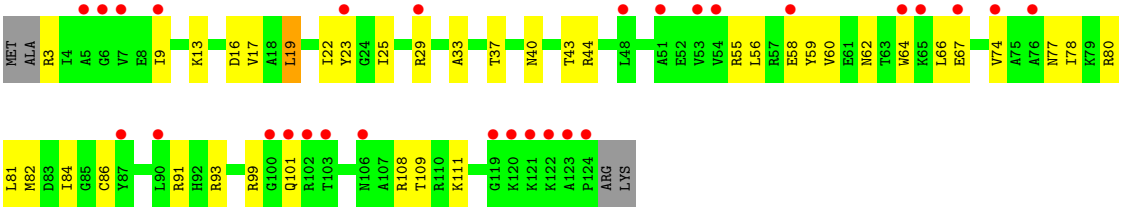

• Molecule 44: 30S ribosomal protein S13

Chain 1m:



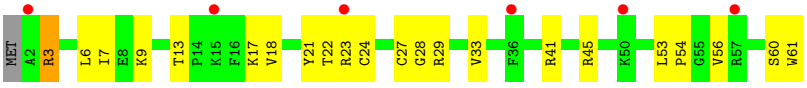

• Molecule 44: 30S ribosomal protein S13

Chain 2m:



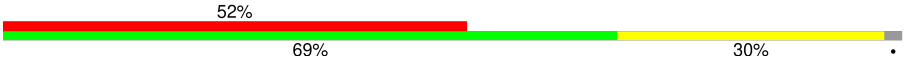

• Molecule 45: 30S ribosomal protein S14 type Z

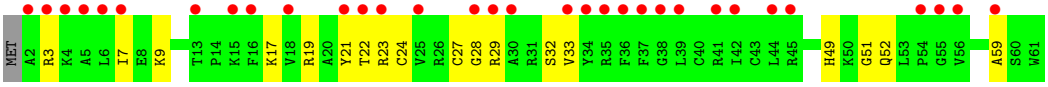
Chain 1n:




• Molecule 45: 30S ribosomal protein S14 type Z

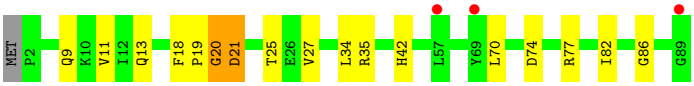
Chain 2n:






• Molecule 46: 30S ribosomal protein S15

Chain 1o:

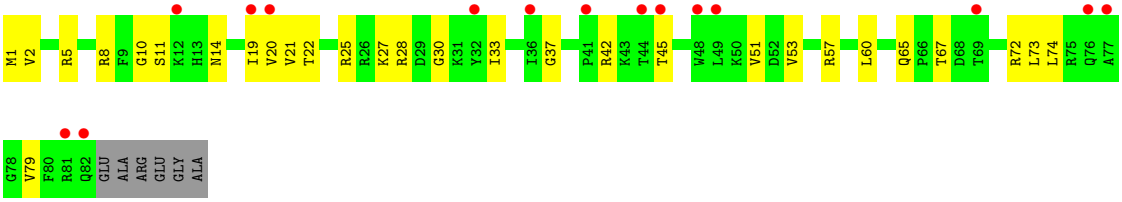



• Molecule 46: 30S ribosomal protein S15

Chain 2o:

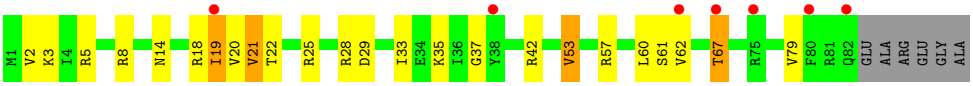
• Molecule 47: 30S ribosomal protein S16

Chain 1p:




• Molecule 47: 30S ribosomal protein S16

Chain 2p:

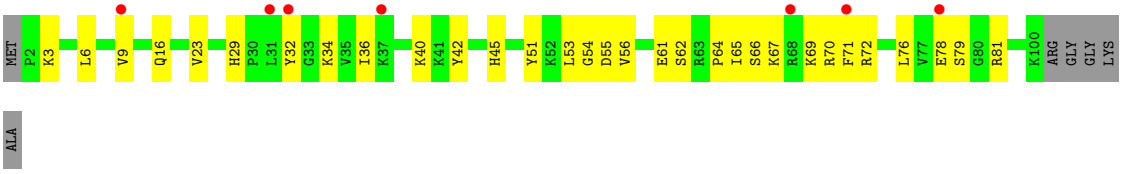



• Molecule 48: 30S ribosomal protein S17

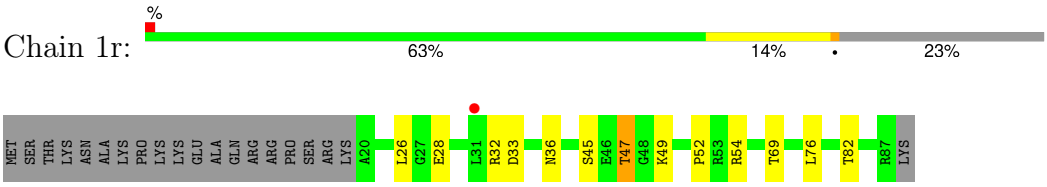
Chain 1q:

• Molecule 48: 30S ribosomal protein S17

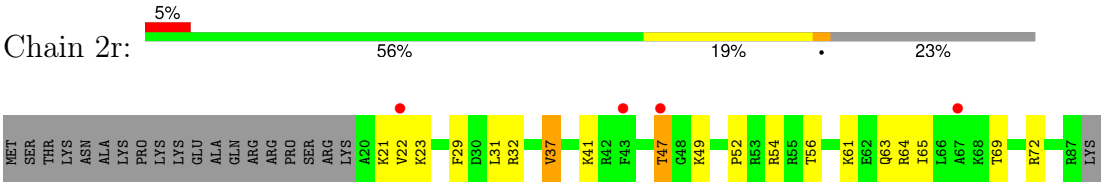
Chain 2q:



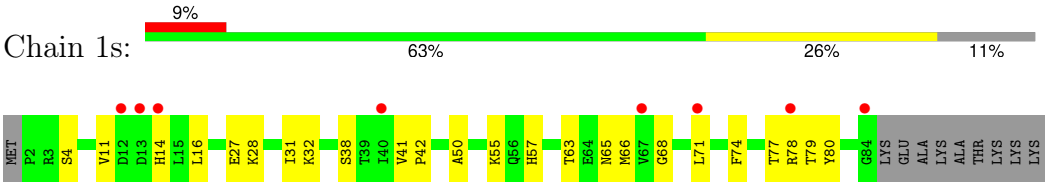

• Molecule 49: 30S ribosomal protein S18



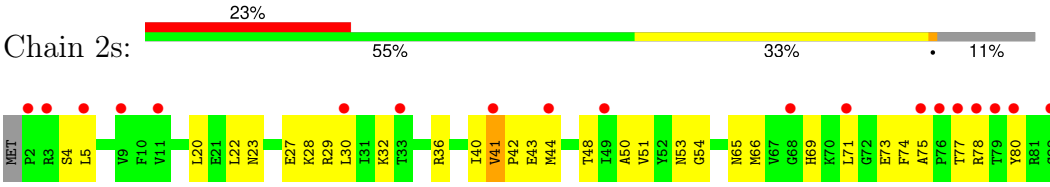

• Molecule 49: 30S ribosomal protein S18



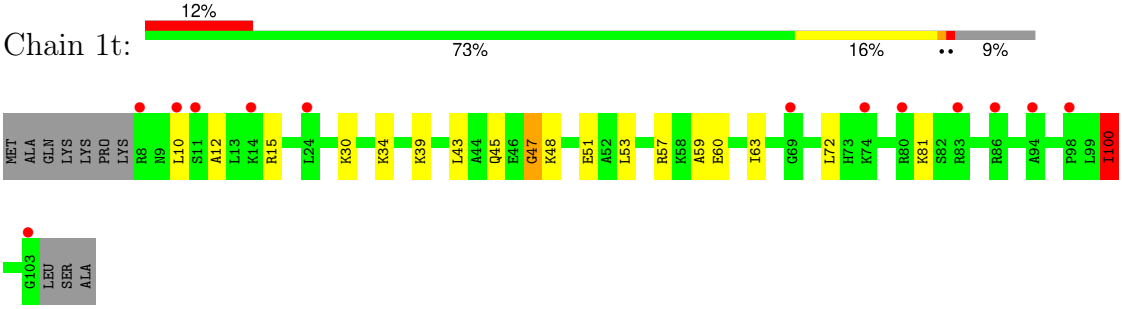

• Molecule 50: 30S ribosomal protein S19




• Molecule 50: 30S ribosomal protein S19

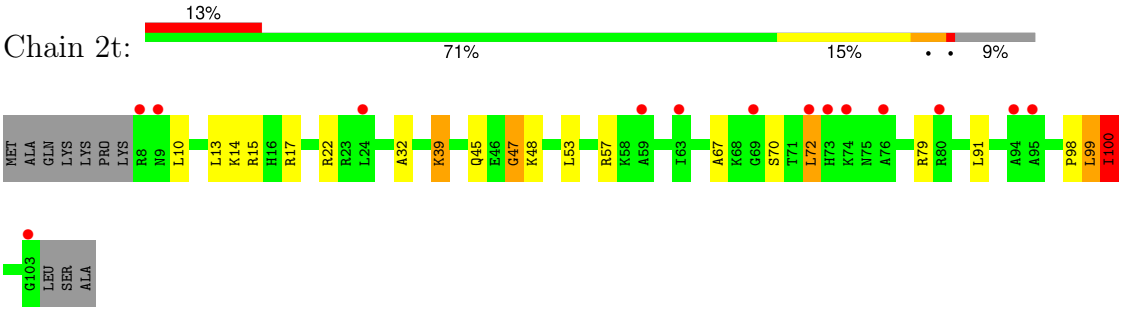



• Molecule 51: 30S ribosomal protein S20




• Molecule 51: 30S ribosomal protein S20

Chain 2t:

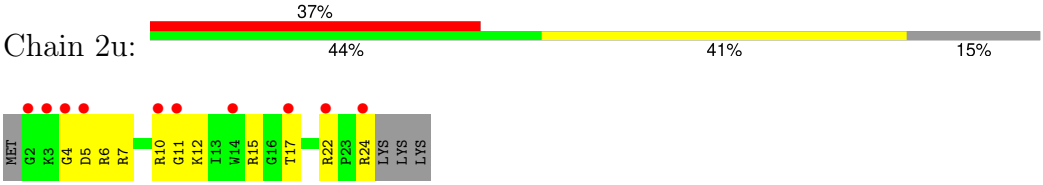



• Molecule 52: 30S ribosomal protein Thx

Chain 1u:

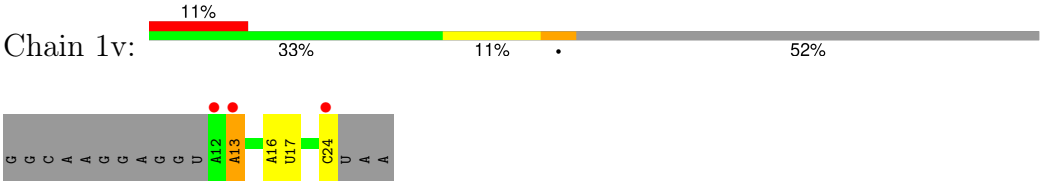
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



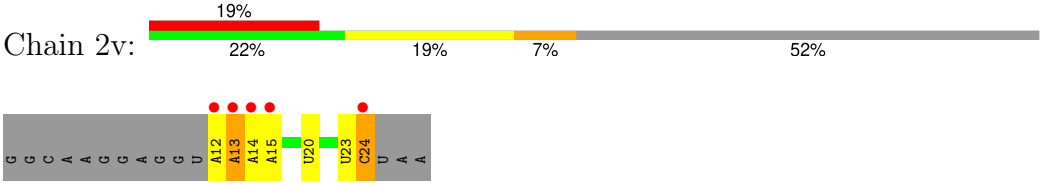

• Molecule 53: mRNA

Chain 1v:



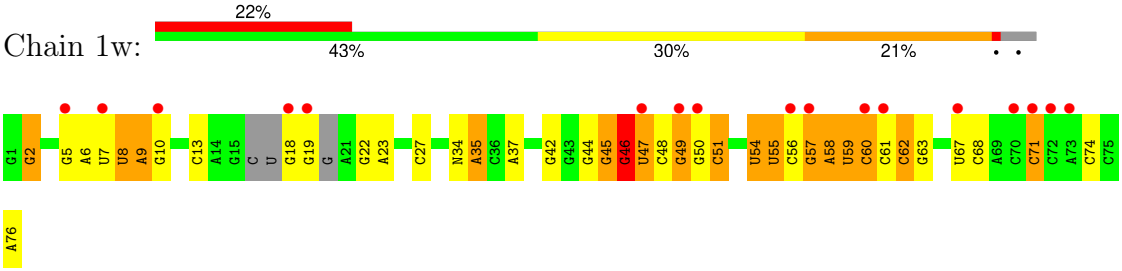

• Molecule 53: mRNA

Chain 2v:



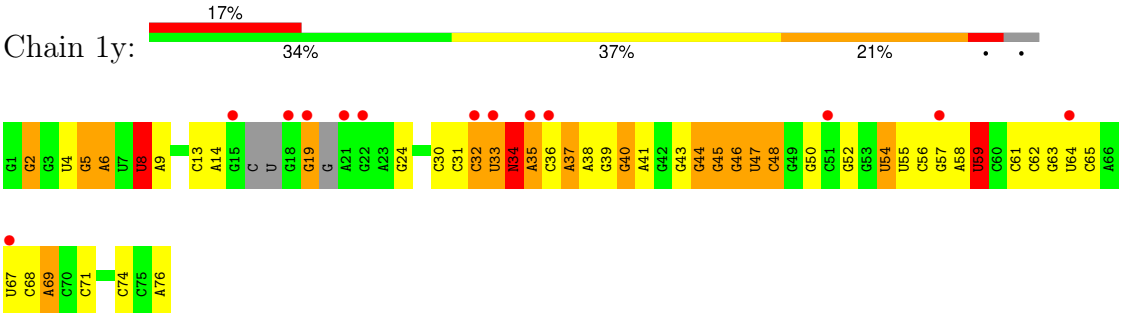

• Molecule 54: A-site and E-site tRNAs

Chain 1w:



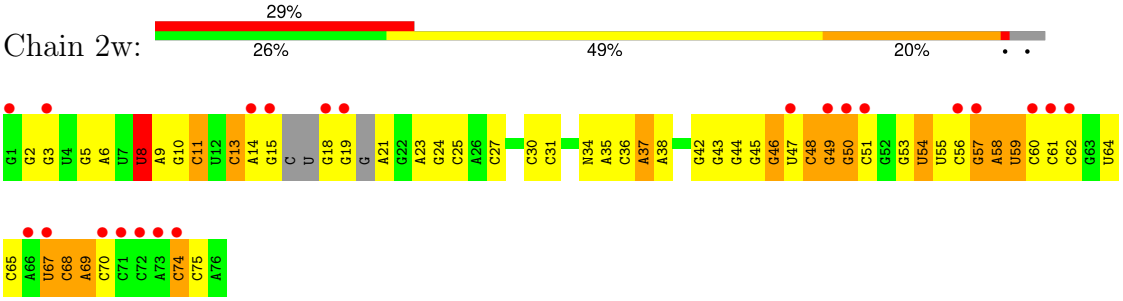

• Molecule 54: A-site and E-site tRNAs

Chain 1y:



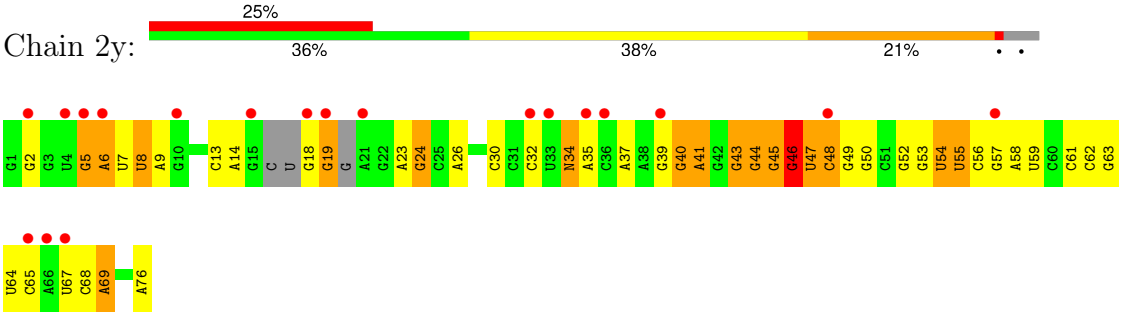

• Molecule 54: A-site and E-site tRNAs

Chain 2w:



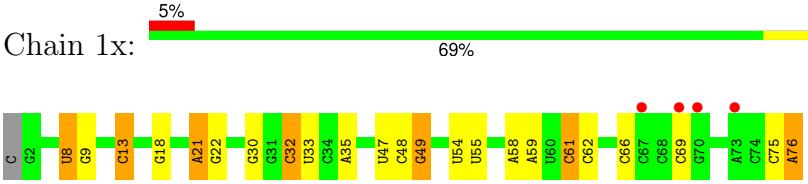

• Molecule 54: A-site and E-site tRNAs

Chain 2y:



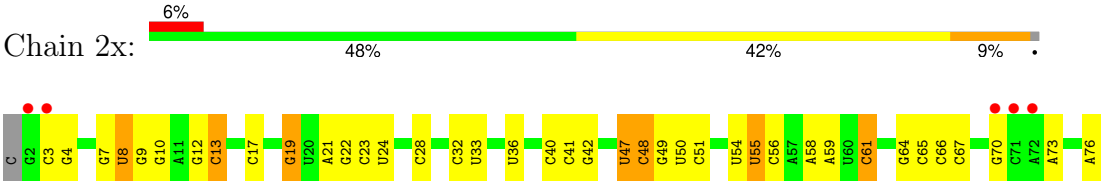

• Molecule 55: P-site tRNA

Chain 1x:




• Molecule 55: P-site tRNA

Chain 2x:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 209.02Å 447.76Å 618.39Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 254.43 – 2.75<br>254.43 – 2.75 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.5 (254.43-2.75)<br>99.5 (254.43-2.75) | Depositor<br>EDS |
| $R_{merge}$ | 0.21 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.16 (at 2.73Å) | Xtriage |
| Refinement program | PHENIX 1.8.2 | Depositor |
| R, $R_{free}$ | 0.235 , 0.284<br>0.237 , 0.282 | Depositor<br>DCC |
| $R_{free}$ test set | 74125 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 52.4 | Xtriage |
| Anisotropy | 0.169 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 60.0 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.39$, $< L^2 > = 0.21$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.88 | EDS |
| Total number of atoms | 300702 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 53.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 4OC, 5MU, 2MG, OMG, 0TD, 4SU, OMU, PSU, OMC, UR3, 2MA, MA6, MG, 7MG, LUJ, ZN, CM0, 6MZ, SF4, K, M2G

