



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:48 am BST

PDB ID : 6O97
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 2.75Å 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

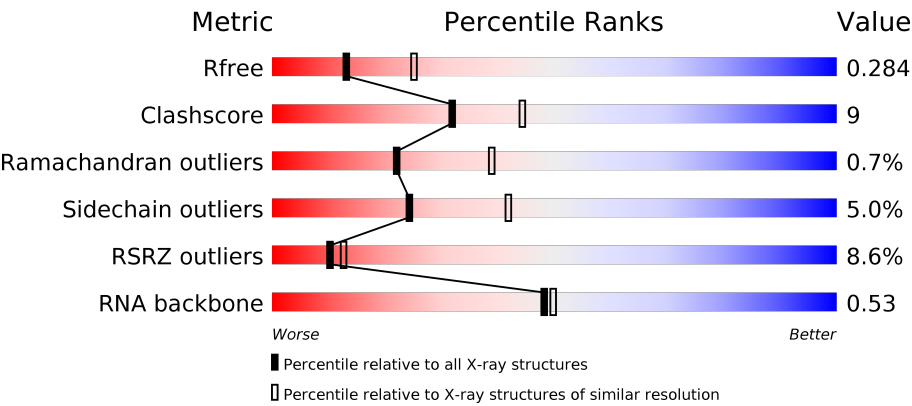
| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

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} | 130704 | 1235 (2.78-2.74) |
| Clashscore | 141614 | 1277 (2.78-2.74) |
| Ramachandran outliers | 138981 | 1257 (2.78-2.74) |
| Sidechain outliers | 138945 | 1257 (2.78-2.74) |
| RSRZ outliers | 127900 | 1207 (2.78-2.74) |
| RNA backbone | 3102 | 1060 (3.02-2.50) |

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 1A | 2915 | <div><div>60%31%7%</div><div></div></div> |
| 1 | 2A | 2915 | <div><div>53%35%8%</div><div></div></div> |
| 2 | 1B | 121 | <div><div>69%26%</div><div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | |
| 14 | 1S | 112 | |
| 14 | 2S | 112 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 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 | |
| 26 | 24 | 71 | |
| 27 | 15 | 60 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 27 | 25 | 60 | <div> <div>8%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div> |
| 28 | 16 | 54 | <div> <div>78%</div> <div>20%</div> <div>•</div> </div> |
| 28 | 26 | 54 | <div> <div>19%</div> <div>74%</div> <div>20%</div> <div>• •</div> </div> |
| 29 | 17 | 49 | <div> <div>10%</div> <div>71%</div> <div>27%</div> <div>•</div> </div> |
| 29 | 27 | 49 | <div> <div>16%</div> <div>69%</div> <div>27%</div> <div>• •</div> </div> |
| 30 | 18 | 65 | <div> <div>5%</div> <div>60%</div> <div>37%</div> <div>• •</div> </div> |
| 30 | 28 | 65 | <div> <div>40%</div> <div>69%</div> <div>28%</div> <div>• •</div> </div> |
| 31 | 19 | 37 | <div> <div>78%</div> <div>19%</div> <div>•</div> </div> |
| 31 | 29 | 37 | <div> <div>30%</div> <div>76%</div> <div>22%</div> <div>•</div> </div> |
| 32 | 1a | 1521 | <div> <div>%</div> <div>82%</div> <div>16%</div> <div>•</div> </div> |
| 32 | 2a | 1521 | <div> <div>3%</div> <div>80%</div> <div>18%</div> <div>• •</div> </div> |
| 33 | 1b | 256 | <div> <div>9%</div> <div>85%</div> <div>• •</div> <div>10%</div> </div> |
| 33 | 2b | 256 | <div> <div>29%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div> |
| 34 | 1c | 239 | <div> <div>8%</div> <div>83%</div> <div>•</div> <div>14%</div> </div> |
| 34 | 2c | 239 | <div> <div>23%</div> <div>84%</div> <div>•</div> <div>14%</div> </div> |
| 35 | 1d | 209 | <div> <div>13%</div> <div>96%</div> <div>•</div> </div> |
| 35 | 2d | 209 | <div> <div>17%</div> <div>96%</div> <div>•</div> </div> |
| 36 | 1e | 162 | <div> <div>11%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div> |
| 36 | 2e | 162 | <div> <div>29%</div> <div>88%</div> <div>•</div> <div>9%</div> </div> |
| 37 | 1f | 101 | <div> <div>2%</div> <div>97%</div> <div>• •</div> </div> |
| 37 | 2f | 101 | <div> <div>2%</div> <div>96%</div> <div>• •</div> </div> |
| 38 | 1g | 156 | <div> <div>14%</div> <div>96%</div> <div>• •</div> </div> |
| 38 | 2g | 156 | <div> <div>18%</div> <div>97%</div> <div>• •</div> </div> |
| 39 | 1h | 138 | <div> <div>16%</div> <div>93%</div> <div>6%</div> <div>•</div> </div> |
| 39 | 2h | 138 | <div> <div>26%</div> <div>96%</div> <div>• •</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40 | 1i | 128 | |
| 40 | 2i | 128 | |
| 41 | 1j | 105 | |
| 41 | 2j | 105 | |
| 42 | 1k | 129 | |
| 42 | 2k | 129 | |
| 43 | 1l | 132 | |
| 43 | 2l | 132 | |
| 44 | 1m | 126 | |
| 44 | 2m | 126 | |
| 45 | 1n | 61 | |
| 45 | 2n | 61 | |
| 46 | 1o | 89 | |
| 46 | 2o | 89 | |
| 47 | 1p | 88 | |
| 47 | 2p | 88 | |
| 48 | 1q | 105 | |
| 48 | 2q | 105 | |
| 49 | 1r | 88 | |
| 49 | 2r | 88 | |
| 50 | 1s | 93 | |
| 50 | 2s | 93 | |
| 51 | 1t | 106 | |
| 51 | 2t | 106 | |
| 52 | 1u | 27 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52 | 2u | 27 | |
| 53 | 1v | 27 | |
| 53 | 2v | 27 | |
| 54 | 1w | 76 | |
| 54 | 1y | 76 | |
| 54 | 2w | 76 | |
| 54 | 2y | 76 | |
| 55 | 1x | 77 | |
| 55 | 2x | 77 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54 | CM0 | 2y | 34 | - | - | - | X |
| 56 | MG | 1A | 3354 | - | - | - | X |
| 56 | MG | 1A | 3360 | - | - | - | X |
| 56 | MG | 1A | 3453 | - | - | - | X |
| 56 | MG | 1A | 3525 | - | - | - | X |
| 56 | MG | 1A | 3948 | - | - | - | X |
| 56 | MG | 1A | 3993 | - | - | - | X |
| 56 | MG | 1A | 4017 | - | - | - | X |
| 56 | MG | 1A | 4053 | - | - | - | X |
| 56 | MG | 1A | 4098 | - | - | - | X |
| 56 | MG | 1E | 302 | - | - | - | X |
| 56 | MG | 1a | 1603 | - | - | - | X |
| 56 | MG | 1a | 1605 | - | - | - | X |
| 56 | MG | 1a | 1622 | - | - | - | X |
| 56 | MG | 1l | 202 | - | - | - | X |
| 56 | MG | 1v | 101 | - | - | - | X |
| 56 | MG | 1y | 105 | - | - | - | X |
| 56 | MG | 2A | 3177 | - | - | - | X |
| 56 | MG | 2A | 3232 | - | - | - | X |
| 56 | MG | 2A | 3251 | - | - | - | X |
| 56 | MG | 2A | 3288 | - | - | - | X |
| 56 | MG | 2A | 3503 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | 2A | 3647 | - | - | - | X |
| 56 | MG | 2A | 3854 | - | - | - | X |
| 56 | MG | 2F | 303 | - | - | - | X |
| 56 | MG | 2a | 3015 | - | - | - | X |
| 56 | MG | 2a | 3016 | - | - | - | X |
| 56 | MG | 2a | 3027 | - | - | - | X |
| 56 | MG | 2a | 3049 | - | - | - | X |
| 56 | MG | 2a | 3091 | - | - | - | X |

2 Entry composition

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 | C | N | O | S | 0 | 0 | 0 |
| | | | 933 | 588 | 171 | 170 | 4 | | | |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

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

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56 | 2E | 8 | Total | Mg | 0 | 0 |
| | | | 8 | 8 | | |
| 56 | 17 | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | 2d | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | 1T | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | 1N | 7 | Total | Mg | 0 | 0 |
| | | | 7 | 7 | | |
| 56 | 20 | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | 18 | 4 | Total | Mg | 0 | 0 |
| | | | 4 | 4 | | |
| 56 | 2W | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|------------|---------|---------|
| 56 | 1Y | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | 13 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1f | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 1P | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | 2B | 18 | Total 18 | Mg 18 | 0 | 0 |
| 56 | 1q | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 2a | 231 | Total 231 | Mg 231 | 0 | 0 |
| 56 | 1E | 7 | Total 7 | Mg 7 | 0 | 0 |
| 56 | 1b | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 2l | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | 2F | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | 16 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 28 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 2e | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1W | 7 | Total 7 | Mg 7 | 0 | 0 |
| 56 | 1A | 1134 | Total 1134 | Mg 1134 | 0 | 0 |
| 56 | 1t | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1n | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 2P | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 1X | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | 2q | 3 | Total 3 | Mg 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 56 | 12 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 1y | 6 | Total 6 | Mg 6 | 0 | 0 |
| 56 | 2i | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1S | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | 25 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 2T | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | 1D | 13 | Total 13 | Mg 13 | 0 | 0 |
| 56 | 2N | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1e | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 2G | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1I | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 29 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 2f | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1V | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 2X | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1w | 8 | Total 8 | Mg 8 | 0 | 0 |
| 56 | 1a | 233 | Total 233 | Mg 233 | 0 | 0 |
| 56 | 2Q | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | 15 | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | 1x | 15 | Total 15 | Mg 15 | 0 | 0 |
| 56 | 2j | 2 | Total 2 | Mg 2 | 0 | 0 |

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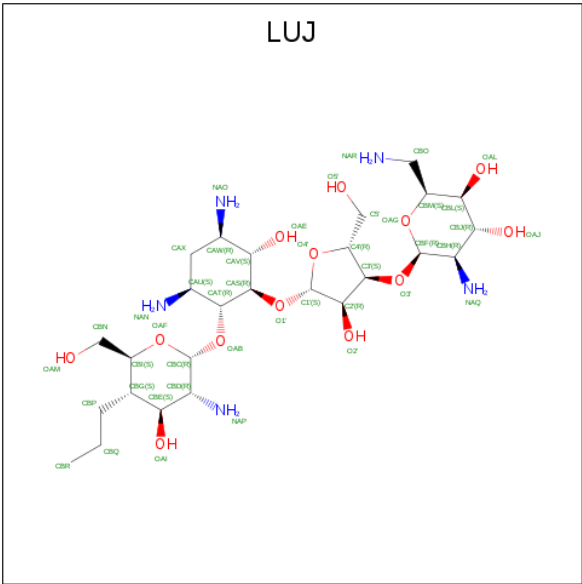
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 56 | 1R | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | 2v | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | 2U | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | 1G | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | 2O | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 11 | 2 | Total 2 | Mg 2 | 0 | 0 |
| 56 | 2r | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 21 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 2Y | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1v | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 2x | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | 2R | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | 1Z | 5 | Total 5 | Mg 5 | 0 | 0 |
| 56 | 2D | 3 | Total 3 | Mg 3 | 0 | 0 |
| 56 | 14 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 2k | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1U | 7 | Total 7 | Mg 7 | 0 | 0 |
| 56 | 1O | 4 | Total 4 | Mg 4 | 0 | 0 |
| 56 | 27 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 19 | 1 | Total 1 | Mg 1 | 0 | 0 |
| 56 | 1l | 3 | Total 3 | Mg 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | 2V | 2 | Total | Mg | 0 | 0 |
| | | | 2 | 2 | | |
| 56 | 1F | 10 | Total | Mg | 0 | 0 |
| | | | 10 | 10 | | |
| 56 | 10 | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 56 | 2t | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | 1Q | 5 | Total | Mg | 0 | 0 |
| | | | 5 | 5 | | |
| 56 | 2A | 860 | Total | Mg | 0 | 0 |
| | | | 860 | 860 | | |
| 56 | 1B | 36 | Total | Mg | 0 | 0 |
| | | | 36 | 36 | | |
| 56 | 2y | 6 | Total | Mg | 0 | 0 |
| | | | 6 | 6 | | |

- 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-hydroxycyclohexyl 2-amino-2,4-dideoxy-4-propyl-alpha-D-glucopyranoside (three-letter code: LUJ) (formula: C₂₆H₅₁N₅O₁₃).



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

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

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

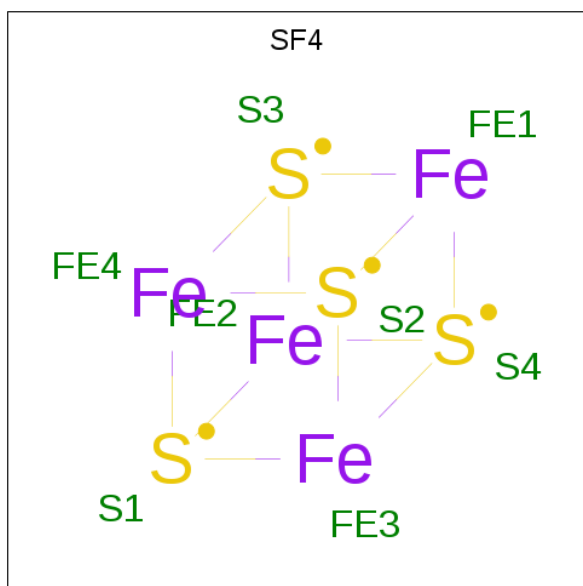
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 59 | 1Y | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 14 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 1n | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 59 | 15 | 1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

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

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



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

- Molecule 61 is water.

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

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

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

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

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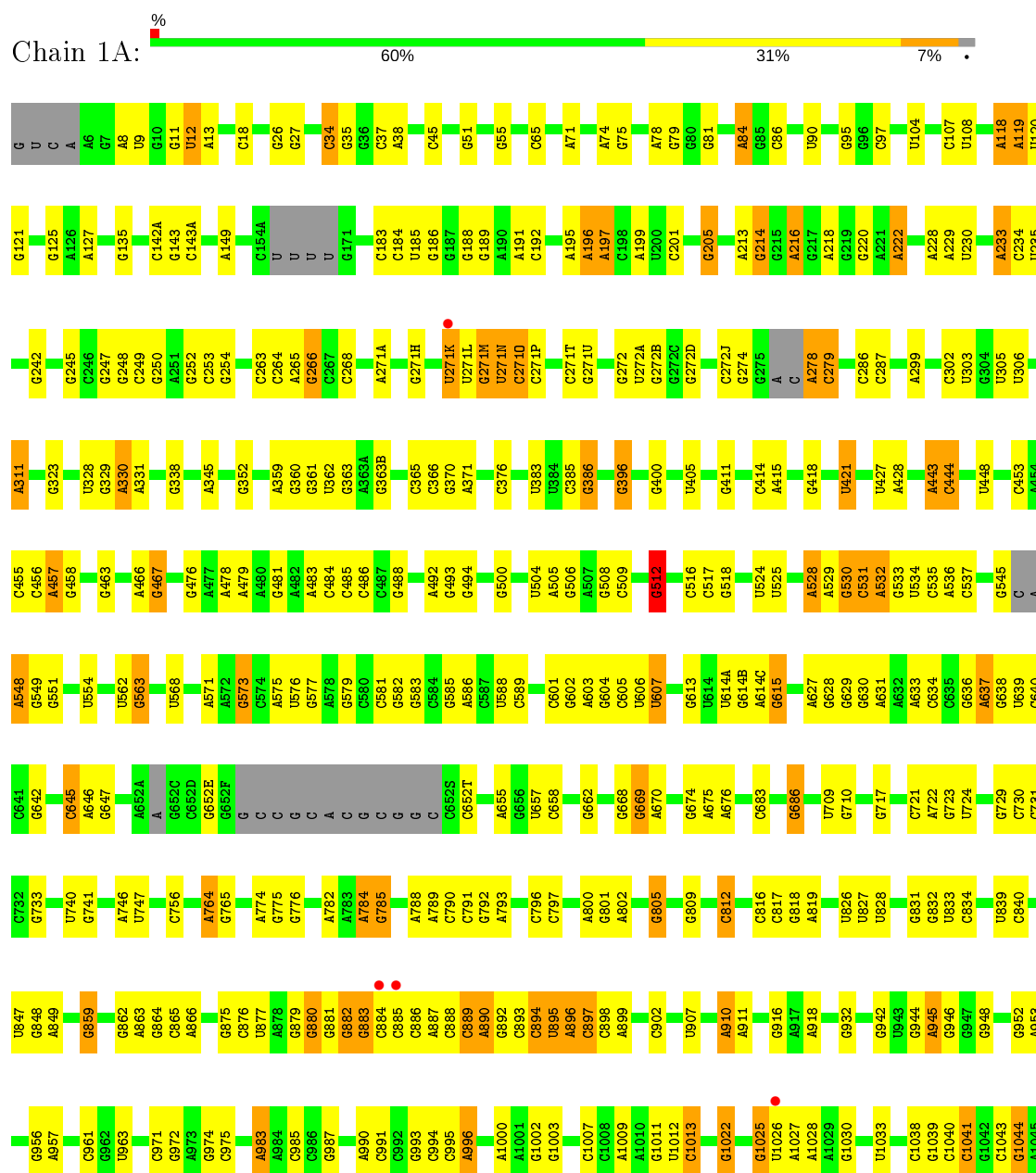
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 61 | 28 | 6 | Total 6 | O 6 | 0 | 0 |
| 61 | 2a | 322 | Total 322 | O 322 | 0 | 0 |
| 61 | 2e | 2 | Total 2 | O 2 |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

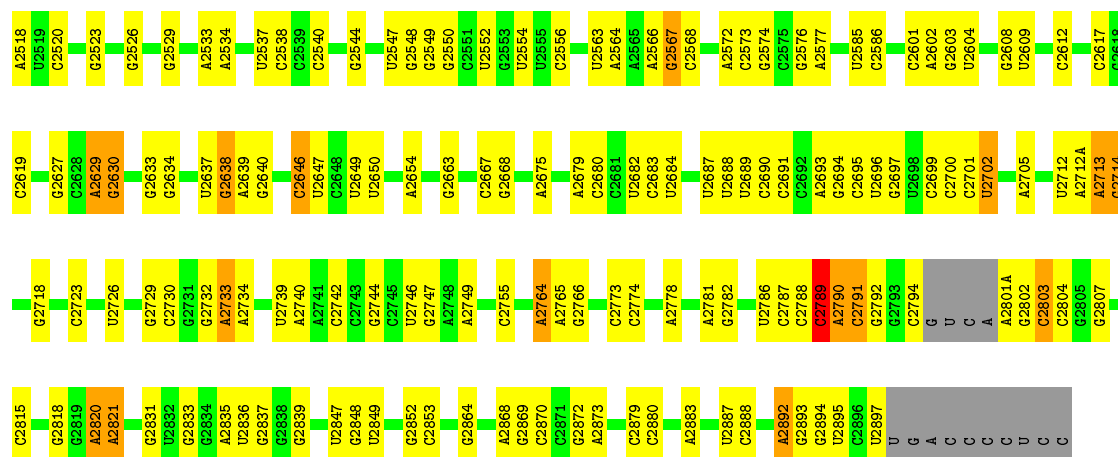
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

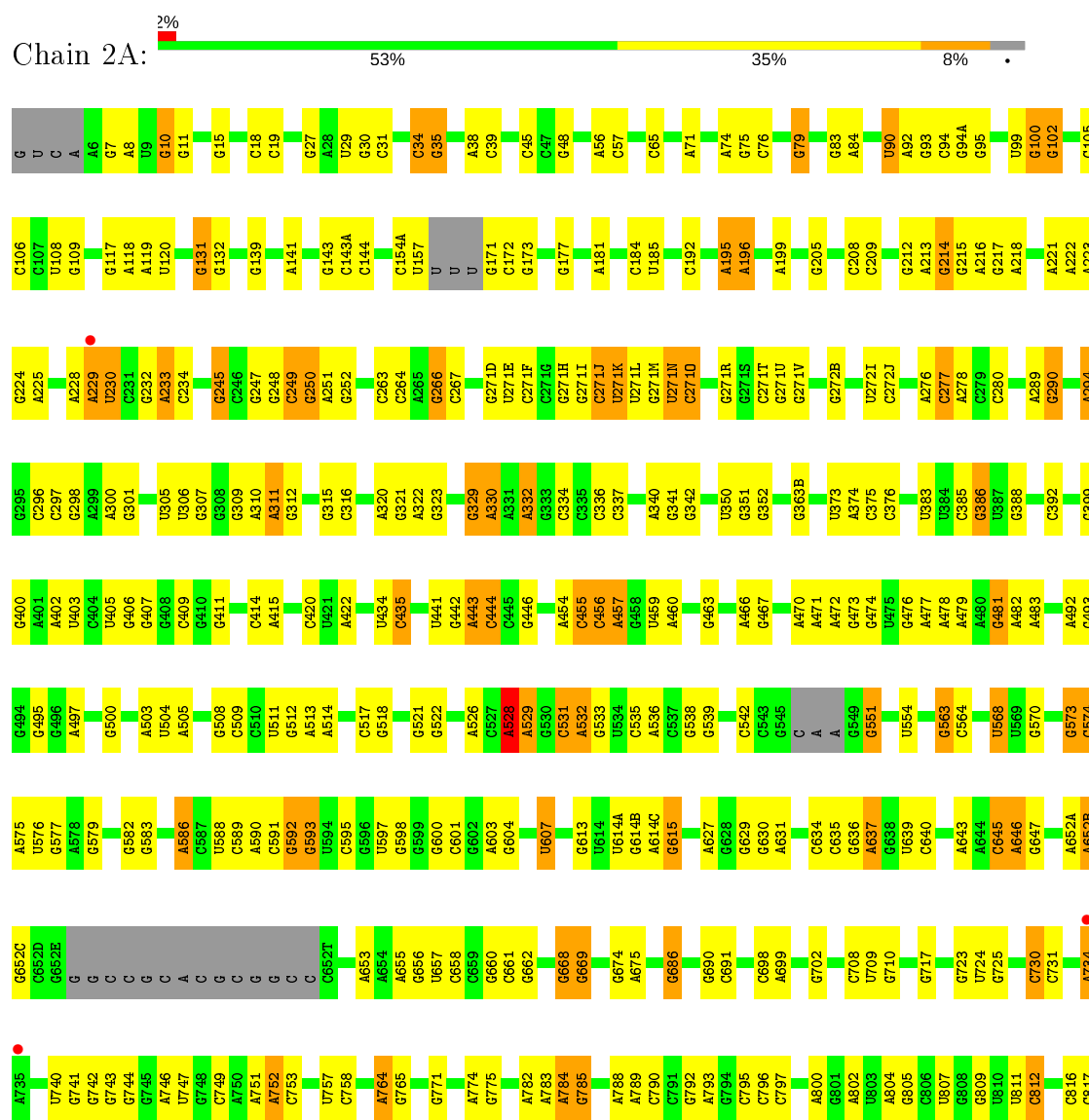
• Molecule 1: 23S Ribosomal RNA



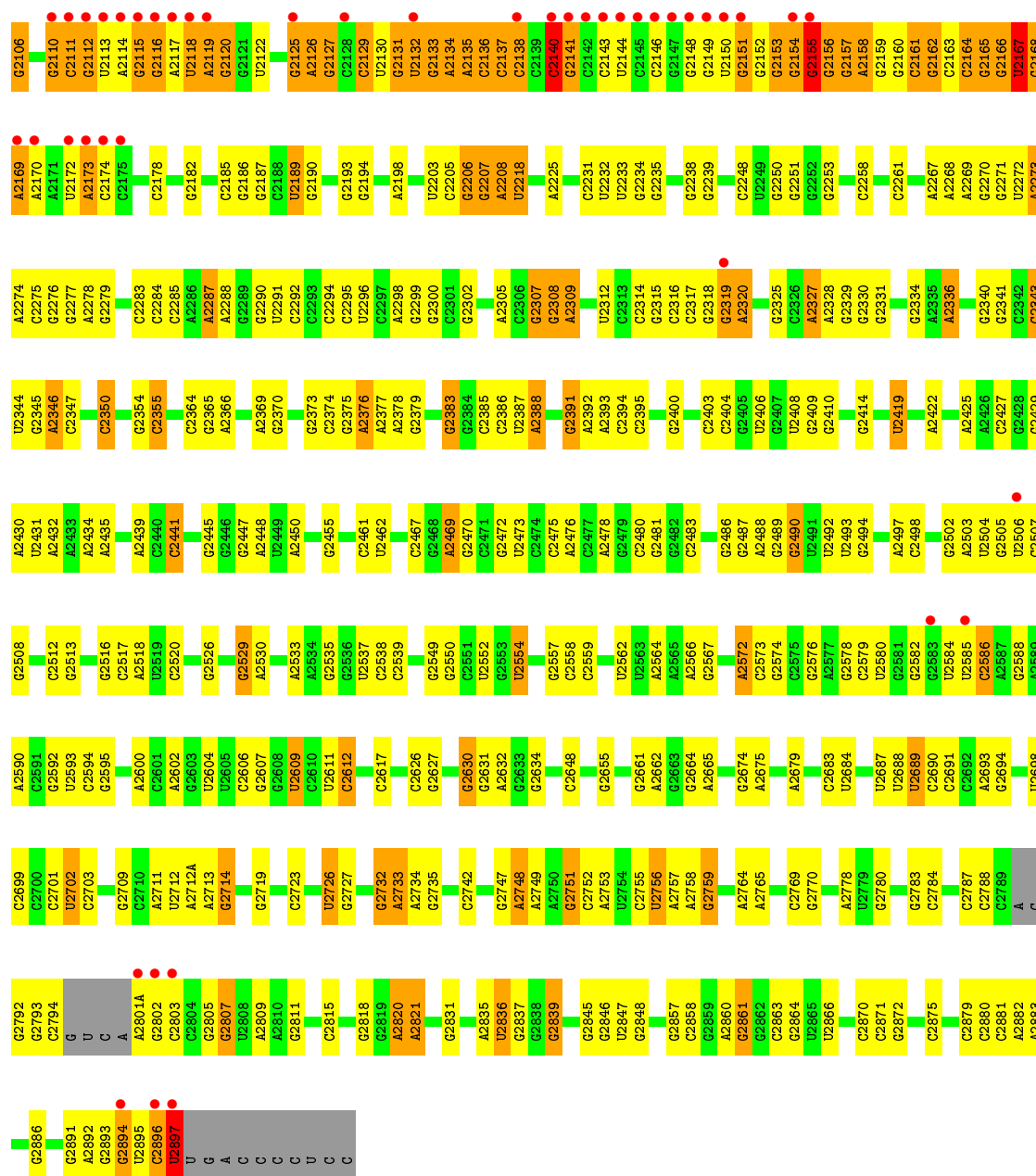
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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| G2409 | G2410 | A2418 | A2419 | C2424 | A2425 | G2428 | G2429 | A2430 | U2431 | A2432 | A2435 | A2439 | C2440 | C2441 | C2442 | C2443 | C2444 | G2445 | A2448 | G2458 | C2464 | G2470 | C2471 | C2472 | U2473 | C2474 | C2475 | A2476 | A2477 | A2478 | C2483 | G2490 | U2491 | U2492 | U2493 | C2496 | C2498 | C2499 | U2500 | C2501 | G2502 | G2505 | U2506 | U2406 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2303 | G2304 | A2305 | C2306 | G2307 | A2308 | A2309 | U2312 | C2313 | C2314 | G2315 | C2316 | G2319 | A2320 | A2321 | G2322 | A2323 | G2324 | G2325 | C2326 | A2327 | C2328 | G2329 | G2330 | G2331 | G2334 | A2335 | A2336 | A2346 | C2347 | U2348 | G2349 | C2350 | A2360 | A2361 | C2364 | G2365 | G2375 | A2376 | A2377 | A2378 | U2379 | C2380 | G2383 | C2384 | C2385 | G2389 | U2390 | A2393 | G2396 | U2406 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2182 | C2183 | G2184 | C2188 | U2189 | G2190 | G2191 | A2198 | C2199 | C2200 | U2201 | A2203 | C2205 | G2206 | G2207 | A2208 | U2218 | G2222 | A2225 | G2238 | U2243 | U2244 | G2247 | G2250 | G2256 | U2257 | U2262 | C2263 | C2264 | A2268 | A2269 | G2270 | G2271 | G2279 | G2280 | C2283 | A2286 | A2287 | U2291 | C2292 | U2296 | G2299 | G2300 | C2301 | G2302 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A2119 | G2120 | G2123 | G2124 | G2125 | A2126 | G2127 | C2128 | C2129 | U2130 | U2131 | U2132 | G2133 | A2134 | A2135 | A2136 | C2137 | C2138 | C2139 | G2140 | G2141 | C2142 | C2143 | U2144 | C2145 | C2146 | G2147 | G2148 | U2149 | U2150 | G2151 | G2152 | G2153 | G2154 | G2155 | G2156 | G2157 | A2158 | G2159 | G2160 | C2161 | G2162 | C2163 | C2164 | C2165 | G2166 | U2167 | C2168 | A2169 | A2170 | U2171 | U2172 | A2173 | C2174 | C2175 | A2176 | C2177 | C2178 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G2020 | C2021 | G2022 | G2023 | A2030 | A2031 | G2032 | A2033 | C2040 | U2041 | A2042 | C2043 | G2053 | A2054 | C2055 | G2056 | A2060 | A2061 | A2062 | C2065 | C2066 | U2067 | U2068 | G2069 | G2070 | A2071 | C2072 | C2073 | U2074 | U2075 | U2076 | U2077 | U2079 | G2080 | U2086 | G2087 | U2098 | U2099 | G2100 | G2101 | U2102 | C2105 | G2106 | C2107 | C2108 | U2109 | G2110 | G2111 | C2112 | U2113 | A2114 | G2115 | C2116 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A1789 | C1790 | A1791 | U1794 | C1795 | U1796 | C1797 | U1798 | A1799 | G1800 | A1801 | A1802 | A1803 | A1812 | A1815 | G1816 | G1817 | U1818 | A1821 | G1822 | C1823 | C1824 | C1825 | C1826 | G1827 | G1828 | A1829 | G1830 | C1831 | C1832 | G1833 | G1834 | U1835 | C1852 | A1853 | A1854 | G1861 | G1862 | G1863 | C1866 | A1876 | G1877 | G1878 | C1881 | C1882 | U1883 | A1889 | G1899 | A1900 | A1786 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| G1906 | A1918 | A1927 | A1928 | G1929 | G1930 | U1931 | A1932 | G1933 | A1936 | A1937 | A1938 | U1939 | U1940 | G1949 | G1950 | A1951 | A1952 | A1953 | G1954 | U1955 | U1963 | G1964 | G1969 | G1970 | A1966 | G1967 | G1968 | A1969 | A1970 | A1971 | A1972 | G1973 | C1988 | U1991 | G1992 | U1993 | C1996 | G1997 | G1998 | C1999 | G2000 | A2001 | G2002 | G2010 | U2011 | G2012 | A2013 | A2014 | G2018 | A2019 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| A2020 | C2021 | G2022 | G2023 | A2030 | A2031 | G2032 | A2033 | C2040 | U2041 | A2042 | C2043 | G2053 | A2054 | C2055 | G2056 | A2060 | A2061 | A2062 | C2065 | C2066 | U2067 | U2068 | G2069 | G2070 | A2071 | C2072 | C2073 | U2074 | U2075 | U2076 | U2077 | U2079 | G2080 | U2086 | G2087 | U2098 | U2099 | G2100 | G2101 | U2102 | C2105 | G2106 | C2107 | C2108 | U2109 | G2110 | G2111 | C2112 | U2113 | A2114 | G2115 | C2116 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
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• Molecule 1: 23S Ribosomal RNA







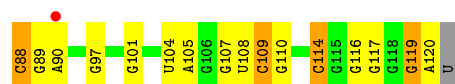
● Molecule 2: 5S Ribosomal RNA

Chain 1B: 69% 26%

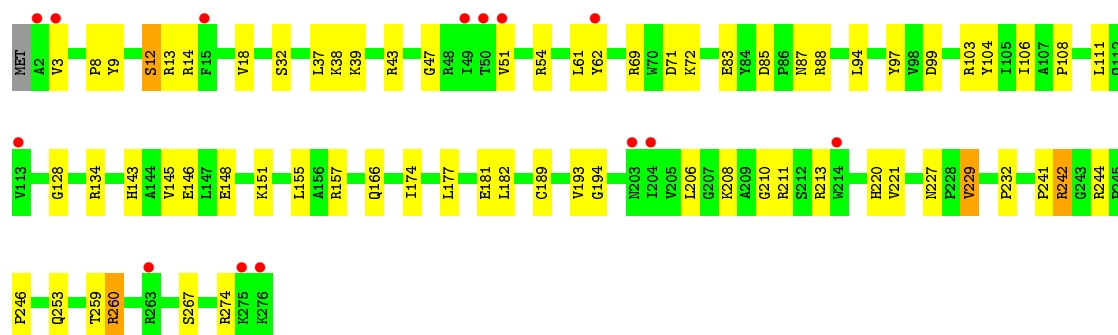
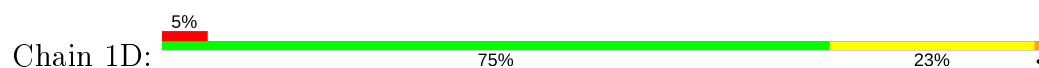
● Molecule 2: 5S Ribosomal RNA

Chain 2B: 51% 37% 11%

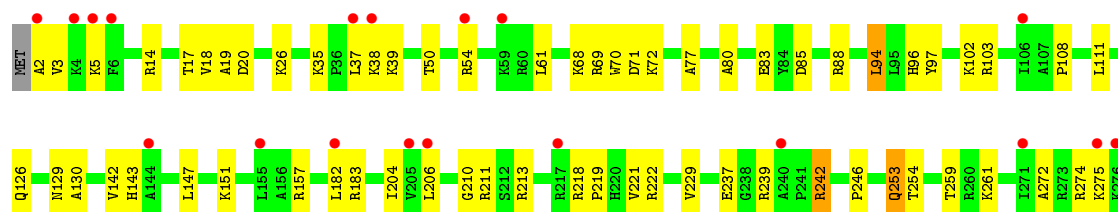
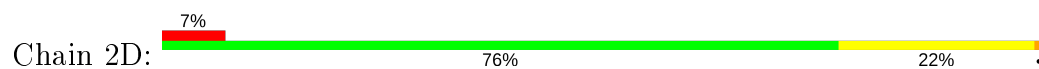




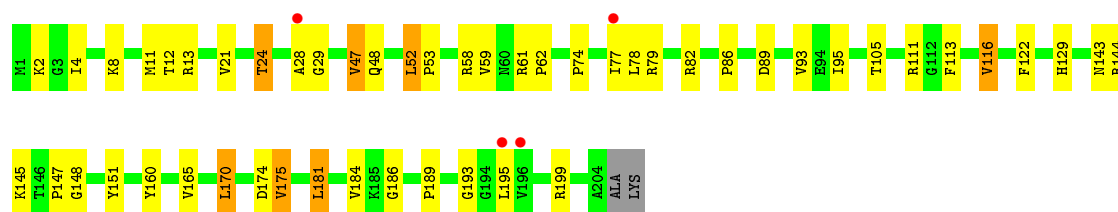
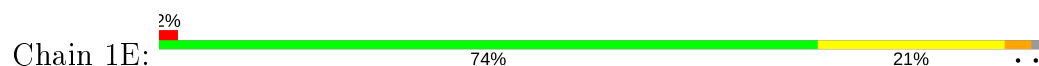
• Molecule 3: 50S ribosomal protein L2



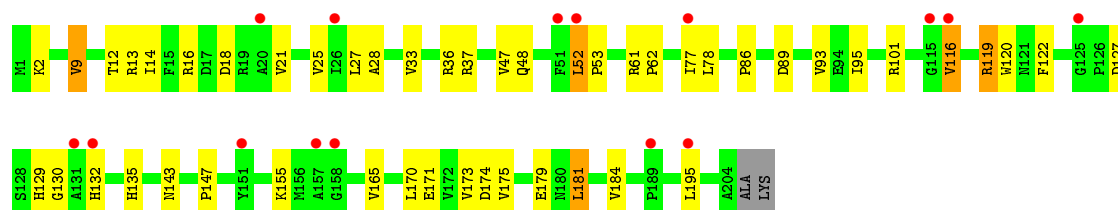
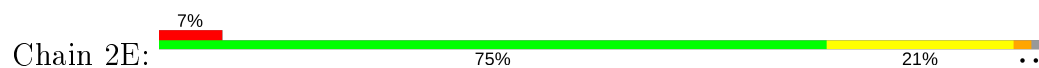
• Molecule 3: 50S ribosomal protein L2



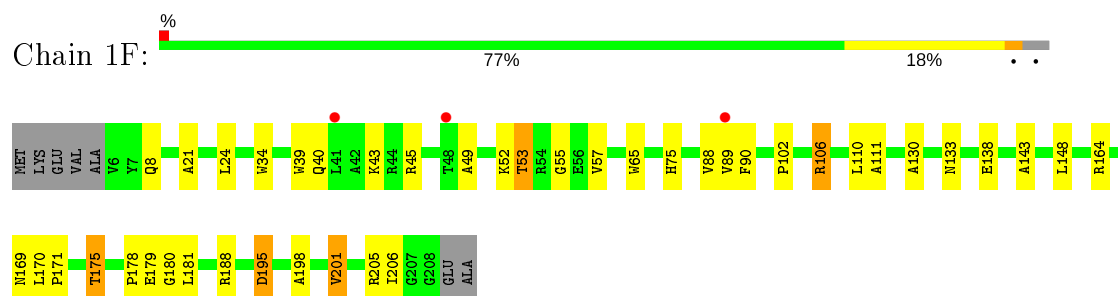
• Molecule 4: 50S ribosomal protein L3



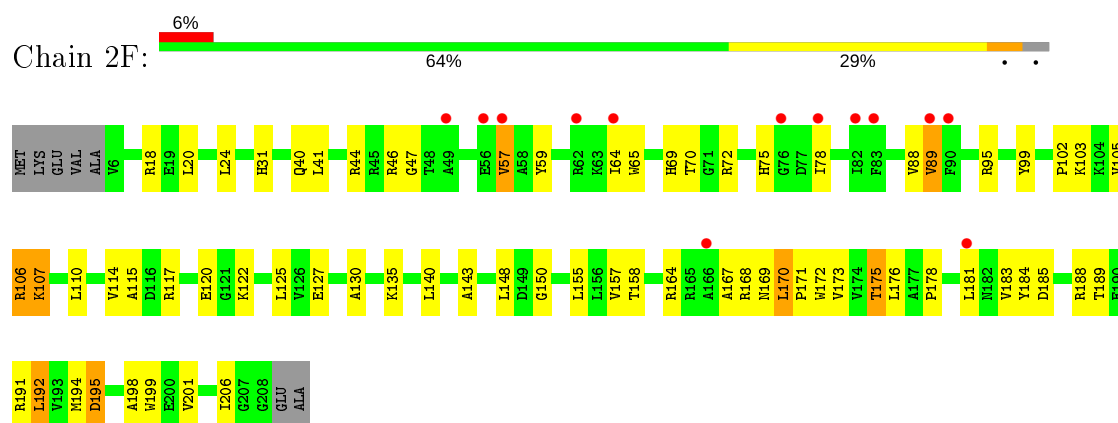
• Molecule 4: 50S ribosomal protein L3



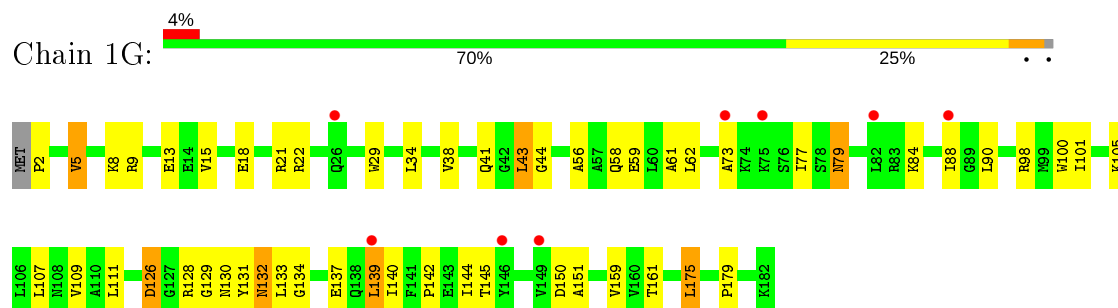
- Molecule 5: 50S ribosomal protein L4



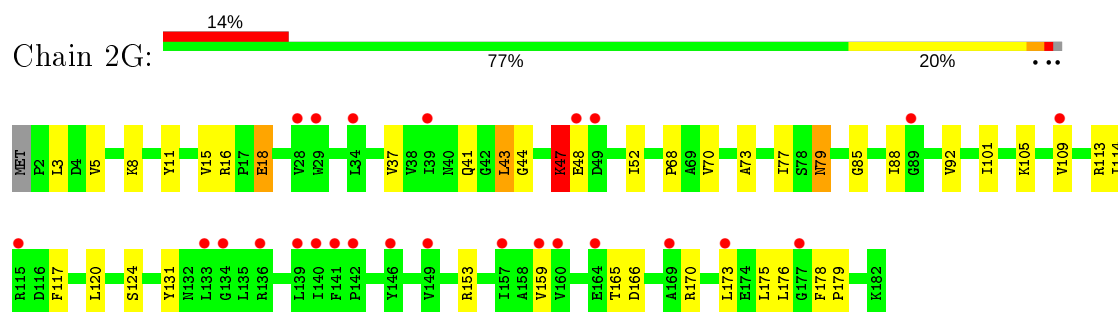
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

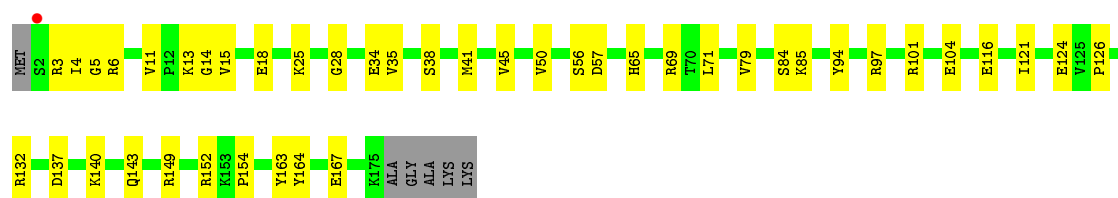


- Molecule 6: 50S ribosomal protein L5



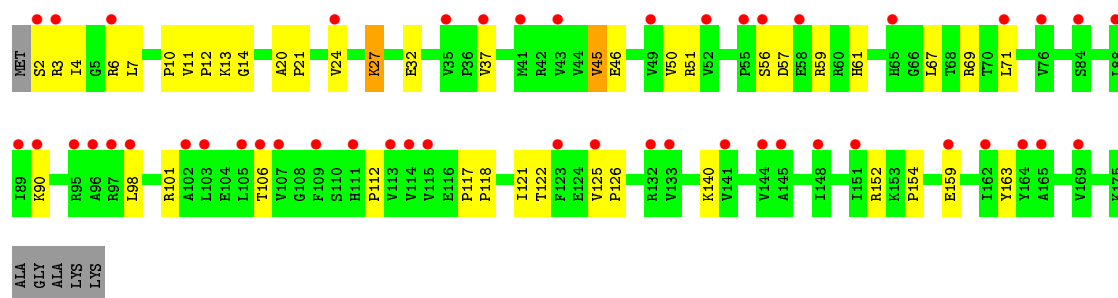
- Molecule 7: 50S ribosomal protein L6





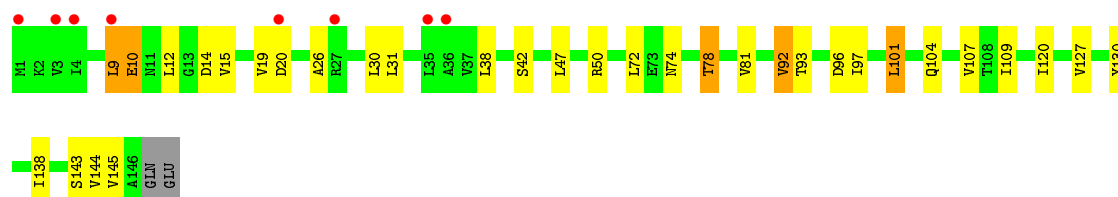
• Molecule 7: 50S ribosomal protein L6

Chain 2H: 27% 73% 23%



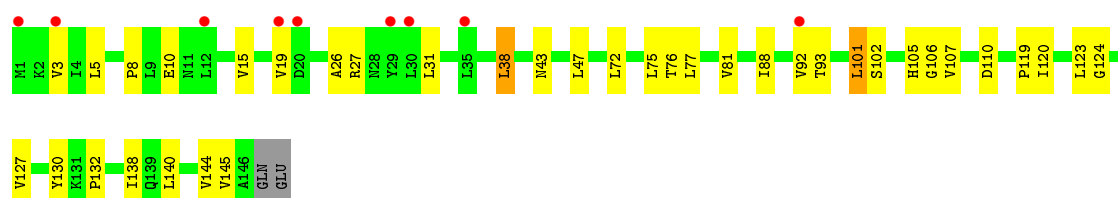
• Molecule 8: 50S ribosomal protein L9

Chain 1I: 5% 76% 19%



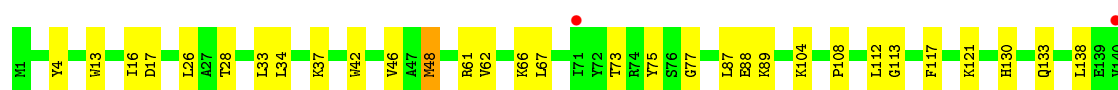
• Molecule 8: 50S ribosomal protein L9

Chain 2I: 6% 74% 24%

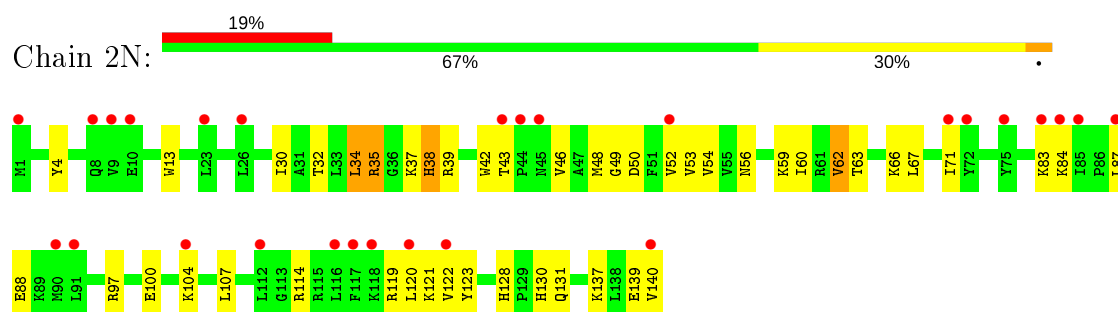


• Molecule 9: 50S ribosomal protein L13

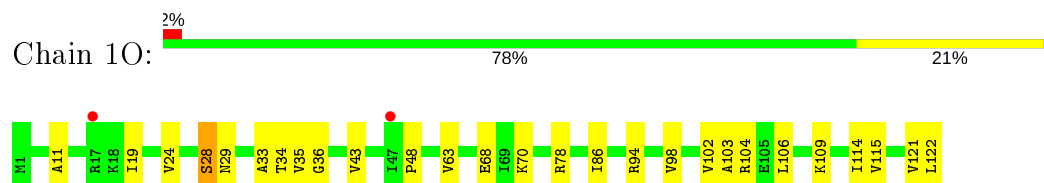
Chain 1N: 78% 21%



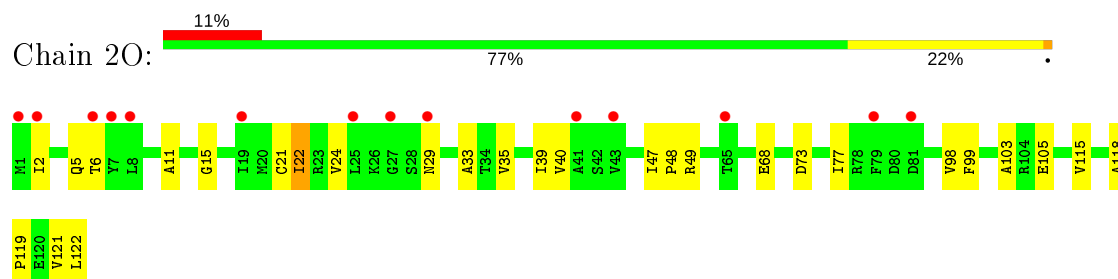
• Molecule 9: 50S ribosomal protein L13



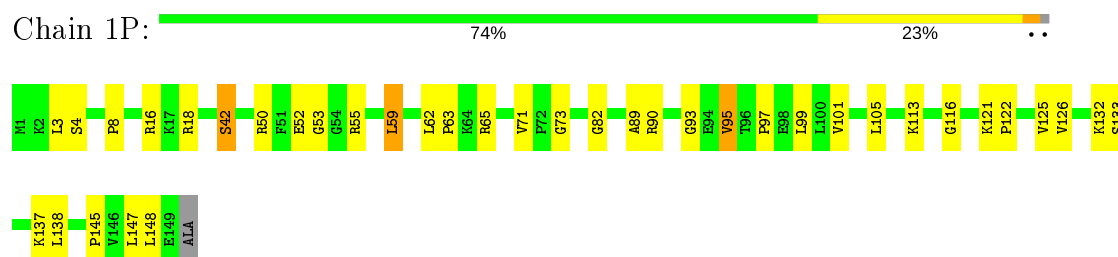
- Molecule 10: 50S ribosomal protein L14



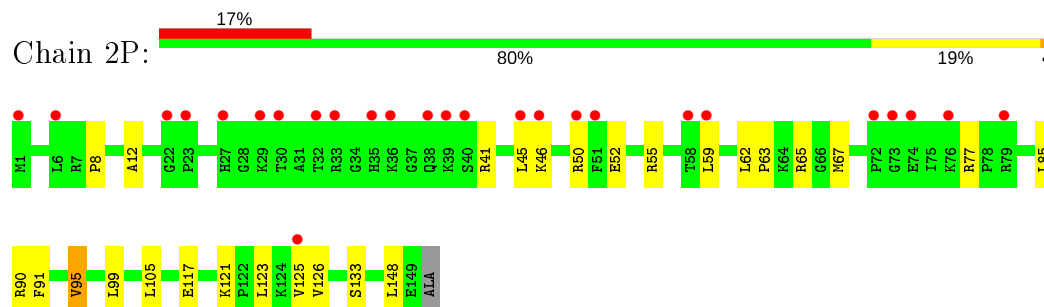
- Molecule 10: 50S ribosomal protein L14



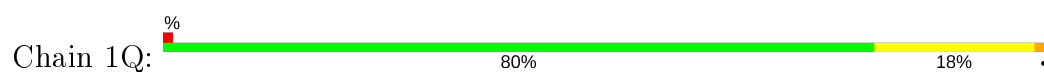
- Molecule 11: 50S ribosomal protein L15



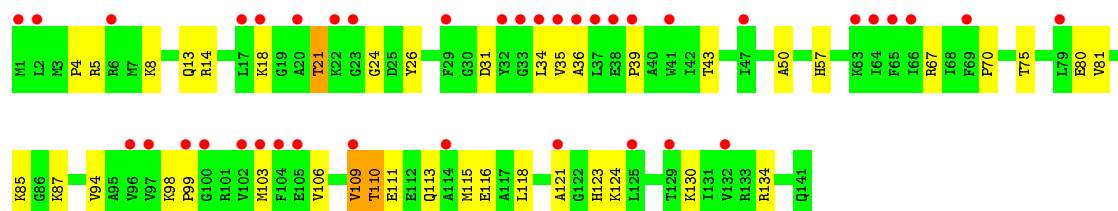
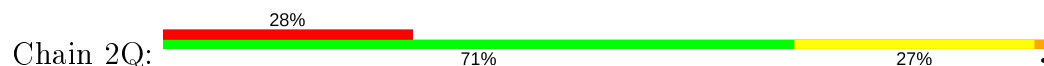
- Molecule 11: 50S ribosomal protein L15



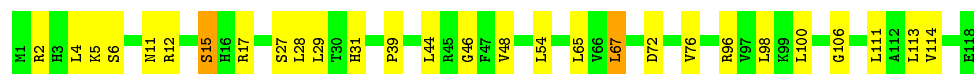
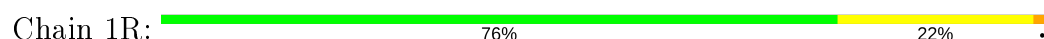
- Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16



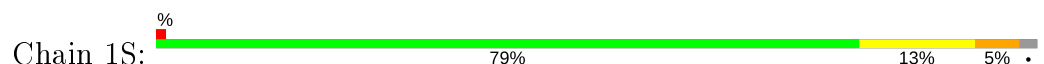
• Molecule 13: 50S ribosomal protein L17



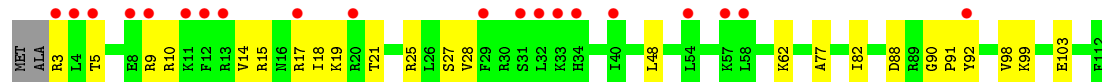
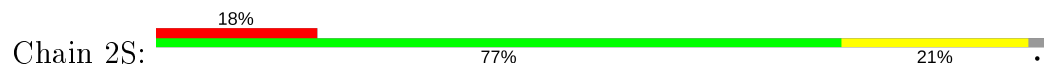
• Molecule 13: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L18

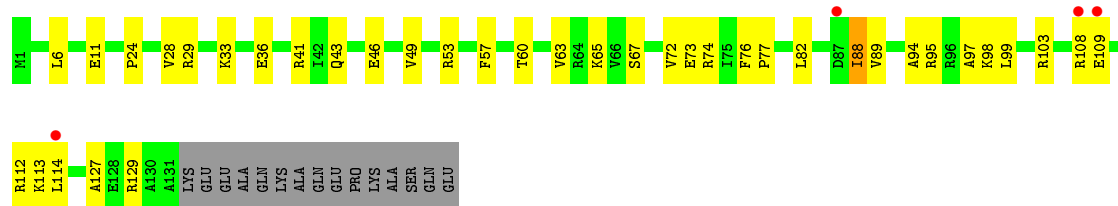


• Molecule 14: 50S ribosomal protein L18

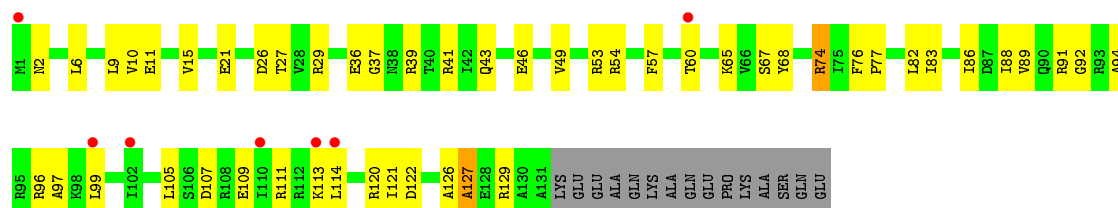


• Molecule 15: 50S ribosomal protein L19

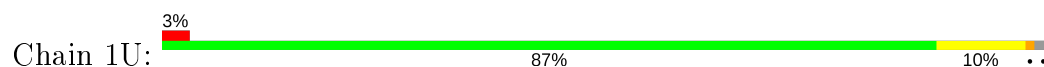




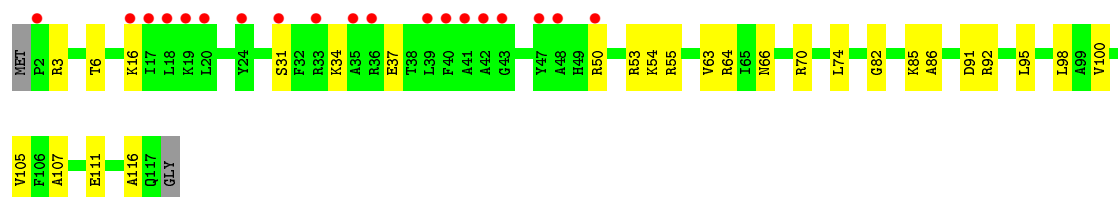
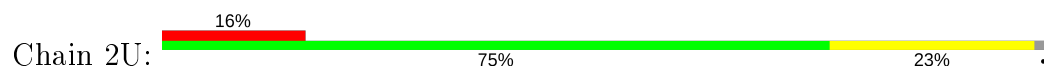
- Molecule 15: 50S ribosomal protein L19



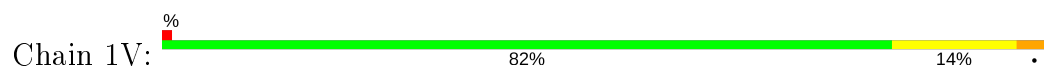
- Molecule 16: 50S ribosomal protein L20



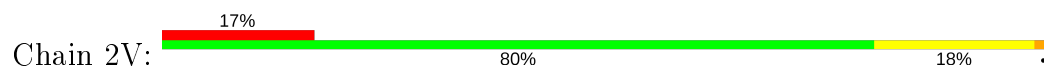
- Molecule 16: 50S ribosomal protein L20



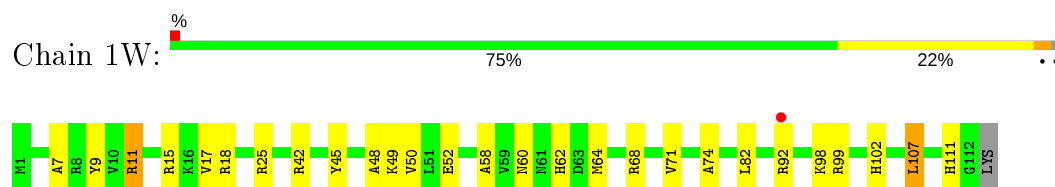
- Molecule 17: 50S ribosomal protein L21



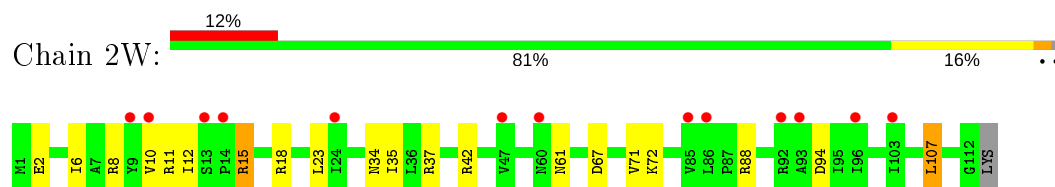
- Molecule 17: 50S ribosomal protein L21



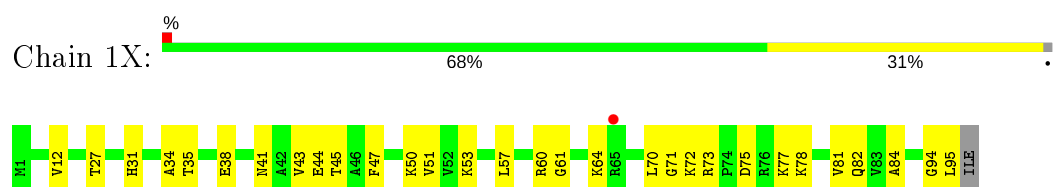
- Molecule 18: 50S ribosomal protein L22



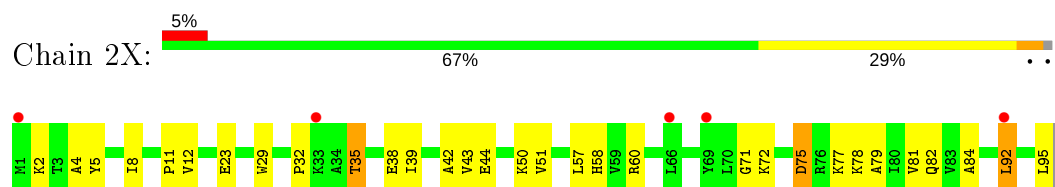
- Molecule 18: 50S ribosomal protein L22



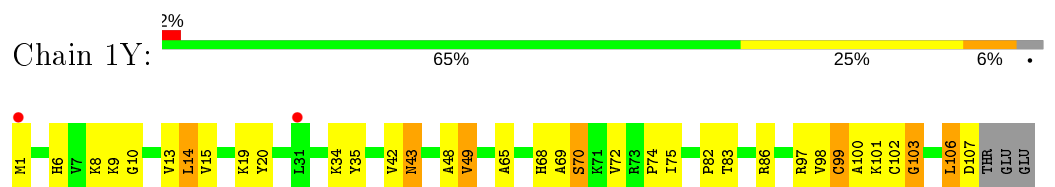
- Molecule 19: 50S ribosomal protein L23



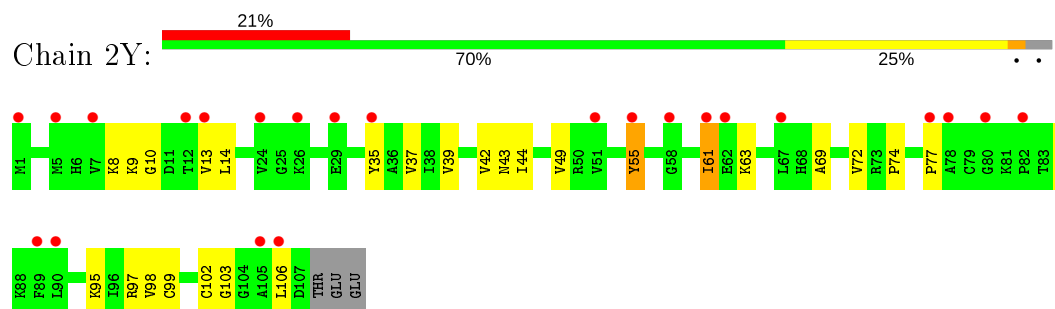
- Molecule 19: 50S ribosomal protein L23



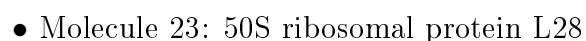
- Molecule 20: 50S ribosomal protein L24

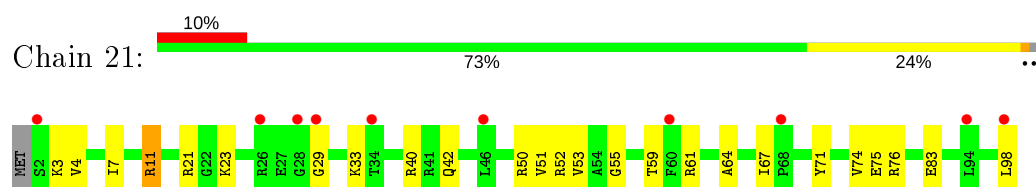


- Molecule 20: 50S ribosomal protein L24

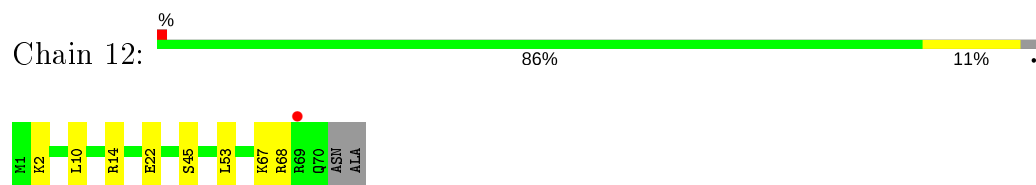


- Molecule 21: 50S ribosomal protein L25

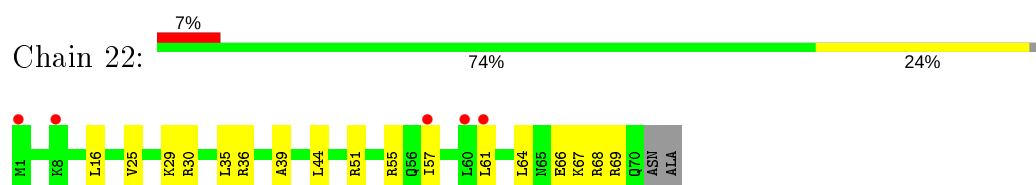




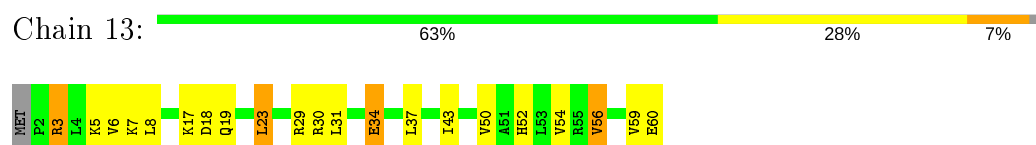
- Molecule 24: 50S ribosomal protein L29



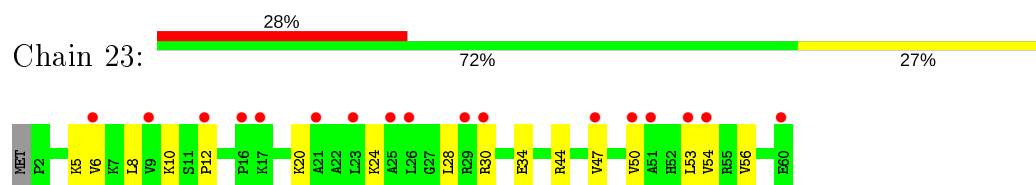
- Molecule 24: 50S ribosomal protein L29



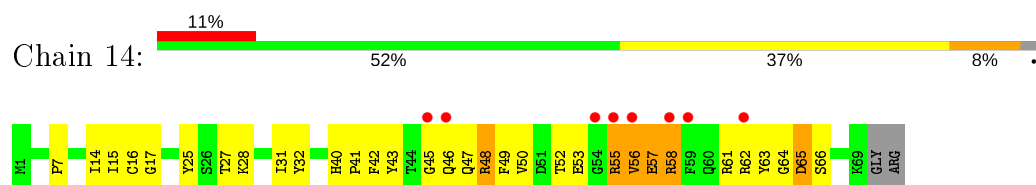
- Molecule 25: 50S ribosomal protein L30



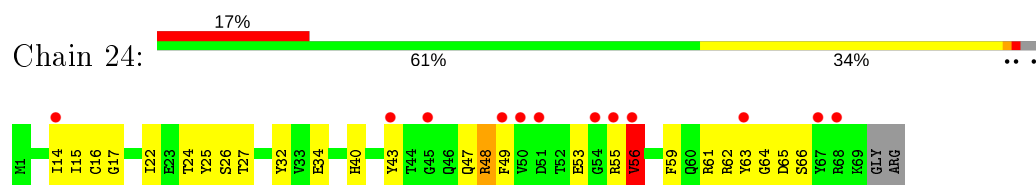
- Molecule 25: 50S ribosomal protein L30



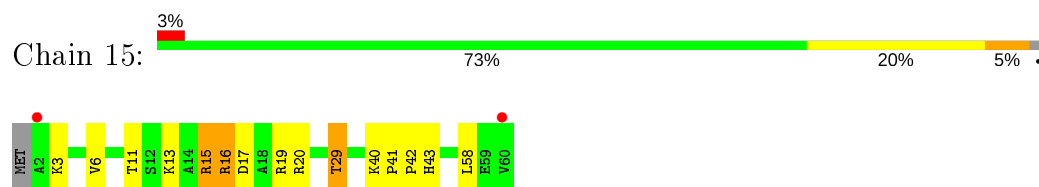
- Molecule 26: 50S ribosomal protein L31



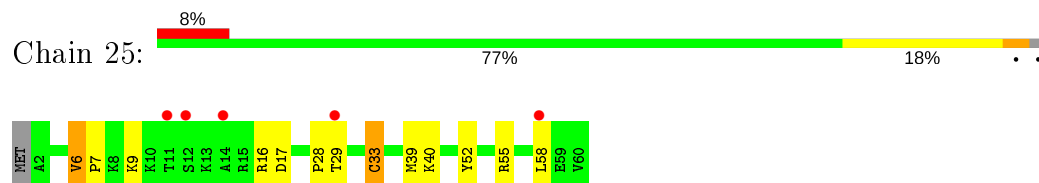
- Molecule 26: 50S ribosomal protein L31



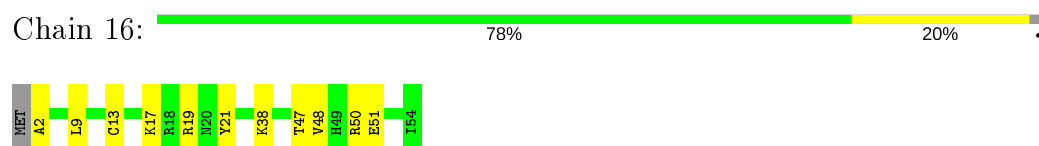
• Molecule 27: 50S ribosomal protein L32



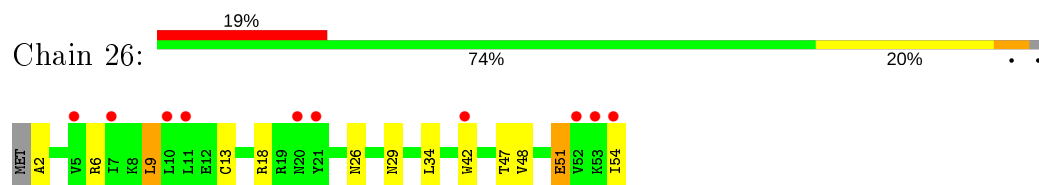
• Molecule 27: 50S ribosomal protein L32



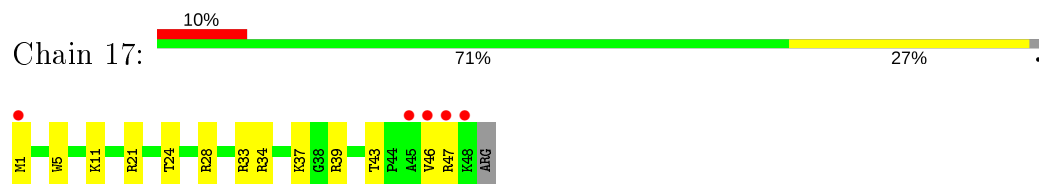
• Molecule 28: 50S ribosomal protein L33



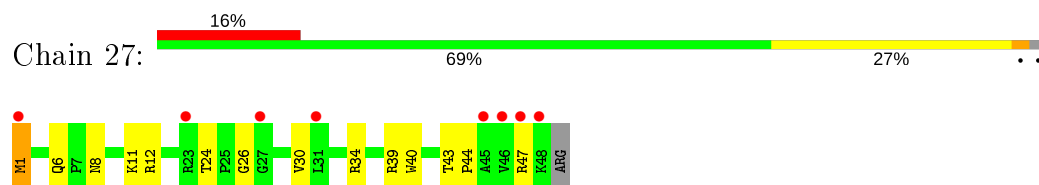
• Molecule 28: 50S ribosomal protein L33



• Molecule 29: 50S ribosomal protein L34



• Molecule 29: 50S ribosomal protein L34

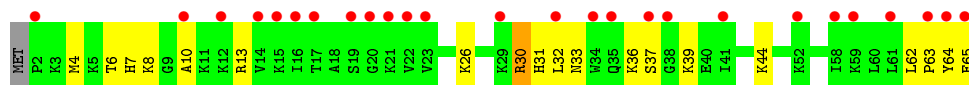
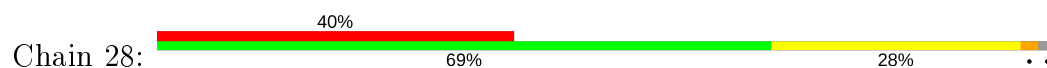


• Molecule 30: 50S ribosomal protein L35





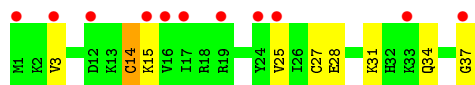
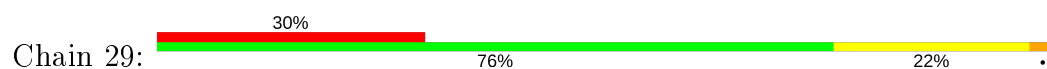
- Molecule 30: 50S ribosomal protein L35



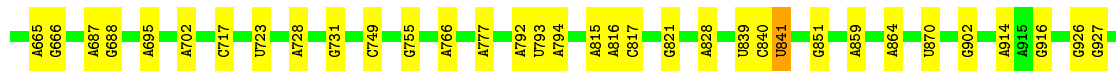
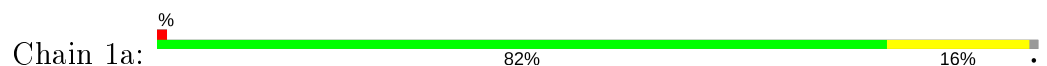
- Molecule 31: 50S ribosomal protein L36

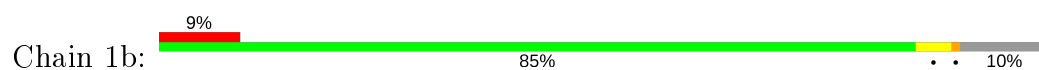


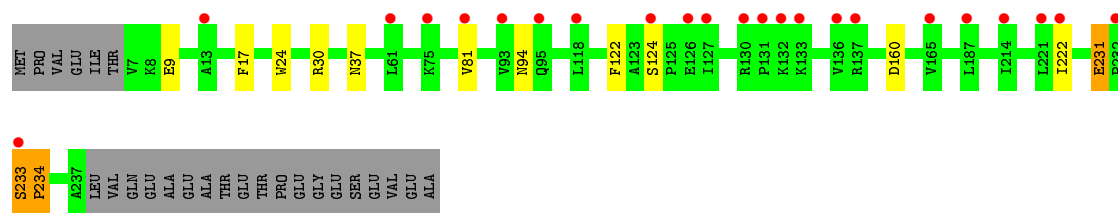
- Molecule 31: 50S ribosomal protein L36



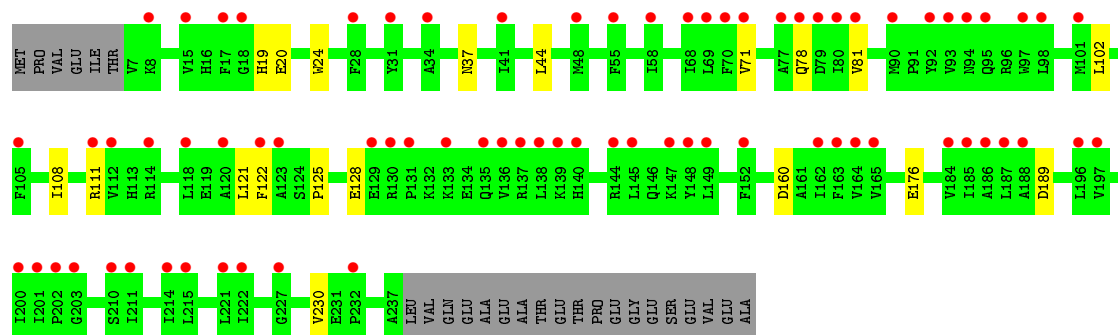
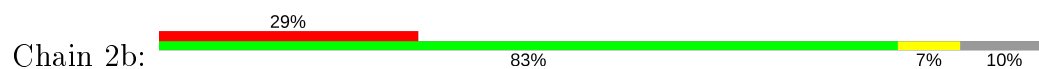
- Molecule 32: 16S Ribosomal RNA



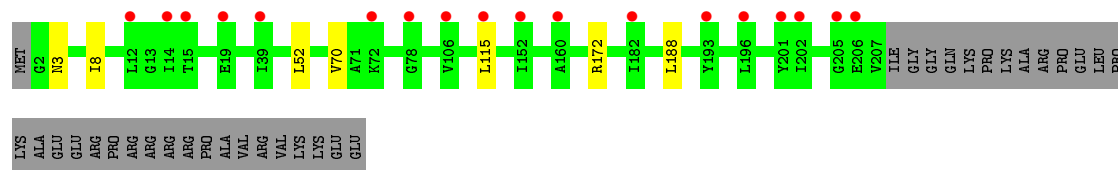
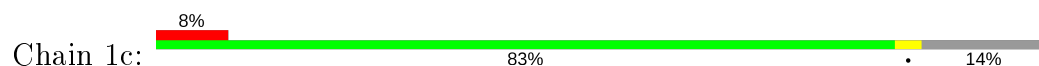




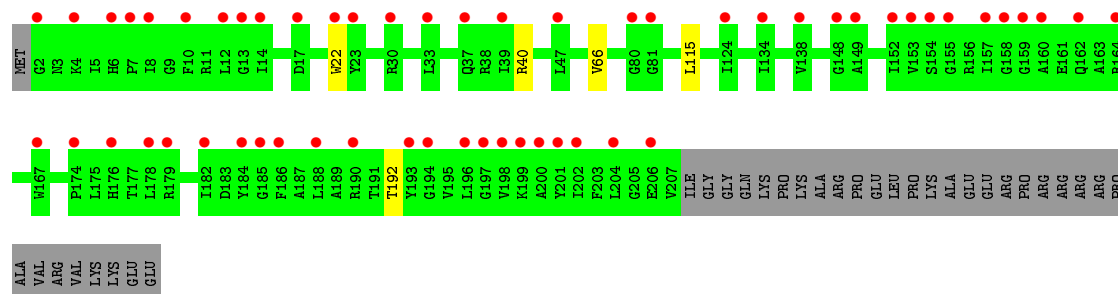
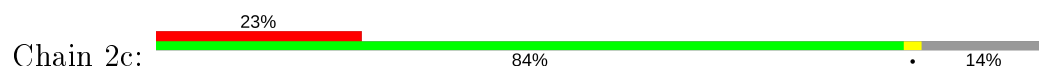
• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3

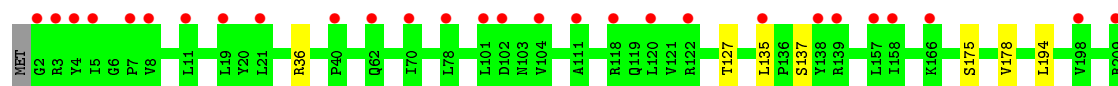


• Molecule 34: 30S ribosomal protein S3

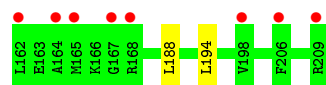
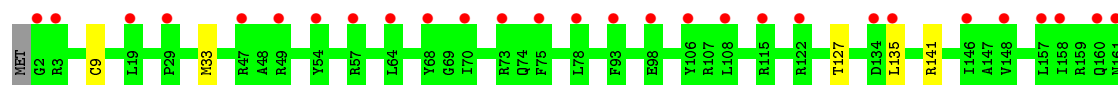


• Molecule 35: 30S ribosomal protein S4

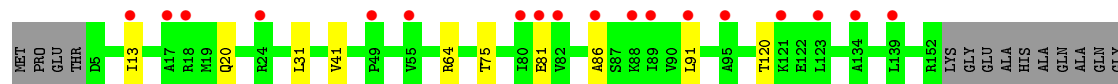
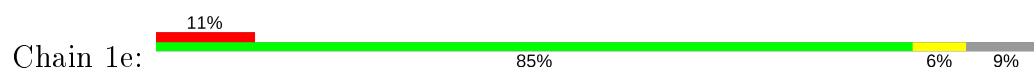




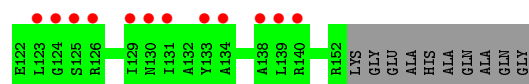
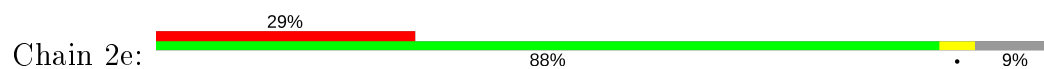
- Molecule 35: 30S ribosomal protein S4



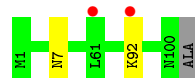
- Molecule 36: 30S ribosomal protein S5



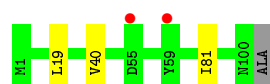
- Molecule 36: 30S ribosomal protein S5



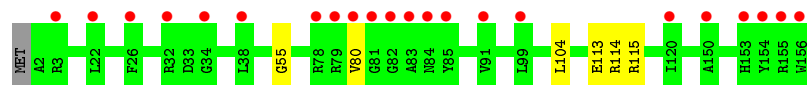
- Molecule 37: 30S ribosomal protein S6



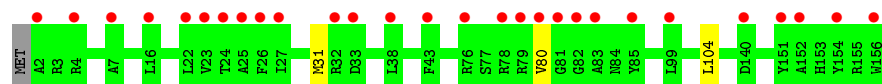
- Molecule 37: 30S ribosomal protein S6



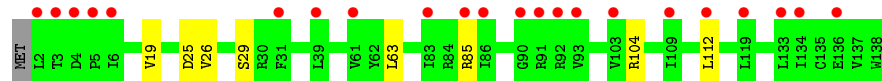
- Molecule 38: 30S ribosomal protein S7



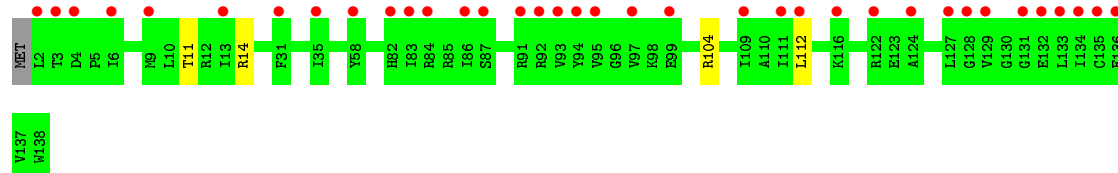
- Molecule 38: 30S ribosomal protein S7



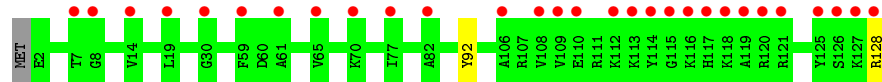
- Molecule 39: 30S ribosomal protein S8



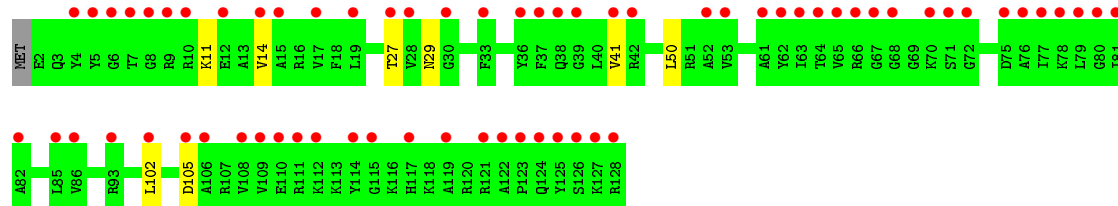
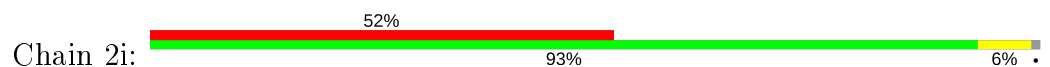
- Molecule 39: 30S ribosomal protein S8



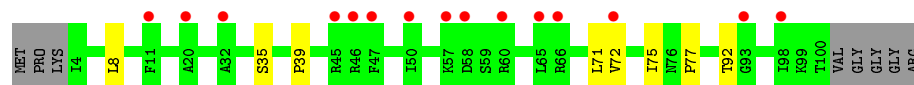
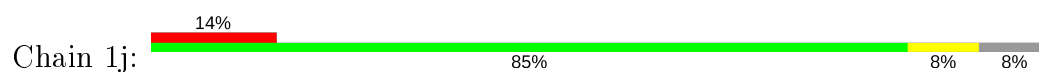
- Molecule 40: 30S ribosomal protein S9



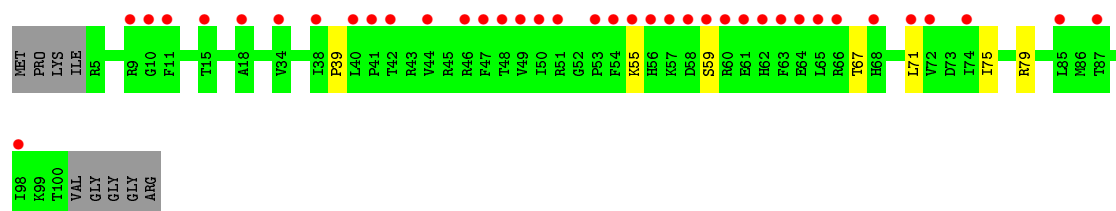
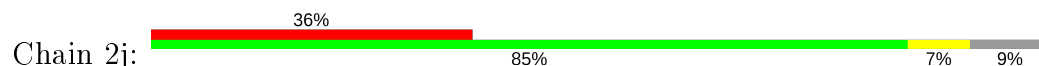
- Molecule 40: 30S ribosomal protein S9



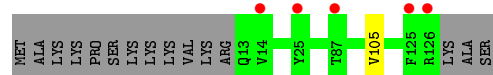
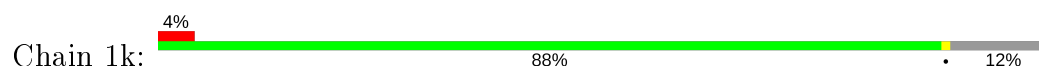
- Molecule 41: 30S ribosomal protein S10



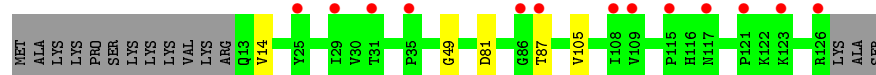
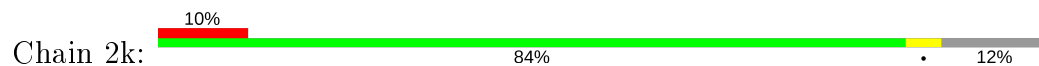
- Molecule 41: 30S ribosomal protein S10



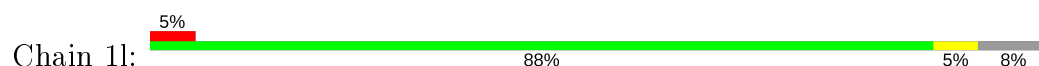
- Molecule 42: 30S ribosomal protein S11



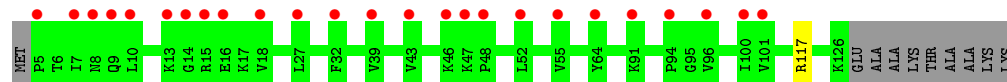
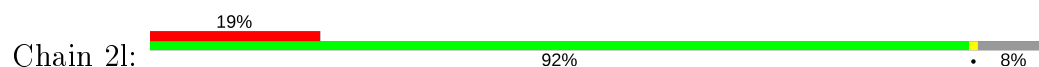
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

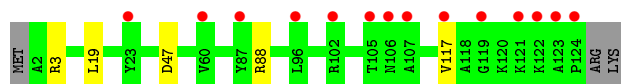


- Molecule 43: 30S ribosomal protein S12

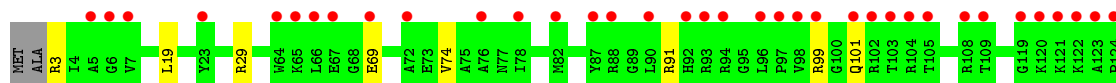


- Molecule 44: 30S ribosomal protein S13

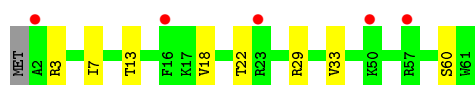
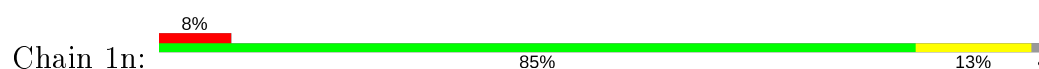




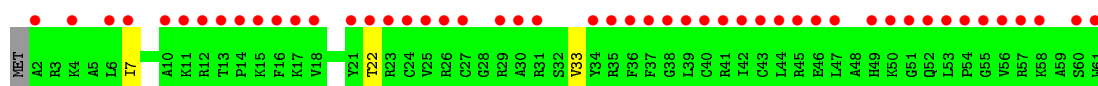
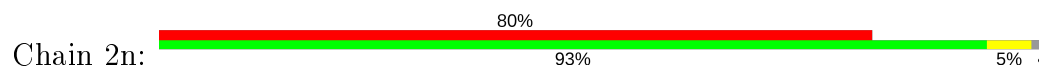
- Molecule 44: 30S ribosomal protein S13



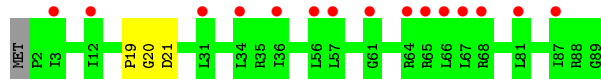
- Molecule 45: 30S ribosomal protein S14 type Z



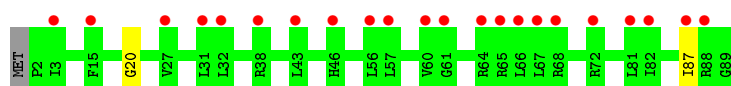
- Molecule 45: 30S ribosomal protein S14 type Z



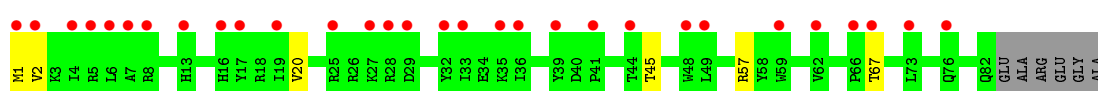
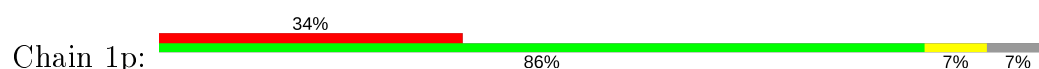
- Molecule 46: 30S ribosomal protein S15



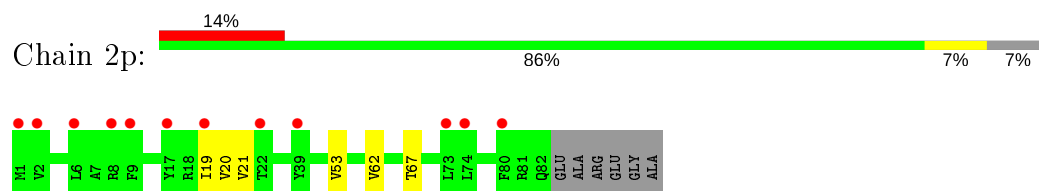
- Molecule 46: 30S ribosomal protein S15



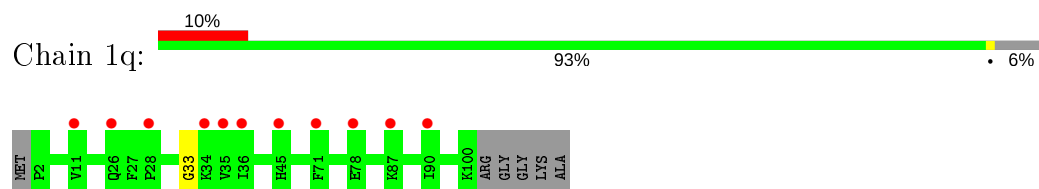
- Molecule 47: 30S ribosomal protein S16



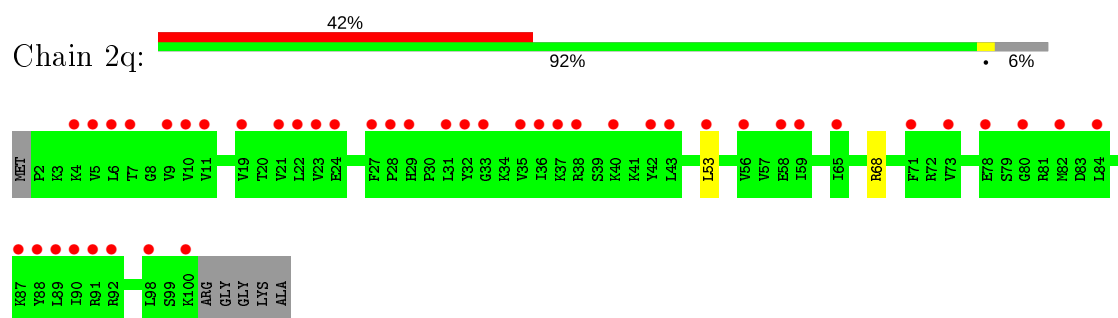
- Molecule 47: 30S ribosomal protein S16



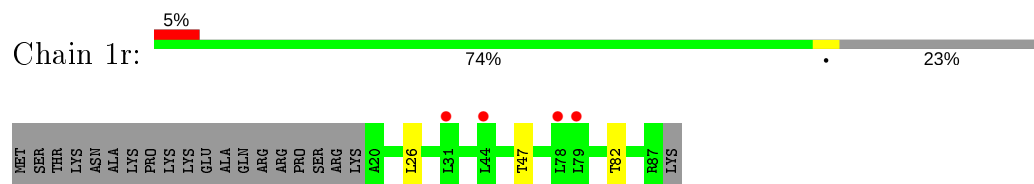
- Molecule 48: 30S ribosomal protein S17



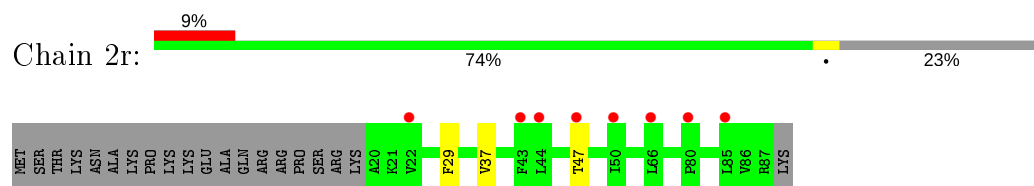
- Molecule 48: 30S ribosomal protein S17



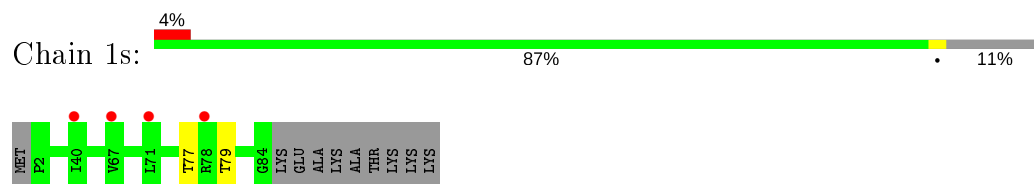
- Molecule 49: 30S ribosomal protein S18



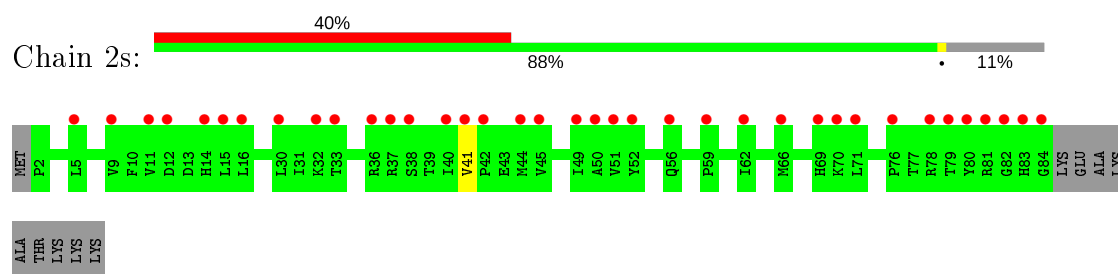
- Molecule 49: 30S ribosomal protein S18



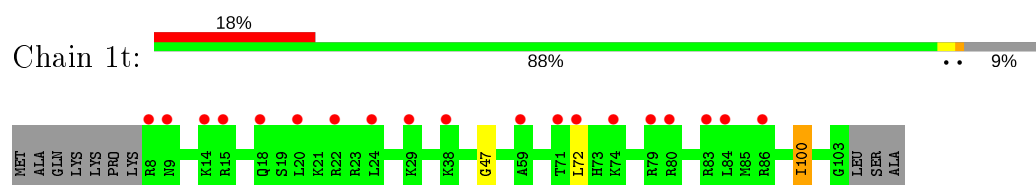
- Molecule 50: 30S ribosomal protein S19



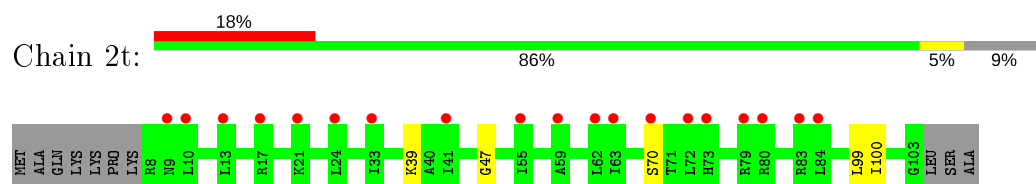
- Molecule 50: 30S ribosomal protein S19



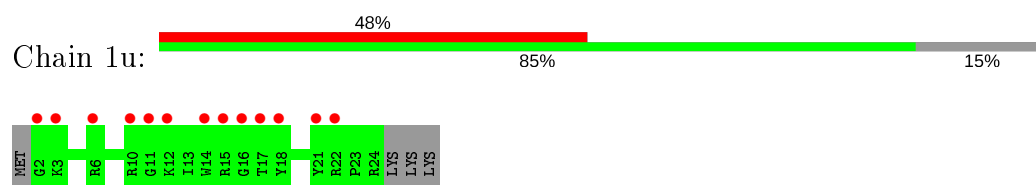
- Molecule 51: 30S ribosomal protein S20



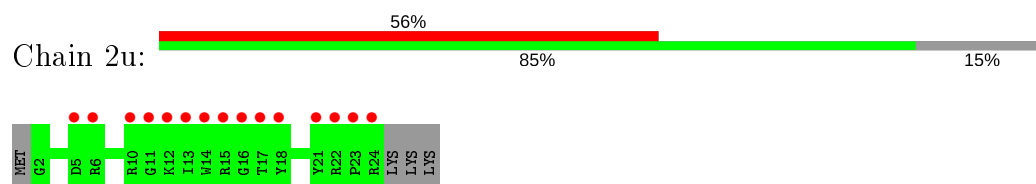
- Molecule 51: 30S ribosomal protein S20



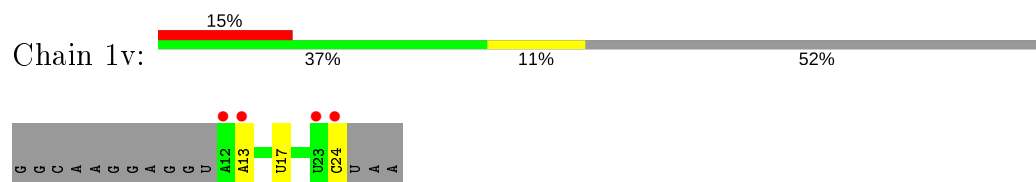
- Molecule 52: 30S ribosomal protein Thx



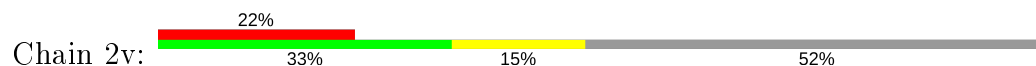
- Molecule 52: 30S ribosomal protein Thx

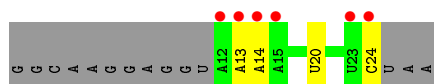


- Molecule 53: mRNA



- Molecule 53: mRNA

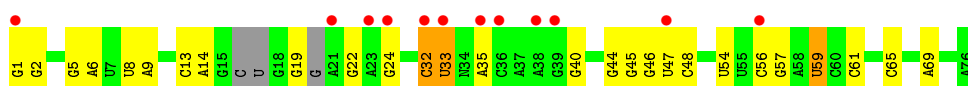




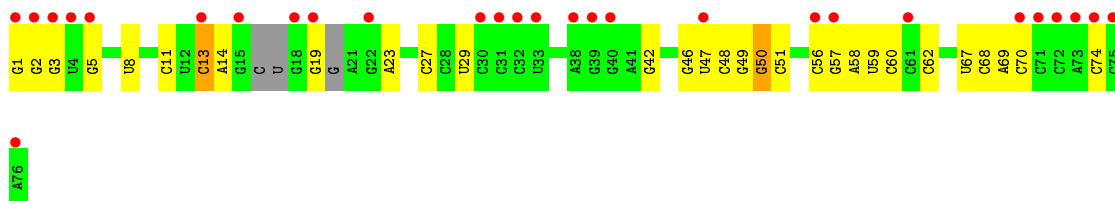
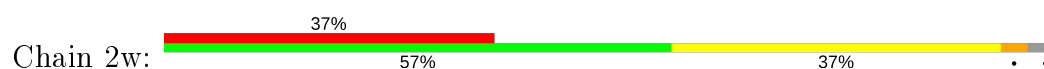
- Molecule 54: A-site and E-site tRNAs



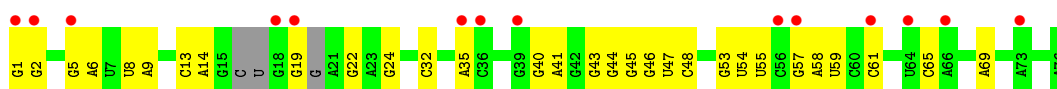
- Molecule 54: A-site and E-site tRNAs



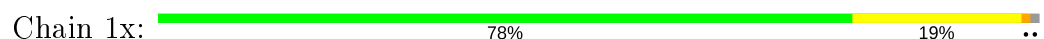
- Molecule 54: A-site and E-site tRNAs



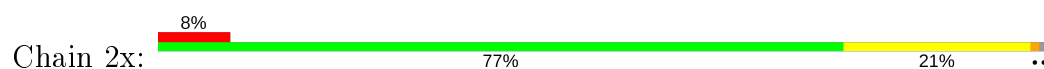
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 209.02Å 447.76Å 618.39Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 254.43 – 2.75 309.19 – 2.75 | Depositor EDS |
| % Data completeness (in resolution range) | 99.5 (254.43-2.75) 99.5 (309.19-2.75) | Depositor EDS |
| R_{merge} | 0.21 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.16 (at 2.73Å) | Xtriage |
| Refinement program | PHENIX 1.8.2 | Depositor |
| R, R_{free} | 0.235 , 0.284 0.236 , 0.284 | Depositor DCC |
| R_{free} test set | 74125 reflections (5.03%) | 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) | 0.28 , 52.5 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.88 | 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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 1A | 0.34 | 0/69011 | 0.82 | 22/107720 (0.0%) |
| 1 | 2A | 0.26 | 0/67295 | 0.79 | 28/105042 (0.0%) |
| 2 | 1B | 0.34 | 1/2882 (0.0%) | 0.76 | 0/4494 |
| 2 | 2B | 0.30 | 1/2879 (0.0%) | 0.77 | 1/4487 (0.0%) |
| 3 | 1D | 0.29 | 0/2186 | 0.52 | 0/2944 |
| 3 | 2D | 0.27 | 0/2186 | 0.49 | 0/2944 |
| 4 | 1E | 0.30 | 0/1592 | 0.48 | 0/2149 |
| 4 | 2E | 0.26 | 0/1592 | 0.47 | 0/2149 |
| 5 | 1F | 0.28 | 0/1619 | 0.47 | 0/2193 |
| 5 | 2F | 0.26 | 0/1615 | 0.44 | 0/2188 |
| 6 | 1G | 0.27 | 0/1448 | 0.45 | 0/1957 |
| 6 | 2G | 0.26 | 0/1453 | 0.46 | 0/1963 |
| 7 | 1H | 0.27 | 0/1356 | 0.45 | 0/1834 |
| 7 | 2H | 0.25 | 0/1356 | 0.43 | 0/1834 |
| 8 | 1I | 0.26 | 0/1112 | 0.45 | 0/1514 |
| 8 | 2I | 0.25 | 0/1079 | 0.44 | 0/1475 |
| 9 | 1N | 0.27 | 0/1144 | 0.46 | 0/1543 |
| 9 | 2N | 0.25 | 0/1144 | 0.43 | 0/1543 |
| 10 | 1O | 0.31 | 0/943 | 0.49 | 0/1269 |
| 10 | 2O | 0.28 | 0/943 | 0.48 | 0/1269 |
| 11 | 1P | 0.28 | 0/1152 | 0.48 | 0/1533 |
| 11 | 2P | 0.26 | 0/1152 | 0.46 | 0/1533 |
| 12 | 1Q | 0.32 | 0/1143 | 0.47 | 0/1527 |
| 12 | 2Q | 0.26 | 0/1143 | 0.45 | 0/1527 |
| 13 | 1R | 0.28 | 0/982 | 0.46 | 0/1312 |
| 13 | 2R | 0.24 | 0/982 | 0.46 | 0/1312 |
| 14 | 1S | 0.26 | 0/883 | 0.45 | 0/1176 |
| 14 | 2S | 0.26 | 0/880 | 0.43 | 0/1172 |
| 15 | 1T | 0.28 | 0/1105 | 0.47 | 0/1477 |
| 15 | 2T | 0.26 | 0/1097 | 0.44 | 0/1468 |
| 16 | 1U | 0.30 | 0/977 | 0.43 | 0/1301 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | 2U | 0.26 | 0/977 | 0.41 | 0/1301 |
| 17 | 1V | 0.29 | 0/782 | 0.49 | 0/1049 |
| 17 | 2V | 0.27 | 0/782 | 0.50 | 0/1049 |
| 18 | 1W | 0.29 | 0/897 | 0.46 | 0/1205 |
| 18 | 2W | 0.26 | 0/897 | 0.42 | 0/1205 |
| 19 | 1X | 0.30 | 0/764 | 0.51 | 0/1025 |
| 19 | 2X | 0.26 | 0/764 | 0.46 | 0/1025 |
| 20 | 1Y | 0.28 | 0/819 | 0.50 | 0/1095 |
| 20 | 2Y | 0.26 | 0/819 | 0.47 | 0/1095 |
| 21 | 1Z | 0.27 | 0/1267 | 0.48 | 0/1717 |
| 21 | 2Z | 0.26 | 0/1299 | 0.48 | 0/1763 |
| 22 | 10 | 0.29 | 0/662 | 0.48 | 0/881 |
| 22 | 20 | 0.27 | 0/662 | 0.46 | 0/881 |
| 23 | 11 | 0.28 | 0/762 | 0.46 | 0/1014 |
| 23 | 21 | 0.26 | 0/762 | 0.47 | 0/1014 |
| 24 | 12 | 0.27 | 0/590 | 0.41 | 0/781 |
| 24 | 22 | 0.25 | 0/590 | 0.38 | 0/781 |
| 25 | 13 | 0.28 | 0/474 | 0.46 | 0/635 |
| 25 | 23 | 0.24 | 0/469 | 0.43 | 0/630 |
| 26 | 14 | 0.30 | 0/565 | 0.55 | 0/761 |
| 26 | 24 | 0.26 | 0/545 | 0.50 | 0/737 |
| 27 | 15 | 0.29 | 0/469 | 0.51 | 0/635 |
| 27 | 25 | 0.29 | 0/469 | 0.47 | 0/635 |
| 28 | 16 | 0.28 | 0/460 | 0.48 | 0/613 |
| 28 | 26 | 0.26 | 0/456 | 0.46 | 0/608 |
| 29 | 17 | 0.26 | 0/426 | 0.47 | 0/561 |
| 29 | 27 | 0.25 | 0/426 | 0.45 | 0/561 |
| 30 | 18 | 0.28 | 0/525 | 0.48 | 0/691 |
| 30 | 28 | 0.25 | 0/525 | 0.45 | 0/691 |
| 31 | 19 | 0.29 | 0/310 | 0.47 | 0/407 |
| 31 | 29 | 0.24 | 0/310 | 0.47 | 0/407 |
| 32 | 1a | 0.26 | 0/35795 | 0.80 | 19/55864 (0.0%) |
| 32 | 2a | 0.26 | 2/35886 (0.0%) | 0.84 | 47/56005 (0.1%) |
| 33 | 1b | 0.32 | 0/1881 | 0.50 | 2/2542 (0.1%) |
| 33 | 2b | 0.26 | 0/1860 | 0.44 | 0/2518 |
| 34 | 1c | 0.26 | 0/1572 | 0.45 | 0/2126 |
| 34 | 2c | 0.25 | 0/1566 | 0.44 | 0/2119 |
| 35 | 1d | 0.29 | 1/1685 (0.1%) | 0.42 | 0/2262 |
| 35 | 2d | 0.27 | 0/1704 | 0.42 | 0/2284 |
| 36 | 1e | 0.26 | 0/1145 | 0.46 | 0/1543 |
| 36 | 2e | 0.26 | 0/1149 | 0.47 | 0/1548 |
| 37 | 1f | 0.25 | 0/823 | 0.43 | 0/1115 |
| 37 | 2f | 0.26 | 0/829 | 0.44 | 0/1123 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | 1g | 0.26 | 0/1250 | 0.41 | 0/1679 |
| 38 | 2g | 0.25 | 0/1254 | 0.39 | 0/1683 |
| 39 | 1h | 0.26 | 0/1108 | 0.45 | 0/1494 |
| 39 | 2h | 0.25 | 0/1108 | 0.44 | 0/1494 |
| 40 | 1i | 0.26 | 0/1002 | 0.47 | 0/1346 |
| 40 | 2i | 0.26 | 0/997 | 0.46 | 0/1343 |
| 41 | 1j | 0.24 | 0/722 | 0.45 | 0/982 |
| 41 | 2j | 0.26 | 0/727 | 0.46 | 0/988 |
| 42 | 1k | 0.25 | 0/844 | 0.44 | 0/1145 |
| 42 | 2k | 0.26 | 0/848 | 0.45 | 0/1149 |
| 43 | 1l | 0.26 | 0/937 | 0.48 | 0/1260 |
| 43 | 2l | 0.26 | 0/937 | 0.48 | 0/1260 |
| 44 | 1m | 0.25 | 0/969 | 0.45 | 0/1302 |
| 44 | 2m | 0.26 | 0/961 | 0.46 | 0/1291 |
| 45 | 1n | 0.26 | 0/501 | 0.43 | 0/664 |
| 45 | 2n | 0.27 | 0/501 | 0.42 | 0/664 |
| 46 | 1o | 0.25 | 0/739 | 0.41 | 0/985 |
| 46 | 2o | 0.23 | 0/739 | 0.43 | 0/985 |
| 47 | 1p | 0.25 | 0/697 | 0.46 | 0/939 |
| 47 | 2p | 0.25 | 0/693 | 0.46 | 0/935 |
| 48 | 1q | 0.24 | 0/836 | 0.45 | 0/1117 |
| 48 | 2q | 0.25 | 0/836 | 0.44 | 0/1117 |
| 49 | 1r | 0.24 | 0/560 | 0.43 | 0/746 |
| 49 | 2r | 0.24 | 0/560 | 0.42 | 0/746 |
| 50 | 1s | 0.26 | 0/667 | 0.50 | 0/900 |
| 50 | 2s | 0.27 | 0/661 | 0.51 | 0/893 |
| 51 | 1t | 0.25 | 0/730 | 0.43 | 0/965 |
| 51 | 2t | 0.25 | 0/729 | 0.42 | 0/965 |
| 52 | 1u | 0.24 | 0/203 | 0.43 | 0/266 |
| 52 | 2u | 0.23 | 0/203 | 0.45 | 0/266 |
| 53 | 1v | 0.36 | 0/308 | 0.95 | 2/477 (0.4%) |
| 53 | 2v | 0.30 | 0/308 | 0.82 | 0/477 |
| 54 | 1w | 0.67 | 5/1600 (0.3%) | 1.24 | 11/2482 (0.4%) |
| 54 | 1y | 0.66 | 5/1600 (0.3%) | 1.20 | 15/2482 (0.6%) |
| 54 | 2w | 0.45 | 1/1600 (0.1%) | 1.06 | 4/2482 (0.2%) |
| 54 | 2y | 0.44 | 1/1600 (0.1%) | 0.96 | 1/2482 (0.0%) |
| 55 | 1x | 0.40 | 0/1725 | 1.03 | 9/2689 (0.3%) |
| 55 | 2x | 0.36 | 0/1725 | 1.03 | 9/2689 (0.3%) |
| All | All | 0.29 | 17/316735 (0.0%) | 0.74 | 170/474180 (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 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 54 | 1w | 59 | U | C4-O4 | 13.16 | 1.34 | 1.23 |
| 54 | 1y | 59 | U | C4-O4 | 13.03 | 1.34 | 1.23 |
| 54 | 1y | 32 | C | C4-N4 | -11.30 | 1.23 | 1.33 |
| 54 | 1w | 60 | C | C4-N4 | -11.27 | 1.23 | 1.33 |
| 54 | 1w | 1 | G | OP3-P | -10.52 | 1.48 | 1.61 |
| 54 | 2w | 1 | G | OP3-P | -10.52 | 1.48 | 1.61 |
| 2 | 2B | 1 | U | OP3-P | -10.49 | 1.48 | 1.61 |
| 54 | 1y | 1 | G | OP3-P | -10.43 | 1.48 | 1.61 |
| 54 | 2y | 1 | G | OP3-P | -10.43 | 1.48 | 1.61 |
| 2 | 1B | 1 | U | OP3-P | -10.17 | 1.49 | 1.61 |
| 32 | 2a | 1272 | G | C6-N1 | -8.23 | 1.33 | 1.39 |
| 32 | 2a | 1272 | G | N1-C2 | -7.84 | 1.31 | 1.37 |
| 54 | 1y | 32 | C | N3-C4 | 6.75 | 1.38 | 1.33 |
| 54 | 1w | 60 | C | N3-C4 | 6.28 | 1.38 | 1.33 |
| 54 | 1w | 59 | U | N3-C4 | -5.45 | 1.33 | 1.38 |
| 35 | 1d | 36 | ARG | C-N | 5.38 | 1.44 | 1.34 |
| 54 | 1y | 59 | U | N3-C4 | -5.34 | 1.33 | 1.38 |

All (170) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 54 | 1w | 60 | C | N3-C4-C5 | -19.32 | 114.17 | 121.90 |
| 32 | 2a | 1272 | G | N3-C2-N2 | 18.90 | 133.13 | 119.90 |
| 54 | 1y | 32 | C | N3-C4-C5 | -18.38 | 114.55 | 121.90 |
| 32 | 2a | 1263 | C | N1-C2-O2 | 17.46 | 129.37 | 118.90 |
| 32 | 2a | 1272 | G | C5-C6-O6 | 17.13 | 138.88 | 128.60 |
| 54 | 1w | 60 | C | C2-N3-C4 | 15.74 | 127.77 | 119.90 |
| 32 | 2a | 1272 | G | N1-C2-N2 | -15.70 | 102.07 | 116.20 |
| 54 | 1y | 32 | C | C2-N3-C4 | 14.18 | 126.99 | 119.90 |
| 32 | 2a | 1272 | G | C6-N1-C2 | 12.54 | 132.62 | 125.10 |
| 54 | 1y | 59 | U | N3-C4-C5 | 11.66 | 121.60 | 114.60 |
| 54 | 1w | 59 | U | N3-C4-C5 | 11.55 | 121.53 | 114.60 |
| 54 | 1y | 59 | U | C2-N3-C4 | -11.48 | 120.11 | 127.00 |
| 54 | 1w | 59 | U | C2-N3-C4 | -11.33 | 120.20 | 127.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-----------|--------|-------------|----------|
| 32 | 2a | 1263 | C | C2-N3-C4 | 11.22 | 125.51 | 119.90 |
| 32 | 2a | 1272 | G | C5-C6-N1 | -10.71 | 106.14 | 111.50 |
| 32 | 2a | 1263 | C | C5-C6-N1 | 10.21 | 126.11 | 121.00 |
| 54 | 1w | 60 | C | N1-C2-O2 | 10.05 | 124.93 | 118.90 |
| 1 | 2A | 2136 | C | N1-C2-O2 | 9.57 | 124.64 | 118.90 |
| 32 | 2a | 1263 | C | N3-C2-O2 | -9.42 | 115.31 | 121.90 |
| 1 | 1A | 1086 | A | N1-C6-N6 | -8.84 | 113.30 | 118.60 |
| 54 | 1y | 59 | U | C5-C4-O4 | -8.60 | 120.74 | 125.90 |
| 54 | 1w | 60 | C | C5-C4-N4 | 8.58 | 126.20 | 120.20 |
| 32 | 2a | 1158 | C | C2-N1-C1' | 8.57 | 128.23 | 118.80 |
| 32 | 2a | 1272 | G | N1-C6-O6 | -8.23 | 114.96 | 119.90 |
| 32 | 2a | 1158 | C | N1-C2-O2 | 8.23 | 123.84 | 118.90 |
| 54 | 1w | 59 | U | C5-C4-O4 | -8.21 | 120.97 | 125.90 |
| 32 | 1a | 1030(B) | C | C2-N1-C1' | 8.04 | 127.64 | 118.80 |
| 54 | 1w | 59 | U | N1-C2-N3 | 7.99 | 119.69 | 114.90 |
| 54 | 1y | 32 | C | C5-C4-N4 | 7.98 | 125.79 | 120.20 |
| 54 | 1y | 59 | U | N1-C2-N3 | 7.93 | 119.66 | 114.90 |
| 32 | 2a | 1272 | G | C2-N3-C4 | -7.91 | 107.94 | 111.90 |
| 54 | 1y | 22 | G | N1-C6-O6 | 7.70 | 124.52 | 119.90 |
| 1 | 1A | 1075 | C | N1-C2-O2 | 7.67 | 123.50 | 118.90 |
| 1 | 1A | 2167 | U | C2-N1-C1' | 7.61 | 126.83 | 117.70 |
| 32 | 2a | 1272 | G | C4-N9-C1' | 7.55 | 136.32 | 126.50 |
| 1 | 1A | 1075 | C | C2-N3-C4 | 7.50 | 123.65 | 119.90 |
| 1 | 2A | 2167 | U | N1-C2-O2 | 7.40 | 127.98 | 122.80 |
| 32 | 2a | 754 | C | C2-N1-C1' | 7.32 | 126.85 | 118.80 |
| 32 | 1a | 1030(B) | C | N1-C2-O2 | 7.31 | 123.28 | 118.90 |
| 32 | 2a | 1263 | C | C6-N1-C2 | -7.24 | 117.40 | 120.30 |
| 1 | 2A | 1313 | U | C2-N1-C1' | 7.23 | 126.38 | 117.70 |
| 32 | 2a | 754 | C | N1-C2-O2 | 7.21 | 123.23 | 118.90 |
| 1 | 1A | 2167 | U | N1-C2-O2 | 7.20 | 127.84 | 122.80 |
| 32 | 2a | 1272 | G | C8-N9-C1' | -7.20 | 117.64 | 127.00 |
| 32 | 1a | 1025 | U | N1-C2-O2 | 7.15 | 127.80 | 122.80 |
| 55 | 2x | 17 | C | N1-C2-O2 | 7.11 | 123.17 | 118.90 |
| 55 | 1x | 46 | G | C6-N1-C2 | -7.10 | 120.84 | 125.10 |
| 32 | 2a | 1263 | C | C2-N1-C1' | 6.98 | 126.48 | 118.80 |
| 32 | 2a | 999 | C | N1-C2-O2 | 6.94 | 123.06 | 118.90 |
| 1 | 1A | 2167 | U | N3-C2-O2 | -6.90 | 117.37 | 122.20 |
| 55 | 2x | 17 | C | C2-N1-C1' | 6.89 | 126.38 | 118.80 |
| 1 | 2A | 2167 | U | C2-N1-C1' | 6.89 | 125.96 | 117.70 |
| 32 | 2a | 1001(A) | G | N3-C4-N9 | 6.85 | 130.11 | 126.00 |
| 32 | 2a | 1039 | C | C5-C4-N4 | -6.85 | 115.41 | 120.20 |
| 1 | 2A | 2167 | U | N3-C2-O2 | -6.78 | 117.46 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 1 | 2A | 2897 | U | C2-N1-C1' | 6.74 | 125.78 | 117.70 |
| 2 | 2B | 80 | U | O4'-C1'-N1 | 6.68 | 113.54 | 108.20 |
| 1 | 1A | 12 | U | C2-N1-C1' | 6.67 | 125.70 | 117.70 |
| 32 | 2a | 1263 | C | C4-C5-C6 | -6.67 | 114.07 | 117.40 |
| 32 | 2a | 1029 | C | N1-C2-O2 | 6.63 | 122.88 | 118.90 |
| 1 | 2A | 2136 | C | N3-C2-O2 | -6.61 | 117.27 | 121.90 |
| 53 | 1v | 17 | U | C2-N3-C4 | 6.55 | 130.93 | 127.00 |
| 1 | 1A | 1063 | G | C5-C6-O6 | 6.55 | 132.53 | 128.60 |
| 1 | 2A | 2473 | U | C2-N1-C1' | 6.50 | 125.51 | 117.70 |
| 1 | 1A | 512 | G | O4'-C1'-N9 | 6.42 | 113.34 | 108.20 |
| 54 | 2w | 50 | G | C5-C6-O6 | -6.36 | 124.78 | 128.60 |
| 55 | 2x | 17 | C | N3-C2-O2 | -6.34 | 117.46 | 121.90 |
| 32 | 1a | 1030(B) | C | C6-N1-C2 | -6.29 | 117.78 | 120.30 |
| 54 | 1w | 49 | G | N3-C4-N9 | 6.28 | 129.76 | 126.00 |
| 32 | 1a | 1027 | C | C6-N1-C1' | 6.25 | 128.30 | 120.80 |
| 32 | 1a | 1030(B) | C | N3-C2-O2 | -6.23 | 117.54 | 121.90 |
| 54 | 1y | 32 | C | N1-C2-O2 | 6.21 | 122.63 | 118.90 |
| 54 | 1y | 22 | G | C6-C5-N7 | -6.21 | 126.68 | 130.40 |
| 32 | 1a | 1025 | U | C2-N1-C1' | 6.19 | 125.13 | 117.70 |
| 32 | 2a | 1054 | C | C2-N1-C1' | 6.19 | 125.61 | 118.80 |
| 53 | 1v | 17 | U | C5-C4-O4 | 6.17 | 129.60 | 125.90 |
| 55 | 1x | 22 | G | N1-C6-O6 | -6.17 | 116.20 | 119.90 |
| 32 | 2a | 1158 | C | C6-N1-C1' | -6.16 | 113.40 | 120.80 |
| 54 | 1w | 60 | C | N1-C2-N3 | -6.12 | 114.92 | 119.20 |
| 32 | 1a | 1002 | G | N3-C4-N9 | 6.11 | 129.66 | 126.00 |
| 55 | 2x | 22 | G | N1-C6-O6 | -6.09 | 116.25 | 119.90 |
| 32 | 2a | 1039 | C | C2-N1-C1' | 6.09 | 125.50 | 118.80 |
| 32 | 2a | 841 | U | C5-C6-N1 | 6.08 | 125.74 | 122.70 |
| 32 | 2a | 1158 | C | N3-C2-O2 | -6.08 | 117.65 | 121.90 |
| 32 | 1a | 1027 | C | C2-N1-C1' | -6.06 | 112.14 | 118.80 |
| 54 | 1y | 32 | C | N1-C2-N3 | -6.05 | 114.97 | 119.20 |
| 1 | 1A | 2789 | C | O4'-C1'-N1 | 5.95 | 112.96 | 108.20 |
| 55 | 1x | 46 | G | N3-C2-N2 | -5.93 | 115.75 | 119.90 |
| 1 | 1A | 1174 | A | OP1-P-O3' | 5.90 | 118.18 | 105.20 |
| 32 | 2a | 1264 | C | N1-C2-O2 | 5.87 | 122.42 | 118.90 |
| 32 | 2a | 1028 | C | C2-N3-C4 | 5.87 | 122.83 | 119.90 |
| 1 | 2A | 528 | A | OP1-P-O3' | 5.86 | 118.09 | 105.20 |
| 32 | 2a | 1039 | C | N3-C4-N4 | 5.78 | 122.05 | 118.00 |
| 1 | 1A | 1063 | G | C6-N1-C2 | 5.78 | 128.57 | 125.10 |
| 32 | 1a | 266 | G | P-O3'-C3' | 5.76 | 126.61 | 119.70 |
| 54 | 1y | 22 | G | C4-C5-C6 | 5.75 | 122.25 | 118.80 |
| 54 | 2w | 29 | U | C5-C4-O4 | 5.74 | 129.34 | 125.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 55 | 1x | 35 | A | C6-N1-C2 | 5.73 | 122.04 | 118.60 |
| 1 | 2A | 1142 | U | C2-N1-C1' | 5.71 | 124.55 | 117.70 |
| 1 | 2A | 2897 | U | N1-C2-O2 | 5.70 | 126.79 | 122.80 |
| 1 | 2A | 2154 | G | C5-C6-O6 | -5.69 | 125.19 | 128.60 |
| 1 | 2A | 2155 | G | N3-C2-N2 | 5.67 | 123.87 | 119.90 |
| 1 | 1A | 1176 | G | OP1-P-O3' | 5.67 | 117.68 | 105.20 |
| 32 | 2a | 1054 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 32 | 1a | 1002 | G | C4-N9-C1' | 5.65 | 133.85 | 126.50 |
| 32 | 2a | 1263 | C | N1-C2-N3 | -5.62 | 115.27 | 119.20 |
| 1 | 1A | 847 | U | C2-N1-C1' | 5.60 | 124.42 | 117.70 |
| 32 | 1a | 1002 | G | N3-C4-C5 | -5.60 | 125.80 | 128.60 |
| 55 | 1x | 35 | A | C5-C6-N6 | 5.60 | 128.18 | 123.70 |
| 32 | 2a | 1025 | U | N1-C2-O2 | 5.59 | 126.71 | 122.80 |
| 32 | 2a | 1029 | C | C2-N3-C4 | 5.58 | 122.69 | 119.90 |
| 33 | 1b | 233 | SER | C-N-CD | 5.51 | 139.97 | 128.40 |
| 32 | 2a | 1395 | C | N1-C2-O2 | 5.51 | 122.20 | 118.90 |
| 1 | 1A | 2789 | C | C2-N1-C1' | -5.50 | 112.75 | 118.80 |
| 55 | 2x | 22 | G | C6-C5-N7 | 5.48 | 133.69 | 130.40 |
| 1 | 2A | 214 | G | O4'-C1'-N9 | 5.46 | 112.57 | 108.20 |
| 54 | 1w | 60 | C | C5-C6-N1 | 5.45 | 123.73 | 121.00 |
| 1 | 2A | 1420 | U | C2-N1-C1' | 5.45 | 124.23 | 117.70 |
| 32 | 2a | 1001(A) | G | C4-N9-C1' | 5.44 | 133.57 | 126.50 |
| 32 | 2a | 754 | C | N3-C2-O2 | -5.43 | 118.10 | 121.90 |
| 1 | 2A | 528 | A | P-O3'-C3' | 5.43 | 126.22 | 119.70 |
| 54 | 2w | 50 | G | N1-C6-O6 | 5.43 | 123.16 | 119.90 |
| 1 | 2A | 2140 | C | N1-C2-O2 | 5.41 | 122.14 | 118.90 |
| 32 | 1a | 1027 | C | N3-C4-C5 | -5.40 | 119.74 | 121.90 |
| 32 | 2a | 754 | C | C6-N1-C1' | -5.40 | 114.32 | 120.80 |
| 54 | 1y | 56 | C | N1-C2-O2 | 5.39 | 122.14 | 118.90 |
| 1 | 2A | 1644 | C | N1-C2-O2 | 5.39 | 122.13 | 118.90 |
| 55 | 1x | 22 | G | C4-C5-C6 | -5.38 | 115.57 | 118.80 |
| 32 | 2a | 1065 | U | P-O3'-C3' | 5.36 | 126.13 | 119.70 |
| 55 | 1x | 14 | A | C4-C5-C6 | 5.32 | 119.66 | 117.00 |
| 1 | 2A | 2155 | G | C6-N1-C2 | 5.30 | 128.28 | 125.10 |
| 1 | 1A | 1313 | U | C2-N1-C1' | 5.29 | 124.05 | 117.70 |
| 32 | 2a | 204 | U | C2-N1-C1' | 5.29 | 124.04 | 117.70 |
| 55 | 1x | 22 | G | C8-N9-C1' | 5.25 | 133.82 | 127.00 |
| 1 | 2A | 2473 | U | N1-C2-O2 | 5.25 | 126.47 | 122.80 |
| 32 | 2a | 1001(A) | G | C6-C5-N7 | -5.25 | 127.25 | 130.40 |
| 32 | 1a | 1067 | A | P-O3'-C3' | 5.24 | 125.99 | 119.70 |
| 32 | 2a | 841 | U | C2-N1-C1' | 5.24 | 123.98 | 117.70 |
| 32 | 2a | 266 | G | P-O3'-C3' | 5.22 | 125.97 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 55 | 2x | 46 | G | C6-N1-C2 | -5.22 | 121.97 | 125.10 |
| 1 | 1A | 1174 | A | P-O3'-C3' | 5.22 | 125.96 | 119.70 |
| 1 | 1A | 1086 | A | C5-C6-N6 | 5.21 | 127.87 | 123.70 |
| 32 | 1a | 1030(B) | C | C6-N1-C1' | -5.21 | 114.55 | 120.80 |
| 54 | 2y | 22 | G | N1-C6-O6 | 5.20 | 123.02 | 119.90 |
| 32 | 1a | 1025 | U | C6-N1-C1' | -5.19 | 113.94 | 121.20 |
| 1 | 1A | 2167 | U | C5-C6-N1 | 5.17 | 125.28 | 122.70 |
| 32 | 1a | 841 | U | C5-C6-N1 | 5.16 | 125.28 | 122.70 |
| 33 | 1b | 231 | GLU | C-N-CD | 5.16 | 139.24 | 128.40 |
| 55 | 2x | 22 | G | N3-C4-N9 | -5.16 | 122.90 | 126.00 |
| 54 | 1y | 22 | G | N3-C4-N9 | 5.16 | 129.09 | 126.00 |
| 1 | 2A | 1210 | A | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | 1A | 548 | A | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 1 | 2A | 1992 | G | P-O3'-C3' | 5.15 | 125.88 | 119.70 |
| 1 | 2A | 1313 | U | N1-C2-O2 | 5.14 | 126.40 | 122.80 |
| 1 | 2A | 1644 | C | C2-N1-C1' | 5.13 | 124.45 | 118.80 |
| 1 | 2A | 928 | G | C6-C5-N7 | -5.13 | 127.32 | 130.40 |
| 55 | 2x | 17 | C | C6-N1-C2 | -5.12 | 118.25 | 120.30 |
| 1 | 2A | 1380 | G | O5'-P-OP2 | -5.12 | 101.09 | 105.70 |
| 55 | 1x | 14 | A | C5-N7-C8 | 5.11 | 106.45 | 103.90 |
| 1 | 1A | 1063 | G | N3-C2-N2 | 5.10 | 123.47 | 119.90 |
| 54 | 2w | 13 | C | P-O3'-C3' | 5.10 | 125.82 | 119.70 |
| 54 | 1y | 33 | U | C2-N1-C1' | 5.10 | 123.82 | 117.70 |
| 1 | 1A | 1992 | G | P-O3'-C3' | 5.09 | 125.81 | 119.70 |
| 55 | 2x | 22 | G | C8-N9-C1' | 5.08 | 133.60 | 127.00 |
| 1 | 2A | 2866 | U | C2-N1-C1' | 5.05 | 123.76 | 117.70 |
| 32 | 1a | 560 | U | C3'-C2'-C1' | 5.05 | 105.54 | 101.50 |
| 32 | 2a | 687 | A | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 1 | 2A | 2136 | C | C2-N1-C1' | 5.03 | 124.34 | 118.80 |
| 32 | 1a | 1158 | C | C2-N1-C1' | 5.01 | 124.32 | 118.80 |
| 32 | 2a | 1039 | C | C6-N1-C1' | -5.00 | 114.79 | 120.80 |