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 1A | 0.19 | 0/69011 | 0.36 | 0/107720 |
| 1 | 2A | 0.15 | 0/67295 | 0.32 | 0/105042 |
| 2 | 1B | 0.16 | 0/2882 | 0.32 | 0/4494 |
| 2 | 2B | 0.13 | 0/2879 | 0.30 | 0/4487 |
| 3 | 1D | 0.18 | 0/2186 | 0.43 | 0/2944 |
| 3 | 2D | 0.16 | 0/2186 | 0.42 | 0/2944 |
| 4 | 1E | 0.20 | 0/1592 | 0.42 | 0/2149 |
| 4 | 2E | 0.15 | 0/1592 | 0.39 | 0/2149 |
| 5 | 1F | 0.17 | 0/1619 | 0.40 | 0/2193 |
| 5 | 2F | 0.15 | 0/1615 | 0.37 | 0/2188 |
| 6 | 1G | 0.16 | 0/1448 | 0.38 | 0/1957 |
| 6 | 2G | 0.15 | 0/1453 | 0.39 | 0/1963 |
| 7 | 1H | 0.16 | 0/1356 | 0.37 | 0/1834 |
| 7 | 2H | 0.14 | 0/1356 | 0.32 | 0/1834 |
| 8 | 1I | 0.14 | 0/1112 | 0.35 | 0/1514 |
| 8 | 2I | 0.13 | 0/1079 | 0.34 | 0/1475 |
| 9 | 1N | 0.17 | 0/1144 | 0.38 | 0/1543 |
| 9 | 2N | 0.15 | 0/1144 | 0.35 | 0/1543 |
| 10 | 1O | 0.18 | 0/943 | 0.38 | 0/1269 |
| 10 | 2O | 0.14 | 0/943 | 0.36 | 0/1269 |
| 11 | 1P | 0.19 | 0/1152 | 0.41 | 0/1533 |
| 11 | 2P | 0.16 | 0/1152 | 0.38 | 0/1533 |
| 12 | 1Q | 0.20 | 0/1143 | 0.38 | 0/1527 |
| 12 | 2Q | 0.14 | 0/1143 | 0.35 | 0/1527 |
| 13 | 1R | 0.21 | 0/982 | 0.40 | 0/1312 |
| 13 | 2R | 0.15 | 0/982 | 0.39 | 0/1312 |
| 14 | 1S | 0.14 | 0/883 | 0.38 | 0/1176 |
| 14 | 2S | 0.14 | 0/880 | 0.37 | 0/1172 |
| 15 | 1T | 0.19 | 0/1105 | 0.48 | 1/1477 (0.1%) |
| 15 | 2T | 0.14 | 0/1097 | 0.38 | 0/1468 |
| 16 | 1U | 0.20 | 0/977 | 0.40 | 0/1301 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 16 | 2U | 0.15 | 0/977 | 0.37 | 0/1301 |
| 17 | 1V | 0.19 | 0/782 | 0.39 | 0/1049 |
| 17 | 2V | 0.14 | 0/782 | 0.35 | 0/1049 |
| 18 | 1W | 0.19 | 0/897 | 0.37 | 0/1205 |
| 18 | 2W | 0.14 | 0/897 | 0.34 | 0/1205 |
| 19 | 1X | 0.19 | 0/764 | 0.45 | 0/1025 |
| 19 | 2X | 0.14 | 0/764 | 0.37 | 0/1025 |
| 20 | 1Y | 0.24 | 0/819 | 0.42 | 0/1095 |
| 20 | 2Y | 0.14 | 0/819 | 0.39 | 0/1095 |
| 21 | 1Z | 0.17 | 0/1267 | 0.44 | 0/1717 |
| 21 | 2Z | 0.17 | 0/1299 | 0.41 | 0/1763 |
| 22 | 10 | 0.18 | 0/662 | 0.43 | 0/881 |
| 22 | 20 | 0.15 | 0/662 | 0.39 | 0/881 |
| 23 | 11 | 0.16 | 0/762 | 0.34 | 0/1014 |
| 23 | 21 | 0.15 | 0/762 | 0.37 | 0/1014 |
| 24 | 12 | 0.20 | 0/590 | 0.42 | 1/781 (0.1%) |
| 24 | 22 | 0.14 | 0/590 | 0.34 | 0/781 |
| 25 | 13 | 0.18 | 0/474 | 0.39 | 0/635 |
| 25 | 23 | 0.13 | 0/469 | 0.35 | 0/630 |
| 26 | 14 | 0.21 | 0/565 | 0.54 | 0/761 |
| 26 | 24 | 0.17 | 0/545 | 0.52 | 0/737 |
| 27 | 15 | 0.22 | 0/469 | 0.44 | 0/635 |
| 27 | 25 | 0.18 | 0/469 | 0.44 | 0/635 |
| 28 | 16 | 0.19 | 0/460 | 0.40 | 0/613 |
| 28 | 26 | 0.16 | 0/456 | 0.41 | 0/608 |
| 29 | 17 | 0.19 | 0/426 | 0.45 | 0/561 |
| 29 | 27 | 0.18 | 0/426 | 0.45 | 0/561 |
| 30 | 18 | 0.19 | 0/525 | 0.37 | 0/691 |
| 30 | 28 | 0.14 | 0/525 | 0.35 | 0/691 |
| 31 | 19 | 0.18 | 0/310 | 0.51 | 0/407 |
| 31 | 29 | 0.13 | 0/310 | 0.36 | 0/407 |
| 32 | 1a | 0.15 | 0/35795 | 0.32 | 0/55864 |
| 32 | 2a | 0.14 | 0/35886 | 0.32 | 0/56005 |
| 33 | 1b | 0.27 | 0/1881 | 0.51 | 2/2542 (0.1%) |
| 33 | 2b | 0.17 | 0/1860 | 0.42 | 0/2518 |
| 34 | 1c | 0.15 | 0/1572 | 0.38 | 0/2126 |
| 34 | 2c | 0.14 | 0/1566 | 0.36 | 0/2119 |
| 35 | 1d | 0.18 | 0/1685 | 0.37 | 0/2262 |
| 35 | 2d | 0.16 | 0/1704 | 0.38 | 0/2284 |
| 36 | 1e | 0.15 | 0/1145 | 0.40 | 0/1543 |
| 36 | 2e | 0.16 | 0/1149 | 0.42 | 0/1548 |
| 37 | 1f | 0.13 | 0/823 | 0.33 | 0/1115 |
| 37 | 2f | 0.15 | 0/829 | 0.35 | 0/1123 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | 1g | 0.15 | 0/1250 | 0.36 | 0/1679 |
| 38 | 2g | 0.14 | 0/1254 | 0.35 | 0/1683 |
| 39 | 1h | 0.14 | 0/1108 | 0.36 | 0/1494 |
| 39 | 2h | 0.13 | 0/1108 | 0.37 | 0/1494 |
| 40 | 1i | 0.16 | 0/1002 | 0.43 | 0/1346 |
| 40 | 2i | 0.17 | 0/997 | 0.46 | 1/1343 (0.1%) |
| 41 | 1j | 0.14 | 0/722 | 0.37 | 0/982 |
| 41 | 2j | 0.19 | 0/727 | 0.42 | 0/988 |
| 42 | 1k | 0.13 | 0/844 | 0.32 | 0/1145 |
| 42 | 2k | 0.15 | 0/848 | 0.33 | 0/1149 |
| 43 | 1l | 0.15 | 0/937 | 0.36 | 0/1260 |
| 43 | 2l | 0.16 | 0/937 | 0.41 | 0/1260 |
| 44 | 1m | 0.15 | 0/969 | 0.39 | 0/1302 |
| 44 | 2m | 0.16 | 0/961 | 0.38 | 0/1291 |
| 45 | 1n | 0.15 | 0/501 | 0.37 | 0/664 |
| 45 | 2n | 0.17 | 0/501 | 0.39 | 0/664 |
| 46 | 1o | 0.15 | 0/739 | 0.35 | 0/985 |
| 46 | 2o | 0.12 | 0/739 | 0.34 | 0/985 |
| 47 | 1p | 0.13 | 0/697 | 0.41 | 0/939 |
| 47 | 2p | 0.14 | 0/693 | 0.40 | 0/935 |
| 48 | 1q | 0.13 | 0/836 | 0.37 | 0/1117 |
| 48 | 2q | 0.15 | 0/836 | 0.36 | 0/1117 |
| 49 | 1r | 0.14 | 0/560 | 0.37 | 0/746 |
| 49 | 2r | 0.14 | 0/560 | 0.34 | 0/746 |
| 50 | 1s | 0.20 | 0/667 | 0.45 | 0/900 |
| 50 | 2s | 0.20 | 0/661 | 0.50 | 0/893 |
| 51 | 1t | 0.16 | 0/730 | 0.44 | 0/965 |
| 51 | 2t | 0.17 | 0/729 | 0.45 | 0/965 |
| 52 | 1u | 0.15 | 0/203 | 0.37 | 0/266 |
| 52 | 2u | 0.15 | 0/203 | 0.40 | 0/266 |
| 53 | 1v | 0.18 | 0/308 | 0.31 | 0/477 |
| 53 | 2v | 0.16 | 0/308 | 0.33 | 0/477 |
| 54 | 1w | 0.30 | 2/1600 (0.1%) | 0.39 | 0/2482 |
| 54 | 1y | 0.30 | 3/1600 (0.2%) | 0.38 | 0/2482 |
| 54 | 2w | 0.22 | 0/1600 | 0.37 | 0/2482 |
| 54 | 2y | 0.22 | 1/1600 (0.1%) | 0.35 | 0/2482 |
| 55 | 1x | 0.21 | 0/1725 | 0.35 | 0/2689 |
| 55 | 2x | 0.20 | 0/1725 | 0.35 | 0/2689 |
| All | All | 0.17 | 6/316735 (0.0%) | 0.35 | 5/474180 (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 |
| 33 | 1b | 0 | 1 |
| All | All | 0 | 2 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | 1y | 8 | 4SU | O3'-P | 5.31 | 1.61 | 1.56 |
| 54 | 1w | 59 | U | C4-O4 | 5.27 | 1.34 | 1.23 |
| 54 | 1y | 59 | U | C4-O4 | 5.21 | 1.34 | 1.23 |
| 54 | 2y | 8 | 4SU | O3'-P | 5.19 | 1.61 | 1.56 |
| 54 | 1y | 32 | C | C4-N4 | -5.08 | 1.23 | 1.33 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 40 | 2i | 53 | VAL | N-CA-C | -7.39 | 105.35 | 112.29 |
| 24 | 12 | 41 | ILE | N-CA-C | -6.21 | 105.66 | 112.80 |
| 15 | 1T | 89 | VAL | N-CA-C | -5.61 | 106.86 | 113.42 |
| 33 | 1b | 231 | GLU | CA-C-N | -5.37 | 114.25 | 119.78 |
| 33 | 1b | 231 | GLU | C-N-CA | -5.37 | 114.25 | 119.78 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 26 | 14 | 63 | TYR | Peptide |
| 33 | 1b | 124 | SER | 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 | 61852 | 0 | 31189 | 746 | 0 |
| 1 | 2A | 60322 | 0 | 30428 | 786 | 0 |
| 2 | 1B | 2577 | 0 | 1305 | 25 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | 2B | 2575 | 0 | 1303 | 29 | 0 |
| 3 | 1D | 2136 | 0 | 2218 | 52 | 0 |
| 3 | 2D | 2136 | 0 | 2218 | 54 | 0 |
| 4 | 1E | 1559 | 0 | 1618 | 41 | 0 |
| 4 | 2E | 1559 | 0 | 1618 | 37 | 0 |
| 5 | 1F | 1584 | 0 | 1625 | 28 | 0 |
| 5 | 2F | 1580 | 0 | 1619 | 43 | 0 |
| 6 | 1G | 1423 | 0 | 1436 | 39 | 0 |
| 6 | 2G | 1428 | 0 | 1438 | 30 | 0 |
| 7 | 1H | 1330 | 0 | 1407 | 26 | 0 |
| 7 | 2H | 1330 | 0 | 1407 | 28 | 0 |
| 8 | 1I | 1097 | 0 | 1140 | 25 | 0 |
| 8 | 2I | 1064 | 0 | 1082 | 17 | 0 |
| 9 | 1N | 1117 | 0 | 1184 | 19 | 0 |
| 9 | 2N | 1117 | 0 | 1184 | 28 | 0 |
| 10 | 1O | 933 | 0 | 996 | 22 | 0 |
| 10 | 2O | 933 | 0 | 996 | 20 | 0 |
| 11 | 1P | 1135 | 0 | 1212 | 33 | 0 |
| 11 | 2P | 1135 | 0 | 1212 | 25 | 0 |
| 12 | 1Q | 1122 | 0 | 1179 | 18 | 0 |
| 12 | 2Q | 1122 | 0 | 1179 | 32 | 0 |
| 13 | 1R | 968 | 0 | 1033 | 19 | 0 |
| 13 | 2R | 968 | 0 | 1033 | 28 | 0 |
| 14 | 1S | 873 | 0 | 927 | 18 | 0 |
| 14 | 2S | 870 | 0 | 923 | 20 | 0 |
| 15 | 1T | 1091 | 0 | 1151 | 29 | 0 |
| 15 | 2T | 1083 | 0 | 1136 | 38 | 0 |
| 16 | 1U | 959 | 0 | 1019 | 13 | 0 |
| 16 | 2U | 959 | 0 | 1019 | 20 | 0 |
| 17 | 1V | 771 | 0 | 830 | 12 | 0 |
| 17 | 2V | 771 | 0 | 830 | 12 | 0 |
| 18 | 1W | 886 | 0 | 940 | 19 | 0 |
| 18 | 2W | 886 | 0 | 940 | 13 | 0 |
| 19 | 1X | 750 | 0 | 814 | 21 | 0 |
| 19 | 2X | 750 | 0 | 814 | 21 | 0 |
| 20 | 1Y | 806 | 0 | 881 | 20 | 0 |
| 20 | 2Y | 806 | 0 | 881 | 16 | 0 |
| 21 | 1Z | 1240 | 0 | 1240 | 29 | 0 |
| 21 | 2Z | 1271 | 0 | 1273 | 36 | 0 |
| 22 | 10 | 653 | 0 | 674 | 13 | 0 |
| 22 | 20 | 653 | 0 | 674 | 19 | 0 |
| 23 | 11 | 755 | 0 | 826 | 19 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 23 | 21 | 755 | 0 | 826 | 22 | 0 |
| 24 | 12 | 588 | 0 | 643 | 5 | 0 |
| 24 | 22 | 588 | 0 | 643 | 11 | 0 |
| 25 | 13 | 469 | 0 | 518 | 13 | 0 |
| 25 | 23 | 464 | 0 | 514 | 6 | 0 |
| 26 | 14 | 552 | 0 | 533 | 23 | 0 |
| 26 | 24 | 532 | 0 | 503 | 20 | 0 |
| 27 | 15 | 455 | 0 | 465 | 12 | 0 |
| 27 | 25 | 455 | 0 | 465 | 9 | 0 |
| 28 | 16 | 453 | 0 | 472 | 5 | 0 |
| 28 | 26 | 449 | 0 | 469 | 10 | 0 |
| 29 | 17 | 418 | 0 | 467 | 7 | 0 |
| 29 | 27 | 418 | 0 | 467 | 11 | 0 |
| 30 | 18 | 517 | 0 | 582 | 23 | 0 |
| 30 | 28 | 517 | 0 | 582 | 18 | 0 |
| 31 | 19 | 307 | 0 | 335 | 6 | 0 |
| 31 | 29 | 307 | 0 | 335 | 7 | 0 |
| 32 | 1a | 32246 | 0 | 16295 | 453 | 0 |
| 32 | 2a | 32327 | 0 | 16338 | 514 | 0 |
| 33 | 1b | 1846 | 0 | 1867 | 69 | 0 |
| 33 | 2b | 1825 | 0 | 1828 | 67 | 0 |
| 34 | 1c | 1548 | 0 | 1535 | 23 | 0 |
| 34 | 2c | 1542 | 0 | 1517 | 46 | 0 |
| 35 | 1d | 1655 | 0 | 1672 | 36 | 0 |
| 35 | 2d | 1674 | 0 | 1714 | 52 | 0 |
| 36 | 1e | 1129 | 0 | 1185 | 32 | 0 |
| 36 | 2e | 1133 | 0 | 1191 | 26 | 0 |
| 37 | 1f | 810 | 0 | 804 | 14 | 0 |
| 37 | 2f | 816 | 0 | 808 | 8 | 0 |
| 38 | 1g | 1231 | 0 | 1238 | 22 | 0 |
| 38 | 2g | 1235 | 0 | 1249 | 23 | 0 |
| 39 | 1h | 1088 | 0 | 1126 | 22 | 0 |
| 39 | 2h | 1088 | 0 | 1126 | 30 | 0 |
| 40 | 1i | 983 | 0 | 986 | 23 | 0 |
| 40 | 2i | 978 | 0 | 966 | 32 | 0 |
| 41 | 1j | 709 | 0 | 650 | 14 | 0 |
| 41 | 2j | 714 | 0 | 672 | 21 | 0 |
| 42 | 1k | 829 | 0 | 825 | 13 | 0 |
| 42 | 2k | 833 | 0 | 836 | 20 | 0 |
| 43 | 1l | 932 | 0 | 981 | 16 | 0 |
| 43 | 2l | 932 | 0 | 981 | 24 | 0 |
| 44 | 1m | 958 | 0 | 1002 | 31 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 44 | 2m | 950 | 0 | 988 | 30 | 0 |
| 45 | 1n | 492 | 0 | 529 | 17 | 0 |
| 45 | 2n | 492 | 0 | 529 | 17 | 0 |
| 46 | 1o | 728 | 0 | 760 | 11 | 0 |
| 46 | 2o | 728 | 0 | 760 | 15 | 0 |
| 47 | 1p | 681 | 0 | 697 | 16 | 0 |
| 47 | 2p | 677 | 0 | 686 | 18 | 0 |
| 48 | 1q | 823 | 0 | 891 | 20 | 0 |
| 48 | 2q | 823 | 0 | 891 | 23 | 0 |
| 49 | 1r | 555 | 0 | 618 | 10 | 0 |
| 49 | 2r | 555 | 0 | 618 | 16 | 0 |
| 50 | 1s | 652 | 0 | 662 | 17 | 0 |
| 50 | 2s | 646 | 0 | 644 | 27 | 0 |
| 51 | 1t | 728 | 0 | 798 | 10 | 0 |
| 51 | 2t | 727 | 0 | 796 | 14 | 0 |
| 52 | 1u | 199 | 0 | 208 | 9 | 0 |
| 52 | 2u | 199 | 0 | 208 | 8 | 0 |
| 53 | 1v | 276 | 0 | 139 | 3 | 0 |
| 53 | 2v | 276 | 0 | 139 | 5 | 0 |
| 54 | 1w | 1568 | 0 | 800 | 28 | 0 |
| 54 | 1y | 1568 | 0 | 800 | 35 | 0 |
| 54 | 2w | 1568 | 0 | 802 | 39 | 0 |
| 54 | 2y | 1568 | 0 | 802 | 28 | 0 |
| 55 | 1x | 1625 | 0 | 827 | 12 | 0 |
| 55 | 2x | 1625 | 0 | 829 | 18 | 0 |
| 56 | 10 | 5 | 0 | 0 | 0 | 0 |
| 56 | 11 | 2 | 0 | 0 | 0 | 0 |
| 56 | 12 | 2 | 0 | 0 | 0 | 0 |
| 56 | 13 | 1 | 0 | 0 | 0 | 0 |
| 56 | 14 | 1 | 0 | 0 | 0 | 0 |
| 56 | 15 | 3 | 0 | 0 | 0 | 0 |
| 56 | 16 | 2 | 0 | 0 | 0 | 0 |
| 56 | 17 | 4 | 0 | 0 | 0 | 0 |
| 56 | 18 | 4 | 0 | 0 | 0 | 0 |
| 56 | 19 | 1 | 0 | 0 | 0 | 0 |
| 56 | 1A | 1134 | 0 | 0 | 0 | 0 |
| 56 | 1B | 36 | 0 | 0 | 0 | 0 |
| 56 | 1D | 13 | 0 | 0 | 0 | 0 |
| 56 | 1E | 7 | 0 | 0 | 0 | 0 |
| 56 | 1F | 10 | 0 | 0 | 0 | 0 |
| 56 | 1G | 5 | 0 | 0 | 0 | 0 |
| 56 | 1I | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 56 | 1N | 7 | 0 | 0 | 0 | 0 |
| 56 | 1O | 4 | 0 | 0 | 0 | 0 |
| 56 | 1P | 3 | 0 | 0 | 0 | 0 |
| 56 | 1Q | 5 | 0 | 0 | 0 | 0 |
| 56 | 1R | 4 | 0 | 0 | 0 | 0 |
| 56 | 1S | 3 | 0 | 0 | 0 | 0 |
| 56 | 1T | 2 | 0 | 0 | 0 | 0 |
| 56 | 1U | 7 | 0 | 0 | 0 | 0 |
| 56 | 1V | 2 | 0 | 0 | 0 | 0 |
| 56 | 1W | 7 | 0 | 0 | 0 | 0 |
| 56 | 1X | 5 | 0 | 0 | 0 | 0 |
| 56 | 1Y | 5 | 0 | 0 | 0 | 0 |
| 56 | 1Z | 5 | 0 | 0 | 0 | 0 |
| 56 | 1a | 233 | 0 | 0 | 0 | 0 |
| 56 | 1b | 2 | 0 | 0 | 0 | 0 |
| 56 | 1e | 2 | 0 | 0 | 0 | 0 |
| 56 | 1f | 2 | 0 | 0 | 0 | 0 |
| 56 | 1l | 3 | 0 | 0 | 0 | 0 |
| 56 | 1n | 1 | 0 | 0 | 0 | 0 |
| 56 | 1q | 1 | 0 | 0 | 0 | 0 |
| 56 | 1t | 1 | 0 | 0 | 0 | 0 |
| 56 | 1v | 1 | 0 | 0 | 0 | 0 |
| 56 | 1w | 8 | 0 | 0 | 0 | 0 |
| 56 | 1x | 15 | 0 | 0 | 0 | 0 |
| 56 | 1y | 6 | 0 | 0 | 0 | 0 |
| 56 | 20 | 2 | 0 | 0 | 0 | 0 |
| 56 | 21 | 1 | 0 | 0 | 0 | 0 |
| 56 | 25 | 2 | 0 | 0 | 0 | 0 |
| 56 | 27 | 1 | 0 | 0 | 0 | 0 |
| 56 | 28 | 1 | 0 | 0 | 0 | 0 |
| 56 | 29 | 1 | 0 | 0 | 0 | 0 |
| 56 | 2A | 860 | 0 | 0 | 0 | 0 |
| 56 | 2B | 18 | 0 | 0 | 0 | 0 |
| 56 | 2D | 3 | 0 | 0 | 0 | 0 |
| 56 | 2E | 8 | 0 | 0 | 0 | 0 |
| 56 | 2F | 5 | 0 | 0 | 0 | 0 |
| 56 | 2G | 1 | 0 | 0 | 0 | 0 |
| 56 | 2N | 1 | 0 | 0 | 0 | 0 |
| 56 | 2O | 2 | 0 | 0 | 0 | 0 |
| 56 | 2P | 2 | 0 | 0 | 0 | 0 |
| 56 | 2Q | 5 | 0 | 0 | 0 | 0 |
| 56 | 2R | 3 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 56 | 2T | 4 | 0 | 0 | 0 | 0 |
| 56 | 2U | 4 | 0 | 0 | 0 | 0 |
| 56 | 2V | 2 | 0 | 0 | 0 | 0 |
| 56 | 2W | 1 | 0 | 0 | 0 | 0 |
| 56 | 2X | 1 | 0 | 0 | 0 | 0 |
| 56 | 2Y | 1 | 0 | 0 | 0 | 0 |
| 56 | 2a | 231 | 0 | 0 | 0 | 0 |
| 56 | 2d | 2 | 0 | 0 | 0 | 0 |
| 56 | 2e | 1 | 0 | 0 | 0 | 0 |
| 56 | 2f | 1 | 0 | 0 | 0 | 0 |
| 56 | 2i | 1 | 0 | 0 | 0 | 0 |
| 56 | 2j | 2 | 0 | 0 | 0 | 0 |
| 56 | 2k | 1 | 0 | 0 | 0 | 0 |
| 56 | 2l | 4 | 0 | 0 | 0 | 0 |
| 56 | 2q | 3 | 0 | 0 | 0 | 0 |
| 56 | 2r | 1 | 0 | 0 | 0 | 0 |
| 56 | 2t | 1 | 0 | 0 | 0 | 0 |
| 56 | 2v | 3 | 0 | 0 | 0 | 0 |
| 56 | 2x | 5 | 0 | 0 | 0 | 0 |
| 56 | 2y | 6 | 0 | 0 | 0 | 0 |
| 57 | 1A | 84 | 0 | 0 | 3 | 0 |
| 57 | 1a | 44 | 0 | 0 | 1 | 0 |
| 57 | 2A | 84 | 0 | 0 | 3 | 0 |
| 57 | 2a | 44 | 0 | 0 | 1 | 0 |
| 58 | 1A | 1 | 0 | 0 | 0 | 0 |
| 58 | 2A | 1 | 0 | 0 | 0 | 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 | 0 | 0 |
| 61 | 10 | 9 | 0 | 0 | 1 | 0 |
| 61 | 11 | 12 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 61 | 12 | 4 | 0 | 0 | 0 | 0 |
| 61 | 13 | 4 | 0 | 0 | 0 | 0 |
| 61 | 14 | 1 | 0 | 0 | 0 | 0 |
| 61 | 15 | 7 | 0 | 0 | 0 | 0 |
| 61 | 16 | 2 | 0 | 0 | 0 | 0 |
| 61 | 17 | 8 | 0 | 0 | 1 | 0 |
| 61 | 18 | 13 | 0 | 0 | 1 | 0 |
| 61 | 19 | 1 | 0 | 0 | 0 | 0 |
| 61 | 1A | 2225 | 0 | 0 | 74 | 0 |
| 61 | 1B | 69 | 0 | 0 | 1 | 0 |
| 61 | 1D | 28 | 0 | 0 | 2 | 0 |
| 61 | 1E | 27 | 0 | 0 | 3 | 0 |
| 61 | 1F | 17 | 0 | 0 | 0 | 0 |
| 61 | 1G | 6 | 0 | 0 | 0 | 0 |
| 61 | 1H | 1 | 0 | 0 | 0 | 0 |
| 61 | 1I | 2 | 0 | 0 | 0 | 0 |
| 61 | 1N | 3 | 0 | 0 | 1 | 0 |
| 61 | 1O | 7 | 0 | 0 | 0 | 0 |
| 61 | 1P | 26 | 0 | 0 | 2 | 0 |
| 61 | 1Q | 12 | 0 | 0 | 0 | 0 |
| 61 | 1R | 14 | 0 | 0 | 1 | 0 |
| 61 | 1S | 4 | 0 | 0 | 0 | 0 |
| 61 | 1T | 7 | 0 | 0 | 0 | 0 |
| 61 | 1U | 13 | 0 | 0 | 0 | 0 |
| 61 | 1V | 8 | 0 | 0 | 2 | 0 |
| 61 | 1W | 9 | 0 | 0 | 1 | 0 |
| 61 | 1X | 7 | 0 | 0 | 1 | 0 |
| 61 | 1Y | 4 | 0 | 0 | 1 | 0 |
| 61 | 1Z | 1 | 0 | 0 | 0 | 0 |
| 61 | 1a | 438 | 0 | 0 | 14 | 0 |
| 61 | 1b | 1 | 0 | 0 | 0 | 0 |
| 61 | 1d | 1 | 0 | 0 | 0 | 0 |
| 61 | 1e | 1 | 0 | 0 | 0 | 0 |
| 61 | 1g | 1 | 0 | 0 | 1 | 0 |
| 61 | 1j | 1 | 0 | 0 | 0 | 0 |
| 61 | 1l | 8 | 0 | 0 | 0 | 0 |
| 61 | 1m | 2 | 0 | 0 | 0 | 0 |
| 61 | 1n | 1 | 0 | 0 | 0 | 0 |
| 61 | 1p | 1 | 0 | 0 | 0 | 0 |
| 61 | 1q | 3 | 0 | 0 | 0 | 0 |
| 61 | 1u | 1 | 0 | 0 | 1 | 0 |
| 61 | 1v | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 61 | 1w | 6 | 0 | 0 | 1 | 0 |
| 61 | 1x | 17 | 0 | 0 | 1 | 0 |
| 61 | 1y | 3 | 0 | 0 | 0 | 0 |
| 61 | 20 | 3 | 0 | 0 | 0 | 0 |
| 61 | 21 | 9 | 0 | 0 | 0 | 0 |
| 61 | 23 | 1 | 0 | 0 | 0 | 0 |
| 61 | 25 | 3 | 0 | 0 | 0 | 0 |
| 61 | 27 | 3 | 0 | 0 | 0 | 0 |
| 61 | 28 | 6 | 0 | 0 | 3 | 0 |
| 61 | 2A | 1163 | 0 | 0 | 40 | 0 |
| 61 | 2B | 20 | 0 | 0 | 0 | 0 |
| 61 | 2D | 23 | 0 | 0 | 1 | 0 |
| 61 | 2E | 10 | 0 | 0 | 2 | 0 |
| 61 | 2F | 13 | 0 | 0 | 0 | 0 |
| 61 | 2I | 2 | 0 | 0 | 0 | 0 |
| 61 | 2N | 1 | 0 | 0 | 0 | 0 |
| 61 | 2O | 2 | 0 | 0 | 0 | 0 |
| 61 | 2P | 6 | 0 | 0 | 0 | 0 |
| 61 | 2Q | 1 | 0 | 0 | 0 | 0 |
| 61 | 2R | 3 | 0 | 0 | 0 | 0 |
| 61 | 2T | 2 | 0 | 0 | 0 | 0 |
| 61 | 2U | 3 | 0 | 0 | 0 | 0 |
| 61 | 2V | 2 | 0 | 0 | 1 | 0 |
| 61 | 2W | 1 | 0 | 0 | 0 | 0 |
| 61 | 2X | 2 | 0 | 0 | 0 | 0 |
| 61 | 2Z | 1 | 0 | 0 | 0 | 0 |
| 61 | 2a | 322 | 0 | 0 | 11 | 0 |
| 61 | 2e | 2 | 0 | 0 | 0 | 0 |
| 61 | 2f | 1 | 0 | 0 | 0 | 0 |
| 61 | 2g | 2 | 0 | 0 | 0 | 0 |
| 61 | 2j | 4 | 0 | 0 | 2 | 0 |
| 61 | 2l | 5 | 0 | 0 | 0 | 0 |
| 61 | 2o | 2 | 0 | 0 | 0 | 0 |
| 61 | 2p | 4 | 0 | 0 | 0 | 0 |
| 61 | 2q | 1 | 0 | 0 | 0 | 0 |
| 61 | 2r | 1 | 0 | 0 | 0 | 0 |
| 61 | 2t | 4 | 0 | 0 | 0 | 0 |
| 61 | 2u | 1 | 0 | 0 | 0 | 0 |
| 61 | 2v | 3 | 0 | 0 | 0 | 0 |
| 61 | 2w | 3 | 0 | 0 | 0 | 0 |
| 61 | 2x | 7 | 0 | 0 | 0 | 0 |
| 61 | 2y | 9 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 300702 | 0 | 196683 | 4265 | 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 4265 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 | 1.30 | 1.28 |
| 1:2A:2137:C:N4 | 1:2A:2154:G:H1 | 1.51 | 1.08 |
| 1:1A:1082:U:O4 | 1:1A:1086:A:N1 | 1.89 | 1.06 |
| 54:1w:51:C:N4 | 54:1w:63:G:H1 | 1.58 | 1.02 |
| 32:2a:997:U:H3 | 32:2a:1044:A:N6 | 1.58 | 1.01 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 3 | 1D | 273/276 (99%) | 255 (93%) | 17 (6%) | 1 (0%) | 30 | 50 |
| 3 | 2D | 273/276 (99%) | 261 (96%) | 11 (4%) | 1 (0%) | 30 | 50 |
| 4 | 1E | 202/206 (98%) | 192 (95%) | 9 (4%) | 1 (0%) | 24 | 43 |
| 4 | 2E | 202/206 (98%) | 196 (97%) | 5 (2%) | 1 (0%) | 24 | 43 |
| 5 | 1F | 201/210 (96%) | 196 (98%) | 4 (2%) | 1 (0%) | 24 | 43 |
| 5 | 2F | 201/210 (96%) | 196 (98%) | 3 (2%) | 2 (1%) | 12 | 24 |
| 6 | 1G | 179/182 (98%) | 163 (91%) | 15 (8%) | 1 (1%) | 21 | 38 |
| 6 | 2G | 179/182 (98%) | 162 (90%) | 15 (8%) | 2 (1%) | 11 | 22 |
| 7 | 1H | 172/180 (96%) | 164 (95%) | 7 (4%) | 1 (1%) | 21 | 38 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 7 | 2H | 172/180 (96%) | 157 (91%) | 14 (8%) | 1 (1%) | 21 38 |
| 8 | 1I | 144/148 (97%) | 134 (93%) | 9 (6%) | 1 (1%) | 18 34 |
| 8 | 2I | 144/148 (97%) | 133 (92%) | 9 (6%) | 2 (1%) | 9 17 |
| 9 | 1N | 138/140 (99%) | 132 (96%) | 6 (4%) | 0 | 100 100 |
| 9 | 2N | 138/140 (99%) | 134 (97%) | 4 (3%) | 0 | 100 100 |
| 10 | 1O | 120/122 (98%) | 113 (94%) | 7 (6%) | 0 | 100 100 |
| 10 | 2O | 120/122 (98%) | 113 (94%) | 7 (6%) | 0 | 100 100 |
| 11 | 1P | 147/150 (98%) | 137 (93%) | 9 (6%) | 1 (1%) | 18 34 |
| 11 | 2P | 147/150 (98%) | 140 (95%) | 7 (5%) | 0 | 100 100 |
| 12 | 1Q | 139/141 (99%) | 134 (96%) | 5 (4%) | 0 | 100 100 |
| 12 | 2Q | 139/141 (99%) | 130 (94%) | 9 (6%) | 0 | 100 100 |
| 13 | 1R | 116/118 (98%) | 112 (97%) | 4 (3%) | 0 | 100 100 |
| 13 | 2R | 116/118 (98%) | 112 (97%) | 4 (3%) | 0 | 100 100 |
| 14 | 1S | 108/112 (96%) | 105 (97%) | 3 (3%) | 0 | 100 100 |
| 14 | 2S | 108/112 (96%) | 101 (94%) | 7 (6%) | 0 | 100 100 |
| 15 | 1T | 129/146 (88%) | 121 (94%) | 8 (6%) | 0 | 100 100 |
| 15 | 2T | 129/146 (88%) | 122 (95%) | 5 (4%) | 2 (2%) | 7 14 |
| 16 | 1U | 114/118 (97%) | 112 (98%) | 2 (2%) | 0 | 100 100 |
| 16 | 2U | 114/118 (97%) | 112 (98%) | 2 (2%) | 0 | 100 100 |
| 17 | 1V | 99/101 (98%) | 92 (93%) | 5 (5%) | 2 (2%) | 6 11 |
| 17 | 2V | 99/101 (98%) | 93 (94%) | 6 (6%) | 0 | 100 100 |
| 18 | 1W | 110/113 (97%) | 109 (99%) | 1 (1%) | 0 | 100 100 |
| 18 | 2W | 110/113 (97%) | 110 (100%) | 0 | 0 | 100 100 |
| 19 | 1X | 93/96 (97%) | 89 (96%) | 4 (4%) | 0 | 100 100 |
| 19 | 2X | 93/96 (97%) | 88 (95%) | 5 (5%) | 0 | 100 100 |
| 20 | 1Y | 105/110 (96%) | 100 (95%) | 4 (4%) | 1 (1%) | 12 24 |
| 20 | 2Y | 105/110 (96%) | 98 (93%) | 7 (7%) | 0 | 100 100 |
| 21 | 1Z | 148/206 (72%) | 131 (88%) | 14 (10%) | 3 (2%) | 6 11 |
| 21 | 2Z | 156/206 (76%) | 137 (88%) | 15 (10%) | 4 (3%) | 4 7 |
| 22 | 10 | 81/85 (95%) | 78 (96%) | 3 (4%) | 0 | 100 100 |
| 22 | 20 | 81/85 (95%) | 78 (96%) | 3 (4%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 23 | 11 | 95/98 (97%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 23 | 21 | 95/98 (97%) | 92 (97%) | 3 (3%) | 0 | 100 | 100 |
| 24 | 12 | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 24 | 22 | 68/72 (94%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | 13 | 57/60 (95%) | 56 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | 23 | 57/60 (95%) | 56 (98%) | 0 | 1 (2%) | 6 | 13 |
| 26 | 14 | 67/71 (94%) | 54 (81%) | 9 (13%) | 4 (6%) | 1 | 1 |
| 26 | 24 | 67/71 (94%) | 54 (81%) | 9 (13%) | 4 (6%) | 1 | 1 |
| 27 | 15 | 57/60 (95%) | 55 (96%) | 2 (4%) | 0 | 100 | 100 |
| 27 | 25 | 57/60 (95%) | 53 (93%) | 4 (7%) | 0 | 100 | 100 |
| 28 | 16 | 51/54 (94%) | 47 (92%) | 4 (8%) | 0 | 100 | 100 |
| 28 | 26 | 51/54 (94%) | 49 (96%) | 2 (4%) | 0 | 100 | 100 |
| 29 | 17 | 46/49 (94%) | 45 (98%) | 1 (2%) | 0 | 100 | 100 |
| 29 | 27 | 46/49 (94%) | 46 (100%) | 0 | 0 | 100 | 100 |
| 30 | 18 | 62/65 (95%) | 62 (100%) | 0 | 0 | 100 | 100 |
| 30 | 28 | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 31 | 19 | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 31 | 29 | 35/37 (95%) | 34 (97%) | 1 (3%) | 0 | 100 | 100 |
| 33 | 1b | 229/256 (90%) | 201 (88%) | 23 (10%) | 5 (2%) | 5 | 10 |
| 33 | 2b | 229/256 (90%) | 203 (89%) | 22 (10%) | 4 (2%) | 7 | 14 |
| 34 | 1c | 204/239 (85%) | 190 (93%) | 14 (7%) | 0 | 100 | 100 |
| 34 | 2c | 204/239 (85%) | 187 (92%) | 16 (8%) | 1 (0%) | 24 | 43 |
| 35 | 1d | 206/209 (99%) | 200 (97%) | 6 (3%) | 0 | 100 | 100 |
| 35 | 2d | 206/209 (99%) | 200 (97%) | 6 (3%) | 0 | 100 | 100 |
| 36 | 1e | 146/162 (90%) | 137 (94%) | 8 (6%) | 1 (1%) | 18 | 34 |
| 36 | 2e | 146/162 (90%) | 137 (94%) | 8 (6%) | 1 (1%) | 18 | 34 |
| 37 | 1f | 98/101 (97%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 37 | 2f | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 38 | 1g | 153/156 (98%) | 147 (96%) | 3 (2%) | 3 (2%) | 6 | 11 |
| 38 | 2g | 153/156 (98%) | 142 (93%) | 10 (6%) | 1 (1%) | 18 | 34 |
| 39 | 1h | 135/138 (98%) | 128 (95%) | 7 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 39 | 2h | 135/138 (98%) | 129 (96%) | 6 (4%) | 0 | 100 100 |
| 40 | 1i | 125/128 (98%) | 115 (92%) | 10 (8%) | 0 | 100 100 |
| 40 | 2i | 125/128 (98%) | 111 (89%) | 13 (10%) | 1 (1%) | 16 30 |
| 41 | 1j | 95/105 (90%) | 83 (87%) | 9 (10%) | 3 (3%) | 3 5 |
| 41 | 2j | 94/105 (90%) | 83 (88%) | 7 (7%) | 4 (4%) | 2 3 |
| 42 | 1k | 112/129 (87%) | 106 (95%) | 5 (4%) | 1 (1%) | 14 28 |
| 42 | 2k | 112/129 (87%) | 103 (92%) | 7 (6%) | 2 (2%) | 6 13 |
| 43 | 1l | 119/132 (90%) | 114 (96%) | 5 (4%) | 0 | 100 100 |
| 43 | 2l | 119/132 (90%) | 113 (95%) | 6 (5%) | 0 | 100 100 |
| 44 | 1m | 121/126 (96%) | 111 (92%) | 10 (8%) | 0 | 100 100 |
| 44 | 2m | 120/126 (95%) | 109 (91%) | 9 (8%) | 2 (2%) | 7 14 |
| 45 | 1n | 58/61 (95%) | 55 (95%) | 3 (5%) | 0 | 100 100 |
| 45 | 2n | 58/61 (95%) | 53 (91%) | 5 (9%) | 0 | 100 100 |
| 46 | 1o | 86/89 (97%) | 83 (96%) | 1 (1%) | 2 (2%) | 5 9 |
| 46 | 2o | 86/89 (97%) | 82 (95%) | 3 (4%) | 1 (1%) | 10 20 |
| 47 | 1p | 80/88 (91%) | 78 (98%) | 2 (2%) | 0 | 100 100 |
| 47 | 2p | 80/88 (91%) | 77 (96%) | 2 (2%) | 1 (1%) | 9 18 |
| 48 | 1q | 97/105 (92%) | 93 (96%) | 3 (3%) | 1 (1%) | 12 24 |
| 48 | 2q | 97/105 (92%) | 91 (94%) | 6 (6%) | 0 | 100 100 |
| 49 | 1r | 66/88 (75%) | 63 (96%) | 3 (4%) | 0 | 100 100 |
| 49 | 2r | 66/88 (75%) | 63 (96%) | 3 (4%) | 0 | 100 100 |
| 50 | 1s | 81/93 (87%) | 72 (89%) | 9 (11%) | 0 | 100 100 |
| 50 | 2s | 81/93 (87%) | 69 (85%) | 12 (15%) | 0 | 100 100 |
| 51 | 1t | 94/106 (89%) | 88 (94%) | 4 (4%) | 2 (2%) | 5 11 |
| 51 | 2t | 94/106 (89%) | 87 (93%) | 5 (5%) | 2 (2%) | 5 11 |
| 52 | 1u | 21/27 (78%) | 21 (100%) | 0 | 0 | 100 100 |
| 52 | 2u | 21/27 (78%) | 20 (95%) | 1 (5%) | 0 | 100 100 |
| All | All | 11370/12128 (94%) | 10699 (94%) | 596 (5%) | 75 (1%) | 18 34 |

5 of 75 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | 1H | 126 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | 1I | 10 | GLU |
| 26 | 14 | 65 | ASP |
| 33 | 1b | 17 | PHE |
| 51 | 1t | 100 | ILE |

### 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 | 215/218 (99%) | 203 (94%) | 12 (6%) | 19 36 |
| 3 | 2D | 215/218 (99%) | 206 (96%) | 9 (4%) | 26 49 |
| 4 | 1E | 164/166 (99%) | 155 (94%) | 9 (6%) | 19 37 |
| 4 | 2E | 164/166 (99%) | 153 (93%) | 11 (7%) | 15 28 |
| 5 | 1F | 160/166 (96%) | 148 (92%) | 12 (8%) | 12 24 |
| 5 | 2F | 159/166 (96%) | 145 (91%) | 14 (9%) | 9 18 |
| 6 | 1G | 143/156 (92%) | 132 (92%) | 11 (8%) | 12 22 |
| 6 | 2G | 143/156 (92%) | 132 (92%) | 11 (8%) | 12 22 |
| 7 | 1H | 144/148 (97%) | 140 (97%) | 4 (3%) | 38 61 |
| 7 | 2H | 144/148 (97%) | 137 (95%) | 7 (5%) | 22 43 |
| 8 | 1I | 113/124 (91%) | 100 (88%) | 13 (12%) | 5 10 |
| 8 | 2I | 105/124 (85%) | 94 (90%) | 11 (10%) | 6 13 |
| 9 | 1N | 118/119 (99%) | 109 (92%) | 9 (8%) | 12 23 |
| 9 | 2N | 118/119 (99%) | 107 (91%) | 11 (9%) | 8 16 |
| 10 | 1O | 100/100 (100%) | 97 (97%) | 3 (3%) | 36 60 |
| 10 | 2O | 100/100 (100%) | 97 (97%) | 3 (3%) | 36 60 |
| 11 | 1P | 115/116 (99%) | 109 (95%) | 6 (5%) | 21 39 |
| 11 | 2P | 115/116 (99%) | 112 (97%) | 3 (3%) | 40 63 |
| 12 | 1Q | 111/111 (100%) | 104 (94%) | 7 (6%) | 16 30 |
| 12 | 2Q | 111/111 (100%) | 106 (96%) | 5 (4%) | 24 46 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 13 | 1R | 101/101 (100%) | 91 (90%) | 10 (10%) | 7 15 |
| 13 | 2R | 101/101 (100%) | 95 (94%) | 6 (6%) | 18 33 |
| 14 | 1S | 86/88 (98%) | 77 (90%) | 9 (10%) | 6 13 |
| 14 | 2S | 85/88 (97%) | 80 (94%) | 5 (6%) | 18 33 |
| 15 | 1T | 115/127 (91%) | 110 (96%) | 5 (4%) | 26 47 |
| 15 | 2T | 113/127 (89%) | 111 (98%) | 2 (2%) | 51 71 |
| 16 | 1U | 93/94 (99%) | 88 (95%) | 5 (5%) | 20 38 |
| 16 | 2U | 93/94 (99%) | 89 (96%) | 4 (4%) | 26 47 |
| 17 | 1V | 80/82 (98%) | 74 (92%) | 6 (8%) | 12 24 |
| 17 | 2V | 80/82 (98%) | 75 (94%) | 5 (6%) | 16 30 |
| 18 | 1W | 90/92 (98%) | 87 (97%) | 3 (3%) | 33 57 |
| 18 | 2W | 90/92 (98%) | 86 (96%) | 4 (4%) | 25 47 |
| 19 | 1X | 77/78 (99%) | 75 (97%) | 2 (3%) | 40 63 |
| 19 | 2X | 77/78 (99%) | 70 (91%) | 7 (9%) | 9 17 |
| 20 | 1Y | 85/91 (93%) | 75 (88%) | 10 (12%) | 5 9 |
| 20 | 2Y | 85/91 (93%) | 78 (92%) | 7 (8%) | 10 20 |
| 21 | 1Z | 135/179 (75%) | 123 (91%) | 12 (9%) | 9 17 |
| 21 | 2Z | 137/179 (76%) | 127 (93%) | 10 (7%) | 13 24 |
| 22 | 10 | 65/67 (97%) | 63 (97%) | 2 (3%) | 35 59 |
| 22 | 20 | 65/67 (97%) | 65 (100%) | 0 | 100 100 |
| 23 | 11 | 80/83 (96%) | 78 (98%) | 2 (2%) | 42 64 |
| 23 | 21 | 80/83 (96%) | 77 (96%) | 3 (4%) | 29 52 |
| 24 | 12 | 65/67 (97%) | 64 (98%) | 1 (2%) | 57 74 |
| 24 | 22 | 65/67 (97%) | 63 (97%) | 2 (3%) | 35 59 |
| 25 | 13 | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 6 |
| 25 | 23 | 50/52 (96%) | 48 (96%) | 2 (4%) | 28 50 |
| 26 | 14 | 59/63 (94%) | 49 (83%) | 10 (17%) | 2 3 |
| 26 | 24 | 53/63 (84%) | 47 (89%) | 6 (11%) | 5 11 |
| 27 | 15 | 50/52 (96%) | 47 (94%) | 3 (6%) | 17 32 |
| 27 | 25 | 50/52 (96%) | 48 (96%) | 2 (4%) | 28 50 |
| 28 | 16 | 51/52 (98%) | 47 (92%) | 4 (8%) | 11 21 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 28 | 26 | 50/52 (96%) | 46 (92%) | 4 (8%) | 11 20 |
| 29 | 17 | 41/42 (98%) | 38 (93%) | 3 (7%) | 13 24 |
| 29 | 27 | 41/42 (98%) | 37 (90%) | 4 (10%) | 7 15 |
| 30 | 18 | 54/55 (98%) | 49 (91%) | 5 (9%) | 8 16 |
| 30 | 28 | 54/55 (98%) | 51 (94%) | 3 (6%) | 19 36 |
| 31 | 19 | 34/34 (100%) | 33 (97%) | 1 (3%) | 37 61 |
| 31 | 29 | 34/34 (100%) | 33 (97%) | 1 (3%) | 37 61 |
| 33 | 1b | 192/220 (87%) | 180 (94%) | 12 (6%) | 16 30 |
| 33 | 2b | 187/220 (85%) | 164 (88%) | 23 (12%) | 4 8 |
| 34 | 1c | 142/188 (76%) | 130 (92%) | 12 (8%) | 10 18 |
| 34 | 2c | 140/188 (74%) | 135 (96%) | 5 (4%) | 31 55 |
| 35 | 1d | 169/181 (93%) | 160 (95%) | 9 (5%) | 20 39 |
| 35 | 2d | 173/181 (96%) | 166 (96%) | 7 (4%) | 28 50 |
| 36 | 1e | 113/123 (92%) | 104 (92%) | 9 (8%) | 11 20 |
| 36 | 2e | 114/123 (93%) | 109 (96%) | 5 (4%) | 25 47 |
| 37 | 1f | 84/90 (93%) | 81 (96%) | 3 (4%) | 31 55 |
| 37 | 2f | 85/90 (94%) | 80 (94%) | 5 (6%) | 18 33 |
| 38 | 1g | 119/127 (94%) | 116 (98%) | 3 (2%) | 42 64 |
| 38 | 2g | 120/127 (94%) | 118 (98%) | 2 (2%) | 53 71 |
| 39 | 1h | 114/119 (96%) | 108 (95%) | 6 (5%) | 20 39 |
| 39 | 2h | 114/119 (96%) | 111 (97%) | 3 (3%) | 40 63 |
| 40 | 1i | 90/99 (91%) | 87 (97%) | 3 (3%) | 33 57 |
| 40 | 2i | 89/99 (90%) | 82 (92%) | 7 (8%) | 11 21 |
| 41 | 1j | 66/92 (72%) | 59 (89%) | 7 (11%) | 6 13 |
| 41 | 2j | 69/92 (75%) | 65 (94%) | 4 (6%) | 18 34 |
| 42 | 1k | 82/99 (83%) | 81 (99%) | 1 (1%) | 63 78 |
| 42 | 2k | 83/99 (84%) | 79 (95%) | 4 (5%) | 23 44 |
| 43 | 1l | 96/108 (89%) | 87 (91%) | 9 (9%) | 8 16 |
| 43 | 2l | 96/108 (89%) | 95 (99%) | 1 (1%) | 68 81 |
| 44 | 1m | 93/101 (92%) | 87 (94%) | 6 (6%) | 15 29 |
| 44 | 2m | 92/101 (91%) | 88 (96%) | 4 (4%) | 26 47 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 45 | 1n | 49/50 (98%) | 41 (84%) | 8 (16%) | 2 3 |
| 45 | 2n | 49/50 (98%) | 46 (94%) | 3 (6%) | 17 31 |
| 46 | 1o | 78/80 (98%) | 76 (97%) | 2 (3%) | 40 63 |
| 46 | 2o | 78/80 (98%) | 77 (99%) | 1 (1%) | 61 76 |
| 47 | 1p | 69/74 (93%) | 63 (91%) | 6 (9%) | 9 18 |
| 47 | 2p | 68/74 (92%) | 62 (91%) | 6 (9%) | 9 18 |
| 48 | 1q | 94/97 (97%) | 92 (98%) | 2 (2%) | 47 67 |
| 48 | 2q | 94/97 (97%) | 93 (99%) | 1 (1%) | 65 79 |
| 49 | 1r | 59/77 (77%) | 56 (95%) | 3 (5%) | 21 40 |
| 49 | 2r | 59/77 (77%) | 57 (97%) | 2 (3%) | 32 57 |
| 50 | 1s | 69/80 (86%) | 67 (97%) | 2 (3%) | 37 61 |
| 50 | 2s | 67/80 (84%) | 64 (96%) | 3 (4%) | 24 46 |
| 51 | 1t | 70/82 (85%) | 67 (96%) | 3 (4%) | 26 47 |
| 51 | 2t | 70/82 (85%) | 65 (93%) | 5 (7%) | 13 25 |
| 52 | 1u | 18/22 (82%) | 18 (100%) | 0 | 100 100 |
| 52 | 2u | 18/22 (82%) | 18 (100%) | 0 | 100 100 |
| All | All | 9303/10064 (92%) | 8758 (94%) | 545 (6%) | 18 33 |