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 ⓘ

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 | 755 | 0 |
| 1 | 2A | 60322 | 0 | 30428 | 813 | 0 |
| 2 | 1B | 2577 | 0 | 1305 | 23 | 0 |
| 2 | 2B | 2575 | 0 | 1303 | 29 | 0 |
| 3 | 1D | 2136 | 0 | 2218 | 51 | 0 |
| 3 | 2D | 2136 | 0 | 2218 | 53 | 0 |
| 4 | 1E | 1559 | 0 | 1618 | 40 | 0 |
| 4 | 2E | 1559 | 0 | 1618 | 37 | 0 |
| 5 | 1F | 1584 | 0 | 1625 | 27 | 0 |
| 5 | 2F | 1580 | 0 | 1619 | 43 | 0 |
| 6 | 1G | 1423 | 0 | 1436 | 39 | 0 |
| 6 | 2G | 1428 | 0 | 1438 | 29 | 0 |
| 7 | 1H | 1330 | 0 | 1407 | 26 | 0 |
| 7 | 2H | 1330 | 0 | 1407 | 27 | 0 |
| 8 | 1I | 1097 | 0 | 1140 | 25 | 0 |
| 8 | 2I | 1064 | 0 | 1082 | 17 | 0 |
| 9 | 1N | 1117 | 0 | 1184 | 18 | 0 |
| 9 | 2N | 1117 | 0 | 1184 | 25 | 0 |
| 10 | 1O | 933 | 0 | 996 | 20 | 0 |
| 10 | 2O | 933 | 0 | 996 | 19 | 0 |
| 11 | 1P | 1135 | 0 | 1212 | 32 | 0 |
| 11 | 2P | 1135 | 0 | 1212 | 24 | 0 |
| 12 | 1Q | 1122 | 0 | 1179 | 19 | 0 |
| 12 | 2Q | 1122 | 0 | 1179 | 30 | 0 |
| 13 | 1R | 968 | 0 | 1033 | 19 | 0 |
| 13 | 2R | 968 | 0 | 1033 | 26 | 0 |
| 14 | 1S | 873 | 0 | 927 | 18 | 0 |
| 14 | 2S | 870 | 0 | 923 | 20 | 0 |
| 15 | 1T | 1091 | 0 | 1151 | 28 | 0 |
| 15 | 2T | 1083 | 0 | 1136 | 35 | 0 |
| 16 | 1U | 959 | 0 | 1019 | 12 | 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 | 12 | 0 |
| 19 | 1X | 750 | 0 | 814 | 19 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19 | 2X | 750 | 0 | 814 | 20 | 0 |
| 20 | 1Y | 806 | 0 | 881 | 21 | 0 |
| 20 | 2Y | 806 | 0 | 881 | 16 | 0 |
| 21 | 1Z | 1240 | 0 | 1240 | 26 | 0 |
| 21 | 2Z | 1271 | 0 | 1273 | 33 | 0 |
| 22 | 10 | 653 | 0 | 674 | 13 | 0 |
| 22 | 20 | 653 | 0 | 674 | 19 | 0 |
| 23 | 11 | 755 | 0 | 826 | 18 | 0 |
| 23 | 21 | 755 | 0 | 826 | 21 | 0 |
| 24 | 12 | 588 | 0 | 643 | 5 | 0 |
| 24 | 22 | 588 | 0 | 643 | 11 | 0 |
| 25 | 13 | 469 | 0 | 518 | 11 | 0 |
| 25 | 23 | 464 | 0 | 514 | 7 | 0 |
| 26 | 14 | 552 | 0 | 533 | 21 | 0 |
| 26 | 24 | 532 | 0 | 503 | 17 | 0 |
| 27 | 15 | 455 | 0 | 465 | 11 | 0 |
| 27 | 25 | 455 | 0 | 465 | 9 | 0 |
| 28 | 16 | 453 | 0 | 472 | 6 | 0 |
| 28 | 26 | 449 | 0 | 469 | 9 | 0 |
| 29 | 17 | 418 | 0 | 467 | 8 | 0 |
| 29 | 27 | 418 | 0 | 467 | 8 | 0 |
| 30 | 18 | 517 | 0 | 582 | 22 | 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 | 0 | 0 |
| 32 | 2a | 32327 | 0 | 16338 | 0 | 0 |
| 33 | 1b | 1846 | 0 | 1867 | 0 | 0 |
| 33 | 2b | 1825 | 0 | 1828 | 0 | 0 |
| 34 | 1c | 1548 | 0 | 1535 | 0 | 0 |
| 34 | 2c | 1542 | 0 | 1517 | 0 | 0 |
| 35 | 1d | 1655 | 0 | 1672 | 0 | 0 |
| 35 | 2d | 1674 | 0 | 1714 | 0 | 0 |
| 36 | 1e | 1129 | 0 | 1185 | 0 | 0 |
| 36 | 2e | 1133 | 0 | 1191 | 0 | 0 |
| 37 | 1f | 810 | 0 | 804 | 0 | 0 |
| 37 | 2f | 816 | 0 | 808 | 0 | 0 |
| 38 | 1g | 1231 | 0 | 1238 | 0 | 0 |
| 38 | 2g | 1235 | 0 | 1249 | 0 | 0 |
| 39 | 1h | 1088 | 0 | 1126 | 0 | 0 |
| 39 | 2h | 1088 | 0 | 1126 | 0 | 0 |
| 40 | 1i | 983 | 0 | 986 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 40 | 2i | 978 | 0 | 966 | 0 | 0 |
| 41 | 1j | 709 | 0 | 650 | 0 | 0 |
| 41 | 2j | 714 | 0 | 672 | 0 | 0 |
| 42 | 1k | 829 | 0 | 825 | 0 | 0 |
| 42 | 2k | 833 | 0 | 836 | 0 | 0 |
| 43 | 1l | 932 | 0 | 981 | 0 | 0 |
| 43 | 2l | 932 | 0 | 981 | 0 | 0 |
| 44 | 1m | 958 | 0 | 1002 | 0 | 0 |
| 44 | 2m | 950 | 0 | 988 | 0 | 0 |
| 45 | 1n | 492 | 0 | 529 | 0 | 0 |
| 45 | 2n | 492 | 0 | 529 | 0 | 0 |
| 46 | 1o | 728 | 0 | 760 | 0 | 0 |
| 46 | 2o | 728 | 0 | 760 | 0 | 0 |
| 47 | 1p | 681 | 0 | 697 | 0 | 0 |
| 47 | 2p | 677 | 0 | 686 | 0 | 0 |
| 48 | 1q | 823 | 0 | 891 | 0 | 0 |
| 48 | 2q | 823 | 0 | 891 | 0 | 0 |
| 49 | 1r | 555 | 0 | 618 | 0 | 0 |
| 49 | 2r | 555 | 0 | 618 | 0 | 0 |
| 50 | 1s | 652 | 0 | 662 | 0 | 0 |
| 50 | 2s | 646 | 0 | 644 | 0 | 0 |
| 51 | 1t | 728 | 0 | 798 | 0 | 0 |
| 51 | 2t | 727 | 0 | 796 | 0 | 0 |
| 52 | 1u | 199 | 0 | 208 | 0 | 0 |
| 52 | 2u | 199 | 0 | 208 | 0 | 0 |
| 53 | 1v | 276 | 0 | 139 | 0 | 0 |
| 53 | 2v | 276 | 0 | 139 | 0 | 0 |
| 54 | 1w | 1568 | 0 | 800 | 0 | 0 |
| 54 | 1y | 1568 | 0 | 800 | 0 | 0 |
| 54 | 2w | 1568 | 0 | 802 | 0 | 0 |
| 54 | 2y | 1568 | 0 | 802 | 0 | 0 |
| 55 | 1x | 1625 | 0 | 827 | 0 | 0 |
| 55 | 2x | 1625 | 0 | 829 | 0 | 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 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 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 |
| 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 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 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 |
| 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 | 0 | 0 |
| 57 | 2A | 84 | 0 | 0 | 3 | 0 |
| 57 | 2a | 44 | 0 | 0 | 0 | 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 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 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 |
| 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 | 72 | 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 | 0 | 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 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6l | 1j | 1 | 0 | 0 | 0 | 0 |
| 6l | 1l | 8 | 0 | 0 | 0 | 0 |
| 6l | 1m | 2 | 0 | 0 | 0 | 0 |
| 6l | 1n | 1 | 0 | 0 | 0 | 0 |
| 6l | 1p | 1 | 0 | 0 | 0 | 0 |
| 6l | 1q | 3 | 0 | 0 | 0 | 0 |
| 6l | 1u | 1 | 0 | 0 | 0 | 0 |
| 6l | 1v | 4 | 0 | 0 | 0 | 0 |
| 6l | 1w | 6 | 0 | 0 | 0 | 0 |
| 6l | 1x | 17 | 0 | 0 | 0 | 0 |
| 6l | 1y | 3 | 0 | 0 | 0 | 0 |
| 6l | 20 | 3 | 0 | 0 | 0 | 0 |
| 6l | 21 | 9 | 0 | 0 | 0 | 0 |
| 6l | 23 | 1 | 0 | 0 | 0 | 0 |
| 6l | 25 | 3 | 0 | 0 | 0 | 0 |
| 6l | 27 | 3 | 0 | 0 | 0 | 0 |
| 6l | 28 | 6 | 0 | 0 | 2 | 0 |
| 6l | 2A | 1163 | 0 | 0 | 40 | 0 |
| 6l | 2B | 20 | 0 | 0 | 0 | 0 |
| 6l | 2D | 23 | 0 | 0 | 1 | 0 |
| 6l | 2E | 10 | 0 | 0 | 2 | 0 |
| 6l | 2F | 13 | 0 | 0 | 0 | 0 |
| 6l | 2I | 2 | 0 | 0 | 0 | 0 |
| 6l | 2N | 1 | 0 | 0 | 0 | 0 |
| 6l | 2O | 2 | 0 | 0 | 0 | 0 |
| 6l | 2P | 6 | 0 | 0 | 0 | 0 |
| 6l | 2Q | 1 | 0 | 0 | 0 | 0 |
| 6l | 2R | 3 | 0 | 0 | 0 | 0 |
| 6l | 2T | 2 | 0 | 0 | 0 | 0 |
| 6l | 2U | 3 | 0 | 0 | 0 | 0 |
| 6l | 2V | 2 | 0 | 0 | 1 | 0 |
| 6l | 2W | 1 | 0 | 0 | 0 | 0 |
| 6l | 2X | 2 | 0 | 0 | 0 | 0 |
| 6l | 2Z | 1 | 0 | 0 | 0 | 0 |
| 6l | 2a | 322 | 0 | 0 | 0 | 0 |
| 6l | 2e | 2 | 0 | 0 | 0 | 0 |
| 6l | 2f | 1 | 0 | 0 | 0 | 0 |
| 6l | 2g | 2 | 0 | 0 | 0 | 0 |
| 6l | 2j | 4 | 0 | 0 | 0 | 0 |
| 6l | 2l | 5 | 0 | 0 | 0 | 0 |
| 6l | 2o | 2 | 0 | 0 | 0 | 0 |
| 6l | 2p | 4 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 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 |
| All | All | 300702 | 0 | 196683 | 2462 | 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.