5 of 545 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 33 | 2b | 119 | GLU |
| 33 | 2b | 230 | VAL |
| 33 | 2b | 112 | VAL |
| 44 | 2m | 19 | LEU |
| 33 | 1b | 160 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 41 | 1j | 68 | HIS |
| 41 | 2j | 56 | HIS |
| 5 | 2F | 69 | HIS |
| 41 | 2j | 33 | GLN |
| 50 | 2s | 69 | HIS |

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | 1A | 2864/2915 (98%) | 448 (15%) | 19 (0%) |
| 1 | 2A | 2791/2915 (95%) | 514 (18%) | 19 (0%) |
| 2 | 1B | 120/121 (99%) | 11 (9%) | 1 (0%) |
| 2 | 2B | 118/121 (97%) | 28 (23%) | 0 |
| 32 | 1a | 1497/1521 (98%) | 251 (16%) | 0 |
| 32 | 2a | 1501/1521 (98%) | 283 (18%) | 0 |
| 53 | 1v | 12/27 (44%) | 2 (16%) | 0 |
| 53 | 2v | 12/27 (44%) | 4 (33%) | 0 |
| 54 | 1w | 70/76 (92%) | 24 (34%) | 0 |
| 54 | 1y | 70/76 (92%) | 25 (35%) | 0 |
| 54 | 2w | 70/76 (92%) | 28 (40%) | 0 |
| 54 | 2y | 70/76 (92%) | 29 (41%) | 0 |
| 55 | 1x | 75/77 (97%) | 13 (17%) | 0 |
| 55 | 2x | 75/77 (97%) | 15 (20%) | 0 |
| All | All | 9345/9626 (97%) | 1675 (17%) | 39 (0%) |

5 of 1675 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 12 | U |
| 1 | 1A | 13 | A |
| 1 | 1A | 34 | C |
| 1 | 1A | 45 | C |
| 1 | 1A | 71 | A |

5 of 39 RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2A | 856 | C |
| 1 | 2A | 1653 | G |
| 1 | 2A | 893 | C |
| 1 | 2A | 1379 | A |
| 1 | 2A | 1992 | G |

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

80 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 | $\#\|Z\| > 2$ |
| 1 | 5MC | 2A | 1962 | 56,1 | 19,22,23 | 1.63 | 3 (15%) | 26,32,35 | 1.11 | 2 (7%) |
| 32 | 4OC | 2a | 1402 | 32 | 20,23,24 | 0.77 | 0 | 25,32,35 | 1.04 | 2 (8%) |
| 54 | 7MG | 1w | 46 | 54 | 23,26,27 | 1.39 | 2 (8%) | 27,39,42 | 2.50 | 8 (29%) |
| 55 | PSU | 1x | 55 | 56,55 | 18,21,22 | 1.40 | 2 (11%) | 21,30,33 | 2.00 | 3 (14%) |
| 1 | OMG | 1A | 2251 | 56,1,55 | 23,26,27 | 1.21 | 3 (13%) | 32,38,41 | 2.05 | 6 (18%) |
| 54 | PSU | 1y | 55 | 54 | 18,21,22 | 1.40 | 2 (11%) | 21,30,33 | 2.06 | 3 (14%) |
| 32 | UR3 | 1a | 1498 | 32 | 19,22,23 | 1.00 | 2 (10%) | 26,32,35 | 1.77 | 3 (11%) |
| 54 | 6MZ | 1w | 37 | 54 | 22,25,26 | 1.53 | 4 (18%) | 29,36,39 | 2.15 | 9 (31%) |
| 32 | MA6 | 2a | 1518 | 32 | 23,26,27 | 1.60 | 4 (17%) | 33,38,41 | 2.32 | 13 (39%) |
| 1 | OMU | 2A | 2552 | 56,1 | 19,22,23 | 1.29 | 3 (15%) | 25,31,34 | 1.90 | 6 (24%) |
| 54 | 4SU | 2y | 8 | 54 | 18,21,22 | 1.83 | 4 (22%) | 25,30,33 | 1.90 | 5 (20%) |
| 32 | MA6 | 1a | 1518 | 32 | 23,26,27 | 1.54 | 5 (21%) | 33,38,41 | 2.28 | 12 (36%) |
| 32 | 5MC | 2a | 1404 | 32 | 19,22,23 | 1.70 | 3 (15%) | 26,32,35 | 1.18 | 3 (11%) |
| 32 | 5MC | 1a | 1400 | 32 | 19,22,23 | 1.60 | 3 (15%) | 26,32,35 | 1.10 | 2 (7%) |
| 1 | OMG | 2A | 2251 | 56,1,55 | 23,26,27 | 1.22 | 3 (13%) | 32,38,41 | 1.96 | 6 (18%) |
| 32 | 5MC | 1a | 1407 | 32 | 19,22,23 | 1.63 | 3 (15%) | 26,32,35 | 1.18 | 3 (11%) |
| 1 | 5MU | 2A | 1939 | 1 | 19,22,23 | 1.40 | 6 (31%) | 27,32,35 | 2.15 | 6 (22%) |
| 55 | 4SU | 2x | 8 | 56,55 | 18,21,22 | 2.00 | 5 (27%) | 25,30,33 | 1.75 | 7 (28%) |
| 32 | 2MG | 1a | 1207 | 32 | 23,26,27 | 1.25 | 2 (8%) | 33,38,41 | 2.14 | 8 (24%) |
| 1 | 5MU | 1A | 1939 | 56,1 | 19,22,23 | 1.42 | 6 (31%) | 27,32,35 | 2.21 | 6 (22%) |
| 32 | MA6 | 1a | 1519 | 32 | 23,26,27 | 1.55 | 4 (17%) | 33,38,41 | 2.31 | 12 (36%) |
| 32 | 7MG | 2a | 527 | 56,32 | 23,26,27 | 1.33 | 3 (13%) | 27,39,42 | 2.60 | 6 (22%) |
| 32 | PSU | 1a | 516 | 56,32 | 18,21,22 | 1.39 | 2 (11%) | 21,30,33 | 2.01 | 4 (19%) |
| 54 | CM0 | 1y | 34 | 54 | 21,26,27 | 1.19 | 3 (14%) | 26,37,40 | 1.88 | 4 (15%) |
| 1 | PSU | 1A | 1917 | 1 | 18,21,22 | 1.38 | 2 (11%) | 21,30,33 | 1.99 | 4 (19%) |
| 1 | PSU | 2A | 1911 | 1 | 18,21,22 | 1.36 | 2 (11%) | 21,30,33 | 1.95 | 3 (14%) |
| 1 | 5MC | 2A | 1942 | 1 | 19,22,23 | 1.66 | 3 (15%) | 26,32,35 | 1.11 | 2 (7%) |
| 1 | 5MU | 2A | 1915 | 1 | 19,22,23 | 1.47 | 5 (26%) | 27,32,35 | 2.09 | 6 (22%) |
| 32 | 5MC | 2a | 1407 | 32 | 19,22,23 | 1.66 | 3 (15%) | 26,32,35 | 1.13 | 3 (11%) |
| 1 | PSU | 1A | 1911 | 1 | 18,21,22 | 1.39 | 3 (16%) | 21,30,33 | 2.07 | 4 (19%) |
| 1 | OMC | 1A | 1920 | 1 | 19,22,23 | 0.78 | 0 | 25,31,34 | 0.95 | 2 (8%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 54 | PSU | 2w | 55 | 54 | 18,21,22 | 1.36 | 2 (11%) | 21,30,33 | 1.96 | 4 (19%) |
| 54 | 5MU | 1y | 54 | 54 | 19,22,23 | 1.45 | 5 (26%) | 27,32,35 | 2.08 | 5 (18%) |
| 1 | OMU | 1A | 2552 | 56,1 | 19,22,23 | 1.29 | 3 (15%) | 25,31,34 | 1.94 | 6 (24%) |
| 54 | 7MG | 1y | 46 | 54 | 23,26,27 | 1.45 | 3 (13%) | 27,39,42 | 2.79 | 6 (22%) |
| 43 | 0TD | 2l | 92 | 43 | 8,9,10 | 4.60 | 1 (12%) | 6,11,13 | 4.81 | 3 (50%) |
| 43 | 0TD | 1l | 92 | 43 | 8,9,10 | 4.69 | 1 (12%) | 6,11,13 | 7.21 | 3 (50%) |
| 54 | CM0 | 1w | 34 | 54 | 21,26,27 | 1.16 | 3 (14%) | 26,37,40 | 1.77 | 5 (19%) |
| 1 | PSU | 1A | 2605 | 56,1 | 18,21,22 | 1.39 | 3 (16%) | 21,30,33 | 1.94 | 4 (19%) |
| 32 | 7MG | 1a | 527 | 56,32 | 23,26,27 | 1.36 | 4 (17%) | 27,39,42 | 2.60 | 6 (22%) |
| 1 | 5MC | 1A | 1942 | 1 | 19,22,23 | 1.63 | 3 (15%) | 26,32,35 | 1.18 | 3 (11%) |
| 54 | 4SU | 1y | 8 | 54 | 18,21,22 | 1.88 | 5 (27%) | 25,30,33 | 2.08 | 5 (20%) |
| 54 | 6MZ | 1y | 37 | 54 | 22,25,26 | 1.54 | 4 (18%) | 29,36,39 | 2.24 | 10 (34%) |
| 55 | 5MU | 2x | 54 | 55 | 19,22,23 | 1.41 | 6 (31%) | 27,32,35 | 2.03 | 6 (22%) |
| 54 | 4SU | 2w | 8 | 54 | 18,21,22 | 1.79 | 4 (22%) | 25,30,33 | 2.09 | 5 (20%) |
| 1 | PSU | 2A | 1917 | 1 | 18,21,22 | 1.37 | 2 (11%) | 21,30,33 | 2.07 | 4 (19%) |
| 54 | 5MU | 2y | 54 | 54 | 19,22,23 | 1.45 | 4 (21%) | 27,32,35 | 2.01 | 8 (29%) |
| 55 | 5MU | 1x | 54 | 55 | 19,22,23 | 1.41 | 5 (26%) | 27,32,35 | 1.81 | 5 (18%) |
| 55 | 4SU | 1x | 8 | 55 | 18,21,22 | 2.08 | 4 (22%) | 25,30,33 | 1.72 | 7 (28%) |
| 32 | 2MG | 2a | 1207 | 32 | 23,26,27 | 1.23 | 2 (8%) | 33,38,41 | 2.23 | 7 (21%) |
| 54 | PSU | 2y | 55 | 54 | 18,21,22 | 1.40 | 2 (11%) | 21,30,33 | 2.01 | 3 (14%) |
| 32 | M2G | 2a | 966 | 32 | 24,27,28 | 1.32 | 4 (16%) | 33,40,43 | 1.88 | 6 (18%) |
| 54 | 6MZ | 2w | 37 | 54 | 22,25,26 | 1.51 | 4 (18%) | 29,36,39 | 2.10 | 8 (27%) |
| 32 | 5MC | 2a | 967 | 32 | 19,22,23 | 1.74 | 3 (15%) | 26,32,35 | 1.09 | 2 (7%) |
| 32 | M2G | 1a | 966 | 32 | 24,27,28 | 1.30 | 3 (12%) | 33,40,43 | 1.83 | 5 (15%) |
| 54 | PSU | 1w | 55 | 54 | 18,21,22 | 1.41 | 1 (5%) | 21,30,33 | 2.04 | 4 (19%) |
| 1 | 2MA | 2A | 2503 | 1 | 22,25,26 | 1.47 | 5 (22%) | 32,37,40 | 2.25 | 9 (28%) |
| 32 | 5MC | 1a | 967 | 32 | 19,22,23 | 1.62 | 3 (15%) | 26,32,35 | 1.18 | 3 (11%) |
| 32 | MA6 | 2a | 1519 | 32 | 23,26,27 | 1.56 | 3 (13%) | 33,38,41 | 2.30 | 12 (36%) |
| 54 | 5MU | 1w | 54 | 54 | 19,22,23 | 1.40 | 5 (26%) | 27,32,35 | 2.17 | 8 (29%) |
| 55 | 5MC | 1x | 32 | 55 | 19,22,23 | 1.69 | 3 (15%) | 26,32,35 | 1.20 | 3 (11%) |
| 1 | 5MC | 1A | 1962 | 1 | 19,22,23 | 1.68 | 3 (15%) | 26,32,35 | 1.15 | 3 (11%) |
| 1 | 5MU | 1A | 1915 | 1 | 19,22,23 | 1.44 | 5 (26%) | 27,32,35 | 2.07 | 6 (22%) |
| 54 | CM0 | 2y | 34 | 54 | 21,26,27 | 1.17 | 2 (9%) | 26,37,40 | 1.87 | 5 (19%) |
| 1 | OMC | 2A | 1920 | 1 | 19,22,23 | 0.80 | 0 | 25,31,34 | 0.99 | 1 (4%) |
| 54 | 7MG | 2y | 46 | 54 | 23,26,27 | 1.40 | 4 (17%) | 27,39,42 | 2.73 | 7 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 32 | 5MC | 2a | 1400 | 32 | 19,22,23 | 1.72 | 3 (15%) | 26,32,35 | 1.18 | 3 (11%) |
| 32 | 5MC | 1a | 1404 | 32 | 19,22,23 | 1.67 | 3 (15%) | 26,32,35 | 1.16 | 3 (11%) |
| 54 | 4SU | 1w | 8 | 54 | 18,21,22 | 1.85 | 5 (27%) | 25,30,33 | 2.04 | 5 (20%) |
| 55 | 5MC | 2x | 32 | 55 | 19,22,23 | 1.74 | 3 (15%) | 26,32,35 | 1.27 | 3 (11%) |
| 1 | 2MA | 1A | 2503 | 56,1 | 22,25,26 | 1.47 | 5 (22%) | 32,37,40 | 2.26 | 9 (28%) |
| 54 | 6MZ | 2y | 37 | 54 | 22,25,26 | 1.55 | 4 (18%) | 29,36,39 | 2.23 | 9 (31%) |
| 55 | PSU | 2x | 55 | 55 | 18,21,22 | 1.33 | 2 (11%) | 21,30,33 | 2.06 | 4 (19%) |
| 32 | 4OC | 1a | 1402 | 32 | 20,23,24 | 0.76 | 0 | 25,32,35 | 0.90 | 1 (4%) |
| 32 | PSU | 2a | 516 | 32 | 18,21,22 | 1.34 | 2 (11%) | 21,30,33 | 1.95 | 3 (14%) |
| 1 | PSU | 2A | 2605 | 1 | 18,21,22 | 1.37 | 3 (16%) | 21,30,33 | 2.00 | 4 (19%) |
| 54 | 5MU | 2w | 54 | 54 | 19,22,23 | 1.39 | 5 (26%) | 27,32,35 | 1.91 | 6 (22%) |
| 54 | CM0 | 2w | 34 | 54 | 21,26,27 | 1.18 | 4 (19%) | 26,37,40 | 1.73 | 4 (15%) |
| 54 | 7MG | 2w | 46 | 54 | 23,26,27 | 1.28 | 3 (13%) | 27,39,42 | 2.65 | 6 (22%) |
| 32 | UR3 | 2a | 1498 | 32 | 19,22,23 | 1.03 | 2 (10%) | 26,32,35 | 1.79 | 4 (15%) |

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 |
|---|---|---|---|---|---|---|---|
| 1 | 5MC | 2A | 1962 | 56,1 | - | 1/7/25/26 | 0/2/2/2 |
| 32 | 4OC | 2a | 1402 | 32 | - | 3/9/29/30 | 0/2/2/2 |
| 54 | 7MG | 1w | 46 | 54 | - | 2/7/37/38 | 0/3/3/3 |
| 55 | PSU | 1x | 55 | 56,55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMG | 1A | 2251 | 56,1,55 | - | 0/9/27/28 | 0/3/3/3 |
| 54 | PSU | 1y | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | UR3 | 1a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 6MZ | 1w | 37 | 54 | - | 0/9/27/28 | 0/3/3/3 |
| 32 | MA6 | 2a | 1518 | 32 | - | 3/11/29/30 | 0/3/3/3 |
| 1 | OMU | 2A | 2552 | 56,1 | - | 0/9/27/28 | 0/2/2/2 |
| 54 | 4SU | 2y | 8 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1518 | 32 | - | 1/11/29/30 | 0/3/3/3 |
| 32 | 5MC | 2a | 1404 | 32 | - | 2/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1400 | 32 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | OMG | 2A | 2251 | 56,1,55 | - | 0/9/27/28 | 0/3/3/3 |
| 32 | 5MC | 1a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1939 | 1 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 55 | 4SU | 2x | 8 | 56,55 | - | 1/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 1a | 1207 | 32 | - | 0/9/27/28 | 0/3/3/3 |
| 1 | 5MU | 1A | 1939 | 56,1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1519 | 32 | - | 4/11/29/30 | 0/3/3/3 |
| 32 | 7MG | 2a | 527 | 56,32 | - | 3/7/37/38 | 0/3/3/3 |
| 32 | PSU | 1a | 516 | 56,32 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | CM0 | 1y | 34 | 54 | - | 4/12/30/31 | 0/2/2/2 |
| 1 | PSU | 1A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1915 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1407 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMC | 1A | 1920 | 1 | - | 1/9/27/28 | 0/2/2/2 |
| 54 | PSU | 2w | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 1y | 54 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 1 | OMU | 1A | 2552 | 56,1 | - | 0/9/27/28 | 0/2/2/2 |
| 54 | 7MG | 1y | 46 | 54 | - | 5/7/37/38 | 0/3/3/3 |
| 43 | 0TD | 2l | 92 | 43 | - | 1/7/12/14 | - |
| 43 | 0TD | 1l | 92 | 43 | - | 3/7/12/14 | - |
| 54 | CM0 | 1w | 34 | 54 | - | 1/12/30/31 | 0/2/2/2 |
| 1 | PSU | 1A | 2605 | 56,1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 7MG | 1a | 527 | 56,32 | - | 3/7/37/38 | 0/3/3/3 |
| 1 | 5MC | 1A | 1942 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 1y | 8 | 54 | - | 3/7/25/26 | 0/2/2/2 |
| 54 | 6MZ | 1y | 37 | 54 | - | 2/9/27/28 | 0/3/3/3 |
| 55 | 5MU | 2x | 54 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 4SU | 2w | 8 | 54 | - | 1/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 2y | 54 | 54 | - | 3/7/25/26 | 0/2/2/2 |
| 55 | 5MU | 1x | 54 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 4SU | 1x | 8 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 2MG | 2a | 1207 | 32 | - | 2/9/27/28 | 0/3/3/3 |
| 54 | PSU | 2y | 55 | 54 | - | 3/7/25/26 | 0/2/2/2 |
| 32 | M2G | 2a | 966 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 54 | 6MZ | 2w | 37 | 54 | - | 2/9/27/28 | 0/3/3/3 |
| 32 | 5MC | 2a | 967 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | M2G | 1a | 966 | 32 | - | 0/11/29/30 | 0/3/3/3 |
| 54 | PSU | 1w | 55 | 54 | - | 1/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | 2MA | 2A | 2503 | 1 | - | 0/7/25/26 | 0/3/3/3 |
| 32 | 5MC | 1a | 967 | 32 | - | 2/7/25/26 | 0/2/2/2 |
| 32 | MA6 | 2a | 1519 | 32 | - | 6/11/29/30 | 0/3/3/3 |
| 54 | 5MU | 1w | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MC | 1x | 32 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 1A | 1962 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1915 | 1 | - | 2/7/25/26 | 0/2/2/2 |
| 54 | CM0 | 2y | 34 | 54 | - | 5/12/30/31 | 0/2/2/2 |
| 1 | OMC | 2A | 1920 | 1 | - | 0/9/27/28 | 0/2/2/2 |
| 54 | 7MG | 2y | 46 | 54 | - | 5/7/37/38 | 0/3/3/3 |
| 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 |
| 54 | 4SU | 1w | 8 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MC | 2x | 32 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 56,1 | - | 1/7/25/26 | 0/3/3/3 |
| 54 | 6MZ | 2y | 37 | 54 | - | 2/9/27/28 | 0/3/3/3 |
| 55 | PSU | 2x | 55 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 4OC | 1a | 1402 | 32 | - | 2/9/29/30 | 0/2/2/2 |
| 32 | PSU | 2a | 516 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | 5MU | 2w | 54 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | CM0 | 2w | 34 | 54 | - | 7/12/30/31 | 0/2/2/2 |
| 54 | 7MG | 2w | 46 | 54 | - | 0/7/37/38 | 0/3/3/3 |
| 32 | UR3 | 2a | 1498 | 32 | - | 0/7/25/26 | 0/2/2/2 |

The worst 5 of 253 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 43 | 1l | 92 | 0TD | CB-SB | -12.87 | 1.69 | 1.82 |
| 43 | 2l | 92 | 0TD | CB-SB | -12.64 | 1.69 | 1.82 |
| 32 | 2a | 967 | 5MC | C5-C4 | 6.37 | 1.48 | 1.44 |
| 32 | 2a | 1400 | 5MC | C5-C4 | 6.36 | 1.48 | 1.44 |
| 55 | 2x | 32 | 5MC | C5-C4 | 6.33 | 1.48 | 1.44 |

The worst 5 of 414 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 43 | 1l | 92 | 0TD | CSB-SB-CB | -17.14 | 71.55 | 102.36 |
| 43 | 2l | 92 | 0TD | CSB-SB-CB | -10.96 | 82.66 | 102.36 |
| 54 | 1y | 46 | 7MG | N9-C4-N3 | 10.14 | 140.32 | 125.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | 2y | 46 | 7MG | N9-C4-N3 | 9.83 | 139.87 | 125.46 |
| 32 | 1a | 527 | 7MG | N9-C4-N3 | 8.96 | 138.59 | 125.46 |

There are no chirality outliers.

5 of 93 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 32 | 1a | 1400 | 5MC | O4'-C4'-C5'-O5' |
| 32 | 1a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 43 | 1l | 92 | 0TD | O-C-CA-CB |
| 32 | 2a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | O4'-C4'-C5'-O5' |

There are no ring outliers.

42 monomers are involved in 62 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | 2A | 1962 | 5MC | 1 | 0 |
| 32 | 2a | 1402 | 4OC | 3 | 0 |
| 54 | 1w | 46 | 7MG | 5 | 0 |
| 32 | 1a | 1498 | UR3 | 1 | 0 |
| 32 | 2a | 1518 | MA6 | 2 | 0 |
| 1 | 2A | 2552 | OMU | 1 | 0 |
| 32 | 1a | 1518 | MA6 | 2 | 0 |
| 32 | 1a | 1400 | 5MC | 1 | 0 |
| 1 | 2A | 2251 | OMG | 1 | 0 |
| 1 | 2A | 1939 | 5MU | 2 | 0 |
| 55 | 2x | 8 | 4SU | 1 | 0 |
| 32 | 1a | 1207 | 2MG | 1 | 0 |
| 1 | 1A | 1939 | 5MU | 1 | 0 |
| 32 | 1a | 1519 | MA6 | 3 | 0 |
| 32 | 2a | 527 | 7MG | 1 | 0 |
| 32 | 1a | 516 | PSU | 1 | 0 |
| 54 | 1y | 34 | CM0 | 2 | 0 |
| 1 | 1A | 1920 | OMC | 1 | 0 |
| 1 | 1A | 2552 | OMU | 1 | 0 |
| 43 | 2l | 92 | 0TD | 2 | 0 |
| 54 | 1y | 8 | 4SU | 1 | 0 |
| 54 | 1y | 37 | 6MZ | 2 | 0 |
| 54 | 2w | 8 | 4SU | 3 | 0 |
| 1 | 2A | 1917 | PSU | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 55 | 1x | 8 | 4SU | 2 | 0 |
| 32 | 2a | 966 | M2G | 1 | 0 |
| 54 | 2w | 37 | 6MZ | 2 | 0 |
| 32 | 2a | 967 | 5MC | 2 | 0 |
| 32 | 1a | 966 | M2G | 1 | 0 |
| 54 | 1w | 55 | PSU | 1 | 0 |
| 1 | 2A | 2503 | 2MA | 1 | 0 |
| 32 | 1a | 967 | 5MC | 1 | 0 |
| 32 | 2a | 1519 | MA6 | 1 | 0 |
| 54 | 1w | 54 | 5MU | 2 | 0 |
| 55 | 1x | 32 | 5MC | 1 | 0 |
| 1 | 2A | 1920 | OMC | 2 | 0 |
| 54 | 2y | 46 | 7MG | 1 | 0 |
| 32 | 1a | 1404 | 5MC | 1 | 0 |
| 54 | 1w | 8 | 4SU | 1 | 0 |
| 55 | 2x | 55 | PSU | 1 | 0 |
| 32 | 1a | 1402 | 4OC | 3 | 0 |
| 54 | 2w | 54 | 5MU | 3 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2778 ligands modelled in this entry, 2770 are monoatomic - leaving 8 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 | $\#\|Z\| > 2$ |
| 57 | LUJ | 1a | 1832 | 56 | 46,47,47 | 0.77 | 1 (2%) | 60,69,69 | 1.21 | 3 (5%) |
| 60 | SF4 | 1d | 501 | 35 | 0,12,12 | - | - | - | | |
| 60 | SF4 | 2d | 303 | 35 | 0,12,12 | - | - | - | | |
| 57 | LUJ | 1A | 4099 | - | 44,45,47 | 0.79 | 1 (2%) | 60,67,69 | 1.51 | 8 (13%) |
| 57 | LUJ | 1A | 4100 | - | 44,45,47 | 0.74 | 1 (2%) | 60,67,69 | 1.14 | 3 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 57 | LUJ | 2a | 3232 | - | 46,47,47 | 0.83 | 3 (6%) | 60,69,69 | 1.36 | 5 (8%) |
| 57 | LUJ | 2A | 3851 | - | 44,45,47 | 0.83 | 2 (4%) | 60,67,69 | 1.57 | 9 (15%) |
| 57 | LUJ | 2A | 3852 | - | 44,45,47 | 0.76 | 1 (2%) | 60,67,69 | 1.21 | 4 (6%) |

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 |
|---|---|---|---|---|---|---|---|
| 57 | LUJ | 1a | 1832 | 56 | - | 5/21/97/97 | 0/4/4/4 |
| 60 | SF4 | 1d | 501 | 35 | - | - | 0/6/5/5 |
| 60 | SF4 | 2d | 303 | 35 | - | - | 0/6/5/5 |
| 57 | LUJ | 1A | 4099 | - | - | 6/18/94/97 | 0/4/4/4 |
| 57 | LUJ | 1A | 4100 | - | - | 5/18/94/97 | 0/4/4/4 |
| 57 | LUJ | 2a | 3232 | - | - | 6/21/97/97 | 0/4/4/4 |
| 57 | LUJ | 2A | 3851 | - | - | 4/18/94/97 | 0/4/4/4 |
| 57 | LUJ | 2A | 3852 | - | - | 4/18/94/97 | 0/4/4/4 |

The worst 5 of 9 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 57 | 2A | 3851 | LUJ | O4'-C1' | 2.76 | 1.46 | 1.41 |
| 57 | 1A | 4100 | LUJ | O4'-C1' | 2.71 | 1.46 | 1.41 |
| 57 | 2A | 3851 | LUJ | CBE-CBD | -2.34 | 1.50 | 1.53 |
| 57 | 1a | 1832 | LUJ | CBG-CBE | -2.30 | 1.50 | 1.53 |
| 57 | 2a | 3232 | LUJ | O4'-C1' | 2.11 | 1.45 | 1.41 |

The worst 5 of 32 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 57 | 2a | 3232 | LUJ | CBF-O3'-C3' | -6.50 | 102.56 | 117.98 |
| 57 | 1A | 4099 | LUJ | O1'-C1'-O4' | -5.62 | 105.63 | 111.37 |
| 57 | 1a | 1832 | LUJ | CBF-O3'-C3' | -5.47 | 105.01 | 117.98 |
| 57 | 2A | 3851 | LUJ | O1'-C1'-O4' | -5.34 | 105.91 | 111.37 |
| 57 | 2A | 3852 | LUJ | CBF-O3'-C3' | -4.91 | 106.35 | 117.98 |

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | 1a | 1832 | LUJ | CBI-CBG-CBP-CBQ |
| 57 | 1a | 1832 | LUJ | CBE-CBG-CBP-CBQ |
| 57 | 2a | 3232 | LUJ | CBI-CBG-CBP-CBQ |
| 57 | 2a | 3232 | LUJ | CBE-CBG-CBP-CBQ |
| 57 | 2a | 3232 | LUJ | O4'-C4'-C5'-O5' |

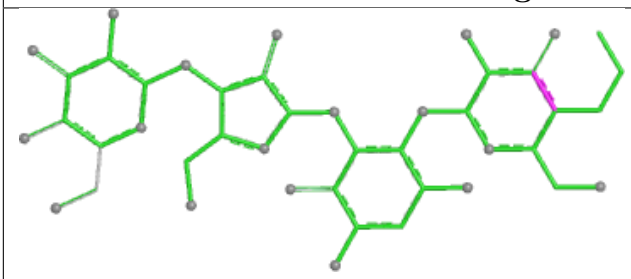
There are no ring outliers.

6 monomers are involved in 8 short contacts:

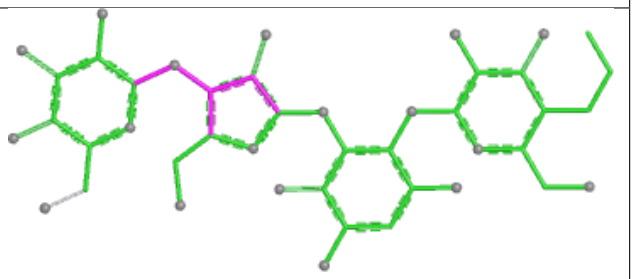
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 57 | 1a | 1832 | LUJ | 1 | 0 |
| 57 | 1A | 4099 | LUJ | 2 | 0 |
| 57 | 1A | 4100 | LUJ | 1 | 0 |
| 57 | 2a | 3232 | LUJ | 1 | 0 |
| 57 | 2A | 3851 | LUJ | 2 | 0 |
| 57 | 2A | 3852 | LUJ | 1 | 0 |

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

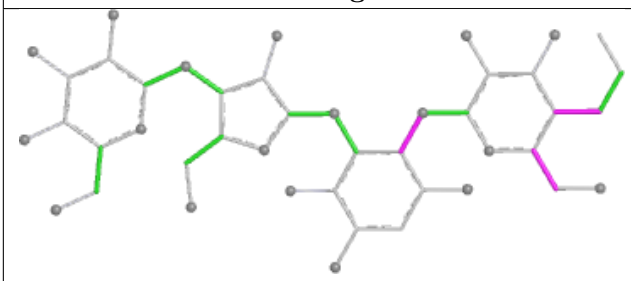
**Ligand LUJ 1a 1832**



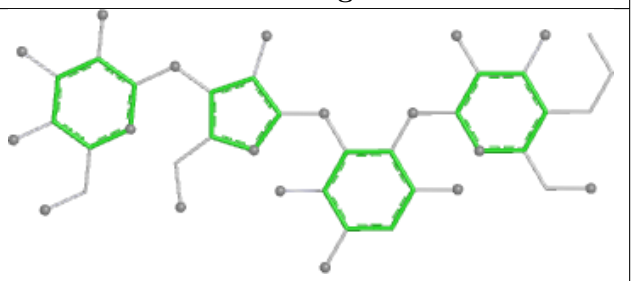
Bond lengths



Bond angles

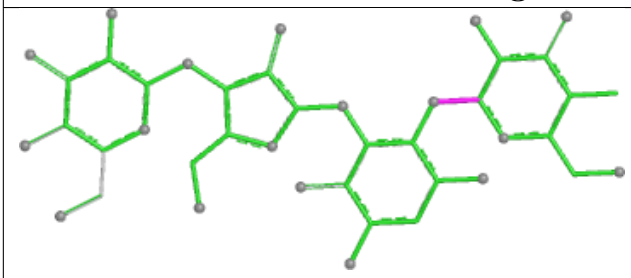


Torsions

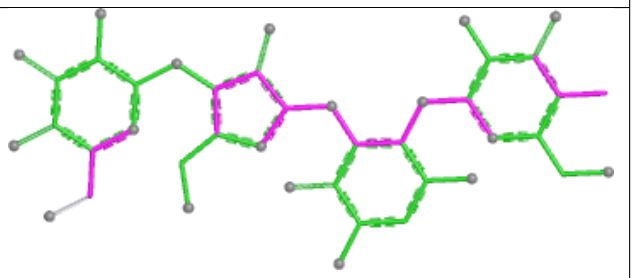


Rings

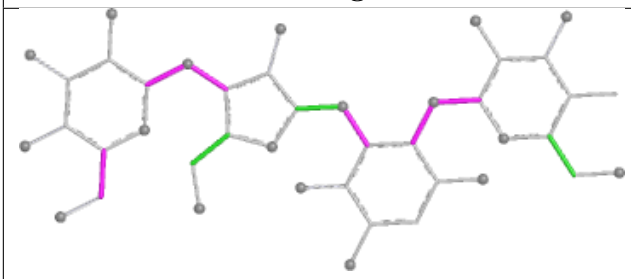
**Ligand LUJ 1A 4099**



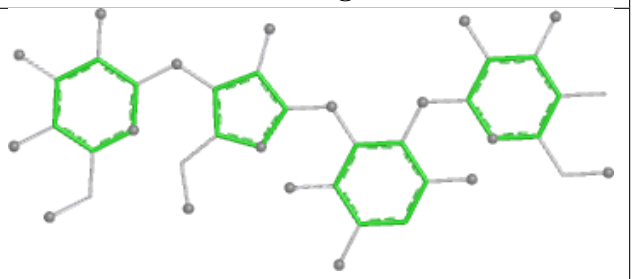
Bond lengths



Bond angles

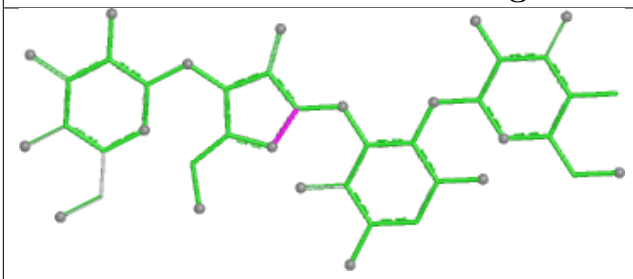


Torsions

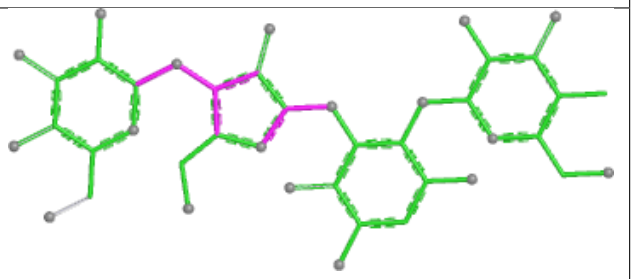


Rings

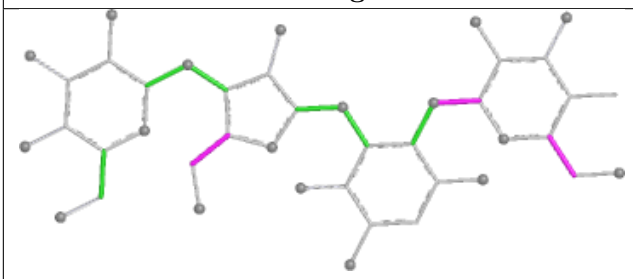
**Ligand LUJ 1A 4100**



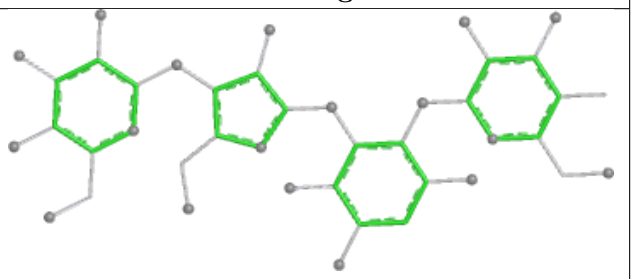
Bond lengths



Bond angles

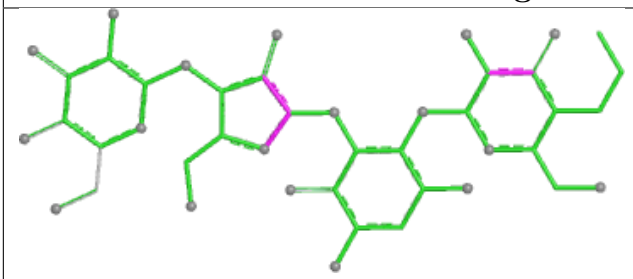


Torsions

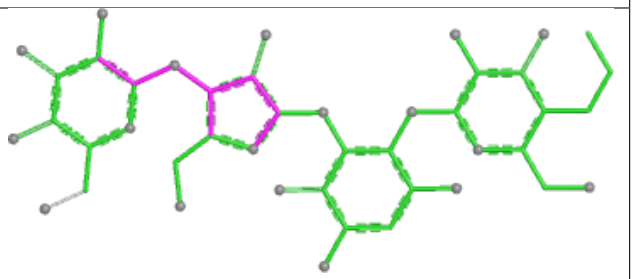


Rings

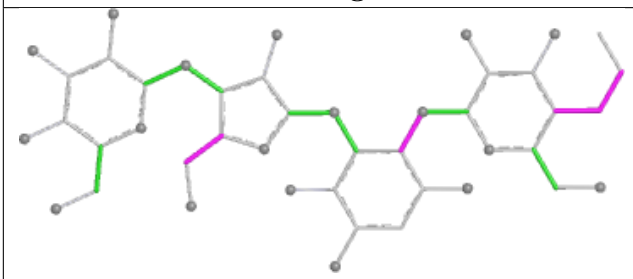
**Ligand LUJ 2a 3232**



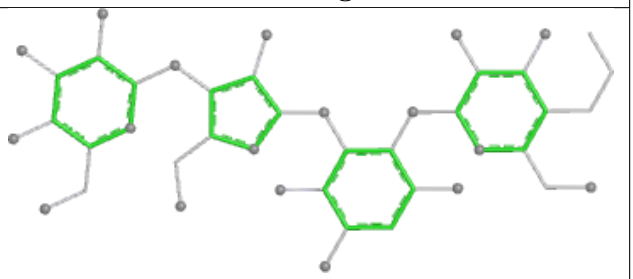
Bond lengths



Bond angles

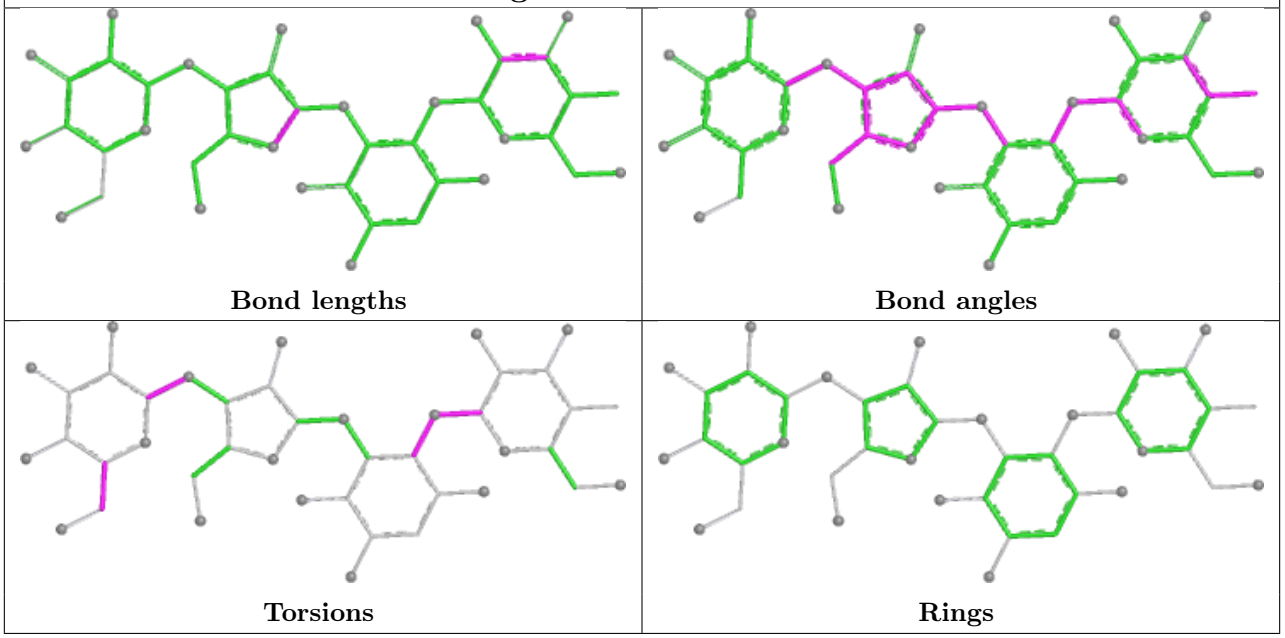


Torsions

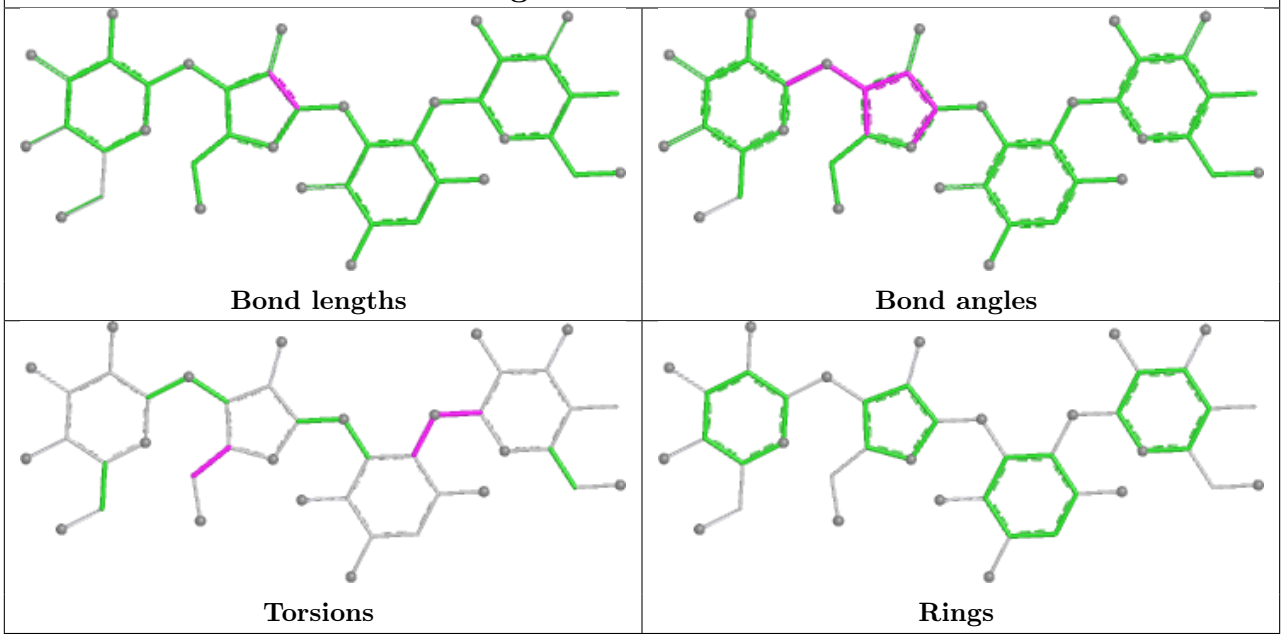


Rings

**Ligand LUJ 2A 3851**




**Ligand LUJ 2A 3852**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | 1A | 2860/2915 (98%) | -0.38 | 97 (3%) 48 46 | 11, 28, 86, 98 | 0 |
| 1 | 2A | 2789/2915 (95%) | 0.17 | 95 (3%) 48 46 | 26, 53, 86, 100 | 0 |
| 2 | 1B | 120/121 (99%) | -0.28 | 0 100 100 | 21, 40, 53, 74 | 0 |
| 2 | 2B | 120/121 (99%) | 0.76 | 1 (0%) 82 82 | 55, 70, 79, 87 | 0 |
| 3 | 1D | 275/276 (99%) | -0.05 | 4 (1%) 72 71 | 13, 31, 45, 74 | 0 |
| 3 | 2D | 275/276 (99%) | 0.37 | 2 (0%) 84 84 | 24, 44, 58, 69 | 0 |
| 4 | 1E | 204/206 (99%) | 0.00 | 0 100 100 | 12, 33, 52, 69 | 0 |
| 4 | 2E | 204/206 (99%) | 0.58 | 8 (3%) 43 40 | 29, 55, 68, 76 | 0 |
| 5 | 1F | 203/210 (96%) | 0.03 | 0 100 100 | 13, 35, 60, 77 | 0 |
| 5 | 2F | 203/210 (96%) | 0.79 | 9 (4%) 39 38 | 31, 61, 75, 79 | 0 |
| 6 | 1G | 181/182 (99%) | 0.80 | 14 (7%) 19 19 | 34, 52, 66, 76 | 0 |
| 6 | 2G | 181/182 (99%) | 1.16 | 22 (12%) 8 7 | 57, 70, 78, 92 | 0 |
| 7 | 1H | 174/180 (96%) | 0.25 | 5 (2%) 53 52 | 31, 45, 57, 63 | 0 |
| 7 | 2H | 174/180 (96%) | 1.52 | 40 (22%) 2 2 | 63, 76, 84, 89 | 0 |
| 8 | 1I | 146/148 (98%) | 0.84 | 6 (4%) 41 39 | 38, 64, 75, 80 | 0 |
| 8 | 2I | 146/148 (98%) | 0.90 | 8 (5%) 30 30 | 53, 65, 74, 78 | 0 |
| 9 | 1N | 140/140 (100%) | 0.01 | 1 (0%) 84 84 | 18, 31, 51, 68 | 0 |
| 9 | 2N | 140/140 (100%) | 0.91 | 5 (3%) 46 44 | 43, 59, 70, 82 | 0 |
| 10 | 1O | 122/122 (100%) | 0.05 | 0 100 100 | 20, 34, 51, 57 | 0 |
| 10 | 2O | 122/122 (100%) | 0.63 | 4 (3%) 49 47 | 43, 55, 65, 67 | 0 |
| 11 | 1P | 149/150 (99%) | 0.13 | 0 100 100 | 13, 39, 62, 68 | 0 |
| 11 | 2P | 149/150 (99%) | 0.77 | 9 (6%) 27 28 | 34, 61, 73, 80 | 0 |
| 12 | 1Q | 141/141 (100%) | 0.07 | 3 (2%) 63 61 | 20, 33, 49, 65 | 0 |
| 12 | 2Q | 141/141 (100%) | 1.17 | 24 (17%) 4 3 | 43, 61, 71, 74 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | 1R | 118/118 (100%) | -0.16 | 0 100 100 | 16, 27, 43, 55 | 0 |
| 13 | 2R | 118/118 (100%) | 0.39 | 2 (1%) 69 67 | 36, 49, 58, 62 | 0 |
| 14 | 1S | 110/112 (98%) | 0.20 | 0 100 100 | 29, 40, 52, 58 | 0 |
| 14 | 2S | 110/112 (98%) | 1.13 | 13 (11%) 9 7 | 52, 63, 75, 79 | 0 |
| 15 | 1T | 131/146 (89%) | 0.26 | 4 (3%) 51 49 | 26, 38, 61, 66 | 0 |
| 15 | 2T | 131/146 (89%) | 0.72 | 1 (0%) 82 82 | 45, 57, 72, 74 | 0 |
| 16 | 1U | 116/118 (98%) | -0.18 | 1 (0%) 81 81 | 14, 23, 36, 60 | 0 |
| 16 | 2U | 116/118 (98%) | 0.78 | 3 (2%) 57 55 | 38, 57, 70, 78 | 0 |
| 17 | 1V | 101/101 (100%) | -0.19 | 0 100 100 | 13, 31, 48, 62 | 0 |
| 17 | 2V | 101/101 (100%) | 0.93 | 7 (6%) 23 22 | 43, 64, 72, 77 | 0 |
| 18 | 1W | 112/113 (99%) | -0.21 | 0 100 100 | 16, 24, 43, 70 | 0 |
| 18 | 2W | 112/113 (99%) | 0.41 | 2 (1%) 67 65 | 37, 46, 60, 75 | 0 |
| 19 | 1X | 95/96 (98%) | -0.02 | 1 (1%) 78 77 | 17, 29, 48, 68 | 0 |
| 19 | 2X | 95/96 (98%) | 0.73 | 4 (4%) 40 39 | 41, 53, 65, 70 | 0 |
| 20 | 1Y | 107/110 (97%) | 0.41 | 2 (1%) 66 64 | 28, 43, 65, 70 | 0 |
| 20 | 2Y | 107/110 (97%) | 1.06 | 12 (11%) 10 9 | 56, 65, 77, 79 | 0 |
| 21 | 1Z | 154/206 (74%) | 0.95 | 16 (10%) 11 11 | 29, 56, 81, 89 | 0 |
| 21 | 2Z | 160/206 (77%) | 1.52 | 43 (26%) 1 1 | 55, 73, 87, 91 | 0 |
| 22 | 10 | 83/85 (97%) | 0.22 | 5 (6%) 27 28 | 20, 28, 53, 69 | 0 |
| 22 | 20 | 83/85 (97%) | 1.15 | 15 (18%) 3 3 | 39, 57, 71, 80 | 0 |
| 23 | 11 | 97/98 (98%) | 0.24 | 1 (1%) 79 79 | 18, 36, 62, 69 | 0 |
| 23 | 21 | 97/98 (98%) | 0.71 | 3 (3%) 51 49 | 30, 52, 69, 74 | 0 |
| 24 | 12 | 70/72 (97%) | 0.28 | 2 (2%) 53 52 | 26, 40, 54, 68 | 0 |
| 24 | 22 | 70/72 (97%) | 0.91 | 7 (10%) 12 12 | 50, 62, 71, 79 | 0 |
| 25 | 13 | 59/60 (98%) | -0.17 | 0 100 100 | 17, 28, 48, 62 | 0 |
| 25 | 23 | 59/60 (98%) | 0.99 | 3 (5%) 33 33 | 50, 61, 75, 82 | 0 |
| 26 | 14 | 69/71 (97%) | 1.21 | 13 (18%) 3 2 | 41, 68, 81, 85 | 0 |
| 26 | 24 | 69/71 (97%) | 1.41 | 17 (24%) 2 1 | 71, 77, 85, 87 | 0 |
| 27 | 15 | 59/60 (98%) | -0.27 | 1 (1%) 69 67 | 12, 24, 44, 55 | 0 |
| 27 | 25 | 59/60 (98%) | 0.39 | 1 (1%) 69 67 | 34, 47, 62, 67 | 0 |
| 28 | 16 | 53/54 (98%) | -0.01 | 0 100 100 | 26, 34, 45, 51 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 28 | 26 | 53/54 (98%) | 0.76 | 4 (7%) 20 20 | 42, 53, 63, 70 | 0 |
| 29 | 17 | 48/49 (97%) | -0.22 | 1 (2%) 63 61 | 14, 19, 50, 59 | 0 |
| 29 | 27 | 48/49 (97%) | 0.23 | 3 (6%) 26 26 | 29, 38, 57, 71 | 0 |
| 30 | 18 | 64/65 (98%) | 0.08 | 1 (1%) 70 69 | 18, 26, 35, 52 | 0 |
| 30 | 28 | 64/65 (98%) | 0.66 | 1 (1%) 70 69 | 39, 49, 56, 66 | 0 |
| 31 | 19 | 37/37 (100%) | -0.03 | 0 100 100 | 22, 32, 46, 47 | 0 |
| 31 | 29 | 37/37 (100%) | 1.06 | 3 (8%) 18 18 | 54, 66, 75, 77 | 0 |
| 32 | 1a | 1488/1521 (97%) | 0.32 | 27 (1%) 67 65 | 29, 57, 83, 98 | 0 |
| 32 | 2a | 1491/1521 (98%) | 0.63 | 66 (4%) 39 38 | 43, 69, 87, 100 | 0 |
| 33 | 1b | 231/256 (90%) | 1.13 | 30 (12%) 7 6 | 54, 70, 78, 84 | 0 |
| 33 | 2b | 231/256 (90%) | 1.46 | 49 (21%) 2 2 | 65, 78, 85, 92 | 0 |
| 34 | 1c | 206/239 (86%) | 0.98 | 12 (5%) 29 29 | 47, 63, 73, 78 | 0 |
| 34 | 2c | 206/239 (86%) | 1.44 | 45 (21%) 2 2 | 64, 75, 81, 88 | 0 |
| 35 | 1d | 208/209 (99%) | 0.92 | 18 (8%) 16 16 | 50, 60, 70, 76 | 0 |
| 35 | 2d | 208/209 (99%) | 0.89 | 11 (5%) 32 31 | 50, 64, 73, 82 | 0 |
| 36 | 1e | 148/162 (91%) | 0.62 | 2 (1%) 73 73 | 45, 56, 65, 71 | 0 |
| 36 | 2e | 148/162 (91%) | 1.15 | 18 (12%) 8 7 | 56, 70, 76, 82 | 0 |
| 37 | 1f | 100/101 (99%) | 0.33 | 0 100 100 | 41, 55, 64, 73 | 0 |
| 37 | 2f | 100/101 (99%) | 0.69 | 5 (5%) 34 34 | 50, 61, 69, 76 | 0 |
| 38 | 1g | 155/156 (99%) | 1.13 | 22 (14%) 6 5 | 52, 63, 75, 83 | 0 |
| 38 | 2g | 155/156 (99%) | 1.13 | 20 (12%) 7 6 | 61, 70, 79, 82 | 0 |
| 39 | 1h | 137/138 (99%) | 0.61 | 3 (2%) 62 60 | 48, 58, 64, 74 | 0 |
| 39 | 2h | 137/138 (99%) | 1.06 | 9 (6%) 24 24 | 61, 69, 75, 79 | 0 |
| 40 | 1i | 127/128 (99%) | 1.35 | 23 (18%) 3 3 | 44, 66, 75, 80 | 0 |
| 40 | 2i | 127/128 (99%) | 1.84 | 49 (38%) 1 0 | 66, 75, 82, 85 | 0 |
| 41 | 1j | 97/105 (92%) | 1.39 | 22 (22%) 2 2 | 49, 70, 80, 90 | 0 |
| 41 | 2j | 96/105 (91%) | 1.98 | 45 (46%) 0 0 | 64, 76, 83, 88 | 0 |
| 42 | 1k | 114/129 (88%) | 0.54 | 2 (1%) 67 65 | 37, 57, 66, 75 | 0 |
| 42 | 2k | 114/129 (88%) | 1.01 | 10 (8%) 15 15 | 51, 65, 74, 76 | 0 |
| 43 | 1l | 121/132 (91%) | 0.29 | 2 (1%) 69 67 | 36, 45, 56, 62 | 0 |
| 43 | 2l | 121/132 (91%) | 0.88 | 11 (9%) 15 14 | 49, 61, 69, 73 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 44 | 1m | 123/126 (97%) | 1.18 | 15 (12%) 8 7 | 47, 62, 72, 85 | 0 |
| 44 | 2m | 122/126 (96%) | 1.78 | 29 (23%) 2 1 | 64, 73, 81, 90 | 0 |
| 45 | 1n | 60/61 (98%) | 1.06 | 6 (10%) 12 12 | 48, 57, 65, 69 | 0 |
| 45 | 2n | 60/61 (98%) | 2.27 | 32 (53%) 0 0 | 66, 76, 80, 81 | 0 |
| 46 | 1o | 88/89 (98%) | 0.55 | 3 (3%) 48 46 | 41, 54, 66, 70 | 0 |
| 46 | 2o | 88/89 (98%) | 0.98 | 8 (9%) 15 14 | 56, 66, 73, 78 | 0 |
| 47 | 1p | 82/88 (93%) | 1.37 | 15 (18%) 3 2 | 48, 59, 70, 79 | 0 |
| 47 | 2p | 82/88 (93%) | 1.01 | 7 (8%) 16 17 | 53, 62, 69, 75 | 0 |
| 48 | 1q | 99/105 (94%) | 0.76 | 5 (5%) 33 33 | 42, 57, 65, 71 | 0 |
| 48 | 2q | 99/105 (94%) | 1.06 | 7 (7%) 22 22 | 55, 66, 74, 76 | 0 |
| 49 | 1r | 68/88 (77%) | 0.35 | 1 (1%) 72 71 | 48, 57, 67, 72 | 0 |
| 49 | 2r | 68/88 (77%) | 0.88 | 4 (5%) 28 28 | 55, 65, 75, 83 | 0 |
| 50 | 1s | 83/93 (89%) | 1.10 | 8 (9%) 13 13 | 50, 61, 72, 78 | 0 |
| 50 | 2s | 83/93 (89%) | 1.69 | 21 (25%) 1 1 | 67, 77, 82, 86 | 0 |
| 51 | 1t | 96/106 (90%) | 1.13 | 13 (13%) 7 5 | 46, 60, 72, 74 | 0 |
| 51 | 2t | 96/106 (90%) | 1.03 | 14 (14%) 6 5 | 53, 64, 75, 77 | 0 |
| 52 | 1u | 23/27 (85%) | 1.66 | 5 (21%) 2 2 | 55, 59, 64, 65 | 0 |
| 52 | 2u | 23/27 (85%) | 2.16 | 10 (43%) 0 0 | 67, 74, 78, 80 | 0 |
| 53 | 1v | 13/27 (48%) | 0.91 | 3 (23%) 2 1 | 40, 50, 82, 92 | 0 |
| 53 | 2v | 13/27 (48%) | 1.40 | 5 (38%) 1 0 | 56, 72, 92, 94 | 0 |
| 54 | 1w | 67/76 (88%) | 1.39 | 17 (25%) 1 1 | 44, 81, 92, 95 | 0 |
| 54 | 1y | 67/76 (88%) | 1.40 | 13 (19%) 3 2 | 31, 89, 96, 96 | 0 |
| 54 | 2w | 67/76 (88%) | 1.64 | 22 (32%) 1 1 | 65, 89, 95, 101 | 0 |
| 54 | 2y | 67/76 (88%) | 1.48 | 19 (28%) 1 1 | 49, 92, 97, 99 | 0 |
| 55 | 1x | 72/77 (93%) | 0.48 | 4 (5%) 30 30 | 30, 60, 74, 80 | 0 |
| 55 | 2x | 72/77 (93%) | 0.84 | 5 (6%) 23 22 | 50, 74, 82, 88 | 0 |
| All | All | 20878/21754 (95%) | 0.48 | 1341 (6%) 25 25 | 11, 57, 82, 101 | 0 |