All (2462) 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 |
| 1:2A:987:G:H1 | 1:2A:1218:C:H42 | 46.66 | 1.01 |
| 1:2A:2104:G:H1 | 1:2A:2185:C:N4 | 1.59 | 1.01 |
| 1:2A:1002:G:H1 | 1:2A:1038:C:N4 | 42.34 | 0.98 |
| 1:2A:2100:G:H1 | 1:2A:2189:U:H3 | 1.12 | 0.96 |
| 1:2A:1120:G:H1 | 1:2A:1153:C:H42 | 34.36 | 0.94 |
| 1:1A:2133:G:HO2' | 1:1A:2157:G:H1 | 1.12 | 0.93 |
| 28:26:34:LEU:H | 28:26:51:GLU:HG2 | 1.32 | 0.92 |
| 1:2A:2138:C:N4 | 1:2A:2153:G:H1 | 1.67 | 0.91 |
| 1:2A:76:C:H42 | 1:2A:93:G:H1 | 26.45 | 0.90 |
| 1:1A:1058:G:H1 | 1:1A:1080:C:N4 | 1.70 | 0.90 |
| 1:2A:1422:G:H5'' | 10:2O:48:PRO:HB3 | 99.57 | 0.89 |
| 1:1A:1058:G:N2 | 1:1A:1080:C:N3 | 2.21 | 0.88 |
| 1:2A:2138:C:N3 | 1:2A:2153:G:N2 | 2.22 | 0.87 |
| 1:1A:1054:A:H61 | 1:1A:1105:U:H3 | 1.23 | 0.87 |
| 1:1A:2807:G:N1 | 1:1A:2893:G:O6 | 2.08 | 0.87 |
| 1:2A:1120:G:H1 | 1:2A:1153:C:N4 | 34.79 | 0.86 |
| 1:1A:2101:G:H1 | 1:1A:2188:C:H42 | 1.23 | 0.85 |
| 1:2A:2129:C:H42 | 1:2A:2159:G:H1 | 1.25 | 0.85 |
| 1:1A:1064:C:N3 | 1:1A:1074:G:O6 | 2.10 | 0.84 |
| 1:2A:882:G:H1 | 1:2A:894:C:H42 | 1.22 | 0.84 |
| 10:2O:35:VAL:HG11 | 10:2O:103:ALA:HB3 | 1.59 | 0.84 |
| 1:1A:1065:U:O2 | 1:1A:1073:A:N6 | 2.10 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:20:10:THR:HG22 | 22:20:12:ASN:H | 1.43 | 0.83 |
| 1:2A:2345:G:H4' | 1:2A:2346:A:H5'' | 1.61 | 0.82 |
| 1:2A:2807:G:N1 | 1:2A:2893:G:O6 | 2.13 | 0.82 |
| 1:1A:1054:A:N6 | 1:1A:1105:U:H3 | 1.77 | 0.82 |
| 1:1A:2124:G:H1 | 1:1A:2174:C:H42 | 1.22 | 0.82 |
| 1:2A:2104:G:H1 | 1:2A:2185:C:H42 | 0.83 | 0.81 |
| 14:1S:25:ARG:NH1 | 14:1S:42:ASP:OD1 | 2.13 | 0.81 |
| 1:2A:2138:C:H42 | 1:2A:2153:G:H1 | 1.21 | 0.81 |
| 26:14:16:CYS:SG | 26:14:17:GLY:N | 2.54 | 0.81 |
| 22:10:11:ARG:O | 22:10:14:ARG:NH2 | 2.14 | 0.81 |
| 1:1A:2099:U:H3 | 1:1A:2190:G:H1 | 1.26 | 0.80 |
| 1:1A:1264:G:OP1 | 27:15:19:ARG:NH2 | 2.14 | 0.80 |
| 1:2A:994:C:OP1 | 16:2U:53:ARG:NH2 | 2.13 | 0.80 |
| 1:2A:1002:G:H1 | 1:2A:1038:C:H42 | 42.74 | 0.80 |
| 1:2A:987:G:H1 | 1:2A:1218:C:N4 | 46.20 | 0.80 |
| 8:1I:92:VAL:HG13 | 8:1I:120:ILE:HB | 1.63 | 0.80 |
| 1:2A:10:G:H1' | 1:2A:2801(A):A:H62 | 1.45 | 0.80 |
| 1:2A:2592:G:N7 | 61:2A:3958:HOH:O | 2.15 | 0.80 |
| 1:2A:1210:A:H4' | 1:2A:1211:U:H5'' | 1.64 | 0.79 |
| 10:1O:35:VAL:HG11 | 10:1O:103:ALA:HB3 | 1.65 | 0.78 |
| 11:1P:42:SER:O | 61:1P:301:HOH:O | 2.00 | 0.78 |
| 1:1A:2135:A:N6 | 1:1A:2156:G:O2' | 2.16 | 0.78 |
| 1:2A:2137:C:N4 | 1:2A:2154:G:N1 | 2.32 | 0.78 |
| 1:2A:2129:C:N4 | 1:2A:2159:G:H1 | 1.80 | 0.78 |
| 1:2A:2137:C:N3 | 1:2A:2154:G:N2 | 2.32 | 0.77 |
| 5:1F:53:THR:HG23 | 5:1F:55:GLY:H | 1.49 | 0.77 |
| 1:1A:1918:A:N6 | 61:1A:4317:HOH:O | 2.18 | 0.77 |
| 1:1A:2125:G:N1 | 1:1A:2172:U:OP1 | 2.18 | 0.77 |
| 1:2A:1032:A:H61 | 1:2A:1122:G:H1 | 1.31 | 0.76 |
| 1:2A:975:C:OP1 | 61:2A:3950:HOH:O | 2.04 | 0.76 |
| 1:2A:2379:G:O2' | 14:2S:17:ARG:NH1 | 2.15 | 0.76 |
| 1:1A:2136:C:N4 | 1:1A:2155:G:N1 | 2.33 | 0.76 |
| 1:1A:2136:C:N3 | 1:1A:2155:G:N2 | 2.33 | 0.76 |
| 16:2U:66:ASN:HD21 | 16:2U:70:ARG:HH21 | 1.34 | 0.76 |
| 1:1A:2690:C:OP2 | 13:1R:17:ARG:NH2 | 2.19 | 0.76 |
| 31:29:25:VAL:HB | 31:29:34:GLN:HB2 | 1.68 | 0.76 |
| 1:1A:1229:G:N7 | 61:1A:4321:HOH:O | 2.18 | 0.76 |
| 4:1E:28:ALA:HB3 | 4:1E:93:VAL:HG12 | 1.68 | 0.76 |
| 21:1Z:102:LEU:HD21 | 21:1Z:171:ILE:HD11 | 1.68 | 0.76 |
| 1:1A:1183:G:O2' | 25:13:29:ARG:NH1 | 2.20 | 0.75 |
| 1:1A:2131:G:H5'' | 1:1A:2132:U:H3' | 1.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:1P:52:GLU:OE1 | 11:1P:55:ARG:NH1 | 2.19 | 0.75 |
| 1:2A:65:C:O2 | 1:2A:456:C:N4 | 2.19 | 0.75 |
| 1:1A:2483:C:N3 | 12:1Q:124:LYS:NZ | 2.35 | 0.75 |
| 1:2A:2287:A:H62 | 1:2A:2344:U:H3 | 1.32 | 0.75 |
| 20:2Y:102:CYS:SG | 20:2Y:103:GLY:N | 2.60 | 0.74 |
| 2:2B:7:G:O6 | 2:2B:114:C:N4 | 2.18 | 0.74 |
| 1:1A:400:G:N7 | 61:1A:4334:HOH:O | 2.20 | 0.74 |
| 1:2A:2150:U:H2' | 1:2A:2151:G:H8 | 1.52 | 0.74 |
| 1:1A:9:U:H3 | 1:1A:2629:A:H2 | 1.35 | 0.74 |
| 17:1V:40:LEU:HB2 | 17:1V:46:VAL:HG13 | 1.70 | 0.74 |
| 1:2A:2133:G:O2' | 1:2A:2157:G:N2 | 2.20 | 0.74 |
| 1:1A:1002:G:H3' | 1:1A:1003:G:H4' | 5.18 | 0.74 |
| 23:11:50:ARG:HG2 | 23:11:59:THR:HG22 | 1.70 | 0.74 |
| 1:1A:1058:G:N1 | 1:1A:1080:C:N4 | 2.30 | 0.74 |
| 4:2E:48:GLN:HE21 | 4:2E:78:LEU:HB3 | 1.53 | 0.74 |
| 1:2A:1219:G:H1 | 1:2A:1230:C:H42 | 1.35 | 0.74 |
| 8:1I:78:THR:H | 8:1I:104:GLN:HE22 | 1.35 | 0.74 |
| 1:2A:83:G:H1 | 1:2A:102:G:HO2' | 1.36 | 0.74 |
| 1:2A:918:A:O2' | 2:2B:97:G:N2 | 2.20 | 0.74 |
| 1:2A:1818:U:H2' | 3:2D:157:ARG:HD2 | 1.70 | 0.74 |
| 26:14:64:GLY:O | 26:14:66:SER:N | 2.21 | 0.73 |
| 1:1A:517:C:OP1 | 27:15:16:ARG:NH2 | 2.21 | 0.73 |
| 1:1A:1064:C:O2 | 1:1A:1074:G:N1 | 2.16 | 0.73 |
| 1:2A:1171:G:H22 | 1:2A:1178:C:H42 | 1.35 | 0.73 |
| 1:1A:1060:U:H3 | 1:1A:1088:A:H8 | 1.35 | 0.73 |
| 3:1D:12:SER:HB3 | 3:1D:208:LYS:HB3 | 1.68 | 0.73 |
| 4:1E:105:THR:OG1 | 4:1E:199:ARG:NH2 | 2.21 | 0.73 |
| 1:2A:1002:G:N2 | 1:2A:1038:C:N3 | 42.05 | 0.73 |
| 1:2A:2104:G:N2 | 1:2A:2185:C:N3 | 2.32 | 0.73 |
| 1:1A:859:G:O2' | 1:1A:916:G:O6 | 2.06 | 0.72 |
| 1:2A:987:G:O2' | 1:2A:1000:A:N3 | 2.22 | 0.72 |
| 1:1A:249:C:O2 | 30:18:12:LYS:NZ | 2.22 | 0.72 |
| 1:1A:279:C:H42 | 1:1A:361:G:H1 | 1.35 | 0.72 |
| 3:1D:8:PRO:HB3 | 3:1D:14:ARG:HB3 | 1.70 | 0.72 |
| 1:2A:2365:G:N7 | 30:28:39:LYS:NZ | 2.38 | 0.72 |
| 1:1A:1798:U:OP2 | 3:1D:274:ARG:NH2 | 2.20 | 0.72 |
| 1:2A:1772:G:OP1 | 61:2A:3951:HOH:O | 2.06 | 0.72 |
| 8:2I:93:THR:HG22 | 8:2I:119:PRO:HB3 | 1.71 | 0.71 |
| 1:1A:880:G:H2' | 1:1A:881:G:H8 | 1.55 | 0.71 |
| 1:1A:488:G:O2' | 18:1W:49:LYS:NZ | 2.22 | 0.71 |
| 7:2H:106:THR:HG22 | 7:2H:112:PRO:HB3 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:76:C:N4 | 1:2A:93:G:H1 | 25.64 | 0.71 |
| 11:2P:91:PHE:O | 11:2P:121:LYS:NZ | 2.22 | 0.71 |
| 25:13:3:ARG:NH1 | 25:13:60:GLU:OE2 | 2.24 | 0.71 |
| 1:2A:1204:A:H2 | 1:2A:1241:A:H62 | 1.39 | 0.71 |
| 1:1A:2837:G:N7 | 61:1A:4351:HOH:O | 2.24 | 0.71 |
| 1:1A:1466:G:HO2' | 1:1A:1546:C:HO2' | 1.36 | 0.70 |
| 1:1A:994:C:OP1 | 16:1U:53:ARG:NH2 | 2.24 | 0.70 |
| 19:1X:35:THR:HG22 | 19:1X:38:GLU:HB2 | 1.73 | 0.70 |
| 1:1A:880:G:H2' | 1:1A:881:G:C8 | 2.27 | 0.70 |
| 1:1A:583:G:N7 | 61:1A:4345:HOH:O | 2.23 | 0.70 |
| 1:1A:1187:G:O6 | 61:1A:4275:HOH:O | 2.07 | 0.70 |
| 1:1A:990:A:OP2 | 61:1A:4218:HOH:O | 2.09 | 0.70 |
| 26:24:64:GLY:O | 26:24:66:SER:N | 2.24 | 0.70 |
| 21:2Z:65:GLN:HE21 | 21:2Z:67:LEU:HD21 | 1.57 | 0.70 |
| 1:1A:1299:G:OP1 | 61:1A:4303:HOH:O | 2.09 | 0.70 |
| 1:2A:1022:G:N2 | 1:2A:1023:U:O4 | 2.25 | 0.70 |
| 1:2A:2343:C:HO2' | 1:2A:2373:G:HO2' | 1.38 | 0.70 |
| 1:1A:2124:G:H1 | 1:1A:2174:C:N4 | 1.90 | 0.69 |
| 22:20:11:ARG:O | 22:20:14:ARG:NH2 | 2.25 | 0.69 |
| 1:1A:1062:G:H1 | 1:1A:1077:A:H61 | 1.39 | 0.69 |
| 27:25:33:CYS:HB2 | 27:25:40:LYS:HD3 | 1.72 | 0.69 |
| 3:2D:26:LYS:HB3 | 3:2D:83:GLU:HG2 | 1.74 | 0.69 |
| 20:1Y:82:PRO:O | 20:1Y:101:LYS:NZ | 2.25 | 0.69 |
| 21:2Z:102:LEU:HD21 | 21:2Z:171:ILE:HD11 | 1.72 | 0.69 |
| 2:2B:22:U:H3 | 2:2B:61:G:H1 | 1.41 | 0.69 |
| 1:2A:2690:C:OP2 | 13:2R:17:ARG:NH2 | 2.25 | 0.69 |
| 19:2X:43:VAL:HG21 | 19:2X:81:VAL:HG11 | 1.74 | 0.69 |
| 1:1A:1173:G:N1 | 1:1A:1176:G:OP2 | 2.25 | 0.69 |
| 1:1A:512:G:N7 | 61:1A:4214:HOH:O | 2.26 | 0.69 |
| 1:1A:733:G:N7 | 61:1A:4363:HOH:O | 2.25 | 0.69 |
| 7:2H:3:ARG:HG2 | 7:2H:6:ARG:HE | 1.58 | 0.69 |
| 1:1A:2688:U:OP1 | 61:1A:4304:HOH:O | 2.11 | 0.69 |
| 1:1A:2292:C:OP1 | 14:1S:17:ARG:NH2 | 2.23 | 0.69 |
| 1:1A:1266:G:O5' | 18:1W:15:ARG:NH2 | 2.26 | 0.69 |
| 1:1A:2101:G:H1 | 1:1A:2188:C:N4 | 1.90 | 0.69 |
| 1:1A:250:G:OP2 | 30:18:13:ARG:NH2 | 2.26 | 0.68 |
| 1:1A:2183:C:H2' | 1:1A:2184:G:H8 | 1.57 | 0.68 |
| 3:1D:242:ARG:NH1 | 61:1D:401:HOH:O | 2.26 | 0.68 |
| 1:2A:2137:C:H42 | 1:2A:2154:G:H1 | 1.37 | 0.68 |
| 1:2A:861:A:N6 | 1:2A:916:G:O2' | 2.26 | 0.68 |
| 5:2F:41:LEU:HD22 | 5:2F:44:ARG:HH11 | 1.59 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:1H:84:SER:OG | 7:1H:132:ARG:NH1 | 2.27 | 0.68 |
| 1:1A:376:C:OP1 | 61:1A:4305:HOH:O | 2.12 | 0.68 |
| 1:2A:2595:G:N7 | 61:2A:4003:HOH:O | 2.26 | 0.68 |
| 17:1V:78:LYS:O | 61:1V:301:HOH:O | 2.12 | 0.68 |
| 1:1A:79:G:N1 | 1:1A:90:U:N3 | 30.15 | 0.68 |
| 23:21:51:VAL:HG11 | 23:21:74:VAL:HG21 | 1.75 | 0.68 |
| 11:2P:62:LEU:O | 30:28:13:ARG:NH1 | 2.26 | 0.68 |
| 1:1A:1447:G:N7 | 61:1A:4373:HOH:O | 2.26 | 0.68 |
| 3:1D:242:ARG:HG3 | 3:1D:242:ARG:HH11 | 1.59 | 0.68 |
| 24:12:14:ARG:O | 24:12:67:LYS:NZ | 2.25 | 0.67 |
| 1:1A:1093:G:H3' | 1:1A:1094:U:H5'' | 1.75 | 0.67 |
| 1:1A:2135:A:H61 | 1:1A:2156:G:HO2' | 1.43 | 0.67 |
| 1:1A:2444:G:N7 | 61:1A:4371:HOH:O | 2.26 | 0.67 |
| 7:1H:164:TYR:HB2 | 7:1H:167:GLU:HB2 | 1.76 | 0.67 |
| 1:2A:783:A:OP2 | 61:2A:3952:HOH:O | 2.12 | 0.67 |
| 1:1A:1395:A:OP1 | 61:1A:4201:HOH:O | 2.13 | 0.67 |
| 1:1A:833:U:O2 | 11:1P:55:ARG:NH2 | 2.28 | 0.67 |
| 1:2A:2150:U:H2' | 1:2A:2151:G:C8 | 2.29 | 0.67 |
| 1:1A:1670:C:OP2 | 61:1A:4260:HOH:O | 2.13 | 0.67 |
| 3:1D:38:LYS:NZ | 3:1D:39:LYS:O | 2.19 | 0.67 |
| 1:1A:746:A:N7 | 61:1A:4386:HOH:O | 2.28 | 0.67 |
| 13:1R:28:LEU:HD23 | 13:1R:48:VAL:HG21 | 1.76 | 0.67 |
| 1:2A:307:G:H21 | 1:2A:330:A:H62 | 1.43 | 0.67 |
| 1:2A:521:G:H2' | 1:2A:522:G:H8 | 1.60 | 0.67 |
| 30:18:33:ASN:HA | 30:18:36:LYS:HD2 | 1.75 | 0.67 |
| 21:1Z:52:SER:HG | 21:1Z:54:HIS:HD1 | 1.41 | 0.67 |
| 1:2A:2116:G:N7 | 1:2A:2166:G:N2 | 2.33 | 0.67 |
| 1:2A:2576:G:OP1 | 61:2A:3953:HOH:O | 2.13 | 0.67 |
| 1:2A:637:A:OP1 | 11:2P:133:SER:OG | 2.11 | 0.67 |
| 1:2A:1783:A:HO2' | 1:2A:2607:G:HO2' | 1.42 | 0.67 |
| 1:2A:276:A:H5'' | 1:2A:277:C:H5' | 1.75 | 0.67 |
| 1:2A:1446:C:H42 | 1:2A:1465:G:H1 | 1.41 | 0.66 |
| 2:2B:24:G:N7 | 2:2B:56:G:H2' | 2.10 | 0.66 |
| 3:1D:85:ASP:OD2 | 3:1D:88:ARG:NH1 | 2.27 | 0.66 |
| 1:1A:1174:A:H4' | 1:1A:1175:U:OP1 | 1.94 | 0.66 |
| 1:1A:2165:G:N2 | 1:1A:2171:A:O2' | 2.28 | 0.66 |
| 1:1A:2441:C:OP2 | 1:1A:2586:C:O2' | 2.13 | 0.66 |
| 1:1A:731:C:OP1 | 61:1A:4306:HOH:O | 2.13 | 0.66 |
| 1:2A:2129:C:N3 | 1:2A:2159:G:N2 | 2.40 | 0.66 |
| 1:2A:2136:C:N4 | 1:2A:2155:G:H1 | 1.92 | 0.66 |
| 1:1A:2296:U:OP2 | 14:1S:9:ARG:NH2 | 2.27 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:2D:72:LYS:HG3 | 3:2D:103:ARG:HH21 | 1.60 | 0.66 |
| 19:2X:72:LYS:NZ | 19:2X:75:ASP:OD1 | 2.25 | 0.66 |
| 1:1A:1055:G:H1 | 1:1A:1104:C:H42 | 1.43 | 0.66 |
| 1:1A:1113:U:H2' | 1:1A:1114:G:H8 | 1.61 | 0.66 |
| 1:1A:1988:C:OP2 | 61:1A:4308:HOH:O | 2.13 | 0.66 |
| 1:1A:530:G:N1 | 1:1A:2023:G:OP1 | 2.28 | 0.66 |
| 19:1X:43:VAL:HG21 | 19:1X:81:VAL:HG11 | 1.77 | 0.66 |
| 1:2A:2140:C:N4 | 1:2A:2151:G:H1 | 1.92 | 0.66 |
| 1:1A:889:C:O2' | 1:1A:890:A:O4' | 2.14 | 0.66 |
| 1:1A:271(M):G:N2 | 8:1I:50:ARG:HH12 | 1.93 | 0.66 |
| 1:2A:2102:U:H3 | 1:2A:2187:G:H1 | 1.44 | 0.66 |
| 1:2A:2126:A:N6 | 1:2A:2162:G:O2' | 2.29 | 0.66 |
| 4:2E:47:VAL:HG11 | 4:2E:86:PRO:HD2 | 1.78 | 0.66 |
| 7:2H:46:GLU:OE2 | 7:2H:51:ARG:NH2 | 2.29 | 0.66 |
| 7:2H:90:LYS:HD3 | 7:2H:159:GLU:HG2 | 1.78 | 0.66 |
| 15:2T:65:LYS:HE3 | 15:2T:67:SER:HB2 | 1.78 | 0.66 |
| 1:1A:2409:G:N7 | 61:1A:4389:HOH:O | 2.29 | 0.65 |
| 6:1G:142:PRO:HB2 | 26:14:31:ILE:HG21 | 1.79 | 0.65 |
| 1:1A:2098:U:H3 | 1:1A:2191:G:H1 | 1.42 | 0.65 |
| 5:2F:24:LEU:HD23 | 5:2F:115:ALA:HA | 1.78 | 0.65 |
| 1:1A:2849:U:OP2 | 15:1T:95:ARG:NH1 | 2.29 | 0.65 |
| 25:23:8:LEU:HB2 | 25:23:28:LEU:HD13 | 1.77 | 0.65 |
| 1:2A:2375:G:N2 | 1:2A:2378:A:OP2 | 2.26 | 0.65 |
| 1:2A:309:G:N3 | 1:2A:329:G:O2' | 2.29 | 0.65 |
| 1:1A:2789:C:O2' | 1:1A:2790:A:O4' | 2.14 | 0.65 |
| 17:1V:76:LYS:HB2 | 17:1V:81:TYR:HB3 | 1.78 | 0.65 |
| 1:2A:2296:U:OP2 | 14:2S:9:ARG:NH2 | 2.30 | 0.65 |
| 9:2N:97:ARG:HA | 9:2N:100:GLU:HB2 | 1.77 | 0.65 |
| 1:2A:2114:A:N6 | 1:2A:2119:A:N7 | 2.44 | 0.65 |
| 1:1A:1071:G:H1' | 1:1A:1089:G:H2' | 1.79 | 0.65 |
| 1:1A:1604:C:OP2 | 61:1A:4201:HOH:O | 2.15 | 0.65 |
| 1:1A:2428:G:OP1 | 61:1A:4236:HOH:O | 2.14 | 0.65 |
| 1:2A:751:A:OP1 | 61:2A:3957:HOH:O | 2.15 | 0.65 |
| 1:2A:2683:C:OP1 | 15:2T:53:ARG:NH2 | 2.29 | 0.65 |
| 1:1A:1047:G:H2' | 1:1A:1110:G:H22 | 1.61 | 0.65 |
| 1:1A:1030:G:OP2 | 12:1Q:128:LYS:NZ | 2.30 | 0.65 |
| 1:2A:2857:G:N2 | 1:2A:2860:A:OP2 | 2.23 | 0.65 |
| 11:1P:116:GLY:O | 11:1P:137:LYS:NZ | 2.30 | 0.65 |
| 1:2A:2441:C:OP2 | 1:2A:2586:C:O2' | 2.14 | 0.65 |
| 1:1A:2585:U:OP1 | 61:1A:4310:HOH:O | 2.15 | 0.64 |
| 3:1D:69:ARG:NH2 | 3:1D:128:GLY:O | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:1Y:102:CYS:SG | 20:1Y:103:GLY:N | 2.62 | 0.64 |
| 4:2E:143:ASN:HD22 | 4:2E:147:PRO:HD3 | 1.62 | 0.64 |
| 12:1Q:85:LYS:HG2 | 22:10:7:LEU:HB3 | 1.77 | 0.64 |
| 1:2A:1019:U:H3 | 1:2A:1142(A):A:H62 | 1.46 | 0.64 |
| 1:2A:2218:U:N3 | 23:21:55:GLY:O | 2.31 | 0.64 |
| 1:2A:568:U:H5' | 1:2A:945:A:N1 | 2.12 | 0.64 |
| 1:2A:852:G:H2' | 1:2A:853:G:H8 | 1.61 | 0.64 |
| 3:2D:69:ARG:HE | 3:2D:130:ALA:HB2 | 1.62 | 0.64 |
| 30:18:6:THR:HG22 | 30:18:63:PRO:HD2 | 1.78 | 0.64 |
| 8:1I:130:TYR:HB3 | 8:1I:138:ILE:HB | 1.77 | 0.64 |
| 1:2A:882:G:H1 | 1:2A:894:C:N4 | 1.93 | 0.64 |
| 1:2A:1363:C:O2' | 1:2A:1809:A:N3 | 2.31 | 0.64 |
| 1:1A:1043:C:H2' | 1:1A:1044:G:H5'' | 1.80 | 0.64 |
| 1:1A:1453:U:O2' | 1:1A:1455:G:N7 | 2.28 | 0.64 |
| 1:1A:2705:A:N3 | 61:1A:4391:HOH:O | 2.29 | 0.64 |
| 1:2A:2787:C:H1' | 4:2E:62:PRO:HG3 | 1.80 | 0.64 |
| 31:19:25:VAL:HB | 31:19:34:GLN:HB2 | 1.79 | 0.64 |
| 1:1A:2331:G:N7 | 61:1A:4401:HOH:O | 2.30 | 0.64 |
| 1:1A:729:G:C6 | 3:1D:208:LYS:HB2 | 2.33 | 0.64 |
| 1:2A:2355:C:H4' | 22:20:24:LYS:HG3 | 1.80 | 0.64 |
| 23:21:4:VAL:HG12 | 23:21:11:ARG:HB2 | 1.80 | 0.64 |
| 1:2A:392:C:H5'' | 1:2A:409:C:H5'' | 1.79 | 0.64 |
| 7:2H:27:LYS:NZ | 7:2H:32:GLU:OE1 | 2.31 | 0.64 |
| 12:2Q:109:VAL:HG22 | 12:2Q:113:GLN:HB3 | 1.79 | 0.64 |
| 16:2U:91:ASP:O | 16:2U:95:LEU:HB2 | 1.98 | 0.64 |
| 1:2A:476:G:OP1 | 61:2A:3955:HOH:O | 2.15 | 0.63 |
| 1:1A:2140:C:H42 | 1:1A:2150:U:H3 | 1.45 | 0.63 |
| 20:2Y:8:LYS:HE3 | 20:2Y:97:ARG:HH11 | 1.64 | 0.63 |
| 31:19:16:VAL:HG22 | 31:19:25:VAL:HG22 | 1.81 | 0.63 |
| 1:2A:79:G:H1 | 1:2A:90:U:H3 | 29.66 | 0.63 |
| 11:2P:87:ASP:O | 11:2P:90:ARG:NH1 | 2.31 | 0.63 |
| 19:2X:32:PRO:O | 19:2X:77:LYS:NZ | 2.30 | 0.63 |
| 1:1A:1771:C:OP1 | 61:1A:4312:HOH:O | 2.15 | 0.63 |
| 1:2A:749:C:OP2 | 61:2A:3959:HOH:O | 2.16 | 0.63 |
| 1:1A:2140:C:N3 | 1:1A:2151:G:O6 | 2.31 | 0.63 |
| 7:1H:149:ARG:NH2 | 7:1H:167:GLU:OE2 | 2.28 | 0.63 |
| 1:2A:1002:G:C2 | 1:2A:1003:G:H1' | 3.15 | 0.63 |
| 1:2A:643:A:N1 | 1:2A:2369:A:O2' | 2.29 | 0.63 |
| 1:2A:463:G:N2 | 1:2A:466:A:OP2 | 2.28 | 0.63 |
| 17:2V:72:VAL:HG13 | 17:2V:85:LYS:HB3 | 1.80 | 0.63 |
| 1:1A:1653:G:N2 | 61:1A:4413:HOH:O | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:2O:115:VAL:HG13 | 10:2O:121:VAL:HG21 | 1.80 | 0.63 |
| 11:2P:59:LEU:HD11 | 30:28:10:ALA:HB2 | 1.81 | 0.63 |
| 1:2A:400:G:N7 | 61:2A:4028:HOH:O | 2.31 | 0.62 |
| 14:2S:15:ARG:HB3 | 14:2S:19:LYS:HE3 | 1.80 | 0.62 |
| 1:1A:895:U:H4' | 1:1A:896:A:OP1 | 2.00 | 0.62 |
| 1:1A:2393:A:H5'' | 11:1P:63:PRO:HB3 | 1.80 | 0.62 |
| 1:2A:1420:U:O2' | 1:2A:1421:G:OP1 | 2.16 | 0.62 |
| 4:1E:77:ILE:HG21 | 4:1E:195:LEU:HD11 | 1.80 | 0.62 |
| 4:2E:28:ALA:HB3 | 4:2E:93:VAL:HG12 | 1.79 | 0.62 |
| 5:2F:103:LYS:HA | 5:2F:106:ARG:HG3 | 1.80 | 0.62 |
| 1:1A:2307:G:O6 | 61:1A:4311:HOH:O | 2.15 | 0.62 |
| 1:1A:2638:G:P | 4:1E:82:ARG:HH12 | 2.21 | 0.62 |
| 18:2W:34:ASN:OD1 | 18:2W:37:ARG:NH2 | 2.32 | 0.62 |
| 19:2X:8:ILE:O | 24:22:36:ARG:NH2 | 2.32 | 0.62 |
| 1:1A:1783:A:N7 | 61:1A:4408:HOH:O | 2.31 | 0.62 |
| 1:2A:857:C:OP2 | 22:20:77:ARG:NH2 | 2.32 | 0.62 |
| 1:2A:1434:A:H61 | 1:2A:1558:A:H62 | 1.45 | 0.62 |
| 1:2A:323:G:OP2 | 57:2A:3851:LUJ:NAP | 2.33 | 0.62 |
| 6:2G:113:ARG:NH1 | 26:24:34:GLU:OE2 | 2.32 | 0.62 |
| 1:1A:1670:C:O2 | 4:1E:129:HIS:NE2 | 2.31 | 0.62 |
| 21:1Z:130:PRO:HA | 21:1Z:133:ILE:HG13 | 1.82 | 0.62 |
| 1:2A:271(U):G:H2' | 1:2A:271(V):G:H8 | 1.63 | 0.62 |
| 22:10:10:THR:HG23 | 22:10:12:ASN:H | 1.65 | 0.62 |
| 1:1A:1842:G:O2' | 3:1D:253:GLN:OE1 | 2.15 | 0.62 |
| 1:2A:1021:A:H62 | 1:2A:1141:U:H3 | 1.48 | 0.62 |
| 6:2G:11:TYR:HA | 6:2G:15:VAL:HB | 1.82 | 0.62 |
| 26:14:41:PRO:HA | 26:14:47:GLN:HB3 | 1.82 | 0.62 |
| 24:22:29:LYS:HG2 | 24:22:57:ILE:HD13 | 1.80 | 0.62 |
| 1:2A:2010:G:H5'' | 18:2W:42:ARG:HB2 | 1.82 | 0.62 |
| 1:1A:615:G:OP2 | 5:1F:43:LYS:NZ | 2.32 | 0.62 |
| 1:2A:2140:C:H42 | 1:2A:2151:G:H1 | 1.47 | 0.62 |
| 1:1A:195:A:N7 | 61:1A:4241:HOH:O | 2.31 | 0.61 |
| 6:1G:34:LEU:HD23 | 6:1G:161:THR:HG22 | 1.81 | 0.61 |
| 19:1X:57:LEU:HD11 | 19:1X:78:LYS:HE2 | 1.80 | 0.61 |
| 4:2E:36:ARG:HG2 | 4:2E:47:VAL:HG12 | 1.82 | 0.61 |
| 1:1A:1090:U:C2 | 1:1A:1102:C:H1' | 2.35 | 0.61 |
| 1:1A:2693:A:H2' | 1:1A:2694:G:H8 | 1.65 | 0.61 |
| 11:1P:59:LEU:HD21 | 30:18:10:ALA:HA | 1.82 | 0.61 |
| 1:2A:652(A):A:H3' | 1:2A:652(B):A:H5'' | 1.82 | 0.61 |
| 1:1A:2430:A:N3 | 1:1A:2430:A:H2' | 2.14 | 0.61 |
| 10:1O:98:VAL:HG11 | 10:1O:114:ILE:HG23 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2A:994:C:O2' | 1:2A:996:A:OP1 | 2.17 | 0.61 |
| 1:1A:2141:G:O6 | 1:1A:2150:U:O2 | 2.18 | 0.61 |
| 3:1D:18:VAL:HG12 | 3:1D:211:ARG:HH12 | 1.65 | 0.61 |
| 1:2A:1379:A:H4' | 1:2A:1380:G:OP2 | 1.99 | 0.61 |
| 1:2A:2839:G:H5' | 13:2R:46:GLY:HA2 | 1.83 | 0.61 |
| 2:2B:14:U:OP2 | 2:2B:70:C:O2' | 2.17 | 0.61 |
| 1:2A:2882:A:OP1 | 13:2R:96:ARG:NH1 | 2.32 | 0.61 |
| 1:2A:301:G:OP2 | 20:2Y:84:ARG:NH2 | 2.34 | 0.61 |
| 1:1A:801:G:O6 | 5:1F:53:THR:OG1 | 2.17 | 0.61 |
| 1:2A:2152:G:C2 | 1:2A:2153:G:H1' | 2.36 | 0.61 |
| 1:2A:2151:G:H2' | 1:2A:2152:G:C8 | 2.35 | 0.61 |
| 1:1A:1385:G:O2' | 1:1A:1396:U:O2 | 2.15 | 0.61 |
| 4:1E:47:VAL:HG11 | 4:1E:86:PRO:HD2 | 1.82 | 0.61 |
| 1:2A:2022:U:O2' | 1:2A:2617:C:H5' | 2.01 | 0.61 |
| 1:2A:2113:U:H3 | 1:2A:2170:A:H61 | 1.48 | 0.61 |
| 3:2D:108:PRO:HB3 | 3:2D:143:HIS:HE1 | 1.65 | 0.61 |
| 1:1A:1038:C:H42 | 1:1A:1117:G:H1 | 1.47 | 0.61 |
| 1:1A:944:G:N7 | 61:1A:4404:HOH:O | 2.30 | 0.61 |
| 25:23:12:PRO:HB2 | 25:23:20:LYS:HG2 | 1.82 | 0.61 |
| 1:2A:1794:U:H2' | 1:2A:1795:C:C6 | 2.36 | 0.61 |
| 1:2A:2404:C:O3' | 11:2P:77:ARG:NH2 | 2.33 | 0.61 |
| 27:15:40:LYS:NZ | 27:15:41:PRO:O | 2.33 | 0.61 |
| 1:1A:266:G:H5'' | 1:1A:268:C:H41 | 11.55 | 0.61 |
| 1:2A:538:G:H2' | 1:2A:539:G:H8 | 1.65 | 0.61 |
| 8:2I:72:LEU:HD21 | 8:2I:107:VAL:HG11 | 1.83 | 0.61 |
| 1:1A:1815:A:OP1 | 61:1A:4315:HOH:O | 2.16 | 0.60 |
| 1:1A:2384:G:N7 | 61:1A:4407:HOH:O | 2.31 | 0.60 |
| 9:2N:49:GLY:O | 9:2N:119:ARG:NH1 | 2.33 | 0.60 |
| 1:1A:1039:G:H1 | 1:1A:1116:C:H42 | 1.47 | 0.60 |
| 1:1A:637:A:OP1 | 11:1P:133:SER:OG | 2.16 | 0.60 |
| 1:2A:2137:C:H1' | 1:2A:2138:C:H5' | 1.83 | 0.60 |
| 1:1A:1105:U:H2' | 1:1A:1106:G:H8 | 1.66 | 0.60 |
| 26:24:59:PHE:O | 26:24:62:ARG:NH1 | 2.34 | 0.60 |
| 4:2E:179:GLU:HG3 | 15:2T:9:LEU:HD21 | 1.82 | 0.60 |
| 21:2Z:17:ALA:HB2 | 21:2Z:20:ARG:HH21 | 1.67 | 0.60 |
| 1:1A:455:C:H42 | 1:1A:476:G:H1 | 22.46 | 0.60 |
| 1:1A:613:G:N2 | 1:1A:614(C):A:O2' | 2.35 | 0.60 |
| 1:1A:993:G:OP1 | 16:1U:50:ARG:NH2 | 2.34 | 0.60 |
| 1:1A:784:A:O4' | 3:1D:227:ASN:ND2 | 2.34 | 0.60 |
| 1:2A:574:C:OP2 | 61:2A:3960:HOH:O | 2.16 | 0.60 |
| 1:2A:668:G:H5' | 1:2A:669:G:OP2 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:2S:27:SER:HA | 14:2S:88:ASP:HB3 | 1.83 | 0.60 |
| 1:1A:1173:G:O2' | 1:1A:1174:A:O4' | 2.19 | 0.60 |
| 23:11:2:SER:HB3 | 23:11:46:LEU:HD12 | 1.82 | 0.60 |
| 1:1A:1422:G:H5'' | 10:1O:48:PRO:HB3 | 99.23 | 0.60 |
| 1:1A:2206:G:H8 | 1:1A:2207:G:N7 | 1.99 | 0.60 |
| 1:2A:2693:A:H2' | 1:2A:2694:G:H8 | 1.65 | 0.60 |
| 1:1A:816:C:OP2 | 61:1A:4314:HOH:O | 2.16 | 0.60 |
| 4:2E:77:ILE:HG21 | 4:2E:195:LEU:HD11 | 1.84 | 0.60 |
| 6:2G:15:VAL:HG22 | 6:2G:175:LEU:HB3 | 1.84 | 0.60 |
| 5:1F:188:ARG:HA | 11:1P:3:LEU:HD11 | 1.83 | 0.60 |
| 13:2R:67:LEU:HD13 | 13:2R:76:VAL:HG21 | 1.83 | 0.60 |
| 1:1A:615:G:OP1 | 5:1F:40:GLN:NE2 | 2.35 | 0.60 |
| 1:2A:2584:U:O4 | 61:2A:3962:HOH:O | 2.17 | 0.60 |
| 18:1W:71:VAL:HA | 18:1W:107:LEU:HD12 | 1.82 | 0.60 |
| 1:2A:845:G:N2 | 1:2A:845:G:OP2 | 2.35 | 0.60 |
| 11:2P:52:GLU:OE1 | 11:2P:55:ARG:NH1 | 2.35 | 0.60 |
| 19:2X:4:ALA:HB1 | 19:2X:42:ALA:HA | 1.83 | 0.60 |
| 1:2A:2319:G:N2 | 14:2S:3:ARG:HD3 | 2.18 | 0.59 |
| 4:2E:12:THR:HG22 | 4:2E:13:ARG:H | 1.67 | 0.59 |
| 4:2E:135:HIS:NE2 | 61:2E:402:HOH:O | 2.30 | 0.59 |
| 15:2T:29:ARG:HG3 | 15:2T:46:GLU:HB2 | 1.84 | 0.59 |
| 1:1A:1506:C:H2' | 1:1A:1507:A:H8 | 1.67 | 0.59 |
| 1:1A:2815:C:H5' | 27:15:29:THR:HG21 | 1.84 | 0.59 |
| 9:1N:67:LEU:HD12 | 9:1N:87:LEU:HD13 | 1.85 | 0.59 |
| 13:1R:12:ARG:O | 13:1R:17:ARG:NH1 | 2.34 | 0.59 |
| 1:2A:1199:U:O2' | 61:2A:3956:HOH:O | 2.15 | 0.59 |
| 1:2A:441:U:O2 | 5:2F:46:ARG:NH2 | 2.35 | 0.59 |
| 1:1A:1321:A:H2' | 1:1A:1322:A:H8 | 1.67 | 0.59 |
| 1:2A:987:G:N2 | 1:2A:1218:C:N3 | 46.76 | 0.59 |
| 1:2A:1826:G:H4' | 3:2D:242:ARG:NH2 | 2.17 | 0.59 |
| 1:2A:1920:OMC:HM22 | 1:2A:1921:G:H5' | 1.84 | 0.59 |
| 1:2A:2203:U:H4' | 3:2D:151:LYS:HG3 | 1.84 | 0.59 |
| 1:1A:2142:C:H2' | 1:1A:2143:C:H6 | 1.66 | 0.59 |
| 8:1I:9:LEU:HD22 | 8:1I:12:LEU:HD12 | 1.84 | 0.59 |
| 1:2A:1113:U:H2' | 1:2A:1114:G:C8 | 2.36 | 0.59 |
| 1:2A:764:A:H5' | 3:2D:210:GLY:HA2 | 1.85 | 0.59 |
| 2:2B:104:U:HO2' | 21:2Z:29:TYR:HH | 1.47 | 0.59 |
| 1:1A:1786:A:H1' | 1:1A:1938:A:N6 | 2.17 | 0.59 |
| 1:1A:2160:G:O6 | 1:1A:2161:C:N4 | 2.34 | 0.59 |
| 1:2A:2600:A:N6 | 61:2A:3942:HOH:O | 2.32 | 0.59 |
| 1:2A:532:A:N6 | 1:2A:1206:G:O2' | 62.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:563:G:OP2 | 61:2A:3961:HOH:O | 2.17 | 0.59 |
| 1:1A:1696:G:N7 | 61:1A:4417:HOH:O | 2.32 | 0.59 |
| 1:1A:987:G:N7 | 61:1A:4411:HOH:O | 2.31 | 0.59 |
| 5:1F:164:ARG:HD2 | 5:1F:175:THR:HG23 | 1.84 | 0.59 |
| 1:1A:2286:A:H4' | 1:1A:2287:A:O4' | 2.02 | 0.59 |
| 21:1Z:52:SER:OG | 21:1Z:54:HIS:ND1 | 2.30 | 0.59 |
| 1:2A:1816:G:O6 | 3:2D:35:LYS:NZ | 2.24 | 0.59 |
| 1:2A:2299:G:H2' | 1:2A:2300:G:H8 | 1.66 | 0.59 |
| 1:2A:2836:U:H2' | 1:2A:2837:G:C8 | 2.38 | 0.59 |
| 1:2A:586:A:H5' | 5:2F:89:VAL:HG21 | 1.84 | 0.59 |
| 1:1A:2746:U:OP1 | 7:1H:85:LYS:NZ | 2.30 | 0.59 |
| 1:1A:882:G:H1 | 1:1A:894:C:H42 | 1.51 | 0.59 |
| 1:2A:2061:G:H5'' | 1:2A:2503:2MA:C2 | 2.33 | 0.59 |
| 1:2A:784:A:OP2 | 61:2A:3952:HOH:O | 2.17 | 0.59 |
| 1:1A:1082:U:H3 | 1:1A:1086:A:H61 | 0.67 | 0.59 |
| 2:1B:105:A:OP1 | 21:1Z:72:ARG:NH1 | 2.36 | 0.59 |
| 7:1H:3:ARG:NH1 | 7:1H:4:ILE:H | 2.00 | 0.59 |
| 11:1P:59:LEU:HD11 | 30:18:10:ALA:HB2 | 1.85 | 0.59 |
| 19:1X:60:ARG:HH22 | 29:17:47:ARG:HH12 | 1.49 | 0.59 |
| 1:2A:2079:U:OP1 | 23:21:21:ARG:NH2 | 2.36 | 0.59 |
| 1:2A:386:G:O2' | 61:2A:3963:HOH:O | 2.17 | 0.59 |
| 6:2G:79:ASN:OD1 | 6:2G:79:ASN:N | 2.36 | 0.59 |
| 28:26:26:ASN:HB3 | 28:26:29:ASN:HB2 | 1.85 | 0.58 |
| 1:2A:473:G:H2' | 1:2A:474:G:H8 | 2.70 | 0.58 |
| 9:2N:123:TYR:OH | 9:2N:130:HIS:NE2 | 2.25 | 0.58 |
| 1:1A:1588:C:H2' | 1:1A:1589:C:H6 | 1.68 | 0.58 |
| 1:1A:220:G:O2' | 1:1A:233:A:N3 | 2.34 | 0.58 |
| 3:1D:108:PRO:HD2 | 3:1D:111:LEU:HD22 | 1.85 | 0.58 |
| 1:2A:1266:G:O5' | 18:2W:15:ARG:NH2 | 2.36 | 0.58 |
| 9:1N:13:TRP:CE2 | 9:1N:133:GLN:HG2 | 2.38 | 0.58 |
| 1:2A:2414:G:N2 | 11:2P:67:MET:SD | 2.73 | 0.58 |
| 1:1A:2432:A:C4 | 23:11:33:LYS:HG2 | 2.38 | 0.58 |
| 26:14:15:ILE:HB | 26:14:32:TYR:HD1 | 1.68 | 0.58 |
| 12:2Q:75:THR:HG21 | 12:2Q:87:LYS:HE3 | 1.84 | 0.58 |
| 21:2Z:33:LEU:HD21 | 21:2Z:90:VAL:HG21 | 1.86 | 0.58 |
| 1:1A:1011:G:OP1 | 16:1U:77:SER:OG | 2.19 | 0.58 |
| 1:1A:1321:A:H2' | 1:1A:1322:A:C8 | 2.38 | 0.58 |
| 26:24:15:ILE:HB | 26:24:32:TYR:HD1 | 1.69 | 0.58 |
| 12:2Q:39:PRO:HD3 | 12:2Q:99:PRO:HG3 | 1.86 | 0.58 |
| 17:1V:14:VAL:HB | 17:1V:96:ILE:HG13 | 1.85 | 0.58 |
| 1:1A:185:U:H2' | 1:1A:186:G:H8 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:1796:U:H2' | 1:2A:1797:C:C6 | 2.38 | 0.58 |
| 1:2A:2232:U:P | 23:21:40:ARG:HH12 | 2.26 | 0.58 |
| 30:18:23:VAL:HG13 | 30:18:47:LYS:HB3 | 1.85 | 0.58 |
| 1:1A:383:U:H2' | 1:1A:385:C:H5 | 1.69 | 0.58 |
| 6:1G:18:GLU:OE2 | 6:1G:21:ARG:NH2 | 2.34 | 0.58 |
| 10:1O:36:GLY:HA3 | 10:1O:109:LYS:HD2 | 1.84 | 0.58 |
| 1:2A:686:G:N2 | 1:2A:788:A:H61 | 2.02 | 0.58 |
| 1:1A:2134:A:O2' | 1:1A:2135:A:OP1 | 2.19 | 0.58 |
| 1:1A:2379:G:O2' | 14:1S:17:ARG:NH1 | 2.22 | 0.58 |
| 1:1A:534:U:H2' | 1:1A:535:C:C6 | 2.39 | 0.58 |
| 11:1P:89:ALA:O | 11:1P:121:LYS:NZ | 2.32 | 0.58 |
| 26:24:24:THR:OG1 | 26:24:25:TYR:N | 2.32 | 0.58 |
| 1:1A:2336:A:H61 | 22:10:43:THR:HG22 | 1.68 | 0.58 |
| 19:1X:34:ALA:O | 19:1X:77:LYS:NZ | 2.31 | 0.58 |
| 1:2A:1265:A:H61 | 1:2A:2013:A:H5'' | 1.69 | 0.58 |
| 1:2A:1937:A:OP1 | 61:2A:3964:HOH:O | 2.17 | 0.58 |
| 1:2A:918:A:H2 | 2:2B:81:G:H5' | 1.69 | 0.58 |
| 1:2A:1120:G:N2 | 1:2A:1153:C:N3 | 33.04 | 0.57 |
| 1:2A:2138:C:N4 | 1:2A:2153:G:N1 | 2.32 | 0.57 |
| 20:2Y:77:PRO:HD2 | 20:2Y:106:LEU:HD23 | 1.84 | 0.57 |
| 4:1E:8:LYS:O | 4:1E:193:GLY:N | 2.32 | 0.57 |
| 1:2A:332:A:O2' | 1:2A:334:C:OP2 | 2.18 | 0.57 |
| 6:1G:126:ASP:HB2 | 6:1G:130:ASN:H | 1.68 | 0.57 |
| 15:1T:60:THR:HG22 | 15:1T:77:PRO:HA | 1.85 | 0.57 |
| 1:2A:1022:G:H22 | 1:2A:1142(A):A:H2 | 1.51 | 0.57 |
| 1:2A:1170:G:O6 | 1:2A:1180:C:N4 | 2.37 | 0.57 |
| 1:2A:1266:G:O2' | 1:2A:2012:G:O6 | 2.13 | 0.57 |
| 6:2G:68:PRO:HB3 | 6:2G:92:VAL:HB | 1.87 | 0.57 |
| 24:12:10:LEU:O | 24:12:14:ARG:HG2 | 2.03 | 0.57 |
| 1:1A:1113:U:H2' | 1:1A:1114:G:C8 | 2.39 | 0.57 |
| 1:2A:2159:G:H2' | 1:2A:2160:G:H8 | 1.70 | 0.57 |
| 3:2D:206:LEU:O | 3:2D:211:ARG:HD3 | 2.05 | 0.57 |
| 5:2F:178:PRO:HB3 | 5:2F:198:ALA:HA | 1.87 | 0.57 |
| 26:14:61:ARG:HG3 | 26:14:62:ARG:N | 2.20 | 0.57 |
| 1:1A:1052:C:H2' | 1:1A:1053:C:H6 | 1.68 | 0.57 |
| 1:1A:1366:A:OP1 | 23:11:3:LYS:NZ | 2.37 | 0.57 |
| 1:1A:1631(A):A:OP1 | 61:1A:4316:HOH:O | 2.18 | 0.57 |
| 1:1A:2136:C:N3 | 1:1A:2155:G:C2 | 2.72 | 0.57 |
| 1:1A:2328:A:H2' | 1:1A:2329:G:C8 | 2.39 | 0.57 |
| 1:2A:2336:A:H61 | 22:20:43:THR:HG22 | 1.69 | 0.57 |
| 30:28:6:THR:HG22 | 30:28:63:PRO:HD2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 21:2Z:141:VAL:HG13 | 21:2Z:142:SER:H | 1.69 | 0.57 |
| 1:1A:2334:G:O6 | 22:10:74:ARG:NH1 | 2.34 | 0.57 |
| 30:28:26:LYS:NZ | 61:28:202:HOH:O | 2.38 | 0.57 |
| 5:2F:143:ALA:HB1 | 5:2F:148:LEU:HB2 | 1.85 | 0.57 |
| 30:18:62:LEU:HB3 | 30:18:65:GLU:HG2 | 1.86 | 0.57 |
| 1:1A:1358:G:O2' | 1:1A:1373:A:N6 | 2.37 | 0.57 |
| 1:1A:2550:G:OP1 | 61:1A:4260:HOH:O | 2.17 | 0.57 |
| 1:1A:918:A:N3 | 2:1B:80:U:O2' | 2.34 | 0.57 |
| 3:1D:242:ARG:HD2 | 3:1D:246:PRO:HG3 | 1.86 | 0.57 |
| 1:2A:832:G:H5' | 11:2P:45:LEU:HD21 | 1.86 | 0.57 |
| 9:2N:4:TYR:O | 16:2U:64:ARG:NH2 | 2.31 | 0.57 |
| 1:1A:79:G:C2 | 1:1A:90:U:O2 | 30.90 | 0.57 |
| 1:2A:131:G:OP1 | 61:2A:3965:HOH:O | 2.17 | 0.57 |
| 17:2V:76:LYS:HB2 | 17:2V:81:TYR:HB3 | 1.87 | 0.57 |
| 8:1I:101:LEU:HD22 | 8:1I:107:VAL:HB | 1.85 | 0.57 |
| 25:13:8:LEU:HG | 25:13:31:LEU:HD23 | 1.86 | 0.57 |
| 1:1A:2790:A:H5'' | 1:1A:2791:C:H5' | 1.85 | 0.57 |
| 1:1A:1800:C:OP1 | 3:1D:260:ARG:NH2 | 2.38 | 0.57 |
| 30:28:33:ASN:HA | 30:28:36:LYS:HD2 | 1.86 | 0.57 |
| 1:2A:2408:U:H2' | 1:2A:2409:G:C8 | 2.40 | 0.57 |
| 21:2Z:138:GLU:HB2 | 21:2Z:156:LYS:HD3 | 1.85 | 0.57 |
| 1:1A:1071:G:H2' | 1:1A:1072:C:H6 | 1.69 | 0.56 |
| 1:1A:639:U:H2' | 1:1A:640:C:C6 | 2.40 | 0.56 |
| 1:1A:2749:A:OP1 | 7:1H:3:ARG:NH1 | 2.38 | 0.56 |
| 15:1T:108:ARG:HH22 | 15:1T:112:ARG:HD3 | 1.69 | 0.56 |
| 1:1A:1588:C:H2' | 1:1A:1589:C:C6 | 2.39 | 0.56 |
| 1:1A:2136:C:N4 | 1:1A:2155:G:C6 | 2.74 | 0.56 |
| 1:1A:2138:C:N4 | 1:1A:2153:G:H1 | 2.03 | 0.56 |
| 18:1W:25:ARG:NH2 | 18:1W:74:ALA:O | 2.36 | 0.56 |
| 1:2A:2137:C:C4 | 1:2A:2154:G:N1 | 2.70 | 0.56 |
| 4:2E:116:VAL:HG13 | 4:2E:122:PHE:HB2 | 1.86 | 0.56 |
| 1:1A:573:G:N2 | 1:1A:2031:A:OP2 | 2.37 | 0.56 |
| 1:1A:2142:C:H2' | 1:1A:2143:C:C6 | 2.39 | 0.56 |
| 1:2A:2066:C:OP1 | 61:2A:3966:HOH:O | 2.18 | 0.56 |
| 1:2A:2110:G:H3' | 1:2A:2111:C:H5' | 1.86 | 0.56 |
| 5:2F:185:ASP:HA | 5:2F:188:ARG:HD3 | 1.87 | 0.56 |
| 1:1A:571:A:O2' | 17:1V:78:LYS:HE2 | 2.05 | 0.56 |
| 1:2A:405:U:OP1 | 1:2A:406:G:O2' | 9.92 | 0.56 |
| 1:2A:18:C:O2' | 1:2A:554:U:OP1 | 2.22 | 0.56 |
| 3:2D:108:PRO:HB3 | 3:2D:143:HIS:CE1 | 2.40 | 0.56 |
| 19:1X:53:LYS:HB3 | 19:1X:82:GLN:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:223:A:O2' | 1:2A:420:C:O2 | 2.22 | 0.56 |
| 9:2N:137:LYS:NZ | 9:2N:139:GLU:OE2 | 2.31 | 0.56 |
| 17:2V:98:GLU:OE2 | 17:2V:100:ARG:NH1 | 2.38 | 0.56 |
| 1:1A:1405:U:H2' | 1:1A:1406:U:C6 | 2.41 | 0.56 |
| 1:1A:1932:A:H2' | 1:1A:1933:G:O4' | 2.06 | 0.56 |
| 3:1D:274:ARG:NH1 | 61:1D:404:HOH:O | 2.37 | 0.56 |
| 14:1S:61:ASN:HD22 | 14:1S:64:GLU:H | 1.54 | 0.56 |
| 1:2A:1824:G:N3 | 3:2D:254:THR:OG1 | 2.38 | 0.56 |
| 3:2D:242:ARG:N | 3:2D:242:ARG:HH11 | 2.03 | 0.56 |
| 1:1A:1002:G:H3' | 1:1A:1003:G:C4' | 4.81 | 0.56 |
| 1:2A:2287:A:N6 | 1:2A:2344:U:H3 | 2.02 | 0.56 |
| 1:2A:639:U:H2' | 1:2A:640:C:C6 | 2.40 | 0.56 |
| 1:2A:2319:G:H22 | 14:2S:3:ARG:HD3 | 1.69 | 0.56 |
| 1:1A:1082:U:N3 | 1:1A:1086:A:N6 | 2.14 | 0.56 |
| 12:1Q:18:LYS:O | 12:1Q:98:LYS:NZ | 2.37 | 0.56 |
| 15:1T:65:LYS:HE3 | 15:1T:67:SER:HB2 | 1.87 | 0.56 |
| 1:2A:2137:C:C2 | 1:2A:2154:G:N2 | 2.71 | 0.56 |
| 1:2A:2630:G:H2' | 1:2A:2631:G:C8 | 2.41 | 0.56 |
| 6:2G:11:TYR:OH | 6:2G:16:ARG:NH1 | 2.39 | 0.56 |
| 3:1D:108:PRO:HB3 | 3:1D:143:HIS:CE1 | 2.41 | 0.56 |
| 13:1R:2:ARG:NH1 | 13:1R:5:LYS:O | 2.38 | 0.56 |
| 1:2A:2794:C:N4 | 1:2A:2802:G:O6 | 2.38 | 0.56 |
| 1:2A:307:G:N1 | 1:2A:310:A:OP2 | 2.35 | 0.56 |
| 23:11:23:LYS:HB3 | 23:11:29:GLY:HA3 | 1.87 | 0.56 |
| 1:1A:1688:U:O2 | 1:1A:1700:A:H5' | 2.06 | 0.56 |
| 1:1A:1187:G:H5'' | 17:1V:81:TYR:CE1 | 2.41 | 0.56 |
| 1:2A:2327:A:H2' | 1:2A:2328:A:C8 | 2.41 | 0.56 |
| 1:2A:245:G:O6 | 30:28:8:LYS:NZ | 2.38 | 0.56 |
| 25:13:6:VAL:HG22 | 25:13:56:VAL:HG13 | 1.88 | 0.56 |
| 1:1A:2375:G:O2' | 1:1A:2377:A:N7 | 2.33 | 0.56 |
| 1:2A:564:C:N4 | 61:2A:3993:HOH:O | 2.35 | 0.56 |
| 15:2T:26:ASP:OD1 | 15:2T:120:ARG:NH2 | 2.32 | 0.56 |
| 23:21:83:GLU:N | 23:21:83:GLU:OE1 | 2.38 | 0.55 |
| 1:2A:1991:U:H2' | 1:2A:1992:G:H5'' | 1.88 | 0.55 |
| 1:2A:2189:U:H2' | 1:2A:2190:G:C8 | 2.41 | 0.55 |
| 1:2A:1252:G:N2 | 16:2U:37:GLU:OE2 | 2.34 | 0.55 |
| 6:1G:179:PRO:HB2 | 26:14:42:PHE:HE2 | 1.72 | 0.55 |
| 23:21:50:ARG:HG2 | 23:21:59:THR:HG22 | 1.88 | 0.55 |
| 1:2A:1600:C:OP1 | 19:2X:58:HIS:NE2 | 2.38 | 0.55 |
| 1:2A:1939:5MU:OP1 | 1:2A:2604:U:O2' | 2.22 | 0.55 |
| 1:2A:900:A:O2' | 1:2A:901:A:OP1 | 2.20 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:2693:A:H2' | 1:1A:2694:G:C8 | 2.42 | 0.55 |
| 1:1A:272(D):G:N7 | 61:1A:4430:HOH:O | 2.33 | 0.55 |
| 4:1E:89:ASP:OD1 | 4:1E:89:ASP:N | 2.37 | 0.55 |
| 1:2A:2134:A:O2' | 1:2A:2159:G:N2 | 2.39 | 0.55 |
| 21:2Z:146:ILE:HD13 | 21:2Z:174:VAL:HG13 | 1.88 | 0.55 |
| 1:1A:2135:A:N6 | 1:1A:2156:G:HO2' | 2.01 | 0.55 |
| 4:1E:59:VAL:HG21 | 4:1E:74:PRO:HB3 | 1.88 | 0.55 |
| 9:1N:121:LYS:HD3 | 9:1N:130:HIS:CE1 | 2.41 | 0.55 |
| 1:2A:1579:A:H2' | 1:2A:1580:A:C8 | 2.41 | 0.55 |
| 1:2A:300:A:OP1 | 20:2Y:86:ARG:NH2 | 2.25 | 0.55 |
| 11:1P:63:PRO:HG2 | 30:18:25:MET:HB2 | 1.89 | 0.55 |
| 2:1B:14:U:O3' | 2:1B:108:U:O2' | 2.24 | 0.55 |
| 1:2A:2161:C:H2' | 1:2A:2162:G:O4' | 2.07 | 0.55 |
| 1:2A:2472:G:H2' | 1:2A:2475:C:H42 | 1.72 | 0.55 |
| 3:2D:242:ARG:HD3 | 3:2D:246:PRO:HG3 | 1.88 | 0.55 |
| 4:2E:89:ASP:N | 4:2E:89:ASP:OD1 | 2.38 | 0.55 |
| 11:2P:121:LYS:HE2 | 11:2P:123:LEU:HD21 | 1.89 | 0.55 |
| 12:2Q:34:LEU:HB2 | 12:2Q:118:LEU:HD22 | 1.87 | 0.55 |
| 20:2Y:13:VAL:HG12 | 20:2Y:74:PRO:HA | 1.88 | 0.55 |
| 1:1A:602:G:O2' | 1:1A:655:A:N6 | 2.40 | 0.55 |
| 7:1H:3:ARG:NH2 | 7:1H:65:HIS:HB3 | 2.21 | 0.55 |
| 1:1A:2577:A:OP2 | 27:15:3:LYS:NZ | 2.39 | 0.55 |
| 1:1A:631:A:OP1 | 11:1P:65:ARG:NE | 2.36 | 0.55 |
| 3:2D:206:LEU:HD23 | 3:2D:211:ARG:HE | 1.71 | 0.55 |
| 9:2N:104:LYS:HA | 9:2N:107:LEU:HD12 | 1.89 | 0.55 |
| 1:1A:2627:G:O2' | 1:1A:2781:A:N1 | 2.35 | 0.55 |
| 1:2A:2140:C:N3 | 1:2A:2151:G:N2 | 2.48 | 0.55 |
| 1:2A:2250:G:OP1 | 12:2Q:85:LYS:NZ | 2.36 | 0.55 |
| 3:2D:80:ALA:HB3 | 3:2D:94:LEU:HB3 | 1.89 | 0.55 |
| 4:2E:9:VAL:HG22 | 4:2E:25:VAL:HB | 1.88 | 0.55 |
| 1:1A:1069:A:H2' | 1:1A:1073:A:N7 | 2.22 | 0.55 |
| 5:1F:111:ALA:HB2 | 5:1F:206:ILE:HG21 | 1.89 | 0.55 |
| 1:1A:956:G:H5'' | 12:1Q:77:LYS:HD2 | 1.89 | 0.55 |
| 1:2A:1502:C:H2' | 1:2A:1503:U:H6 | 1.72 | 0.55 |
| 4:2E:127:ASP:OD2 | 61:2E:401:HOH:O | 2.18 | 0.55 |
| 10:2O:11:ALA:O | 10:2O:99:PHE:N | 2.34 | 0.55 |
| 13:2R:33:ARG:NH2 | 13:2R:115:GLU:OE1 | 2.33 | 0.55 |
| 1:1A:2162:G:H1' | 1:1A:2173:A:H1' | 1.89 | 0.55 |
| 1:1A:657:U:H2' | 1:1A:658:C:C6 | 2.42 | 0.55 |
| 1:2A:517:C:OP1 | 27:25:16:ARG:NH2 | 2.40 | 0.55 |
| 1:2A:271(D):G:H1 | 1:2A:271(T):C:H42 | 1.54 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:2Z:73:GLN:H | 21:2Z:87:ASP:HB2 | 1.72 | 0.55 |
| 1:1A:1930:G:O2' | 1:1A:1968:G:O6 | 2.21 | 0.54 |
| 1:1A:2011:U:OP1 | 18:1W:42:ARG:NH1 | 2.40 | 0.54 |
| 1:2A:2632:A:HO2' | 1:2A:2811:G:HO2' | 1.41 | 0.54 |
| 1:2A:521:G:H2' | 1:2A:522:G:C8 | 2.42 | 0.54 |
| 1:1A:2138:C:H42 | 1:1A:2153:G:H1 | 1.54 | 0.54 |
| 1:1A:848:G:H2' | 1:1A:849:A:C8 | 2.42 | 0.54 |
| 1:2A:1514:U:H2' | 1:2A:1515:G:H8 | 1.73 | 0.54 |
| 5:2F:150:GLY:HA2 | 5:2F:172:TRP:CD2 | 2.43 | 0.54 |
| 9:2N:128:HIS:O | 9:2N:131:GLN:NE2 | 2.41 | 0.54 |
| 2:1B:66:A:H61 | 2:1B:108:U:H2' | 1.71 | 0.54 |
| 6:1G:131:TYR:HB3 | 6:1G:159:VAL:HG22 | 1.89 | 0.54 |
| 3:2D:108:PRO:HD2 | 3:2D:111:LEU:HD22 | 1.88 | 0.54 |
| 1:1A:674:G:H2' | 1:1A:675:A:H8 | 4.72 | 0.54 |
| 10:1O:86:ILE:HG22 | 10:1O:94:ARG:HD3 | 1.89 | 0.54 |
| 1:2A:1639:U:H2' | 1:2A:1640:C:H5'' | 1.88 | 0.54 |
| 1:2A:1714:G:H2' | 1:2A:1717:G:H8 | 1.72 | 0.54 |
| 1:2A:1817:G:OP1 | 3:2D:88:ARG:NH2 | 2.40 | 0.54 |
| 10:1O:68:GLU:OE1 | 10:1O:78:ARG:NH1 | 2.36 | 0.54 |
| 1:1A:1243:G:O2' | 11:1P:4:SER:O | 2.24 | 0.54 |
| 1:2A:2258:C:O2' | 1:2A:2427:C:OP2 | 2.24 | 0.54 |
| 1:2A:800:A:OP1 | 1:2A:800:A:H8 | 1.89 | 0.54 |
| 2:2B:40:U:H1' | 2:2B:45:A:H61 | 1.71 | 0.54 |
| 5:2F:120:GLU:HB2 | 5:2F:122:LYS:HG2 | 1.90 | 0.54 |
| 8:2I:3:VAL:HG12 | 8:2I:38:LEU:HA | 1.88 | 0.54 |
| 1:2A:1155:A:H5'' | 16:2U:55:ARG:HH11 | 1.71 | 0.54 |
| 19:2X:57:LEU:HD11 | 19:2X:78:LYS:HE2 | 1.89 | 0.54 |
| 1:1A:1071:G:H2' | 1:1A:1072:C:C6 | 2.42 | 0.54 |
| 1:1A:2106:G:H2' | 1:1A:2107:C:C6 | 2.43 | 0.54 |
| 1:2A:1423:G:H2' | 1:2A:1424:G:C8 | 2.43 | 0.54 |
| 1:2A:1711:C:H2' | 1:2A:1712:C:H6 | 1.73 | 0.54 |
| 1:2A:251:A:C5 | 1:2A:252:G:H1' | 2.43 | 0.54 |
| 1:2A:881:G:H1 | 1:2A:895:U:H3 | 1.55 | 0.54 |
| 12:2Q:31:ASP:N | 12:2Q:106:VAL:O | 2.37 | 0.54 |
| 1:1A:2127:G:H2' | 1:1A:2128:C:C6 | 2.43 | 0.54 |
| 1:1A:668:G:N7 | 61:1A:4425:HOH:O | 2.32 | 0.54 |
| 21:1Z:123:ASP:N | 21:1Z:123:ASP:OD1 | 2.39 | 0.54 |
| 21:1Z:92:SER:O | 21:1Z:130:PRO:HG2 | 2.08 | 0.54 |
| 1:2A:1506:C:H2' | 1:2A:1507:A:H5' | 1.89 | 0.54 |
| 1:2A:2529:G:O6 | 31:29:31:LYS:NZ | 2.41 | 0.54 |
| 1:2A:27:G:N2 | 1:2A:512:G:H1' | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:910:A:N1 | 1:2A:2277:G:H1' | 2.22 | 0.54 |
| 1:1A:1218:C:H42 | 1:1A:1231:G:H1 | 1.55 | 0.54 |
| 1:1A:2347:C:OP1 | 28:16:38:LYS:NZ | 2.36 | 0.54 |
| 1:1A:242:G:C8 | 30:18:5:LYS:HG2 | 2.43 | 0.54 |
| 1:1A:2563:U:H4' | 10:1O:28:SER:HA | 1.88 | 0.54 |
| 16:1U:50:ARG:HH12 | 17:1V:72:VAL:HA | 1.72 | 0.54 |
| 1:2A:108:U:H2' | 1:2A:109:G:C8 | 2.43 | 0.54 |
| 1:2A:2060:A:N3 | 61:2A:4045:HOH:O | 2.34 | 0.54 |
| 1:2A:455:C:H42 | 1:2A:476:G:H1 | 22.57 | 0.54 |
| 5:2F:184:TYR:CE2 | 5:2F:188:ARG:HD2 | 2.43 | 0.54 |
| 1:1A:863:A:H2' | 1:1A:864:G:C8 | 2.42 | 0.54 |
| 1:1A:1799:G:O2' | 3:1D:181:GLU:OE2 | 2.22 | 0.54 |
| 3:1D:143:HIS:ND1 | 3:1D:194:GLY:O | 2.38 | 0.54 |
| 4:1E:122:PHE:O | 61:1E:401:HOH:O | 2.18 | 0.54 |
| 15:1T:29:ARG:HG3 | 15:1T:46:GLU:HB2 | 1.90 | 0.54 |
| 1:2A:1423:G:H2' | 1:2A:1424:G:H8 | 1.72 | 0.54 |
| 1:1A:1185:C:OP2 | 61:1A:4320:HOH:O | 2.18 | 0.53 |
| 1:1A:1499:C:H2' | 1:1A:1500:G:H8 | 1.73 | 0.53 |
| 1:1A:2839:G:H5' | 13:1R:46:GLY:HA2 | 1.90 | 0.53 |
| 1:1A:2887:U:H2' | 1:1A:2888:C:C6 | 2.43 | 0.53 |
| 6:1G:126:ASP:N | 6:1G:130:ASN:O | 2.37 | 0.53 |
| 11:1P:63:PRO:HD3 | 30:18:27:THR:HG22 | 1.90 | 0.53 |
| 1:2A:2278:A:OP2 | 22:20:12:ASN:ND2 | 2.39 | 0.53 |
| 1:2A:2295:C:OP1 | 14:2S:10:ARG:NH1 | 2.40 | 0.53 |
| 1:2A:2748:A:H5' | 7:2H:4:ILE:HD12 | 1.89 | 0.53 |
| 16:2U:85:LYS:HB2 | 16:2U:116:ALA:HB1 | 1.89 | 0.53 |
| 2:1B:66:A:H61 | 2:1B:109:C:H5'' | 1.72 | 0.53 |
| 1:2A:2291:U:H2' | 1:2A:2292:C:C6 | 2.43 | 0.53 |
| 1:2A:2759:G:OP2 | 61:2A:3968:HOH:O | 2.19 | 0.53 |
| 1:2A:740:U:H2' | 1:2A:741:G:C8 | 2.43 | 0.53 |
| 1:1A:2327:A:H2' | 1:1A:2328:A:C8 | 2.43 | 0.53 |
| 3:1D:206:LEU:O | 3:1D:211:ARG:HD3 | 2.09 | 0.53 |
| 1:1A:2314:C:H5'' | 6:1G:38:VAL:HG21 | 1.89 | 0.53 |
| 18:1W:58:ALA:HB1 | 18:1W:64:MET:HB2 | 1.89 | 0.53 |
| 1:2A:1237:A:OP1 | 61:2A:3967:HOH:O | 2.18 | 0.53 |
| 1:2A:2135:A:C8 | 1:2A:2136:C:H5 | 2.26 | 0.53 |
| 1:2A:793:A:OP2 | 1:2A:2071:A:O2' | 2.25 | 0.53 |
| 1:2A:1826:G:H4' | 3:2D:242:ARG:HH21 | 1.72 | 0.53 |
| 9:2N:30:ILE:HG23 | 9:2N:52:VAL:HG11 | 1.89 | 0.53 |
| 12:2Q:85:LYS:HD3 | 22:20:7:LEU:HD13 | 1.90 | 0.53 |
| 1:1A:1051:G:H2' | 1:1A:1052:C:O4' | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2572:A:OP1 | 1:1A:2574:G:O2' | 2.24 | 0.53 |
| 1:2A:849:A:N6 | 1:2A:928:G:O2' | 2.36 | 0.53 |
| 1:2A:1800:C:OP2 | 3:2D:183:ARG:NH2 | 2.42 | 0.53 |
| 6:2G:44:GLY:N | 6:2G:88:ILE:O | 2.41 | 0.53 |
| 1:1A:1213:A:N3 | 1:1A:1238:G:O2' | 2.37 | 0.53 |
| 1:1A:2127:G:H2' | 1:1A:2128:C:H6 | 1.73 | 0.53 |
| 1:1A:97:C:OP1 | 24:12:2:LYS:NZ | 2.41 | 0.53 |
| 20:1Y:15:VAL:HG21 | 20:1Y:42:VAL:HG11 | 1.88 | 0.53 |
| 3:1D:83:GLU:OE1 | 3:1D:104:TYR:OH | 2.26 | 0.53 |
| 25:23:5:LYS:NZ | 25:23:34:GLU:OE2 | 2.37 | 0.53 |
| 1:2A:1171:G:H22 | 1:2A:1178:C:N4 | 2.06 | 0.53 |
| 1:2A:1829:A:OP1 | 61:2A:3969:HOH:O | 2.19 | 0.53 |
| 1:2A:1962:5MC:O2' | 1:2A:1964:G:OP2 | 2.25 | 0.53 |
| 1:2A:271(E):U:H2' | 1:2A:271(F):C:C6 | 2.44 | 0.53 |
| 1:2A:1287:A:H8 | 13:2R:104:ARG:HD3 | 1.73 | 0.53 |
| 1:1A:1991:U:H2' | 1:1A:1992:G:H5'' | 1.90 | 0.53 |
| 1:1A:2849:U:H4' | 1:1A:2868:A:C2 | 2.44 | 0.53 |
| 3:1D:71:ASP:OD1 | 3:1D:71:ASP:N | 2.40 | 0.53 |
| 4:1E:111:ARG:HD2 | 4:1E:160:TYR:CE2 | 2.44 | 0.53 |
| 61:1A:4467:HOH:O | 15:1T:98:LYS:NZ | 2.37 | 0.53 |
| 24:22:66:GLU:HA | 24:22:69:ARG:NH1 | 2.24 | 0.53 |
| 3:2D:242:ARG:H | 3:2D:242:ARG:HH11 | 1.55 | 0.53 |
| 11:2P:87:ASP:HB3 | 11:2P:105:LEU:HD13 | 1.90 | 0.53 |
| 21:2Z:17:ALA:HA | 21:2Z:20:ARG:HE | 1.74 | 0.53 |
| 1:1A:1794:U:H2' | 1:1A:1795:C:C6 | 2.44 | 0.53 |
| 7:1H:124:GLU:HG2 | 7:1H:132:ARG:HB3 | 1.90 | 0.53 |
| 1:2A:816:C:OP1 | 1:2A:1185:C:O2' | 2.21 | 0.53 |
| 3:2D:108:PRO:HG2 | 3:2D:111:LEU:HB2 | 1.90 | 0.53 |
| 1:2A:1815:A:P | 3:2D:54:ARG:HH12 | 2.32 | 0.53 |
| 6:1G:101:ILE:HD13 | 26:14:25:TYR:HB2 | 1.91 | 0.53 |
| 1:1A:642:G:N2 | 1:1A:645:C:OP2 | 2.37 | 0.53 |
| 14:1S:83:LYS:HB3 | 14:1S:111:GLU:HG3 | 1.91 | 0.53 |
| 1:2A:2070:G:H2' | 1:2A:2071:A:C8 | 2.44 | 0.53 |
| 1:1A:1105:U:H2' | 1:1A:1106:G:C8 | 2.44 | 0.53 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:HG22 | 1.91 | 0.53 |
| 1:1A:2291:U:H2' | 1:1A:2292:C:C6 | 2.44 | 0.53 |
| 1:1A:800:A:OP1 | 1:1A:800:A:H8 | 1.92 | 0.53 |
| 1:2A:785:G:N2 | 1:2A:797:C:O2 | 28.43 | 0.53 |
| 6:2G:41:GLN:HB3 | 6:2G:43:LEU:HD22 | 1.90 | 0.53 |
| 9:2N:38:HIS:NE2 | 9:2N:50:ASP:OD2 | 2.32 | 0.53 |
| 19:2X:11:PRO:HB3 | 19:2X:92:LEU:HD11 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:1297:C:O2' | 1:1A:1302:A:N1 | 2.40 | 0.52 |
| 1:1A:2114:A:N6 | 1:1A:2119:A:N7 | 2.57 | 0.52 |
| 6:1G:109:VAL:HG11 | 26:14:14:ILE:HG21 | 1.91 | 0.52 |
| 1:2A:857:C:H1' | 22:20:26:TYR:HE1 | 1.74 | 0.52 |
| 23:21:23:LYS:HB3 | 23:21:29:GLY:HA3 | 1.89 | 0.52 |
| 1:2A:1507:A:O2' | 1:2A:1508:A:O4' | 2.27 | 0.52 |
| 1:2A:579:G:O2' | 1:2A:2019:A:OP1 | 2.23 | 0.52 |
| 3:2D:274:ARG:O | 3:2D:275:LYS:HD2 | 2.09 | 0.52 |
| 6:2G:173:LEU:HB3 | 6:2G:178:PHE:CG | 2.44 | 0.52 |
| 1:1A:2701:C:H2' | 1:1A:2702:U:H2' | 1.92 | 0.52 |
| 6:1G:79:ASN:N | 6:1G:79:ASN:OD1 | 2.41 | 0.52 |
| 12:1Q:138:ASP:OD1 | 12:1Q:138:ASP:N | 2.42 | 0.52 |
| 1:2A:2143:C:H42 | 1:2A:2148:G:H1 | 1.55 | 0.52 |
| 1:2A:796:C:H2' | 1:2A:797:C:C6 | 2.45 | 0.52 |
| 1:1A:2222:G:OP2 | 61:1A:4323:HOH:O | 2.19 | 0.52 |
| 1:1A:588:U:H2' | 1:1A:589:C:C6 | 2.44 | 0.52 |
| 1:2A:132:G:O6 | 61:2A:3954:HOH:O | 2.14 | 0.52 |
| 1:2A:2317:C:N4 | 1:2A:2318:G:O6 | 2.43 | 0.52 |
| 5:2F:140:LEU:HD11 | 5:2F:170:LEU:HD11 | 1.91 | 0.52 |
| 13:2R:97:VAL:HG22 | 13:2R:114:VAL:HG22 | 1.91 | 0.52 |
| 17:2V:18:LEU:HD21 | 17:2V:20:LEU:HB2 | 1.92 | 0.52 |
| 23:11:77:ALA:HA | 23:11:80:LEU:HD13 | 1.92 | 0.52 |
| 1:1A:1048:A:OP2 | 1:1A:1109:C:N4 | 2.41 | 0.52 |
| 1:1A:2126:A:N6 | 1:1A:2162:G:O2' | 2.40 | 0.52 |
| 1:1A:2163:C:OP1 | 1:1A:2165:G:N2 | 2.39 | 0.52 |
| 1:1A:2299:G:H2' | 1:1A:2300:G:H8 | 1.73 | 0.52 |
| 1:1A:2821:A:N1 | 61:1A:4448:HOH:O | 2.34 | 0.52 |
| 8:1I:93:THR:H | 8:1I:96:ASP:HB2 | 1.74 | 0.52 |
| 1:2A:330:A:H2 | 1:2A:1210:A:HO2' | 1.55 | 0.52 |
| 1:2A:34:C:H2' | 1:2A:35:G:C8 | 5.16 | 0.52 |
| 1:2A:859:G:O2' | 1:2A:916:G:O6 | 2.27 | 0.52 |
| 8:2I:110:ASP:N | 8:2I:130:TYR:OH | 2.43 | 0.52 |
| 12:2Q:24:GLY:HA2 | 12:2Q:67:ARG:NH2 | 2.24 | 0.52 |
| 1:1A:2206:G:H5'' | 1:1A:2207:G:C5 | 2.44 | 0.52 |
| 1:1A:601:C:O2' | 1:1A:605:C:OP1 | 2.23 | 0.52 |
| 1:1A:1796:U:H2' | 1:1A:1797:C:C6 | 2.44 | 0.52 |
| 6:1G:126:ASP:HB3 | 6:1G:128:ARG:H | 1.74 | 0.52 |
| 28:26:9:LEU:HA | 28:26:54:ILE:HB | 1.91 | 0.52 |
| 1:2A:1385:G:O2' | 1:2A:1396:U:O2 | 2.23 | 0.52 |
| 1:2A:2110:G:O2' | 1:2A:2120:G:OP2 | 2.22 | 0.52 |
| 1:2A:2136:C:N4 | 1:2A:2155:G:N1 | 2.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2131:G:H1 | 1:2A:2158:A:N6 | 2.08 | 0.52 |
| 1:2A:2290:G:N2 | 1:2A:2373:G:O2' | 2.41 | 0.52 |
| 6:2G:18:GLU:HG2 | 6:2G:175:LEU:HD21 | 1.92 | 0.52 |
| 1:2A:1751:C:HO2' | 1:2A:2861:G:HO2' | 1.53 | 0.52 |
| 1:2A:2805:G:H2' | 1:2A:2807:G:C8 | 2.44 | 0.52 |
| 1:2A:1790:C:H5'' | 1:2A:1791:A:OP1 | 2.10 | 0.52 |
| 1:2A:2152:G:N3 | 1:2A:2153:G:H1' | 2.24 | 0.52 |
| 1:2A:2163:C:C5 | 1:2A:2164:C:H1' | 2.45 | 0.52 |
| 1:2A:2470:G:O6 | 1:2A:2481:G:N2 | 2.43 | 0.52 |
| 1:2A:321:G:OP1 | 5:2F:135:LYS:NZ | 2.40 | 0.52 |
| 1:2A:597:U:H2' | 1:2A:598:G:C8 | 2.45 | 0.52 |
| 4:2E:119:ARG:HG2 | 4:2E:120:TRP:CD1 | 2.45 | 0.52 |
| 1:1A:142(A):C:H2' | 1:1A:143:G:O4' | 2.10 | 0.52 |
| 1:1A:185:U:H2' | 1:1A:186:G:C8 | 2.45 | 0.52 |
| 1:1A:2022:U:O2' | 1:1A:2617:C:H5' | 2.10 | 0.52 |
| 1:1A:796:C:H2' | 1:1A:797:C:C6 | 2.45 | 0.52 |
| 1:1A:586:A:H5' | 5:1F:89:VAL:HG21 | 1.92 | 0.52 |
| 1:2A:1006:C:H2' | 1:2A:1007:C:O4' | 3.34 | 0.52 |
| 1:2A:1539:G:H2' | 1:2A:1540:U:O4' | 2.09 | 0.52 |
| 6:2G:101:ILE:HG22 | 6:2G:105:LYS:HE2 | 1.91 | 0.52 |
| 16:2U:50:ARG:O | 16:2U:54:LYS:NZ | 2.42 | 0.52 |
| 1:2A:993:G:N3 | 17:2V:89:GLN:NE2 | 2.58 | 0.52 |
| 1:1A:1145:C:O2 | 1:1A:1147:C:N4 | 7.98 | 0.52 |
| 1:1A:2787:C:H1' | 4:1E:62:PRO:HG3 | 1.92 | 0.52 |
| 1:1A:668:G:H5' | 1:1A:669:G:OP2 | 2.10 | 0.52 |
| 4:1E:12:THR:HG21 | 15:1T:11:GLU:HG2 | 1.92 | 0.52 |
| 15:1T:11:GLU:OE1 | 15:1T:57:PHE:HB3 | 2.10 | 0.52 |
| 26:24:64:GLY:C | 26:24:66:SER:H | 2.12 | 0.52 |
| 1:2A:1231:G:H2' | 1:2A:1232:G:C8 | 2.45 | 0.52 |
| 11:2P:95:VAL:HG13 | 11:2P:125:VAL:HA | 1.92 | 0.52 |
| 6:1G:15:VAL:HG22 | 6:1G:175:LEU:HB3 | 1.93 | 0.51 |
| 23:21:40:ARG:NH2 | 23:21:42:GLN:HG2 | 2.25 | 0.51 |
| 18:2W:35:ILE:HG23 | 27:25:28:PRO:HD2 | 1.91 | 0.51 |
| 1:2A:1514:U:H2' | 1:2A:1515:G:C8 | 2.45 | 0.51 |
| 6:2G:120:LEU:N | 6:2G:179:PRO:O | 2.33 | 0.51 |
| 7:2H:11:VAL:HG21 | 7:2H:50:VAL:HG23 | 1.91 | 0.51 |
| 1:1A:2853:C:H42 | 1:1A:2864:G:H1 | 1.58 | 0.51 |
| 1:1A:532:A:N6 | 1:1A:1206:G:O2' | 62.11 | 0.51 |
| 1:2A:479:A:N3 | 1:2A:481:G:H5'' | 2.24 | 0.51 |
| 13:2R:2:ARG:NH1 | 13:2R:5:LYS:O | 2.43 | 0.51 |
| 21:2Z:131:ARG:HG3 | 21:2Z:132:ASN:HD22 | 1.76 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:793:A:OP2 | 1:1A:2071:A:O2' | 2.27 | 0.51 |
| 1:1A:222:A:H5'' | 1:1A:421:U:OP1 | 2.10 | 0.51 |
| 1:1A:709:U:H2' | 1:1A:710:G:C8 | 2.45 | 0.51 |
| 1:1A:765:G:N1 | 1:1A:812:C:O2' | 83.99 | 0.51 |
| 1:1A:876:C:H2' | 1:1A:877:U:O4' | 2.11 | 0.51 |
| 9:1N:108:PRO:O | 9:1N:113:GLY:HA3 | 2.10 | 0.51 |
| 27:25:16:ARG:NH1 | 27:25:17:ASP:OD1 | 2.43 | 0.51 |
| 1:2A:106:C:O2 | 1:2A:294:A:O2' | 2.28 | 0.51 |
| 1:1A:1063:G:C5 | 1:1A:1064:C:N4 | 2.78 | 0.51 |
| 1:1A:2348:U:OP2 | 30:18:42:ARG:NH2 | 2.44 | 0.51 |
| 1:1A:245:G:O5' | 11:1P:73:GLY:HA2 | 2.10 | 0.51 |
| 1:1A:2499:C:OP1 | 61:1A:4327:HOH:O | 2.19 | 0.51 |
| 1:1A:2646:C:H2' | 1:1A:2647:U:O4' | 2.10 | 0.51 |
| 1:2A:1782:C:H1' | 1:2A:2609:U:H5'' | 1.93 | 0.51 |
| 1:2A:2483:C:N3 | 12:2Q:124:LYS:NZ | 2.55 | 0.51 |
| 1:2A:2590:A:O3' | 3:2D:239:ARG:NH2 | 2.43 | 0.51 |
| 1:2A:340:A:H2' | 1:2A:341:G:O4' | 2.09 | 0.51 |
| 1:2A:984:A:H5'' | 1:2A:985:C:H5 | 1.75 | 0.51 |
| 1:1A:2183:C:H2' | 1:1A:2184:G:C8 | 2.43 | 0.51 |
| 1:1A:2537:U:H2' | 1:1A:2538:C:C6 | 2.46 | 0.51 |
| 1:1A:271(H):G:H1 | 1:1A:271(P):C:H42 | 1.58 | 0.51 |
| 3:1D:37:LEU:HD13 | 3:1D:62:TYR:HB2 | 1.92 | 0.51 |
| 10:1O:104:ARG:HD3 | 15:1T:36:GLU:HG2 | 1.92 | 0.51 |
| 10:1O:24:VAL:HG13 | 10:1O:33:ALA:HB2 | 1.92 | 0.51 |
| 11:2P:50:ARG:HD3 | 30:28:7:HIS:CD2 | 2.46 | 0.51 |
| 1:2A:1005:C:H2' | 1:2A:1006:C:C6 | 2.46 | 0.51 |
| 1:2A:108:U:H2' | 1:2A:109:G:H8 | 1.75 | 0.51 |
| 1:2A:266:G:H2' | 1:2A:266:G:N3 | 3.09 | 0.51 |
| 2:2B:8:U:O3' | 14:2S:25:ARG:NH2 | 2.38 | 0.51 |
| 1:1A:1068:G:O2' | 1:1A:1070:A:N7 | 2.40 | 0.51 |
| 1:1A:2464:C:H1' | 61:1A:5662:HOH:O | 2.11 | 0.51 |
| 1:1A:266:G:H2' | 1:1A:266:G:N3 | 3.30 | 0.51 |
| 1:1A:2701:C:OP1 | 61:1A:4330:HOH:O | 2.19 | 0.51 |
| 19:1X:94:GLY:H | 19:1X:95:LEU:HB2 | 1.75 | 0.51 |
| 1:2A:2112:G:C6 | 1:2A:2113:U:H1' | 2.46 | 0.51 |
| 22:10:14:ARG:NH2 | 61:10:203:HOH:O | 2.43 | 0.51 |
| 1:1A:1009:A:OP2 | 9:1N:37:LYS:NZ | 2.23 | 0.51 |
| 1:1A:1426:G:O2' | 1:1A:1572:A:N6 | 2.42 | 0.51 |
| 1:1A:2567:G:H2' | 1:1A:2568:C:C6 | 2.46 | 0.51 |
| 1:1A:2696:U:H2' | 1:1A:2697:G:C8 | 2.46 | 0.51 |
| 3:1D:146:GLU:HB2 | 3:1D:189:CYS:HB3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:22:39:ALA:HB2 | 24:22:44:LEU:HD23 | 1.92 | 0.51 |
| 1:2A:751:A:H2 | 1:2A:789:A:HO2' | 1.58 | 0.51 |
| 1:1A:1086:A:H4' | 1:1A:1103:A:H2 | 1.74 | 0.51 |
| 1:1A:121:G:H4' | 1:1A:149:A:H5' | 1.93 | 0.51 |
| 1:1A:1593:G:H2' | 1:1A:1594:G:C8 | 2.46 | 0.51 |
| 1:1A:271(T):C:H2' | 1:1A:271(U):G:H8 | 1.76 | 0.51 |
| 1:2A:247:G:H4' | 1:2A:386:G:C5 | 2.46 | 0.51 |
| 1:2A:2630:G:H2' | 1:2A:2631:G:H8 | 1.75 | 0.51 |
| 1:2A:774:A:N3 | 1:2A:774:A:H2' | 2.26 | 0.51 |
| 4:2E:174:ASP:OD1 | 4:2E:175:VAL:N | 2.41 | 0.51 |
| 1:1A:2108:C:H2' | 1:1A:2109:U:H6 | 1.76 | 0.51 |
| 1:1A:1818:U:OP2 | 3:1D:157:ARG:HD2 | 2.11 | 0.51 |
| 7:1H:3:ARG:HH21 | 7:1H:65:HIS:HB3 | 1.76 | 0.51 |
| 1:1A:581:C:OP1 | 16:1U:33:ARG:HG3 | 2.11 | 0.51 |
| 1:2A:1119:C:H2' | 1:2A:1120:G:C8 | 3.10 | 0.51 |
| 5:2F:184:TYR:CZ | 5:2F:188:ARG:HD2 | 2.46 | 0.51 |
| 19:2X:35:THR:HG23 | 19:2X:38:GLU:HB2 | 1.92 | 0.51 |
| 1:1A:184:C:H2' | 1:1A:185:U:C6 | 2.46 | 0.51 |
| 1:1A:2079:U:O3' | 23:11:35:THR:OG1 | 2.24 | 0.51 |
| 1:1A:2848:G:C8 | 15:1T:97:ALA:HB2 | 2.45 | 0.51 |
| 4:1E:2:LYS:HB2 | 4:1E:95:ILE:HD12 | 1.92 | 0.51 |
| 15:1T:108:ARG:NH2 | 15:1T:112:ARG:HD3 | 2.26 | 0.51 |
| 1:2A:1248:G:C5 | 16:2U:3:ARG:HB2 | 2.46 | 0.51 |
| 4:2E:2:LYS:HB2 | 4:2E:95:ILE:HD12 | 1.92 | 0.51 |
| 5:2F:110:LEU:HD11 | 5:2F:181:LEU:HG | 1.93 | 0.51 |
| 5:2F:18:ARG:NH2 | 5:2F:127:GLU:OE1 | 2.38 | 0.51 |
| 12:2Q:110:THR:HG23 | 12:2Q:113:GLN:HB2 | 1.92 | 0.51 |
| 1:1A:1826:G:H4' | 3:1D:242:ARG:NH1 | 2.26 | 0.50 |
| 1:1A:214:G:N3 | 1:1A:216:A:O2' | 2.39 | 0.50 |
| 1:1A:2577:A:OP1 | 61:1A:4331:HOH:O | 2.20 | 0.50 |
| 1:1A:361:G:OP1 | 61:1A:4318:HOH:O | 2.18 | 0.50 |
| 4:1E:111:ARG:HD2 | 4:1E:160:TYR:CD2 | 2.46 | 0.50 |
| 25:23:44:ARG:HA | 25:23:47:VAL:HB | 1.93 | 0.50 |
| 1:2A:1007:C:N3 | 1:2A:1022:G:O6 | 17.06 | 0.50 |
| 1:2A:582:G:H2' | 1:2A:583:G:C8 | 2.46 | 0.50 |
| 1:2A:90:U:H1' | 1:2A:92:A:C8 | 2.45 | 0.50 |
| 10:2O:21:CYS:HB2 | 10:2O:39:ILE:HD12 | 1.93 | 0.50 |
| 1:1A:197:A:N6 | 1:1A:2430:A:O2' | 2.44 | 0.50 |
| 13:1R:67:LEU:HD13 | 13:1R:76:VAL:HG21 | 1.93 | 0.50 |
| 18:1W:92:ARG:NH2 | 61:1W:301:HOH:O | 2.41 | 0.50 |
| 20:1Y:34:LYS:NZ | 61:1Y:301:HOH:O | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:483:A:O2' | 20:1Y:49:VAL:O | 2.25 | 0.50 |
| 1:2A:2701:C:H2' | 1:2A:2702:U:H2' | 1.93 | 0.50 |
| 1:2A:2734:A:H2' | 1:2A:2735:G:O4' | 2.11 | 0.50 |
| 1:2A:660:G:H5' | 5:2F:99:TYR:CE1 | 2.46 | 0.50 |
| 1:2A:686:G:H21 | 1:2A:788:A:H61 | 1.58 | 0.50 |
| 1:2A:1652:A:OP1 | 13:2R:8:ARG:NH1 | 2.44 | 0.50 |
| 1:1A:1082:U:C4 | 1:1A:1086:A:N1 | 2.75 | 0.50 |
| 1:1A:27:G:N2 | 1:1A:512:G:H1' | 2.27 | 0.50 |
| 1:1A:686:G:N2 | 1:1A:788:A:H61 | 2.09 | 0.50 |
| 1:1A:863:A:H2' | 1:1A:864:G:H8 | 1.76 | 0.50 |
| 1:1A:875:G:H1 | 1:1A:902:C:H42 | 1.59 | 0.50 |
| 5:1F:179:GLU:HA | 5:1F:205:ARG:HH22 | 1.76 | 0.50 |
| 15:1T:49:VAL:HG12 | 15:1T:63:VAL:HG22 | 1.93 | 0.50 |
| 16:1U:58:ARG:HA | 16:1U:61:TRP:CE3 | 2.47 | 0.50 |
| 1:2A:1015:G:H2' | 1:2A:1016:G:C8 | 2.47 | 0.50 |
| 1:2A:271(U):G:H2' | 1:2A:271(V):G:C8 | 2.45 | 0.50 |
| 3:2D:237:GLU:OE2 | 61:2D:401:HOH:O | 2.18 | 0.50 |
| 1:1A:2390:U:P | 30:18:35:GLN:HE22 | 2.34 | 0.50 |
| 1:1A:942:G:O2' | 1:1A:1189:A:N3 | 2.38 | 0.50 |
| 1:2A:597:U:H2' | 1:2A:598:G:H8 | 1.77 | 0.50 |
| 15:2T:26:ASP:HA | 15:2T:92:GLY:H | 1.76 | 0.50 |
| 26:14:64:GLY:C | 26:14:66:SER:H | 2.15 | 0.50 |
| 1:1A:1268:A:H2' | 1:1A:1269:A:O4' | 2.11 | 0.50 |
| 8:1I:92:VAL:HG22 | 8:1I:120:ILE:HD12 | 1.94 | 0.50 |
| 24:22:25:VAL:HG13 | 24:22:57:ILE:HG23 | 1.93 | 0.50 |
| 6:2G:179:PRO:HG3 | 26:24:43:TYR:OH | 2.12 | 0.50 |
| 1:2A:503:A:H4' | 1:2A:504:U:H5'' | 1.93 | 0.50 |
| 6:2G:166:ASP:O | 6:2G:170:ARG:N | 2.41 | 0.50 |
| 9:2N:54:VAL:HB | 9:2N:122:VAL:HG22 | 1.93 | 0.50 |
| 1:1A:2136:C:N4 | 1:1A:2155:G:H1 | 2.08 | 0.50 |
| 1:1A:2747:G:O6 | 1:1A:2755:C:H5'' | 2.12 | 0.50 |
| 1:1A:484:C:H2' | 1:1A:485:C:C6 | 2.47 | 0.50 |
| 4:1E:116:VAL:HG13 | 4:1E:122:PHE:HB2 | 1.92 | 0.50 |
| 13:1R:11:ASN:ND2 | 61:1R:304:HOH:O | 2.44 | 0.50 |
| 1:2A:1149:G:H2' | 1:2A:1150:C:C6 | 2.46 | 0.50 |
| 1:2A:1268:A:H2' | 1:2A:1269:A:O4' | 2.12 | 0.50 |
| 1:2A:2431:U:OP1 | 61:2A:3970:HOH:O | 2.19 | 0.50 |
| 1:2A:2576:G:O2' | 1:2A:2579:C:OP2 | 2.20 | 0.50 |
| 10:2O:15:GLY:O | 10:2O:47:ILE:HG12 | 2.11 | 0.50 |
| 19:2X:12:VAL:HG22 | 19:2X:29:TRP:CE2 | 2.46 | 0.50 |
| 19:2X:44:GLU:HG3 | 19:2X:51:VAL:HG23 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2030:A:OP2 | 61:1A:4332:HOH:O | 2.20 | 0.50 |
| 1:1A:2533:A:H2' | 1:1A:2534:A:O4' | 2.12 | 0.50 |
| 1:1A:274:G:N3 | 1:1A:274:G:H2' | 2.26 | 0.50 |
| 23:21:53:VAL:HG22 | 23:21:74:VAL:HG13 | 1.94 | 0.50 |
| 1:2A:2136:C:N3 | 1:2A:2155:G:N2 | 2.50 | 0.50 |
| 1:2A:564:C:N4 | 1:2A:573:G:OP1 | 2.41 | 0.50 |
| 14:2S:77:ALA:O | 14:2S:82:ILE:N | 2.43 | 0.50 |
| 18:2W:34:ASN:ND2 | 27:25:39:MET:HG3 | 2.26 | 0.50 |
| 1:1A:1108:U:H2' | 1:1A:1109:C:O4' | 2.12 | 0.50 |
| 1:1A:1667:G:O2' | 1:1A:1991:U:O4 | 2.26 | 0.50 |
| 1:1A:881:G:C2 | 1:1A:882:G:H1' | 2.46 | 0.50 |
| 3:1D:51:VAL:HG11 | 3:1D:54:ARG:HE | 1.76 | 0.50 |
| 5:1F:110:LEU:HD11 | 5:1F:181:LEU:HG | 1.93 | 0.50 |
| 15:1T:74:ARG:HG2 | 15:1T:76:PHE:CZ | 2.47 | 0.50 |
| 23:21:7:ILE:HG23 | 23:21:98:LEU:HD11 | 1.94 | 0.50 |
| 1:2A:1231:G:H2' | 1:2A:1232:G:H8 | 1.77 | 0.50 |
| 1:2A:518:G:O5' | 18:2W:18:ARG:NH1 | 2.45 | 0.50 |
| 30:18:62:LEU:HB3 | 30:18:65:GLU:CG | 2.42 | 0.50 |
| 1:1A:1052:C:H2' | 1:1A:1053:C:C6 | 2.46 | 0.50 |
| 1:1A:2687:U:H2' | 1:1A:2688:U:O4' | 2.12 | 0.50 |
| 1:1A:740:U:H2' | 1:1A:741:G:C8 | 2.47 | 0.50 |
| 1:1A:862:G:H2' | 1:1A:863:A:O4' | 2.12 | 0.50 |
| 1:1A:910:A:N3 | 1:1A:2264:C:O2' | 2.40 | 0.50 |
| 11:1P:62:LEU:O | 30:18:13:ARG:HD3 | 2.12 | 0.50 |
| 1:2A:1405:U:H2' | 1:2A:1406:U:C6 | 2.46 | 0.50 |
| 13:2R:44:LEU:HD22 | 13:2R:48:VAL:HG23 | 1.93 | 0.50 |
| 1:1A:1025:G:C4 | 1:1A:1135:C:H1' | 2.46 | 0.49 |
| 1:1A:1094:U:H2' | 1:1A:1095:A:C8 | 2.47 | 0.49 |
| 1:1A:1608:A:H1' | 1:1A:1610:A:OP2 | 2.11 | 0.49 |
| 1:1A:636:G:OP1 | 11:1P:132:LYS:NZ | 2.44 | 0.49 |
| 2:1B:31:C:H4' | 6:1G:29:TRP:CH2 | 2.47 | 0.49 |
| 4:1E:11:MET:HG2 | 4:1E:24:THR:HB | 1.93 | 0.49 |
| 1:1A:323:G:C8 | 5:1F:171:PRO:HG3 | 2.46 | 0.49 |
| 1:2A:2539:C:H4' | 31:29:3:VAL:HG21 | 1.94 | 0.49 |
| 1:2A:2749:A:N3 | 7:2H:59:ARG:NH2 | 2.60 | 0.49 |
| 1:1A:1047:G:HO2' | 1:1A:1048:A:P | 2.35 | 0.49 |
| 1:1A:1359:A:H2' | 1:1A:1360:A:H5' | 1.94 | 0.49 |
| 1:1A:2523:G:H21 | 1:1A:2764:A:H1' | 1.78 | 0.49 |
| 1:1A:1817:G:OP1 | 3:1D:88:ARG:NH2 | 2.44 | 0.49 |
| 7:1H:35:VAL:HG11 | 7:1H:71:LEU:HB3 | 1.94 | 0.49 |
| 26:24:14:ILE:HB | 26:24:22:ILE:HB | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2393:A:H5'' | 11:2P:63:PRO:HB3 | 1.94 | 0.49 |
| 6:2G:47:LYS:HG3 | 6:2G:48:GLU:H | 1.76 | 0.49 |
| 10:2O:48:PRO:HB2 | 10:2O:49:ARG:NH1 | 2.27 | 0.49 |
| 21:2Z:30:ASN:HB3 | 21:2Z:90:VAL:HB | 1.92 | 0.49 |
| 30:18:63:PRO:HG2 | 30:18:64:TYR:CE2 | 2.48 | 0.49 |
| 1:1A:1851:U:H2' | 1:1A:1852:C:O4' | 2.11 | 0.49 |
| 1:1A:338:G:N7 | 61:1A:4439:HOH:O | 2.33 | 0.49 |
| 8:1I:14:ASP:OD1 | 8:1I:15:VAL:N | 2.45 | 0.49 |
| 15:1T:73:GLU:OE2 | 15:1T:103:ARG:NE | 2.44 | 0.49 |
| 19:1X:12:VAL:HG21 | 19:1X:27:THR:HG22 | 1.94 | 0.49 |
| 1:2A:1352:U:OP1 | 61:2A:3971:HOH:O | 2.19 | 0.49 |
| 1:2A:2143:C:H2' | 1:2A:2144:U:O4' | 2.12 | 0.49 |
| 1:2A:858:U:H1' | 1:2A:2268:A:H2' | 1.94 | 0.49 |
| 1:2A:2533:A:OP1 | 1:2A:2665:A:O2' | 2.28 | 0.49 |
| 15:2T:94:ALA:HB1 | 15:2T:99:LEU:HD21 | 1.92 | 0.49 |
| 1:1A:247:G:H4' | 1:1A:386:G:C5 | 2.47 | 0.49 |
| 1:1A:2564:A:C2 | 1:1A:2647:U:H4' | 2.47 | 0.49 |
| 1:1A:764:A:O4' | 3:1D:213:ARG:HG3 | 2.13 | 0.49 |
| 6:1G:61:ALA:HB1 | 26:14:7:PRO:HG3 | 1.94 | 0.49 |
| 12:1Q:35:VAL:HG13 | 12:1Q:130:LYS:HB3 | 1.93 | 0.49 |
| 1:2A:1264:G:H2' | 1:2A:2014:A:N6 | 2.27 | 0.49 |
| 1:2A:2292:C:OP1 | 14:2S:17:ARG:NH2 | 2.39 | 0.49 |
| 10:2O:24:VAL:HG13 | 10:2O:33:ALA:HB2 | 1.94 | 0.49 |
| 26:14:55:ARG:H | 26:14:56:VAL:HA | 1.77 | 0.49 |
| 1:1A:218:A:C2 | 1:1A:235:U:H4' | 2.48 | 0.49 |
| 1:1A:662:G:OP1 | 11:1P:16:ARG:NE | 2.34 | 0.49 |
| 10:1O:34:THR:OG1 | 10:1O:35:VAL:N | 2.44 | 0.49 |
| 14:1S:61:ASN:HD22 | 14:1S:64:GLU:HG3 | 1.78 | 0.49 |
| 8:2I:27:ARG:HG2 | 23:21:71:TYR:CZ | 2.48 | 0.49 |
| 1:2A:1410:G:H2' | 1:2A:1411:C:C6 | 2.47 | 0.49 |
| 9:2N:34:LEU:HD21 | 9:2N:120:LEU:HB2 | 1.94 | 0.49 |
| 10:2O:2:ILE:HD12 | 10:2O:6:THR:HG21 | 1.95 | 0.49 |
| 15:2T:91:ARG:HB2 | 15:2T:121:ILE:HG12 | 1.95 | 0.49 |
| 21:2Z:79:ARG:HD2 | 21:2Z:80:ARG:HH21 | 1.77 | 0.49 |
| 1:1A:1153:C:H2' | 1:1A:1154:G:O4' | 2.13 | 0.49 |
| 1:1A:1165:U:H2' | 1:1A:1166:C:C6 | 2.48 | 0.49 |
| 1:1A:1325:G:OP1 | 1:1A:1647:G:O2' | 2.24 | 0.49 |
| 1:1A:2136:C:C2 | 1:1A:2155:G:N2 | 2.80 | 0.49 |
| 1:1A:818:G:O6 | 61:1A:4325:HOH:O | 2.19 | 0.49 |
| 1:2A:2168:G:H2' | 1:2A:2170:A:N7 | 2.27 | 0.49 |
| 1:2A:2314:C:H2' | 1:2A:2315:G:H8 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:807:U:OP2 | 11:2P:41:ARG:NH2 | 2.46 | 0.49 |
| 10:2O:119:PRO:HB2 | 15:2T:68:TYR:CE2 | 2.46 | 0.49 |
| 1:1A:1406:U:H2' | 1:1A:1407:C:C6 | 2.47 | 0.49 |
| 1:1A:1881:C:H2' | 1:1A:1882:C:H6 | 1.77 | 0.49 |
| 6:1G:137:GLU:HB2 | 6:1G:140:ILE:HG12 | 1.94 | 0.49 |
| 25:23:10:LYS:HB3 | 25:23:53:LEU:HA | 1.95 | 0.49 |
| 1:2A:1711:C:H2' | 1:2A:1712:C:C6 | 2.47 | 0.49 |
| 5:2F:65:TRP:HH2 | 5:2F:72:ARG:HH21 | 1.59 | 0.49 |
| 9:2N:71:ILE:HG21 | 9:2N:84:LYS:HB3 | 1.94 | 0.49 |
| 25:13:5:LYS:NZ | 25:13:34:GLU:OE2 | 2.37 | 0.49 |
| 1:1A:1013:C:OP2 | 61:1A:4232:HOH:O | 2.18 | 0.49 |
| 1:1A:443:A:H1' | 1:1A:1201:C:O4' | 2.12 | 0.49 |
| 1:1A:2683:C:OP1 | 15:1T:53:ARG:NH2 | 2.44 | 0.49 |
| 1:1A:2839:G:OP1 | 61:1A:4329:HOH:O | 2.19 | 0.49 |
| 11:1P:95:VAL:HG13 | 11:1P:125:VAL:HA | 1.95 | 0.49 |
| 15:1T:127:ALA:C | 15:1T:129:ARG:H | 2.15 | 0.49 |
| 15:1T:73:GLU:OE1 | 15:1T:103:ARG:NH2 | 2.39 | 0.49 |
| 1:2A:1945:G:O6 | 1:2A:1960:A:N6 | 2.46 | 0.49 |
| 1:2A:212:G:H2' | 1:2A:213:A:O4' | 2.13 | 0.49 |
| 1:2A:473:G:H2' | 1:2A:474:G:C8 | 3.37 | 0.49 |
| 1:2A:903:C:H2' | 1:2A:904:C:C6 | 2.48 | 0.49 |
| 1:2A:918:A:C2 | 2:2B:81:G:H5' | 2.47 | 0.49 |
| 6:2G:73:ALA:HB3 | 6:2G:85:GLY:H | 1.76 | 0.49 |
| 30:18:23:VAL:HG11 | 30:18:47:LYS:HD3 | 1.95 | 0.49 |
| 1:1A:1176:G:H1' | 1:1A:1177:A:H5'' | 1.95 | 0.49 |
| 1:1A:1506:C:H2' | 1:1A:1507:A:C8 | 2.47 | 0.49 |
| 1:1A:1970:A:OP1 | 61:1A:4333:HOH:O | 2.20 | 0.49 |
| 1:1A:2243:U:H2' | 1:1A:2244:U:C6 | 2.48 | 0.49 |
| 1:1A:2649:U:H2' | 1:1A:2650:U:C6 | 2.48 | 0.49 |
| 6:2G:11:TYR:HB2 | 6:2G:176:LEU:HD21 | 1.95 | 0.49 |
| 12:2Q:26:TYR:O | 12:2Q:67:ARG:NH1 | 2.40 | 0.49 |
| 1:2A:144:C:H5' | 19:2X:2:LYS:HZ2 | 1.78 | 0.49 |
| 1:1A:1485:G:OP2 | 61:1A:4324:HOH:O | 2.19 | 0.49 |
| 1:1A:1508:A:HO2' | 1:1A:1509:C:P | 2.35 | 0.49 |
| 1:1A:467:G:OP1 | 29:17:33:ARG:NH1 | 2.46 | 0.49 |
| 1:1A:971:C:H2' | 1:1A:972:G:O4' | 2.13 | 0.49 |
| 1:1A:323:G:H5' | 5:1F:169:ASN:HD21 | 1.78 | 0.49 |
| 8:2I:43:ASN:ND2 | 23:21:75:GLU:OE2 | 2.46 | 0.49 |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:C8 | 2.47 | 0.49 |
| 11:2P:126:VAL:HG12 | 11:2P:148:LEU:HD23 | 1.95 | 0.49 |
| 16:2U:82:GLY:O | 16:2U:86:ALA:N | 2.35 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:10:18:ALA:HB3 | 22:10:20:ARG:NH1 | 2.27 | 0.48 |
| 1:1A:2336:A:H61 | 22:10:43:THR:CG2 | 2.25 | 0.48 |
| 1:1A:1292:U:H2' | 1:1A:1293:C:C6 | 2.48 | 0.48 |
| 15:1T:29:ARG:HH21 | 15:1T:89:VAL:HG12 | 1.78 | 0.48 |
| 20:1Y:68:HIS:ND1 | 20:1Y:70:SER:HB3 | 2.28 | 0.48 |
| 1:2A:1786:A:H1' | 1:2A:1938:A:N6 | 2.27 | 0.48 |
| 1:2A:1918:A:O2' | 1:2A:1920:OMC:N4 | 2.45 | 0.48 |
| 1:2A:336:C:H2' | 1:2A:337:C:H6 | 2.12 | 0.48 |
| 1:2A:709:U:H2' | 1:2A:710:G:C8 | 2.47 | 0.48 |
| 6:2G:131:TYR:HB3 | 6:2G:159:VAL:HG23 | 1.95 | 0.48 |
| 1:2A:1669:A:C8 | 10:2O:5:GLN:HG3 | 2.48 | 0.48 |
| 12:2Q:111:GLU:O | 12:2Q:115:MET:HG2 | 2.13 | 0.48 |
| 1:1A:1587:A:H2' | 1:1A:1588:C:C6 | 2.47 | 0.48 |
| 1:1A:18:C:O2' | 1:1A:554:U:OP1 | 2.31 | 0.48 |
| 1:1A:34:C:H2' | 1:1A:35:G:C8 | 5.65 | 0.48 |
| 1:1A:196:A:O2' | 1:1A:805:G:O6 | 2.29 | 0.48 |
| 7:1H:137:ASP:HB3 | 7:1H:140:LYS:HB3 | 1.94 | 0.48 |
| 1:2A:1013:C:H2' | 1:2A:1014:U:C6 | 2.48 | 0.48 |
| 1:2A:1019:U:O2' | 1:2A:1021:A:H2 | 1.96 | 0.48 |
| 1:2A:1354:A:H5" | 3:2D:38:LYS:HD3 | 1.95 | 0.48 |
| 1:2A:2168:G:H8 | 1:2A:2170:A:N7 | 2.11 | 0.48 |
| 7:2H:154:PRO:HB3 | 7:2H:163:TYR:CE1 | 2.48 | 0.48 |
| 1:2A:2882:A:OP1 | 13:2R:96:ARG:HD3 | 2.13 | 0.48 |
| 17:2V:43:GLU:OE1 | 17:2V:43:GLU:N | 2.46 | 0.48 |
| 20:2Y:87:LYS:HD2 | 20:2Y:95:LYS:HD2 | 1.95 | 0.48 |
| 21:2Z:52:SER:OG | 21:2Z:54:HIS:ND1 | 2.39 | 0.48 |
| 1:1A:2683:C:O2 | 10:1O:70:LYS:NZ | 2.33 | 0.48 |
| 2:1B:82:G:N2 | 61:1B:312:HOH:O | 2.46 | 0.48 |
| 7:1H:101:ARG:NH2 | 7:1H:116:GLU:OE2 | 2.46 | 0.48 |
| 9:1N:16:ILE:HG21 | 9:1N:26:LEU:HD11 | 1.95 | 0.48 |
| 14:1S:20:ARG:HD2 | 14:1S:20:ARG:HA | 1.56 | 0.48 |
| 19:1X:43:VAL:HG13 | 19:1X:47:PHE:HD2 | 1.79 | 0.48 |
| 1:2A:1423:G:OP1 | 1:2A:1492:G:O2' | 2.31 | 0.48 |
| 3:2D:85:ASP:OD2 | 3:2D:88:ARG:NH1 | 2.43 | 0.48 |
| 15:2T:127:ALA:C | 15:2T:129:ARG:H | 2.16 | 0.48 |
| 1:1A:1899:G:N3 | 1:1A:1899:G:H2' | 2.29 | 0.48 |
| 1:1A:747:U:O2 | 1:1A:2014:A:H1' | 2.13 | 0.48 |
| 1:1A:2105:C:H2' | 1:1A:2106:G:C8 | 2.49 | 0.48 |
| 1:1A:2148:G:C2 | 1:1A:2149:G:H1' | 2.49 | 0.48 |
| 22:20:48:GLY:HA3 | 22:20:80:HIS:ND1 | 2.28 | 0.48 |
| 1:2A:1152:C:H2' | 1:2A:1153:C:H6 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:2011:U:H2' | 1:2A:2012:G:O4' | 2.13 | 0.48 |
| 1:2A:2166:G:H5' | 1:2A:2167:U:OP2 | 2.14 | 0.48 |
| 1:2A:542:C:H42 | 1:2A:551:G:H1 | 1.61 | 0.48 |
| 1:2A:690:G:H2' | 1:2A:691:C:C6 | 2.48 | 0.48 |
| 5:2F:117:ARG:NH2 | 5:2F:189:THR:O | 2.44 | 0.48 |
| 1:1A:1653:G:H3' | 13:1R:2:ARG:HD3 | 1.95 | 0.48 |
| 1:1A:1668:A:H4' | 1:1A:1669:A:O5' | 2.13 | 0.48 |
| 1:1A:1955:U:OP2 | 61:1A:4326:HOH:O | 2.19 | 0.48 |
| 1:1A:881:G:H1 | 1:1A:897:C:N4 | 2.10 | 0.48 |
| 1:1A:2831:G:P | 4:1E:58:ARG:HH21 | 2.36 | 0.48 |
| 7:1H:3:ARG:HH11 | 7:1H:4:ILE:H | 1.61 | 0.48 |
| 10:1O:68:GLU:H | 10:1O:68:GLU:CD | 2.17 | 0.48 |
| 15:2T:74:ARG:HG2 | 15:2T:76:PHE:CZ | 2.48 | 0.48 |
| 21:2Z:55:HIS:CE1 | 21:2Z:135:GLU:HG3 | 2.48 | 0.48 |
| 21:2Z:77:ASP:OD2 | 21:2Z:80:ARG:HG2 | 2.13 | 0.48 |
| 1:1A:1936:A:OP1 | 1:1A:1937:A:H5' | 2.12 | 0.48 |
| 1:1A:2107:C:H42 | 1:1A:2182:G:H1 | 1.61 | 0.48 |
| 1:1A:576:U:H2' | 1:1A:577:G:C8 | 2.48 | 0.48 |
| 4:1E:170:LEU:HB3 | 4:1E:184:VAL:HG22 | 1.96 | 0.48 |
| 7:1H:11:VAL:HG21 | 7:1H:50:VAL:HG23 | 1.96 | 0.48 |
| 21:1Z:124:ILE:HD11 | 21:1Z:171:ILE:HD12 | 1.94 | 0.48 |
| 1:2A:2058:A:N7 | 61:2A:4056:HOH:O | 2.35 | 0.48 |
| 1:2A:724:U:H2' | 1:2A:725:G:O4' | 2.14 | 0.48 |
| 1:2A:2467:C:H4' | 12:2Q:123:HIS:CD2 | 2.49 | 0.48 |
| 22:10:27:GLU:HG3 | 22:10:68:GLU:HA | 1.95 | 0.48 |
| 25:13:37:LEU:HB3 | 25:13:43:ILE:HD13 | 1.96 | 0.48 |
| 1:1A:1518:U:H2' | 1:1A:1519:G:O4' | 2.14 | 0.48 |
| 1:1A:2127:G:N2 | 1:1A:2173:A:O2' | 2.46 | 0.48 |
| 1:1A:832:G:OP1 | 61:1A:4328:HOH:O | 2.19 | 0.48 |
| 21:1Z:7:ALA:HB2 | 21:1Z:59:LEU:HD22 | 1.94 | 0.48 |
| 1:2A:1485:G:H2' | 1:2A:1486:A:C8 | 2.48 | 0.48 |
| 1:2A:2207:G:H3' | 1:2A:2208:A:H5'' | 1.95 | 0.48 |
| 31:19:29:ASN:HD22 | 31:19:32:HIS:CE1 | 2.31 | 0.48 |
| 1:1A:1086:A:H3' | 1:1A:1086:A:N3 | 2.29 | 0.48 |
| 1:1A:1364:G:P | 23:11:3:LYS:HG3 | 2.54 | 0.48 |
| 1:1A:1499:C:H2' | 1:1A:1500:G:C8 | 2.49 | 0.48 |
| 1:1A:1866:C:H2' | 1:1A:1876:A:O4' | 2.13 | 0.48 |
| 1:1A:2167:U:O2 | 1:1A:2167:U:H2' | 2.13 | 0.48 |
| 1:1A:637:A:H4' | 1:1A:638:G:O5' | 2.14 | 0.48 |
| 1:1A:1009:A:P | 9:1N:37:LYS:HZ3 | 2.33 | 0.48 |
| 19:1X:44:GLU:HG3 | 19:1X:51:VAL:HG23 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2135:A:H2' | 1:2A:2136:C:C5 | 2.49 | 0.48 |
| 1:2A:2376:A:H2' | 1:2A:2377:A:O4' | 2.14 | 0.48 |
| 7:2H:45:VAL:HG12 | 7:2H:50:VAL:HG22 | 1.96 | 0.48 |
| 21:2Z:45:ASP:OD1 | 21:2Z:49:ARG:NE | 2.44 | 0.48 |
| 25:13:59:VAL:O | 25:13:60:GLU:HG2 | 2.14 | 0.48 |
| 1:1A:1056:G:H4' | 1:1A:1086:A:H8 | 1.79 | 0.48 |
| 1:1A:2377:A:H2' | 1:1A:2378:A:C8 | 2.49 | 0.48 |
| 1:1A:2679:A:H4' | 4:1E:165:VAL:HG11 | 1.95 | 0.48 |
| 1:1A:883:G:H21 | 1:1A:893:C:H42 | 1.62 | 0.48 |
| 3:1D:166:GLN:HB2 | 3:1D:174:ILE:HG22 | 1.96 | 0.48 |
| 4:1E:143:ASN:HD22 | 4:1E:147:PRO:HD2 | 1.79 | 0.48 |
| 9:1N:75:TYR:CE2 | 9:1N:77:GLY:HA2 | 2.49 | 0.48 |
| 1:1A:826:U:H4' | 11:1P:55:ARG:HB3 | 1.94 | 0.48 |
| 14:1S:61:ASN:HB3 | 14:1S:64:GLU:HB2 | 1.95 | 0.48 |
| 29:27:8:ASN:HB3 | 29:27:11:LYS:HB3 | 1.95 | 0.48 |
| 1:2A:2391:G:O2' | 1:2A:2422:A:N7 | 2.47 | 0.48 |
| 1:2A:34:C:H2' | 1:2A:35:G:H8 | 4.30 | 0.48 |
| 10:2O:105:GLU:N | 10:2O:105:GLU:OE1 | 2.40 | 0.48 |
| 15:2T:60:THR:HG22 | 15:2T:77:PRO:HA | 1.94 | 0.48 |
| 1:2A:997:G:H5'' | 16:2U:92:ARG:NH1 | 2.29 | 0.48 |
| 1:2A:483:A:O2' | 20:2Y:49:VAL:O | 2.21 | 0.48 |
| 21:2Z:121:HIS:HB2 | 21:2Z:171:ILE:HG13 | 1.94 | 0.48 |
| 27:15:11:THR:HG23 | 27:15:15:ARG:HB3 | 1.96 | 0.48 |
| 1:1A:1790:C:H2' | 1:1A:1791:A:C5 | 2.48 | 0.48 |
| 1:1A:1783:A:H5' | 1:1A:2608:G:H4' | 1.96 | 0.48 |
| 1:1A:330:A:N7 | 1:1A:1210:A:O2' | 2.34 | 0.48 |
| 1:1A:8:A:H2' | 1:1A:9:U:C6 | 2.49 | 0.48 |
| 3:1D:62:TYR:HA | 3:1D:87:ASN:OD1 | 2.13 | 0.48 |
| 1:2A:1159:U:O2' | 1:2A:1160:G:OP2 | 4.85 | 0.48 |
| 1:2A:172:C:H2' | 1:2A:173:G:H8 | 1.78 | 0.48 |
| 1:2A:2809:A:H62 | 1:2A:2891:G:H2' | 1.78 | 0.48 |
| 15:2T:83:ILE:HD13 | 15:2T:86:ILE:HD11 | 1.95 | 0.48 |
| 28:16:13:CYS:SG | 28:16:47:THR:HG21 | 2.54 | 0.47 |
| 1:1A:1301:A:O2' | 1:1A:1302:A:H3' | 2.13 | 0.47 |
| 1:1A:1268:A:C2 | 1:1A:2013:A:C4 | 3.02 | 0.47 |
| 1:1A:2072:G:N2 | 61:1A:4572:HOH:O | 2.46 | 0.47 |
| 1:1A:2477:C:N4 | 31:19:10:ILE:HG23 | 2.29 | 0.47 |
| 1:1A:2821:A:OP2 | 61:1A:4278:HOH:O | 2.19 | 0.47 |
| 21:1Z:93:ASP:HA | 21:1Z:131:ARG:HH22 | 1.79 | 0.47 |
| 30:28:30:ARG:HD3 | 30:28:30:ARG:HA | 1.50 | 0.47 |
| 1:2A:1010:A:O2' | 1:2A:1152:C:O2 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:1388:G:H2' | 1:2A:1389:G:H8 | 1.77 | 0.47 |
| 1:2A:482:A:O2' | 1:2A:497:A:N1 | 2.46 | 0.47 |
| 1:2A:531:C:H4' | 1:2A:532:A:H5'' | 1.96 | 0.47 |
| 2:2B:49:C:H2' | 2:2B:50:G:C8 | 2.49 | 0.47 |
| 6:2G:11:TYR:O | 6:2G:16:ARG:HG3 | 2.14 | 0.47 |
| 7:2H:56:SER:HB3 | 7:2H:61:HIS:ND1 | 2.29 | 0.47 |
| 8:2I:77:LEU:HD13 | 8:2I:101:LEU:HD12 | 1.96 | 0.47 |
| 9:2N:35:ARG:HG2 | 9:2N:37:LYS:HG3 | 1.96 | 0.47 |
| 1:1A:1210:A:H5'' | 1:1A:1212:G:O4' | 2.14 | 0.47 |
| 12:1Q:65:PHE:HB2 | 12:1Q:105:GLU:HB2 | 1.96 | 0.47 |
| 61:1A:4748:HOH:O | 13:1R:15:SER:HB2 | 2.15 | 0.47 |
| 1:2A:1019:U:OP1 | 1:2A:1035:U:O2' | 2.27 | 0.47 |
| 1:2A:2059:A:C8 | 1:2A:2503:2MA:HM23 | 2.49 | 0.47 |
| 1:2A:2355:C:H6 | 1:2A:2355:C:O5' | 1.97 | 0.47 |
| 15:2T:6:LEU:O | 15:2T:10:VAL:HG23 | 2.15 | 0.47 |
| 29:17:21:ARG:NH1 | 61:17:201:HOH:O | 2.37 | 0.47 |
| 1:1A:1066:U:N3 | 1:1A:1069:A:OP2 | 2.46 | 0.47 |
| 1:1A:2126:A:H4' | 1:1A:2127:G:OP1 | 2.14 | 0.47 |
| 1:1A:271(K):U:H1' | 8:1I:50:ARG:CZ | 2.44 | 0.47 |
| 1:1A:299:A:H5'' | 20:1Y:86:ARG:HH12 | 1.78 | 0.47 |
| 4:1E:79:ARG:NH1 | 61:1E:407:HOH:O | 2.46 | 0.47 |
| 7:1H:97:ARG:NE | 7:1H:104:GLU:OE1 | 2.44 | 0.47 |
| 8:1I:12:LEU:HD22 | 8:1I:19:VAL:HG21 | 1.96 | 0.47 |
| 10:1O:63:VAL:HG12 | 10:1O:106:LEU:HD11 | 1.97 | 0.47 |
| 20:1Y:83:THR:HG21 | 20:1Y:99:CYS:HB2 | 1.97 | 0.47 |
| 5:2F:167:ALA:HB1 | 5:2F:173:VAL:HG11 | 1.95 | 0.47 |
| 9:2N:67:LEU:HB3 | 9:2N:88:GLU:HG3 | 1.96 | 0.47 |
| 15:2T:105:LEU:HD22 | 15:2T:109:GLU:HB3 | 1.96 | 0.47 |
| 21:2Z:79:ARG:HD2 | 21:2Z:80:ARG:NH2 | 2.29 | 0.47 |
| 1:1A:1418:G:N7 | 61:1A:4461:HOH:O | 2.36 | 0.47 |
| 1:1A:2124:G:N2 | 1:1A:2174:C:N3 | 2.54 | 0.47 |
| 18:1W:82:LEU:HB2 | 18:1W:98:LYS:HB2 | 1.96 | 0.47 |
| 19:1X:31:HIS:NE2 | 61:1X:201:HOH:O | 2.35 | 0.47 |
| 19:1X:61:GLY:HA3 | 19:1X:73:ARG:O | 2.14 | 0.47 |
| 1:2A:1019:U:H3 | 1:2A:1142(A):A:N6 | 2.12 | 0.47 |
| 1:2A:1882:C:H2' | 1:2A:1883:G:O4' | 2.15 | 0.47 |
| 1:2A:2314:C:H2' | 1:2A:2315:G:C8 | 2.50 | 0.47 |
| 6:2G:5:VAL:HG23 | 6:2G:8:LYS:H | 1.78 | 0.47 |
| 1:2A:2493:U:O2' | 12:2Q:80:GLU:OE2 | 2.21 | 0.47 |
| 19:2X:5:TYR:CE2 | 24:22:30:ARG:HB2 | 2.49 | 0.47 |
| 1:1A:686:G:P | 29:17:11:LYS:HZ3 | 2.37 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:1086:A:H4' | 1:1A:1103:A:C2 | 2.49 | 0.47 |
| 1:1A:1295:C:H2' | 1:1A:1296:G:H8 | 1.79 | 0.47 |
| 1:1A:573:G:N1 | 1:1A:2031:A:OP2 | 2.47 | 0.47 |
| 1:1A:2176:A:H2' | 1:1A:2177:C:C6 | 2.50 | 0.47 |
| 1:1A:588:U:O4 | 1:1A:670:A:H1' | 2.14 | 0.47 |
| 4:1E:24:THR:HG22 | 4:1E:186:GLY:O | 2.14 | 0.47 |
| 11:1P:97:PRO:HD3 | 11:1P:126:VAL:O | 2.15 | 0.47 |
| 1:2A:323:G:HO2' | 1:2A:1205:U:H3 | 1.62 | 0.47 |
| 1:2A:2529:G:H5'' | 1:2A:2530:A:H5'' | 1.96 | 0.47 |
| 1:2A:854:G:H2' | 1:2A:855:G:C8 | 2.49 | 0.47 |
| 1:2A:848:G:C4 | 1:2A:933:A:H8 | 2.32 | 0.47 |
| 1:1A:2347:C:O2' | 28:16:21:TYR:OH | 2.32 | 0.47 |
| 1:1A:1300:U:H4' | 1:1A:1301:A:H5'' | 1.97 | 0.47 |
| 1:1A:1465:G:O2' | 1:1A:1545:A:N1 | 2.48 | 0.47 |
| 1:1A:579:G:O2' | 1:1A:2019:A:OP1 | 2.30 | 0.47 |
| 1:1A:2406:U:OP2 | 1:1A:2406:U:H2' | 2.15 | 0.47 |
| 1:1A:582:G:H2' | 1:1A:583:G:C8 | 2.50 | 0.47 |
| 26:24:15:ILE:HB | 26:24:32:TYR:CD1 | 2.48 | 0.47 |
| 1:2A:1636:C:H2' | 1:2A:1637:A:C8 | 2.50 | 0.47 |
| 1:2A:1889:A:H2' | 1:2A:1890:A:C8 | 2.49 | 0.47 |
| 1:2A:2870:C:H2' | 1:2A:2871:C:O4' | 2.14 | 0.47 |
| 4:2E:119:ARG:HG2 | 4:2E:120:TRP:NE1 | 2.29 | 0.47 |
| 1:2A:322:A:OP2 | 5:2F:169:ASN:HB2 | 2.14 | 0.47 |
| 8:2I:92:VAL:HG13 | 8:2I:120:ILE:HB | 1.95 | 0.47 |
| 13:2R:12:ARG:HB3 | 13:2R:16:HIS:HB3 | 1.97 | 0.47 |
| 15:2T:107:ASP:OD2 | 15:2T:111:ARG:NH1 | 2.47 | 0.47 |
| 1:1A:944:G:N1 | 1:1A:1338:G:OP2 | 84.53 | 0.47 |
| 1:1A:2031:A:C6 | 1:1A:2498:C:H1' | 2.49 | 0.47 |
| 1:1A:2203:U:H4' | 3:1D:151:LYS:HG3 | 1.97 | 0.47 |
| 1:1A:2312:U:H5' | 6:1G:88:ILE:HD11 | 1.96 | 0.47 |
| 1:1A:2791:C:H2' | 1:1A:2792:G:H8 | 1.79 | 0.47 |
| 1:1A:585:G:O6 | 1:1A:756:C:N4 | 56.92 | 0.47 |
| 2:1B:91:C:OP2 | 12:1Q:16:ARG:NH1 | 2.48 | 0.47 |
| 6:1G:129:GLY:O | 6:1G:161:THR:OG1 | 2.32 | 0.47 |
| 10:1O:115:VAL:HG13 | 10:1O:121:VAL:HG21 | 1.95 | 0.47 |
| 1:2A:1400:G:H2' | 1:2A:1401:G:H8 | 1.80 | 0.47 |
| 1:2A:1714:G:H2' | 1:2A:1717:G:C8 | 2.49 | 0.47 |
| 1:2A:2557:G:H2' | 1:2A:2558:C:C6 | 2.49 | 0.47 |
| 1:2A:2564:A:OP1 | 1:2A:2648:C:H4' | 2.15 | 0.47 |
| 1:2A:2848:G:C8 | 15:2T:97:ALA:HB2 | 2.49 | 0.47 |
| 1:2A:631:A:OP1 | 11:2P:65:ARG:NE | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:2F:57:VAL:HG13 | 5:2F:59:TYR:H | 1.79 | 0.47 |
| 1:2A:910:A:C5 | 12:2Q:13:GLN:HG3 | 2.50 | 0.47 |
| 1:1A:1103:A:H8 | 1:1A:1103:A:O5' | 1.97 | 0.47 |
| 1:1A:2140:C:N4 | 1:1A:2149:G:O6 | 2.48 | 0.47 |
| 1:1A:721:C:H2' | 1:1A:722:A:C8 | 2.50 | 0.47 |
| 2:1B:33:G:H5' | 6:1G:2:PRO:HD3 | 1.97 | 0.47 |
| 1:1A:2744:G:N2 | 7:1H:143:GLN:OE1 | 2.47 | 0.47 |
| 18:1W:68:ARG:HH11 | 18:1W:111:HIS:HA | 1.80 | 0.47 |
| 23:21:64:ALA:HA | 23:21:67:ILE:HG13 | 1.96 | 0.47 |
| 1:2A:577:G:O2' | 1:2A:1254:A:OP1 | 2.28 | 0.47 |
| 1:2A:2149:G:H2' | 1:2A:2150:U:O4' | 2.14 | 0.47 |
| 1:2A:2330:G:H2' | 1:2A:2331:G:O4' | 2.14 | 0.47 |
| 1:2A:765:G:N1 | 1:2A:812:C:O2' | 83.57 | 0.47 |
| 1:2A:900:A:HO2' | 1:2A:901:A:P | 2.35 | 0.47 |
| 4:2E:14:ILE:HD11 | 4:2E:173:VAL:HG11 | 1.95 | 0.47 |
| 19:2X:50:LYS:O | 19:2X:84:ALA:N | 2.48 | 0.47 |
| 10:1O:11:ALA:O | 10:1O:98:VAL:HA | 2.15 | 0.47 |
| 1:2A:990:A:C6 | 1:2A:1186:G:H1' | 2.50 | 0.47 |
| 1:2A:1608:A:H1' | 1:2A:1610:A:OP2 | 2.15 | 0.47 |
| 1:2A:2461:C:H2' | 1:2A:2462:U:C6 | 2.49 | 0.47 |
| 1:2A:576:U:H2' | 1:2A:577:G:C8 | 2.49 | 0.47 |
| 1:2A:1693:U:H1' | 3:2D:14:ARG:NH2 | 2.29 | 0.47 |
| 1:1A:2334:G:H5' | 14:1S:9:ARG:HG2 | 1.97 | 0.47 |
| 1:1A:948:G:N2 | 1:1A:985:C:OP2 | 2.48 | 0.47 |
| 21:1Z:155:LEU:HD12 | 21:1Z:155:LEU:HA | 1.82 | 0.47 |
| 26:24:48:ARG:HA | 26:24:48:ARG:HD3 | 1.38 | 0.47 |
| 31:29:27:CYS:SG | 31:29:28:GLU:N | 2.88 | 0.47 |
| 1:2A:2001:A:H2' | 1:2A:2002:G:C8 | 2.50 | 0.47 |
| 1:2A:2693:A:H2' | 1:2A:2694:G:C8 | 2.49 | 0.47 |
| 1:2A:2752:C:H2' | 1:2A:2753:A:O4' | 2.14 | 0.47 |
| 1:2A:336:C:H2' | 1:2A:337:C:C6 | 2.60 | 0.47 |
| 1:2A:495:G:N3 | 18:2W:61:ASN:ND2 | 2.62 | 0.47 |
| 1:2A:747:U:O2 | 1:2A:2014:A:H1' | 2.14 | 0.47 |
| 2:2B:66:A:N6 | 2:2B:109:C:H5'' | 2.30 | 0.47 |
| 8:2I:81:VAL:HG21 | 8:2I:88:ILE:HD13 | 1.96 | 0.47 |
| 1:2A:1153:C:OP1 | 16:2U:92:ARG:NH2 | 2.47 | 0.47 |
| 1:1A:2086:U:H2' | 1:1A:2087:G:C8 | 2.50 | 0.47 |
| 6:1G:9:ARG:NH1 | 6:1G:13:GLU:OE2 | 2.48 | 0.47 |
| 11:1P:90:ARG:NH1 | 11:1P:105:LEU:HD11 | 2.30 | 0.47 |
| 1:2A:2549:G:H2' | 1:2A:2550:G:H8 | 1.80 | 0.47 |
| 1:2A:933:A:OP1 | 25:23:24:LYS:NZ | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2B:3:C:H1' | 2:2B:119:G:N2 | 2.30 | 0.47 |
| 1:1A:1047:G:H2' | 1:1A:1110:G:N2 | 2.29 | 0.46 |
| 1:1A:1971:A:C4 | 3:1D:241:PRO:HD3 | 2.50 | 0.46 |
| 1:1A:453:C:O2 | 1:1A:457:A:O2' | 2.27 | 0.46 |
| 1:1A:486:C:O2' | 18:1W:60:ASN:ND2 | 2.49 | 0.46 |
| 1:1A:674:G:H2' | 1:1A:675:A:C8 | 5.02 | 0.46 |
| 5:1F:143:ALA:HB1 | 5:1F:148:LEU:HB2 | 1.97 | 0.46 |
| 7:1H:38:SER:HB3 | 7:1H:41:MET:HG2 | 1.98 | 0.46 |
| 7:1H:4:ILE:O | 7:1H:69:ARG:HD2 | 2.15 | 0.46 |
| 1:1A:1152:C:H4' | 16:1U:77:SER:HA | 1.97 | 0.46 |
| 1:1A:81:G:H21 | 20:1Y:1:MET:HE2 | 1.80 | 0.46 |
| 1:2A:1502:C:H2' | 1:2A:1503:U:C6 | 2.50 | 0.46 |
| 1:2A:1794:U:H2' | 1:2A:1795:C:H6 | 1.79 | 0.46 |
| 1:2A:1851:U:H2' | 1:2A:1852:C:O4' | 2.15 | 0.46 |
| 1:2A:2674:G:H2' | 1:2A:2675:A:C8 | 2.50 | 0.46 |
| 1:2A:2788:C:OP1 | 4:2E:61:ARG:NH2 | 2.48 | 0.46 |
| 1:2A:2893:G:H5'' | 1:2A:2894:G:O4' | 2.15 | 0.46 |
| 5:2F:64:ILE:HG21 | 5:2F:78:ILE:HG23 | 1.97 | 0.46 |
| 9:2N:34:LEU:HD23 | 9:2N:107:LEU:HD21 | 1.97 | 0.46 |
| 21:2Z:25:PRO:O | 21:2Z:85:HIS:HA | 2.15 | 0.46 |
| 1:1A:1756:G:H4' | 1:1A:1758:G:O4' | 2.14 | 0.46 |
| 1:1A:2162:G:H4' | 1:1A:2172:U:H2' | 1.96 | 0.46 |
| 2:1B:1:U:HO2' | 2:1B:2:C:P | 2.37 | 0.46 |
| 2:1B:24:G:N7 | 2:1B:56:G:H2' | 2.30 | 0.46 |
| 7:1H:25:LYS:HG2 | 7:1H:34:GLU:HG2 | 1.97 | 0.46 |
| 1:2A:1296:G:OP1 | 1:2A:2709:G:O2' | 2.20 | 0.46 |
| 1:2A:1400:G:H2' | 1:2A:1401:G:C8 | 2.50 | 0.46 |
| 1:2A:1946:U:H2' | 1:2A:1947:C:C6 | 2.50 | 0.46 |
| 1:2A:2136:C:O2' | 1:2A:2137:C:O5' | 2.33 | 0.46 |
| 1:2A:2169:A:H2' | 1:2A:2170:A:C8 | 2.49 | 0.46 |
| 1:2A:538:G:H2' | 1:2A:539:G:C8 | 2.49 | 0.46 |
| 7:2H:101:ARG:HH12 | 7:2H:122:THR:HG23 | 1.81 | 0.46 |
| 20:2Y:9:LYS:HA | 20:2Y:10:GLY:HA2 | 1.59 | 0.46 |
| 1:1A:1939:5MU:OP1 | 1:1A:2604:U:O2' | 2.31 | 0.46 |
| 1:1A:2110:G:C2 | 1:1A:2120:G:H1' | 2.50 | 0.46 |
| 1:1A:2238:G:H2' | 1:1A:2238:G:N3 | 2.30 | 0.46 |
| 1:1A:1789:A:H5'' | 3:1D:220:HIS:O | 2.15 | 0.46 |
| 4:1E:29:GLY:HA3 | 61:1E:408:HOH:O | 2.14 | 0.46 |
| 6:1G:5:VAL:HG22 | 6:1G:8:LYS:H | 1.80 | 0.46 |
| 12:1Q:32:TYR:OH | 12:1Q:111:GLU:OE1 | 2.32 | 0.46 |
| 21:1Z:149:SER:OG | 21:1Z:150:LEU:N | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:2A:1449:A:O2' | 1:2A:1529:G:N2 | 2.38 | 0.46 |
| 1:2A:2469:A:H2' | 1:2A:2470:G:O4' | 2.15 | 0.46 |
| 1:2A:2896:C:H2' | 1:2A:2897:U:C6 | 2.51 | 0.46 |
| 1:2A:614(A):U:O4 | 5:2F:175:THR:N | 2.40 | 0.46 |
| 10:2O:77:ILE:HB | 15:2T:74:ARG:HD2 | 1.96 | 0.46 |
| 1:1A:1055:G:H1 | 1:1A:1104:C:N4 | 2.10 | 0.46 |
| 1:1A:1062:G:N2 | 1:1A:1088:A:C6 | 2.83 | 0.46 |
| 1:1A:1442:G:H2' | 1:1A:1442:G:N3 | 2.89 | 0.46 |
| 1:1A:2303:G:O2' | 6:1G:132:ASN:ND2 | 2.44 | 0.46 |
| 1:1A:2492:U:H2' | 1:1A:2493:U:C6 | 2.51 | 0.46 |
| 1:1A:370:G:H4' | 1:1A:371:A:OP2 | 2.15 | 0.46 |
| 1:1A:993:G:H2' | 1:1A:995:C:H41 | 14.53 | 0.46 |
| 10:1O:68:GLU:HB3 | 10:1O:78:ARG:HB2 | 1.97 | 0.46 |
| 24:22:51:ARG:O | 24:22:55:ARG:HG2 | 2.14 | 0.46 |
| 1:2A:2030:A:H4' | 1:2A:2031:A:C8 | 2.51 | 0.46 |
| 1:2A:373:U:H2' | 1:2A:374:A:H8 | 1.80 | 0.46 |
| 1:2A:414:C:H2' | 1:2A:415:A:C8 | 2.51 | 0.46 |
| 1:2A:476:G:H2' | 1:2A:477:A:H8 | 3.89 | 0.46 |
| 1:2A:586:A:N1 | 1:2A:809:G:O2' | 2.38 | 0.46 |
| 1:2A:918:A:N3 | 2:2B:80:U:O2' | 2.42 | 0.46 |
| 2:2B:51:G:N7 | 14:2S:62:LYS:NZ | 2.56 | 0.46 |
| 26:14:15:ILE:HB | 26:14:32:TYR:CD1 | 2.49 | 0.46 |
| 1:1A:2572:A:N7 | 4:1E:145:LYS:HB2 | 2.30 | 0.46 |
| 1:1A:911:A:H2' | 12:1Q:9:TYR:OH | 2.15 | 0.46 |
| 26:24:16:CYS:SG | 26:24:17:GLY:N | 2.88 | 0.46 |
| 1:2A:1336:A:H2' | 1:2A:1337:G:C8 | 2.50 | 0.46 |
| 1:2A:1364:G:P | 23:21:3:LYS:HG3 | 2.56 | 0.46 |
| 1:2A:2070:G:H2' | 1:2A:2071:A:H8 | 1.79 | 0.46 |
| 1:2A:2284:C:P | 28:26:6:ARG:HG3 | 2.56 | 0.46 |
| 1:2A:741:G:H2' | 1:2A:742:G:O4' | 2.59 | 0.46 |
| 2:2B:74:U:H2' | 2:2B:75:G:O4' | 2.15 | 0.46 |
| 1:2A:918:A:HO2' | 2:2B:97:G:H22 | 1.60 | 0.46 |
| 6:2G:41:GLN:HG2 | 6:2G:43:LEU:HD13 | 1.96 | 0.46 |
| 4:2E:181:LEU:HD11 | 15:2T:6:LEU:HD23 | 1.98 | 0.46 |
| 25:13:23:LEU:HD13 | 25:13:50:VAL:HG11 | 1.97 | 0.46 |
| 1:1A:1064:C:N3 | 1:1A:1074:G:C6 | 2.81 | 0.46 |
| 1:1A:1504:C:H2' | 1:1A:1505:C:C6 | 2.51 | 0.46 |
| 1:1A:252:G:OP1 | 11:1P:50:ARG:NH1 | 2.39 | 0.46 |
| 1:1A:34:C:H2' | 1:1A:35:G:H8 | 4.95 | 0.46 |
| 1:1A:65:C:H5' | 19:1X:71:GLY:HA3 | 1.97 | 0.46 |
| 20:1Y:9:LYS:HA | 20:1Y:10:GLY:HA2 | 1.61 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:1Z:124:ILE:HG22 | 21:1Z:126:VAL:HG23 | 1.97 | 0.46 |
| 1:2A:2285:C:OP2 | 28:26:6:ARG:HD3 | 2.16 | 0.46 |
| 1:2A:2769:C:H2' | 1:2A:2770:G:O4' | 2.16 | 0.46 |
| 1:2A:881:G:H2' | 1:2A:882:G:C8 | 2.50 | 0.46 |
| 4:2E:170:LEU:HB3 | 4:2E:184:VAL:HG22 | 1.97 | 0.46 |
| 5:2F:24:LEU:HD21 | 5:2F:114:VAL:HG12 | 1.98 | 0.46 |
| 13:2R:70:LEU:HD12 | 13:2R:76:VAL:HG22 | 1.98 | 0.46 |
| 1:1A:11:G:O2' | 1:1A:506:G:N2 | 53.62 | 0.46 |
| 1:1A:1400:G:H2' | 1:1A:1401:G:C8 | 2.50 | 0.46 |
| 1:1A:2316:C:O2' | 6:1G:128:ARG:NH2 | 2.49 | 0.46 |
| 1:1A:2869:G:H2' | 1:1A:2870:C:O4' | 2.16 | 0.46 |
| 1:1A:396:G:H1' | 23:11:42:GLN:HB3 | 1.97 | 0.46 |
| 1:1A:816:C:H2' | 1:1A:817:C:H6 | 1.80 | 0.46 |
| 1:1A:518:G:H4' | 18:1W:18:ARG:NE | 2.31 | 0.46 |
| 1:2A:2492:U:H2' | 1:2A:2493:U:C6 | 2.51 | 0.46 |
| 1:2A:1983:C:H4' | 1:2A:2606:C:H4' | 1.97 | 0.46 |
| 1:2A:263:C:H2' | 1:2A:264:C:O4' | 2.15 | 0.46 |
| 5:2F:157:VAL:HB | 5:2F:194:MET:HG2 | 1.96 | 0.46 |
| 9:2N:53:VAL:HA | 9:2N:121:LYS:O | 2.15 | 0.46 |
| 15:2T:36:GLU:OE2 | 15:2T:41:ARG:NH2 | 2.49 | 0.46 |
| 1:1A:2577:A:H5' | 27:15:3:LYS:NZ | 2.30 | 0.46 |
| 1:1A:1427:A:H4' | 1:1A:1428:C:O4' | 2.16 | 0.46 |
| 1:1A:191:A:H2' | 1:1A:192:C:C6 | 2.51 | 0.46 |
| 1:1A:2128:C:C2 | 1:1A:2129:C:H1' | 2.51 | 0.46 |
| 1:1A:883:G:N2 | 1:1A:893:C:H42 | 2.13 | 0.46 |
| 2:1B:1:U:O2' | 2:1B:2:C:OP1 | 2.33 | 0.46 |
| 1:1A:784:A:C6 | 3:1D:229:VAL:HG11 | 2.50 | 0.46 |
| 19:1X:72:LYS:NZ | 19:1X:75:ASP:OD1 | 2.46 | 0.46 |
| 19:1X:50:LYS:HB3 | 19:1X:84:ALA:HB2 | 1.97 | 0.46 |
| 30:28:30:ARG:NH1 | 61:28:203:HOH:O | 2.48 | 0.46 |
| 1:2A:105:C:H2' | 1:2A:106:C:C6 | 2.51 | 0.46 |
| 1:2A:1316:U:H2' | 1:2A:1317:A:H8 | 1.80 | 0.46 |
| 1:2A:1406:U:H2' | 1:2A:1407:C:C6 | 2.50 | 0.46 |
| 1:2A:2127:G:N1 | 1:2A:2161:C:C2 | 2.84 | 0.46 |
| 1:2A:2863:C:H2' | 1:2A:2864:G:C8 | 2.51 | 0.46 |
| 1:2A:708:C:H42 | 1:2A:723:G:H1 | 1.62 | 0.46 |
| 1:2A:795:C:H2' | 1:2A:796:C:C6 | 2.51 | 0.46 |
| 2:2B:4:C:H42 | 2:2B:117:G:H1 | 1.64 | 0.46 |
| 1:1A:1355:G:H2' | 1:1A:1356:G:C8 | 2.99 | 0.46 |
| 1:1A:1853:A:H2' | 1:1A:1854:A:C8 | 2.51 | 0.46 |
| 1:1A:188:G:H5" | 23:11:14:VAL:HG21 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:1A:2470:G:O6 | 1:1A:2476:A:O2' | 2.21 | 0.46 |
| 1:1A:323:G:OP2 | 57:1A:4099:LUJ:NAP | 2.48 | 0.46 |
| 1:1A:531:C:H4' | 1:1A:532:A:H5'' | 1.97 | 0.46 |
| 1:1A:881:G:H1 | 1:1A:897:C:H42 | 1.63 | 0.46 |
| 2:1B:72:G:O2' | 2:1B:105:A:N6 | 2.48 | 0.46 |
| 3:1D:9:TYR:CE1 | 3:1D:13:ARG:HG3 | 2.51 | 0.46 |
| 5:1F:133:ASN:N | 5:1F:138:GLU:OE1 | 2.32 | 0.46 |
| 1:1A:443:A:C5 | 5:1F:45:ARG:HD2 | 2.51 | 0.46 |
| 14:1S:10:ARG:O | 14:1S:14:VAL:HG13 | 2.16 | 0.46 |
| 1:2A:1015:G:H2' | 1:2A:1016:G:H8 | 1.80 | 0.46 |
| 1:2A:1023:U:O2' | 1:2A:1122:G:H5' | 2.16 | 0.46 |
| 1:2A:1783:A:N7 | 61:2A:4059:HOH:O | 2.36 | 0.46 |
| 1:2A:2086:U:H2' | 1:2A:2087:G:C8 | 2.51 | 0.46 |
| 1:2A:2447:G:N2 | 1:2A:2450:A:OP2 | 2.49 | 0.46 |
| 1:2A:434:U:H2' | 1:2A:435:C:C6 | 6.32 | 0.46 |
| 1:2A:958:U:O2 | 2:2B:90:A:O2' | 2.22 | 0.46 |
| 2:2B:72:G:O2' | 2:2B:105:A:N6 | 2.49 | 0.46 |
| 12:2Q:36:ALA:HB2 | 12:2Q:103:MET:SD | 2.56 | 0.46 |
| 1:1A:1359:A:H2 | 1:1A:1372:U:O4 | 1.99 | 0.46 |
| 1:1A:1429:G:H2' | 1:1A:1430:C:C6 | 2.50 | 0.46 |
| 1:1A:1794:U:H2' | 1:1A:1795:C:H6 | 1.80 | 0.46 |
| 1:1A:2123:G:H1 | 1:1A:2175:C:H42 | 1.64 | 0.46 |
| 1:1A:2168:G:O6 | 1:1A:2171:A:H5'' | 2.16 | 0.46 |
| 1:1A:686:G:H21 | 1:1A:788:A:H61 | 1.63 | 0.46 |
| 1:1A:78:A:H2' | 1:1A:79:G:H8 | 1.81 | 0.46 |
| 4:1E:12:THR:HG22 | 4:1E:13:ARG:H | 1.80 | 0.46 |
| 8:1I:9:LEU:HB3 | 8:1I:12:LEU:HB2 | 1.98 | 0.46 |
| 15:1T:109:GLU:O | 15:1T:113:LYS:HG2 | 2.15 | 0.46 |
| 15:1T:94:ALA:HB1 | 15:1T:99:LEU:HD21 | 1.98 | 0.46 |
| 1:2A:570:G:H2' | 1:2A:2030:A:C5 | 2.51 | 0.46 |
| 1:2A:249:C:H4' | 1:2A:250:G:O5' | 2.16 | 0.46 |
| 1:2A:947:G:H2' | 1:2A:948:G:C8 | 2.51 | 0.46 |
| 3:2D:96:HIS:HD2 | 3:2D:102:LYS:HG2 | 1.81 | 0.46 |
| 1:1A:1826:G:H2' | 1:1A:1827:C:O4' | 2.17 | 0.45 |
| 1:1A:2183:C:HO2' | 1:1A:2184:G:P | 2.39 | 0.45 |
| 1:1A:2639:A:H2' | 1:1A:2640:G:O4' | 2.17 | 0.45 |
| 1:1A:463:G:N2 | 1:1A:466:A:OP2 | 2.44 | 0.45 |
| 17:1V:50:PRO:HG2 | 17:1V:51:VAL:HG12 | 1.97 | 0.45 |
| 24:22:25:VAL:HG11 | 24:22:61:LEU:HD21 | 1.99 | 0.45 |
| 1:2A:1993:U:H2' | 1:2A:1994:C:O4' | 2.16 | 0.45 |
| 1:2A:2117:A:O2' | 1:2A:2118:U:H5'' | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2A:2131:G:H4' | 1:2A:2132:U:H3' | 1.98 | 0.45 |
| 1:2A:2507:C:H2' | 1:2A:2508:G:O4' | 2.16 | 0.45 |
| 1:2A:457:A:H5'' | 61:2A:4527:HOH:O | 2.15 | 0.45 |
| 1:2A:783:A:O2' | 1:2A:785:G:OP1 | 2.30 | 0.45 |
| 1:2A:192:C:O2' | 1:2A:802:A:N3 | 2.44 | 0.45 |
| 6:2G:41:GLN:HE21 | 6:2G:153:ARG:HB3 | 1.81 | 0.45 |
| 8:2I:75:LEU:HD13 | 8:2I:105:HIS:CE1 | 2.51 | 0.45 |
| 11:2P:121:LYS:O | 11:2P:123:LEU:N | 2.48 | 0.45 |
| 1:1A:1000:A:H62 | 1:1A:1154:G:H2' | 1.81 | 0.45 |
| 1:1A:2188:C:H2' | 1:1A:2189:U:O4' | 2.16 | 0.45 |
| 1:1A:2695:C:H2' | 1:1A:2696:U:C6 | 2.51 | 0.45 |
| 1:1A:2773:C:H2' | 1:1A:2774:C:H6 | 1.81 | 0.45 |
| 1:1A:628:G:H2' | 1:1A:629:G:C8 | 2.51 | 0.45 |
| 4:1E:174:ASP:OD1 | 4:1E:175:VAL:N | 2.48 | 0.45 |
| 8:1I:78:THR:H | 8:1I:104:GLN:NE2 | 2.10 | 0.45 |
| 24:22:39:ALA:HA | 24:22:44:LEU:HB3 | 1.99 | 0.45 |
| 1:2A:1131:G:O6 | 1:2A:2040:C:H1' | 2.17 | 0.45 |
| 1:2A:2115:G:H2' | 1:2A:2116:G:H3' | 1.97 | 0.45 |
| 1:2A:2309:A:OP1 | 1:2A:2309:A:H8 | 1.99 | 0.45 |
| 1:2A:297:C:H2' | 1:2A:298:G:O4' | 2.17 | 0.45 |
| 1:2A:2875:C:O2' | 15:2T:2:ASN:OD1 | 2.25 | 0.45 |
| 1:1A:2271:G:OP1 | 22:10:18:ALA:HB1 | 2.17 | 0.45 |
| 25:13:19:GLN:OE1 | 25:13:52:HIS:NE2 | 2.40 | 0.45 |
| 25:13:7:LYS:HB2 | 25:13:34:GLU:HG3 | 1.98 | 0.45 |
| 1:1A:1149:G:H2' | 1:1A:1150:C:C6 | 2.51 | 0.45 |
| 1:1A:2010:G:H5'' | 18:1W:42:ARG:HB2 | 1.98 | 0.45 |
| 1:1A:524:U:H2' | 1:1A:525:U:C6 | 2.51 | 0.45 |
| 1:1A:536:A:H2' | 1:1A:537:C:C6 | 2.51 | 0.45 |
| 1:1A:839:U:H2' | 1:1A:840:C:C6 | 2.51 | 0.45 |
| 3:1D:148:GLU:OE1 | 3:1D:151:LYS:NZ | 2.37 | 0.45 |
| 21:1Z:137:ILE:HA | 21:1Z:156:LYS:HE2 | 1.98 | 0.45 |
| 1:2A:1479:G:H5' | 1:2A:1558:A:H2 | 1.81 | 0.45 |
| 1:2A:1557:C:OP2 | 1:2A:1558:A:O2' | 2.18 | 0.45 |
| 1:2A:320:A:H4' | 1:2A:322:A:N7 | 2.31 | 0.45 |
| 1:2A:661:C:H2' | 1:2A:662:G:C8 | 2.51 | 0.45 |
| 1:2A:927:G:O6 | 1:2A:928:G:N2 | 2.49 | 0.45 |
| 1:1A:1882:C:H2' | 1:1A:1883:G:O4' | 2.15 | 0.45 |
| 1:1A:785:G:N2 | 1:1A:797:C:O2 | 28.27 | 0.45 |
| 26:24:26:SER:OG | 26:24:27:THR:N | 2.49 | 0.45 |
| 1:2A:1670:C:O2 | 4:2E:129:HIS:NE2 | 2.42 | 0.45 |
| 1:2A:2157:G:O2' | 1:2A:2158:A:OP2 | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:2815:C:H5' | 27:25:29:THR:HG21 | 1.98 | 0.45 |
| 1:2A:698:C:H4' | 1:2A:734:A:H61 | 1.82 | 0.45 |
| 1:2A:817:C:O2' | 1:2A:839:U:H5'' | 2.17 | 0.45 |
| 3:2D:77:ALA:HA | 3:2D:97:TYR:HA | 1.98 | 0.45 |
| 10:2O:122:LEU:HD23 | 15:2T:43:GLN:NE2 | 2.31 | 0.45 |
| 1:2A:2845:G:H5'' | 15:2T:54:ARG:O | 2.17 | 0.45 |
| 1:1A:330:A:H8 | 1:1A:1210:A:C4 | 2.35 | 0.45 |
| 1:1A:2409:G:N3 | 61:1A:4468:HOH:O | 2.36 | 0.45 |
| 1:1A:466:A:N3 | 1:1A:683:C:H1' | 2.32 | 0.45 |
| 2:1B:13:A:O2' | 2:1B:15:A:H5'' | 2.17 | 0.45 |
| 5:1F:195:ASP:HB3 | 5:1F:198:ALA:H | 1.80 | 0.45 |
| 6:1G:56:ALA:O | 6:1G:59:GLU:HG2 | 2.16 | 0.45 |
| 7:1H:154:PRO:HB3 | 7:1H:163:TYR:CZ | 2.52 | 0.45 |
| 9:1N:77:GLY:O | 61:1N:301:HOH:O | 2.21 | 0.45 |
| 9:1N:67:LEU:O | 9:1N:88:GLU:HG3 | 2.16 | 0.45 |
| 1:2A:1165:U:H2' | 1:2A:1166:C:C6 | 2.52 | 0.45 |
| 1:2A:2105:C:H2' | 1:2A:2106:G:C8 | 2.52 | 0.45 |
| 1:2A:2340:G:H2' | 1:2A:2341:G:H8 | 1.81 | 0.45 |
| 1:2A:233:A:H2' | 1:2A:234:C:O4' | 2.17 | 0.45 |
| 1:2A:478:A:N1 | 1:2A:500:G:H4' | 2.32 | 0.45 |
| 1:2A:674:G:H2' | 1:2A:675:A:H8 | 4.80 | 0.45 |
| 1:2A:892:G:H3' | 1:2A:893:C:H4' | 1.97 | 0.45 |
| 26:14:58:ARG:N | 26:14:58:ARG:HD2 | 2.30 | 0.45 |
| 1:1A:1040:C:H2' | 1:1A:1041:C:O4' | 2.16 | 0.45 |
| 1:1A:2130:U:H2' | 1:1A:2158:A:N1 | 2.31 | 0.45 |
| 1:1A:2680:C:H5' | 4:1E:189:PRO:HA | 1.98 | 0.45 |
| 19:1X:41:ASN:O | 19:1X:45:THR:HG23 | 2.16 | 0.45 |
| 20:1Y:86:ARG:HB2 | 20:1Y:98:VAL:HG23 | 1.98 | 0.45 |
| 1:2A:2152:G:C4 | 1:2A:2153:G:H1' | 2.52 | 0.45 |
| 1:2A:2846:G:H2' | 1:2A:2847:U:O4' | 2.16 | 0.45 |
| 1:2A:598:G:HO2' | 5:2F:31:HIS:CE1 | 2.35 | 0.45 |
| 9:2N:42:TRP:HA | 9:2N:48:MET:SD | 2.57 | 0.45 |
| 12:2Q:57:HIS:CE1 | 12:2Q:116:GLU:HG2 | 2.52 | 0.45 |
| 1:1A:2206:G:H4' | 1:1A:2206:G:OP2 | 2.15 | 0.45 |
| 16:1U:86:ALA:O | 17:1V:49:THR:HG23 | 2.17 | 0.45 |
| 25:23:6:VAL:HG13 | 25:23:56:VAL:HG22 | 1.99 | 0.45 |
| 1:2A:184:C:H2' | 1:2A:185:U:C6 | 2.51 | 0.45 |
| 1:2A:2096:U:H3 | 1:2A:2193:G:H1 | 1.65 | 0.45 |
| 1:2A:2203:U:H2' | 1:2A:2205:C:C6 | 2.52 | 0.45 |
| 1:2A:2386:C:H2' | 1:2A:2387:U:C6 | 2.51 | 0.45 |
| 1:2A:590:A:H2' | 1:2A:591:C:C6 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1009:A:OP2 | 9:2N:37:LYS:NZ | 2.50 | 0.45 |
| 14:2S:28:VAL:HG11 | 14:2S:98:VAL:HG13 | 1.99 | 0.45 |
| 22:10:10:THR:CG2 | 22:10:12:ASN:H | 2.29 | 0.45 |
| 1:1A:143:G:H2' | 1:1A:143(A):C:C6 | 2.52 | 0.45 |
| 1:1A:2101:G:H2' | 1:1A:2102:U:C6 | 2.51 | 0.45 |
| 1:2A:1161:C:H2' | 1:2A:1162:G:C8 | 2.52 | 0.45 |
| 1:2A:1428:C:N4 | 1:2A:1570:A:OP2 | 2.44 | 0.45 |
| 1:2A:2689:U:OP2 | 1:2A:2719:G:N2 | 2.36 | 0.45 |
| 1:2A:2831:G:H2' | 61:2A:4405:HOH:O | 2.16 | 0.45 |
| 1:2A:656:G:H2' | 1:2A:657:U:O4' | 2.15 | 0.45 |
| 3:2D:5:LYS:HG2 | 3:2D:17:THR:HG22 | 1.98 | 0.45 |
| 5:2F:164:ARG:O | 5:2F:168:ARG:HB2 | 2.16 | 0.45 |
| 15:2T:11:GLU:O | 15:2T:15:VAL:HG23 | 2.17 | 0.45 |
| 1:1A:1028:A:N6 | 1:1A:1125:G:H2' | 2.31 | 0.45 |
| 1:1A:1086:A:O2' | 1:1A:1087:G:N7 | 2.45 | 0.45 |
| 1:1A:1424:G:H2' | 1:1A:1425:G:O4' | 2.17 | 0.45 |
| 1:1A:26:G:C6 | 1:1A:27:G:N1 | 2.85 | 0.45 |
| 1:1A:607:U:OP1 | 5:1F:102:PRO:HA | 2.17 | 0.45 |
| 5:1F:106:ARG:HG2 | 5:1F:106:ARG:H | 1.44 | 0.45 |
| 5:1F:178:PRO:HB2 | 5:1F:201:VAL:HG21 | 1.98 | 0.45 |
| 30:28:26:LYS:HB2 | 30:28:44:LYS:O | 2.16 | 0.45 |
| 1:2A:143(A):C:O2' | 19:2X:2:LYS:NZ | 2.50 | 0.45 |
| 1:2A:1581:G:H2' | 1:2A:1582:C:O4' | 2.17 | 0.45 |
| 1:2A:271(H):G:H2' | 1:2A:271(I):G:H8 | 1.80 | 0.45 |
| 1:2A:446:G:OP1 | 16:2U:3:ARG:HD3 | 2.17 | 0.45 |
| 1:1A:2164:C:H2' | 1:1A:2165:G:H5' | 1.98 | 0.45 |
| 1:1A:2262:U:OP2 | 22:10:19:LYS:NZ | 2.48 | 0.45 |
| 1:1A:278:A:H2 | 1:1A:362:U:H3 | 1.65 | 0.45 |
| 1:1A:2801(A):A:N3 | 1:1A:2895:U:H1' | 2.32 | 0.45 |
| 1:1A:895:U:O2' | 1:1A:896:A:H5' | 2.16 | 0.45 |
| 6:1G:107:LEU:HA | 6:1G:111:LEU:HD12 | 1.98 | 0.45 |
| 5:1F:34:TRP:CH2 | 11:1P:8:PRO:HB3 | 2.52 | 0.45 |
| 1:2A:1149:G:H2' | 1:2A:1150:C:H6 | 1.81 | 0.45 |
| 1:2A:1614:A:P | 1:2A:1614:A:H8 | 2.39 | 0.45 |
| 1:2A:2151:G:H2' | 1:2A:2152:G:H8 | 1.79 | 0.45 |
| 1:2A:2369:A:H2' | 1:2A:2370:G:H8 | 1.82 | 0.45 |
| 1:2A:629:G:H2' | 1:2A:630:G:O4' | 2.53 | 0.45 |
| 1:2A:757:U:OP2 | 57:2A:3852:LUJ:NAP | 2.50 | 0.45 |
| 2:2B:78:A:H2' | 2:2B:79:C:O4' | 2.17 | 0.45 |
| 3:2D:18:VAL:HG12 | 3:2D:211:ARG:HH12 | 1.82 | 0.45 |
| 1:1A:1779:U:H2' | 61:1A:4408:HOH:O | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:2136:C:C4 | 1:1A:2155:G:N1 | 2.85 | 0.44 |
| 1:1A:2803:C:H2' | 1:1A:2804:C:C6 | 2.51 | 0.44 |
| 1:1A:1799:G:C8 | 3:1D:177:LEU:HD12 | 2.53 | 0.44 |
| 15:1T:88:ILE:HG12 | 15:1T:88:ILE:H | 1.59 | 0.44 |
| 1:2A:83:G:O2' | 1:2A:102:G:N2 | 2.49 | 0.44 |
| 1:2A:2364:C:OP1 | 22:20:55:ARG:NH1 | 2.47 | 0.44 |
| 1:2A:921:G:H4' | 1:2A:2269:A:C5 | 2.52 | 0.44 |
| 3:2D:19:ALA:HB2 | 3:2D:204:ILE:HD11 | 1.99 | 0.44 |
| 5:2F:155:LEU:HD11 | 5:2F:176:LEU:HD12 | 1.97 | 0.44 |
| 8:2I:5:LEU:HD11 | 8:2I:19:VAL:HG22 | 1.99 | 0.44 |
| 23:11:89:GLU:O | 23:11:93:GLU:HG2 | 2.18 | 0.44 |
| 1:1A:1048:A:N1 | 1:1A:1112:G:O2' | 2.42 | 0.44 |
| 1:1A:1665:A:H2' | 1:1A:1666:G:O4' | 2.17 | 0.44 |
| 1:1A:2151:G:H2' | 1:1A:2152:G:C8 | 2.52 | 0.44 |
| 1:1A:2106:G:H1 | 1:1A:2183:C:H42 | 1.64 | 0.44 |
| 1:1A:2848:G:H8 | 15:1T:97:ALA:HB2 | 1.82 | 0.44 |
| 1:1A:86:C:H4' | 1:1A:104:U:H1' | 1.99 | 0.44 |
| 7:1H:28:GLY:HA3 | 7:1H:79:VAL:HB | 1.99 | 0.44 |
| 17:1V:80:GLN:HA | 17:1V:82:ARG:NH1 | 2.32 | 0.44 |
| 6:2G:109:VAL:HG11 | 26:24:14:ILE:HG21 | 1.99 | 0.44 |
| 1:2A:1239:G:H2' | 1:2A:1240:U:O4' | 2.17 | 0.44 |
| 1:2A:1364:G:OP2 | 23:21:61:ARG:NH2 | 2.47 | 0.44 |
| 1:2A:2114:A:O2' | 1:2A:2167:U:H1' | 2.17 | 0.44 |
| 1:2A:2284:C:OP2 | 28:26:2:ALA:N | 2.51 | 0.44 |
| 1:2A:592:G:H2' | 1:2A:593:G:C8 | 3.73 | 0.44 |
| 1:2A:613:G:O2' | 1:2A:614(C):A:N1 | 2.43 | 0.44 |
| 1:2A:657:U:H2' | 1:2A:658:C:C6 | 2.52 | 0.44 |
| 1:2A:746:A:H2' | 1:2A:2612:C:H5'' | 1.99 | 0.44 |
| 1:2A:925:C:H2' | 1:2A:926:A:C8 | 2.53 | 0.44 |
| 1:2A:744:G:OP1 | 4:2E:132:HIS:ND1 | 2.49 | 0.44 |
| 14:2S:10:ARG:HG2 | 14:2S:91:PRO:HA | 1.99 | 0.44 |
| 28:16:2:ALA:HB2 | 30:18:34:TRP:CZ2 | 2.53 | 0.44 |
| 1:1A:2250:G:O2' | 1:1A:2496:C:OP1 | 2.31 | 0.44 |
| 1:1A:286:C:H2' | 1:1A:287:C:C6 | 2.53 | 0.44 |
| 3:1D:208:LYS:HG3 | 3:1D:210:GLY:H | 1.83 | 0.44 |
| 11:1P:18:ARG:NE | 61:1P:307:HOH:O | 2.48 | 0.44 |
| 1:2A:171:G:H2' | 1:2A:172:C:C6 | 2.52 | 0.44 |
| 1:2A:2023:G:H5' | 1:2A:2617:C:H4' | 1.99 | 0.44 |
| 1:2A:946:G:OP1 | 61:2A:3973:HOH:O | 2.21 | 0.44 |
| 12:2Q:85:LYS:HG2 | 22:20:7:LEU:HB3 | 2.00 | 0.44 |
| 20:2Y:35:TYR:CE2 | 20:2Y:69:ALA:HB3 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 21:2Z:54:HIS:CD2 | 21:2Z:101:PRO:HG3 | 2.53 | 0.44 |
| 1:1A:1972:A:H2' | 1:1A:1973:G:H8 | 1.82 | 0.44 |
| 1:1A:2331:G:O2' | 1:1A:2336:A:N1 | 2.40 | 0.44 |
| 1:1A:816:C:H2' | 1:1A:817:C:C6 | 2.52 | 0.44 |
| 1:2A:1482:G:H1 | 1:2A:1506:C:H42 | 1.65 | 0.44 |
| 1:2A:1551:C:H2' | 1:2A:1552:G:O4' | 2.16 | 0.44 |
| 1:2A:2343:C:O2' | 1:2A:2373:G:O2' | 2.16 | 0.44 |
| 1:2A:457:A:H61 | 1:2A:470:A:H5'' | 1.82 | 0.44 |
| 1:2A:646:A:H2' | 1:2A:647:G:O4' | 2.18 | 0.44 |
| 1:2A:893:C:H2' | 1:2A:894:C:C5 | 2.53 | 0.44 |
| 1:2A:912:C:OP1 | 12:2Q:8:LYS:NZ | 2.40 | 0.44 |
| 4:2E:170:LEU:HB3 | 4:2E:184:VAL:CG2 | 2.48 | 0.44 |
| 7:2H:4:ILE:O | 7:2H:69:ARG:HD2 | 2.17 | 0.44 |
| 9:2N:56:ASN:HB3 | 9:2N:59:LYS:HD2 | 1.98 | 0.44 |
| 14:2S:14:VAL:O | 14:2S:18:ILE:HG12 | 2.16 | 0.44 |
| 10:2O:73:ASP:HB2 | 15:2T:82:LEU:HD12 | 1.99 | 0.44 |
| 1:1A:1056:G:H5'' | 1:1A:1057:A:O4' | 2.18 | 0.44 |
| 1:1A:1802:A:H2' | 1:1A:1803:A:C8 | 2.53 | 0.44 |
| 1:1A:1803:A:O2' | 3:1D:259:THR:HG21 | 2.17 | 0.44 |
| 1:1A:234:C:H2' | 1:1A:235:U:H6 | 1.83 | 0.44 |
| 1:1A:2418:A:H2' | 1:1A:2419:U:C6 | 2.52 | 0.44 |
| 1:1A:2781:A:H5'' | 1:1A:2782:G:H5' | 2.00 | 0.44 |
| 1:1A:2305:A:H5'' | 6:1G:134:GLY:HA3 | 1.98 | 0.44 |
| 21:1Z:103:ARG:N | 21:1Z:137:ILE:O | 2.49 | 0.44 |
| 1:2A:99:U:H4' | 1:2A:100:G:H5' | 1.97 | 0.44 |
| 1:2A:1469:A:H2' | 1:2A:1470:G:O4' | 2.18 | 0.44 |
| 1:2A:1495:A:H2' | 1:2A:1496:A:C8 | 2.52 | 0.44 |
| 1:2A:1667:G:O2' | 1:2A:1991:U:O4 | 2.26 | 0.44 |
| 1:2A:2319:G:N2 | 14:2S:3:ARG:HA | 2.32 | 0.44 |
| 1:2A:2557:G:H2' | 1:2A:2558:C:H6 | 1.83 | 0.44 |
| 1:2A:529:A:H62 | 1:2A:2041:U:H3 | 1.64 | 0.44 |
| 1:2A:661:C:H2' | 1:2A:662:G:H8 | 1.82 | 0.44 |
| 1:2A:1649:G:O2' | 13:2R:107:ASP:OD2 | 2.26 | 0.44 |
| 21:2Z:73:GLN:HB3 | 21:2Z:87:ASP:OD2 | 2.18 | 0.44 |
| 1:1A:1653:G:O3' | 13:1R:2:ARG:HB2 | 2.18 | 0.44 |
| 1:1A:1689:A:OP2 | 1:1A:1698:A:N6 | 2.42 | 0.44 |
| 1:1A:2067:G:O2' | 1:1A:2069:G:H5' | 2.17 | 0.44 |
| 1:1A:2637:U:H5'' | 4:1E:82:ARG:NH1 | 2.33 | 0.44 |
| 1:1A:2705:A:O2' | 1:1A:2852:G:OP1 | 2.26 | 0.44 |
| 1:1A:952:G:OP1 | 12:1Q:16:ARG:NH2 | 2.50 | 0.44 |
| 9:1N:104:LYS:HB2 | 9:1N:117:PHE:CE1 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 20:1Y:14:LEU:HB2 | 20:1Y:75:ILE:HD11 | 2.00 | 0.44 |
| 1:2A:1203:G:O2' | 1:2A:1242:A:N6 | 2.48 | 0.44 |
| 1:2A:1265:A:N6 | 1:2A:2013:A:H5'' | 2.32 | 0.44 |
| 1:2A:143:G:H2' | 1:2A:143(A):C:C6 | 2.53 | 0.44 |
| 1:2A:1823:G:OP1 | 3:2D:54:ARG:NH2 | 2.49 | 0.44 |
| 1:2A:2186:G:H2' | 1:2A:2187:G:C8 | 2.53 | 0.44 |
| 1:2A:250:G:C6 | 1:2A:251:A:C6 | 3.06 | 0.44 |
| 1:2A:2753:A:N3 | 31:29:15:LYS:NZ | 2.56 | 0.44 |
| 1:2A:385:C:O2' | 1:2A:388:G:N2 | 2.50 | 0.44 |
| 2:2B:38:C:H2' | 2:2B:39:A:H8 | 1.83 | 0.44 |
| 6:2G:37:VAL:HG22 | 6:2G:159:VAL:HG12 | 2.00 | 0.44 |
| 13:2R:79:LEU:HA | 13:2R:83:ILE:HD12 | 1.98 | 0.44 |
| 17:2V:82:ARG:NH2 | 61:2V:301:HOH:O | 2.51 | 0.44 |
| 23:11:8:SER:HB3 | 23:11:66:HIS:CD2 | 2.53 | 0.44 |
| 25:13:18:ASP:OD1 | 25:13:18:ASP:N | 2.49 | 0.44 |
| 1:1A:305:U:H2' | 1:1A:306:U:C6 | 2.53 | 0.44 |
| 4:1E:181:LEU:HA | 4:1E:181:LEU:HD12 | 1.78 | 0.44 |
| 5:1F:102:PRO:O | 5:1F:106:ARG:HG2 | 2.17 | 0.44 |
| 10:1O:19:ILE:HG22 | 10:1O:43:VAL:HG22 | 1.99 | 0.44 |
| 1:2A:1516:C:H2' | 1:2A:1517:G:C8 | 2.53 | 0.44 |
| 1:2A:1916:A:H2' | 1:2A:1917:PSU:O4' | 2.17 | 0.44 |
| 1:2A:2140:C:C2 | 1:2A:2152:G:N2 | 2.86 | 0.44 |
| 1:2A:2233:U:H2' | 1:2A:2234:G:C8 | 2.53 | 0.44 |
| 1:2A:848:G:H2' | 1:2A:849:A:C8 | 2.53 | 0.44 |
| 1:2A:2679:A:H4' | 4:2E:165:VAL:HG11 | 1.99 | 0.44 |
| 12:2Q:39:PRO:HB3 | 12:2Q:99:PRO:HD3 | 1.98 | 0.44 |
| 1:2A:2839:G:H5' | 13:2R:46:GLY:CA | 2.48 | 0.44 |
| 13:2R:96:ARG:NH2 | 13:2R:117:VAL:HG13 | 2.33 | 0.44 |
| 17:2V:3:ALA:HB3 | 17:2V:14:VAL:HG23 | 2.00 | 0.44 |
| 23:11:59:THR:O | 23:11:91:LYS:NZ | 2.42 | 0.44 |
| 26:14:40:HIS:HB3 | 26:14:43:TYR:HD2 | 1.83 | 0.44 |
| 26:14:58:ARG:HD2 | 26:14:58:ARG:H | 1.83 | 0.44 |
| 1:1A:1274:A:N3 | 1:1A:1297:C:H1' | 2.33 | 0.44 |
| 1:1A:2376:A:H2' | 1:1A:2377:A:O4' | 2.17 | 0.44 |
| 1:1A:2820:A:C5 | 13:1R:4:LEU:HD11 | 2.53 | 0.44 |
| 18:1W:62:HIS:O | 18:1W:64:MET:HG3 | 2.18 | 0.44 |
| 20:1Y:19:LYS:HE3 | 20:1Y:20:TYR:CE2 | 2.53 | 0.44 |
| 1:2A:1199:U:H2' | 1:2A:1200:C:C6 | 2.53 | 0.44 |
| 1:2A:2144:U:H1' | 1:2A:2148:G:N2 | 2.33 | 0.44 |
| 1:2A:289:A:H2' | 1:2A:290:G:O4' | 2.17 | 0.44 |
| 1:2A:323:G:C8 | 5:2F:171:PRO:HG3 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:645:C:H5' | 1:2A:646:A:OP2 | 2.17 | 0.44 |
| 3:2D:2:ALA:HA | 3:2D:20:ASP:HB3 | 2.00 | 0.44 |
| 4:2E:16:ARG:NH1 | 4:2E:171:GLU:OE2 | 2.49 | 0.44 |
| 10:2O:22:ILE:HG12 | 10:2O:40:VAL:O | 2.17 | 0.44 |
| 18:2W:88:ARG:NH1 | 18:2W:94:ASP:OD2 | 2.50 | 0.44 |
| 1:1A:135:G:N7 | 61:1A:4471:HOH:O | 2.36 | 0.44 |
| 1:1A:414:C:H2' | 1:1A:415:A:C8 | 2.53 | 0.44 |
| 6:1G:41:GLN:HG2 | 6:1G:43:LEU:HD13 | 2.00 | 0.44 |
| 21:1Z:158:PRO:O | 21:1Z:161:VAL:HG12 | 2.17 | 0.44 |
| 1:2A:1184:G:H3' | 1:2A:1184:G:OP1 | 4.73 | 0.44 |
| 1:2A:2626:C:H2' | 1:2A:2627:G:C8 | 2.53 | 0.44 |
| 1:2A:2784:C:H1' | 4:2E:37:ARG:HH12 | 1.83 | 0.44 |
| 1:2A:974:G:OP1 | 1:2A:1187:G:O2' | 2.24 | 0.44 |
| 1:1A:1094:U:N3 | 1:1A:1097:U:OP2 | 2.51 | 0.43 |
| 1:1A:2552:OMU:H6 | 1:1A:2552:OMU:O5' | 2.18 | 0.43 |
| 1:1A:2729:G:H2' | 1:1A:2730:C:O4' | 2.17 | 0.43 |
| 1:1A:34:C:H5'' | 1:1A:35:G:OP2 | 2.17 | 0.43 |
| 3:1D:232:PRO:HB3 | 3:1D:244:ARG:CZ | 2.48 | 0.43 |
| 8:1I:72:LEU:HD12 | 8:1I:138:ILE:HG21 | 1.99 | 0.43 |
| 26:24:53:GLU:HG2 | 26:24:56:VAL:HG13 | 2.00 | 0.43 |
| 1:2A:2400:G:H4' | 28:26:18:ARG:HG2 | 2.00 | 0.43 |
| 1:2A:1472:A:H61 | 1:2A:1519:G:H1' | 1.83 | 0.43 |
| 1:2A:1747(A):G:H2' | 1:2A:1748:G:H8 | 1.82 | 0.43 |
| 1:2A:2140:C:H3' | 1:2A:2141:G:H5'' | 1.99 | 0.43 |
| 1:2A:229:A:H5' | 1:2A:230:U:OP1 | 2.17 | 0.43 |
| 1:2A:305:U:H2' | 1:2A:306:U:C6 | 2.53 | 0.43 |
| 1:2A:373:U:H2' | 1:2A:374:A:C8 | 2.53 | 0.43 |
| 1:2A:932:G:H4' | 1:2A:933:A:O5' | 2.18 | 0.43 |
| 13:2R:118:GLU:CD | 13:2R:118:GLU:H | 2.20 | 0.43 |
| 1:2A:994:C:H3' | 16:2U:54:LYS:HE3 | 2.00 | 0.43 |
| 17:2V:61:VAL:HA | 17:2V:94:LEU:HD23 | 1.99 | 0.43 |
| 26:14:56:VAL:HG23 | 26:14:57:GLU:H | 1.84 | 0.43 |
| 1:1A:1218:C:N4 | 1:1A:1231:G:H1 | 2.15 | 0.43 |
| 1:1A:1541:G:H3' | 1:1A:1542:A:H2' | 2.00 | 0.43 |
| 1:1A:1685:C:H2' | 1:1A:1686:C:H6 | 1.83 | 0.43 |
| 1:1A:2156:G:H2' | 1:1A:2157:G:C2 | 2.53 | 0.43 |
| 3:1D:145:VAL:HB | 3:1D:155:LEU:HB2 | 1.99 | 0.43 |
| 5:1F:39:TRP:O | 5:1F:43:LYS:HG2 | 2.18 | 0.43 |
| 14:1S:39:ILE:HB | 14:1S:49:VAL:HG12 | 1.99 | 0.43 |
| 10:1O:122:LEU:HD13 | 15:1T:72:VAL:HG11 | 2.00 | 0.43 |
| 24:22:16:LEU:O | 24:22:67:LYS:HE2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:24:62:ARG:HA | 26:24:62:ARG:HD3 | 1.79 | 0.43 |
| 1:2A:1481:U:H2' | 1:2A:1482:G:C8 | 6.85 | 0.43 |
| 1:2A:1778:U:OP1 | 61:2A:3972:HOH:O | 2.21 | 0.43 |
| 1:2A:1637:A:H4' | 1:2A:2711:A:O2' | 2.18 | 0.43 |
| 1:2A:330:A:H2 | 1:2A:1210:A:H2' | 1.83 | 0.43 |
| 1:2A:730:C:H2' | 1:2A:731:C:H6 | 1.83 | 0.43 |
| 1:2A:941:A:H3' | 1:2A:942:G:H8 | 1.83 | 0.43 |
| 1:2A:980:A:N3 | 1:2A:2037:G:O2' | 2.42 | 0.43 |
| 15:2T:122:ASP:O | 15:2T:126:ALA:N | 2.45 | 0.43 |
| 21:2Z:99:TYR:HA | 21:2Z:124:ILE:O | 2.18 | 0.43 |
| 1:1A:1039:G:H1 | 1:1A:1116:C:N4 | 2.14 | 0.43 |
| 1:1A:1068:G:OP2 | 1:1A:1068:G:H8 | 4.24 | 0.43 |
| 1:1A:2667:C:H2' | 1:1A:2668:G:O4' | 2.18 | 0.43 |
| 1:1A:2791:C:H2' | 1:1A:2792:G:C8 | 2.53 | 0.43 |
| 1:1A:385:C:O2 | 11:1P:71:VAL:HG21 | 2.18 | 0.43 |
| 1:1A:991:C:OP2 | 61:1A:4218:HOH:O | 2.21 | 0.43 |
| 2:1B:79:C:H2' | 2:1B:80:U:O4' | 2.18 | 0.43 |
| 13:1R:67:LEU:HD13 | 13:1R:67:LEU:HA | 1.82 | 0.43 |
| 1:2A:1002:G:N3 | 1:2A:1003:G:H1' | 3.19 | 0.43 |
| 1:2A:1525:G:H2' | 1:2A:1526:G:O4' | 2.47 | 0.43 |
| 1:2A:2140:C:N4 | 1:2A:2151:G:N1 | 2.53 | 0.43 |
| 1:2A:443:A:H5'' | 1:2A:444:C:OP1 | 2.18 | 0.43 |
| 1:2A:817:C:H3' | 1:2A:818:G:H8 | 1.83 | 0.43 |
| 1:2A:848:G:OP2 | 1:2A:928:G:N2 | 2.51 | 0.43 |
| 1:2A:856:C:H2' | 1:2A:857:C:C6 | 2.53 | 0.43 |
| 2:2B:14:U:O4' | 2:2B:107:G:N2 | 2.51 | 0.43 |
| 3:2D:69:ARG:HH21 | 3:2D:130:ALA:N | 2.15 | 0.43 |
| 21:2Z:102:LEU:HD23 | 21:2Z:139:VAL:HG21 | 2.01 | 0.43 |
| 1:1A:1508:A:O2' | 1:1A:1509:C:OP1 | 2.27 | 0.43 |
| 1:1A:2011:U:H2' | 1:1A:2012:G:O4' | 2.18 | 0.43 |
| 1:1A:2544:G:H1' | 1:1A:2646:C:H4' | 2.01 | 0.43 |
| 1:1A:278:A:H2' | 1:1A:279:C:C6 | 2.53 | 0.43 |
| 1:1A:359:A:H2' | 1:1A:360:G:O4' | 2.19 | 0.43 |
| 1:1A:562:U:O2' | 1:1A:563:G:OP2 | 2.33 | 0.43 |
| 1:1A:723:G:H2' | 1:1A:724:U:O4' | 2.19 | 0.43 |
| 1:1A:788:A:OP1 | 1:1A:791:C:N4 | 2.45 | 0.43 |
| 6:1G:18:GLU:O | 6:1G:22:ARG:HG3 | 2.19 | 0.43 |
| 12:1Q:30:GLY:HA2 | 12:1Q:107:ALA:HB2 | 1.99 | 0.43 |
| 1:1A:1252:G:O4' | 16:1U:33:ARG:HD2 | 2.17 | 0.43 |
| 18:1W:9:TYR:H | 18:1W:102:HIS:CE1 | 2.37 | 0.43 |
| 1:2A:2432:A:C4 | 23:21:33:LYS:HG2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:27:26:GLY:O | 29:27:30:VAL:HG23 | 2.18 | 0.43 |
| 1:2A:1002:G:N1 | 1:2A:1003:G:H8 | 5.02 | 0.43 |
| 1:2A:1006:C:N4 | 1:2A:1022:G:O6 | 13.36 | 0.43 |
| 1:2A:1593:G:H2' | 1:2A:1594:G:C8 | 2.54 | 0.43 |
| 1:2A:1756:G:H4' | 1:2A:1758:G:O4' | 2.18 | 0.43 |
| 1:2A:1899:G:N3 | 1:2A:1899:G:H2' | 2.32 | 0.43 |
| 1:2A:2592:G:H2' | 1:2A:2593:U:O4' | 2.17 | 0.43 |
| 1:2A:271(T):C:H2' | 1:2A:271(U):G:C8 | 2.53 | 0.43 |
| 1:2A:1999:C:H5'' | 1:2A:2723:C:O2' | 2.18 | 0.43 |
| 1:2A:29:U:H2' | 1:2A:30:G:C8 | 2.53 | 0.43 |
| 1:2A:588:U:H2' | 1:2A:589:C:C6 | 2.53 | 0.43 |
| 3:2D:37:LEU:HA | 3:2D:37:LEU:HD12 | 1.85 | 0.43 |
| 7:2H:98:LEU:HD13 | 7:2H:125:VAL:HG23 | 2.00 | 0.43 |
| 21:2Z:155:LEU:HD12 | 21:2Z:155:LEU:HA | 1.89 | 0.43 |
| 1:1A:1540:U:H2' | 1:1A:1541:G:O4' | 2.18 | 0.43 |
| 57:1A:4099:LUJ:NAQ | 57:1A:4099:LUJ:OAL | 2.51 | 0.43 |
| 1:1A:568:U:O5' | 1:1A:945:A:N6 | 2.52 | 0.43 |
| 1:1A:686:G:OP1 | 29:17:11:LYS:NZ | 2.51 | 0.43 |
| 1:1A:1803:A:H4' | 3:1D:259:THR:HG23 | 2.00 | 0.43 |
| 5:1F:8:GLN:HE22 | 5:1F:21:ALA:HB2 | 1.82 | 0.43 |
| 61:1A:4395:HOH:O | 13:1R:15:SER:HB3 | 2.18 | 0.43 |
| 14:1S:110:LEU:HA | 14:1S:110:LEU:HD12 | 1.80 | 0.43 |
| 20:1Y:97:ARG:HB3 | 20:1Y:106:LEU:HD12 | 2.00 | 0.43 |
| 23:21:3:LYS:HB2 | 23:21:61:ARG:NH2 | 2.33 | 0.43 |
| 1:2A:1448:G:H4' | 1:2A:1542:A:OP1 | 2.17 | 0.43 |
| 1:2A:2129:C:H5' | 1:2A:2130:U:OP2 | 2.19 | 0.43 |
| 1:2A:2136:C:O2' | 1:2A:2137:C:C6 | 2.69 | 0.43 |
| 1:2A:526:A:N3 | 1:2A:2044:C:H1' | 2.33 | 0.43 |
| 1:2A:992:C:O4' | 17:2V:85:LYS:NZ | 2.51 | 0.43 |
| 4:2E:120:TRP:CD1 | 4:2E:155:LYS:HB3 | 2.54 | 0.43 |
| 1:2A:607:U:OP1 | 5:2F:102:PRO:HA | 2.18 | 0.43 |
| 12:2Q:18:LYS:O | 12:2Q:98:LYS:NZ | 2.34 | 0.43 |
| 12:2Q:35:VAL:HG12 | 12:2Q:130:LYS:O | 2.17 | 0.43 |
| 21:2Z:150:LEU:O | 21:2Z:171:ILE:HG22 | 2.18 | 0.43 |
| 1:1A:2695:C:H2' | 1:1A:2696:U:H6 | 1.82 | 0.43 |
| 1:1A:79:G:C6 | 1:1A:90:U:N3 | 29.96 | 0.43 |
| 1:1A:84:A:OP2 | 20:1Y:8:LYS:NZ | 2.37 | 0.43 |
| 6:1G:43:LEU:HB3 | 6:1G:44:GLY:H | 1.70 | 0.43 |
| 2:1B:8:U:O3' | 14:1S:25:ARG:NH2 | 2.52 | 0.43 |
| 22:20:52:GLY:O | 22:20:59:LEU:HA | 2.19 | 0.43 |
| 1:2A:1124:C:H2' | 1:2A:1125:G:O4' | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1316:U:H2' | 1:2A:1317:A:C8 | 2.53 | 0.43 |
| 1:2A:1594:G:H2' | 1:2A:1595:G:C8 | 2.53 | 0.43 |
| 1:2A:1668:A:O2' | 1:2A:1674:G:N7 | 2.33 | 0.43 |
| 1:2A:48:G:N1 | 1:2A:177:G:OP2 | 2.41 | 0.43 |
| 1:2A:1941:C:C5 | 1:2A:1942:5MC:HM52 | 2.53 | 0.43 |
| 1:2A:223:A:N1 | 1:2A:407:G:O2' | 2.47 | 0.43 |
| 2:2B:41:U:H5 | 6:2G:70:VAL:H | 1.67 | 0.43 |
| 2:2B:88:C:H2' | 2:2B:89:G:O4' | 2.18 | 0.43 |
| 4:2E:179:GLU:HG3 | 15:2T:9:LEU:CD2 | 2.48 | 0.43 |
| 6:2G:15:VAL:HA | 6:2G:175:LEU:HD23 | 2.00 | 0.43 |
| 1:1A:2364:C:H4' | 22:10:56:ASP:OD1 | 2.19 | 0.43 |
| 1:1A:1131:G:O6 | 1:1A:2040:C:H1' | 2.18 | 0.43 |
| 1:1A:1178:C:H2' | 1:1A:1179:C:C6 | 2.54 | 0.43 |
| 1:1A:1844:C:H2' | 1:1A:1845:G:H8 | 1.83 | 0.43 |
| 1:1A:2123:G:H2' | 1:1A:2124:G:C8 | 2.54 | 0.43 |
| 1:1A:528:A:O2' | 1:1A:529:A:H5' | 2.18 | 0.43 |
| 1:1A:774:A:N3 | 1:1A:774:A:H2' | 2.34 | 0.43 |
| 8:1I:78:THR:HA | 8:1I:143:SER:O | 2.19 | 0.43 |
| 2:1B:96:U:OP1 | 21:1Z:14:LYS:NZ | 2.51 | 0.43 |
| 19:2X:60:ARG:HH22 | 29:27:47:ARG:NH1 | 2.16 | 0.43 |
| 1:2A:2026:C:H2' | 1:2A:2027:G:O4' | 2.18 | 0.43 |
| 1:2A:2364:C:H2' | 1:2A:2365:G:O4' | 2.19 | 0.43 |
| 1:2A:927:G:H2' | 1:2A:928:G:O4' | 2.40 | 0.43 |
| 5:2F:102:PRO:HB2 | 5:2F:105:VAL:HG23 | 2.00 | 0.43 |
| 8:2I:130:TYR:HB3 | 8:2I:138:ILE:HB | 2.00 | 0.43 |
| 10:2O:68:GLU:CD | 10:2O:68:GLU:H | 2.21 | 0.43 |
| 27:15:42:PRO:HB2 | 27:15:43:HIS:ND1 | 2.34 | 0.43 |
| 1:1A:1783:A:OP1 | 61:1A:4337:HOH:O | 2.21 | 0.43 |
| 1:1A:2675:A:H5' | 10:1O:29:ASN:O | 2.18 | 0.43 |
| 1:1A:271(O):C:H2' | 1:1A:271(P):C:C6 | 2.53 | 0.43 |
| 1:1A:657:U:H2' | 1:1A:658:C:H6 | 1.81 | 0.43 |
| 1:1A:78:A:H2' | 1:1A:79:G:C8 | 2.54 | 0.43 |
| 3:1D:71:ASP:OD2 | 3:1D:103:ARG:NH1 | 2.42 | 0.43 |
| 1:1A:2682:U:O2' | 4:1E:13:ARG:HD3 | 2.19 | 0.43 |
| 20:1Y:43:ASN:O | 20:1Y:65:ALA:N | 2.40 | 0.43 |
| 1:2A:1479:G:H5' | 1:2A:1558:A:C2 | 2.54 | 0.43 |
| 1:2A:1683:C:H2' | 1:2A:1684:C:C6 | 2.54 | 0.43 |
| 1:2A:224:G:H2' | 1:2A:225:A:O4' | 2.19 | 0.43 |
| 1:2A:647:G:N3 | 1:2A:2350:C:O2' | 2.51 | 0.43 |
| 1:2A:2393:A:H2' | 1:2A:2394:C:O4' | 2.19 | 0.43 |
| 1:2A:615:G:OP1 | 5:2F:40:GLN:NE2 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:2A:902:C:H2' | 1:2A:903:C:C6 | 2.54 | 0.43 |
| 11:2P:85:LEU:HA | 11:2P:88:LEU:HD12 | 2.01 | 0.43 |
| 12:2Q:50:ALA:HB1 | 12:2Q:121:ALA:HB1 | 2.00 | 0.43 |
| 15:2T:27:THR:HB | 15:2T:89:VAL:HG23 | 2.00 | 0.43 |
| 21:2Z:141:VAL:HG22 | 21:2Z:142:SER:N | 2.34 | 0.43 |
| 21:2Z:6:LYS:HE3 | 21:2Z:8:TYR:HE2 | 1.84 | 0.43 |
| 27:15:16:ARG:HD2 | 27:15:20:ARG:NH1 | 2.33 | 0.43 |
| 1:1A:1366:A:H2' | 1:1A:1367:A:O4' | 2.19 | 0.43 |
| 1:1A:2364:C:H2' | 1:1A:2365:G:O4' | 2.18 | 0.43 |
| 1:1A:2788:C:OP1 | 4:1E:61:ARG:NH2 | 2.51 | 0.43 |
| 11:1P:121:LYS:HG2 | 11:1P:122:PRO:HD2 | 2.00 | 0.43 |
| 1:2A:1147:C:H2' | 1:2A:1148:A:H8 | 1.84 | 0.43 |
| 1:2A:1932:A:H2' | 1:2A:1933:G:O4' | 2.19 | 0.43 |
| 1:2A:2082:A:H2' | 1:2A:2083:G:O4' | 2.19 | 0.43 |
| 1:2A:2273:A:H2' | 1:2A:2274:A:C8 | 2.53 | 0.43 |
| 1:2A:38:A:H2' | 1:2A:39:C:C6 | 2.54 | 0.43 |
| 1:2A:471:A:H2' | 1:2A:472:A:O4' | 2.19 | 0.43 |
| 1:2A:918:A:C6 | 1:2A:919:G:H1' | 2.54 | 0.43 |
| 1:1A:1007:C:OP1 | 9:1N:37:LYS:NZ | 2.48 | 0.43 |
| 1:1A:1230:C:H2' | 1:1A:1231:G:C8 | 2.54 | 0.43 |
| 1:1A:2101:G:N2 | 1:1A:2188:C:N3 | 2.55 | 0.43 |
| 1:1A:2630:G:N3 | 1:1A:2892:A:O2' | 2.51 | 0.43 |
| 1:1A:606:U:H4' | 1:1A:658:C:H4' | 1.99 | 0.43 |
| 11:1P:95:VAL:HA | 11:1P:99:LEU:HD23 | 2.01 | 0.43 |
| 12:1Q:1:MET:HB3 | 12:1Q:2:LEU:H | 1.65 | 0.43 |
| 1:2A:2751:G:H8 | 7:2H:2:SER:HA | 1.83 | 0.43 |
| 1:2A:592:G:H2' | 1:2A:593:G:H8 | 3.16 | 0.43 |
| 5:2F:110:LEU:HD21 | 5:2F:181:LEU:HD23 | 2.01 | 0.43 |
| 8:2I:102:SER:O | 8:2I:106:GLY:N | 2.52 | 0.43 |
| 12:2Q:4:PRO:HD3 | 12:2Q:70:PRO:O | 2.18 | 0.43 |
| 1:1A:1087:G:H2' | 1:1A:1089:G:C8 | 2.53 | 0.42 |
| 1:1A:323:G:H1' | 1:1A:1205:U:O2 | 2.19 | 0.42 |
| 1:1A:1721:G:H3' | 1:1A:1722:A:H5'' | 2.01 | 0.42 |
| 1:1A:957:A:N1 | 1:1A:2458:G:H4' | 2.34 | 0.42 |
| 12:1Q:66:ILE:HG12 | 12:1Q:104:PHE:HD1 | 1.84 | 0.42 |
| 20:1Y:86:ARG:HG3 | 20:1Y:100:ALA:HB2 | 2.01 | 0.42 |
| 22:20:82:ARG:HE | 22:20:82:ARG:HB2 | 1.66 | 0.42 |
| 1:2A:1186:G:H2' | 1:2A:1187:G:O4' | 2.19 | 0.42 |
| 1:2A:1464:C:H2' | 1:2A:1465:G:C8 | 2.54 | 0.42 |
| 1:2A:1742:G:H2' | 1:2A:1743:C:O4' | 2.18 | 0.42 |
| 1:2A:1779:U:H2' | 61:2A:4059:HOH:O | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:1798:U:H5' | 3:2D:259:THR:HG23 | 2.01 | 0.42 |
| 1:2A:2164:C:C5 | 1:2A:2165:G:H1' | 2.54 | 0.42 |
| 1:2A:2298:A:H62 | 1:2A:2318:G:H8 | 1.67 | 0.42 |
| 1:2A:876:C:H2' | 1:2A:877:U:H6 | 1.84 | 0.42 |
| 1:2A:892:G:H3' | 1:2A:893:C:C4' | 2.49 | 0.42 |
| 4:2E:181:LEU:HA | 4:2E:181:LEU:HD12 | 1.72 | 0.42 |
| 8:2I:8:PRO:HD3 | 8:2I:15:VAL:HB | 2.01 | 0.42 |
| 26:14:46:GLN:HG2 | 26:14:46:GLN:O | 2.19 | 0.42 |
| 1:1A:1612:C:O2' | 29:17:5:TRP:O | 2.32 | 0.42 |
| 1:1A:1038:C:N4 | 1:1A:1117:G:H1 | 2.15 | 0.42 |
| 1:1A:1337:G:H2' | 1:1A:1338:G:O4' | 2.19 | 0.42 |
| 1:1A:1372:U:H2' | 1:1A:1373:A:O4' | 2.18 | 0.42 |
| 1:1A:1482:G:H2' | 1:1A:1484:G:H8 | 1.84 | 0.42 |
| 1:1A:2144:U:H3' | 1:1A:2146:C:N4 | 2.33 | 0.42 |
| 1:1A:647:G:N3 | 1:1A:2350:C:O2' | 2.52 | 0.42 |
| 1:1A:2471:C:H2' | 1:1A:2472:G:O4' | 2.19 | 0.42 |
| 1:1A:516:C:OP1 | 27:15:13:LYS:NZ | 2.38 | 0.42 |
| 3:1D:182:LEU:HD23 | 3:1D:182:LEU:HA | 1.85 | 0.42 |
| 3:1D:242:ARG:HG3 | 3:1D:242:ARG:NH1 | 2.27 | 0.42 |
| 6:1G:150:ASP:OD1 | 6:1G:151:ALA:N | 2.52 | 0.42 |
| 8:1I:109:ILE:HG23 | 8:1I:130:TYR:CE1 | 2.53 | 0.42 |
| 15:1T:24:PRO:HA | 15:1T:49:VAL:HG23 | 2.01 | 0.42 |
| 1:2A:1630:G:N7 | 61:2A:4063:HOH:O | 2.37 | 0.42 |
| 1:2A:1821:A:H2' | 1:2A:1822:G:C8 | 2.54 | 0.42 |
| 1:2A:2318:G:N2 | 14:2S:3:ARG:HE | 2.17 | 0.42 |
| 1:2A:56:A:H2' | 1:2A:57:C:O4' | 2.18 | 0.42 |
| 5:2F:41:LEU:HA | 5:2F:44:ARG:HD3 | 2.01 | 0.42 |
| 5:2F:47:GLY:HA3 | 5:2F:95:ARG:O | 2.19 | 0.42 |
| 7:2H:10:PRO:O | 7:2H:12:PRO:HD3 | 2.18 | 0.42 |
| 7:2H:3:ARG:NH1 | 7:2H:4:ILE:H | 2.17 | 0.42 |
| 9:2N:67:LEU:HA | 9:2N:87:LEU:HD22 | 2.01 | 0.42 |
| 11:2P:95:VAL:HA | 11:2P:99:LEU:HD23 | 2.00 | 0.42 |
| 12:2Q:130:LYS:HB3 | 12:2Q:130:LYS:HE2 | 1.80 | 0.42 |
| 13:2R:24:GLN:HB3 | 13:2R:44:LEU:HD11 | 2.00 | 0.42 |
| 16:2U:98:LEU:HD22 | 16:2U:105:VAL:HG11 | 2.00 | 0.42 |
| 1:1A:1614:A:H8 | 1:1A:1614:A:P | 2.43 | 0.42 |
| 1:1A:2125:G:N2 | 1:1A:2172:U:O5' | 2.50 | 0.42 |
| 1:1A:2526:G:H5' | 1:1A:2742:C:O2' | 2.19 | 0.42 |
| 1:1A:2732:G:H3' | 1:1A:2733:A:O4' | 2.19 | 0.42 |
| 1:1A:37:C:H2' | 1:1A:38:A:C8 | 2.54 | 0.42 |
| 1:1A:563:G:OP2 | 61:1A:4336:HOH:O | 2.21 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1F:65:TRP:CZ2 | 5:1F:75:HIS:HD2 | 2.38 | 0.42 |
| 13:1R:72:ASP:O | 13:1R:76:VAL:HG23 | 2.19 | 0.42 |
| 20:1Y:6:HIS:CD2 | 20:1Y:6:HIS:H | 2.37 | 0.42 |
| 21:1Z:126:VAL:HG13 | 21:1Z:161:VAL:HG23 | 2.01 | 0.42 |
| 1:2A:1359:A:H2' | 1:2A:1360:A:H5' | 2.01 | 0.42 |
| 1:2A:2031:A:N3 | 1:2A:2455:G:O2' | 2.37 | 0.42 |
| 1:2A:208:C:H2' | 1:2A:209:C:C6 | 2.54 | 0.42 |
| 1:2A:2055:C:O2 | 1:2A:2572:A:N6 | 2.53 | 0.42 |
| 1:2A:816:C:H2' | 1:2A:817:C:H6 | 1.85 | 0.42 |
| 1:2A:854:G:H2' | 1:2A:855:G:H8 | 1.84 | 0.42 |
| 1:2A:2684:U:OP1 | 15:2T:53:ARG:HD3 | 2.20 | 0.42 |
| 1:1A:1557:C:H5'' | 1:1A:1558:A:OP2 | 2.19 | 0.42 |
| 1:1A:234:C:H2' | 1:1A:235:U:C6 | 2.53 | 0.42 |
| 1:1A:2699:C:H2' | 1:1A:2700:C:O4' | 2.19 | 0.42 |
| 1:1A:2712:U:OP1 | 1:1A:2714:G:H4' | 2.20 | 0.42 |
| 1:1A:302:C:H2' | 1:1A:303:U:C6 | 2.54 | 0.42 |
| 1:1A:27:G:C2 | 1:1A:512:G:N3 | 2.88 | 0.42 |
| 1:1A:993:G:H2' | 1:1A:993:G:N3 | 3.04 | 0.42 |
| 7:1H:3:ARG:NH1 | 7:1H:5:GLY:H | 2.17 | 0.42 |
| 20:1Y:35:TYR:CE2 | 20:1Y:69:ALA:HB3 | 2.54 | 0.42 |
| 1:2A:1530:C:O2' | 1:2A:1531:C:O5' | 2.30 | 0.42 |
| 1:2A:251:A:C4 | 1:2A:252:G:H1' | 2.53 | 0.42 |
| 1:2A:2802:G:H2' | 1:2A:2803:C:O4' | 2.20 | 0.42 |
| 3:2D:126:GLN:O | 3:2D:129:ASN:ND2 | 2.49 | 0.42 |
| 15:2T:39:ARG:HH12 | 15:2T:41:ARG:HD3 | 1.84 | 0.42 |
| 16:2U:107:ALA:O | 16:2U:111:GLU:HG2 | 2.18 | 0.42 |
| 18:2W:10:VAL:HG12 | 18:2W:12:ILE:HG22 | 2.00 | 0.42 |
| 26:14:46:GLN:HB2 | 26:14:48:ARG:HH21 | 1.85 | 0.42 |
| 1:1A:1028:A:H61 | 1:1A:1125:G:H2' | 1.85 | 0.42 |
| 1:1A:1364:G:OP2 | 23:11:61:ARG:NH2 | 2.53 | 0.42 |
| 1:1A:1651:G:H4' | 13:1R:39:PRO:HG2 | 2.01 | 0.42 |
| 1:1A:1655:A:H3' | 1:1A:1656:C:C6 | 2.54 | 0.42 |
| 1:1A:1927:A:H2' | 1:1A:1928:A:C8 | 2.55 | 0.42 |
| 1:1A:2141:G:H3' | 1:1A:2142:C:O4' | 2.19 | 0.42 |
| 1:1A:2312:U:OP1 | 6:1G:73:ALA:HA | 2.19 | 0.42 |
| 1:1A:265:A:N1 | 1:1A:427:U:O2' | 2.46 | 0.42 |
| 9:1N:4:TYR:CE2 | 16:1U:100:VAL:HG11 | 2.55 | 0.42 |
| 9:1N:61:ARG:HD3 | 9:1N:61:ARG:HA | 1.74 | 0.42 |
| 16:1U:46:ALA:O | 16:1U:50:ARG:HG3 | 2.19 | 0.42 |
| 30:28:4:MET:HE3 | 30:28:63:PRO:HG3 | 2.00 | 0.42 |
| 1:2A:1006:C:C4 | 1:2A:1007:C:C4 | 3.89 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:2A:511:U:H4' | 1:2A:1235:G:H4' | 2.01 | 0.42 |
| 1:2A:2203:U:H2' | 1:2A:2205:C:H6 | 1.84 | 0.42 |
| 1:2A:492:A:H2' | 1:2A:493:G:O4' | 2.19 | 0.42 |
| 1:2A:65:C:H5' | 19:2X:71:GLY:HA3 | 2.02 | 0.42 |
| 1:2A:855:G:H2' | 1:2A:856:C:C6 | 2.54 | 0.42 |
| 1:2A:864:G:H1' | 1:2A:914:C:N4 | 2.34 | 0.42 |
| 1:2A:892:G:H2' | 1:2A:892:G:N3 | 2.34 | 0.42 |
| 1:2A:992:C:H2' | 1:2A:993:G:H8 | 1.84 | 0.42 |
| 14:2S:14:VAL:HG21 | 14:2S:90:GLY:O | 2.20 | 0.42 |
| 12:2Q:21:THR:O | 21:2Z:78:LYS:HD3 | 2.19 | 0.42 |
| 1:1A:1080:C:H5' | 1:1A:1081:U:OP2 | 2.19 | 0.42 |
| 1:1A:1821:A:H2' | 1:1A:1822:G:C8 | 2.55 | 0.42 |
| 1:1A:529:A:H62 | 1:1A:2041:U:H3 | 1.65 | 0.42 |
| 1:1A:493:G:H2' | 1:1A:494:G:O4' | 2.19 | 0.42 |
| 4:1E:144:ARG:O | 4:1E:148:GLY:HA2 | 2.20 | 0.42 |
| 26:24:61:ARG:HG3 | 26:24:62:ARG:N | 2.35 | 0.42 |
| 1:2A:1028:A:N3 | 1:2A:2486:G:O2' | 2.44 | 0.42 |
| 1:2A:1409:C:O2 | 1:2A:1491:G:N2 | 43.16 | 0.42 |
| 1:2A:1897:G:H2' | 1:2A:1898:U:C6 | 2.55 | 0.42 |
| 1:2A:635:C:H2' | 1:2A:636:G:O4' | 2.18 | 0.42 |
| 5:2F:64:ILE:HD11 | 5:2F:75:HIS:HB2 | 2.02 | 0.42 |
| 7:2H:24:VAL:HG13 | 7:2H:37:VAL:HG21 | 2.00 | 0.42 |
| 9:2N:38:HIS:CE1 | 9:2N:39:ARG:HG3 | 2.55 | 0.42 |
| 11:2P:8:PRO:HB2 | 11:2P:12:ALA:HB3 | 2.02 | 0.42 |
| 1:1A:1283:G:N2 | 1:1A:1285:G:H3' | 2.35 | 0.42 |
| 1:1A:483:A:O4' | 20:1Y:48:ALA:HB1 | 2.19 | 0.42 |
| 1:1A:628:G:H2' | 1:1A:629:G:H8 | 1.85 | 0.42 |
| 3:1D:260:ARG:NH1 | 3:1D:267:SER:OG | 2.52 | 0.42 |
| 7:1H:121:ILE:HD11 | 7:1H:140:LYS:HG2 | 2.00 | 0.42 |
| 8:1I:109:ILE:HG23 | 8:1I:130:TYR:CZ | 2.54 | 0.42 |
| 21:1Z:150:LEU:HG | 21:1Z:151:HIS:H | 1.84 | 0.42 |
| 21:1Z:45:ASP:CG | 21:1Z:49:ARG:HE | 2.23 | 0.42 |
| 1:2A:2019:A:N7 | 27:25:9:LYS:HE2 | 2.34 | 0.42 |
| 30:28:63:PRO:HG2 | 30:28:64:TYR:CE2 | 2.55 | 0.42 |
| 1:2A:1580:A:H3' | 1:2A:1581:G:H8 | 1.85 | 0.42 |
| 1:2A:1686:C:H2' | 1:2A:1687:G:O4' | 2.19 | 0.42 |
| 1:2A:2274:A:C5 | 1:2A:2276:G:C8 | 3.08 | 0.42 |
| 1:2A:2320:A:H2' | 1:2A:2320:A:N3 | 2.34 | 0.42 |
| 1:2A:2537:U:H2' | 1:2A:2538:C:C6 | 2.55 | 0.42 |
| 1:2A:2051:A:H5' | 1:2A:2578:G:O4' | 2.20 | 0.42 |
| 1:2A:2689:U:H4' | 1:2A:2690:C:H5' | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:2A:2881:C:H2' | 1:2A:2882:A:O4' | 2.18 | 0.42 |
| 15:2T:113:LYS:O | 15:2T:114:LEU:HD23 | 2.20 | 0.42 |
| 1:2A:1009:A:H5'' | 16:2U:63:VAL:CG2 | 2.49 | 0.42 |
| 21:2Z:55:HIS:HE1 | 21:2Z:135:GLU:HG3 | 1.84 | 0.42 |
| 1:1A:1740:G:H2' | 1:1A:1741:A:C8 | 2.55 | 0.42 |
| 1:1A:1996:C:H4' | 1:1A:1997:G:OP1 | 2.19 | 0.42 |
| 1:1A:2061:G:H2' | 1:1A:2501:C:O2' | 2.19 | 0.42 |
| 1:1A:2299:G:H2' | 1:1A:2300:G:C8 | 2.55 | 0.42 |
| 1:1A:2347:C:H2' | 1:1A:2348:U:C6 | 2.55 | 0.42 |
| 1:1A:2633:G:H2' | 1:1A:2634:G:O4' | 2.20 | 0.42 |
| 1:1A:956:G:H2' | 1:1A:957:A:H2' | 2.01 | 0.42 |
| 6:1G:131:TYR:HE2 | 6:1G:133:LEU:HD23 | 1.85 | 0.42 |
| 9:1N:62:VAL:HG13 | 9:1N:66:LYS:HD2 | 2.01 | 0.42 |
| 1:1A:1288:U:O4 | 13:1R:106:GLY:HA3 | 2.20 | 0.42 |
| 15:1T:99:LEU:HD13 | 15:1T:114:LEU:HD11 | 2.01 | 0.42 |
| 18:1W:45:TYR:OH | 18:1W:49:LYS:HE3 | 2.20 | 0.42 |
| 1:2A:467:G:OP2 | 29:27:34:ARG:HD3 | 2.20 | 0.42 |
| 1:2A:1263:U:C4 | 1:2A:1264:G:C6 | 3.07 | 0.42 |
| 1:2A:196:A:N3 | 1:2A:196:A:H2' | 2.35 | 0.42 |
| 1:2A:1853:A:N1 | 1:2A:2087:G:H1' | 2.35 | 0.42 |
| 1:2A:2328:A:H2' | 1:2A:2329:G:C8 | 2.54 | 0.42 |
| 1:2A:2712:U:OP1 | 1:2A:2714:G:H4' | 2.19 | 0.42 |
| 1:2A:573:G:O6 | 1:2A:2029:G:H2' | 2.19 | 0.42 |
| 1:2A:945:A:H2 | 61:2A:4541:HOH:O | 2.03 | 0.42 |
| 5:2F:195:ASP:HB3 | 5:2F:198:ALA:H | 1.85 | 0.42 |
| 9:2N:62:VAL:HG11 | 9:2N:66:LYS:HB2 | 2.01 | 0.42 |
| 1:1A:1364:G:P | 23:11:61:ARG:HH12 | 2.42 | 0.42 |
| 1:1A:1066:U:H2' | 1:1A:1068:G:OP2 | 2.20 | 0.42 |
| 1:1A:1417:C:H2' | 1:1A:1418:G:O4' | 2.20 | 0.42 |
| 1:1A:586:A:N1 | 1:1A:809:G:O2' | 2.38 | 0.42 |
| 1:1A:1278:A:O2' | 13:1R:27:SER:HB3 | 2.20 | 0.42 |
| 12:1Q:141:GLN:NE2 | 21:1Z:74:VAL:O | 2.51 | 0.42 |
| 1:2A:459:U:H5'' | 29:27:40:TRP:CD2 | 2.55 | 0.42 |
| 1:2A:1478:G:H2' | 1:2A:1479:G:H8 | 1.84 | 0.42 |
| 1:2A:1833:U:OP1 | 61:2A:3975:HOH:O | 2.22 | 0.42 |
| 1:2A:1877:A:H5' | 1:2A:1878:G:OP2 | 2.19 | 0.42 |
| 1:2A:195:A:H5'' | 1:2A:196:A:O5' | 2.19 | 0.42 |
| 1:2A:321:G:C2 | 1:2A:341:G:H4' | 2.55 | 0.42 |
| 2:2B:39:A:O2' | 2:2B:40:U:H5' | 2.19 | 0.42 |
| 7:2H:56:SER:OG | 7:2H:57:ASP:N | 2.53 | 0.42 |
| 14:2S:99:LYS:HE2 | 14:2S:103:GLU:OE2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:2E:18:ASP:HB3 | 15:2T:82:LEU:HD21 | 2.00 | 0.42 |
| 23:11:46:LEU:HA | 23:11:63:ALA:HA | 2.01 | 0.42 |
| 1:1A:1360:A:OP1 | 1:1A:1360:A:H8 | 5.14 | 0.42 |
| 1:1A:2074:U:H2' | 1:1A:2075:U:C6 | 2.55 | 0.42 |
| 1:1A:2138:C:N3 | 1:1A:2153:G:N2 | 2.67 | 0.42 |
| 1:1A:2346:A:C5 | 1:1A:2383:G:C2 | 3.07 | 0.42 |
| 1:1A:676:A:HO2' | 1:1A:2442:C:HO2' | 1.63 | 0.42 |
| 1:1A:271(P):C:H4' | 8:1I:42:SER:O | 2.20 | 0.42 |
| 1:1A:833:U:H2' | 1:1A:834:C:C6 | 2.65 | 0.42 |
| 2:1B:43:C:H4' | 6:1G:98:ARG:HH21 | 1.85 | 0.42 |
| 8:1I:109:ILE:HD12 | 8:1I:130:TYR:CZ | 2.54 | 0.42 |
| 14:1S:65:VAL:O | 14:1S:69:VAL:HG12 | 2.20 | 0.42 |
| 15:1T:33:LYS:HE3 | 15:1T:82:LEU:HD22 | 2.02 | 0.42 |
| 19:1X:94:GLY:N | 19:1X:95:LEU:HB2 | 2.35 | 0.42 |
| 1:2A:1128:A:N7 | 1:2A:2489:G:O2' | 2.53 | 0.42 |
| 1:2A:1472:A:N6 | 1:2A:1519:G:H1' | 2.35 | 0.42 |
| 1:2A:2125:G:H1' | 1:2A:2173:A:N6 | 2.35 | 0.42 |
| 1:2A:2270:G:H2' | 1:2A:2271:G:O4' | 2.20 | 0.42 |
| 1:2A:2687:U:H2' | 1:2A:2688:U:O4' | 2.20 | 0.42 |
| 1:2A:2698:U:H2' | 1:2A:2699:C:C6 | 2.55 | 0.42 |
| 1:2A:2726:U:O2' | 1:2A:2727:G:H8 | 2.02 | 0.42 |
| 1:2A:30:G:H2' | 1:2A:31:C:C6 | 2.55 | 0.42 |
| 1:2A:350:U:H2' | 1:2A:351:G:O4' | 2.20 | 0.42 |
| 1:2A:757:U:H2' | 1:2A:758:C:O4' | 2.20 | 0.42 |
| 2:2B:38:C:H2' | 2:2B:39:A:C8 | 2.54 | 0.42 |
| 8:2I:26:ALA:O | 8:2I:31:LEU:HB2 | 2.20 | 0.42 |
| 14:2S:92:TYR:HB3 | 14:2S:98:VAL:HG21 | 2.02 | 0.42 |
| 16:2U:16:LYS:HB3 | 16:2U:16:LYS:HE2 | 1.81 | 0.42 |
| 24:12:22:GLU:OE2 | 24:12:68:ARG:NH2 | 2.53 | 0.41 |
| 30:18:38:GLY:O | 30:18:42:ARG:HB2 | 2.20 | 0.41 |
| 1:1A:2360:A:H2' | 1:1A:2361:A:O4' | 2.20 | 0.41 |
| 1:1A:2601:C:H2' | 1:1A:2603:G:C8 | 2.55 | 0.41 |
| 4:1E:4:ILE:HD13 | 4:1E:28:ALA:HB1 | 2.01 | 0.41 |
| 4:1E:79:ARG:HD3 | 4:1E:79:ARG:HA | 1.81 | 0.41 |
| 17:1V:79:VAL:HG23 | 61:1V:301:HOH:O | 2.19 | 0.41 |
| 11:2P:63:PRO:HB2 | 30:28:30:ARG:NH2 | 2.35 | 0.41 |
| 30:28:62:LEU:HB3 | 30:28:65:GLU:HG2 | 2.02 | 0.41 |
| 1:2A:1357:U:H2' | 1:2A:1358:G:O4' | 2.20 | 0.41 |
| 1:2A:1415:U:H3 | 1:2A:1587:A:H61 | 1.67 | 0.41 |
| 1:2A:2513:G:N2 | 4:2E:143:ASN:OD1 | 2.52 | 0.41 |
| 1:2A:1662:C:O2' | 1:2A:2687:U:OP1 | 2.30 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:457:A:N6 | 1:2A:470:A:H5'' | 2.35 | 0.41 |
| 7:2H:101:ARG:NH2 | 7:2H:121:ILE:O | 2.52 | 0.41 |
| 20:2Y:86:ARG:HB2 | 20:2Y:98:VAL:HG23 | 2.01 | 0.41 |
| 26:14:40:HIS:HB3 | 26:14:43:TYR:CD2 | 2.55 | 0.41 |
| 1:1A:1862:G:H2' | 1:1A:1863:G:H8 | 1.85 | 0.41 |
| 1:1A:2540:C:O2' | 1:1A:2740:A:N3 | 2.50 | 0.41 |
| 1:1A:2790:A:C5' | 1:1A:2893:G:H21 | 2.34 | 0.41 |
| 1:1A:311:A:C6 | 1:1A:328:U:C4 | 3.08 | 0.41 |
| 1:1A:957:A:H5' | 12:1Q:76:LYS:HG3 | 2.01 | 0.41 |
| 26:24:40:HIS:HB3 | 26:24:43:TYR:HD2 | 1.84 | 0.41 |
| 1:2A:2783:G:H2' | 1:2A:2784:C:C6 | 2.55 | 0.41 |
| 1:2A:2820:A:O2' | 1:2A:2821:A:OP1 | 2.34 | 0.41 |
| 1:2A:2870:C:H5'' | 13:2R:65:LEU:HD21 | 2.01 | 0.41 |
| 1:2A:296:C:O3' | 20:2Y:95:LYS:NZ | 2.52 | 0.41 |
| 1:2A:848:G:C2 | 1:2A:933:A:H1' | 2.55 | 0.41 |
| 1:2A:1803:A:O2' | 3:2D:259:THR:HG21 | 2.21 | 0.41 |
| 7:2H:117:PRO:HA | 7:2H:118:PRO:HD3 | 1.91 | 0.41 |
| 12:2Q:31:ASP:HA | 12:2Q:134:ARG:HH11 | 1.85 | 0.41 |
| 21:2Z:30:ASN:OD1 | 21:2Z:33:LEU:N | 2.51 | 0.41 |
| 1:1A:1180:C:H2' | 1:1A:1181:C:C6 | 2.55 | 0.41 |
| 1:1A:55:G:O2' | 1:1A:127:A:N1 | 2.46 | 0.41 |
| 1:1A:1485:G:C2 | 1:1A:1486:A:C4 | 3.08 | 0.41 |
| 1:1A:1636:C:H2' | 1:1A:1637:A:C8 | 2.55 | 0.41 |
| 1:1A:2072:G:H2' | 1:1A:2073:C:O4' | 2.19 | 0.41 |
| 1:1A:2443:C:H2' | 1:1A:2444:G:C8 | 2.55 | 0.41 |
| 1:1A:263:C:H2' | 1:1A:264:C:O4' | 2.19 | 0.41 |
| 1:1A:2836:U:H2' | 1:1A:2837:G:C8 | 2.55 | 0.41 |
| 1:1A:2718:G:O2' | 1:1A:2847:U:OP1 | 2.26 | 0.41 |
| 1:1A:831:G:N2 | 11:1P:53:GLY:O | 2.52 | 0.41 |
| 1:1A:944:G:O6 | 1:1A:1337:G:H8 | 83.19 | 0.41 |
| 1:1A:271(M):G:H21 | 8:1I:50:ARG:HH12 | 1.68 | 0.41 |
| 21:1Z:128:VAL:HG23 | 21:1Z:160:GLY:O | 2.20 | 0.41 |
| 21:1Z:150:LEU:HG | 21:1Z:151:HIS:N | 2.35 | 0.41 |
| 1:2A:1527:G:HO2' | 1:2A:1544:A:H62 | 1.67 | 0.41 |
| 1:2A:2019:A:H4' | 16:2U:34:LYS:HD2 | 2.01 | 0.41 |
| 1:2A:2065:C:H4' | 1:2A:2251:OMG:HM22 | 2.02 | 0.41 |
| 1:2A:2272:U:H5'' | 1:2A:2273:A:OP1 | 2.20 | 0.41 |
| 1:2A:2261:C:H1' | 1:2A:2388:A:N3 | 2.34 | 0.41 |
| 1:2A:2490:G:H8 | 1:2A:2490:G:OP2 | 2.02 | 0.41 |
| 1:2A:1966:A:H2 | 1:2A:2592:G:N3 | 2.18 | 0.41 |
| 1:2A:743:G:OP1 | 4:2E:130:GLY:HA2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:925:C:H2' | 1:2A:926:A:H8 | 1.85 | 0.41 |
| 1:2A:1805:U:O2 | 3:2D:50:THR:HB | 2.20 | 0.41 |
| 14:2S:48:LEU:HD23 | 14:2S:82:ILE:HD11 | 2.01 | 0.41 |
| 17:2V:40:LEU:HB2 | 17:2V:46:VAL:HG12 | 2.02 | 0.41 |
| 24:12:53:LEU:HA | 24:12:53:LEU:HD23 | 1.84 | 0.41 |
| 1:1A:1056:G:O2' | 1:1A:1086:A:H1' | 2.20 | 0.41 |
| 1:1A:492:A:H2' | 1:1A:493:G:O4' | 2.21 | 0.41 |
| 7:1H:13:LYS:HA | 7:1H:14:GLY:HA2 | 1.57 | 0.41 |
| 7:1H:94:TYR:OH | 7:1H:152:ARG:NH1 | 2.54 | 0.41 |
| 9:1N:138:LEU:HA | 9:1N:138:LEU:HD23 | 1.88 | 0.41 |
| 1:2A:1274:A:N3 | 1:2A:1297:C:H1' | 2.36 | 0.41 |
| 1:2A:172:C:H2' | 1:2A:173:G:C8 | 2.55 | 0.41 |
| 1:2A:2065:C:H2' | 1:2A:2066:C:C6 | 2.55 | 0.41 |
| 1:2A:2253:G:O6 | 22:20:4:LYS:NZ | 2.53 | 0.41 |
| 1:2A:2558:C:H2' | 1:2A:2559:C:O4' | 2.21 | 0.41 |
| 57:2A:3851:LUJ:OAL | 57:2A:3851:LUJ:NAQ | 2.54 | 0.41 |
| 6:2G:124:SER:HB2 | 6:2G:131:TYR:CE1 | 2.55 | 0.41 |
| 1:2A:1187:G:H5' | 17:2V:81:TYR:CE1 | 2.55 | 0.41 |
| 20:2Y:39:VAL:HB | 20:2Y:42:VAL:HB | 2.03 | 0.41 |
| 20:2Y:55:TYR:CZ | 20:2Y:61:ILE:HG21 | 2.56 | 0.41 |
| 1:1A:1054:A:H4' | 1:1A:1054:A:OP1 | 2.21 | 0.41 |
| 1:1A:1663:C:O2' | 1:1A:1664:A:O5' | 2.31 | 0.41 |
| 1:1A:2001:A:H2' | 1:1A:2002:G:C8 | 2.55 | 0.41 |
| 1:1A:2319:G:H22 | 14:1S:3:ARG:CD | 2.33 | 0.41 |
| 1:1A:272(J):C:H2' | 1:1A:274:G:C8 | 2.55 | 0.41 |
| 1:1A:952:G:P | 12:1Q:16:ARG:HH21 | 2.43 | 0.41 |
| 2:1B:41:U:P | 2:1B:43:C:H41 | 2.42 | 0.41 |
| 1:1A:444:C:H4' | 5:1F:49:ALA:HB2 | 2.02 | 0.41 |
| 12:2Q:81:VAL:HB | 22:20:7:LEU:HD21 | 2.02 | 0.41 |
| 27:25:52:TYR:O | 27:25:55:ARG:HG2 | 2.21 | 0.41 |
| 1:2A:2383:G:OP2 | 30:28:37:SER:HB2 | 2.20 | 0.41 |
| 1:2A:2392:A:OP2 | 30:28:31:HIS:NE2 | 2.53 | 0.41 |
| 1:2A:2512:C:H2' | 1:2A:2513:G:O4' | 2.19 | 0.41 |
| 1:2A:2732:G:H3' | 1:2A:2733:A:O4' | 2.21 | 0.41 |
| 1:2A:2747:G:O6 | 1:2A:2755:C:H5'' | 2.21 | 0.41 |
| 1:2A:686:G:H8 | 29:27:6:GLN:O | 2.04 | 0.41 |
| 1:2A:698:C:O2' | 1:2A:734:A:N6 | 2.54 | 0.41 |
| 1:2A:94(A):G:H2' | 1:2A:95:G:O4' | 2.20 | 0.41 |
| 3:2D:182:LEU:HB2 | 3:2D:272:ALA:HB3 | 2.02 | 0.41 |
| 3:2D:97:TYR:HE2 | 3:2D:103:ARG:HB2 | 1.85 | 0.41 |
| 1:1A:51:G:N3 | 1:1A:119:A:C2 | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1527:G:H3' | 61:1A:4755:HOH:O | 2.20 | 0.41 |
| 1:1A:1590:U:H2' | 1:1A:1591:G:C8 | 2.55 | 0.41 |
| 1:1A:1655:A:H3' | 1:1A:1656:C:H6 | 1.85 | 0.41 |
| 1:1A:1790:C:H5'' | 1:1A:1791:A:OP1 | 2.20 | 0.41 |
| 1:1A:2547:U:H2' | 1:1A:2548:G:C8 | 2.56 | 0.41 |
| 1:1A:2831:G:H1' | 1:1A:2883:A:H2' | 2.01 | 0.41 |
| 1:1A:614(C):A:C4 | 5:1F:180:GLY:HA2 | 2.56 | 0.41 |
| 6:1G:101:ILE:HG22 | 6:1G:105:LYS:HE2 | 2.03 | 0.41 |
| 6:1G:179:PRO:HB2 | 26:14:42:PHE:CE2 | 2.55 | 0.41 |
| 22:20:68:GLU:OE1 | 22:20:82:ARG:HD3 | 2.21 | 0.41 |
| 28:26:13:CYS:SG | 28:26:47:THR:HG21 | 2.61 | 0.41 |
| 1:2A:1213:A:N3 | 1:2A:1238:G:O2' | 2.46 | 0.41 |
| 1:2A:1388:G:H4' | 1:2A:1525:G:O2' | 2.20 | 0.41 |
| 1:2A:2232:U:OP1 | 23:21:42:GLN:NE2 | 2.53 | 0.41 |
| 1:2A:1027:A:C2 | 1:2A:2488:A:H5' | 2.56 | 0.41 |
| 1:2A:2792:G:N3 | 1:2A:2792:G:H2' | 2.36 | 0.41 |
| 1:2A:528:A:H8 | 9:2N:114:ARG:NH2 | 2.19 | 0.41 |
| 13:2R:29:LEU:HA | 13:2R:29:LEU:HD12 | 1.83 | 0.41 |
| 1:2A:2848:G:H8 | 15:2T:97:ALA:HB2 | 1.85 | 0.41 |
| 18:2W:2:GLU:OE2 | 18:2W:72:LYS:NZ | 2.40 | 0.41 |
| 23:11:3:LYS:HB2 | 23:11:61:ARG:NH2 | 2.35 | 0.41 |
| 29:17:24:THR:O | 29:17:28:ARG:HG3 | 2.20 | 0.41 |
| 1:1A:1062:G:H5'' | 1:1A:1070:A:O2' | 2.21 | 0.41 |
| 1:1A:1239:G:H2' | 1:1A:1240:U:O4' | 2.21 | 0.41 |
| 1:1A:1881:C:H2' | 1:1A:1882:C:C6 | 2.56 | 0.41 |
| 1:1A:2291:U:OP1 | 1:1A:2380:C:O2' | 2.35 | 0.41 |
| 2:1B:48:A:H2' | 2:1B:49:C:C6 | 2.55 | 0.41 |
| 2:1B:88:C:H2' | 2:1B:89:G:O4' | 2.20 | 0.41 |
| 4:1E:48:GLN:NE2 | 4:1E:78:LEU:HD13 | 2.35 | 0.41 |
| 8:1I:10:GLU:HG2 | 8:1I:10:GLU:H | 1.70 | 0.41 |
| 11:1P:82:GLY:HA2 | 11:1P:113:LYS:O | 2.20 | 0.41 |
| 1:2A:1161:C:H2' | 1:2A:1162:G:H8 | 1.86 | 0.41 |
| 1:2A:117:G:OP2 | 1:2A:119:A:O2' | 2.31 | 0.41 |
| 1:2A:1477:A:H2' | 1:2A:1478:G:O4' | 2.21 | 0.41 |
| 1:2A:2307:G:H4' | 1:2A:2308:G:O4' | 2.20 | 0.41 |
| 1:2A:2497:A:H5'' | 61:2A:4136:HOH:O | 2.20 | 0.41 |
| 1:2A:2031:A:C6 | 1:2A:2498:C:H1' | 2.56 | 0.41 |
| 1:2A:2896:C:H2' | 1:2A:2897:U:H6 | 1.84 | 0.41 |
| 1:2A:702:G:C2 | 1:2A:731:C:C2 | 3.08 | 0.41 |
| 1:2A:828:U:H4' | 1:2A:831:G:N1 | 2.36 | 0.41 |
| 4:2E:120:TRP:CG | 4:2E:155:LYS:HB3 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:2I:124:GLY:H | 8:2I:144:VAL:HG23 | 1.86 | 0.41 |
| 1:2A:7:G:H4' | 9:2N:13:TRP:CH2 | 2.56 | 0.41 |
| 10:2O:29:ASN:OD1 | 10:2O:29:ASN:N | 2.53 | 0.41 |
| 1:2A:2820:A:C5 | 13:2R:4:LEU:HD11 | 2.55 | 0.41 |
| 21:2Z:77:ASP:OD1 | 21:2Z:80:ARG:NH1 | 2.54 | 0.41 |
| 1:1A:1041:C:H42 | 1:1A:1114:G:H1 | 1.69 | 0.41 |
| 1:1A:1258:C:H2' | 1:1A:1259:G:O4' | 2.20 | 0.41 |
| 1:1A:1952:A:C6 | 1:1A:1953:A:N1 | 2.89 | 0.41 |
| 1:1A:2079:U:H2' | 1:1A:2080:G:O4' | 2.20 | 0.41 |
| 1:1A:330:A:HO2' | 1:1A:331:A:H8 | 1.65 | 0.41 |
| 1:1A:272:G:O2' | 1:1A:421:U:OP2 | 2.32 | 0.41 |
| 5:1F:89:VAL:HG12 | 5:1F:90:PHE:CD2 | 2.55 | 0.41 |
| 8:1I:109:ILE:HD13 | 8:1I:109:ILE:HA | 1.85 | 0.41 |
| 14:1S:51:ALA:HB3 | 14:1S:73:LEU:HB2 | 2.03 | 0.41 |
| 19:1X:64:LYS:HD3 | 19:1X:64:LYS:HA | 1.88 | 0.41 |
| 21:1Z:154:ASP:OD1 | 21:1Z:154:ASP:N | 2.52 | 0.41 |
| 1:2A:752:A:H3' | 29:27:1:MET:CE | 2.50 | 0.41 |
| 1:2A:1164:G:H2' | 1:2A:1165:U:C6 | 2.56 | 0.41 |
| 1:2A:1448:G:H2' | 1:2A:1449:A:C8 | 2.55 | 0.41 |
| 1:2A:1351:C:O2' | 1:2A:1571:A:N3 | 2.44 | 0.41 |
| 1:2A:1592:C:H2' | 1:2A:1593:G:H8 | 1.85 | 0.41 |
| 1:2A:18:C:H2' | 1:2A:19:C:C6 | 2.56 | 0.41 |
| 1:2A:2378:A:C5 | 1:2A:2379:G:H1' | 2.56 | 0.41 |
| 1:2A:2572:A:OP1 | 1:2A:2574:G:O2' | 2.24 | 0.41 |
| 1:2A:2580:U:OP1 | 61:2A:3977:HOH:O | 2.22 | 0.41 |
| 1:2A:271(J):C:O2' | 1:2A:271(K):U:OP2 | 2.32 | 0.41 |
| 1:2A:320:A:H4' | 1:2A:322:A:C8 | 2.56 | 0.41 |
| 1:2A:652(B):A:N6 | 1:2A:655:A:H1' | 2.36 | 0.41 |
| 1:2A:928:G:H3' | 1:2A:928:G:H8 | 1.86 | 0.41 |
| 2:2B:5:C:H42 | 2:2B:116:G:H1 | 1.69 | 0.41 |
| 3:2D:96:HIS:CD2 | 3:2D:102:LYS:HG2 | 2.56 | 0.41 |
| 3:2D:71:ASP:N | 3:2D:71:ASP:OD1 | 2.51 | 0.41 |
| 5:2F:107:LYS:HG3 | 5:2F:206:ILE:HA | 2.02 | 0.41 |
| 1:1A:107:C:H2' | 1:1A:108:U:C6 | 2.56 | 0.41 |
| 1:1A:1682:G:H1' | 1:1A:1762:A:C6 | 2.55 | 0.41 |
| 1:1A:196:A:N3 | 1:1A:196:A:H2' | 2.35 | 0.41 |
| 1:1A:2108:C:H2' | 1:1A:2109:U:C6 | 2.55 | 0.41 |
| 1:1A:2786:U:H2' | 1:1A:2787:C:H6 | 1.85 | 0.41 |
| 1:1A:365:C:H2' | 1:1A:366:C:O4' | 2.21 | 0.41 |
| 12:1Q:56:ARG:HD2 | 12:1Q:56:ARG:HA | 1.71 | 0.41 |
| 13:1R:98:LEU:HB2 | 13:1R:113:LEU:HD11 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:1W:48:ALA:O | 18:1W:52:GLU:HG2 | 2.20 | 0.41 |
| 22:20:19:LYS:HD3 | 22:20:19:LYS:HA | 1.96 | 0.41 |
| 28:26:18:ARG:HD2 | 28:26:42:TRP:CG | 2.56 | 0.41 |
| 29:27:12:ARG:NH2 | 29:27:44:PRO:HB3 | 2.36 | 0.41 |
| 1:2A:1418:G:OP1 | 1:2A:1588:C:O2' | 2.39 | 0.41 |
| 1:2A:1499:C:H2' | 1:2A:1500:G:C8 | 2.55 | 0.41 |
| 1:2A:2369:A:H2' | 1:2A:2370:G:C8 | 2.56 | 0.41 |
| 1:2A:2291:U:O2' | 1:2A:2374:C:O2 | 2.34 | 0.41 |
| 1:2A:2552:OMU:H2' | 1:2A:2554:U:OP2 | 2.21 | 0.41 |
| 1:2A:271(R):G:OP1 | 23:21:76:ARG:NH1 | 2.54 | 0.41 |
| 2:2B:17:C:H2' | 2:2B:18:G:O4' | 2.20 | 0.41 |
| 3:2D:68:LYS:C | 3:2D:70:TRP:H | 2.23 | 0.41 |
| 4:2E:52:LEU:HA | 4:2E:53:PRO:HD3 | 1.95 | 0.41 |
| 7:2H:20:ALA:HB1 | 7:2H:21:PRO:HD2 | 2.02 | 0.41 |
| 1:2A:637:A:H2' | 11:2P:117:GLU:OE1 | 2.21 | 0.41 |
| 30:18:34:TRP:CG | 30:18:35:GLN:N | 2.88 | 0.41 |
| 1:1A:1062:G:H5'' | 1:1A:1070:A:H1' | 2.03 | 0.41 |
| 1:1A:118:A:H3' | 1:1A:119:A:C5' | 2.51 | 0.41 |
| 1:1A:271(M):G:O2' | 1:1A:271(N):U:H5'' | 2.21 | 0.41 |
| 1:1A:630:G:N2 | 1:1A:633:A:OP2 | 2.48 | 0.41 |
| 1:1A:882:G:H3' | 1:1A:883:G:H8 | 1.85 | 0.41 |
| 1:1A:971:C:O2' | 1:1A:983:A:N3 | 2.45 | 0.41 |
| 6:1G:34:LEU:HD12 | 6:1G:100:TRP:CH2 | 2.56 | 0.41 |
| 15:1T:41:ARG:HH22 | 15:1T:43:GLN:NE2 | 2.19 | 0.41 |
| 1:1A:996:A:O3' | 16:1U:91:ASP:HB2 | 2.20 | 0.41 |
| 20:1Y:13:VAL:HG12 | 20:1Y:74:PRO:HA | 2.03 | 0.41 |
| 1:2A:2078:C:C4 | 1:2A:2079:U:C4 | 3.09 | 0.41 |
| 1:2A:2689:U:P | 1:2A:2719:G:H22 | 2.43 | 0.41 |
| 1:2A:311:A:H8 | 1:2A:311:A:OP1 | 2.03 | 0.41 |
| 1:2A:315:G:H2' | 1:2A:316:C:C6 | 2.55 | 0.41 |
| 1:2A:535:C:H2' | 1:2A:536:A:C8 | 2.56 | 0.41 |
| 1:2A:928:G:H3' | 1:2A:928:G:C8 | 2.56 | 0.41 |
| 1:2A:1842:G:O2' | 3:2D:253:GLN:OE1 | 2.37 | 0.41 |
| 4:2E:101:ARG:CZ | 4:2E:171:GLU:HB2 | 2.51 | 0.41 |
| 5:2F:192:LEU:HD22 | 5:2F:194:MET:HG3 | 2.03 | 0.41 |
| 8:2I:130:TYR:CE2 | 8:2I:132:PRO:HB3 | 2.56 | 0.41 |
| 1:2A:196:A:C8 | 11:2P:46:LYS:HD2 | 2.55 | 0.41 |
| 13:2R:55:ALA:HA | 13:2R:80:PHE:CE1 | 2.56 | 0.41 |
| 19:2X:39:ILE:HD13 | 19:2X:79:ALA:HB2 | 2.02 | 0.41 |
| 21:2Z:98:MET:O | 21:2Z:126:VAL:N | 2.54 | 0.41 |
| 31:19:7:VAL:HG12 | 31:19:34:GLN:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:1A:1394:U:H2' | 1:1A:1395:A:O4' | 2.21 | 0.41 |
| 1:1A:1999:C:H4' | 1:1A:2723:C:O2 | 2.20 | 0.41 |
| 1:1A:2065:C:H2' | 1:1A:2066:C:C6 | 2.56 | 0.41 |
| 1:1A:2206:G:H3' | 1:1A:2207:G:C8 | 2.56 | 0.41 |
| 1:1A:2683:C:H2' | 1:1A:2684:U:H6 | 1.86 | 0.41 |
| 1:1A:476:G:N1 | 1:1A:479:A:OP2 | 2.49 | 0.41 |
| 3:1D:43:ARG:HG2 | 3:1D:47:GLY:O | 2.21 | 0.41 |
| 61:1A:5262:HOH:O | 4:1E:145:LYS:HD3 | 2.20 | 0.41 |
| 1:1A:1279:G:H4' | 13:1R:31:HIS:CD2 | 2.56 | 0.41 |
| 19:1X:94:GLY:H | 19:1X:95:LEU:C | 2.24 | 0.41 |
| 1:2A:2271:G:OP1 | 22:20:18:ALA:HB1 | 2.21 | 0.41 |
| 1:2A:857:C:H4' | 22:20:23:VAL:HG21 | 2.03 | 0.41 |
| 31:29:14:CYS:HA | 31:29:27:CYS:HB2 | 2.03 | 0.41 |
| 1:2A:1153:C:H2' | 1:2A:1154:G:O4' | 2.21 | 0.41 |
| 7:2H:140:LYS:HB2 | 7:2H:140:LYS:HE3 | 1.80 | 0.41 |
| 13:2R:13:HIS:CE1 | 13:2R:16:HIS:HB2 | 2.56 | 0.41 |
| 15:2T:88:ILE:HG21 | 15:2T:91:ARG:NE | 2.36 | 0.41 |
| 1:1A:1060:U:C2 | 1:1A:1062:G:H1' | 2.57 | 0.40 |
| 1:1A:1295:C:H2' | 1:1A:1296:G:C8 | 2.56 | 0.40 |
| 1:1A:1668:A:N1 | 1:1A:1675:C:N4 | 2.67 | 0.40 |
| 1:1A:2018:G:H2' | 1:1A:2019:A:C8 | 2.55 | 0.40 |
| 1:1A:2053:G:H5' | 4:1E:144:ARG:O | 2.21 | 0.40 |
| 1:1A:2115:G:O5' | 1:1A:2115:G:H8 | 2.04 | 0.40 |
| 1:1A:183:C:N4 | 1:1A:213:A:H61 | 2.19 | 0.40 |
| 1:1A:2302:G:H2' | 1:1A:2303:G:H8 | 1.87 | 0.40 |
| 1:1A:2472:G:O2' | 1:1A:2478:A:N6 | 2.51 | 0.40 |
| 1:1A:253:C:H2' | 1:1A:254:G:O4' | 2.21 | 0.40 |
| 1:1A:2619:C:H4' | 4:1E:151:TYR:O | 2.21 | 0.40 |
| 1:1A:330:A:H2' | 1:1A:330:A:N3 | 2.37 | 0.40 |
| 1:1A:467:G:OP2 | 1:1A:467:G:H8 | 2.04 | 0.40 |
| 1:1A:478:A:N1 | 1:1A:500:G:H4' | 2.36 | 0.40 |
| 4:1E:52:LEU:HA | 4:1E:53:PRO:HD3 | 1.94 | 0.40 |
| 6:1G:58:GLN:O | 6:1G:62:LEU:HG | 2.21 | 0.40 |
| 17:1V:97:LYS:HD2 | 17:1V:97:LYS:HA | 1.90 | 0.40 |
| 18:1W:11:ARG:NH1 | 18:1W:99:ARG:O | 2.54 | 0.40 |
| 18:1W:7:ALA:HB2 | 18:1W:50:VAL:HG22 | 2.03 | 0.40 |
| 1:2A:1641:A:H2' | 1:2A:1642:G:O4' | 2.21 | 0.40 |
| 1:2A:1834:U:H4' | 1:2A:1969:A:C6 | 2.56 | 0.40 |
| 1:2A:2059:A:O3' | 5:2F:69:HIS:HA | 2.21 | 0.40 |
| 1:2A:271(N):U:O2' | 1:2A:271(O):C:H5' | 2.21 | 0.40 |
| 1:2A:443:A:H1' | 1:2A:1201:C:O4' | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:2A:764:A:O4' | 3:2D:213:ARG:HG3 | 2.21 | 0.40 |
| 3:2D:147:LEU:HD11 | 3:2D:183:ARG:NE | 2.35 | 0.40 |
| 3:2D:218:ARG:HB3 | 3:2D:219:PRO:HD2 | 2.03 | 0.40 |
| 1:1A:1365:A:O4' | 23:11:41:ARG:NH2 | 2.54 | 0.40 |
| 1:1A:1526:G:C6 | 1:1A:1527:G:C2 | 3.09 | 0.40 |
| 1:1A:1754:C:H2' | 1:1A:1755:A:O4' | 2.21 | 0.40 |
| 1:1A:1798:U:H5' | 3:1D:259:THR:CG2 | 2.51 | 0.40 |
| 1:1A:1949:G:C6 | 1:1A:1950:G:C6 | 3.09 | 0.40 |
| 1:1A:1963:U:H4' | 1:1A:1964:G:OP1 | 2.21 | 0.40 |
| 2:1B:4:C:H2' | 2:1B:5:C:O4' | 2.22 | 0.40 |
| 8:1I:26:ALA:HA | 8:1I:30:LEU:HB2 | 2.03 | 0.40 |
| 8:1I:92:VAL:HG11 | 8:1I:144:VAL:HG11 | 2.02 | 0.40 |
| 11:1P:147:LEU:HD23 | 11:1P:148:LEU:N | 2.36 | 0.40 |
| 21:1Z:31:ARG:H | 21:1Z:31:ARG:HG3 | 1.72 | 0.40 |
| 1:2A:2419:U:H5'' | 30:28:33:ASN:HB2 | 2.03 | 0.40 |
| 1:2A:1442:G:N3 | 1:2A:1442:G:H2' | 2.85 | 0.40 |
| 1:2A:2050:C:N4 | 1:2A:2051:A:C6 | 2.89 | 0.40 |
| 1:2A:217:G:H2' | 1:2A:218:A:O4' | 2.20 | 0.40 |
| 1:2A:2231:C:H2' | 1:2A:2232:U:O4' | 2.21 | 0.40 |
| 1:2A:2516:G:C6 | 1:2A:2517:C:C4 | 3.09 | 0.40 |
| 1:2A:993:G:N3 | 1:2A:993:G:H2' | 2.81 | 0.40 |
| 7:2H:13:LYS:HA | 7:2H:14:GLY:HA2 | 1.74 | 0.40 |
| 7:2H:59:ARG:HD2 | 7:2H:59:ARG:HA | 1.91 | 0.40 |
| 13:2R:28:LEU:HD23 | 13:2R:48:VAL:HG21 | 2.03 | 0.40 |
| 13:2R:96:ARG:HH21 | 13:2R:117:VAL:HG13 | 1.85 | 0.40 |
| 18:2W:6:ILE:HG22 | 18:2W:8:ARG:HG3 | 2.02 | 0.40 |
| 20:2Y:61:ILE:O | 20:2Y:61:ILE:HG13 | 2.16 | 0.40 |
| 28:16:38:LYS:HE3 | 28:16:38:LYS:HB3 | 1.96 | 0.40 |
| 30:18:30:ARG:NH1 | 61:18:202:HOH:O | 2.51 | 0.40 |
| 30:18:63:PRO:HG2 | 30:18:64:TYR:CD2 | 2.56 | 0.40 |
| 31:19:11:CYS:HB3 | 31:19:32:HIS:CE1 | 2.56 | 0.40 |
| 1:1A:1685:C:H2' | 1:1A:1686:C:C6 | 2.56 | 0.40 |
| 1:1A:189:G:H2' | 1:1A:205:G:N2 | 2.37 | 0.40 |
| 1:1A:2576:G:H1' | 61:1A:5158:HOH:O | 2.21 | 0.40 |
| 1:1A:2712:U:O2' | 1:1A:2713:A:H5' | 2.21 | 0.40 |
| 1:1A:518:G:H4' | 18:1W:18:ARG:HE | 1.86 | 0.40 |
| 6:1G:139:LEU:HA | 6:1G:144:ILE:HB | 2.03 | 0.40 |
| 7:1H:3:ARG:HG2 | 7:1H:6:ARG:NE | 2.36 | 0.40 |
| 8:1I:97:ILE:O | 8:1I:101:LEU:HB2 | 2.21 | 0.40 |
| 10:1O:102:VAL:HB | 10:1O:106:LEU:HD12 | 2.03 | 0.40 |
| 11:1P:138:LEU:HD23 | 11:1P:145:PRO:HB3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1S:10:ARG:HG2 | 14:1S:91:PRO:HA | 2.03 | 0.40 |
| 24:22:64:LEU:O | 24:22:68:ARG:HG3 | 2.22 | 0.40 |
| 1:2A:1125:G:H5' | 31:29:37:GLY:HA2 | 2.03 | 0.40 |
| 1:2A:1032:A:N6 | 1:2A:1122:G:H1 | 2.09 | 0.40 |
| 1:2A:2156:G:H2' | 1:2A:2157:G:C6 | 2.56 | 0.40 |
| 1:2A:2312:U:H5' | 6:2G:88:ILE:HD11 | 2.02 | 0.40 |
| 1:2A:2375:G:O2' | 1:2A:2377:A:N7 | 2.36 | 0.40 |
| 1:2A:249:C:OP2 | 1:2A:2394:C:O2' | 2.30 | 0.40 |
| 1:2A:479:A:O2' | 1:2A:481:G:H5' | 2.21 | 0.40 |
| 5:2F:125:LEU:HD11 | 5:2F:199:TRP:CE3 | 2.55 | 0.40 |
| 7:2H:7:LEU:O | 7:2H:69:ARG:NE | 2.43 | 0.40 |
| 10:2O:98:VAL:HG23 | 10:2O:118:ALA:HA | 2.02 | 0.40 |
| 1:2A:1340:U:H3' | 19:2X:57:LEU:HD22 | 2.04 | 0.40 |
| 19:2X:95:LEU:H | 19:2X:95:LEU:HD12 | 1.86 | 0.40 |
| 20:2Y:44:ILE:HA | 20:2Y:63:LYS:O | 2.22 | 0.40 |
| 28:16:17:LYS:HA | 28:16:17:LYS:HD3 | 1.95 | 0.40 |
| 1:1A:458:G:H8 | 29:17:37:LYS:O | 2.04 | 0.40 |
| 1:1A:107:C:H2' | 1:1A:108:U:H6 | 1.86 | 0.40 |
| 1:1A:1607:C:H4' | 1:1A:1608:A:O5' | 2.21 | 0.40 |
| 1:1A:1927:A:C6 | 1:1A:1928:A:C6 | 3.10 | 0.40 |
| 1:1A:185:U:H4' | 1:1A:218:A:H4' | 2.03 | 0.40 |
| 1:1A:2256:G:H2' | 1:1A:2257:U:O4' | 2.20 | 0.40 |
| 3:1D:72:LYS:HD3 | 3:1D:97:TYR:CE1 | 2.56 | 0.40 |
| 6:1G:139:LEU:H | 6:1G:139:LEU:HG | 1.66 | 0.40 |
| 9:1N:42:TRP:HA | 9:1N:48:MET:SD | 2.61 | 0.40 |
| 1:2A:1348:G:O6 | 1:2A:1349:A:N6 | 2.54 | 0.40 |
| 1:2A:1913:A:H4' | 1:2A:1914:C:O5' | 2.20 | 0.40 |
| 1:2A:2655:G:O2' | 1:2A:2664:G:O6 | 2.35 | 0.40 |
| 1:2A:2756:U:H3 | 1:2A:2758:A:H62 | 1.69 | 0.40 |
| 1:2A:383:U:H2' | 1:2A:385:C:H5 | 1.86 | 0.40 |
| 1:2A:600:G:H2' | 1:2A:601:C:C6 | 2.57 | 0.40 |
| 3:2D:38:LYS:HE2 | 3:2D:39:LYS:O | 2.21 | 0.40 |
| 5:2F:41:LEU:HD22 | 5:2F:44:ARG:NH1 | 2.29 | 0.40 |
| 6:2G:114:ILE:HB | 6:2G:117:PHE:HD1 | 1.87 | 0.40 |
| 9:2N:4:TYR:CE2 | 16:2U:100:VAL:HG11 | 2.56 | 0.40 |
| 27:15:16:ARG:NH1 | 27:15:17:ASP:OD1 | 2.55 | 0.40 |
| 1:1A:1022:G:C5 | 1:1A:1140:C:C4 | 3.09 | 0.40 |
| 57:1A:4100:LUJ:OAL | 57:1A:4100:LUJ:NAQ | 2.54 | 0.40 |
| 2:1B:15:A:H1' | 2:1B:110:G:C5 | 2.56 | 0.40 |
| 9:1N:89:LYS:HB2 | 9:1N:89:LYS:HE2 | 1.93 | 0.40 |
| 15:1T:108:ARG:HG3 | 15:1T:109:GLU:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:1Z:121:HIS:HB3 | 21:1Z:123:ASP:O | 2.21 | 0.40 |
| 23:21:23:LYS:HB2 | 23:21:23:LYS:HE3 | 1.85 | 0.40 |
| 27:25:6:VAL:HG22 | 27:25:7:PRO:HD2 | 2.04 | 0.40 |
| 1:2A:1028:A:H2' | 1:2A:1029:A:C8 | 2.56 | 0.40 |
| 1:2A:1193:G:H2' | 1:2A:1194:A:H8 | 1.86 | 0.40 |
| 1:2A:1342:A:H2 | 1:2A:1396:U:HO2' | 1.67 | 0.40 |
| 1:2A:1827:C:OP2 | 3:2D:222:ARG:HD2 | 2.22 | 0.40 |
| 1:2A:2206:G:OP2 | 1:2A:2206:G:H4' | 2.21 | 0.40 |
| 1:2A:2593:U:H2' | 1:2A:2594:C:C6 | 2.56 | 0.40 |
| 1:2A:2526:G:H5' | 1:2A:2742:C:O2' | 2.22 | 0.40 |
| 1:2A:375:C:H2' | 1:2A:376:C:C6 | 2.56 | 0.40 |
| 1:2A:460:A:C2 | 1:2A:470:A:C4 | 3.10 | 0.40 |
| 1:2A:730:C:H2' | 1:2A:731:C:C6 | 2.57 | 0.40 |
| 7:2H:152:ARG:HD3 | 7:2H:152:ARG:HA | 1.83 | 0.40 |
| 1:2A:958:U:H5'' | 12:2Q:14:ARG:HD3 | 2.04 | 0.40 |
| 12:2Q:43:THR:HA | 12:2Q:94:VAL:HG12 | 2.03 | 0.40 |
| 15:2T:21:GLU:O | 15:2T:91:ARG:NH1 | 2.50 | 0.40 |
| 18:2W:71:VAL:HA | 18:2W:107:LEU:HD12 | 2.02 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 3 | 1D | 273/276 (99%) | 255 (93%) | 17 (6%) | 1 (0%) | 34 | 53 |
| 3 | 2D | 273/276 (99%) | 261 (96%) | 11 (4%) | 1 (0%) | 34 | 53 |
| 4 | 1E | 202/206 (98%) | 192 (95%) | 9 (4%) | 1 (0%) | 29 | 47 |
| 4 | 2E | 202/206 (98%) | 196 (97%) | 5 (2%) | 1 (0%) | 29 | 47 |
| 5 | 1F | 201/210 (96%) | 196 (98%) | 4 (2%) | 1 (0%) | 29 | 47 |
| 5 | 2F | 201/210 (96%) | 196 (98%) | 3 (2%) | 2 (1%) | 15 | 27 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 6 | 1G | 179/182 (98%) | 163 (91%) | 15 (8%) | 1 (1%) | 25 | 42 |
| 6 | 2G | 179/182 (98%) | 162 (90%) | 15 (8%) | 2 (1%) | 14 | 25 |
| 7 | 1H | 172/180 (96%) | 164 (95%) | 7 (4%) | 1 (1%) | 25 | 42 |
| 7 | 2H | 172/180 (96%) | 157 (91%) | 14 (8%) | 1 (1%) | 25 | 42 |
| 8 | 1I | 144/148 (97%) | 134 (93%) | 9 (6%) | 1 (1%) | 22 | 39 |
| 8 | 2I | 144/148 (97%) | 133 (92%) | 9 (6%) | 2 (1%) | 11 | 19 |
| 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%) | 22 | 39 |
| 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%) | 9 | 16 |
| 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%) | 7 | 13 |
| 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%) | 15 | 27 |
| 20 | 2Y | 105/110 (96%) | 98 (93%) | 7 (7%) | 0 | 100 | 100 |
| 21 | 1Z | 148/206 (72%) | 131 (88%) | 14 (10%) | 3 (2%) | 7 | 13 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 21 | 2Z | 156/206 (76%) | 137 (88%) | 15 (10%) | 4 (3%) | 5 | 8 |
| 22 | 10 | 81/85 (95%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 22 | 20 | 81/85 (95%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 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%) | 8 | 15 |
| 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%) | 6 | 11 |
| 33 | 2b | 229/256 (90%) | 203 (89%) | 22 (10%) | 4 (2%) | 9 | 16 |
| 34 | 1c | 204/239 (85%) | 190 (93%) | 14 (7%) | 0 | 100 | 100 |
| 34 | 2c | 204/239 (85%) | 187 (92%) | 16 (8%) | 1 (0%) | 29 | 47 |
| 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%) | 22 | 39 |
| 36 | 2e | 146/162 (90%) | 137 (94%) | 8 (6%) | 1 (1%) | 22 | 39 |
| 37 | 1f | 98/101 (97%) | 93 (95%) | 5 (5%) | 0 | 100 | 100 |
| 37 | 2f | 98/101 (97%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 38 | 1g | 153/156 (98%) | 147 (96%) | 3 (2%) | 3 (2%) | 7 | 13 |
| 38 | 2g | 153/156 (98%) | 142 (93%) | 10 (6%) | 1 (1%) | 22 | 39 |
| 39 | 1h | 135/138 (98%) | 128 (95%) | 7 (5%) | 0 | 100 | 100 |
| 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%) | 19 | 34 |
| 41 | 1j | 95/105 (90%) | 83 (87%) | 9 (10%) | 3 (3%) | 4 | 6 |
| 41 | 2j | 94/105 (90%) | 83 (88%) | 7 (7%) | 4 (4%) | 2 | 3 |
| 42 | 1k | 112/129 (87%) | 106 (95%) | 5 (4%) | 1 (1%) | 17 | 31 |
| 42 | 2k | 112/129 (87%) | 103 (92%) | 7 (6%) | 2 (2%) | 8 | 15 |
| 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%) | 9 | 16 |
| 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%) | 6 | 10 |
| 46 | 2o | 86/89 (97%) | 82 (95%) | 3 (4%) | 1 (1%) | 13 | 23 |
| 47 | 1p | 80/88 (91%) | 78 (98%) | 2 (2%) | 0 | 100 | 100 |
| 47 | 2p | 80/88 (91%) | 77 (96%) | 2 (2%) | 1 (1%) | 12 | 21 |
| 48 | 1q | 97/105 (92%) | 93 (96%) | 3 (3%) | 1 (1%) | 15 | 27 |
| 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%) | 7 | 12 |
| 51 | 2t | 94/106 (89%) | 87 (93%) | 5 (5%) | 2 (2%) | 7 | 12 |
| 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%) | 22 | 39 |