The worst 5 of 1341 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 44 | 2m | 123 | ALA | 12.6 |
| 44 | 1m | 124 | PRO | 10.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 44 | 2m | 124 | PRO | 10.7 |
| 44 | 2m | 122 | LYS | 9.7 |
| 44 | 1m | 123 | ALA | 8.2 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ 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 |
|---|---|---|---|---|---|---|---|---|
| 54 | 6MZ | 2y | 37 | 23/24 | 0.34 | 0.19 | 82,87,100,116 | 0 |
| 54 | 7MG | 2w | 46 | 24/25 | 0.52 | 0.16 | 80,90,102,117 | 0 |
| 54 | 7MG | 2y | 46 | 24/25 | 0.53 | 0.16 | 87,98,104,119 | 0 |
| 54 | CM0 | 2y | 34 | 25/26 | 0.55 | 0.18 | 82,94,105,114 | 0 |
| 54 | 4SU | 2y | 8 | 20/21 | 0.55 | 0.14 | 92,97,104,113 | 0 |
| 54 | PSU | 2w | 55 | 20/21 | 0.57 | 0.17 | 74,91,97,99 | 0 |
| 54 | 4SU | 2w | 8 | 20/21 | 0.60 | 0.16 | 84,94,99,102 | 0 |
| 54 | 4SU | 1y | 8 | 20/21 | 0.64 | 0.13 | 82,91,101,109 | 0 |
| 54 | 7MG | 1y | 46 | 24/25 | 0.65 | 0.16 | 82,91,96,99 | 0 |
| 54 | CM0 | 1y | 34 | 25/26 | 0.68 | 0.17 | 79,86,99,109 | 0 |
| 54 | PSU | 1w | 55 | 20/21 | 0.69 | 0.16 | 63,85,89,91 | 0 |
| 54 | 7MG | 1w | 46 | 24/25 | 0.70 | 0.15 | 74,82,92,94 | 0 |
| 54 | 5MU | 2y | 54 | 21/22 | 0.71 | 0.13 | 82,90,102,115 | 0 |
| 54 | PSU | 2y | 55 | 20/21 | 0.71 | 0.15 | 85,91,95,96 | 0 |
| 54 | 6MZ | 1y | 37 | 23/24 | 0.72 | 0.17 | 77,82,92,107 | 0 |
| 54 | PSU | 1y | 55 | 20/21 | 0.74 | 0.14 | 79,88,95,98 | 0 |
| 54 | 5MU | 2w | 54 | 21/22 | 0.76 | 0.15 | 74,81,87,90 | 0 |
| 54 | 5MU | 1y | 54 | 21/22 | 0.79 | 0.12 | 70,80,88,93 | 0 |
| 54 | 4SU | 1w | 8 | 20/21 | 0.80 | 0.12 | 72,81,90,90 | 0 |
| 55 | PSU | 2x | 55 | 20/21 | 0.84 | 0.10 | 67,73,86,93 | 0 |
| 55 | 5MU | 1x | 54 | 21/22 | 0.85 | 0.14 | 54,62,70,75 | 0 |
| 32 | 2MG | 2a | 1207 | 24/25 | 0.85 | 0.12 | 54,77,82,86 | 0 |
| 54 | CM0 | 2w | 34 | 25/26 | 0.86 | 0.13 | 60,71,78,90 | 0 |
| 55 | 4SU | 2x | 8 | 20/21 | 0.86 | 0.10 | 71,76,79,87 | 0 |
| 32 | PSU | 2a | 516 | 20/21 | 0.86 | 0.11 | 63,68,72,80 | 0 |
| 55 | 5MU | 2x | 54 | 21/22 | 0.86 | 0.10 | 72,76,83,85 | 0 |
| 54 | 5MU | 1w | 54 | 21/22 | 0.86 | 0.12 | 52,67,79,83 | 0 |
| 43 | 0TD | 1l | 92 | 10/11 | 0.87 | 0.13 | 35,41,44,49 | 0 |
| 1 | 5MU | 2A | 1915 | 21/22 | 0.88 | 0.11 | 62,68,77,81 | 0 |
| 43 | 0TD | 2l | 92 | 10/11 | 0.89 | 0.13 | 56,61,66,79 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 32 | 5MC | 2a | 1407 | 21/22 | 0.90 | 0.15 | 46,54,61,74 | 0 |
| 32 | M2G | 2a | 966 | 25/26 | 0.90 | 0.15 | 53,63,72,76 | 0 |
| 54 | CM0 | 1w | 34 | 25/26 | 0.90 | 0.14 | 53,60,68,73 | 0 |
| 55 | 4SU | 1x | 8 | 20/21 | 0.91 | 0.12 | 47,62,75,77 | 0 |
| 32 | 7MG | 2a | 527 | 24/25 | 0.91 | 0.12 | 54,62,69,71 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.91 | 0.10 | 48,58,66,68 | 0 |
| 32 | 5MC | 2a | 967 | 21/22 | 0.91 | 0.14 | 58,65,74,77 | 0 |
| 55 | PSU | 1x | 55 | 20/21 | 0.91 | 0.10 | 50,62,65,72 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.91 | 0.12 | 46,52,58,60 | 0 |
| 32 | 5MC | 2a | 1400 | 21/22 | 0.92 | 0.14 | 56,62,67,67 | 0 |
| 55 | 5MC | 2x | 32 | 21/22 | 0.92 | 0.12 | 60,67,74,75 | 0 |
| 54 | 6MZ | 2w | 37 | 23/24 | 0.92 | 0.11 | 62,69,76,77 | 0 |
| 55 | 5MC | 1x | 32 | 21/22 | 0.93 | 0.12 | 36,49,52,56 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.94 | 0.09 | 53,58,60,63 | 0 |
| 32 | 4OC | 2a | 1402 | 22/23 | 0.94 | 0.11 | 45,58,61,62 | 0 |
| 32 | 5MC | 2a | 1404 | 21/22 | 0.94 | 0.10 | 46,51,57,58 | 0 |
| 32 | PSU | 1a | 516 | 20/21 | 0.94 | 0.09 | 40,49,51,54 | 0 |
| 32 | 2MG | 1a | 1207 | 24/25 | 0.94 | 0.10 | 51,59,62,69 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.94 | 0.09 | 37,47,51,52 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.95 | 0.10 | 47,56,62,68 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.95 | 0.09 | 39,50,54,56 | 0 |
| 1 | PSU | 1A | 1911 | 20/21 | 0.95 | 0.08 | 37,44,51,53 | 0 |
| 32 | 7MG | 1a | 527 | 24/25 | 0.95 | 0.09 | 28,38,44,47 | 0 |
| 32 | MA6 | 2a | 1518 | 24/25 | 0.95 | 0.13 | 43,54,61,63 | 0 |
| 32 | MA6 | 2a | 1519 | 24/25 | 0.95 | 0.15 | 43,57,63,65 | 0 |
| 54 | 6MZ | 1w | 37 | 23/24 | 0.95 | 0.10 | 40,46,53,54 | 0 |
| 32 | M2G | 1a | 966 | 25/26 | 0.95 | 0.10 | 37,45,51,55 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.95 | 0.09 | 32,38,44,52 | 0 |
| 1 | OMC | 2A | 1920 | 21/22 | 0.95 | 0.10 | 49,58,60,62 | 0 |
| 32 | UR3 | 2a | 1498 | 21/22 | 0.96 | 0.12 | 39,53,60,64 | 0 |
| 32 | 4OC | 1a | 1402 | 22/23 | 0.96 | 0.09 | 27,41,47,53 | 0 |
| 32 | MA6 | 1a | 1519 | 24/25 | 0.96 | 0.10 | 28,33,42,44 | 0 |
| 1 | 5MU | 2A | 1939 | 21/22 | 0.96 | 0.09 | 38,40,42,50 | 0 |
| 32 | 5MC | 1a | 967 | 21/22 | 0.96 | 0.08 | 40,46,50,53 | 0 |
| 1 | OMC | 1A | 1920 | 21/22 | 0.96 | 0.08 | 30,40,46,51 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.96 | 0.08 | 33,39,43,46 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.96 | 0.09 | 25,29,36,40 | 0 |
| 32 | 5MC | 1a | 1400 | 21/22 | 0.96 | 0.10 | 30,40,46,48 | 0 |
| 32 | 5MC | 1a | 1407 | 21/22 | 0.97 | 0.09 | 31,35,39,44 | 0 |
| 1 | OMU | 2A | 2552 | 21/22 | 0.97 | 0.07 | 27,37,43,48 | 0 |
| 1 | PSU | 2A | 2605 | 20/21 | 0.97 | 0.07 | 29,38,42,46 | 0 |
| 32 | MA6 | 1a | 1518 | 24/25 | 0.97 | 0.09 | 26,33,37,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | 5MC | 1A | 1962 | 21/22 | 0.97 | 0.08 | 26,32,35,45 | 0 |
| 1 | OMU | 1A | 2552 | 21/22 | 0.97 | 0.07 | 18,26,30,31 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.97 | 0.08 | 15,23,26,36 | 0 |
| 32 | 5MC | 1a | 1404 | 21/22 | 0.97 | 0.08 | 28,31,36,37 | 0 |
| 32 | UR3 | 1a | 1498 | 21/22 | 0.98 | 0.07 | 26,33,37,41 | 0 |
| 1 | 2MA | 1A | 2503 | 23/24 | 0.98 | 0.06 | 11,14,17,18 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.98 | 0.05 | 14,19,20,21 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.98 | 0.07 | 16,22,30,30 | 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, 95$^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3993 | 1/1 | 0.31 | 0.30 | 86,86,86,86 | 0 |
| 56 | MG | 1x | 114 | 1/1 | 0.35 | 0.17 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3649 | 1/1 | 0.49 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3046 | 1/1 | 0.54 | 0.19 | 72,72,72,72 | 0 |
| 56 | MG | 2B | 212 | 1/1 | 0.58 | 0.19 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 3106 | 1/1 | 0.58 | 0.21 | 74,74,74,74 | 0 |
| 56 | MG | 2y | 105 | 1/1 | 0.59 | 0.21 | 85,85,85,85 | 0 |
| 56 | MG | 1a | 1786 | 1/1 | 0.61 | 0.15 | 84,84,84,84 | 0 |
| 56 | MG | 2a | 3049 | 1/1 | 0.61 | 0.21 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3503 | 1/1 | 0.62 | 0.24 | 50,50,50,50 | 0 |
| 56 | MG | 1w | 106 | 1/1 | 0.62 | 0.16 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3662 | 1/1 | 0.62 | 0.29 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1662 | 1/1 | 0.62 | 0.33 | 66,66,66,66 | 0 |
| 56 | MG | 2y | 102 | 1/1 | 0.63 | 0.25 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 4053 | 1/1 | 0.63 | 0.61 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3219 | 1/1 | 0.64 | 0.27 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3355 | 1/1 | 0.64 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3731 | 1/1 | 0.64 | 0.23 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3722 | 1/1 | 0.65 | 0.19 | 53,53,53,53 | 0 |
| 56 | MG | 2y | 101 | 1/1 | 0.65 | 0.22 | 67,67,67,67 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1y | 104 | 1/1 | 0.65 | 0.22 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3671 | 1/1 | 0.65 | 0.24 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 4044 | 1/1 | 0.66 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3702 | 1/1 | 0.66 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3735 | 1/1 | 0.67 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3259 | 1/1 | 0.68 | 0.20 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3629 | 1/1 | 0.68 | 0.23 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3416 | 1/1 | 0.68 | 0.26 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3187 | 1/1 | 0.68 | 0.22 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1777 | 1/1 | 0.68 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3635 | 1/1 | 0.68 | 0.23 | 72,72,72,72 | 0 |
| 56 | MG | 1B | 218 | 1/1 | 0.68 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3001 | 1/1 | 0.68 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3224 | 1/1 | 0.69 | 0.20 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3647 | 1/1 | 0.69 | 0.18 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3204 | 1/1 | 0.69 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4032 | 1/1 | 0.69 | 0.13 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3024 | 1/1 | 0.70 | 0.16 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1776 | 1/1 | 0.70 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3268 | 1/1 | 0.70 | 0.23 | 69,69,69,69 | 0 |
| 56 | MG | 1x | 112 | 1/1 | 0.70 | 0.28 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 3016 | 1/1 | 0.70 | 0.21 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1782 | 1/1 | 0.71 | 0.12 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3466 | 1/1 | 0.71 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3836 | 1/1 | 0.71 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1y | 105 | 1/1 | 0.71 | 0.18 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3779 | 1/1 | 0.72 | 0.22 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3948 | 1/1 | 0.72 | 0.20 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3044 | 1/1 | 0.72 | 0.23 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3333 | 1/1 | 0.72 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 2y | 104 | 1/1 | 0.72 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3603 | 1/1 | 0.72 | 0.17 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1672 | 1/1 | 0.73 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3425 | 1/1 | 0.73 | 0.18 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3712 | 1/1 | 0.74 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3975 | 1/1 | 0.74 | 0.22 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3077 | 1/1 | 0.74 | 0.26 | 66,66,66,66 | 0 |
| 56 | MG | 1B | 231 | 1/1 | 0.74 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3608 | 1/1 | 0.74 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3766 | 1/1 | 0.74 | 0.17 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3771 | 1/1 | 0.74 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | 1l | 202 | 1/1 | 0.74 | 0.18 | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3367 | 1/1 | 0.74 | 0.24 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3140 | 1/1 | 0.74 | 0.24 | 54,54,54,54 | 0 |
| 56 | MG | 1v | 101 | 1/1 | 0.74 | 0.18 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3477 | 1/1 | 0.74 | 0.27 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1801 | 1/1 | 0.75 | 0.13 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3837 | 1/1 | 0.75 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3669 | 1/1 | 0.75 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3779 | 1/1 | 0.75 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3827 | 1/1 | 0.75 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1B | 230 | 1/1 | 0.75 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3841 | 1/1 | 0.75 | 0.18 | 42,42,42,42 | 0 |
| 56 | MG | 2B | 206 | 1/1 | 0.75 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3721 | 1/1 | 0.75 | 0.24 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 4036 | 1/1 | 0.75 | 0.21 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3821 | 1/1 | 0.75 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3029 | 1/1 | 0.75 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3571 | 1/1 | 0.76 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3596 | 1/1 | 0.76 | 0.21 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3865 | 1/1 | 0.76 | 0.26 | 42,42,42,42 | 0 |
| 56 | MG | 1B | 234 | 1/1 | 0.76 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3625 | 1/1 | 0.76 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1603 | 1/1 | 0.76 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3340 | 1/1 | 0.76 | 0.22 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3228 | 1/1 | 0.76 | 0.21 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3015 | 1/1 | 0.76 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3318 | 1/1 | 0.76 | 0.23 | 77,77,77,77 | 0 |
| 56 | MG | 1a | 1784 | 1/1 | 0.76 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3778 | 1/1 | 0.76 | 0.14 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3276 | 1/1 | 0.77 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3735 | 1/1 | 0.77 | 0.16 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3719 | 1/1 | 0.77 | 0.13 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3720 | 1/1 | 0.77 | 0.17 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3176 | 1/1 | 0.77 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3106 | 1/1 | 0.77 | 0.30 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3197 | 1/1 | 0.77 | 0.10 | 72,72,72,72 | 0 |
| 56 | MG | 1a | 1762 | 1/1 | 0.77 | 0.26 | 60,60,60,60 | 0 |
| 56 | MG | 2B | 209 | 1/1 | 0.77 | 0.16 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3594 | 1/1 | 0.77 | 0.20 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3442 | 1/1 | 0.77 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3231 | 1/1 | 0.77 | 0.21 | 73,73,73,73 | 0 |
| 56 | MG | 2x | 104 | 1/1 | 0.77 | 0.19 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3008 | 1/1 | 0.77 | 0.23 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3739 | 1/1 | 0.77 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3667 | 1/1 | 0.77 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3240 | 1/1 | 0.77 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 4110 | 1/1 | 0.78 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 1a | 1628 | 1/1 | 0.78 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3725 | 1/1 | 0.78 | 0.19 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3337 | 1/1 | 0.78 | 0.24 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3919 | 1/1 | 0.78 | 0.11 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3411 | 1/1 | 0.78 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3097 | 1/1 | 0.78 | 0.19 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3642 | 1/1 | 0.78 | 0.15 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3759 | 1/1 | 0.78 | 0.12 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3424 | 1/1 | 0.78 | 0.29 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3188 | 1/1 | 0.78 | 0.14 | 71,71,71,71 | 0 |
| 56 | MG | 1w | 104 | 1/1 | 0.78 | 0.23 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3232 | 1/1 | 0.78 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3469 | 1/1 | 0.78 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3670 | 1/1 | 0.78 | 0.15 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3845 | 1/1 | 0.78 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 1O | 204 | 1/1 | 0.78 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2t | 201 | 1/1 | 0.78 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3684 | 1/1 | 0.78 | 0.22 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3572 | 1/1 | 0.78 | 0.28 | 75,75,75,75 | 0 |
| 56 | MG | 2Q | 202 | 1/1 | 0.78 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3591 | 1/1 | 0.78 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 1V | 202 | 1/1 | 0.78 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3095 | 1/1 | 0.79 | 0.31 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3837 | 1/1 | 0.79 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1706 | 1/1 | 0.79 | 0.23 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3141 | 1/1 | 0.79 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3641 | 1/1 | 0.79 | 0.12 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4017 | 1/1 | 0.79 | 0.20 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3314 | 1/1 | 0.79 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3567 | 1/1 | 0.79 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 1Z | 304 | 1/1 | 0.79 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3482 | 1/1 | 0.79 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4045 | 1/1 | 0.79 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | 1E | 302 | 1/1 | 0.79 | 0.26 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3172 | 1/1 | 0.79 | 0.26 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3027 | 1/1 | 0.79 | 0.16 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3368 | 1/1 | 0.79 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3043 | 1/1 | 0.79 | 0.10 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3809 | 1/1 | 0.79 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | 1B | 220 | 1/1 | 0.79 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | 1y | 103 | 1/1 | 0.79 | 0.21 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3353 | 1/1 | 0.80 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3624 | 1/1 | 0.80 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3166 | 1/1 | 0.80 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3065 | 1/1 | 0.80 | 0.22 | 55,55,55,55 | 0 |
| 56 | MG | 2F | 303 | 1/1 | 0.80 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4052 | 1/1 | 0.80 | 0.12 | 21,21,21,21 | 0 |
| 56 | MG | 1x | 108 | 1/1 | 0.80 | 0.18 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3408 | 1/1 | 0.80 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3212 | 1/1 | 0.80 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3379 | 1/1 | 0.80 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3784 | 1/1 | 0.80 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3702 | 1/1 | 0.80 | 0.10 | 29,29,29,29 | 0 |
| 56 | MG | 2j | 201 | 1/1 | 0.80 | 0.15 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3937 | 1/1 | 0.80 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3828 | 1/1 | 0.80 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1B | 204 | 1/1 | 0.80 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1809 | 1/1 | 0.80 | 0.17 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3238 | 1/1 | 0.80 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3499 | 1/1 | 0.80 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 2y | 106 | 1/1 | 0.80 | 0.19 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3086 | 1/1 | 0.81 | 0.31 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3103 | 1/1 | 0.81 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3017 | 1/1 | 0.81 | 0.18 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1612 | 1/1 | 0.81 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3539 | 1/1 | 0.81 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3112 | 1/1 | 0.81 | 0.24 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3465 | 1/1 | 0.81 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1636 | 1/1 | 0.81 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3071 | 1/1 | 0.81 | 0.23 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3190 | 1/1 | 0.81 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3093 | 1/1 | 0.81 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1b | 302 | 1/1 | 0.81 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | 1f | 202 | 1/1 | 0.81 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3102 | 1/1 | 0.81 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3241 | 1/1 | 0.81 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3694 | 1/1 | 0.81 | 0.13 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1667 | 1/1 | 0.81 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3789 | 1/1 | 0.81 | 0.13 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3186 | 1/1 | 0.81 | 0.18 | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1E | 305 | 1/1 | 0.81 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3310 | 1/1 | 0.81 | 0.17 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1675 | 1/1 | 0.81 | 0.25 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3199 | 1/1 | 0.81 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 1x | 101 | 1/1 | 0.81 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3595 | 1/1 | 0.81 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 1a | 1709 | 1/1 | 0.81 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1735 | 1/1 | 0.81 | 0.22 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3849 | 1/1 | 0.81 | 0.15 | 70,70,70,70 | 0 |
| 56 | MG | 1a | 1748 | 1/1 | 0.81 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1T | 202 | 1/1 | 0.81 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3470 | 1/1 | 0.81 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 2B | 214 | 1/1 | 0.81 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3756 | 1/1 | 0.81 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 10 | 105 | 1/1 | 0.81 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3708 | 1/1 | 0.81 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3890 | 1/1 | 0.81 | 0.17 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1679 | 1/1 | 0.82 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4086 | 1/1 | 0.82 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3624 | 1/1 | 0.82 | 0.20 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3094 | 1/1 | 0.82 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3776 | 1/1 | 0.82 | 0.21 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3810 | 1/1 | 0.82 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3197 | 1/1 | 0.82 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3999 | 1/1 | 0.82 | 0.13 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3827 | 1/1 | 0.82 | 0.18 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3157 | 1/1 | 0.82 | 0.19 | 67,67,67,67 | 0 |
| 56 | MG | 1B | 227 | 1/1 | 0.82 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3411 | 1/1 | 0.82 | 0.27 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3155 | 1/1 | 0.82 | 0.13 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3177 | 1/1 | 0.82 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3457 | 1/1 | 0.82 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3202 | 1/1 | 0.82 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3680 | 1/1 | 0.82 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3266 | 1/1 | 0.82 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3072 | 1/1 | 0.82 | 0.18 | 54,54,54,54 | 0 |
| 56 | MG | 2B | 207 | 1/1 | 0.82 | 0.25 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3202 | 1/1 | 0.82 | 0.24 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3625 | 1/1 | 0.82 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1670 | 1/1 | 0.82 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3713 | 1/1 | 0.82 | 0.12 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3432 | 1/1 | 0.82 | 0.17 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2F | 305 | 1/1 | 0.82 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3275 | 1/1 | 0.82 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3806 | 1/1 | 0.82 | 0.35 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3007 | 1/1 | 0.82 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3278 | 1/1 | 0.82 | 0.21 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3281 | 1/1 | 0.82 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3727 | 1/1 | 0.82 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3288 | 1/1 | 0.82 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3734 | 1/1 | 0.82 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3886 | 1/1 | 0.83 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3273 | 1/1 | 0.83 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3733 | 1/1 | 0.83 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3014 | 1/1 | 0.83 | 0.21 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1793 | 1/1 | 0.83 | 0.12 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3888 | 1/1 | 0.83 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1U | 207 | 1/1 | 0.83 | 0.58 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 3055 | 1/1 | 0.83 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4026 | 1/1 | 0.83 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3306 | 1/1 | 0.83 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3085 | 1/1 | 0.83 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 1e | 201 | 1/1 | 0.83 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1693 | 1/1 | 0.83 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3029 | 1/1 | 0.83 | 0.16 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3360 | 1/1 | 0.83 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3794 | 1/1 | 0.83 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3138 | 1/1 | 0.83 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3340 | 1/1 | 0.83 | 0.26 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3659 | 1/1 | 0.83 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3347 | 1/1 | 0.83 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1717 | 1/1 | 0.83 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3750 | 1/1 | 0.83 | 0.17 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3445 | 1/1 | 0.83 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3176 | 1/1 | 0.83 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 1x | 103 | 1/1 | 0.83 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3184 | 1/1 | 0.83 | 0.31 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3698 | 1/1 | 0.83 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3210 | 1/1 | 0.83 | 0.14 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3215 | 1/1 | 0.83 | 0.18 | 71,71,71,71 | 0 |
| 56 | MG | 1x | 105 | 1/1 | 0.83 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3951 | 1/1 | 0.83 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2B | 216 | 1/1 | 0.83 | 0.28 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3541 | 1/1 | 0.83 | 0.11 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3480 | 1/1 | 0.83 | 0.23 | 67,67,67,67 | 0 |
| 56 | MG | 2j | 202 | 1/1 | 0.83 | 0.10 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3556 | 1/1 | 0.83 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1666 | 1/1 | 0.83 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3006 | 1/1 | 0.83 | 0.31 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3248 | 1/1 | 0.83 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3548 | 1/1 | 0.83 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3014 | 1/1 | 0.83 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | 1I | 201 | 1/1 | 0.83 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3313 | 1/1 | 0.84 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1712 | 1/1 | 0.84 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3750 | 1/1 | 0.84 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3764 | 1/1 | 0.84 | 0.08 | 62,62,62,62 | 0 |
| 56 | MG | 1G | 202 | 1/1 | 0.84 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3035 | 1/1 | 0.84 | 0.23 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3321 | 1/1 | 0.84 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3628 | 1/1 | 0.84 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3142 | 1/1 | 0.84 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1733 | 1/1 | 0.84 | 0.33 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3168 | 1/1 | 0.84 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3075 | 1/1 | 0.84 | 0.28 | 53,53,53,53 | 0 |
| 56 | MG | 1B | 206 | 1/1 | 0.84 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1637 | 1/1 | 0.84 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3359 | 1/1 | 0.84 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3366 | 1/1 | 0.84 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1653 | 1/1 | 0.84 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 2a | 3098 | 1/1 | 0.84 | 0.22 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4040 | 1/1 | 0.84 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1664 | 1/1 | 0.84 | 0.17 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3124 | 1/1 | 0.84 | 0.27 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3130 | 1/1 | 0.84 | 0.23 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3200 | 1/1 | 0.84 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3844 | 1/1 | 0.84 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3156 | 1/1 | 0.84 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3164 | 1/1 | 0.84 | 0.12 | 83,83,83,83 | 0 |
| 56 | MG | 1A | 3121 | 1/1 | 0.84 | 0.29 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3170 | 1/1 | 0.84 | 0.10 | 84,84,84,84 | 0 |
| 56 | MG | 1U | 204 | 1/1 | 0.84 | 0.15 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3180 | 1/1 | 0.84 | 0.19 | 83,83,83,83 | 0 |
| 56 | MG | 2A | 3850 | 1/1 | 0.84 | 0.24 | 70,70,70,70 | 0 |
| 56 | MG | 1a | 1669 | 1/1 | 0.84 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3467 | 1/1 | 0.84 | 0.23 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2B | 208 | 1/1 | 0.84 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1790 | 1/1 | 0.84 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3646 | 1/1 | 0.84 | 0.13 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3869 | 1/1 | 0.84 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3047 | 1/1 | 0.84 | 0.22 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 3214 | 1/1 | 0.84 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 2E | 307 | 1/1 | 0.84 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2E | 308 | 1/1 | 0.84 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3220 | 1/1 | 0.84 | 0.26 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3052 | 1/1 | 0.84 | 0.23 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3778 | 1/1 | 0.84 | 0.11 | 17,17,17,17 | 0 |
| 56 | MG | 2G | 201 | 1/1 | 0.84 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3070 | 1/1 | 0.84 | 0.22 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3344 | 1/1 | 0.84 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 2r | 101 | 1/1 | 0.84 | 0.10 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3004 | 1/1 | 0.84 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3962 | 1/1 | 0.84 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1699 | 1/1 | 0.84 | 0.25 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3969 | 1/1 | 0.84 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 2y | 103 | 1/1 | 0.84 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 2a | 3009 | 1/1 | 0.84 | 0.23 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3013 | 1/1 | 0.84 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1627 | 1/1 | 0.84 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3519 | 1/1 | 0.85 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3759 | 1/1 | 0.85 | 0.15 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3045 | 1/1 | 0.85 | 0.25 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3253 | 1/1 | 0.85 | 0.07 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3391 | 1/1 | 0.85 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3770 | 1/1 | 0.85 | 0.11 | 77,77,77,77 | 0 |
| 56 | MG | 2a | 3062 | 1/1 | 0.85 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3069 | 1/1 | 0.85 | 0.14 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3553 | 1/1 | 0.85 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3701 | 1/1 | 0.85 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1812 | 1/1 | 0.85 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 1U | 206 | 1/1 | 0.85 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3271 | 1/1 | 0.85 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3190 | 1/1 | 0.85 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3603 | 1/1 | 0.85 | 0.12 | 8,8,8,8 | 0 |
| 56 | MG | 2A | 3107 | 1/1 | 0.85 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3604 | 1/1 | 0.85 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3298 | 1/1 | 0.85 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3122 | 1/1 | 0.85 | 0.28 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3830 | 1/1 | 0.85 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3832 | 1/1 | 0.85 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3017 | 1/1 | 0.85 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3308 | 1/1 | 0.85 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3121 | 1/1 | 0.85 | 0.27 | 63,63,63,63 | 0 |
| 56 | MG | 1w | 103 | 1/1 | 0.85 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3878 | 1/1 | 0.85 | 0.11 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 4005 | 1/1 | 0.85 | 0.09 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3151 | 1/1 | 0.85 | 0.33 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3329 | 1/1 | 0.85 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1622 | 1/1 | 0.85 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3334 | 1/1 | 0.85 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3666 | 1/1 | 0.85 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4014 | 1/1 | 0.85 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3884 | 1/1 | 0.85 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3175 | 1/1 | 0.85 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3351 | 1/1 | 0.85 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3263 | 1/1 | 0.85 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1B | 233 | 1/1 | 0.85 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3179 | 1/1 | 0.85 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3218 | 1/1 | 0.85 | 0.14 | 69,69,69,69 | 0 |
| 56 | MG | 1a | 1640 | 1/1 | 0.85 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4027 | 1/1 | 0.85 | 0.14 | 80,80,80,80 | 0 |
| 56 | MG | 2T | 204 | 1/1 | 0.85 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3374 | 1/1 | 0.85 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3194 | 1/1 | 0.85 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3382 | 1/1 | 0.85 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3196 | 1/1 | 0.85 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3225 | 1/1 | 0.85 | 0.17 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3633 | 1/1 | 0.85 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3912 | 1/1 | 0.85 | 0.18 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3431 | 1/1 | 0.85 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3214 | 1/1 | 0.85 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3229 | 1/1 | 0.85 | 0.31 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3805 | 1/1 | 0.85 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3500 | 1/1 | 0.85 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1794 | 1/1 | 0.85 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1652 | 1/1 | 0.86 | 0.19 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3663 | 1/1 | 0.86 | 0.10 | 17,17,17,17 | 0 |
| 56 | MG | 1a | 1657 | 1/1 | 0.86 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3178 | 1/1 | 0.86 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3040 | 1/1 | 0.86 | 0.28 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1660 | 1/1 | 0.86 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 1e | 202 | 1/1 | 0.86 | 0.10 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3985 | 1/1 | 0.86 | 0.10 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3193 | 1/1 | 0.86 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3754 | 1/1 | 0.86 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3476 | 1/1 | 0.86 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3670 | 1/1 | 0.86 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3687 | 1/1 | 0.86 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3842 | 1/1 | 0.86 | 0.23 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3862 | 1/1 | 0.86 | 0.22 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3398 | 1/1 | 0.86 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3544 | 1/1 | 0.86 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3094 | 1/1 | 0.86 | 0.22 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3160 | 1/1 | 0.86 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3722 | 1/1 | 0.86 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1688 | 1/1 | 0.86 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3885 | 1/1 | 0.86 | 0.26 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3798 | 1/1 | 0.86 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3577 | 1/1 | 0.86 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3100 | 1/1 | 0.86 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3425 | 1/1 | 0.86 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3621 | 1/1 | 0.86 | 0.11 | 26,26,26,26 | 0 |
| 56 | MG | 1a | 1713 | 1/1 | 0.86 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3052 | 1/1 | 0.86 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3162 | 1/1 | 0.86 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1718 | 1/1 | 0.86 | 0.32 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4075 | 1/1 | 0.86 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3286 | 1/1 | 0.86 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3626 | 1/1 | 0.86 | 0.25 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3048 | 1/1 | 0.86 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3634 | 1/1 | 0.86 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3291 | 1/1 | 0.86 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | 13 | 101 | 1/1 | 0.86 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3191 | 1/1 | 0.86 | 0.14 | 66,66,66,66 | 0 |
| 56 | MG | 14 | 101 | 1/1 | 0.86 | 0.24 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1749 | 1/1 | 0.86 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | 2B | 210 | 1/1 | 0.86 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3080 | 1/1 | 0.86 | 0.20 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1752 | 1/1 | 0.86 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1601 | 1/1 | 0.86 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1767 | 1/1 | 0.86 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3365 | 1/1 | 0.86 | 0.14 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2F | 301 | 1/1 | 0.86 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 4101 | 1/1 | 0.86 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3108 | 1/1 | 0.86 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3939 | 1/1 | 0.86 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3787 | 1/1 | 0.86 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | 2d | 301 | 1/1 | 0.86 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3124 | 1/1 | 0.86 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1785 | 1/1 | 0.86 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3242 | 1/1 | 0.86 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3516 | 1/1 | 0.86 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | 1B | 219 | 1/1 | 0.86 | 0.22 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1639 | 1/1 | 0.86 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3714 | 1/1 | 0.86 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3162 | 1/1 | 0.86 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1795 | 1/1 | 0.86 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3370 | 1/1 | 0.86 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3518 | 1/1 | 0.86 | 0.08 | 43,43,43,43 | 0 |
| 57 | LUJ | 2A | 3851 | 42/44 | 0.86 | 0.16 | 50,62,75,82 | 0 |
| 56 | MG | 1A | 3817 | 1/1 | 0.87 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3350 | 1/1 | 0.87 | 0.28 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3677 | 1/1 | 0.87 | 0.15 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3554 | 1/1 | 0.87 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 1x | 113 | 1/1 | 0.87 | 0.23 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3010 | 1/1 | 0.87 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3357 | 1/1 | 0.87 | 0.25 | 48,48,48,48 | 0 |
| 56 | MG | 1B | 221 | 1/1 | 0.87 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 1x | 115 | 1/1 | 0.87 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3710 | 1/1 | 0.87 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3468 | 1/1 | 0.87 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3019 | 1/1 | 0.87 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3191 | 1/1 | 0.87 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3028 | 1/1 | 0.87 | 0.28 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3831 | 1/1 | 0.87 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3420 | 1/1 | 0.87 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1648 | 1/1 | 0.87 | 0.27 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3041 | 1/1 | 0.87 | 0.23 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3380 | 1/1 | 0.87 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3390 | 1/1 | 0.87 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3018 | 1/1 | 0.87 | 0.16 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3726 | 1/1 | 0.87 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | 2a | 3050 | 1/1 | 0.87 | 0.09 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3726 | 1/1 | 0.87 | 0.15 | 55,55,55,55 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3423 | 1/1 | 0.87 | 0.24 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3065 | 1/1 | 0.87 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3868 | 1/1 | 0.87 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3223 | 1/1 | 0.87 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3429 | 1/1 | 0.87 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3489 | 1/1 | 0.87 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3082 | 1/1 | 0.87 | 0.11 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3334 | 1/1 | 0.87 | 0.20 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3091 | 1/1 | 0.87 | 0.17 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3234 | 1/1 | 0.87 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3407 | 1/1 | 0.87 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3478 | 1/1 | 0.87 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3242 | 1/1 | 0.87 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3245 | 1/1 | 0.87 | 0.20 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3100 | 1/1 | 0.87 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3101 | 1/1 | 0.87 | 0.21 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3335 | 1/1 | 0.87 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3504 | 1/1 | 0.87 | 0.22 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 3107 | 1/1 | 0.87 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3514 | 1/1 | 0.87 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3522 | 1/1 | 0.87 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3539 | 1/1 | 0.87 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3545 | 1/1 | 0.87 | 0.15 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3790 | 1/1 | 0.87 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3267 | 1/1 | 0.87 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3797 | 1/1 | 0.87 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1671 | 1/1 | 0.87 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3781 | 1/1 | 0.87 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3824 | 1/1 | 0.87 | 0.12 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3904 | 1/1 | 0.87 | 0.10 | 11,11,11,11 | 0 |
| 56 | MG | 1Y | 202 | 1/1 | 0.87 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3589 | 1/1 | 0.87 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3831 | 1/1 | 0.87 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1680 | 1/1 | 0.87 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3114 | 1/1 | 0.87 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3192 | 1/1 | 0.87 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3118 | 1/1 | 0.87 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3905 | 1/1 | 0.87 | 0.15 | 17,17,17,17 | 0 |
| 56 | MG | 2A | 3289 | 1/1 | 0.87 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3907 | 1/1 | 0.87 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3613 | 1/1 | 0.87 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3296 | 1/1 | 0.87 | 0.12 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3857 | 1/1 | 0.87 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3861 | 1/1 | 0.87 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 11 | 102 | 1/1 | 0.87 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 1t | 201 | 1/1 | 0.87 | 0.19 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3247 | 1/1 | 0.87 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3632 | 1/1 | 0.87 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1708 | 1/1 | 0.87 | 0.14 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3155 | 1/1 | 0.87 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3413 | 1/1 | 0.87 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3317 | 1/1 | 0.87 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3159 | 1/1 | 0.87 | 0.23 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3674 | 1/1 | 0.87 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3651 | 1/1 | 0.87 | 0.22 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3165 | 1/1 | 0.87 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3660 | 1/1 | 0.87 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3807 | 1/1 | 0.87 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3809 | 1/1 | 0.87 | 0.11 | 12,12,12,12 | 0 |
| 56 | MG | 2A | 3173 | 1/1 | 0.87 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 2U | 203 | 1/1 | 0.87 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3682 | 1/1 | 0.87 | 0.11 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3356 | 1/1 | 0.88 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3304 | 1/1 | 0.88 | 0.13 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3525 | 1/1 | 0.88 | 0.30 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3531 | 1/1 | 0.88 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1792 | 1/1 | 0.88 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 2T | 201 | 1/1 | 0.88 | 0.26 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3312 | 1/1 | 0.88 | 0.11 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3534 | 1/1 | 0.88 | 0.24 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3943 | 1/1 | 0.88 | 0.12 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 3003 | 1/1 | 0.88 | 0.33 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3316 | 1/1 | 0.88 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1656 | 1/1 | 0.88 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3815 | 1/1 | 0.88 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3153 | 1/1 | 0.88 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3295 | 1/1 | 0.88 | 0.27 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3331 | 1/1 | 0.88 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3012 | 1/1 | 0.88 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3307 | 1/1 | 0.88 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3203 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3335 | 1/1 | 0.88 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3970 | 1/1 | 0.88 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3215 | 1/1 | 0.88 | 0.13 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3979 | 1/1 | 0.88 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3679 | 1/1 | 0.88 | 0.07 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3983 | 1/1 | 0.88 | 0.10 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3026 | 1/1 | 0.88 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3034 | 1/1 | 0.88 | 0.18 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3488 | 1/1 | 0.88 | 0.33 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3038 | 1/1 | 0.88 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3117 | 1/1 | 0.88 | 0.11 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3599 | 1/1 | 0.88 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3042 | 1/1 | 0.88 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3365 | 1/1 | 0.88 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 1w | 105 | 1/1 | 0.88 | 0.20 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3731 | 1/1 | 0.88 | 0.10 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3180 | 1/1 | 0.88 | 0.10 | 61,61,61,61 | 0 |
| 56 | MG | 1w | 108 | 1/1 | 0.88 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3053 | 1/1 | 0.88 | 0.20 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3187 | 1/1 | 0.88 | 0.23 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3377 | 1/1 | 0.88 | 0.19 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1682 | 1/1 | 0.88 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3496 | 1/1 | 0.88 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3871 | 1/1 | 0.88 | 0.08 | 14,14,14,14 | 0 |
| 56 | MG | 2a | 3072 | 1/1 | 0.88 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3397 | 1/1 | 0.88 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3400 | 1/1 | 0.88 | 0.30 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3078 | 1/1 | 0.88 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3403 | 1/1 | 0.88 | 0.19 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3405 | 1/1 | 0.88 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3875 | 1/1 | 0.88 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1703 | 1/1 | 0.88 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3745 | 1/1 | 0.88 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3199 | 1/1 | 0.88 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4031 | 1/1 | 0.88 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3876 | 1/1 | 0.88 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3208 | 1/1 | 0.88 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3765 | 1/1 | 0.88 | 0.11 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3611 | 1/1 | 0.88 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3767 | 1/1 | 0.88 | 0.23 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3432 | 1/1 | 0.88 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3116 | 1/1 | 0.88 | 0.22 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3445 | 1/1 | 0.88 | 0.49 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3774 | 1/1 | 0.88 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3612 | 1/1 | 0.88 | 0.12 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3620 | 1/1 | 0.88 | 0.19 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3154 | 1/1 | 0.88 | 0.10 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 3777 | 1/1 | 0.88 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3448 | 1/1 | 0.88 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3788 | 1/1 | 0.88 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3016 | 1/1 | 0.88 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3483 | 1/1 | 0.88 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3489 | 1/1 | 0.88 | 0.29 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3173 | 1/1 | 0.88 | 0.14 | 86,86,86,86 | 0 |