All (75) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | 1H | 126 | PRO |
| 8 | 1I | 10 | GLU |
| 26 | 14 | 65 | ASP |
| 33 | 1b | 17 | PHE |
| 51 | 1t | 100 | ILE |
| 5 | 2F | 130 | ALA |
| 7 | 2H | 126 | PRO |
| 8 | 2I | 10 | GLU |
| 26 | 24 | 55 | ARG |
| 26 | 24 | 56 | VAL |
| 33 | 2b | 125 | PRO |
| 33 | 2b | 128 | GLU |
| 5 | 1F | 130 | ALA |
| 26 | 14 | 45 | GLY |
| 38 | 1g | 114 | ARG |
| 41 | 1j | 75 | ILE |
| 6 | 2G | 47 | LYS |
| 21 | 2Z | 146 | ILE |
| 26 | 24 | 47 | GLN |
| 26 | 24 | 65 | ASP |
| 41 | 2j | 75 | ILE |
| 42 | 2k | 49 | GLY |
| 17 | 1V | 53 | GLU |
| 21 | 1Z | 2 | GLU |
| 33 | 1b | 234 | PRO |
| 33 | 2b | 20 | GLU |
| 41 | 2j | 79 | ARG |
| 4 | 1E | 52 | LEU |
| 6 | 1G | 84 | LYS |
| 20 | 1Y | 103 | GLY |
| 26 | 14 | 53 | GLU |
| 33 | 1b | 9 | GLU |
| 46 | 1o | 20 | GLY |
| 51 | 1t | 47 | GLY |
| 5 | 2F | 89 | VAL |
| 51 | 2t | 47 | GLY |
| 51 | 2t | 100 | ILE |
| 3 | 1D | 3 | VAL |
| 17 | 1V | 43 | GLU |
| 26 | 14 | 55 | ARG |
| 33 | 1b | 233 | SER |
| 36 | 1e | 86 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 2D | 3 | VAL |
| 8 | 2I | 145 | VAL |
| 15 | 2T | 37 | GLY |
| 21 | 2Z | 141 | VAL |
| 41 | 2j | 55 | LYS |
| 44 | 2m | 99 | ARG |
| 44 | 2m | 101 | GLN |
| 46 | 2o | 20 | GLY |
| 21 | 1Z | 134 | PRO |
| 38 | 1g | 80 | VAL |
| 4 | 2E | 52 | LEU |
| 15 | 2T | 127 | ALA |
| 33 | 2b | 78 | GLN |
| 34 | 2c | 66 | VAL |
| 36 | 2e | 85 | GLY |
| 40 | 2i | 11 | LYS |
| 21 | 1Z | 165 | VAL |
| 33 | 1b | 231 | GLU |
| 11 | 1P | 93 | GLY |
| 38 | 2g | 80 | VAL |
| 38 | 1g | 55 | GLY |
| 41 | 1j | 39 | PRO |
| 21 | 2Z | 165 | VAL |
| 25 | 23 | 50 | VAL |
| 41 | 2j | 39 | PRO |
| 42 | 1k | 105 | VAL |
| 46 | 1o | 19 | PRO |
| 48 | 1q | 33 | GLY |
| 6 | 2G | 52 | ILE |
| 21 | 2Z | 134 | PRO |
| 42 | 2k | 105 | VAL |
| 41 | 1j | 77 | PRO |
| 47 | 2p | 53 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3 | 1D | 215/218 (99%) | 203 (94%) | 12 (6%) | 21 | 36 |
| 3 | 2D | 215/218 (99%) | 207 (96%) | 8 (4%) | 34 | 54 |
| 4 | 1E | 164/166 (99%) | 156 (95%) | 8 (5%) | 25 | 43 |
| 4 | 2E | 164/166 (99%) | 157 (96%) | 7 (4%) | 29 | 48 |
| 5 | 1F | 160/166 (96%) | 150 (94%) | 10 (6%) | 18 | 31 |
| 5 | 2F | 159/166 (96%) | 145 (91%) | 14 (9%) | 10 | 17 |
| 6 | 1G | 143/156 (92%) | 133 (93%) | 10 (7%) | 15 | 26 |
| 6 | 2G | 143/156 (92%) | 136 (95%) | 7 (5%) | 25 | 43 |
| 7 | 1H | 144/148 (97%) | 139 (96%) | 5 (4%) | 36 | 56 |
| 7 | 2H | 144/148 (97%) | 140 (97%) | 4 (3%) | 43 | 63 |
| 8 | 1I | 113/124 (91%) | 101 (89%) | 12 (11%) | 6 | 11 |
| 8 | 2I | 105/124 (85%) | 98 (93%) | 7 (7%) | 16 | 28 |
| 9 | 1N | 118/119 (99%) | 110 (93%) | 8 (7%) | 16 | 28 |
| 9 | 2N | 118/119 (99%) | 107 (91%) | 11 (9%) | 9 | 15 |
| 10 | 1O | 100/100 (100%) | 99 (99%) | 1 (1%) | 76 | 85 |
| 10 | 2O | 100/100 (100%) | 99 (99%) | 1 (1%) | 76 | 85 |
| 11 | 1P | 115/116 (99%) | 111 (96%) | 4 (4%) | 36 | 56 |
| 11 | 2P | 115/116 (99%) | 114 (99%) | 1 (1%) | 78 | 87 |
| 12 | 1Q | 111/111 (100%) | 104 (94%) | 7 (6%) | 18 | 31 |
| 12 | 2Q | 111/111 (100%) | 107 (96%) | 4 (4%) | 35 | 55 |
| 13 | 1R | 101/101 (100%) | 90 (89%) | 11 (11%) | 6 | 10 |
| 13 | 2R | 101/101 (100%) | 95 (94%) | 6 (6%) | 19 | 34 |
| 14 | 1S | 86/88 (98%) | 79 (92%) | 7 (8%) | 11 | 21 |
| 14 | 2S | 85/88 (97%) | 83 (98%) | 2 (2%) | 49 | 68 |
| 15 | 1T | 115/127 (91%) | 112 (97%) | 3 (3%) | 46 | 66 |
| 15 | 2T | 113/127 (89%) | 109 (96%) | 4 (4%) | 36 | 56 |
| 16 | 1U | 93/94 (99%) | 89 (96%) | 4 (4%) | 29 | 48 |
| 16 | 2U | 93/94 (99%) | 90 (97%) | 3 (3%) | 39 | 59 |
| 17 | 1V | 80/82 (98%) | 75 (94%) | 5 (6%) | 18 | 31 |
| 17 | 2V | 80/82 (98%) | 75 (94%) | 5 (6%) | 18 | 31 |
| 18 | 1W | 90/92 (98%) | 87 (97%) | 3 (3%) | 38 | 58 |
| 18 | 2W | 90/92 (98%) | 85 (94%) | 5 (6%) | 21 | 36 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 19 | 1X | 77/78 (99%) | 76 (99%) | 1 (1%) | 69 | 81 |
| 19 | 2X | 77/78 (99%) | 72 (94%) | 5 (6%) | 17 | 30 |
| 20 | 1Y | 85/91 (93%) | 77 (91%) | 8 (9%) | 8 | 15 |
| 20 | 2Y | 85/91 (93%) | 77 (91%) | 8 (9%) | 8 | 15 |
| 21 | 1Z | 135/179 (75%) | 125 (93%) | 10 (7%) | 13 | 24 |
| 21 | 2Z | 137/179 (76%) | 130 (95%) | 7 (5%) | 24 | 41 |
| 22 | 10 | 65/67 (97%) | 63 (97%) | 2 (3%) | 40 | 60 |
| 22 | 20 | 65/67 (97%) | 65 (100%) | 0 | 100 | 100 |
| 23 | 11 | 80/83 (96%) | 78 (98%) | 2 (2%) | 47 | 67 |
| 23 | 21 | 80/83 (96%) | 78 (98%) | 2 (2%) | 47 | 67 |
| 24 | 12 | 65/67 (97%) | 64 (98%) | 1 (2%) | 65 | 78 |
| 24 | 22 | 65/67 (97%) | 64 (98%) | 1 (2%) | 65 | 78 |
| 25 | 13 | 51/52 (98%) | 44 (86%) | 7 (14%) | 3 | 5 |
| 25 | 23 | 50/52 (96%) | 48 (96%) | 2 (4%) | 31 | 51 |
| 26 | 14 | 59/63 (94%) | 49 (83%) | 10 (17%) | 2 | 3 |
| 26 | 24 | 53/63 (84%) | 49 (92%) | 4 (8%) | 13 | 23 |
| 27 | 15 | 50/52 (96%) | 45 (90%) | 5 (10%) | 7 | 13 |
| 27 | 25 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 33 |
| 28 | 16 | 51/52 (98%) | 46 (90%) | 5 (10%) | 8 | 13 |
| 28 | 26 | 50/52 (96%) | 47 (94%) | 3 (6%) | 19 | 33 |
| 29 | 17 | 41/42 (98%) | 36 (88%) | 5 (12%) | 5 | 7 |
| 29 | 27 | 41/42 (98%) | 37 (90%) | 4 (10%) | 8 | 13 |
| 30 | 18 | 54/55 (98%) | 48 (89%) | 6 (11%) | 6 | 10 |
| 30 | 28 | 54/55 (98%) | 52 (96%) | 2 (4%) | 34 | 54 |
| 31 | 19 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 62 |
| 31 | 29 | 34/34 (100%) | 33 (97%) | 1 (3%) | 42 | 62 |
| 33 | 1b | 192/220 (87%) | 183 (95%) | 9 (5%) | 26 | 45 |
| 33 | 2b | 187/220 (85%) | 172 (92%) | 15 (8%) | 12 | 21 |
| 34 | 1c | 142/188 (76%) | 135 (95%) | 7 (5%) | 25 | 43 |
| 34 | 2c | 140/188 (74%) | 136 (97%) | 4 (3%) | 42 | 62 |
| 35 | 1d | 169/181 (93%) | 163 (96%) | 6 (4%) | 35 | 55 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 35 | 2d | 173/181 (96%) | 166 (96%) | 7 (4%) | 31 | 51 |
| 36 | 1e | 113/123 (92%) | 104 (92%) | 9 (8%) | 12 | 21 |
| 36 | 2e | 114/123 (93%) | 109 (96%) | 5 (4%) | 28 | 47 |
| 37 | 1f | 84/90 (93%) | 82 (98%) | 2 (2%) | 49 | 68 |
| 37 | 2f | 85/90 (94%) | 82 (96%) | 3 (4%) | 36 | 56 |
| 38 | 1g | 119/127 (94%) | 116 (98%) | 3 (2%) | 47 | 67 |
| 38 | 2g | 120/127 (94%) | 118 (98%) | 2 (2%) | 60 | 76 |
| 39 | 1h | 114/119 (96%) | 106 (93%) | 8 (7%) | 15 | 26 |
| 39 | 2h | 114/119 (96%) | 110 (96%) | 4 (4%) | 36 | 56 |
| 40 | 1i | 90/99 (91%) | 88 (98%) | 2 (2%) | 52 | 70 |
| 40 | 2i | 89/99 (90%) | 82 (92%) | 7 (8%) | 12 | 22 |
| 41 | 1j | 66/92 (72%) | 61 (92%) | 5 (8%) | 13 | 23 |
| 41 | 2j | 69/92 (75%) | 66 (96%) | 3 (4%) | 29 | 48 |
| 42 | 1k | 82/99 (83%) | 82 (100%) | 0 | 100 | 100 |
| 42 | 2k | 83/99 (84%) | 80 (96%) | 3 (4%) | 35 | 55 |
| 43 | 1l | 96/108 (89%) | 90 (94%) | 6 (6%) | 18 | 31 |
| 43 | 2l | 96/108 (89%) | 95 (99%) | 1 (1%) | 76 | 85 |
| 44 | 1m | 93/101 (92%) | 88 (95%) | 5 (5%) | 22 | 38 |
| 44 | 2m | 92/101 (91%) | 86 (94%) | 6 (6%) | 17 | 30 |
| 45 | 1n | 49/50 (98%) | 41 (84%) | 8 (16%) | 2 | 3 |
| 45 | 2n | 49/50 (98%) | 46 (94%) | 3 (6%) | 18 | 33 |
| 46 | 1o | 78/80 (98%) | 77 (99%) | 1 (1%) | 69 | 81 |
| 46 | 2o | 78/80 (98%) | 77 (99%) | 1 (1%) | 69 | 81 |
| 47 | 1p | 69/74 (93%) | 63 (91%) | 6 (9%) | 10 | 18 |
| 47 | 2p | 68/74 (92%) | 63 (93%) | 5 (7%) | 13 | 24 |
| 48 | 1q | 94/97 (97%) | 94 (100%) | 0 | 100 | 100 |
| 48 | 2q | 94/97 (97%) | 92 (98%) | 2 (2%) | 53 | 71 |
| 49 | 1r | 59/77 (77%) | 56 (95%) | 3 (5%) | 24 | 41 |
| 49 | 2r | 59/77 (77%) | 56 (95%) | 3 (5%) | 24 | 41 |
| 50 | 1s | 69/80 (86%) | 67 (97%) | 2 (3%) | 42 | 62 |
| 50 | 2s | 67/80 (84%) | 66 (98%) | 1 (2%) | 65 | 78 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 51 | 1t | 70/82 (85%) | 68 (97%) | 2 (3%) | 42 | 62 |
| 51 | 2t | 70/82 (85%) | 67 (96%) | 3 (4%) | 29 | 48 |
| 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%) | 8837 (95%) | 466 (5%) | 24 | 42 |

All (466) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1D | 12 | SER |
| 3 | 1D | 32 | SER |
| 3 | 1D | 61 | LEU |
| 3 | 1D | 94 | LEU |
| 3 | 1D | 99 | ASP |
| 3 | 1D | 106 | ILE |
| 3 | 1D | 134 | ARG |
| 3 | 1D | 193 | VAL |
| 3 | 1D | 221 | VAL |
| 3 | 1D | 229 | VAL |
| 3 | 1D | 242 | ARG |
| 3 | 1D | 260 | ARG |
| 4 | 1E | 21 | VAL |
| 4 | 1E | 24 | THR |
| 4 | 1E | 47 | VAL |
| 4 | 1E | 113 | PHE |
| 4 | 1E | 116 | VAL |
| 4 | 1E | 170 | LEU |
| 4 | 1E | 175 | VAL |
| 4 | 1E | 181 | LEU |
| 5 | 1F | 24 | LEU |
| 5 | 1F | 52 | LYS |
| 5 | 1F | 53 | THR |
| 5 | 1F | 57 | VAL |
| 5 | 1F | 88 | VAL |
| 5 | 1F | 106 | ARG |
| 5 | 1F | 170 | LEU |
| 5 | 1F | 175 | THR |
| 5 | 1F | 195 | ASP |
| 5 | 1F | 201 | VAL |
| 6 | 1G | 5 | VAL |
| 6 | 1G | 43 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | 1G | 77 | ILE |
| 6 | 1G | 79 | ASN |
| 6 | 1G | 90 | LEU |
| 6 | 1G | 126 | ASP |
| 6 | 1G | 132 | ASN |
| 6 | 1G | 139 | LEU |
| 6 | 1G | 145 | THR |
| 6 | 1G | 175 | LEU |
| 7 | 1H | 15 | VAL |
| 7 | 1H | 18 | GLU |
| 7 | 1H | 45 | VAL |
| 7 | 1H | 56 | SER |
| 7 | 1H | 57 | ASP |
| 8 | 1I | 9 | LEU |
| 8 | 1I | 20 | ASP |
| 8 | 1I | 31 | LEU |
| 8 | 1I | 38 | LEU |
| 8 | 1I | 47 | LEU |
| 8 | 1I | 74 | ASN |
| 8 | 1I | 78 | THR |
| 8 | 1I | 81 | VAL |
| 8 | 1I | 92 | VAL |
| 8 | 1I | 101 | LEU |
| 8 | 1I | 127 | VAL |
| 8 | 1I | 145 | VAL |
| 9 | 1N | 17 | ASP |
| 9 | 1N | 28 | THR |
| 9 | 1N | 33 | LEU |
| 9 | 1N | 34 | LEU |
| 9 | 1N | 46 | VAL |
| 9 | 1N | 48 | MET |
| 9 | 1N | 73 | THR |
| 9 | 1N | 112 | LEU |
| 10 | 1O | 28 | SER |
| 11 | 1P | 42 | SER |
| 11 | 1P | 59 | LEU |
| 11 | 1P | 95 | VAL |
| 11 | 1P | 101 | VAL |
| 12 | 1Q | 8 | LYS |
| 12 | 1Q | 35 | VAL |
| 12 | 1Q | 98 | LYS |
| 12 | 1Q | 101 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | 1Q | 109 | VAL |
| 12 | 1Q | 110 | THR |
| 12 | 1Q | 138 | ASP |
| 13 | 1R | 6 | SER |
| 13 | 1R | 15 | SER |
| 13 | 1R | 29 | LEU |
| 13 | 1R | 44 | LEU |
| 13 | 1R | 54 | LEU |
| 13 | 1R | 65 | LEU |
| 13 | 1R | 67 | LEU |
| 13 | 1R | 96 | ARG |
| 13 | 1R | 100 | LEU |
| 13 | 1R | 111 | LEU |
| 13 | 1R | 114 | VAL |
| 14 | 1S | 3 | ARG |
| 14 | 1S | 14 | VAL |
| 14 | 1S | 20 | ARG |
| 14 | 1S | 25 | ARG |
| 14 | 1S | 69 | VAL |
| 14 | 1S | 75 | GLU |
| 14 | 1S | 110 | LEU |
| 15 | 1T | 6 | LEU |
| 15 | 1T | 28 | VAL |
| 15 | 1T | 88 | ILE |
| 16 | 1U | 8 | VAL |
| 16 | 1U | 59 | ARG |
| 16 | 1U | 74 | LEU |
| 16 | 1U | 77 | SER |
| 17 | 1V | 46 | VAL |
| 17 | 1V | 51 | VAL |
| 17 | 1V | 52 | VAL |
| 17 | 1V | 72 | VAL |
| 17 | 1V | 79 | VAL |
| 18 | 1W | 11 | ARG |
| 18 | 1W | 17 | VAL |
| 18 | 1W | 107 | LEU |
| 19 | 1X | 70 | LEU |
| 20 | 1Y | 14 | LEU |
| 20 | 1Y | 43 | ASN |
| 20 | 1Y | 49 | VAL |
| 20 | 1Y | 70 | SER |
| 20 | 1Y | 72 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20 | 1Y | 99 | CYS |
| 20 | 1Y | 106 | LEU |
| 20 | 1Y | 107 | ASP |
| 21 | 1Z | 61 | LEU |
| 21 | 1Z | 70 | LEU |
| 21 | 1Z | 76 | LEU |
| 21 | 1Z | 81 | ARG |
| 21 | 1Z | 91 | LEU |
| 21 | 1Z | 126 | VAL |
| 21 | 1Z | 141 | VAL |
| 21 | 1Z | 153 | SER |
| 21 | 1Z | 165 | VAL |
| 21 | 1Z | 171 | ILE |
| 22 | 10 | 10 | THR |
| 22 | 10 | 14 | ARG |
| 23 | 11 | 30 | VAL |
| 23 | 11 | 35 | THR |
| 24 | 12 | 45 | SER |
| 25 | 13 | 3 | ARG |
| 25 | 13 | 17 | LYS |
| 25 | 13 | 23 | LEU |
| 25 | 13 | 30 | ARG |
| 25 | 13 | 34 | GLU |
| 25 | 13 | 54 | VAL |
| 25 | 13 | 56 | VAL |
| 26 | 14 | 27 | THR |
| 26 | 14 | 28 | LYS |
| 26 | 14 | 48 | ARG |
| 26 | 14 | 49 | PHE |
| 26 | 14 | 50 | VAL |
| 26 | 14 | 52 | THR |
| 26 | 14 | 56 | VAL |
| 26 | 14 | 57 | GLU |
| 26 | 14 | 58 | ARG |
| 26 | 14 | 65 | ASP |
| 27 | 15 | 6 | VAL |
| 27 | 15 | 15 | ARG |
| 27 | 15 | 16 | ARG |
| 27 | 15 | 29 | THR |
| 27 | 15 | 58 | LEU |
| 28 | 16 | 9 | LEU |
| 28 | 16 | 19 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28 | 16 | 48 | VAL |
| 28 | 16 | 50 | ARG |
| 28 | 16 | 51 | GLU |
| 29 | 17 | 1 | MET |
| 29 | 17 | 34 | ARG |
| 29 | 17 | 39 | ARG |
| 29 | 17 | 43 | THR |
| 29 | 17 | 46 | VAL |
| 30 | 18 | 14 | VAL |
| 30 | 18 | 31 | HIS |
| 30 | 18 | 32 | LEU |
| 30 | 18 | 34 | TRP |
| 30 | 18 | 43 | GLN |
| 30 | 18 | 58 | ILE |
| 31 | 19 | 7 | VAL |
| 33 | 1b | 24 | TRP |
| 33 | 1b | 30 | ARG |
| 33 | 1b | 37 | ASN |
| 33 | 1b | 81 | VAL |
| 33 | 1b | 94 | ASN |
| 33 | 1b | 122 | PHE |
| 33 | 1b | 160 | ASP |
| 33 | 1b | 222 | ILE |
| 33 | 1b | 234 | PRO |
| 34 | 1c | 3 | ASN |
| 34 | 1c | 8 | ILE |
| 34 | 1c | 52 | LEU |
| 34 | 1c | 70 | VAL |
| 34 | 1c | 115 | LEU |
| 34 | 1c | 172 | ARG |
| 34 | 1c | 188 | LEU |
| 35 | 1d | 127 | THR |
| 35 | 1d | 135 | LEU |
| 35 | 1d | 137 | SER |
| 35 | 1d | 175 | SER |
| 35 | 1d | 178 | VAL |
| 35 | 1d | 194 | LEU |
| 36 | 1e | 13 | ILE |
| 36 | 1e | 20 | GLN |
| 36 | 1e | 31 | LEU |
| 36 | 1e | 41 | VAL |
| 36 | 1e | 64 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | 1e | 75 | THR |
| 36 | 1e | 81 | GLU |
| 36 | 1e | 91 | LEU |
| 36 | 1e | 120 | THR |
| 37 | 1f | 7 | ASN |
| 37 | 1f | 92 | LYS |
| 38 | 1g | 104 | LEU |
| 38 | 1g | 113 | GLU |
| 38 | 1g | 115 | ARG |
| 39 | 1h | 19 | VAL |
| 39 | 1h | 25 | ASP |
| 39 | 1h | 26 | VAL |
| 39 | 1h | 29 | SER |
| 39 | 1h | 63 | LEU |
| 39 | 1h | 85 | ARG |
| 39 | 1h | 104 | ARG |
| 39 | 1h | 112 | LEU |
| 40 | 1i | 92 | TYR |
| 40 | 1i | 128 | ARG |
| 41 | 1j | 8 | LEU |
| 41 | 1j | 35 | SER |
| 41 | 1j | 71 | LEU |
| 41 | 1j | 72 | VAL |
| 41 | 1j | 92 | THR |
| 43 | 1l | 27 | LEU |
| 43 | 1l | 28 | LYS |
| 43 | 1l | 54 | LYS |
| 43 | 1l | 58 | VAL |
| 43 | 1l | 70 | ILE |
| 43 | 1l | 113 | ARG |
| 44 | 1m | 3 | ARG |
| 44 | 1m | 19 | LEU |
| 44 | 1m | 47 | ASP |
| 44 | 1m | 88 | ARG |
| 44 | 1m | 117 | VAL |
| 45 | 1n | 3 | ARG |
| 45 | 1n | 7 | ILE |
| 45 | 1n | 13 | THR |
| 45 | 1n | 18 | VAL |
| 45 | 1n | 22 | THR |
| 45 | 1n | 29 | ARG |
| 45 | 1n | 33 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45 | 1n | 60 | SER |
| 46 | 1o | 21 | ASP |
| 47 | 1p | 1 | MET |
| 47 | 1p | 2 | VAL |
| 47 | 1p | 20 | VAL |
| 47 | 1p | 45 | THR |
| 47 | 1p | 57 | ARG |
| 47 | 1p | 67 | THR |
| 49 | 1r | 26 | LEU |
| 49 | 1r | 47 | THR |
| 49 | 1r | 82 | THR |
| 50 | 1s | 77 | THR |
| 50 | 1s | 79 | THR |
| 51 | 1t | 72 | LEU |
| 51 | 1t | 100 | ILE |
| 3 | 2D | 61 | LEU |
| 3 | 2D | 94 | LEU |
| 3 | 2D | 142 | VAL |
| 3 | 2D | 221 | VAL |
| 3 | 2D | 229 | VAL |
| 3 | 2D | 242 | ARG |
| 3 | 2D | 253 | GLN |
| 3 | 2D | 261 | LYS |
| 4 | 2E | 9 | VAL |
| 4 | 2E | 21 | VAL |
| 4 | 2E | 27 | LEU |
| 4 | 2E | 33 | VAL |
| 4 | 2E | 116 | VAL |
| 4 | 2E | 119 | ARG |
| 4 | 2E | 181 | LEU |
| 5 | 2F | 20 | LEU |
| 5 | 2F | 57 | VAL |
| 5 | 2F | 70 | THR |
| 5 | 2F | 88 | VAL |
| 5 | 2F | 106 | ARG |
| 5 | 2F | 107 | LYS |
| 5 | 2F | 158 | THR |
| 5 | 2F | 170 | LEU |
| 5 | 2F | 175 | THR |
| 5 | 2F | 183 | VAL |
| 5 | 2F | 191 | ARG |
| 5 | 2F | 192 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | 2F | 195 | ASP |
| 5 | 2F | 201 | VAL |
| 6 | 2G | 3 | LEU |
| 6 | 2G | 18 | GLU |
| 6 | 2G | 43 | LEU |
| 6 | 2G | 47 | LYS |
| 6 | 2G | 77 | ILE |
| 6 | 2G | 79 | ASN |
| 6 | 2G | 165 | THR |
| 7 | 2H | 27 | LYS |
| 7 | 2H | 45 | VAL |
| 7 | 2H | 67 | LEU |
| 7 | 2H | 71 | LEU |
| 8 | 2I | 38 | LEU |
| 8 | 2I | 47 | LEU |
| 8 | 2I | 76 | THR |
| 8 | 2I | 101 | LEU |
| 8 | 2I | 123 | LEU |
| 8 | 2I | 127 | VAL |
| 8 | 2I | 140 | LEU |
| 9 | 2N | 32 | THR |
| 9 | 2N | 34 | LEU |
| 9 | 2N | 35 | ARG |
| 9 | 2N | 38 | HIS |
| 9 | 2N | 43 | THR |
| 9 | 2N | 46 | VAL |
| 9 | 2N | 60 | ILE |
| 9 | 2N | 62 | VAL |
| 9 | 2N | 63 | THR |
| 9 | 2N | 83 | LYS |
| 9 | 2N | 140 | VAL |
| 10 | 2O | 22 | ILE |
| 11 | 2P | 95 | VAL |
| 12 | 2Q | 5 | ARG |
| 12 | 2Q | 21 | THR |
| 12 | 2Q | 109 | VAL |
| 12 | 2Q | 110 | THR |
| 13 | 2R | 6 | SER |
| 13 | 2R | 29 | LEU |
| 13 | 2R | 44 | LEU |
| 13 | 2R | 65 | LEU |
| 13 | 2R | 67 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | 2R | 111 | LEU |
| 14 | 2S | 5 | THR |
| 14 | 2S | 21 | THR |
| 15 | 2T | 49 | VAL |
| 15 | 2T | 57 | PHE |
| 15 | 2T | 74 | ARG |
| 15 | 2T | 96 | ARG |
| 16 | 2U | 6 | THR |
| 16 | 2U | 31 | SER |
| 16 | 2U | 74 | LEU |
| 17 | 2V | 7 | THR |
| 17 | 2V | 51 | VAL |
| 17 | 2V | 61 | VAL |
| 17 | 2V | 62 | LEU |
| 17 | 2V | 72 | VAL |
| 18 | 2W | 11 | ARG |
| 18 | 2W | 15 | ARG |
| 18 | 2W | 23 | LEU |
| 18 | 2W | 67 | ASP |
| 18 | 2W | 107 | LEU |
| 19 | 2X | 23 | GLU |
| 19 | 2X | 35 | THR |
| 19 | 2X | 75 | ASP |
| 19 | 2X | 82 | GLN |
| 19 | 2X | 92 | LEU |
| 20 | 2Y | 14 | LEU |
| 20 | 2Y | 37 | VAL |
| 20 | 2Y | 43 | ASN |
| 20 | 2Y | 55 | TYR |
| 20 | 2Y | 61 | ILE |
| 20 | 2Y | 72 | VAL |
| 20 | 2Y | 85 | VAL |
| 20 | 2Y | 99 | CYS |
| 21 | 2Z | 19 | ARG |
| 21 | 2Z | 42 | VAL |
| 21 | 2Z | 67 | LEU |
| 21 | 2Z | 70 | LEU |
| 21 | 2Z | 155 | LEU |
| 21 | 2Z | 157 | LEU |
| 21 | 2Z | 174 | VAL |
| 23 | 21 | 11 | ARG |
| 23 | 21 | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | 22 | 35 | LEU |
| 25 | 23 | 30 | ARG |
| 25 | 23 | 54 | VAL |
| 26 | 24 | 48 | ARG |
| 26 | 24 | 49 | PHE |
| 26 | 24 | 56 | VAL |
| 26 | 24 | 63 | TYR |
| 27 | 25 | 6 | VAL |
| 27 | 25 | 33 | CYS |
| 27 | 25 | 58 | LEU |
| 28 | 26 | 9 | LEU |
| 28 | 26 | 48 | VAL |
| 28 | 26 | 51 | GLU |
| 29 | 27 | 1 | MET |
| 29 | 27 | 24 | THR |
| 29 | 27 | 39 | ARG |
| 29 | 27 | 43 | THR |
| 30 | 28 | 30 | ARG |
| 30 | 28 | 32 | LEU |
| 31 | 29 | 14 | CYS |
| 33 | 2b | 19 | HIS |
| 33 | 2b | 24 | TRP |
| 33 | 2b | 37 | ASN |
| 33 | 2b | 44 | LEU |
| 33 | 2b | 71 | VAL |
| 33 | 2b | 81 | VAL |
| 33 | 2b | 102 | LEU |
| 33 | 2b | 108 | ILE |
| 33 | 2b | 111 | ARG |
| 33 | 2b | 121 | LEU |
| 33 | 2b | 122 | PHE |
| 33 | 2b | 160 | ASP |
| 33 | 2b | 176 | GLU |
| 33 | 2b | 189 | ASP |
| 33 | 2b | 230 | VAL |
| 34 | 2c | 22 | TRP |
| 34 | 2c | 40 | ARG |
| 34 | 2c | 115 | LEU |
| 34 | 2c | 192 | THR |
| 35 | 2d | 9 | CYS |
| 35 | 2d | 33 | MET |
| 35 | 2d | 127 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | 2d | 135 | LEU |
| 35 | 2d | 141 | ARG |
| 35 | 2d | 188 | LEU |
| 35 | 2d | 194 | LEU |
| 36 | 2e | 41 | VAL |
| 36 | 2e | 64 | ARG |
| 36 | 2e | 81 | GLU |
| 36 | 2e | 91 | LEU |
| 36 | 2e | 120 | THR |
| 37 | 2f | 19 | LEU |
| 37 | 2f | 40 | VAL |
| 37 | 2f | 81 | ILE |
| 38 | 2g | 31 | MET |
| 38 | 2g | 104 | LEU |
| 39 | 2h | 11 | THR |
| 39 | 2h | 14 | ARG |
| 39 | 2h | 104 | ARG |
| 39 | 2h | 112 | LEU |
| 40 | 2i | 14 | VAL |
| 40 | 2i | 27 | THR |
| 40 | 2i | 29 | ASN |
| 40 | 2i | 41 | VAL |
| 40 | 2i | 50 | LEU |
| 40 | 2i | 102 | LEU |
| 40 | 2i | 105 | ASP |
| 41 | 2j | 59 | SER |
| 41 | 2j | 67 | THR |
| 41 | 2j | 71 | LEU |
| 42 | 2k | 14 | VAL |
| 42 | 2k | 81 | ASP |
| 42 | 2k | 87 | THR |
| 43 | 2l | 117 | ARG |
| 44 | 2m | 3 | ARG |
| 44 | 2m | 19 | LEU |
| 44 | 2m | 29 | ARG |
| 44 | 2m | 69 | GLU |
| 44 | 2m | 74 | VAL |
| 44 | 2m | 91 | ARG |
| 45 | 2n | 7 | ILE |
| 45 | 2n | 22 | THR |
| 45 | 2n | 33 | VAL |
| 46 | 2o | 87 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47 | 2p | 19 | ILE |
| 47 | 2p | 20 | VAL |
| 47 | 2p | 21 | VAL |
| 47 | 2p | 62 | VAL |
| 47 | 2p | 67 | THR |
| 48 | 2q | 53 | LEU |
| 48 | 2q | 68 | ARG |
| 49 | 2r | 29 | PHE |
| 49 | 2r | 37 | VAL |
| 49 | 2r | 47 | THR |
| 50 | 2s | 41 | VAL |
| 51 | 2t | 39 | LYS |
| 51 | 2t | 70 | SER |
| 51 | 2t | 99 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | 1D | 116 | GLN |
| 3 | 1D | 126 | GLN |
| 5 | 1F | 169 | ASN |
| 8 | 1I | 11 | ASN |
| 8 | 1I | 104 | GLN |
| 10 | 1O | 3 | GLN |
| 14 | 1S | 38 | GLN |
| 14 | 1S | 61 | ASN |
| 16 | 1U | 81 | HIS |
| 18 | 1W | 60 | ASN |
| 19 | 1X | 31 | HIS |
| 20 | 1Y | 6 | HIS |
| 21 | 1Z | 55 | HIS |
| 21 | 1Z | 73 | GLN |
| 22 | 10 | 50 | ASN |
| 30 | 18 | 35 | GLN |
| 31 | 19 | 34 | GLN |
| 33 | 1b | 16 | HIS |
| 33 | 1b | 37 | ASN |
| 33 | 1b | 78 | GLN |
| 33 | 1b | 94 | ASN |
| 34 | 1c | 110 | ASN |
| 35 | 1d | 77 | ASN |
| 35 | 1d | 116 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35 | 1d | 123 | HIS |
| 35 | 1d | 125 | HIS |
| 36 | 1e | 20 | GLN |
| 36 | 1e | 78 | HIS |
| 38 | 1g | 28 | ASN |
| 38 | 1g | 51 | GLN |
| 38 | 1g | 110 | GLN |
| 40 | 1i | 3 | GLN |
| 40 | 1i | 34 | ASN |
| 40 | 1i | 58 | HIS |
| 40 | 1i | 73 | GLN |
| 41 | 1j | 56 | HIS |
| 43 | 1l | 99 | HIS |
| 44 | 1m | 92 | HIS |
| 46 | 1o | 62 | GLN |
| 47 | 1p | 14 | ASN |
| 48 | 1q | 26 | GLN |
| 49 | 1r | 63 | GLN |
| 50 | 1s | 23 | ASN |
| 50 | 1s | 83 | HIS |
| 51 | 1t | 16 | HIS |
| 4 | 2E | 48 | GLN |
| 5 | 2F | 69 | HIS |
| 5 | 2F | 203 | GLN |
| 6 | 2G | 123 | ASN |
| 12 | 2Q | 123 | HIS |
| 12 | 2Q | 141 | GLN |
| 15 | 2T | 79 | HIS |
| 16 | 2U | 66 | ASN |
| 20 | 2Y | 43 | ASN |
| 21 | 2Z | 34 | ASN |
| 21 | 2Z | 55 | HIS |
| 21 | 2Z | 65 | GLN |
| 21 | 2Z | 132 | ASN |
| 33 | 2b | 37 | ASN |
| 33 | 2b | 94 | ASN |
| 33 | 2b | 212 | GLN |
| 35 | 2d | 74 | GLN |
| 35 | 2d | 77 | ASN |
| 35 | 2d | 116 | GLN |
| 35 | 2d | 119 | GLN |
| 35 | 2d | 125 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | 2e | 73 | ASN |
| 36 | 2e | 78 | HIS |
| 37 | 2f | 100 | ASN |
| 38 | 2g | 68 | ASN |
| 38 | 2g | 86 | GLN |
| 39 | 2h | 78 | GLN |
| 40 | 2i | 3 | GLN |
| 40 | 2i | 58 | HIS |
| 40 | 2i | 73 | GLN |
| 41 | 2j | 21 | GLN |
| 41 | 2j | 56 | HIS |
| 43 | 2l | 99 | HIS |
| 49 | 2r | 63 | GLN |
| 50 | 2s | 23 | ASN |
| 50 | 2s | 69 | HIS |
| 50 | 2s | 83 | HIS |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | 1A | 2863/2915 (98%) | 448 (15%) | 19 (0%) |
| 1 | 2A | 2790/2915 (95%) | 514 (18%) | 19 (0%) |
| 2 | 1B | 120/121 (99%) | 11 (9%) | 1 (0%) |
| 2 | 2B | 118/121 (97%) | 28 (23%) | 0 |
| 32 | 1a | 1494/1521 (98%) | 250 (16%) | 0 |
| 32 | 2a | 1498/1521 (98%) | 281 (18%) | 0 |
| 53 | 1v | 12/27 (44%) | 2 (16%) | 0 |
| 53 | 2v | 12/27 (44%) | 4 (33%) | 0 |
| 54 | 1w | 68/76 (89%) | 24 (35%) | 0 |
| 54 | 1y | 68/76 (89%) | 24 (35%) | 0 |
| 54 | 2w | 68/76 (89%) | 28 (41%) | 0 |
| 54 | 2y | 68/76 (89%) | 28 (41%) | 0 |
| 55 | 1x | 75/77 (97%) | 13 (17%) | 0 |
| 55 | 2x | 75/77 (97%) | 15 (20%) | 0 |
| All | All | 9329/9626 (96%) | 1670 (17%) | 39 (0%) |