| 56 | MG | 1a | 1722 | 1/1 | 0.88 | 0.27 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1724 | 1/1 | 0.88 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 15 | 103 | 1/1 | 0.88 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3813 | 1/1 | 0.88 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3510 | 1/1 | 0.88 | 0.10 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3513 | 1/1 | 0.88 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1734 | 1/1 | 0.88 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3049 | 1/1 | 0.88 | 0.31 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3534 | 1/1 | 0.88 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3201 | 1/1 | 0.88 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3050 | 1/1 | 0.88 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 18 | 104 | 1/1 | 0.88 | 0.21 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3504 | 1/1 | 0.88 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3271 | 1/1 | 0.88 | 0.25 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3561 | 1/1 | 0.88 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3216 | 1/1 | 0.88 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4061 | 1/1 | 0.88 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3847 | 1/1 | 0.88 | 0.22 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1605 | 1/1 | 0.88 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1760 | 1/1 | 0.88 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3227 | 1/1 | 0.88 | 0.25 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3582 | 1/1 | 0.88 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3229 | 1/1 | 0.88 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3277 | 1/1 | 0.88 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2B | 201 | 1/1 | 0.88 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | 2B | 204 | 1/1 | 0.88 | 0.13 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4068 | 1/1 | 0.88 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3280 | 1/1 | 0.88 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3096 | 1/1 | 0.88 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 2v | 101 | 1/1 | 0.88 | 0.22 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3451 | 1/1 | 0.88 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 4080 | 1/1 | 0.88 | 0.11 | 11,11,11,11 | 0 |
| 56 | MG | 1A | 3627 | 1/1 | 0.88 | 0.10 | 15,15,15,15 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3090 | 1/1 | 0.88 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3615 | 1/1 | 0.88 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2E | 302 | 1/1 | 0.88 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3622 | 1/1 | 0.88 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 4103 | 1/1 | 0.88 | 0.09 | 17,17,17,17 | 0 |
| 56 | MG | 1a | 1787 | 1/1 | 0.89 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3465 | 1/1 | 0.89 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3140 | 1/1 | 0.89 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3474 | 1/1 | 0.89 | 0.18 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3737 | 1/1 | 0.89 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3036 | 1/1 | 0.89 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3062 | 1/1 | 0.89 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3987 | 1/1 | 0.89 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3746 | 1/1 | 0.89 | 0.11 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3754 | 1/1 | 0.89 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3537 | 1/1 | 0.89 | 0.05 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3756 | 1/1 | 0.89 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3120 | 1/1 | 0.89 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3048 | 1/1 | 0.89 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3436 | 1/1 | 0.89 | 0.28 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3438 | 1/1 | 0.89 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3136 | 1/1 | 0.89 | 0.22 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3881 | 1/1 | 0.89 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | 2a | 3056 | 1/1 | 0.89 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3506 | 1/1 | 0.89 | 0.22 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3290 | 1/1 | 0.89 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3067 | 1/1 | 0.89 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4023 | 1/1 | 0.89 | 0.14 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3187 | 1/1 | 0.89 | 0.08 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3148 | 1/1 | 0.89 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3528 | 1/1 | 0.89 | 0.19 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3300 | 1/1 | 0.89 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3494 | 1/1 | 0.89 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3305 | 1/1 | 0.89 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3655 | 1/1 | 0.89 | 0.07 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3392 | 1/1 | 0.89 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3309 | 1/1 | 0.89 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3156 | 1/1 | 0.89 | 0.12 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3808 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3561 | 1/1 | 0.89 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3810 | 1/1 | 0.89 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3229 | 1/1 | 0.89 | 0.10 | 10,10,10,10 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1689 | 1/1 | 0.89 | 0.08 | 35,35,35,35 | 0 |
| 56 | MG | 1a | 1690 | 1/1 | 0.89 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3593 | 1/1 | 0.89 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3343 | 1/1 | 0.89 | 0.18 | 24,24,24,24 | 0 |
| 56 | MG | 2a | 3110 | 1/1 | 0.89 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3319 | 1/1 | 0.89 | 0.16 | 60,60,60,60 | 0 |
| 56 | MG | 10 | 103 | 1/1 | 0.89 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3323 | 1/1 | 0.89 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3129 | 1/1 | 0.89 | 0.25 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4050 | 1/1 | 0.89 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3611 | 1/1 | 0.89 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3143 | 1/1 | 0.89 | 0.12 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 3692 | 1/1 | 0.89 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3269 | 1/1 | 0.89 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1711 | 1/1 | 0.89 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3936 | 1/1 | 0.89 | 0.15 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3601 | 1/1 | 0.89 | 0.09 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3182 | 1/1 | 0.89 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3346 | 1/1 | 0.89 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3630 | 1/1 | 0.89 | 0.35 | 40,40,40,40 | 0 |
| 56 | MG | 2B | 202 | 1/1 | 0.89 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3179 | 1/1 | 0.89 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3107 | 1/1 | 0.89 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3182 | 1/1 | 0.89 | 0.27 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3822 | 1/1 | 0.89 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3947 | 1/1 | 0.89 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4097 | 1/1 | 0.89 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1727 | 1/1 | 0.89 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3711 | 1/1 | 0.89 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3194 | 1/1 | 0.89 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3361 | 1/1 | 0.89 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3364 | 1/1 | 0.89 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1615 | 1/1 | 0.89 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 2B | 217 | 1/1 | 0.89 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3294 | 1/1 | 0.89 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3040 | 1/1 | 0.89 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3211 | 1/1 | 0.89 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1626 | 1/1 | 0.89 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3723 | 1/1 | 0.89 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 1B | 201 | 1/1 | 0.89 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3375 | 1/1 | 0.89 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1759 | 1/1 | 0.89 | 0.10 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1631 | 1/1 | 0.89 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3129 | 1/1 | 0.89 | 0.13 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3062 | 1/1 | 0.89 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3844 | 1/1 | 0.89 | 0.08 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3238 | 1/1 | 0.89 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3239 | 1/1 | 0.89 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3706 | 1/1 | 0.89 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 1B | 215 | 1/1 | 0.89 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3078 | 1/1 | 0.89 | 0.25 | 54,54,54,54 | 0 |
| 56 | MG | 2k | 201 | 1/1 | 0.89 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3971 | 1/1 | 0.89 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3419 | 1/1 | 0.89 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3422 | 1/1 | 0.89 | 0.29 | 45,45,45,45 | 0 |
| 56 | MG | 2v | 103 | 1/1 | 0.89 | 0.10 | 69,69,69,69 | 0 |
| 56 | MG | 2x | 102 | 1/1 | 0.89 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3730 | 1/1 | 0.89 | 0.13 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3528 | 1/1 | 0.89 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3258 | 1/1 | 0.89 | 0.23 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3980 | 1/1 | 0.89 | 0.20 | 72,72,72,72 | 0 |
| 56 | MG | 1B | 224 | 1/1 | 0.89 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3105 | 1/1 | 0.89 | 0.31 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3439 | 1/1 | 0.89 | 0.08 | 63,63,63,63 | 0 |
| 56 | MG | 2a | 3024 | 1/1 | 0.89 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3447 | 1/1 | 0.90 | 0.28 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3967 | 1/1 | 0.90 | 0.12 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3854 | 1/1 | 0.90 | 0.24 | 39,39,39,39 | 0 |
| 56 | MG | 1N | 201 | 1/1 | 0.90 | 0.29 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3469 | 1/1 | 0.90 | 0.26 | 52,52,52,52 | 0 |
| 56 | MG | 1N | 206 | 1/1 | 0.90 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 1O | 201 | 1/1 | 0.90 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3495 | 1/1 | 0.90 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 1P | 203 | 1/1 | 0.90 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3479 | 1/1 | 0.90 | 0.36 | 56,56,56,56 | 0 |
| 56 | MG | 1Q | 204 | 1/1 | 0.90 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3482 | 1/1 | 0.90 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 1Q | 205 | 1/1 | 0.90 | 0.11 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3350 | 1/1 | 0.90 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 1U | 201 | 1/1 | 0.90 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 2B | 215 | 1/1 | 0.90 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3500 | 1/1 | 0.90 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3422 | 1/1 | 0.90 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3501 | 1/1 | 0.90 | 0.15 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2E | 303 | 1/1 | 0.90 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3626 | 1/1 | 0.90 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3351 | 1/1 | 0.90 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3814 | 1/1 | 0.90 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1Y | 203 | 1/1 | 0.90 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3515 | 1/1 | 0.90 | 0.24 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3984 | 1/1 | 0.90 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | 2O | 202 | 1/1 | 0.90 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3524 | 1/1 | 0.90 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 2Q | 203 | 1/1 | 0.90 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 2Q | 204 | 1/1 | 0.90 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3505 | 1/1 | 0.90 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | 2T | 202 | 1/1 | 0.90 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3506 | 1/1 | 0.90 | 0.12 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3536 | 1/1 | 0.90 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 2V | 202 | 1/1 | 0.90 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3218 | 1/1 | 0.90 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3542 | 1/1 | 0.90 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3990 | 1/1 | 0.90 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1804 | 1/1 | 0.90 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3549 | 1/1 | 0.90 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3427 | 1/1 | 0.90 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3292 | 1/1 | 0.90 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1815 | 1/1 | 0.90 | 0.09 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1817 | 1/1 | 0.90 | 0.11 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3099 | 1/1 | 0.90 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 18 | 102 | 1/1 | 0.90 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3586 | 1/1 | 0.90 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4008 | 1/1 | 0.90 | 0.07 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3247 | 1/1 | 0.90 | 0.27 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3018 | 1/1 | 0.90 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3592 | 1/1 | 0.90 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4010 | 1/1 | 0.90 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 1a | 1602 | 1/1 | 0.90 | 0.28 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3599 | 1/1 | 0.90 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3255 | 1/1 | 0.90 | 0.20 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4012 | 1/1 | 0.90 | 0.10 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3829 | 1/1 | 0.90 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3260 | 1/1 | 0.90 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3037 | 1/1 | 0.90 | 0.13 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3265 | 1/1 | 0.90 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 1w | 102 | 1/1 | 0.90 | 0.16 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3665 | 1/1 | 0.90 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3269 | 1/1 | 0.90 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4021 | 1/1 | 0.90 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3358 | 1/1 | 0.90 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1623 | 1/1 | 0.90 | 0.23 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3047 | 1/1 | 0.90 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1624 | 1/1 | 0.90 | 0.24 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3838 | 1/1 | 0.90 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | 1x | 102 | 1/1 | 0.90 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3052 | 1/1 | 0.90 | 0.16 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3840 | 1/1 | 0.90 | 0.07 | 12,12,12,12 | 0 |
| 56 | MG | 1A | 4028 | 1/1 | 0.90 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | 1x | 106 | 1/1 | 0.90 | 0.19 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3060 | 1/1 | 0.90 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3526 | 1/1 | 0.90 | 0.16 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3681 | 1/1 | 0.90 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3847 | 1/1 | 0.90 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3068 | 1/1 | 0.90 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3848 | 1/1 | 0.90 | 0.33 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3295 | 1/1 | 0.90 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3661 | 1/1 | 0.90 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3253 | 1/1 | 0.90 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3663 | 1/1 | 0.90 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3257 | 1/1 | 0.90 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4048 | 1/1 | 0.90 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3668 | 1/1 | 0.90 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3688 | 1/1 | 0.90 | 0.17 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3010 | 1/1 | 0.90 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3447 | 1/1 | 0.90 | 0.18 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3672 | 1/1 | 0.90 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 2a | 3096 | 1/1 | 0.90 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3372 | 1/1 | 0.90 | 0.11 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3020 | 1/1 | 0.90 | 0.27 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3022 | 1/1 | 0.90 | 0.36 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3696 | 1/1 | 0.90 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3692 | 1/1 | 0.90 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4066 | 1/1 | 0.90 | 0.23 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1663 | 1/1 | 0.90 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3324 | 1/1 | 0.90 | 0.21 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3111 | 1/1 | 0.90 | 0.19 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3453 | 1/1 | 0.90 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3325 | 1/1 | 0.90 | 0.10 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3462 | 1/1 | 0.90 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3126 | 1/1 | 0.90 | 0.24 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3320 | 1/1 | 0.90 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3258 | 1/1 | 0.90 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3715 | 1/1 | 0.90 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3322 | 1/1 | 0.90 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3146 | 1/1 | 0.90 | 0.11 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3058 | 1/1 | 0.90 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3032 | 1/1 | 0.90 | 0.34 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3330 | 1/1 | 0.90 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3157 | 1/1 | 0.90 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3724 | 1/1 | 0.90 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3563 | 1/1 | 0.90 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3165 | 1/1 | 0.90 | 0.14 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1674 | 1/1 | 0.90 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3071 | 1/1 | 0.90 | 0.19 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3406 | 1/1 | 0.90 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1678 | 1/1 | 0.90 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3339 | 1/1 | 0.90 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4116 | 1/1 | 0.90 | 0.21 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3343 | 1/1 | 0.90 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3087 | 1/1 | 0.90 | 0.17 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3088 | 1/1 | 0.90 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3349 | 1/1 | 0.90 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3090 | 1/1 | 0.90 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4118 | 1/1 | 0.90 | 0.38 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3193 | 1/1 | 0.90 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3894 | 1/1 | 0.90 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3734 | 1/1 | 0.90 | 0.10 | 8,8,8,8 | 0 |
| 56 | MG | 1A | 3583 | 1/1 | 0.90 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | 1B | 209 | 1/1 | 0.90 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1692 | 1/1 | 0.90 | 0.19 | 34,34,34,34 | 0 |
| 56 | MG | 1B | 211 | 1/1 | 0.90 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3208 | 1/1 | 0.90 | 0.17 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3769 | 1/1 | 0.90 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1695 | 1/1 | 0.90 | 0.25 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1698 | 1/1 | 0.90 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3115 | 1/1 | 0.90 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3592 | 1/1 | 0.90 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1702 | 1/1 | 0.90 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3179 | 1/1 | 0.90 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3342 | 1/1 | 0.90 | 0.50 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3922 | 1/1 | 0.90 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3225 | 1/1 | 0.90 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3757 | 1/1 | 0.90 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3139 | 1/1 | 0.90 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3476 | 1/1 | 0.90 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3772 | 1/1 | 0.90 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3226 | 1/1 | 0.90 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3150 | 1/1 | 0.90 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3245 | 1/1 | 0.90 | 0.27 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3413 | 1/1 | 0.90 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 2q | 201 | 1/1 | 0.90 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3415 | 1/1 | 0.90 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3416 | 1/1 | 0.90 | 0.11 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3421 | 1/1 | 0.90 | 0.26 | 43,43,43,43 | 0 |
| 56 | MG | 1D | 312 | 1/1 | 0.90 | 0.13 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3953 | 1/1 | 0.90 | 0.08 | 25,25,25,25 | 0 |
| 56 | MG | 1a | 1729 | 1/1 | 0.90 | 0.32 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1730 | 1/1 | 0.90 | 0.42 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3782 | 1/1 | 0.90 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3430 | 1/1 | 0.90 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1F | 304 | 1/1 | 0.90 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3965 | 1/1 | 0.90 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1736 | 1/1 | 0.90 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1740 | 1/1 | 0.90 | 0.12 | 61,61,61,61 | 0 |
| 57 | LUJ | 2A | 3852 | 42/44 | 0.90 | 0.16 | 38,59,68,75 | 0 |
| 56 | MG | 1A | 3319 | 1/1 | 0.91 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 4083 | 1/1 | 0.91 | 0.09 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3808 | 1/1 | 0.91 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4088 | 1/1 | 0.91 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1750 | 1/1 | 0.91 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3621 | 1/1 | 0.91 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | 20 | 102 | 1/1 | 0.91 | 0.22 | 59,59,59,59 | 0 |
| 56 | MG | 25 | 101 | 1/1 | 0.91 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3109 | 1/1 | 0.91 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 4089 | 1/1 | 0.91 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1756 | 1/1 | 0.91 | 0.30 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1757 | 1/1 | 0.91 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 4092 | 1/1 | 0.91 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1604 | 1/1 | 0.91 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4095 | 1/1 | 0.91 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3633 | 1/1 | 0.91 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3011 | 1/1 | 0.91 | 0.31 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3323 | 1/1 | 0.91 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1772 | 1/1 | 0.91 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3464 | 1/1 | 0.91 | 0.13 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1621 | 1/1 | 0.91 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3813 | 1/1 | 0.91 | 0.08 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3209 | 1/1 | 0.91 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3650 | 1/1 | 0.91 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3143 | 1/1 | 0.91 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3657 | 1/1 | 0.91 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 2a | 3026 | 1/1 | 0.91 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3255 | 1/1 | 0.91 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3678 | 1/1 | 0.91 | 0.09 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 4133 | 1/1 | 0.91 | 0.30 | 24,24,24,24 | 0 |
| 56 | MG | 2a | 3033 | 1/1 | 0.91 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3819 | 1/1 | 0.91 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | 1B | 203 | 1/1 | 0.91 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3348 | 1/1 | 0.91 | 0.21 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1633 | 1/1 | 0.91 | 0.28 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1635 | 1/1 | 0.91 | 0.28 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3150 | 1/1 | 0.91 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3160 | 1/1 | 0.91 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | 1B | 205 | 1/1 | 0.91 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3547 | 1/1 | 0.91 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3223 | 1/1 | 0.91 | 0.34 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3412 | 1/1 | 0.91 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3082 | 1/1 | 0.91 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3836 | 1/1 | 0.91 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3690 | 1/1 | 0.91 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3414 | 1/1 | 0.91 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3695 | 1/1 | 0.91 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3565 | 1/1 | 0.91 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1658 | 1/1 | 0.91 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3373 | 1/1 | 0.91 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3566 | 1/1 | 0.91 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1B | 222 | 1/1 | 0.91 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3064 | 1/1 | 0.91 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3376 | 1/1 | 0.91 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3841 | 1/1 | 0.91 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3177 | 1/1 | 0.91 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3185 | 1/1 | 0.91 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3186 | 1/1 | 0.91 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3390 | 1/1 | 0.91 | 0.22 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1w | 101 | 1/1 | 0.91 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1665 | 1/1 | 0.91 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3267 | 1/1 | 0.91 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3081 | 1/1 | 0.91 | 0.23 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3591 | 1/1 | 0.91 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3407 | 1/1 | 0.91 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3090 | 1/1 | 0.91 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3996 | 1/1 | 0.91 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3007 | 1/1 | 0.91 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3093 | 1/1 | 0.91 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3728 | 1/1 | 0.91 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3420 | 1/1 | 0.91 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3126 | 1/1 | 0.91 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3205 | 1/1 | 0.91 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3099 | 1/1 | 0.91 | 0.24 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3741 | 1/1 | 0.91 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3742 | 1/1 | 0.91 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1E | 306 | 1/1 | 0.91 | 0.30 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3103 | 1/1 | 0.91 | 0.10 | 63,63,63,63 | 0 |
| 56 | MG | 1x | 104 | 1/1 | 0.91 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3213 | 1/1 | 0.91 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3596 | 1/1 | 0.91 | 0.13 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3216 | 1/1 | 0.91 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3001 | 1/1 | 0.91 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3120 | 1/1 | 0.91 | 0.35 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3220 | 1/1 | 0.91 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1G | 204 | 1/1 | 0.91 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3431 | 1/1 | 0.91 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3127 | 1/1 | 0.91 | 0.30 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3446 | 1/1 | 0.91 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1684 | 1/1 | 0.91 | 0.23 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3135 | 1/1 | 0.91 | 0.09 | 78,78,78,78 | 0 |
| 56 | MG | 2A | 3450 | 1/1 | 0.91 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3451 | 1/1 | 0.91 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3455 | 1/1 | 0.91 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3233 | 1/1 | 0.91 | 0.25 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1685 | 1/1 | 0.91 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3468 | 1/1 | 0.91 | 0.19 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3781 | 1/1 | 0.91 | 0.09 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3236 | 1/1 | 0.91 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3354 | 1/1 | 0.91 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3751 | 1/1 | 0.91 | 0.10 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4024 | 1/1 | 0.91 | 0.14 | 70,70,70,70 | 0 |
| 56 | MG | 1a | 1691 | 1/1 | 0.91 | 0.23 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3006 | 1/1 | 0.91 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3200 | 1/1 | 0.91 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3481 | 1/1 | 0.91 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | 1P | 202 | 1/1 | 0.91 | 0.06 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3181 | 1/1 | 0.91 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3251 | 1/1 | 0.91 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3812 | 1/1 | 0.91 | 0.08 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3486 | 1/1 | 0.91 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3823 | 1/1 | 0.91 | 0.08 | 24,24,24,24 | 0 |
| 56 | MG | 2a | 3189 | 1/1 | 0.91 | 0.11 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3297 | 1/1 | 0.91 | 0.21 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3490 | 1/1 | 0.91 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3493 | 1/1 | 0.91 | 0.24 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3515 | 1/1 | 0.91 | 0.07 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3302 | 1/1 | 0.91 | 0.18 | 35,35,35,35 | 0 |
| 56 | MG | 1S | 203 | 1/1 | 0.91 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3039 | 1/1 | 0.91 | 0.24 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3766 | 1/1 | 0.91 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 1a | 1705 | 1/1 | 0.91 | 0.36 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3205 | 1/1 | 0.91 | 0.23 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3517 | 1/1 | 0.91 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3892 | 1/1 | 0.91 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3303 | 1/1 | 0.91 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3517 | 1/1 | 0.91 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3900 | 1/1 | 0.91 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3051 | 1/1 | 0.91 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3856 | 1/1 | 0.91 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3519 | 1/1 | 0.91 | 0.06 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3532 | 1/1 | 0.91 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3221 | 1/1 | 0.91 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3223 | 1/1 | 0.91 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3053 | 1/1 | 0.91 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3054 | 1/1 | 0.91 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3279 | 1/1 | 0.91 | 0.23 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3540 | 1/1 | 0.91 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3369 | 1/1 | 0.91 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1716 | 1/1 | 0.91 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3283 | 1/1 | 0.91 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3063 | 1/1 | 0.91 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3049 | 1/1 | 0.91 | 0.13 | 22,22,22,22 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3560 | 1/1 | 0.91 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | 2l | 201 | 1/1 | 0.91 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 1Y | 204 | 1/1 | 0.91 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 1Y | 205 | 1/1 | 0.91 | 0.18 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3911 | 1/1 | 0.91 | 0.13 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3294 | 1/1 | 0.91 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3632 | 1/1 | 0.91 | 0.08 | 33,33,33,33 | 0 |
| 56 | MG | 1a | 1728 | 1/1 | 0.91 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | 2x | 103 | 1/1 | 0.91 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3310 | 1/1 | 0.91 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3640 | 1/1 | 0.91 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | 2F | 302 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 12 | 3701 | 1/1 | 0.91 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3093 | 1/1 | 0.91 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 4073 | 1/1 | 0.91 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3313 | 1/1 | 0.91 | 0.23 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3600 | 1/1 | 0.91 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3097 | 1/1 | 0.91 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2R | 3001 | 1/1 | 0.92 | 0.36 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3326 | 1/1 | 0.92 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3617 | 1/1 | 0.92 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1625 | 1/1 | 0.92 | 0.21 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3680 | 1/1 | 0.92 | 0.08 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 4098 | 1/1 | 0.92 | 0.26 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3367 | 1/1 | 0.92 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | 21 | 101 | 1/1 | 0.92 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3368 | 1/1 | 0.92 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3627 | 1/1 | 0.92 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3002 | 1/1 | 0.92 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3949 | 1/1 | 0.92 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3573 | 1/1 | 0.92 | 0.22 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3575 | 1/1 | 0.92 | 0.30 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1800 | 1/1 | 0.92 | 0.08 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3955 | 1/1 | 0.92 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3956 | 1/1 | 0.92 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3638 | 1/1 | 0.92 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1B | 202 | 1/1 | 0.92 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 1a | 1643 | 1/1 | 0.92 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3643 | 1/1 | 0.92 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3646 | 1/1 | 0.92 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3820 | 1/1 | 0.92 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1649 | 1/1 | 0.92 | 0.22 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1828 | 1/1 | 0.92 | 0.25 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1834 | 1/1 | 0.92 | 0.06 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3656 | 1/1 | 0.92 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3022 | 1/1 | 0.92 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3964 | 1/1 | 0.92 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3358 | 1/1 | 0.92 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3111 | 1/1 | 0.92 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1654 | 1/1 | 0.92 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3966 | 1/1 | 0.92 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3244 | 1/1 | 0.92 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3968 | 1/1 | 0.92 | 0.11 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3825 | 1/1 | 0.92 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3159 | 1/1 | 0.92 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3697 | 1/1 | 0.92 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3372 | 1/1 | 0.92 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3973 | 1/1 | 0.92 | 0.12 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3699 | 1/1 | 0.92 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3675 | 1/1 | 0.92 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3336 | 1/1 | 0.92 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3678 | 1/1 | 0.92 | 0.07 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3060 | 1/1 | 0.92 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3982 | 1/1 | 0.92 | 0.08 | 10,10,10,10 | 0 |
| 56 | MG | 1B | 229 | 1/1 | 0.92 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3704 | 1/1 | 0.92 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3175 | 1/1 | 0.92 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3512 | 1/1 | 0.92 | 0.20 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3391 | 1/1 | 0.92 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3054 | 1/1 | 0.92 | 0.06 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3396 | 1/1 | 0.92 | 0.06 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3597 | 1/1 | 0.92 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3398 | 1/1 | 0.92 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3061 | 1/1 | 0.92 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 1B | 236 | 1/1 | 0.92 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 1x | 107 | 1/1 | 0.92 | 0.09 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3404 | 1/1 | 0.92 | 0.29 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3066 | 1/1 | 0.92 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3298 | 1/1 | 0.92 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | 1x | 110 | 1/1 | 0.92 | 0.17 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3036 | 1/1 | 0.92 | 0.21 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3224 | 1/1 | 0.92 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3414 | 1/1 | 0.92 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3074 | 1/1 | 0.92 | 0.12 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3211 | 1/1 | 0.92 | 0.23 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3998 | 1/1 | 0.92 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3853 | 1/1 | 0.92 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 4001 | 1/1 | 0.92 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3859 | 1/1 | 0.92 | 0.12 | 20,20,20,20 | 0 |
| 56 | MG | 2a | 3084 | 1/1 | 0.92 | 0.19 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3217 | 1/1 | 0.92 | 0.11 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3607 | 1/1 | 0.92 | 0.08 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3219 | 1/1 | 0.92 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3092 | 1/1 | 0.92 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3002 | 1/1 | 0.92 | 0.25 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3003 | 1/1 | 0.92 | 0.24 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3228 | 1/1 | 0.92 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3004 | 1/1 | 0.92 | 0.23 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3005 | 1/1 | 0.92 | 0.17 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3744 | 1/1 | 0.92 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3443 | 1/1 | 0.92 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3444 | 1/1 | 0.92 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3749 | 1/1 | 0.92 | 0.09 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 4009 | 1/1 | 0.92 | 0.09 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3863 | 1/1 | 0.92 | 0.25 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3235 | 1/1 | 0.92 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3758 | 1/1 | 0.92 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3449 | 1/1 | 0.92 | 0.28 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3455 | 1/1 | 0.92 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3065 | 1/1 | 0.92 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3117 | 1/1 | 0.92 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3260 | 1/1 | 0.92 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3456 | 1/1 | 0.92 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3021 | 1/1 | 0.92 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3024 | 1/1 | 0.92 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3244 | 1/1 | 0.92 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3128 | 1/1 | 0.92 | 0.24 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3773 | 1/1 | 0.92 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3023 | 1/1 | 0.92 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3355 | 1/1 | 0.92 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 2a | 3140 | 1/1 | 0.92 | 0.10 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3026 | 1/1 | 0.92 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3249 | 1/1 | 0.92 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3030 | 1/1 | 0.92 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3150 | 1/1 | 0.92 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3037 | 1/1 | 0.92 | 0.21 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3786 | 1/1 | 0.92 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3134 | 1/1 | 0.92 | 0.41 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3256 | 1/1 | 0.92 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3160 | 1/1 | 0.92 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3320 | 1/1 | 0.92 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3793 | 1/1 | 0.92 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3041 | 1/1 | 0.92 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3418 | 1/1 | 0.92 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3168 | 1/1 | 0.92 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3261 | 1/1 | 0.92 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3264 | 1/1 | 0.92 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3174 | 1/1 | 0.92 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3046 | 1/1 | 0.92 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3177 | 1/1 | 0.92 | 0.09 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3359 | 1/1 | 0.92 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3767 | 1/1 | 0.92 | 0.09 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3771 | 1/1 | 0.92 | 0.08 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 4035 | 1/1 | 0.92 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 1V | 201 | 1/1 | 0.92 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3507 | 1/1 | 0.92 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3474 | 1/1 | 0.92 | 0.22 | 30,30,30,30 | 0 |
| 56 | MG | 1X | 104 | 1/1 | 0.92 | 0.18 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3192 | 1/1 | 0.92 | 0.26 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 4042 | 1/1 | 0.92 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3477 | 1/1 | 0.92 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3546 | 1/1 | 0.92 | 0.28 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3839 | 1/1 | 0.92 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3899 | 1/1 | 0.92 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3842 | 1/1 | 0.92 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3067 | 1/1 | 0.92 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3651 | 1/1 | 0.92 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3287 | 1/1 | 0.92 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3206 | 1/1 | 0.92 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3848 | 1/1 | 0.92 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3652 | 1/1 | 0.92 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3538 | 1/1 | 0.92 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3075 | 1/1 | 0.92 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3481 | 1/1 | 0.92 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 4054 | 1/1 | 0.92 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3860 | 1/1 | 0.92 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4056 | 1/1 | 0.92 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3906 | 1/1 | 0.92 | 0.08 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3791 | 1/1 | 0.92 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 4067 | 1/1 | 0.92 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3554 | 1/1 | 0.92 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3797 | 1/1 | 0.92 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3657 | 1/1 | 0.92 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3564 | 1/1 | 0.92 | 0.21 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3913 | 1/1 | 0.92 | 0.09 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3230 | 1/1 | 0.92 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3568 | 1/1 | 0.92 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4076 | 1/1 | 0.92 | 0.15 | 8,8,8,8 | 0 |
| 56 | MG | 2e | 201 | 1/1 | 0.92 | 0.07 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3100 | 1/1 | 0.92 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3101 | 1/1 | 0.92 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3914 | 1/1 | 0.92 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | 2E | 301 | 1/1 | 0.92 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3553 | 1/1 | 0.92 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1606 | 1/1 | 0.92 | 0.25 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4085 | 1/1 | 0.92 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3315 | 1/1 | 0.92 | 0.10 | 63,63,63,63 | 0 |
| 56 | MG | 2v | 102 | 1/1 | 0.92 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3424 | 1/1 | 0.92 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1616 | 1/1 | 0.92 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1773 | 1/1 | 0.92 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3926 | 1/1 | 0.92 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3006 | 1/1 | 0.92 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 2N | 201 | 1/1 | 0.92 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2O | 201 | 1/1 | 0.92 | 0.08 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1780 | 1/1 | 0.92 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 2P | 201 | 1/1 | 0.92 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3609 | 1/1 | 0.92 | 0.10 | 43,43,43,43 | 0 |
| 57 | LUJ | 1A | 4099 | 42/44 | 0.92 | 0.12 | 32,44,54,57 | 0 |
| 57 | LUJ | 1A | 4100 | 42/44 | 0.92 | 0.14 | 23,39,54,62 | 0 |
| 56 | MG | 1A | 3426 | 1/1 | 0.92 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3493 | 1/1 | 0.92 | 0.11 | 22,22,22,22 | 0 |
| 58 | K | 2A | 3434 | 1/1 | 0.92 | 0.09 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3480 | 1/1 | 0.93 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 2T | 203 | 1/1 | 0.93 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3251 | 1/1 | 0.93 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | 2U | 202 | 1/1 | 0.93 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1726 | 1/1 | 0.93 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3605 | 1/1 | 0.93 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3567 | 1/1 | 0.93 | 0.10 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4011 | 1/1 | 0.93 | 0.08 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3569 | 1/1 | 0.93 | 0.30 | 36,36,36,36 | 0 |
| 56 | MG | 27 | 101 | 1/1 | 0.93 | 0.38 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3091 | 1/1 | 0.93 | 0.27 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3860 | 1/1 | 0.93 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | 1a | 1732 | 1/1 | 0.93 | 0.34 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3305 | 1/1 | 0.93 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3484 | 1/1 | 0.93 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3623 | 1/1 | 0.93 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3081 | 1/1 | 0.93 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3325 | 1/1 | 0.93 | 0.18 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3867 | 1/1 | 0.93 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3579 | 1/1 | 0.93 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1742 | 1/1 | 0.93 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3582 | 1/1 | 0.93 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3254 | 1/1 | 0.93 | 0.28 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4029 | 1/1 | 0.93 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3725 | 1/1 | 0.93 | 0.26 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3584 | 1/1 | 0.93 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3587 | 1/1 | 0.93 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3640 | 1/1 | 0.93 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 10 | 102 | 1/1 | 0.93 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3023 | 1/1 | 0.93 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3118 | 1/1 | 0.93 | 0.29 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3344 | 1/1 | 0.93 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3644 | 1/1 | 0.93 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3345 | 1/1 | 0.93 | 0.18 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3882 | 1/1 | 0.93 | 0.09 | 15,15,15,15 | 0 |
| 56 | MG | 1a | 1766 | 1/1 | 0.93 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3883 | 1/1 | 0.93 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3125 | 1/1 | 0.93 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3654 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3161 | 1/1 | 0.93 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3361 | 1/1 | 0.93 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1774 | 1/1 | 0.93 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3362 | 1/1 | 0.93 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3744 | 1/1 | 0.93 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3216 | 1/1 | 0.93 | 0.24 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3430 | 1/1 | 0.93 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3366 | 1/1 | 0.93 | 0.23 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3896 | 1/1 | 0.93 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3897 | 1/1 | 0.93 | 0.08 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4062 | 1/1 | 0.93 | 0.07 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3755 | 1/1 | 0.93 | 0.10 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3168 | 1/1 | 0.93 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3371 | 1/1 | 0.93 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1607 | 1/1 | 0.93 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3901 | 1/1 | 0.93 | 0.26 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3161 | 1/1 | 0.93 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3058 | 1/1 | 0.93 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3433 | 1/1 | 0.93 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3508 | 1/1 | 0.93 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3682 | 1/1 | 0.93 | 0.18 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3063 | 1/1 | 0.93 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3765 | 1/1 | 0.93 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3686 | 1/1 | 0.93 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3095 | 1/1 | 0.93 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3125 | 1/1 | 0.93 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3381 | 1/1 | 0.93 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3174 | 1/1 | 0.93 | 0.05 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3070 | 1/1 | 0.93 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3384 | 1/1 | 0.93 | 0.18 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3703 | 1/1 | 0.93 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3387 | 1/1 | 0.93 | 0.23 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1810 | 1/1 | 0.93 | 0.12 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3769 | 1/1 | 0.93 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3393 | 1/1 | 0.93 | 0.28 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3618 | 1/1 | 0.93 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 4087 | 1/1 | 0.93 | 0.08 | 33,33,33,33 | 0 |
| 56 | MG | 2a | 3083 | 1/1 | 0.93 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1819 | 1/1 | 0.93 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1823 | 1/1 | 0.93 | 0.12 | 76,76,76,76 | 0 |
| 56 | MG | 2a | 3088 | 1/1 | 0.93 | 0.26 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1825 | 1/1 | 0.93 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3326 | 1/1 | 0.93 | 0.04 | 18,18,18,18 | 0 |
| 56 | MG | 1a | 1829 | 1/1 | 0.93 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3917 | 1/1 | 0.93 | 0.08 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3408 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 1b | 301 | 1/1 | 0.93 | 0.21 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3188 | 1/1 | 0.93 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3729 | 1/1 | 0.93 | 0.16 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1630 | 1/1 | 0.93 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3378 | 1/1 | 0.93 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3418 | 1/1 | 0.93 | 0.18 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3623 | 1/1 | 0.93 | 0.08 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3736 | 1/1 | 0.93 | 0.12 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1634 | 1/1 | 0.93 | 0.26 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3381 | 1/1 | 0.93 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3930 | 1/1 | 0.93 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3386 | 1/1 | 0.93 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3389 | 1/1 | 0.93 | 0.07 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3114 | 1/1 | 0.93 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3115 | 1/1 | 0.93 | 0.30 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3203 | 1/1 | 0.93 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3204 | 1/1 | 0.93 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3118 | 1/1 | 0.93 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3785 | 1/1 | 0.93 | 0.11 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 4113 | 1/1 | 0.93 | 0.30 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3123 | 1/1 | 0.93 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1645 | 1/1 | 0.93 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3125 | 1/1 | 0.93 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3020 | 1/1 | 0.93 | 0.06 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3788 | 1/1 | 0.93 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3454 | 1/1 | 0.93 | 0.27 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3630 | 1/1 | 0.93 | 0.06 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3631 | 1/1 | 0.93 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3133 | 1/1 | 0.93 | 0.08 | 76,76,76,76 | 0 |
| 56 | MG | 1a | 1655 | 1/1 | 0.93 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3448 | 1/1 | 0.93 | 0.25 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3227 | 1/1 | 0.93 | 0.21 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3529 | 1/1 | 0.93 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3638 | 1/1 | 0.93 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | 2a | 3148 | 1/1 | 0.93 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 3149 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3453 | 1/1 | 0.93 | 0.27 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3227 | 1/1 | 0.93 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3775 | 1/1 | 0.93 | 0.14 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 3960 | 1/1 | 0.93 | 0.08 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3458 | 1/1 | 0.93 | 0.25 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3461 | 1/1 | 0.93 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3161 | 1/1 | 0.93 | 0.07 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1661 | 1/1 | 0.93 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3230 | 1/1 | 0.93 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 1x | 109 | 1/1 | 0.93 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3182 | 1/1 | 0.93 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3473 | 1/1 | 0.93 | 0.07 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1B | 210 | 1/1 | 0.93 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3475 | 1/1 | 0.93 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3460 | 1/1 | 0.93 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3175 | 1/1 | 0.93 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3285 | 1/1 | 0.93 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3463 | 1/1 | 0.93 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3400 | 1/1 | 0.93 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3542 | 1/1 | 0.93 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3543 | 1/1 | 0.93 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3243 | 1/1 | 0.93 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3185 | 1/1 | 0.93 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 1y | 106 | 1/1 | 0.93 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3402 | 1/1 | 0.93 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3667 | 1/1 | 0.93 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3669 | 1/1 | 0.93 | 0.07 | 20,20,20,20 | 0 |
| 56 | MG | 2a | 3190 | 1/1 | 0.93 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3492 | 1/1 | 0.93 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3184 | 1/1 | 0.93 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3498 | 1/1 | 0.93 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3977 | 1/1 | 0.93 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3195 | 1/1 | 0.93 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3835 | 1/1 | 0.93 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3978 | 1/1 | 0.93 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 1B | 232 | 1/1 | 0.93 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3838 | 1/1 | 0.93 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3203 | 1/1 | 0.93 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1681 | 1/1 | 0.93 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3505 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3826 | 1/1 | 0.93 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3089 | 1/1 | 0.93 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3508 | 1/1 | 0.93 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3509 | 1/1 | 0.93 | 0.18 | 25,25,25,25 | 0 |
| 56 | MG | 2a | 3213 | 1/1 | 0.93 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3675 | 1/1 | 0.93 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1686 | 1/1 | 0.93 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1687 | 1/1 | 0.93 | 0.26 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3217 | 1/1 | 0.93 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | 1D | 301 | 1/1 | 0.93 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3855 | 1/1 | 0.93 | 0.08 | 29,29,29,29 | 0 |
| 56 | MG | 1D | 304 | 1/1 | 0.93 | 0.32 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3032 | 1/1 | 0.93 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3034 | 1/1 | 0.93 | 0.06 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3525 | 1/1 | 0.93 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1D | 306 | 1/1 | 0.93 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3552 | 1/1 | 0.93 | 0.17 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3103 | 1/1 | 0.93 | 0.07 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3348 | 1/1 | 0.93 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3555 | 1/1 | 0.93 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1696 | 1/1 | 0.93 | 0.23 | 37,37,37,37 | 0 |
| 56 | MG | 1F | 302 | 1/1 | 0.93 | 0.16 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3839 | 1/1 | 0.93 | 0.12 | 14,14,14,14 | 0 |
| 56 | MG | 2i | 201 | 1/1 | 0.93 | 0.28 | 49,49,49,49 | 0 |
| 56 | MG | 1F | 305 | 1/1 | 0.93 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1F | 308 | 1/1 | 0.93 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1F | 310 | 1/1 | 0.93 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3992 | 1/1 | 0.93 | 0.20 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1707 | 1/1 | 0.93 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | 2q | 203 | 1/1 | 0.93 | 0.06 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3685 | 1/1 | 0.93 | 0.07 | 15,15,15,15 | 0 |
| 56 | MG | 1G | 205 | 1/1 | 0.93 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3563 | 1/1 | 0.93 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3055 | 1/1 | 0.93 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3566 | 1/1 | 0.93 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3147 | 1/1 | 0.93 | 0.13 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3092 | 1/1 | 0.93 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3066 | 1/1 | 0.93 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3845 | 1/1 | 0.93 | 0.10 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3575 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3069 | 1/1 | 0.93 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3303 | 1/1 | 0.93 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3846 | 1/1 | 0.93 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 4007 | 1/1 | 0.93 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3072 | 1/1 | 0.93 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3074 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1721 | 1/1 | 0.93 | 0.20 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3598 | 1/1 | 0.93 | 0.08 | 50,50,50,50 | 0 |
| 57 | LUJ | 2a | 3232 | 44/44 | 0.93 | 0.12 | 40,55,62,65 | 0 |
| 56 | MG | 2A | 3076 | 1/1 | 0.93 | 0.06 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3145 | 1/1 | 0.94 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3146 | 1/1 | 0.94 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3988 | 1/1 | 0.94 | 0.07 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 3727 | 1/1 | 0.94 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3114 | 1/1 | 0.94 | 0.17 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3005 | 1/1 | 0.94 | 0.16 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3152 | 1/1 | 0.94 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3861 | 1/1 | 0.94 | 0.15 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3154 | 1/1 | 0.94 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3143 | 1/1 | 0.94 | 0.07 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3610 | 1/1 | 0.94 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3636 | 1/1 | 0.94 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3116 | 1/1 | 0.94 | 0.07 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3308 | 1/1 | 0.94 | 0.20 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1659 | 1/1 | 0.94 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4004 | 1/1 | 0.94 | 0.17 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 3615 | 1/1 | 0.94 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3748 | 1/1 | 0.94 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3645 | 1/1 | 0.94 | 0.07 | 25,25,25,25 | 0 |
| 56 | MG | 1f | 201 | 1/1 | 0.94 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3020 | 1/1 | 0.94 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3171 | 1/1 | 0.94 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3648 | 1/1 | 0.94 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3078 | 1/1 | 0.94 | 0.05 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3874 | 1/1 | 0.94 | 0.12 | 22,22,22,22 | 0 |
| 56 | MG | 1l | 203 | 1/1 | 0.94 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3311 | 1/1 | 0.94 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3753 | 1/1 | 0.94 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3523 | 1/1 | 0.94 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1668 | 1/1 | 0.94 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3370 | 1/1 | 0.94 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3378 | 1/1 | 0.94 | 0.07 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3449 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 1F | 303 | 1/1 | 0.94 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3039 | 1/1 | 0.94 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3665 | 1/1 | 0.94 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3183 | 1/1 | 0.94 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3450 | 1/1 | 0.94 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1673 | 1/1 | 0.94 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3386 | 1/1 | 0.94 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3758 | 1/1 | 0.94 | 0.06 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3388 | 1/1 | 0.94 | 0.26 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3371 | 1/1 | 0.94 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3674 | 1/1 | 0.94 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3761 | 1/1 | 0.94 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3392 | 1/1 | 0.94 | 0.20 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3452 | 1/1 | 0.94 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 1G | 203 | 1/1 | 0.94 | 0.07 | 61,61,61,61 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3156 | 1/1 | 0.94 | 0.17 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3317 | 1/1 | 0.94 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 2a | 3057 | 1/1 | 0.94 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1683 | 1/1 | 0.94 | 0.13 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3197 | 1/1 | 0.94 | 0.13 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3198 | 1/1 | 0.94 | 0.06 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3691 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3538 | 1/1 | 0.94 | 0.20 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3693 | 1/1 | 0.94 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3198 | 1/1 | 0.94 | 0.11 | 17,17,17,17 | 0 |
| 56 | MG | 2A | 3697 | 1/1 | 0.94 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1N | 202 | 1/1 | 0.94 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 1N | 203 | 1/1 | 0.94 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3385 | 1/1 | 0.94 | 0.21 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3774 | 1/1 | 0.94 | 0.06 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3415 | 1/1 | 0.94 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3061 | 1/1 | 0.94 | 0.17 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3120 | 1/1 | 0.94 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3208 | 1/1 | 0.94 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3076 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3647 | 1/1 | 0.94 | 0.07 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 4047 | 1/1 | 0.94 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3215 | 1/1 | 0.94 | 0.14 | 58,58,58,58 | 0 |
| 56 | MG | 1S | 201 | 1/1 | 0.94 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3042 | 1/1 | 0.94 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3211 | 1/1 | 0.94 | 0.26 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3428 | 1/1 | 0.94 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1700 | 1/1 | 0.94 | 0.21 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3908 | 1/1 | 0.94 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3551 | 1/1 | 0.94 | 0.25 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3224 | 1/1 | 0.94 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3433 | 1/1 | 0.94 | 0.21 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3656 | 1/1 | 0.94 | 0.06 | 9,9,9,9 | 0 |
| 56 | MG | 1A | 3327 | 1/1 | 0.94 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3331 | 1/1 | 0.94 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3801 | 1/1 | 0.94 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 1W | 201 | 1/1 | 0.94 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | 1W | 205 | 1/1 | 0.94 | 0.14 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3803 | 1/1 | 0.94 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3028 | 1/1 | 0.94 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | 1X | 105 | 1/1 | 0.94 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1715 | 1/1 | 0.94 | 0.06 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3104 | 1/1 | 0.94 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3212 | 1/1 | 0.94 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3240 | 1/1 | 0.94 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3036 | 1/1 | 0.94 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3403 | 1/1 | 0.94 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3112 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3259 | 1/1 | 0.94 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3463 | 1/1 | 0.94 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1720 | 1/1 | 0.94 | 0.31 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3761 | 1/1 | 0.94 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3763 | 1/1 | 0.94 | 0.06 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3934 | 1/1 | 0.94 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3246 | 1/1 | 0.94 | 0.07 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3043 | 1/1 | 0.94 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | 1Z | 302 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3165 | 1/1 | 0.94 | 0.19 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1725 | 1/1 | 0.94 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3252 | 1/1 | 0.94 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3166 | 1/1 | 0.94 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3254 | 1/1 | 0.94 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3478 | 1/1 | 0.94 | 0.08 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3410 | 1/1 | 0.94 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3134 | 1/1 | 0.94 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3217 | 1/1 | 0.94 | 0.09 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3218 | 1/1 | 0.94 | 0.08 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3780 | 1/1 | 0.94 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 12 | 3702 | 1/1 | 0.94 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3485 | 1/1 | 0.94 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3483 | 1/1 | 0.94 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3487 | 1/1 | 0.94 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3262 | 1/1 | 0.94 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3950 | 1/1 | 0.94 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3060 | 1/1 | 0.94 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3061 | 1/1 | 0.94 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3796 | 1/1 | 0.94 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3220 | 1/1 | 0.94 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 18 | 101 | 1/1 | 0.94 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3801 | 1/1 | 0.94 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3064 | 1/1 | 0.94 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1737 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3274 | 1/1 | 0.94 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3811 | 1/1 | 0.94 | 0.07 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3169 | 1/1 | 0.94 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3347 | 1/1 | 0.94 | 0.05 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4096 | 1/1 | 0.94 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1743 | 1/1 | 0.94 | 0.06 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3064 | 1/1 | 0.94 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3825 | 1/1 | 0.94 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3826 | 1/1 | 0.94 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3689 | 1/1 | 0.94 | 0.08 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3275 | 1/1 | 0.94 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3512 | 1/1 | 0.94 | 0.08 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1751 | 1/1 | 0.94 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3059 | 1/1 | 0.94 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3833 | 1/1 | 0.94 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3834 | 1/1 | 0.94 | 0.07 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3284 | 1/1 | 0.94 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3516 | 1/1 | 0.94 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1753 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3288 | 1/1 | 0.94 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3521 | 1/1 | 0.94 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3128 | 1/1 | 0.94 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3081 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3083 | 1/1 | 0.94 | 0.45 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3531 | 1/1 | 0.94 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4114 | 1/1 | 0.94 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3292 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3293 | 1/1 | 0.94 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3589 | 1/1 | 0.94 | 0.07 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1613 | 1/1 | 0.94 | 0.26 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1763 | 1/1 | 0.94 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3835 | 1/1 | 0.94 | 0.07 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3207 | 1/1 | 0.94 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4120 | 1/1 | 0.94 | 0.29 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3858 | 1/1 | 0.94 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3301 | 1/1 | 0.94 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1618 | 1/1 | 0.94 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3863 | 1/1 | 0.94 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4121 | 1/1 | 0.94 | 0.27 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 4125 | 1/1 | 0.94 | 0.29 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 4129 | 1/1 | 0.94 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3307 | 1/1 | 0.94 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4130 | 1/1 | 0.94 | 0.29 | 19,19,19,19 | 0 |
| 56 | MG | 1a | 1779 | 1/1 | 0.94 | 0.09 | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3700 | 1/1 | 0.94 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 4134 | 1/1 | 0.94 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3091 | 1/1 | 0.94 | 0.09 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3570 | 1/1 | 0.94 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3043 | 1/1 | 0.94 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3357 | 1/1 | 0.94 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3573 | 1/1 | 0.94 | 0.08 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3296 | 1/1 | 0.94 | 0.17 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3580 | 1/1 | 0.94 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3113 | 1/1 | 0.94 | 0.11 | 29,29,29,29 | 0 |
| 56 | MG | 2d | 302 | 1/1 | 0.94 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 2E | 304 | 1/1 | 0.94 | 0.08 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3583 | 1/1 | 0.94 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3713 | 1/1 | 0.94 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3714 | 1/1 | 0.94 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3117 | 1/1 | 0.94 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3843 | 1/1 | 0.94 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3119 | 1/1 | 0.94 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3718 | 1/1 | 0.94 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3183 | 1/1 | 0.94 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1796 | 1/1 | 0.94 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3327 | 1/1 | 0.94 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3230 | 1/1 | 0.94 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3127 | 1/1 | 0.94 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3130 | 1/1 | 0.94 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3724 | 1/1 | 0.94 | 0.07 | 25,25,25,25 | 0 |
| 56 | MG | 2Q | 205 | 1/1 | 0.94 | 0.19 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3233 | 1/1 | 0.94 | 0.39 | 29,29,29,29 | 0 |
| 56 | MG | 1a | 1808 | 1/1 | 0.94 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3612 | 1/1 | 0.94 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3513 | 1/1 | 0.94 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3614 | 1/1 | 0.94 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3338 | 1/1 | 0.94 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1646 | 1/1 | 0.94 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3620 | 1/1 | 0.94 | 0.07 | 34,34,34,34 | 0 |
| 57 | LUJ | 1a | 1832 | 44/44 | 0.94 | 0.11 | 29,39,44,48 | 0 |
| 56 | MG | 2W | 201 | 1/1 | 0.94 | 0.04 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3857 | 1/1 | 0.94 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3341 | 1/1 | 0.94 | 0.06 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3144 | 1/1 | 0.94 | 0.26 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3503 | 1/1 | 0.95 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3518 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4127 | 1/1 | 0.95 | 0.28 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3520 | 1/1 | 0.95 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3617 | 1/1 | 0.95 | 0.06 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3762 | 1/1 | 0.95 | 0.07 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3921 | 1/1 | 0.95 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3273 | 1/1 | 0.95 | 0.18 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3530 | 1/1 | 0.95 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | 2B | 218 | 1/1 | 0.95 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 2D | 303 | 1/1 | 0.95 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3417 | 1/1 | 0.95 | 0.08 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3098 | 1/1 | 0.95 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3533 | 1/1 | 0.95 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3276 | 1/1 | 0.95 | 0.19 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3009 | 1/1 | 0.95 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3278 | 1/1 | 0.95 | 0.31 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3257 | 1/1 | 0.95 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3011 | 1/1 | 0.95 | 0.06 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3349 | 1/1 | 0.95 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 2F | 304 | 1/1 | 0.95 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3514 | 1/1 | 0.95 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3017 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3018 | 1/1 | 0.95 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3263 | 1/1 | 0.95 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 1B | 208 | 1/1 | 0.95 | 0.24 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3284 | 1/1 | 0.95 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3945 | 1/1 | 0.95 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3562 | 1/1 | 0.95 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3628 | 1/1 | 0.95 | 0.07 | 8,8,8,8 | 0 |
| 56 | MG | 1B | 212 | 1/1 | 0.95 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3565 | 1/1 | 0.95 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 2R | 3003 | 1/1 | 0.95 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3025 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3272 | 1/1 | 0.95 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3176 | 1/1 | 0.95 | 0.19 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3569 | 1/1 | 0.95 | 0.06 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3287 | 1/1 | 0.95 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3034 | 1/1 | 0.95 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3031 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3783 | 1/1 | 0.95 | 0.10 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3289 | 1/1 | 0.95 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3578 | 1/1 | 0.95 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3521 | 1/1 | 0.95 | 0.08 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3634 | 1/1 | 0.95 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3636 | 1/1 | 0.95 | 0.13 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3961 | 1/1 | 0.95 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3587 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3792 | 1/1 | 0.95 | 0.05 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3042 | 1/1 | 0.95 | 0.14 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3796 | 1/1 | 0.95 | 0.31 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3593 | 1/1 | 0.95 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3290 | 1/1 | 0.95 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3045 | 1/1 | 0.95 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3798 | 1/1 | 0.95 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3799 | 1/1 | 0.95 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3800 | 1/1 | 0.95 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3639 | 1/1 | 0.95 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3127 | 1/1 | 0.95 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3644 | 1/1 | 0.95 | 0.09 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3606 | 1/1 | 0.95 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | 1D | 311 | 1/1 | 0.95 | 0.23 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3293 | 1/1 | 0.95 | 0.07 | 21,21,21,21 | 0 |
| 56 | MG | 1D | 313 | 1/1 | 0.95 | 0.14 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3056 | 1/1 | 0.95 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3057 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1697 | 1/1 | 0.95 | 0.25 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3180 | 1/1 | 0.95 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3025 | 1/1 | 0.95 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | 1E | 304 | 1/1 | 0.95 | 0.10 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3441 | 1/1 | 0.95 | 0.10 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1701 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3057 | 1/1 | 0.95 | 0.06 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3654 | 1/1 | 0.95 | 0.08 | 18,18,18,18 | 0 |
| 56 | MG | 1a | 1704 | 1/1 | 0.95 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3811 | 1/1 | 0.95 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3444 | 1/1 | 0.95 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3080 | 1/1 | 0.95 | 0.16 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3536 | 1/1 | 0.95 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 1F | 309 | 1/1 | 0.95 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3631 | 1/1 | 0.95 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1710 | 1/1 | 0.95 | 0.16 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3662 | 1/1 | 0.95 | 0.05 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3986 | 1/1 | 0.95 | 0.08 | 18,18,18,18 | 0 |
| 56 | MG | 2a | 3044 | 1/1 | 0.95 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3077 | 1/1 | 0.95 | 0.08 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3818 | 1/1 | 0.95 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3637 | 1/1 | 0.95 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3132 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3639 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3105 | 1/1 | 0.95 | 0.30 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3051 | 1/1 | 0.95 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3234 | 1/1 | 0.95 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3540 | 1/1 | 0.95 | 0.16 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1719 | 1/1 | 0.95 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3994 | 1/1 | 0.95 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3995 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 1N | 204 | 1/1 | 0.95 | 0.26 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1723 | 1/1 | 0.95 | 0.20 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3059 | 1/1 | 0.95 | 0.05 | 48,48,48,48 | 0 |
| 56 | MG | 1N | 205 | 1/1 | 0.95 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3095 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3824 | 1/1 | 0.95 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3235 | 1/1 | 0.95 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3653 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3098 | 1/1 | 0.95 | 0.08 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3655 | 1/1 | 0.95 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 1O | 203 | 1/1 | 0.95 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3673 | 1/1 | 0.95 | 0.06 | 12,12,12,12 | 0 |
| 56 | MG | 1A | 3058 | 1/1 | 0.95 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3104 | 1/1 | 0.95 | 0.24 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3110 | 1/1 | 0.95 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 1a | 1731 | 1/1 | 0.95 | 0.32 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3044 | 1/1 | 0.95 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3834 | 1/1 | 0.95 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3679 | 1/1 | 0.95 | 0.09 | 7,7,7,7 | 0 |
| 56 | MG | 2A | 3111 | 1/1 | 0.95 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 1S | 202 | 1/1 | 0.95 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3080 | 1/1 | 0.95 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3148 | 1/1 | 0.95 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3045 | 1/1 | 0.95 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | 1a | 1738 | 1/1 | 0.95 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3360 | 1/1 | 0.95 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3116 | 1/1 | 0.95 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3087 | 1/1 | 0.95 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3202 | 1/1 | 0.95 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1U | 202 | 1/1 | 0.95 | 0.25 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3458 | 1/1 | 0.95 | 0.09 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1747 | 1/1 | 0.95 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3459 | 1/1 | 0.95 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3380 | 1/1 | 0.95 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3683 | 1/1 | 0.95 | 0.08 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3153 | 1/1 | 0.95 | 0.05 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3126 | 1/1 | 0.95 | 0.10 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3690 | 1/1 | 0.95 | 0.08 | 7,7,7,7 | 0 |
| 56 | MG | 2A | 3129 | 1/1 | 0.95 | 0.16 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3318 | 1/1 | 0.95 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3131 | 1/1 | 0.95 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3694 | 1/1 | 0.95 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3132 | 1/1 | 0.95 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3133 | 1/1 | 0.95 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3135 | 1/1 | 0.95 | 0.05 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3699 | 1/1 | 0.95 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3700 | 1/1 | 0.95 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 4025 | 1/1 | 0.95 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3137 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3206 | 1/1 | 0.95 | 0.30 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3707 | 1/1 | 0.95 | 0.09 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3154 | 1/1 | 0.95 | 0.05 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3385 | 1/1 | 0.95 | 0.22 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3321 | 1/1 | 0.95 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3141 | 1/1 | 0.95 | 0.11 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3698 | 1/1 | 0.95 | 0.05 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3389 | 1/1 | 0.95 | 0.20 | 30,30,30,30 | 0 |
| 56 | MG | 1a | 1761 | 1/1 | 0.95 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3849 | 1/1 | 0.95 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3852 | 1/1 | 0.95 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3322 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3723 | 1/1 | 0.95 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3147 | 1/1 | 0.95 | 0.11 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3048 | 1/1 | 0.95 | 0.06 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3149 | 1/1 | 0.95 | 0.05 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1771 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3401 | 1/1 | 0.95 | 0.28 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3136 | 1/1 | 0.95 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3256 | 1/1 | 0.95 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3572 | 1/1 | 0.95 | 0.28 | 33,33,33,33 | 0 |
| 56 | MG | 10 | 104 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3144 | 1/1 | 0.95 | 0.06 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3703 | 1/1 | 0.95 | 0.06 | 10,10,10,10 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3147 | 1/1 | 0.95 | 0.10 | 71,71,71,71 | 0 |
| 56 | MG | 11 | 101 | 1/1 | 0.95 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3471 | 1/1 | 0.95 | 0.05 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3412 | 1/1 | 0.95 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3151 | 1/1 | 0.95 | 0.06 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3152 | 1/1 | 0.95 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3399 | 1/1 | 0.95 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3864 | 1/1 | 0.95 | 0.20 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3743 | 1/1 | 0.95 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1783 | 1/1 | 0.95 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3159 | 1/1 | 0.95 | 0.06 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3475 | 1/1 | 0.95 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3578 | 1/1 | 0.95 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3748 | 1/1 | 0.95 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3163 | 1/1 | 0.95 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3715 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3166 | 1/1 | 0.95 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3167 | 1/1 | 0.95 | 0.05 | 39,39,39,39 | 0 |
| 56 | MG | 16 | 102 | 1/1 | 0.95 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3169 | 1/1 | 0.95 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3760 | 1/1 | 0.95 | 0.06 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1788 | 1/1 | 0.95 | 0.06 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3427 | 1/1 | 0.95 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1789 | 1/1 | 0.95 | 0.07 | 66,66,66,66 | 0 |
| 56 | MG | 17 | 101 | 1/1 | 0.95 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3178 | 1/1 | 0.95 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3716 | 1/1 | 0.95 | 0.06 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3019 | 1/1 | 0.95 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | 18 | 103 | 1/1 | 0.95 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 4060 | 1/1 | 0.95 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3184 | 1/1 | 0.95 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3437 | 1/1 | 0.95 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3772 | 1/1 | 0.95 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 19 | 101 | 1/1 | 0.95 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3441 | 1/1 | 0.95 | 0.47 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1799 | 1/1 | 0.95 | 0.07 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3721 | 1/1 | 0.95 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3401 | 1/1 | 0.95 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 1a | 1803 | 1/1 | 0.95 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4064 | 1/1 | 0.95 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4065 | 1/1 | 0.95 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3783 | 1/1 | 0.95 | 0.15 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3063 | 1/1 | 0.95 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | 2a | 3198 | 1/1 | 0.95 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3785 | 1/1 | 0.95 | 0.07 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3213 | 1/1 | 0.95 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3880 | 1/1 | 0.95 | 0.10 | 14,14,14,14 | 0 |
| 56 | MG | 1a | 1611 | 1/1 | 0.95 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3454 | 1/1 | 0.95 | 0.27 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3792 | 1/1 | 0.95 | 0.08 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 4069 | 1/1 | 0.95 | 0.11 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3585 | 1/1 | 0.95 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 1a | 1822 | 1/1 | 0.95 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3459 | 1/1 | 0.95 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3586 | 1/1 | 0.95 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3404 | 1/1 | 0.95 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3464 | 1/1 | 0.95 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3405 | 1/1 | 0.95 | 0.07 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3466 | 1/1 | 0.95 | 0.25 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1619 | 1/1 | 0.95 | 0.07 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1833 | 1/1 | 0.95 | 0.17 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1620 | 1/1 | 0.95 | 0.21 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3820 | 1/1 | 0.95 | 0.05 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3821 | 1/1 | 0.95 | 0.06 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4082 | 1/1 | 0.95 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3330 | 1/1 | 0.95 | 0.07 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3214 | 1/1 | 0.95 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3207 | 1/1 | 0.95 | 0.19 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3332 | 1/1 | 0.95 | 0.05 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3889 | 1/1 | 0.95 | 0.05 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3829 | 1/1 | 0.95 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3409 | 1/1 | 0.95 | 0.16 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3737 | 1/1 | 0.95 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3738 | 1/1 | 0.95 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1a | 1629 | 1/1 | 0.95 | 0.30 | 41,41,41,41 | 0 |
| 56 | MG | 2f | 201 | 1/1 | 0.95 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4093 | 1/1 | 0.95 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3484 | 1/1 | 0.95 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3492 | 1/1 | 0.95 | 0.07 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3745 | 1/1 | 0.95 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3747 | 1/1 | 0.95 | 0.09 | 9,9,9,9 | 0 |
| 56 | MG | 2l | 202 | 1/1 | 0.95 | 0.07 | 50,50,50,50 | 0 |
| 56 | MG | 2l | 204 | 1/1 | 0.95 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3011 | 1/1 | 0.95 | 0.10 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3598 | 1/1 | 0.95 | 0.12 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3491 | 1/1 | 0.95 | 0.27 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3843 | 1/1 | 0.95 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3053 | 1/1 | 0.95 | 0.05 | 25,25,25,25 | 0 |
| 56 | MG | 1a | 1638 | 1/1 | 0.95 | 0.21 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 4104 | 1/1 | 0.95 | 0.15 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 4106 | 1/1 | 0.95 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1641 | 1/1 | 0.95 | 0.32 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1642 | 1/1 | 0.95 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4109 | 1/1 | 0.95 | 0.23 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3752 | 1/1 | 0.95 | 0.08 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3122 | 1/1 | 0.95 | 0.18 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3337 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3237 | 1/1 | 0.95 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3859 | 1/1 | 0.95 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3497 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1651 | 1/1 | 0.95 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3124 | 1/1 | 0.95 | 0.22 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 4119 | 1/1 | 0.95 | 0.06 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3219 | 1/1 | 0.95 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3502 | 1/1 | 0.95 | 0.05 | 33,33,33,33 | 0 |
| 58 | K | 1A | 4137 | 1/1 | 0.95 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1y | 101 | 1/1 | 0.95 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3079 | 1/1 | 0.96 | 0.18 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3099 | 1/1 | 0.96 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 1Z | 301 | 1/1 | 0.96 | 0.15 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3576 | 1/1 | 0.96 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3236 | 1/1 | 0.96 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | 2E | 305 | 1/1 | 0.96 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 1Z | 303 | 1/1 | 0.96 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 4055 | 1/1 | 0.96 | 0.05 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3097 | 1/1 | 0.96 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 4059 | 1/1 | 0.96 | 0.05 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3887 | 1/1 | 0.96 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3588 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3155 | 1/1 | 0.96 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3590 | 1/1 | 0.96 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3324 | 1/1 | 0.96 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3241 | 1/1 | 0.96 | 0.12 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3110 | 1/1 | 0.96 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3437 | 1/1 | 0.96 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | 2P | 202 | 1/1 | 0.96 | 0.06 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3595 | 1/1 | 0.96 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3891 | 1/1 | 0.96 | 0.09 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3028 | 1/1 | 0.96 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3520 | 1/1 | 0.96 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3332 | 1/1 | 0.96 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 2R | 3002 | 1/1 | 0.96 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3601 | 1/1 | 0.96 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3895 | 1/1 | 0.96 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 15 | 101 | 1/1 | 0.96 | 0.27 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3440 | 1/1 | 0.96 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3336 | 1/1 | 0.96 | 0.21 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3607 | 1/1 | 0.96 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1775 | 1/1 | 0.96 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 2V | 201 | 1/1 | 0.96 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4071 | 1/1 | 0.96 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3610 | 1/1 | 0.96 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3157 | 1/1 | 0.96 | 0.12 | 21,21,21,21 | 0 |
| 56 | MG | 17 | 102 | 1/1 | 0.96 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 17 | 104 | 1/1 | 0.96 | 0.05 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3342 | 1/1 | 0.96 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 28 | 101 | 1/1 | 0.96 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 29 | 101 | 1/1 | 0.96 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1781 | 1/1 | 0.96 | 0.05 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4074 | 1/1 | 0.96 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3618 | 1/1 | 0.96 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3004 | 1/1 | 0.96 | 0.04 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3443 | 1/1 | 0.96 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 4077 | 1/1 | 0.96 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 4079 | 1/1 | 0.96 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3246 | 1/1 | 0.96 | 0.12 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3770 | 1/1 | 0.96 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3363 | 1/1 | 0.96 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3352 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3353 | 1/1 | 0.96 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3635 | 1/1 | 0.96 | 0.05 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3356 | 1/1 | 0.96 | 0.23 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3446 | 1/1 | 0.96 | 0.18 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3530 | 1/1 | 0.96 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3304 | 1/1 | 0.96 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1609 | 1/1 | 0.96 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3532 | 1/1 | 0.96 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3362 | 1/1 | 0.96 | 0.10 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3363 | 1/1 | 0.96 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1798 | 1/1 | 0.96 | 0.05 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4090 | 1/1 | 0.96 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3780 | 1/1 | 0.96 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1614 | 1/1 | 0.96 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3641 | 1/1 | 0.96 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3369 | 1/1 | 0.96 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3915 | 1/1 | 0.96 | 0.06 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3032 | 1/1 | 0.96 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1617 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3642 | 1/1 | 0.96 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3207 | 1/1 | 0.96 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3645 | 1/1 | 0.96 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3535 | 1/1 | 0.96 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3923 | 1/1 | 0.96 | 0.11 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3652 | 1/1 | 0.96 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3248 | 1/1 | 0.96 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1820 | 1/1 | 0.96 | 0.06 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3648 | 1/1 | 0.96 | 0.09 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3932 | 1/1 | 0.96 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1824 | 1/1 | 0.96 | 0.05 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3658 | 1/1 | 0.96 | 0.09 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3933 | 1/1 | 0.96 | 0.06 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1826 | 1/1 | 0.96 | 0.06 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1827 | 1/1 | 0.96 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4111 | 1/1 | 0.96 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3164 | 1/1 | 0.96 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3664 | 1/1 | 0.96 | 0.08 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3249 | 1/1 | 0.96 | 0.10 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1830 | 1/1 | 0.96 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3793 | 1/1 | 0.96 | 0.07 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 4115 | 1/1 | 0.96 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3054 | 1/1 | 0.96 | 0.08 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1632 | 1/1 | 0.96 | 0.08 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3395 | 1/1 | 0.96 | 0.14 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3653 | 1/1 | 0.96 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3673 | 1/1 | 0.96 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3940 | 1/1 | 0.96 | 0.05 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3942 | 1/1 | 0.96 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3676 | 1/1 | 0.96 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3399 | 1/1 | 0.96 | 0.26 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3085 | 1/1 | 0.96 | 0.09 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1l | 201 | 1/1 | 0.96 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3312 | 1/1 | 0.96 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3210 | 1/1 | 0.96 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1q | 201 | 1/1 | 0.96 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3376 | 1/1 | 0.96 | 0.19 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3660 | 1/1 | 0.96 | 0.09 | 9,9,9,9 | 0 |