All (1670) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1A | 12 | U |
| 1 | 1A | 13 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1A | 34 | C |
| 1 | 1A | 45 | C |
| 1 | 1A | 71 | A |
| 1 | 1A | 74 | A |
| 1 | 1A | 75 | G |
| 1 | 1A | 84 | A |
| 1 | 1A | 95 | G |
| 1 | 1A | 118 | A |
| 1 | 1A | 119 | A |
| 1 | 1A | 120 | U |
| 1 | 1A | 125 | G |
| 1 | 1A | 196 | A |
| 1 | 1A | 197 | A |
| 1 | 1A | 199 | A |
| 1 | 1A | 201 | C |
| 1 | 1A | 205 | G |
| 1 | 1A | 214 | G |
| 1 | 1A | 216 | A |
| 1 | 1A | 222 | A |
| 1 | 1A | 228 | A |
| 1 | 1A | 229 | A |
| 1 | 1A | 230 | U |
| 1 | 1A | 233 | A |
| 1 | 1A | 248 | G |
| 1 | 1A | 266 | G |
| 1 | 1A | 271(A) | A |
| 1 | 1A | 271(K) | U |
| 1 | 1A | 271(L) | U |
| 1 | 1A | 271(M) | G |
| 1 | 1A | 271(N) | U |
| 1 | 1A | 271(O) | C |
| 1 | 1A | 272(A) | U |
| 1 | 1A | 272(B) | G |
| 1 | 1A | 279 | C |
| 1 | 1A | 311 | A |
| 1 | 1A | 329 | G |
| 1 | 1A | 330 | A |
| 1 | 1A | 345 | A |
| 1 | 1A | 352 | G |
| 1 | 1A | 363 | G |
| 1 | 1A | 363(B) | G |
| 1 | 1A | 386 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1A | 396 | G |
| 1 | 1A | 405 | U |
| 1 | 1A | 411 | G |
| 1 | 1A | 418 | G |
| 1 | 1A | 421 | U |
| 1 | 1A | 428 | A |
| 1 | 1A | 443 | A |
| 1 | 1A | 444 | C |
| 1 | 1A | 448 | U |
| 1 | 1A | 456 | C |
| 1 | 1A | 457 | A |
| 1 | 1A | 467 | G |
| 1 | 1A | 481 | G |
| 1 | 1A | 504 | U |
| 1 | 1A | 505 | A |
| 1 | 1A | 508 | G |
| 1 | 1A | 509 | C |
| 1 | 1A | 512 | G |
| 1 | 1A | 528 | A |
| 1 | 1A | 530 | G |
| 1 | 1A | 531 | C |
| 1 | 1A | 532 | A |
| 1 | 1A | 533 | G |
| 1 | 1A | 545 | G |
| 1 | 1A | 549 | G |
| 1 | 1A | 551 | G |
| 1 | 1A | 563 | G |
| 1 | 1A | 573 | G |
| 1 | 1A | 575 | A |
| 1 | 1A | 603 | A |
| 1 | 1A | 604 | G |
| 1 | 1A | 607 | U |
| 1 | 1A | 614(A) | U |
| 1 | 1A | 614(B) | G |
| 1 | 1A | 615 | G |
| 1 | 1A | 627 | A |
| 1 | 1A | 634 | C |
| 1 | 1A | 637 | A |
| 1 | 1A | 645 | C |
| 1 | 1A | 646 | A |
| 1 | 1A | 652(E) | G |
| 1 | 1A | 652(T) | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1A | 669 | G |
| 1 | 1A | 686 | G |
| 1 | 1A | 717 | G |
| 1 | 1A | 730 | C |
| 1 | 1A | 764 | A |
| 1 | 1A | 775 | G |
| 1 | 1A | 776 | G |
| 1 | 1A | 782 | A |
| 1 | 1A | 784 | A |
| 1 | 1A | 785 | G |
| 1 | 1A | 789 | A |
| 1 | 1A | 790 | C |
| 1 | 1A | 792 | G |
| 1 | 1A | 802 | A |
| 1 | 1A | 805 | G |
| 1 | 1A | 812 | C |
| 1 | 1A | 819 | A |
| 1 | 1A | 827 | U |
| 1 | 1A | 828 | U |
| 1 | 1A | 859 | G |
| 1 | 1A | 865 | C |
| 1 | 1A | 866 | A |
| 1 | 1A | 879 | G |
| 1 | 1A | 880 | G |
| 1 | 1A | 882 | G |
| 1 | 1A | 883 | G |
| 1 | 1A | 884 | C |
| 1 | 1A | 885 | C |
| 1 | 1A | 886 | C |
| 1 | 1A | 887 | A |
| 1 | 1A | 888 | C |
| 1 | 1A | 889 | C |
| 1 | 1A | 890 | A |
| 1 | 1A | 892 | G |
| 1 | 1A | 894 | C |
| 1 | 1A | 895 | U |
| 1 | 1A | 896 | A |
| 1 | 1A | 897 | C |
| 1 | 1A | 898 | C |
| 1 | 1A | 899 | A |
| 1 | 1A | 907 | U |
| 1 | 1A | 910 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 932 | G |
| 1 | 1A | 945 | A |
| 1 | 1A | 946 | G |
| 1 | 1A | 953 | A |
| 1 | 1A | 961 | C |
| 1 | 1A | 963 | U |
| 1 | 1A | 974 | G |
| 1 | 1A | 975 | C |
| 1 | 1A | 983 | A |
| 1 | 1A | 996 | A |
| 1 | 1A | 1012 | U |
| 1 | 1A | 1013 | C |
| 1 | 1A | 1022 | G |
| 1 | 1A | 1025 | G |
| 1 | 1A | 1026 | U |
| 1 | 1A | 1027 | A |
| 1 | 1A | 1033 | U |
| 1 | 1A | 1041 | C |
| 1 | 1A | 1044 | G |
| 1 | 1A | 1046 | A |
| 1 | 1A | 1047 | G |
| 1 | 1A | 1048 | A |
| 1 | 1A | 1054 | A |
| 1 | 1A | 1055 | G |
| 1 | 1A | 1058 | G |
| 1 | 1A | 1059 | G |
| 1 | 1A | 1064 | C |
| 1 | 1A | 1066 | U |
| 1 | 1A | 1068 | G |
| 1 | 1A | 1071 | G |
| 1 | 1A | 1073 | A |
| 1 | 1A | 1074 | G |
| 1 | 1A | 1075 | C |
| 1 | 1A | 1076 | C |
| 1 | 1A | 1078 | U |
| 1 | 1A | 1079 | C |
| 1 | 1A | 1081 | U |
| 1 | 1A | 1088 | A |
| 1 | 1A | 1089 | G |
| 1 | 1A | 1090 | U |
| 1 | 1A | 1093 | G |
| 1 | 1A | 1094 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 1097 | U |
| 1 | 1A | 1098 | A |
| 1 | 1A | 1100 | C |
| 1 | 1A | 1101 | U |
| 1 | 1A | 1109 | C |
| 1 | 1A | 1111 | A |
| 1 | 1A | 1112 | G |
| 1 | 1A | 1128 | A |
| 1 | 1A | 1130 | U |
| 1 | 1A | 1135 | C |
| 1 | 1A | 1136 | G |
| 1 | 1A | 1171 | G |
| 1 | 1A | 1173 | G |
| 1 | 1A | 1174 | A |
| 1 | 1A | 1175 | U |
| 1 | 1A | 1176 | G |
| 1 | 1A | 1177 | A |
| 1 | 1A | 1178 | C |
| 1 | 1A | 1211 | U |
| 1 | 1A | 1212 | G |
| 1 | 1A | 1220 | A |
| 1 | 1A | 1227 | G |
| 1 | 1A | 1229 | G |
| 1 | 1A | 1237 | A |
| 1 | 1A | 1244 | G |
| 1 | 1A | 1248 | G |
| 1 | 1A | 1253 | A |
| 1 | 1A | 1256 | G |
| 1 | 1A | 1267 | U |
| 1 | 1A | 1271 | G |
| 1 | 1A | 1272 | A |
| 1 | 1A | 1300 | U |
| 1 | 1A | 1301 | A |
| 1 | 1A | 1303 | G |
| 1 | 1A | 1320 | C |
| 1 | 1A | 1352 | U |
| 1 | 1A | 1359 | A |
| 1 | 1A | 1360 | A |
| 1 | 1A | 1365 | A |
| 1 | 1A | 1379 | A |
| 1 | 1A | 1384 | A |
| 1 | 1A | 1385 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 1A | 1395 | A |
| 1 | 1A | 1396 | U |
| 1 | 1A | 1416 | G |
| 1 | 1A | 1417 | C |
| 1 | 1A | 1420 | U |
| 1 | 1A | 1421 | G |
| 1 | 1A | 1428 | C |
| 1 | 1A | 1437 | C |
| 1 | 1A | 1445 | A |
| 1 | 1A | 1450 | G |
| 1 | 1A | 1455 | G |
| 1 | 1A | 1467 | C |
| 1 | 1A | 1478 | G |
| 1 | 1A | 1482 | G |
| 1 | 1A | 1490 | A |
| 1 | 1A | 1493 | C |
| 1 | 1A | 1494 | A |
| 1 | 1A | 1497 | U |
| 1 | 1A | 1508 | A |
| 1 | 1A | 1509 | C |
| 1 | 1A | 1509(A) | A |
| 1 | 1A | 1542 | A |
| 1 | 1A | 1554 | A |
| 1 | 1A | 1558 | A |
| 1 | 1A | 1566 | A |
| 1 | 1A | 1569 | A |
| 1 | 1A | 1578 | U |
| 1 | 1A | 1579 | A |
| 1 | 1A | 1580 | A |
| 1 | 1A | 1581 | G |
| 1 | 1A | 1584 | C |
| 1 | 1A | 1586 | A |
| 1 | 1A | 1608 | A |
| 1 | 1A | 1610 | A |
| 1 | 1A | 1612 | C |
| 1 | 1A | 1646 | C |
| 1 | 1A | 1647 | G |
| 1 | 1A | 1648 | C |
| 1 | 1A | 1654 | A |
| 1 | 1A | 1664 | A |
| 1 | 1A | 1667 | G |
| 1 | 1A | 1671 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 1674 | G |
| 1 | 1A | 1696 | G |
| 1 | 1A | 1700 | A |
| 1 | 1A | 1701 | A |
| 1 | 1A | 1703 | G |
| 1 | 1A | 1722 | A |
| 1 | 1A | 1740 | G |
| 1 | 1A | 1756 | G |
| 1 | 1A | 1762 | A |
| 1 | 1A | 1763 | G |
| 1 | 1A | 1764 | G |
| 1 | 1A | 1773 | A |
| 1 | 1A | 1780 | A |
| 1 | 1A | 1782 | C |
| 1 | 1A | 1791 | A |
| 1 | 1A | 1800 | C |
| 1 | 1A | 1801 | G |
| 1 | 1A | 1812 | A |
| 1 | 1A | 1816 | G |
| 1 | 1A | 1828 | G |
| 1 | 1A | 1847 | A |
| 1 | 1A | 1861 | G |
| 1 | 1A | 1877 | A |
| 1 | 1A | 1878 | G |
| 1 | 1A | 1889 | A |
| 1 | 1A | 1900 | A |
| 1 | 1A | 1906 | G |
| 1 | 1A | 1929 | G |
| 1 | 1A | 1930 | G |
| 1 | 1A | 1937 | A |
| 1 | 1A | 1938 | A |
| 1 | 1A | 1940 | U |
| 1 | 1A | 1955 | U |
| 1 | 1A | 1963 | U |
| 1 | 1A | 1965 | C |
| 1 | 1A | 1967 | C |
| 1 | 1A | 1970 | A |
| 1 | 1A | 1971 | A |
| 1 | 1A | 1972 | A |
| 1 | 1A | 1992 | G |
| 1 | 1A | 1993 | U |
| 1 | 1A | 1997 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 2020 | A |
| 1 | 1A | 2023 | G |
| 1 | 1A | 2031 | A |
| 1 | 1A | 2032 | G |
| 1 | 1A | 2033 | A |
| 1 | 1A | 2043 | C |
| 1 | 1A | 2055 | C |
| 1 | 1A | 2056 | G |
| 1 | 1A | 2060 | A |
| 1 | 1A | 2061 | G |
| 1 | 1A | 2062 | A |
| 1 | 1A | 2069 | G |
| 1 | 1A | 2080 | G |
| 1 | 1A | 2101 | G |
| 1 | 1A | 2107 | C |
| 1 | 1A | 2110 | G |
| 1 | 1A | 2113 | U |
| 1 | 1A | 2116 | G |
| 1 | 1A | 2125 | G |
| 1 | 1A | 2127 | G |
| 1 | 1A | 2129 | C |
| 1 | 1A | 2130 | U |
| 1 | 1A | 2131 | G |
| 1 | 1A | 2132 | U |
| 1 | 1A | 2133 | G |
| 1 | 1A | 2134 | A |
| 1 | 1A | 2135 | A |
| 1 | 1A | 2136 | C |
| 1 | 1A | 2138 | C |
| 1 | 1A | 2140 | C |
| 1 | 1A | 2142 | C |
| 1 | 1A | 2144 | U |
| 1 | 1A | 2146 | C |
| 1 | 1A | 2147 | G |
| 1 | 1A | 2149 | G |
| 1 | 1A | 2150 | U |
| 1 | 1A | 2151 | G |
| 1 | 1A | 2152 | G |
| 1 | 1A | 2155 | G |
| 1 | 1A | 2157 | G |
| 1 | 1A | 2158 | A |
| 1 | 1A | 2159 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 2162 | G |
| 1 | 1A | 2163 | C |
| 1 | 1A | 2164 | C |
| 1 | 1A | 2165 | G |
| 1 | 1A | 2166 | G |
| 1 | 1A | 2167 | U |
| 1 | 1A | 2169 | A |
| 1 | 1A | 2171 | A |
| 1 | 1A | 2172 | U |
| 1 | 1A | 2174 | C |
| 1 | 1A | 2178 | C |
| 1 | 1A | 2184 | G |
| 1 | 1A | 2198 | A |
| 1 | 1A | 2206 | G |
| 1 | 1A | 2207 | G |
| 1 | 1A | 2208 | A |
| 1 | 1A | 2218 | U |
| 1 | 1A | 2225 | A |
| 1 | 1A | 2238 | G |
| 1 | 1A | 2249 | U |
| 1 | 1A | 2268 | A |
| 1 | 1A | 2269 | A |
| 1 | 1A | 2279 | G |
| 1 | 1A | 2280 | G |
| 1 | 1A | 2283 | C |
| 1 | 1A | 2287 | A |
| 1 | 1A | 2305 | A |
| 1 | 1A | 2307 | G |
| 1 | 1A | 2308 | G |
| 1 | 1A | 2309 | A |
| 1 | 1A | 2314 | C |
| 1 | 1A | 2320 | A |
| 1 | 1A | 2325 | G |
| 1 | 1A | 2334 | G |
| 1 | 1A | 2336 | A |
| 1 | 1A | 2347 | C |
| 1 | 1A | 2350 | C |
| 1 | 1A | 2361 | A |
| 1 | 1A | 2383 | G |
| 1 | 1A | 2385 | C |
| 1 | 1A | 2389 | G |
| 1 | 1A | 2396 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 1A | 2406 | U |
| 1 | 1A | 2410 | G |
| 1 | 1A | 2424 | C |
| 1 | 1A | 2425 | A |
| 1 | 1A | 2429 | G |
| 1 | 1A | 2430 | A |
| 1 | 1A | 2435 | A |
| 1 | 1A | 2439 | A |
| 1 | 1A | 2441 | C |
| 1 | 1A | 2445 | G |
| 1 | 1A | 2448 | A |
| 1 | 1A | 2474 | C |
| 1 | 1A | 2476 | A |
| 1 | 1A | 2490 | G |
| 1 | 1A | 2491 | U |
| 1 | 1A | 2502 | G |
| 1 | 1A | 2505 | G |
| 1 | 1A | 2506 | U |
| 1 | 1A | 2518 | A |
| 1 | 1A | 2520 | C |
| 1 | 1A | 2529 | G |
| 1 | 1A | 2549 | G |
| 1 | 1A | 2554 | U |
| 1 | 1A | 2556 | C |
| 1 | 1A | 2566 | A |
| 1 | 1A | 2567 | G |
| 1 | 1A | 2573 | C |
| 1 | 1A | 2602 | A |
| 1 | 1A | 2609 | U |
| 1 | 1A | 2612 | C |
| 1 | 1A | 2629 | A |
| 1 | 1A | 2630 | G |
| 1 | 1A | 2638 | G |
| 1 | 1A | 2646 | C |
| 1 | 1A | 2654 | A |
| 1 | 1A | 2663 | G |
| 1 | 1A | 2689 | U |
| 1 | 1A | 2691 | C |
| 1 | 1A | 2702 | U |
| 1 | 1A | 2712(A) | A |
| 1 | 1A | 2713 | A |
| 1 | 1A | 2714 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 1A | 2726 | U |
| 1 | 1A | 2733 | A |
| 1 | 1A | 2734 | A |
| 1 | 1A | 2739 | U |
| 1 | 1A | 2764 | A |
| 1 | 1A | 2765 | A |
| 1 | 1A | 2766 | G |
| 1 | 1A | 2778 | A |
| 1 | 1A | 2789 | C |
| 1 | 1A | 2790 | A |
| 1 | 1A | 2791 | C |
| 1 | 1A | 2794 | C |
| 1 | 1A | 2802 | G |
| 1 | 1A | 2803 | C |
| 1 | 1A | 2818 | G |
| 1 | 1A | 2820 | A |
| 1 | 1A | 2821 | A |
| 1 | 1A | 2833 | G |
| 1 | 1A | 2835 | A |
| 1 | 1A | 2872 | G |
| 1 | 1A | 2873 | A |
| 1 | 1A | 2879 | C |
| 1 | 1A | 2880 | C |
| 1 | 1A | 2892 | A |
| 1 | 1A | 2894 | G |
| 1 | 1A | 2897 | U |
| 2 | 1B | 2 | C |
| 2 | 1B | 15 | A |
| 2 | 1B | 25 | A |
| 2 | 1B | 35 | U |
| 2 | 1B | 42 | C |
| 2 | 1B | 50 | G |
| 2 | 1B | 56 | G |
| 2 | 1B | 73 | A |
| 2 | 1B | 85 | G |
| 2 | 1B | 110 | G |
| 2 | 1B | 120 | A |
| 32 | 1a | 9 | G |
| 32 | 1a | 39 | G |
| 32 | 1a | 47 | C |
| 32 | 1a | 48 | C |
| 32 | 1a | 51 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 32 | 1a | 52 | G |
| 32 | 1a | 54 | C |
| 32 | 1a | 55 | A |
| 32 | 1a | 61 | G |
| 32 | 1a | 77 | G |
| 32 | 1a | 79 | G |
| 32 | 1a | 91 | C |
| 32 | 1a | 92 | C |
| 32 | 1a | 98 | G |
| 32 | 1a | 101 | A |
| 32 | 1a | 105 | G |
| 32 | 1a | 111 | G |
| 32 | 1a | 116 | A |
| 32 | 1a | 121 | C |
| 32 | 1a | 131 | C |
| 32 | 1a | 144 | G |
| 32 | 1a | 159 | G |
| 32 | 1a | 162 | A |
| 32 | 1a | 164 | U |
| 32 | 1a | 174 | C |
| 32 | 1a | 180 | U |
| 32 | 1a | 182 | U |
| 32 | 1a | 189(F) | U |
| 32 | 1a | 189(G) | G |
| 32 | 1a | 189(H) | G |
| 32 | 1a | 189(J) | G |
| 32 | 1a | 195 | A |
| 32 | 1a | 197 | A |
| 32 | 1a | 201 | C |
| 32 | 1a | 202 | U |
| 32 | 1a | 203 | U |
| 32 | 1a | 204 | U |
| 32 | 1a | 216 | G |
| 32 | 1a | 231 | G |
| 32 | 1a | 247 | G |
| 32 | 1a | 251 | G |
| 32 | 1a | 258 | G |
| 32 | 1a | 266 | G |
| 32 | 1a | 267 | C |
| 32 | 1a | 289 | G |
| 32 | 1a | 316 | G |
| 32 | 1a | 321 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 1a | 328 | C |
| 32 | 1a | 332 | G |
| 32 | 1a | 352 | C |
| 32 | 1a | 353 | A |
| 32 | 1a | 354 | G |
| 32 | 1a | 367 | U |
| 32 | 1a | 372 | C |
| 32 | 1a | 373 | A |
| 32 | 1a | 382 | A |
| 32 | 1a | 384 | G |
| 32 | 1a | 397 | A |
| 32 | 1a | 398 | C |
| 32 | 1a | 406 | G |
| 32 | 1a | 412 | A |
| 32 | 1a | 413 | G |
| 32 | 1a | 421 | U |
| 32 | 1a | 424 | G |
| 32 | 1a | 429 | U |
| 32 | 1a | 430 | A |
| 32 | 1a | 435 | C |
| 32 | 1a | 439 | A |
| 32 | 1a | 451 | A |
| 32 | 1a | 452 | A |
| 32 | 1a | 461 | A |
| 32 | 1a | 484 | G |
| 32 | 1a | 485 | G |
| 32 | 1a | 496 | A |
| 32 | 1a | 498 | U |
| 32 | 1a | 509 | A |
| 32 | 1a | 510 | A |
| 32 | 1a | 511 | C |
| 32 | 1a | 518 | C |
| 32 | 1a | 524 | G |
| 32 | 1a | 531 | U |
| 32 | 1a | 532 | A |
| 32 | 1a | 534 | U |
| 32 | 1a | 539 | A |
| 32 | 1a | 547 | A |
| 32 | 1a | 559 | A |
| 32 | 1a | 560 | U |
| 32 | 1a | 561 | U |
| 32 | 1a | 568 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | 1a | 572 | A |
| 32 | 1a | 573 | A |
| 32 | 1a | 576 | G |
| 32 | 1a | 577 | G |
| 32 | 1a | 596 | C |
| 32 | 1a | 628 | G |
| 32 | 1a | 630 | G |
| 32 | 1a | 653 | A |
| 32 | 1a | 665 | A |
| 32 | 1a | 666 | G |
| 32 | 1a | 687 | A |
| 32 | 1a | 688 | G |
| 32 | 1a | 695 | A |
| 32 | 1a | 702 | A |
| 32 | 1a | 717 | C |
| 32 | 1a | 723 | U |
| 32 | 1a | 728 | A |
| 32 | 1a | 731 | G |
| 32 | 1a | 749 | C |
| 32 | 1a | 755 | G |
| 32 | 1a | 766 | A |
| 32 | 1a | 777 | A |
| 32 | 1a | 792 | A |
| 32 | 1a | 793 | U |
| 32 | 1a | 794 | A |
| 32 | 1a | 815 | A |
| 32 | 1a | 816 | A |
| 32 | 1a | 817 | C |
| 32 | 1a | 821 | G |
| 32 | 1a | 828 | A |
| 32 | 1a | 839 | U |
| 32 | 1a | 840 | C |
| 32 | 1a | 841 | U |
| 32 | 1a | 851 | G |
| 32 | 1a | 859 | A |
| 32 | 1a | 864 | A |
| 32 | 1a | 870 | U |
| 32 | 1a | 902 | G |
| 32 | 1a | 914 | A |
| 32 | 1a | 916 | G |
| 32 | 1a | 926 | G |
| 32 | 1a | 927 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | 1a | 932 | C |
| 32 | 1a | 934 | C |
| 32 | 1a | 935 | A |
| 32 | 1a | 960 | U |
| 32 | 1a | 961 | U |
| 32 | 1a | 968 | A |
| 32 | 1a | 969 | A |
| 32 | 1a | 971 | G |
| 32 | 1a | 972 | C |
| 32 | 1a | 974 | A |
| 32 | 1a | 975 | A |
| 32 | 1a | 976 | G |
| 32 | 1a | 977 | A |
| 32 | 1a | 992 | U |
| 32 | 1a | 993 | G |
| 32 | 1a | 997 | U |
| 32 | 1a | 1000 | U |
| 32 | 1a | 1002 | G |
| 32 | 1a | 1003 | G |
| 32 | 1a | 1005 | A |
| 32 | 1a | 1006 | C |
| 32 | 1a | 1007 | C |
| 32 | 1a | 1008 | C |
| 32 | 1a | 1011 | G |
| 32 | 1a | 1020 | U |
| 32 | 1a | 1022 | G |
| 32 | 1a | 1023 | G |
| 32 | 1a | 1024 | G |
| 32 | 1a | 1025 | U |
| 32 | 1a | 1026 | G |
| 32 | 1a | 1027 | C |
| 32 | 1a | 1028 | C |
| 32 | 1a | 1029 | C |
| 32 | 1a | 1030 | C |
| 32 | 1a | 1030(A) | G |
| 32 | 1a | 1030(C) | G |
| 32 | 1a | 1031 | G |
| 32 | 1a | 1033 | G |
| 32 | 1a | 1037 | C |
| 32 | 1a | 1039 | C |
| 32 | 1a | 1043 | C |
| 32 | 1a | 1044 | A |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 32 | 1a | 1054 | C |
| 32 | 1a | 1055 | A |
| 32 | 1a | 1065 | U |
| 32 | 1a | 1066 | C |
| 32 | 1a | 1068 | G |
| 32 | 1a | 1070 | U |
| 32 | 1a | 1094 | G |
| 32 | 1a | 1095 | U |
| 32 | 1a | 1101 | A |
| 32 | 1a | 1108 | G |
| 32 | 1a | 1124 | G |
| 32 | 1a | 1125 | U |
| 32 | 1a | 1131 | G |
| 32 | 1a | 1134 | G |
| 32 | 1a | 1136 | U |
| 32 | 1a | 1137 | C |
| 32 | 1a | 1138 | G |
| 32 | 1a | 1139 | G |
| 32 | 1a | 1141 | C |
| 32 | 1a | 1146 | A |
| 32 | 1a | 1152 | A |
| 32 | 1a | 1154 | G |
| 32 | 1a | 1157 | A |
| 32 | 1a | 1159 | U |
| 32 | 1a | 1160 | G |
| 32 | 1a | 1182 | G |
| 32 | 1a | 1184 | G |
| 32 | 1a | 1196 | U |
| 32 | 1a | 1197 | G |
| 32 | 1a | 1202 | G |
| 32 | 1a | 1212 | U |
| 32 | 1a | 1213 | A |
| 32 | 1a | 1214 | C |
| 32 | 1a | 1227 | A |
| 32 | 1a | 1238 | A |
| 32 | 1a | 1256 | A |
| 32 | 1a | 1257 | U |
| 32 | 1a | 1270 | C |
| 32 | 1a | 1275 | A |
| 32 | 1a | 1278 | U |
| 32 | 1a | 1279 | A |
| 32 | 1a | 1280 | A |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | 1a | 1286 | A |
| 32 | 1a | 1287 | A |
| 32 | 1a | 1299 | A |
| 32 | 1a | 1300 | G |
| 32 | 1a | 1302 | U |
| 32 | 1a | 1305 | G |
| 32 | 1a | 1312 | G |
| 32 | 1a | 1320 | C |
| 32 | 1a | 1346 | A |
| 32 | 1a | 1347 | G |
| 32 | 1a | 1353 | G |
| 32 | 1a | 1363 | C |
| 32 | 1a | 1363(A) | A |
| 32 | 1a | 1364 | U |
| 32 | 1a | 1370 | G |
| 32 | 1a | 1397 | C |
| 32 | 1a | 1400 | 5MC |
| 32 | 1a | 1416 | G |
| 32 | 1a | 1419 | G |
| 32 | 1a | 1442 | G |
| 32 | 1a | 1442(A) | G |
| 32 | 1a | 1442(B) | A |
| 32 | 1a | 1447 | A |
| 32 | 1a | 1456 | G |
| 32 | 1a | 1487 | G |
| 32 | 1a | 1492 | A |
| 32 | 1a | 1497 | G |
| 32 | 1a | 1503 | A |
| 32 | 1a | 1504 | G |
| 32 | 1a | 1505 | G |
| 32 | 1a | 1506 | U |
| 32 | 1a | 1507 | A |
| 32 | 1a | 1517 | G |
| 32 | 1a | 1529 | G |
| 32 | 1a | 1530 | G |
| 53 | 1v | 13 | A |
| 53 | 1v | 24 | C |
| 54 | 1w | 2 | G |
| 54 | 1w | 9 | A |
| 54 | 1w | 13 | C |
| 54 | 1w | 19 | G |
| 54 | 1w | 23 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54 | 1w | 27 | C |
| 54 | 1w | 35 | A |
| 54 | 1w | 42 | G |
| 54 | 1w | 45 | G |
| 54 | 1w | 46 | 7MG |
| 54 | 1w | 47 | U |
| 54 | 1w | 48 | C |
| 54 | 1w | 49 | G |
| 54 | 1w | 50 | G |
| 54 | 1w | 51 | C |
| 54 | 1w | 57 | G |
| 54 | 1w | 58 | A |
| 54 | 1w | 59 | U |
| 54 | 1w | 60 | C |
| 54 | 1w | 61 | C |
| 54 | 1w | 62 | C |
| 54 | 1w | 68 | C |
| 54 | 1w | 71 | C |
| 54 | 1w | 74 | C |
| 55 | 1x | 9 | G |
| 55 | 1x | 13 | C |
| 55 | 1x | 18 | G |
| 55 | 1x | 21 | A |
| 55 | 1x | 22 | G |
| 55 | 1x | 47 | U |
| 55 | 1x | 48 | C |
| 55 | 1x | 49 | G |
| 55 | 1x | 58 | A |
| 55 | 1x | 59 | A |
| 55 | 1x | 61 | C |
| 55 | 1x | 69 | C |
| 55 | 1x | 76 | A |
| 54 | 1y | 2 | G |
| 54 | 1y | 5 | G |
| 54 | 1y | 6 | A |
| 54 | 1y | 8 | 4SU |
| 54 | 1y | 9 | A |
| 54 | 1y | 13 | C |
| 54 | 1y | 14 | A |
| 54 | 1y | 19 | G |
| 54 | 1y | 24 | G |
| 54 | 1y | 32 | C |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 54 | 1y | 33 | U |
| 54 | 1y | 35 | A |
| 54 | 1y | 40 | G |
| 54 | 1y | 44 | G |
| 54 | 1y | 45 | G |
| 54 | 1y | 46 | 7MG |
| 54 | 1y | 47 | U |
| 54 | 1y | 48 | C |
| 54 | 1y | 54 | 5MU |
| 54 | 1y | 57 | G |
| 54 | 1y | 59 | U |
| 54 | 1y | 61 | C |
| 54 | 1y | 65 | C |
| 54 | 1y | 69 | A |
| 1 | 2A | 8 | A |
| 1 | 2A | 10 | G |
| 1 | 2A | 11 | G |
| 1 | 2A | 15 | G |
| 1 | 2A | 34 | C |
| 1 | 2A | 35 | G |
| 1 | 2A | 45 | C |
| 1 | 2A | 71 | A |
| 1 | 2A | 74 | A |
| 1 | 2A | 75 | G |
| 1 | 2A | 79 | G |
| 1 | 2A | 84 | A |
| 1 | 2A | 90 | U |
| 1 | 2A | 94 | C |
| 1 | 2A | 100 | G |
| 1 | 2A | 102 | G |
| 1 | 2A | 118 | A |
| 1 | 2A | 120 | U |
| 1 | 2A | 131 | G |
| 1 | 2A | 139 | G |
| 1 | 2A | 141 | A |
| 1 | 2A | 154(A) | C |
| 1 | 2A | 157 | U |
| 1 | 2A | 181 | A |
| 1 | 2A | 196 | A |
| 1 | 2A | 199 | A |
| 1 | 2A | 205 | G |
| 1 | 2A | 214 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 2A | 215 | G |
| 1 | 2A | 216 | A |
| 1 | 2A | 221 | A |
| 1 | 2A | 222 | A |
| 1 | 2A | 228 | A |
| 1 | 2A | 229 | A |
| 1 | 2A | 230 | U |
| 1 | 2A | 232 | G |
| 1 | 2A | 233 | A |
| 1 | 2A | 245 | G |
| 1 | 2A | 248 | G |
| 1 | 2A | 249 | C |
| 1 | 2A | 250 | G |
| 1 | 2A | 266 | G |
| 1 | 2A | 267 | C |
| 1 | 2A | 271(J) | C |
| 1 | 2A | 271(K) | U |
| 1 | 2A | 271(L) | U |
| 1 | 2A | 271(M) | G |
| 1 | 2A | 271(N) | U |
| 1 | 2A | 271(O) | C |
| 1 | 2A | 272(B) | G |
| 1 | 2A | 272(I) | U |
| 1 | 2A | 272(J) | C |
| 1 | 2A | 277 | C |
| 1 | 2A | 278 | A |
| 1 | 2A | 280 | C |
| 1 | 2A | 290 | G |
| 1 | 2A | 294 | A |
| 1 | 2A | 311 | A |
| 1 | 2A | 312 | G |
| 1 | 2A | 329 | G |
| 1 | 2A | 330 | A |
| 1 | 2A | 332 | A |
| 1 | 2A | 342 | G |
| 1 | 2A | 352 | G |
| 1 | 2A | 363(B) | G |
| 1 | 2A | 386 | G |
| 1 | 2A | 399 | G |
| 1 | 2A | 402 | A |
| 1 | 2A | 403 | U |
| 1 | 2A | 411 | G |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 2A | 422 | A |
| 1 | 2A | 435 | C |
| 1 | 2A | 442 | G |
| 1 | 2A | 443 | A |
| 1 | 2A | 444 | C |
| 1 | 2A | 454 | A |
| 1 | 2A | 455 | C |
| 1 | 2A | 456 | C |
| 1 | 2A | 457 | A |
| 1 | 2A | 481 | G |
| 1 | 2A | 505 | A |
| 1 | 2A | 508 | G |
| 1 | 2A | 509 | C |
| 1 | 2A | 513 | A |
| 1 | 2A | 514 | A |
| 1 | 2A | 528 | A |
| 1 | 2A | 529 | A |
| 1 | 2A | 531 | C |
| 1 | 2A | 532 | A |
| 1 | 2A | 533 | G |
| 1 | 2A | 551 | G |
| 1 | 2A | 563 | G |
| 1 | 2A | 568 | U |
| 1 | 2A | 573 | G |
| 1 | 2A | 574 | C |
| 1 | 2A | 575 | A |
| 1 | 2A | 586 | A |
| 1 | 2A | 592 | G |
| 1 | 2A | 593 | G |
| 1 | 2A | 595 | C |
| 1 | 2A | 603 | A |
| 1 | 2A | 604 | G |
| 1 | 2A | 607 | U |
| 1 | 2A | 614(B) | G |
| 1 | 2A | 615 | G |
| 1 | 2A | 627 | A |
| 1 | 2A | 634 | C |
| 1 | 2A | 637 | A |
| 1 | 2A | 645 | C |
| 1 | 2A | 646 | A |
| 1 | 2A | 652(B) | A |
| 1 | 2A | 652(C) | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2A | 653 | A |
| 1 | 2A | 668 | G |
| 1 | 2A | 669 | G |
| 1 | 2A | 686 | G |
| 1 | 2A | 699 | A |
| 1 | 2A | 717 | G |
| 1 | 2A | 730 | C |
| 1 | 2A | 734 | A |
| 1 | 2A | 753 | C |
| 1 | 2A | 764 | A |
| 1 | 2A | 771 | G |
| 1 | 2A | 775 | G |
| 1 | 2A | 782 | A |
| 1 | 2A | 784 | A |
| 1 | 2A | 785 | G |
| 1 | 2A | 790 | C |
| 1 | 2A | 792 | G |
| 1 | 2A | 804 | A |
| 1 | 2A | 805 | G |
| 1 | 2A | 811 | U |
| 1 | 2A | 812 | C |
| 1 | 2A | 819 | A |
| 1 | 2A | 827 | U |
| 1 | 2A | 832 | G |
| 1 | 2A | 854 | G |
| 1 | 2A | 857 | C |
| 1 | 2A | 859 | G |
| 1 | 2A | 869 | G |
| 1 | 2A | 878 | A |
| 1 | 2A | 879 | G |
| 1 | 2A | 883 | G |
| 1 | 2A | 884 | C |
| 1 | 2A | 886 | C |
| 1 | 2A | 887 | A |
| 1 | 2A | 888 | C |
| 1 | 2A | 892 | G |
| 1 | 2A | 893 | C |
| 1 | 2A | 894 | C |
| 1 | 2A | 895 | U |
| 1 | 2A | 896 | A |
| 1 | 2A | 897 | C |
| 1 | 2A | 898 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 2A | 900 | A |
| 1 | 2A | 901 | A |
| 1 | 2A | 910 | A |
| 1 | 2A | 914 | C |
| 1 | 2A | 915 | C |
| 1 | 2A | 917 | A |
| 1 | 2A | 932 | G |
| 1 | 2A | 933 | A |
| 1 | 2A | 941 | A |
| 1 | 2A | 945 | A |
| 1 | 2A | 946 | G |
| 1 | 2A | 953 | A |
| 1 | 2A | 958 | U |
| 1 | 2A | 959 | A |
| 1 | 2A | 961 | C |
| 1 | 2A | 974 | G |
| 1 | 2A | 975 | C |
| 1 | 2A | 980 | A |
| 1 | 2A | 983 | A |
| 1 | 2A | 990 | A |
| 1 | 2A | 996 | A |
| 1 | 2A | 997 | G |
| 1 | 2A | 1003 | G |
| 1 | 2A | 1012 | U |
| 1 | 2A | 1013 | C |
| 1 | 2A | 1017 | G |
| 1 | 2A | 1022 | G |
| 1 | 2A | 1025 | G |
| 1 | 2A | 1026 | U |
| 1 | 2A | 1033 | U |
| 1 | 2A | 1038 | C |
| 1 | 2A | 1043 | C |
| 1 | 2A | 1117 | G |
| 1 | 2A | 1122 | G |
| 1 | 2A | 1130 | U |
| 1 | 2A | 1135 | C |
| 1 | 2A | 1136 | G |
| 1 | 2A | 1139 | G |
| 1 | 2A | 1142(A) | A |
| 1 | 2A | 1143 | A |
| 1 | 2A | 1144 | G |
| 1 | 2A | 1155 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 1171 | G |
| 1 | 2A | 1210 | A |
| 1 | 2A | 1211 | U |
| 1 | 2A | 1212 | G |
| 1 | 2A | 1220 | A |
| 1 | 2A | 1225 | G |
| 1 | 2A | 1242 | A |
| 1 | 2A | 1248 | G |
| 1 | 2A | 1250 | G |
| 1 | 2A | 1253 | A |
| 1 | 2A | 1256 | G |
| 1 | 2A | 1271 | G |
| 1 | 2A | 1272 | A |
| 1 | 2A | 1273 | U |
| 1 | 2A | 1300 | U |
| 1 | 2A | 1301 | A |
| 1 | 2A | 1314 | C |
| 1 | 2A | 1320 | C |
| 1 | 2A | 1342 | A |
| 1 | 2A | 1345 | C |
| 1 | 2A | 1352 | U |
| 1 | 2A | 1359 | A |
| 1 | 2A | 1360 | A |
| 1 | 2A | 1365 | A |
| 1 | 2A | 1368 | G |
| 1 | 2A | 1370 | C |
| 1 | 2A | 1380 | G |
| 1 | 2A | 1384 | A |
| 1 | 2A | 1385 | G |
| 1 | 2A | 1386 | C |
| 1 | 2A | 1416 | G |
| 1 | 2A | 1417 | C |
| 1 | 2A | 1420 | U |
| 1 | 2A | 1421 | G |
| 1 | 2A | 1427 | A |
| 1 | 2A | 1428 | C |
| 1 | 2A | 1436 | G |
| 1 | 2A | 1437 | C |
| 1 | 2A | 1445 | A |
| 1 | 2A | 1449 | A |
| 1 | 2A | 1450 | G |
| 1 | 2A | 1451 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 2A | 1455 | G |
| 1 | 2A | 1459 | G |
| 1 | 2A | 1460 | A |
| 1 | 2A | 1461 | G |
| 1 | 2A | 1467 | C |
| 1 | 2A | 1471 | A |
| 1 | 2A | 1482 | G |
| 1 | 2A | 1490 | A |
| 1 | 2A | 1493 | C |
| 1 | 2A | 1494 | A |
| 1 | 2A | 1495 | A |
| 1 | 2A | 1496 | A |
| 1 | 2A | 1497 | U |
| 1 | 2A | 1508 | A |
| 1 | 2A | 1509 | C |
| 1 | 2A | 1509(A) | A |
| 1 | 2A | 1514 | U |
| 1 | 2A | 1531 | C |
| 1 | 2A | 1532 | C |
| 1 | 2A | 1541 | G |
| 1 | 2A | 1542 | A |
| 1 | 2A | 1543 | C |
| 1 | 2A | 1547 | C |
| 1 | 2A | 1553 | A |
| 1 | 2A | 1558 | A |
| 1 | 2A | 1566 | A |
| 1 | 2A | 1569 | A |
| 1 | 2A | 1578 | U |
| 1 | 2A | 1580 | A |
| 1 | 2A | 1582 | C |
| 1 | 2A | 1584 | C |
| 1 | 2A | 1586 | A |
| 1 | 2A | 1588 | C |
| 1 | 2A | 1608 | A |
| 1 | 2A | 1609 | A |
| 1 | 2A | 1610 | A |
| 1 | 2A | 1616 | A |
| 1 | 2A | 1640 | C |
| 1 | 2A | 1648 | C |
| 1 | 2A | 1654 | A |
| 1 | 2A | 1664 | A |
| 1 | 2A | 1674 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 1695 | G |
| 1 | 2A | 1696 | G |
| 1 | 2A | 1700 | A |
| 1 | 2A | 1703 | G |
| 1 | 2A | 1721 | G |
| 1 | 2A | 1722 | A |
| 1 | 2A | 1740 | G |
| 1 | 2A | 1746 | G |
| 1 | 2A | 1756 | G |
| 1 | 2A | 1762 | A |
| 1 | 2A | 1763 | G |
| 1 | 2A | 1764 | G |
| 1 | 2A | 1773 | A |
| 1 | 2A | 1778 | U |
| 1 | 2A | 1780 | A |
| 1 | 2A | 1782 | C |
| 1 | 2A | 1791 | A |
| 1 | 2A | 1800 | C |
| 1 | 2A | 1801 | G |
| 1 | 2A | 1812 | A |
| 1 | 2A | 1816 | G |
| 1 | 2A | 1829 | A |
| 1 | 2A | 1847 | A |
| 1 | 2A | 1877 | A |
| 1 | 2A | 1878 | G |
| 1 | 2A | 1900 | A |
| 1 | 2A | 1906 | G |
| 1 | 2A | 1913 | A |
| 1 | 2A | 1914 | C |
| 1 | 2A | 1929 | G |
| 1 | 2A | 1930 | G |
| 1 | 2A | 1931 | U |
| 1 | 2A | 1936 | A |
| 1 | 2A | 1938 | A |
| 1 | 2A | 1955 | U |
| 1 | 2A | 1963 | U |
| 1 | 2A | 1965 | C |
| 1 | 2A | 1967 | C |
| 1 | 2A | 1970 | A |
| 1 | 2A | 1971 | A |
| 1 | 2A | 1972 | A |
| 1 | 2A | 1984 | G |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 2A | 1990 | C |
| 1 | 2A | 1992 | G |
| 1 | 2A | 1993 | U |
| 1 | 2A | 1996 | C |
| 1 | 2A | 1997 | G |
| 1 | 2A | 2020 | A |
| 1 | 2A | 2023 | G |
| 1 | 2A | 2031 | A |
| 1 | 2A | 2032 | G |
| 1 | 2A | 2033 | A |
| 1 | 2A | 2036 | C |
| 1 | 2A | 2043 | C |
| 1 | 2A | 2055 | C |
| 1 | 2A | 2056 | G |
| 1 | 2A | 2060 | A |
| 1 | 2A | 2061 | G |
| 1 | 2A | 2062 | A |
| 1 | 2A | 2069 | G |
| 1 | 2A | 2093 | G |
| 1 | 2A | 2102 | U |
| 1 | 2A | 2106 | G |
| 1 | 2A | 2110 | G |
| 1 | 2A | 2111 | C |
| 1 | 2A | 2112 | G |
| 1 | 2A | 2115 | G |
| 1 | 2A | 2116 | G |
| 1 | 2A | 2118 | U |
| 1 | 2A | 2119 | A |
| 1 | 2A | 2120 | G |
| 1 | 2A | 2122 | U |
| 1 | 2A | 2125 | G |
| 1 | 2A | 2126 | A |
| 1 | 2A | 2127 | G |
| 1 | 2A | 2129 | C |
| 1 | 2A | 2131 | G |
| 1 | 2A | 2132 | U |
| 1 | 2A | 2133 | G |
| 1 | 2A | 2134 | A |
| 1 | 2A | 2135 | A |
| 1 | 2A | 2137 | C |
| 1 | 2A | 2138 | C |
| 1 | 2A | 2140 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 2141 | G |
| 1 | 2A | 2146 | C |
| 1 | 2A | 2151 | G |
| 1 | 2A | 2153 | G |
| 1 | 2A | 2155 | G |
| 1 | 2A | 2156 | G |
| 1 | 2A | 2157 | G |
| 1 | 2A | 2158 | A |
| 1 | 2A | 2161 | C |
| 1 | 2A | 2162 | G |
| 1 | 2A | 2164 | C |
| 1 | 2A | 2165 | G |
| 1 | 2A | 2166 | G |
| 1 | 2A | 2167 | U |
| 1 | 2A | 2168 | G |
| 1 | 2A | 2169 | A |
| 1 | 2A | 2172 | U |
| 1 | 2A | 2173 | A |
| 1 | 2A | 2174 | C |
| 1 | 2A | 2178 | C |
| 1 | 2A | 2182 | G |
| 1 | 2A | 2189 | U |
| 1 | 2A | 2194 | G |
| 1 | 2A | 2198 | A |
| 1 | 2A | 2206 | G |
| 1 | 2A | 2207 | G |
| 1 | 2A | 2208 | A |
| 1 | 2A | 2218 | U |
| 1 | 2A | 2225 | A |
| 1 | 2A | 2235 | G |
| 1 | 2A | 2238 | G |
| 1 | 2A | 2239 | G |
| 1 | 2A | 2248 | C |
| 1 | 2A | 2267 | A |
| 1 | 2A | 2273 | A |
| 1 | 2A | 2275 | C |
| 1 | 2A | 2279 | G |
| 1 | 2A | 2283 | C |
| 1 | 2A | 2287 | A |
| 1 | 2A | 2288 | A |
| 1 | 2A | 2294 | C |
| 1 | 2A | 2302 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 2305 | A |
| 1 | 2A | 2307 | G |
| 1 | 2A | 2308 | G |
| 1 | 2A | 2309 | A |
| 1 | 2A | 2316 | C |
| 1 | 2A | 2319 | G |
| 1 | 2A | 2320 | A |
| 1 | 2A | 2325 | G |
| 1 | 2A | 2327 | A |
| 1 | 2A | 2334 | G |
| 1 | 2A | 2336 | A |
| 1 | 2A | 2343 | C |
| 1 | 2A | 2346 | A |
| 1 | 2A | 2347 | C |
| 1 | 2A | 2350 | C |
| 1 | 2A | 2354 | G |
| 1 | 2A | 2355 | C |
| 1 | 2A | 2366 | A |
| 1 | 2A | 2376 | A |
| 1 | 2A | 2383 | G |
| 1 | 2A | 2385 | C |
| 1 | 2A | 2388 | A |
| 1 | 2A | 2391 | G |
| 1 | 2A | 2395 | C |
| 1 | 2A | 2403 | C |
| 1 | 2A | 2406 | U |
| 1 | 2A | 2410 | G |
| 1 | 2A | 2419 | U |
| 1 | 2A | 2425 | A |
| 1 | 2A | 2429 | G |
| 1 | 2A | 2430 | A |
| 1 | 2A | 2434 | A |
| 1 | 2A | 2435 | A |
| 1 | 2A | 2439 | A |
| 1 | 2A | 2441 | C |
| 1 | 2A | 2445 | G |
| 1 | 2A | 2448 | A |
| 1 | 2A | 2469 | A |
| 1 | 2A | 2476 | A |
| 1 | 2A | 2478 | A |
| 1 | 2A | 2480 | C |
| 1 | 2A | 2487 | G |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 1 | 2A | 2490 | G |
| 1 | 2A | 2494 | G |
| 1 | 2A | 2502 | G |
| 1 | 2A | 2504 | U |
| 1 | 2A | 2505 | G |
| 1 | 2A | 2506 | U |
| 1 | 2A | 2518 | A |
| 1 | 2A | 2520 | C |
| 1 | 2A | 2529 | G |
| 1 | 2A | 2535 | G |
| 1 | 2A | 2554 | U |
| 1 | 2A | 2562 | U |
| 1 | 2A | 2566 | A |
| 1 | 2A | 2567 | G |
| 1 | 2A | 2572 | A |
| 1 | 2A | 2573 | C |
| 1 | 2A | 2582 | G |
| 1 | 2A | 2585 | U |
| 1 | 2A | 2586 | C |
| 1 | 2A | 2588 | G |
| 1 | 2A | 2602 | A |
| 1 | 2A | 2609 | U |
| 1 | 2A | 2611 | U |
| 1 | 2A | 2612 | C |
| 1 | 2A | 2630 | G |
| 1 | 2A | 2634 | G |
| 1 | 2A | 2661 | G |
| 1 | 2A | 2662 | A |
| 1 | 2A | 2689 | U |
| 1 | 2A | 2691 | C |
| 1 | 2A | 2702 | U |
| 1 | 2A | 2703 | C |
| 1 | 2A | 2712(A) | A |
| 1 | 2A | 2713 | A |
| 1 | 2A | 2714 | G |
| 1 | 2A | 2726 | U |
| 1 | 2A | 2732 | G |
| 1 | 2A | 2733 | A |
| 1 | 2A | 2748 | A |
| 1 | 2A | 2751 | G |
| 1 | 2A | 2757 | A |
| 1 | 2A | 2759 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | 2A | 2764 | A |
| 1 | 2A | 2765 | A |
| 1 | 2A | 2778 | A |
| 1 | 2A | 2780 | G |
| 1 | 2A | 2793 | G |
| 1 | 2A | 2807 | G |
| 1 | 2A | 2818 | G |
| 1 | 2A | 2820 | A |
| 1 | 2A | 2821 | A |
| 1 | 2A | 2835 | A |
| 1 | 2A | 2836 | U |
| 1 | 2A | 2839 | G |
| 1 | 2A | 2858 | C |
| 1 | 2A | 2861 | G |
| 1 | 2A | 2872 | G |
| 1 | 2A | 2879 | C |
| 1 | 2A | 2880 | C |
| 1 | 2A | 2883 | A |
| 1 | 2A | 2886 | G |
| 1 | 2A | 2892 | A |
| 1 | 2A | 2894 | G |
| 1 | 2A | 2895 | U |
| 1 | 2A | 2896 | C |
| 1 | 2A | 2897 | U |
| 2 | 2B | 2 | C |
| 2 | 2B | 3 | C |
| 2 | 2B | 7 | G |
| 2 | 2B | 8 | U |
| 2 | 2B | 9 | G |
| 2 | 2B | 13 | A |
| 2 | 2B | 19 | G |
| 2 | 2B | 20 | C |
| 2 | 2B | 40 | U |
| 2 | 2B | 42 | C |
| 2 | 2B | 53 | A |
| 2 | 2B | 56 | G |
| 2 | 2B | 63 | G |
| 2 | 2B | 66 | A |
| 2 | 2B | 67 | G |
| 2 | 2B | 69 | G |
| 2 | 2B | 73 | A |
| 2 | 2B | 74 | U |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 2 | 2B | 75 | G |
| 2 | 2B | 85 | G |
| 2 | 2B | 88 | C |
| 2 | 2B | 101 | G |
| 2 | 2B | 108 | U |
| 2 | 2B | 109 | C |
| 2 | 2B | 110 | G |
| 2 | 2B | 114 | C |
| 2 | 2B | 119 | G |
| 2 | 2B | 120 | A |
| 32 | 2a | 7 | G |
| 32 | 2a | 9 | G |
| 32 | 2a | 32 | A |
| 32 | 2a | 39 | G |
| 32 | 2a | 47 | C |
| 32 | 2a | 48 | C |
| 32 | 2a | 51 | A |
| 32 | 2a | 52 | G |
| 32 | 2a | 54 | C |
| 32 | 2a | 66 | G |
| 32 | 2a | 73 | G |
| 32 | 2a | 78 | G |
| 32 | 2a | 80 | G |
| 32 | 2a | 89 | C |
| 32 | 2a | 101 | A |
| 32 | 2a | 116 | A |
| 32 | 2a | 117 | G |
| 32 | 2a | 120 | A |
| 32 | 2a | 121 | C |
| 32 | 2a | 129(A) | G |
| 32 | 2a | 131 | C |
| 32 | 2a | 144 | G |
| 32 | 2a | 163 | C |
| 32 | 2a | 174 | C |
| 32 | 2a | 182 | U |
| 32 | 2a | 189(E) | U |
| 32 | 2a | 189(F) | U |
| 32 | 2a | 189(J) | G |
| 32 | 2a | 195 | A |
| 32 | 2a | 197 | A |
| 32 | 2a | 201 | C |
| 32 | 2a | 202 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 2a | 203 | U |
| 32 | 2a | 204 | U |
| 32 | 2a | 216 | G |
| 32 | 2a | 222 | U |
| 32 | 2a | 247 | G |
| 32 | 2a | 249 | U |
| 32 | 2a | 250 | A |
| 32 | 2a | 251 | G |
| 32 | 2a | 258 | G |
| 32 | 2a | 266 | G |
| 32 | 2a | 267 | C |
| 32 | 2a | 289 | G |
| 32 | 2a | 301 | G |
| 32 | 2a | 321 | A |
| 32 | 2a | 328 | C |
| 32 | 2a | 332 | G |
| 32 | 2a | 342 | C |
| 32 | 2a | 345 | C |
| 32 | 2a | 348 | G |
| 32 | 2a | 352 | C |
| 32 | 2a | 353 | A |
| 32 | 2a | 354 | G |
| 32 | 2a | 367 | U |
| 32 | 2a | 372 | C |
| 32 | 2a | 373 | A |
| 32 | 2a | 384 | G |
| 32 | 2a | 397 | A |
| 32 | 2a | 398 | C |
| 32 | 2a | 406 | G |
| 32 | 2a | 412 | A |
| 32 | 2a | 413 | G |
| 32 | 2a | 415 | A |
| 32 | 2a | 421 | U |
| 32 | 2a | 423 | G |
| 32 | 2a | 424 | G |
| 32 | 2a | 429 | U |
| 32 | 2a | 430 | A |
| 32 | 2a | 439 | A |
| 32 | 2a | 442 | C |
| 32 | 2a | 452 | A |
| 32 | 2a | 461 | A |
| 32 | 2a | 470 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 2a | 485 | G |
| 32 | 2a | 496 | A |
| 32 | 2a | 498 | U |
| 32 | 2a | 505 | G |
| 32 | 2a | 509 | A |
| 32 | 2a | 510 | A |
| 32 | 2a | 511 | C |
| 32 | 2a | 518 | C |
| 32 | 2a | 521 | G |
| 32 | 2a | 527 | 7MG |
| 32 | 2a | 531 | U |
| 32 | 2a | 532 | A |
| 32 | 2a | 533 | A |
| 32 | 2a | 547 | A |
| 32 | 2a | 559 | A |
| 32 | 2a | 560 | U |
| 32 | 2a | 561 | U |
| 32 | 2a | 562 | C |
| 32 | 2a | 564 | C |
| 32 | 2a | 568 | G |
| 32 | 2a | 572 | A |
| 32 | 2a | 573 | A |
| 32 | 2a | 574 | A |
| 32 | 2a | 576 | G |
| 32 | 2a | 577 | G |
| 32 | 2a | 596 | C |
| 32 | 2a | 602 | A |
| 32 | 2a | 607 | A |
| 32 | 2a | 619 | U |
| 32 | 2a | 630 | G |
| 32 | 2a | 650 | G |
| 32 | 2a | 653 | A |
| 32 | 2a | 655 | A |
| 32 | 2a | 665 | A |
| 32 | 2a | 671 | G |
| 32 | 2a | 687 | A |
| 32 | 2a | 688 | G |
| 32 | 2a | 693 | G |
| 32 | 2a | 695 | A |
| 32 | 2a | 702 | A |
| 32 | 2a | 703 | G |
| 32 | 2a | 723 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32 | 2a | 724 | G |
| 32 | 2a | 729 | A |
| 32 | 2a | 731 | G |
| 32 | 2a | 735 | C |
| 32 | 2a | 749 | C |
| 32 | 2a | 754 | C |
| 32 | 2a | 755 | G |
| 32 | 2a | 777 | A |
| 32 | 2a | 793 | U |
| 32 | 2a | 794 | A |
| 32 | 2a | 812 | C |
| 32 | 2a | 815 | A |
| 32 | 2a | 817 | C |
| 32 | 2a | 818 | G |
| 32 | 2a | 819 | A |
| 32 | 2a | 821 | G |
| 32 | 2a | 828 | A |
| 32 | 2a | 840 | C |
| 32 | 2a | 841 | U |
| 32 | 2a | 853 | G |
| 32 | 2a | 855 | G |
| 32 | 2a | 859 | A |
| 32 | 2a | 874 | G |
| 32 | 2a | 891 | U |
| 32 | 2a | 902 | G |
| 32 | 2a | 914 | A |
| 32 | 2a | 926 | G |
| 32 | 2a | 927 | G |
| 32 | 2a | 934 | C |
| 32 | 2a | 960 | U |
| 32 | 2a | 961 | U |
| 32 | 2a | 968 | A |
| 32 | 2a | 969 | A |
| 32 | 2a | 971 | G |
| 32 | 2a | 974 | A |
| 32 | 2a | 975 | A |
| 32 | 2a | 976 | G |
| 32 | 2a | 977 | A |
| 32 | 2a | 982 | U |
| 32 | 2a | 992 | U |
| 32 | 2a | 993 | G |
| 32 | 2a | 997 | U |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | 2a | 999 | C |
| 32 | 2a | 1001(A) | G |
| 32 | 2a | 1002 | G |
| 32 | 2a | 1003 | G |
| 32 | 2a | 1004 | A |
| 32 | 2a | 1005 | A |
| 32 | 2a | 1006 | C |
| 32 | 2a | 1009 | G |
| 32 | 2a | 1014 | A |
| 32 | 2a | 1020 | U |
| 32 | 2a | 1022 | G |
| 32 | 2a | 1023 | G |
| 32 | 2a | 1024 | G |
| 32 | 2a | 1025 | U |
| 32 | 2a | 1027 | C |
| 32 | 2a | 1028 | C |
| 32 | 2a | 1029 | C |
| 32 | 2a | 1030 | C |
| 32 | 2a | 1030(A) | G |
| 32 | 2a | 1033 | G |
| 32 | 2a | 1034 | G |
| 32 | 2a | 1035 | A |
| 32 | 2a | 1036 | G |
| 32 | 2a | 1037 | C |
| 32 | 2a | 1039 | C |
| 32 | 2a | 1040 | U |
| 32 | 2a | 1042 | G |
| 32 | 2a | 1046 | A |
| 32 | 2a | 1065 | U |
| 32 | 2a | 1066 | C |
| 32 | 2a | 1068 | G |
| 32 | 2a | 1077 | G |
| 32 | 2a | 1081 | G |
| 32 | 2a | 1085 | U |
| 32 | 2a | 1094 | G |
| 32 | 2a | 1095 | U |
| 32 | 2a | 1101 | A |
| 32 | 2a | 1108 | G |
| 32 | 2a | 1116 | C |
| 32 | 2a | 1117 | G |
| 32 | 2a | 1122 | U |
| 32 | 2a | 1124 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 32 | 2a | 1125 | U |
| 32 | 2a | 1128 | C |
| 32 | 2a | 1129 | C |
| 32 | 2a | 1130 | A |
| 32 | 2a | 1132 | C |
| 32 | 2a | 1136 | U |
| 32 | 2a | 1137 | C |
| 32 | 2a | 1138 | G |
| 32 | 2a | 1139 | G |
| 32 | 2a | 1140 | C |
| 32 | 2a | 1141 | C |
| 32 | 2a | 1146 | A |
| 32 | 2a | 1152 | A |
| 32 | 2a | 1157 | A |
| 32 | 2a | 1159 | U |
| 32 | 2a | 1160 | G |
| 32 | 2a | 1181 | G |
| 32 | 2a | 1182 | G |
| 32 | 2a | 1184 | G |
| 32 | 2a | 1191 | A |
| 32 | 2a | 1196 | U |
| 32 | 2a | 1197 | G |
| 32 | 2a | 1201 | A |
| 32 | 2a | 1202 | G |
| 32 | 2a | 1207 | 2MG |
| 32 | 2a | 1208 | C |
| 32 | 2a | 1211 | U |
| 32 | 2a | 1212 | U |
| 32 | 2a | 1213 | A |
| 32 | 2a | 1214 | C |
| 32 | 2a | 1215 | G |
| 32 | 2a | 1220 | G |
| 32 | 2a | 1226 | C |
| 32 | 2a | 1227 | A |
| 32 | 2a | 1238 | A |
| 32 | 2a | 1246 | C |
| 32 | 2a | 1256 | A |
| 32 | 2a | 1257 | U |
| 32 | 2a | 1258 | G |
| 32 | 2a | 1260 | C |
| 32 | 2a | 1261 | A |
| 32 | 2a | 1270 | C |