| 56 | MG | 2A | 3687 | 1/1 | 0.96 | 0.06 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3073 | 1/1 | 0.96 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3410 | 1/1 | 0.96 | 0.26 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 4132 | 1/1 | 0.96 | 0.18 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3316 | 1/1 | 0.96 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3379 | 1/1 | 0.96 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | 1a | 1644 | 1/1 | 0.96 | 0.05 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3545 | 1/1 | 0.96 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3954 | 1/1 | 0.96 | 0.05 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3417 | 1/1 | 0.96 | 0.05 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3163 | 1/1 | 0.96 | 0.06 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3088 | 1/1 | 0.96 | 0.08 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3701 | 1/1 | 0.96 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3086 | 1/1 | 0.96 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3957 | 1/1 | 0.96 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3549 | 1/1 | 0.96 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3705 | 1/1 | 0.96 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3195 | 1/1 | 0.96 | 0.05 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3550 | 1/1 | 0.96 | 0.24 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3384 | 1/1 | 0.96 | 0.26 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3709 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3963 | 1/1 | 0.96 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3426 | 1/1 | 0.96 | 0.23 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3106 | 1/1 | 0.96 | 0.12 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3066 | 1/1 | 0.96 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3816 | 1/1 | 0.96 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3717 | 1/1 | 0.96 | 0.04 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3718 | 1/1 | 0.96 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3172 | 1/1 | 0.96 | 0.08 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3109 | 1/1 | 0.96 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3467 | 1/1 | 0.96 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3559 | 1/1 | 0.96 | 0.17 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3436 | 1/1 | 0.96 | 0.05 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3108 | 1/1 | 0.96 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3109 | 1/1 | 0.96 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3261 | 1/1 | 0.96 | 0.06 | 28,28,28,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3209 | 1/1 | 0.96 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3210 | 1/1 | 0.96 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3442 | 1/1 | 0.96 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3728 | 1/1 | 0.96 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3562 | 1/1 | 0.96 | 0.18 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3730 | 1/1 | 0.96 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | 1y | 102 | 1/1 | 0.96 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3732 | 1/1 | 0.96 | 0.08 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3121 | 1/1 | 0.96 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | 1B | 226 | 1/1 | 0.96 | 0.06 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3027 | 1/1 | 0.96 | 0.15 | 17,17,17,17 | 0 |
| 56 | MG | 1B | 228 | 1/1 | 0.96 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3976 | 1/1 | 0.96 | 0.06 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3393 | 1/1 | 0.96 | 0.18 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3396 | 1/1 | 0.96 | 0.10 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3473 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3452 | 1/1 | 0.96 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3693 | 1/1 | 0.96 | 0.06 | 9,9,9,9 | 0 |
| 56 | MG | 2a | 3131 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3132 | 1/1 | 0.96 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3264 | 1/1 | 0.96 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3832 | 1/1 | 0.96 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3225 | 1/1 | 0.96 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3747 | 1/1 | 0.96 | 0.07 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3139 | 1/1 | 0.96 | 0.11 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3076 | 1/1 | 0.96 | 0.15 | 33,33,33,33 | 0 |
| 56 | MG | 1a | 1676 | 1/1 | 0.96 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3012 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3752 | 1/1 | 0.96 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3178 | 1/1 | 0.96 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3755 | 1/1 | 0.96 | 0.07 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3574 | 1/1 | 0.96 | 0.04 | 25,25,25,25 | 0 |
| 56 | MG | 1D | 308 | 1/1 | 0.96 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 1D | 309 | 1/1 | 0.96 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1D | 310 | 1/1 | 0.96 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3328 | 1/1 | 0.96 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3762 | 1/1 | 0.96 | 0.06 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3329 | 1/1 | 0.96 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3470 | 1/1 | 0.96 | 0.18 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3472 | 1/1 | 0.96 | 0.16 | 30,30,30,30 | 0 |
| 56 | MG | 2a | 3158 | 1/1 | 0.96 | 0.07 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3136 | 1/1 | 0.96 | 0.08 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3270 | 1/1 | 0.96 | 0.25 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3768 | 1/1 | 0.96 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3580 | 1/1 | 0.96 | 0.07 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3112 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3706 | 1/1 | 0.96 | 0.05 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3029 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3167 | 1/1 | 0.96 | 0.05 | 67,67,67,67 | 0 |
| 56 | MG | 1E | 307 | 1/1 | 0.96 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3709 | 1/1 | 0.96 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3272 | 1/1 | 0.96 | 0.06 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3181 | 1/1 | 0.96 | 0.05 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 4000 | 1/1 | 0.96 | 0.09 | 15,15,15,15 | 0 |
| 56 | MG | 1F | 306 | 1/1 | 0.96 | 0.19 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3486 | 1/1 | 0.96 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4002 | 1/1 | 0.96 | 0.08 | 11,11,11,11 | 0 |
| 56 | MG | 1A | 3113 | 1/1 | 0.96 | 0.18 | 36,36,36,36 | 0 |
| 56 | MG | 1G | 201 | 1/1 | 0.96 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3146 | 1/1 | 0.96 | 0.22 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 4006 | 1/1 | 0.96 | 0.05 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3851 | 1/1 | 0.96 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3183 | 1/1 | 0.96 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3490 | 1/1 | 0.96 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3494 | 1/1 | 0.96 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3496 | 1/1 | 0.96 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3338 | 1/1 | 0.96 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3854 | 1/1 | 0.96 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3795 | 1/1 | 0.96 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3856 | 1/1 | 0.96 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3501 | 1/1 | 0.96 | 0.06 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3502 | 1/1 | 0.96 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3799 | 1/1 | 0.96 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3339 | 1/1 | 0.96 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3807 | 1/1 | 0.96 | 0.06 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3196 | 1/1 | 0.96 | 0.11 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3858 | 1/1 | 0.96 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3077 | 1/1 | 0.96 | 0.09 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3594 | 1/1 | 0.96 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3266 | 1/1 | 0.96 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 1N | 207 | 1/1 | 0.96 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3055 | 1/1 | 0.96 | 0.05 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3818 | 1/1 | 0.96 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3819 | 1/1 | 0.96 | 0.09 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 4022 | 1/1 | 0.96 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1714 | 1/1 | 0.96 | 0.18 | 44,44,44,44 | 0 |
| 56 | MG | 1O | 202 | 1/1 | 0.96 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3059 | 1/1 | 0.96 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3341 | 1/1 | 0.96 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3212 | 1/1 | 0.96 | 0.23 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3279 | 1/1 | 0.96 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3280 | 1/1 | 0.96 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3228 | 1/1 | 0.96 | 0.08 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3346 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3033 | 1/1 | 0.96 | 0.24 | 28,28,28,28 | 0 |
| 56 | MG | 1R | 202 | 1/1 | 0.96 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 1R | 204 | 1/1 | 0.96 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3068 | 1/1 | 0.96 | 0.18 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3527 | 1/1 | 0.96 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3222 | 1/1 | 0.96 | 0.17 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3286 | 1/1 | 0.96 | 0.11 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4030 | 1/1 | 0.96 | 0.05 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3606 | 1/1 | 0.96 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3226 | 1/1 | 0.96 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3189 | 1/1 | 0.96 | 0.19 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 4033 | 1/1 | 0.96 | 0.06 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3840 | 1/1 | 0.96 | 0.05 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3872 | 1/1 | 0.96 | 0.05 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3535 | 1/1 | 0.96 | 0.07 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3609 | 1/1 | 0.96 | 0.07 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3231 | 1/1 | 0.96 | 0.10 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3094 | 1/1 | 0.96 | 0.14 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3079 | 1/1 | 0.96 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3541 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3507 | 1/1 | 0.96 | 0.07 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3543 | 1/1 | 0.96 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3544 | 1/1 | 0.96 | 0.05 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3879 | 1/1 | 0.96 | 0.05 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3546 | 1/1 | 0.96 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3297 | 1/1 | 0.96 | 0.06 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3082 | 1/1 | 0.96 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 2q | 202 | 1/1 | 0.96 | 0.07 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3550 | 1/1 | 0.96 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3299 | 1/1 | 0.96 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4046 | 1/1 | 0.96 | 0.05 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3556 | 1/1 | 0.96 | 0.06 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3557 | 1/1 | 0.96 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3558 | 1/1 | 0.96 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | 2B | 203 | 1/1 | 0.96 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3084 | 1/1 | 0.96 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 2B | 205 | 1/1 | 0.96 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | 2x | 105 | 1/1 | 0.96 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 1W | 204 | 1/1 | 0.96 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3613 | 1/1 | 0.96 | 0.08 | 16,16,16,16 | 0 |
| 56 | MG | 1W | 207 | 1/1 | 0.96 | 0.08 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3352 | 1/1 | 0.96 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1741 | 1/1 | 0.96 | 0.21 | 36,36,36,36 | 0 |
| 56 | MG | 2B | 211 | 1/1 | 0.96 | 0.19 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4049 | 1/1 | 0.96 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 2B | 213 | 1/1 | 0.96 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 1Y | 201 | 1/1 | 0.96 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3509 | 1/1 | 0.96 | 0.22 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3311 | 1/1 | 0.96 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4051 | 1/1 | 0.96 | 0.12 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3151 | 1/1 | 0.96 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 2D | 301 | 1/1 | 0.96 | 0.06 | 27,27,27,27 | 0 |
| 59 | ZN | 2n | 501 | 1/1 | 0.96 | 0.07 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 3590 | 1/1 | 0.97 | 0.04 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3740 | 1/1 | 0.97 | 0.05 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3686 | 1/1 | 0.97 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3523 | 1/1 | 0.97 | 0.05 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3909 | 1/1 | 0.97 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3910 | 1/1 | 0.97 | 0.05 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3526 | 1/1 | 0.97 | 0.06 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3328 | 1/1 | 0.97 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3382 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3802 | 1/1 | 0.97 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3237 | 1/1 | 0.97 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3282 | 1/1 | 0.97 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3333 | 1/1 | 0.97 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3916 | 1/1 | 0.97 | 0.05 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3387 | 1/1 | 0.97 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3918 | 1/1 | 0.97 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3051 | 1/1 | 0.97 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 4057 | 1/1 | 0.97 | 0.05 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 4058 | 1/1 | 0.97 | 0.04 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3025 | 1/1 | 0.97 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3695 | 1/1 | 0.97 | 0.06 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3158 | 1/1 | 0.97 | 0.47 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3925 | 1/1 | 0.97 | 0.05 | 12,12,12,12 | 0 |
| 56 | MG | 2A | 3158 | 1/1 | 0.97 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3812 | 1/1 | 0.97 | 0.05 | 18,18,18,18 | 0 |
| 56 | MG | 1P | 201 | 1/1 | 0.97 | 0.17 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3927 | 1/1 | 0.97 | 0.04 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3205 | 1/1 | 0.97 | 0.06 | 26,26,26,26 | 0 |
| 56 | MG | 1Q | 203 | 1/1 | 0.97 | 0.05 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3101 | 1/1 | 0.97 | 0.17 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3602 | 1/1 | 0.97 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3395 | 1/1 | 0.97 | 0.10 | 29,29,29,29 | 0 |
| 56 | MG | 1x | 111 | 1/1 | 0.97 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3559 | 1/1 | 0.97 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3354 | 1/1 | 0.97 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3777 | 1/1 | 0.97 | 0.06 | 58,58,58,58 | 0 |
| 56 | MG | 2a | 3079 | 1/1 | 0.97 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 1R | 203 | 1/1 | 0.97 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3605 | 1/1 | 0.97 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3456 | 1/1 | 0.97 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3010 | 1/1 | 0.97 | 0.11 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3782 | 1/1 | 0.97 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3608 | 1/1 | 0.97 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3941 | 1/1 | 0.97 | 0.04 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3104 | 1/1 | 0.97 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3527 | 1/1 | 0.97 | 0.19 | 27,27,27,27 | 0 |
| 56 | MG | 2a | 3089 | 1/1 | 0.97 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1U | 203 | 1/1 | 0.97 | 0.21 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3944 | 1/1 | 0.97 | 0.05 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 4081 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3291 | 1/1 | 0.97 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3712 | 1/1 | 0.97 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3574 | 1/1 | 0.97 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 4084 | 1/1 | 0.97 | 0.05 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3162 | 1/1 | 0.97 | 0.20 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3007 | 1/1 | 0.97 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3008 | 1/1 | 0.97 | 0.08 | 30,30,30,30 | 0 |
| 56 | MG | 1W | 203 | 1/1 | 0.97 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3800 | 1/1 | 0.97 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3461 | 1/1 | 0.97 | 0.11 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3189 | 1/1 | 0.97 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3828 | 1/1 | 0.97 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 1W | 206 | 1/1 | 0.97 | 0.16 | 23,23,23,23 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3083 | 1/1 | 0.97 | 0.08 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3015 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 1X | 101 | 1/1 | 0.97 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3952 | 1/1 | 0.97 | 0.04 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3041 | 1/1 | 0.97 | 0.12 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3019 | 1/1 | 0.97 | 0.04 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3113 | 1/1 | 0.97 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3383 | 1/1 | 0.97 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3717 | 1/1 | 0.97 | 0.06 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3822 | 1/1 | 0.97 | 0.04 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3597 | 1/1 | 0.97 | 0.05 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3833 | 1/1 | 0.97 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3119 | 1/1 | 0.97 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3201 | 1/1 | 0.97 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4094 | 1/1 | 0.97 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3345 | 1/1 | 0.97 | 0.26 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3602 | 1/1 | 0.97 | 0.07 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3619 | 1/1 | 0.97 | 0.05 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3958 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3206 | 1/1 | 0.97 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3250 | 1/1 | 0.97 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3086 | 1/1 | 0.97 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3394 | 1/1 | 0.97 | 0.21 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 4102 | 1/1 | 0.97 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 1Z | 305 | 1/1 | 0.97 | 0.05 | 32,32,32,32 | 0 |
| 56 | MG | 10 | 101 | 1/1 | 0.97 | 0.04 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3622 | 1/1 | 0.97 | 0.06 | 9,9,9,9 | 0 |
| 56 | MG | 2A | 3033 | 1/1 | 0.97 | 0.05 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3252 | 1/1 | 0.97 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3035 | 1/1 | 0.97 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3402 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 4105 | 1/1 | 0.97 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3619 | 1/1 | 0.97 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3003 | 1/1 | 0.97 | 0.08 | 17,17,17,17 | 0 |
| 56 | MG | 2A | 3038 | 1/1 | 0.97 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3406 | 1/1 | 0.97 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3301 | 1/1 | 0.97 | 0.15 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3169 | 1/1 | 0.97 | 0.23 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3135 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3068 | 1/1 | 0.97 | 0.11 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3732 | 1/1 | 0.97 | 0.09 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3226 | 1/1 | 0.97 | 0.08 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3629 | 1/1 | 0.97 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3070 | 1/1 | 0.97 | 0.16 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3141 | 1/1 | 0.97 | 0.20 | 25,25,25,25 | 0 |
| 56 | MG | 15 | 102 | 1/1 | 0.97 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3862 | 1/1 | 0.97 | 0.05 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 4117 | 1/1 | 0.97 | 0.11 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1739 | 1/1 | 0.97 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 16 | 101 | 1/1 | 0.97 | 0.06 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3736 | 1/1 | 0.97 | 0.05 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3163 | 1/1 | 0.97 | 0.04 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3142 | 1/1 | 0.97 | 0.11 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3850 | 1/1 | 0.97 | 0.07 | 33,33,33,33 | 0 |
| 56 | MG | 1a | 1744 | 1/1 | 0.97 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1746 | 1/1 | 0.97 | 0.07 | 36,36,36,36 | 0 |
| 56 | MG | 17 | 103 | 1/1 | 0.97 | 0.07 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3015 | 1/1 | 0.97 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 4124 | 1/1 | 0.97 | 0.05 | 27,27,27,27 | 0 |
| 56 | MG | 2a | 3171 | 1/1 | 0.97 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3739 | 1/1 | 0.97 | 0.07 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3741 | 1/1 | 0.97 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3221 | 1/1 | 0.97 | 0.10 | 12,12,12,12 | 0 |
| 56 | MG | 1A | 3981 | 1/1 | 0.97 | 0.06 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3855 | 1/1 | 0.97 | 0.06 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3479 | 1/1 | 0.97 | 0.09 | 26,26,26,26 | 0 |
| 56 | MG | 1a | 1758 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3262 | 1/1 | 0.97 | 0.24 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4136 | 1/1 | 0.97 | 0.10 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3440 | 1/1 | 0.97 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3144 | 1/1 | 0.97 | 0.21 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3419 | 1/1 | 0.97 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3315 | 1/1 | 0.97 | 0.17 | 14,14,14,14 | 0 |
| 56 | MG | 1a | 1764 | 1/1 | 0.97 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1608 | 1/1 | 0.97 | 0.25 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3421 | 1/1 | 0.97 | 0.05 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3073 | 1/1 | 0.97 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1768 | 1/1 | 0.97 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1610 | 1/1 | 0.97 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3485 | 1/1 | 0.97 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3991 | 1/1 | 0.97 | 0.11 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3073 | 1/1 | 0.97 | 0.05 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3487 | 1/1 | 0.97 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3423 | 1/1 | 0.97 | 0.07 | 45,45,45,45 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3265 | 1/1 | 0.97 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3364 | 1/1 | 0.97 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3457 | 1/1 | 0.97 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3200 | 1/1 | 0.97 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3075 | 1/1 | 0.97 | 0.16 | 22,22,22,22 | 0 |
| 56 | MG | 1B | 217 | 1/1 | 0.97 | 0.05 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3460 | 1/1 | 0.97 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3270 | 1/1 | 0.97 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3085 | 1/1 | 0.97 | 0.04 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3870 | 1/1 | 0.97 | 0.05 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3649 | 1/1 | 0.97 | 0.06 | 11,11,11,11 | 0 |
| 56 | MG | 1A | 3021 | 1/1 | 0.97 | 0.04 | 28,28,28,28 | 0 |
| 56 | MG | 2a | 3209 | 1/1 | 0.97 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3764 | 1/1 | 0.97 | 0.05 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3429 | 1/1 | 0.97 | 0.16 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3092 | 1/1 | 0.97 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 1B | 223 | 1/1 | 0.97 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 2U | 201 | 1/1 | 0.97 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3568 | 1/1 | 0.97 | 0.33 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3685 | 1/1 | 0.97 | 0.08 | 28,28,28,28 | 0 |
| 56 | MG | 2U | 204 | 1/1 | 0.97 | 0.03 | 37,37,37,37 | 0 |
| 56 | MG | 1B | 225 | 1/1 | 0.97 | 0.06 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3149 | 1/1 | 0.97 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3688 | 1/1 | 0.97 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 2Y | 201 | 1/1 | 0.97 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | 1a | 1791 | 1/1 | 0.97 | 0.06 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3570 | 1/1 | 0.97 | 0.21 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3285 | 1/1 | 0.97 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 25 | 102 | 1/1 | 0.97 | 0.04 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3185 | 1/1 | 0.97 | 0.12 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3031 | 1/1 | 0.97 | 0.11 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3658 | 1/1 | 0.97 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3773 | 1/1 | 0.97 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1797 | 1/1 | 0.97 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3498 | 1/1 | 0.97 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3188 | 1/1 | 0.97 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 4015 | 1/1 | 0.97 | 0.05 | 23,23,23,23 | 0 |
| 56 | MG | 1B | 235 | 1/1 | 0.97 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3576 | 1/1 | 0.97 | 0.05 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3488 | 1/1 | 0.97 | 0.06 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 4020 | 1/1 | 0.97 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1805 | 1/1 | 0.97 | 0.09 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1807 | 1/1 | 0.97 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 1D | 302 | 1/1 | 0.97 | 0.14 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3435 | 1/1 | 0.97 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 2l | 203 | 1/1 | 0.97 | 0.06 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3666 | 1/1 | 0.97 | 0.05 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3302 | 1/1 | 0.97 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3497 | 1/1 | 0.97 | 0.05 | 45,45,45,45 | 0 |
| 56 | MG | 1D | 307 | 1/1 | 0.97 | 0.23 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3716 | 1/1 | 0.97 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3096 | 1/1 | 0.97 | 0.12 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3274 | 1/1 | 0.97 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | 2a | 3021 | 1/1 | 0.97 | 0.04 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3374 | 1/1 | 0.97 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 2x | 101 | 1/1 | 0.97 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3672 | 1/1 | 0.97 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3893 | 1/1 | 0.97 | 0.21 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3123 | 1/1 | 0.97 | 0.06 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3786 | 1/1 | 0.97 | 0.07 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3581 | 1/1 | 0.97 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3152 | 1/1 | 0.97 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3790 | 1/1 | 0.97 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 2a | 3030 | 1/1 | 0.97 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3119 | 1/1 | 0.97 | 0.05 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3277 | 1/1 | 0.97 | 0.45 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3511 | 1/1 | 0.97 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 1F | 301 | 1/1 | 0.97 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3022 | 1/1 | 0.97 | 0.06 | 11,11,11,11 | 0 |
| 56 | MG | 1a | 1831 | 1/1 | 0.97 | 0.05 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3134 | 1/1 | 0.97 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3002 | 1/1 | 0.97 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4037 | 1/1 | 0.97 | 0.06 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3510 | 1/1 | 0.97 | 0.26 | 33,33,33,33 | 0 |
| 59 | ZN | 14 | 102 | 1/1 | 0.97 | 0.05 | 94,94,94,94 | 0 |
| 59 | ZN | 24 | 501 | 1/1 | 0.97 | 0.08 | 113,113,113,113 | 0 |
| 59 | ZN | 29 | 102 | 1/1 | 0.97 | 0.06 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3511 | 1/1 | 0.97 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1770 | 1/1 | 0.98 | 0.03 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3989 | 1/1 | 0.98 | 0.08 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3222 | 1/1 | 0.98 | 0.03 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3306 | 1/1 | 0.98 | 0.03 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3069 | 1/1 | 0.98 | 0.04 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3181 | 1/1 | 0.98 | 0.17 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1647 | 1/1 | 0.98 | 0.16 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3014 | 1/1 | 0.98 | 0.11 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3309 | 1/1 | 0.98 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1778 | 1/1 | 0.98 | 0.05 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1650 | 1/1 | 0.98 | 0.05 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3056 | 1/1 | 0.98 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3643 | 1/1 | 0.98 | 0.04 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3186 | 1/1 | 0.98 | 0.18 | 18,18,18,18 | 0 |
| 56 | MG | 1Q | 201 | 1/1 | 0.98 | 0.12 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3495 | 1/1 | 0.98 | 0.05 | 55,55,55,55 | 0 |
| 56 | MG | 1Q | 202 | 1/1 | 0.98 | 0.04 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3192 | 1/1 | 0.98 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 4107 | 1/1 | 0.98 | 0.19 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 4108 | 1/1 | 0.98 | 0.12 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3008 | 1/1 | 0.98 | 0.03 | 12,12,12,12 | 0 |
| 56 | MG | 2a | 3105 | 1/1 | 0.98 | 0.08 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3853 | 1/1 | 0.98 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3108 | 1/1 | 0.98 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3314 | 1/1 | 0.98 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 4112 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3074 | 1/1 | 0.98 | 0.04 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3130 | 1/1 | 0.98 | 0.04 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3733 | 1/1 | 0.98 | 0.05 | 28,28,28,28 | 0 |
| 56 | MG | 1T | 201 | 1/1 | 0.98 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3191 | 1/1 | 0.98 | 0.04 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3823 | 1/1 | 0.98 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3232 | 1/1 | 0.98 | 0.16 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3131 | 1/1 | 0.98 | 0.11 | 11,11,11,11 | 0 |
| 56 | MG | 1A | 3193 | 1/1 | 0.98 | 0.17 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3524 | 1/1 | 0.98 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4122 | 1/1 | 0.98 | 0.12 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1802 | 1/1 | 0.98 | 0.07 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4123 | 1/1 | 0.98 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3196 | 1/1 | 0.98 | 0.04 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3588 | 1/1 | 0.98 | 0.03 | 24,24,24,24 | 0 |
| 56 | MG | 1a | 1806 | 1/1 | 0.98 | 0.04 | 58,58,58,58 | 0 |
| 56 | MG | 1W | 202 | 1/1 | 0.98 | 0.09 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3689 | 1/1 | 0.98 | 0.05 | 25,25,25,25 | 0 |
| 56 | MG | 1a | 1677 | 1/1 | 0.98 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3522 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4126 | 1/1 | 0.98 | 0.05 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3830 | 1/1 | 0.98 | 0.10 | 37,37,37,37 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1a | 1811 | 1/1 | 0.98 | 0.04 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3743 | 1/1 | 0.98 | 0.04 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3696 | 1/1 | 0.98 | 0.03 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3221 | 1/1 | 0.98 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 2D | 302 | 1/1 | 0.98 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3138 | 1/1 | 0.98 | 0.08 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3222 | 1/1 | 0.98 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3529 | 1/1 | 0.98 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1813 | 1/1 | 0.98 | 0.06 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1814 | 1/1 | 0.98 | 0.04 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4018 | 1/1 | 0.98 | 0.04 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1816 | 1/1 | 0.98 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 2E | 306 | 1/1 | 0.98 | 0.17 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4131 | 1/1 | 0.98 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | 1a | 1818 | 1/1 | 0.98 | 0.05 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3016 | 1/1 | 0.98 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3537 | 1/1 | 0.98 | 0.03 | 47,47,47,47 | 0 |
| 56 | MG | 1X | 103 | 1/1 | 0.98 | 0.10 | 19,19,19,19 | 0 |
| 56 | MG | 2a | 3153 | 1/1 | 0.98 | 0.05 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3231 | 1/1 | 0.98 | 0.06 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3711 | 1/1 | 0.98 | 0.06 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3920 | 1/1 | 0.98 | 0.04 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3659 | 1/1 | 0.98 | 0.03 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3472 | 1/1 | 0.98 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3661 | 1/1 | 0.98 | 0.05 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3089 | 1/1 | 0.98 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3133 | 1/1 | 0.98 | 0.05 | 15,15,15,15 | 0 |
| 56 | MG | 2Q | 201 | 1/1 | 0.98 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3009 | 1/1 | 0.98 | 0.04 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3547 | 1/1 | 0.98 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3239 | 1/1 | 0.98 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3929 | 1/1 | 0.98 | 0.04 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3201 | 1/1 | 0.98 | 0.07 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3551 | 1/1 | 0.98 | 0.06 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1694 | 1/1 | 0.98 | 0.22 | 39,39,39,39 | 0 |
| 56 | MG | 1B | 207 | 1/1 | 0.98 | 0.05 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3555 | 1/1 | 0.98 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3172 | 1/1 | 0.98 | 0.05 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3931 | 1/1 | 0.98 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3281 | 1/1 | 0.98 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3533 | 1/1 | 0.98 | 0.12 | 12,12,12,12 | 0 |
| 56 | MG | 1A | 3373 | 1/1 | 0.98 | 0.04 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3047 | 1/1 | 0.98 | 0.10 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3102 | 1/1 | 0.98 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3250 | 1/1 | 0.98 | 0.05 | 47,47,47,47 | 0 |
| 56 | MG | 1B | 213 | 1/1 | 0.98 | 0.04 | 41,41,41,41 | 0 |
| 56 | MG | 1B | 214 | 1/1 | 0.98 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | 2X | 101 | 1/1 | 0.98 | 0.11 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3283 | 1/1 | 0.98 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 20 | 101 | 1/1 | 0.98 | 0.05 | 55,55,55,55 | 0 |
| 56 | MG | 1B | 216 | 1/1 | 0.98 | 0.09 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3738 | 1/1 | 0.98 | 0.14 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3938 | 1/1 | 0.98 | 0.04 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 4039 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3377 | 1/1 | 0.98 | 0.04 | 12,12,12,12 | 0 |
| 56 | MG | 1A | 4041 | 1/1 | 0.98 | 0.10 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3760 | 1/1 | 0.98 | 0.03 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3409 | 1/1 | 0.98 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3035 | 1/1 | 0.98 | 0.05 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3676 | 1/1 | 0.98 | 0.06 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3243 | 1/1 | 0.98 | 0.05 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3604 | 1/1 | 0.98 | 0.07 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3577 | 1/1 | 0.98 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3164 | 1/1 | 0.98 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3751 | 1/1 | 0.98 | 0.04 | 42,42,42,42 | 0 |
| 56 | MG | 1w | 107 | 1/1 | 0.98 | 0.03 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3753 | 1/1 | 0.98 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3946 | 1/1 | 0.98 | 0.05 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3138 | 1/1 | 0.98 | 0.16 | 9,9,9,9 | 0 |
| 56 | MG | 1A | 3434 | 1/1 | 0.98 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3757 | 1/1 | 0.98 | 0.05 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3684 | 1/1 | 0.98 | 0.05 | 10,10,10,10 | 0 |
| 56 | MG | 2A | 3122 | 1/1 | 0.98 | 0.04 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3139 | 1/1 | 0.98 | 0.06 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3383 | 1/1 | 0.98 | 0.12 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3013 | 1/1 | 0.98 | 0.21 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3115 | 1/1 | 0.98 | 0.12 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3776 | 1/1 | 0.98 | 0.03 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3128 | 1/1 | 0.98 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3491 | 1/1 | 0.98 | 0.17 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3548 | 1/1 | 0.98 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3691 | 1/1 | 0.98 | 0.04 | 9,9,9,9 | 0 |
| 56 | MG | 1D | 303 | 1/1 | 0.98 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3439 | 1/1 | 0.98 | 0.16 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2A | 3282 | 1/1 | 0.98 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3616 | 1/1 | 0.98 | 0.04 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3435 | 1/1 | 0.98 | 0.14 | 19,19,19,19 | 0 |
| 56 | MG | 2a | 3031 | 1/1 | 0.98 | 0.22 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 4063 | 1/1 | 0.98 | 0.05 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3170 | 1/1 | 0.98 | 0.22 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3438 | 1/1 | 0.98 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3866 | 1/1 | 0.98 | 0.17 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3171 | 1/1 | 0.98 | 0.05 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3050 | 1/1 | 0.98 | 0.19 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3173 | 1/1 | 0.98 | 0.09 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3037 | 1/1 | 0.98 | 0.13 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3001 | 1/1 | 0.98 | 0.22 | 34,34,34,34 | 0 |
| 56 | MG | 1E | 301 | 1/1 | 0.98 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 4070 | 1/1 | 0.98 | 0.07 | 19,19,19,19 | 0 |
| 56 | MG | 1E | 303 | 1/1 | 0.98 | 0.10 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3038 | 1/1 | 0.98 | 0.04 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3787 | 1/1 | 0.98 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3616 | 1/1 | 0.98 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4072 | 1/1 | 0.98 | 0.04 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3789 | 1/1 | 0.98 | 0.04 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3791 | 1/1 | 0.98 | 0.08 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3499 | 1/1 | 0.98 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3557 | 1/1 | 0.98 | 0.05 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1745 | 1/1 | 0.98 | 0.04 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3558 | 1/1 | 0.98 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3972 | 1/1 | 0.98 | 0.06 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3013 | 1/1 | 0.98 | 0.04 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3877 | 1/1 | 0.98 | 0.04 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3974 | 1/1 | 0.98 | 0.06 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3145 | 1/1 | 0.98 | 0.23 | 23,23,23,23 | 0 |
| 56 | MG | 1F | 307 | 1/1 | 0.98 | 0.13 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3802 | 1/1 | 0.98 | 0.07 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3803 | 1/1 | 0.98 | 0.04 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3804 | 1/1 | 0.98 | 0.05 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3805 | 1/1 | 0.98 | 0.04 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3795 | 1/1 | 0.98 | 0.03 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3560 | 1/1 | 0.98 | 0.15 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1754 | 1/1 | 0.98 | 0.03 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3705 | 1/1 | 0.98 | 0.07 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3394 | 1/1 | 0.98 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3708 | 1/1 | 0.98 | 0.04 | 33,33,33,33 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3039 | 1/1 | 0.98 | 0.05 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3816 | 1/1 | 0.98 | 0.05 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3817 | 1/1 | 0.98 | 0.04 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3300 | 1/1 | 0.98 | 0.06 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3564 | 1/1 | 0.98 | 0.26 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3471 | 1/1 | 0.98 | 0.08 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3027 | 1/1 | 0.98 | 0.04 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3084 | 1/1 | 0.98 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3170 | 1/1 | 0.98 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 4091 | 1/1 | 0.98 | 0.05 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3804 | 1/1 | 0.98 | 0.07 | 19,19,19,19 | 0 |
| 59 | ZN | 2Y | 202 | 1/1 | 0.98 | 0.04 | 88,88,88,88 | 0 |
| 56 | MG | 1A | 3102 | 1/1 | 0.98 | 0.06 | 23,23,23,23 | 0 |
| 59 | ZN | 25 | 103 | 1/1 | 0.98 | 0.03 | 51,51,51,51 | 0 |
| 59 | ZN | 26 | 501 | 1/1 | 0.98 | 0.04 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3030 | 1/1 | 0.98 | 0.08 | 9,9,9,9 | 0 |
| 56 | MG | 1A | 3123 | 1/1 | 0.98 | 0.05 | 34,34,34,34 | 0 |
| 60 | SF4 | 2d | 303 | 8/8 | 0.98 | 0.04 | 55,66,68,68 | 0 |
| 56 | MG | 1A | 3677 | 1/1 | 0.99 | 0.03 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3749 | 1/1 | 0.99 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3388 | 1/1 | 0.99 | 0.05 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3600 | 1/1 | 0.99 | 0.06 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3924 | 1/1 | 0.99 | 0.03 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3650 | 1/1 | 0.99 | 0.04 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3794 | 1/1 | 0.99 | 0.02 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3012 | 1/1 | 0.99 | 0.04 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3928 | 1/1 | 0.99 | 0.06 | 15,15,15,15 | 0 |
| 56 | MG | 1a | 1755 | 1/1 | 0.99 | 0.03 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3194 | 1/1 | 0.99 | 0.09 | 11,11,11,11 | 0 |
| 56 | MG | 1a | 1821 | 1/1 | 0.99 | 0.03 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3683 | 1/1 | 0.99 | 0.05 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3195 | 1/1 | 0.99 | 0.06 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3087 | 1/1 | 0.99 | 0.06 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 4034 | 1/1 | 0.99 | 0.02 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3137 | 1/1 | 0.99 | 0.03 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3719 | 1/1 | 0.99 | 0.04 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3046 | 1/1 | 0.99 | 0.05 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3935 | 1/1 | 0.99 | 0.04 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 4038 | 1/1 | 0.99 | 0.03 | 13,13,13,13 | 0 |
| 56 | MG | 2a | 3142 | 1/1 | 0.99 | 0.04 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3552 | 1/1 | 0.99 | 0.04 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1765 | 1/1 | 0.99 | 0.05 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 2a | 3145 | 1/1 | 0.99 | 0.03 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3375 | 1/1 | 0.99 | 0.07 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3846 | 1/1 | 0.99 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3174 | 1/1 | 0.99 | 0.03 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3199 | 1/1 | 0.99 | 0.08 | 12,12,12,12 | 0 |
| 56 | MG | 1a | 1769 | 1/1 | 0.99 | 0.04 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3763 | 1/1 | 0.99 | 0.03 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 4043 | 1/1 | 0.99 | 0.04 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3704 | 1/1 | 0.99 | 0.04 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3397 | 1/1 | 0.99 | 0.13 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3137 | 1/1 | 0.99 | 0.05 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3067 | 1/1 | 0.99 | 0.09 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3023 | 1/1 | 0.99 | 0.07 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3768 | 1/1 | 0.99 | 0.03 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3729 | 1/1 | 0.99 | 0.03 | 37,37,37,37 | 0 |
| 56 | MG | 1n | 101 | 1/1 | 0.99 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3637 | 1/1 | 0.99 | 0.10 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3664 | 1/1 | 0.99 | 0.07 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3167 | 1/1 | 0.99 | 0.06 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3997 | 1/1 | 0.99 | 0.03 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3614 | 1/1 | 0.99 | 0.04 | 39,39,39,39 | 0 |
| 56 | MG | 1R | 201 | 1/1 | 0.99 | 0.04 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3903 | 1/1 | 0.99 | 0.02 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3204 | 1/1 | 0.99 | 0.03 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3775 | 1/1 | 0.99 | 0.03 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3668 | 1/1 | 0.99 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 4003 | 1/1 | 0.99 | 0.03 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3005 | 1/1 | 0.99 | 0.04 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3579 | 1/1 | 0.99 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3571 | 1/1 | 0.99 | 0.06 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3581 | 1/1 | 0.99 | 0.06 | 51,51,51,51 | 0 |
| 56 | MG | 1D | 305 | 1/1 | 0.99 | 0.04 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3671 | 1/1 | 0.99 | 0.08 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3585 | 1/1 | 0.99 | 0.04 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3040 | 1/1 | 0.99 | 0.17 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3740 | 1/1 | 0.99 | 0.03 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3959 | 1/1 | 0.99 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 1U | 205 | 1/1 | 0.99 | 0.07 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3806 | 1/1 | 0.99 | 0.02 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3299 | 1/1 | 0.99 | 0.07 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3071 | 1/1 | 0.99 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3784 | 1/1 | 0.99 | 0.08 | 11,11,11,11 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 56 | MG | 1A | 3268 | 1/1 | 0.99 | 0.16 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 4128 | 1/1 | 0.99 | 0.03 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3707 | 1/1 | 0.99 | 0.04 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4016 | 1/1 | 0.99 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3814 | 1/1 | 0.99 | 0.06 | 22,22,22,22 | 0 |
| 59 | ZN | 1Y | 206 | 1/1 | 0.99 | 0.02 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3815 | 1/1 | 0.99 | 0.04 | 59,59,59,59 | 0 |
| 59 | ZN | 16 | 103 | 1/1 | 0.99 | 0.04 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3746 | 1/1 | 0.99 | 0.04 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3428 | 1/1 | 0.99 | 0.02 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 4019 | 1/1 | 0.99 | 0.02 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3873 | 1/1 | 0.99 | 0.03 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3462 | 1/1 | 0.99 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 4135 | 1/1 | 0.99 | 0.04 | 15,15,15,15 | 0 |
| 60 | SF4 | 1d | 501 | 8/8 | 0.99 | 0.04 | 38,50,55,61 | 0 |
| 56 | MG | 1X | 102 | 1/1 | 0.99 | 0.05 | 17,17,17,17 | 0 |
| 59 | ZN | 15 | 104 | 1/1 | 1.00 | 0.05 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3681 | 1/1 | 1.00 | 0.02 | 44,44,44,44 | 0 |
| 59 | ZN | 19 | 102 | 1/1 | 1.00 | 0.03 | 33,33,33,33 | 0 |
| 59 | ZN | 1n | 102 | 1/1 | 1.00 | 0.02 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3710 | 1/1 | 1.00 | 0.04 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 4078 | 1/1 | 1.00 | 0.09 | 6,6,6,6 | 0 |
| 56 | MG | 1A | 3902 | 1/1 | 1.00 | 0.02 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 4013 | 1/1 | 1.00 | 0.02 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3898 | 1/1 | 1.00 | 0.05 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3742 | 1/1 | 1.00 | 0.04 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3720 | 1/1 | 1.00 | 0.06 | 9,9,9,9 | 0 |
| 56 | MG | 2A | 3584 | 1/1 | 1.00 | 0.09 | 31,31,31,31 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.