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| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 32 | 2a | 1272 | G |
| 32 | 2a | 1273 | G |
| 32 | 2a | 1277 | C |
| 32 | 2a | 1279 | A |
| 32 | 2a | 1280 | A |
| 32 | 2a | 1282 | C |
| 32 | 2a | 1286 | A |
| 32 | 2a | 1287 | A |
| 32 | 2a | 1299 | A |
| 32 | 2a | 1300 | G |
| 32 | 2a | 1302 | U |
| 32 | 2a | 1303 | C |
| 32 | 2a | 1305 | G |
| 32 | 2a | 1323 | G |
| 32 | 2a | 1340 | A |
| 32 | 2a | 1346 | A |
| 32 | 2a | 1347 | G |
| 32 | 2a | 1363 | C |
| 32 | 2a | 1368 | G |
| 32 | 2a | 1370 | G |
| 32 | 2a | 1378 | C |
| 32 | 2a | 1404 | 5MC |
| 32 | 2a | 1419 | G |
| 32 | 2a | 1442 | G |
| 32 | 2a | 1442(A) | G |
| 32 | 2a | 1446 | U |
| 32 | 2a | 1447 | A |
| 32 | 2a | 1452 | C |
| 32 | 2a | 1456 | G |
| 32 | 2a | 1487 | G |
| 32 | 2a | 1492 | A |
| 32 | 2a | 1503 | A |
| 32 | 2a | 1504 | G |
| 32 | 2a | 1506 | U |
| 32 | 2a | 1517 | G |
| 32 | 2a | 1520 | G |
| 32 | 2a | 1529 | G |
| 32 | 2a | 1530 | G |
| 32 | 2a | 1531 | A |
| 53 | 2v | 13 | A |
| 53 | 2v | 14 | A |
| 53 | 2v | 20 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | 2v | 24 | C |
| 54 | 2w | 2 | G |
| 54 | 2w | 3 | G |
| 54 | 2w | 5 | G |
| 54 | 2w | 8 | 4SU |
| 54 | 2w | 11 | C |
| 54 | 2w | 13 | C |
| 54 | 2w | 14 | A |
| 54 | 2w | 19 | G |
| 54 | 2w | 23 | A |
| 54 | 2w | 27 | C |
| 54 | 2w | 42 | G |
| 54 | 2w | 46 | 7MG |
| 54 | 2w | 47 | U |
| 54 | 2w | 48 | C |
| 54 | 2w | 49 | G |
| 54 | 2w | 50 | G |
| 54 | 2w | 51 | C |
| 54 | 2w | 56 | C |
| 54 | 2w | 57 | G |
| 54 | 2w | 58 | A |
| 54 | 2w | 59 | U |
| 54 | 2w | 60 | C |
| 54 | 2w | 62 | C |
| 54 | 2w | 67 | U |
| 54 | 2w | 68 | C |
| 54 | 2w | 69 | A |
| 54 | 2w | 70 | C |
| 54 | 2w | 74 | C |
| 55 | 2x | 4 | G |
| 55 | 2x | 9 | G |
| 55 | 2x | 10 | G |
| 55 | 2x | 13 | C |
| 55 | 2x | 19 | G |
| 55 | 2x | 21 | A |
| 55 | 2x | 22 | G |
| 55 | 2x | 28 | C |
| 55 | 2x | 42 | G |
| 55 | 2x | 47 | U |
| 55 | 2x | 48 | C |
| 55 | 2x | 51 | C |
| 55 | 2x | 61 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55 | 2x | 73 | A |
| 55 | 2x | 76 | A |
| 54 | 2y | 2 | G |
| 54 | 2y | 5 | G |
| 54 | 2y | 6 | A |
| 54 | 2y | 8 | 4SU |
| 54 | 2y | 9 | A |
| 54 | 2y | 13 | C |
| 54 | 2y | 14 | A |
| 54 | 2y | 19 | G |
| 54 | 2y | 24 | G |
| 54 | 2y | 32 | C |
| 54 | 2y | 35 | A |
| 54 | 2y | 40 | G |
| 54 | 2y | 41 | A |
| 54 | 2y | 43 | G |
| 54 | 2y | 44 | G |
| 54 | 2y | 45 | G |
| 54 | 2y | 46 | 7MG |
| 54 | 2y | 47 | U |
| 54 | 2y | 48 | C |
| 54 | 2y | 53 | G |
| 54 | 2y | 54 | 5MU |
| 54 | 2y | 55 | PSU |
| 54 | 2y | 57 | G |
| 54 | 2y | 58 | A |
| 54 | 2y | 59 | U |
| 54 | 2y | 61 | C |
| 54 | 2y | 65 | C |
| 54 | 2y | 69 | A |

All (39) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1A | 266 | G |
| 1 | 1A | 271(K) | U |
| 1 | 1A | 278 | A |
| 1 | 1A | 548 | A |
| 1 | 1A | 895 | U |
| 1 | 1A | 1047 | G |
| 1 | 1A | 1065 | U |
| 1 | 1A | 1067 | A |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | 1A | 1174 | A |
| 1 | 1A | 1176 | G |
| 1 | 1A | 1210 | A |
| 1 | 1A | 1442 | G |
| 1 | 1A | 1508 | A |
| 1 | 1A | 1653 | G |
| 1 | 1A | 1663 | C |
| 1 | 1A | 1992 | G |
| 1 | 1A | 2126 | A |
| 1 | 1A | 2134 | A |
| 1 | 1A | 2183 | C |
| 2 | 1B | 1 | U |
| 1 | 2A | 195 | A |
| 1 | 2A | 228 | A |
| 1 | 2A | 266 | G |
| 1 | 2A | 271(M) | G |
| 1 | 2A | 277 | C |
| 1 | 2A | 528 | A |
| 1 | 2A | 752 | A |
| 1 | 2A | 827 | U |
| 1 | 2A | 856 | C |
| 1 | 2A | 893 | C |
| 1 | 2A | 900 | A |
| 1 | 2A | 1210 | A |
| 1 | 2A | 1379 | A |
| 1 | 2A | 1420 | U |
| 1 | 2A | 1608 | A |
| 1 | 2A | 1653 | G |
| 1 | 2A | 1913 | A |
| 1 | 2A | 1992 | G |
| 1 | 2A | 2756 | U |

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 |
| 32 | UR3 | 1a | 1498 | 32 | 14,22,23 | 0.75 | 0 | 15,32,35 | 0.69 | 0 |
| 32 | 5MC | 2a | 967 | 32 | 15,22,23 | 1.36 | 1 (6%) | 19,32,35 | 1.30 | 3 (15%) |
| 54 | 4SU | 1w | 8 | 54 | 14,21,22 | 1.33 | 1 (7%) | 15,30,33 | 1.54 | 2 (13%) |
| 43 | 0TD | 1l | 92 | 43 | 4,9,10 | 3.23 | 1 (25%) | 3,11,13 | 8.92 | 1 (33%) |
| 55 | 4SU | 2x | 8 | 55,56 | 14,21,22 | 1.35 | 2 (14%) | 15,30,33 | 2.00 | 2 (13%) |
| 1 | 5MU | 2A | 1939 | 1 | 15,22,23 | 1.06 | 1 (6%) | 16,32,35 | 1.85 | 2 (12%) |
| 1 | PSU | 2A | 1911 | 1 | 17,21,22 | 1.54 | 2 (11%) | 20,30,33 | 3.21 | 6 (30%) |
| 1 | 5MU | 2A | 1915 | 1 | 15,22,23 | 1.10 | 1 (6%) | 16,32,35 | 1.84 | 2 (12%) |
| 32 | 5MC | 1a | 1407 | 32 | 15,22,23 | 1.34 | 1 (6%) | 19,32,35 | 1.42 | 3 (15%) |
| 54 | PSU | 2y | 55 | 54 | 17,21,22 | 1.47 | 2 (11%) | 20,30,33 | 3.11 | 6 (30%) |
| 32 | M2G | 2a | 966 | 32 | 20,27,28 | 1.43 | 3 (15%) | 22,40,43 | 2.13 | 6 (27%) |
| 1 | 5MC | 1A | 1942 | 1 | 15,22,23 | 1.29 | 1 (6%) | 19,32,35 | 1.32 | 3 (15%) |
| 54 | 4SU | 2y | 8 | 54 | 14,21,22 | 1.26 | 1 (7%) | 15,30,33 | 1.65 | 2 (13%) |
| 1 | OMU | 1A | 2552 | 1,56 | 14,22,23 | 0.90 | 1 (7%) | 14,31,34 | 0.73 | 0 |
| 32 | 5MC | 1a | 1400 | 32 | 15,22,23 | 1.29 | 1 (6%) | 19,32,35 | 1.40 | 3 (15%) |
| 54 | CM0 | 1w | 34 | 54 | 16,26,27 | 1.12 | 1 (6%) | 18,37,40 | 2.00 | 4 (22%) |
| 1 | 2MA | 1A | 2503 | 1,56 | 17,25,26 | 1.40 | 2 (11%) | 19,37,40 | 2.19 | 3 (15%) |
| 32 | PSU | 1a | 516 | 32,56 | 17,21,22 | 1.51 | 3 (17%) | 20,30,33 | 3.05 | 6 (30%) |
| 32 | M2G | 1a | 966 | 32 | 20,27,28 | 1.42 | 3 (15%) | 22,40,43 | 2.20 | 5 (22%) |
| 1 | OMC | 1A | 1920 | 1 | 15,22,23 | 0.63 | 0 | 17,31,34 | 1.50 | 2 (11%) |
| 54 | PSU | 2w | 55 | 54 | 17,21,22 | 1.36 | 2 (11%) | 20,30,33 | 3.20 | 6 (30%) |
| 1 | 5MU | 1A | 1915 | 1 | 15,22,23 | 1.08 | 1 (6%) | 16,32,35 | 1.88 | 1 (6%) |
| 54 | CM0 | 1y | 34 | 54 | 16,26,27 | 1.08 | 1 (6%) | 18,37,40 | 1.97 | 4 (22%) |
| 54 | PSU | 1w | 55 | 54 | 17,21,22 | 1.36 | 2 (11%) | 20,30,33 | 3.17 | 6 (30%) |
| 32 | PSU | 2a | 516 | 32 | 17,21,22 | 1.47 | 2 (11%) | 20,30,33 | 3.13 | 5 (25%) |
| 32 | 4OC | 2a | 1402 | 32 | 16,23,24 | 0.63 | 0 | 17,32,35 | 1.41 | 1 (5%) |
| 55 | PSU | 1x | 55 | 55,56 | 17,21,22 | 1.53 | 2 (11%) | 20,30,33 | 3.13 | 6 (30%) |
| 54 | PSU | 1y | 55 | 54 | 17,21,22 | 1.52 | 2 (11%) | 20,30,33 | 3.20 | 6 (30%) |
| 43 | 0TD | 2l | 92 | 43 | 4,9,10 | 3.14 | 1 (25%) | 3,11,13 | 5.69 | 1 (33%) |
| 1 | PSU | 2A | 2605 | 1 | 17,21,22 | 1.51 | 3 (17%) | 20,30,33 | 3.15 | 6 (30%) |
| 1 | 5MC | 2A | 1962 | 1,56 | 15,22,23 | 1.30 | 1 (6%) | 19,32,35 | 1.41 | 3 (15%) |
| 1 | PSU | 2A | 1917 | 1 | 17,21,22 | 1.62 | 2 (11%) | 20,30,33 | 3.18 | 6 (30%) |
| 32 | 5MC | 1a | 1404 | 32 | 15,22,23 | 1.31 | 1 (6%) | 19,32,35 | 1.34 | 2 (10%) |
| 54 | CM0 | 2w | 34 | 54 | 16,26,27 | 1.04 | 1 (6%) | 18,37,40 | 1.83 | 3 (16%) |
| 55 | 5MC | 2x | 32 | 55 | 15,22,23 | 1.36 | 1 (6%) | 19,32,35 | 1.35 | 3 (15%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|---------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 55 | 4SU | 1x | 8 | 55 | 14,21,22 | 1.46 | 2 (14%) | 15,30,33 | 2.11 | 2 (13%) |
| 1 | 5MU | 1A | 1939 | 1,56 | 15,22,23 | 1.07 | 2 (13%) | 16,32,35 | 1.82 | 2 (12%) |
| 32 | 2MG | 2a | 1207 | 32 | 19,26,27 | 1.29 | 2 (10%) | 21,38,41 | 2.31 | 7 (33%) |
| 1 | OMC | 2A | 1920 | 1 | 15,22,23 | 0.69 | 0 | 17,31,34 | 1.37 | 2 (11%) |
| 1 | OMG | 2A | 2251 | 1,55,56 | 18,26,27 | 1.15 | 2 (11%) | 20,38,41 | 2.09 | 6 (30%) |
| 32 | 5MC | 2a | 1400 | 32 | 15,22,23 | 1.37 | 1 (6%) | 19,32,35 | 1.30 | 3 (15%) |
| 32 | 4OC | 1a | 1402 | 32 | 16,23,24 | 0.62 | 0 | 17,32,35 | 1.23 | 1 (5%) |
| 54 | 5MU | 2y | 54 | 54 | 15,22,23 | 1.05 | 1 (6%) | 16,32,35 | 1.97 | 1 (6%) |
| 1 | PSU | 1A | 1911 | 1 | 17,21,22 | 1.54 | 3 (17%) | 20,30,33 | 3.05 | 6 (30%) |
| 55 | 5MC | 1x | 32 | 55 | 15,22,23 | 1.31 | 1 (6%) | 19,32,35 | 1.45 | 3 (15%) |
| 55 | 5MU | 1x | 54 | 55 | 15,22,23 | 1.07 | 2 (13%) | 16,32,35 | 2.13 | 2 (12%) |
| 54 | 5MU | 1y | 54 | 54 | 15,22,23 | 1.10 | 1 (6%) | 16,32,35 | 1.81 | 2 (12%) |
| 32 | 2MG | 1a | 1207 | 32 | 19,26,27 | 1.21 | 2 (10%) | 21,38,41 | 2.40 | 8 (38%) |
| 54 | 7MG | 1y | 46 | 54 | 22,26,27 | 1.87 | 5 (22%) | 28,39,42 | 3.25 | 12 (42%) |
| 54 | 6MZ | 1y | 37 | 54 | 18,25,26 | 0.97 | 1 (5%) | 16,36,39 | 2.16 | 4 (25%) |
| 55 | PSU | 2x | 55 | 55 | 17,21,22 | 1.57 | 2 (11%) | 20,30,33 | 3.19 | 7 (35%) |
| 32 | 7MG | 2a | 527 | 32,56 | 22,26,27 | 1.77 | 4 (18%) | 28,39,42 | 2.73 | 9 (32%) |
| 54 | CM0 | 2y | 34 | 54 | 16,26,27 | 1.10 | 1 (6%) | 18,37,40 | 2.01 | 4 (22%) |
| 32 | MA6 | 2a | 1519 | 32 | 19,26,27 | 1.01 | 1 (5%) | 18,38,41 | 1.61 | 3 (16%) |
| 54 | 4SU | 1y | 8 | 54 | 14,21,22 | 1.29 | 1 (7%) | 15,30,33 | 1.55 | 2 (13%) |
| 54 | 6MZ | 1w | 37 | 54 | 18,25,26 | 0.92 | 1 (5%) | 16,36,39 | 2.05 | 4 (25%) |
| 32 | 7MG | 1a | 527 | 32,56 | 22,26,27 | 1.81 | 4 (18%) | 28,39,42 | 2.76 | 8 (28%) |
| 32 | MA6 | 1a | 1519 | 32 | 19,26,27 | 1.04 | 1 (5%) | 18,38,41 | 1.66 | 4 (22%) |
| 1 | PSU | 1A | 1917 | 1 | 17,21,22 | 1.60 | 3 (17%) | 20,30,33 | 3.15 | 6 (30%) |
| 1 | OMU | 2A | 2552 | 1,56 | 14,22,23 | 0.89 | 0 | 14,31,34 | 0.84 | 1 (7%) |
| 32 | MA6 | 2a | 1518 | 32 | 19,26,27 | 1.04 | 1 (5%) | 18,38,41 | 1.68 | 4 (22%) |
| 54 | 5MU | 1w | 54 | 54 | 15,22,23 | 1.10 | 1 (6%) | 16,32,35 | 1.74 | 2 (12%) |
| 32 | MA6 | 1a | 1518 | 32 | 19,26,27 | 0.99 | 1 (5%) | 18,38,41 | 1.68 | 6 (33%) |
| 54 | 7MG | 1w | 46 | 54 | 22,26,27 | 1.80 | 4 (18%) | 28,39,42 | 2.58 | 9 (32%) |
| 1 | OMG | 1A | 2251 | 1,55,56 | 18,26,27 | 1.25 | 2 (11%) | 20,38,41 | 2.20 | 6 (30%) |
| 54 | 7MG | 2w | 46 | 54 | 22,26,27 | 1.80 | 3 (13%) | 28,39,42 | 2.71 | 8 (28%) |
| 1 | 5MC | 1A | 1962 | 1 | 15,22,23 | 1.35 | 1 (6%) | 19,32,35 | 1.30 | 3 (15%) |
| 54 | 4SU | 2w | 8 | 54 | 14,21,22 | 1.24 | 1 (7%) | 15,30,33 | 1.56 | 2 (13%) |
| 54 | 6MZ | 2y | 37 | 54 | 18,25,26 | 0.96 | 1 (5%) | 16,36,39 | 2.09 | 4 (25%) |
| 32 | 5MC | 2a | 1407 | 32 | 15,22,23 | 1.33 | 1 (6%) | 19,32,35 | 1.38 | 2 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 32 | UR3 | 2a | 1498 | 32 | 14,22,23 | 0.75 | 1 (7%) | 15,32,35 | 0.71 | 0 |
| 1 | 2MA | 2A | 2503 | 1 | 17,25,26 | 1.33 | 2 (11%) | 19,37,40 | 2.16 | 3 (15%) |
| 32 | 5MC | 1a | 967 | 32 | 15,22,23 | 1.29 | 1 (6%) | 19,32,35 | 1.33 | 3 (15%) |
| 54 | 6MZ | 2w | 37 | 54 | 18,25,26 | 0.93 | 1 (5%) | 16,36,39 | 1.87 | 3 (18%) |
| 1 | PSU | 1A | 2605 | 1,56 | 17,21,22 | 1.60 | 4 (23%) | 20,30,33 | 3.21 | 6 (30%) |
| 55 | 5MU | 2x | 54 | 55 | 15,22,23 | 1.11 | 1 (6%) | 16,32,35 | 1.90 | 2 (12%) |
| 1 | 5MC | 2A | 1942 | 1 | 15,22,23 | 1.33 | 1 (6%) | 19,32,35 | 1.29 | 3 (15%) |
| 32 | 5MC | 2a | 1404 | 32 | 15,22,23 | 1.34 | 1 (6%) | 19,32,35 | 1.31 | 3 (15%) |
| 54 | 7MG | 2y | 46 | 54 | 22,26,27 | 1.81 | 4 (18%) | 28,39,42 | 3.13 | 11 (39%) |
| 54 | 5MU | 2w | 54 | 54 | 15,22,23 | 1.00 | 1 (6%) | 16,32,35 | 2.04 | 2 (12%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|-----------|---------|
| 32 | UR3 | 1a | 1498 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 967 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 54 | 4SU | 1w | 8 | 54 | - | 0/5/25/26 | 0/2/2/2 |
| 43 | 0TD | 1l | 92 | 43 | - | 2/3/12/14 | - |
| 55 | 4SU | 2x | 8 | 55,56 | - | 1/5/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1939 | 1 | - | 2/5/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 2A | 1915 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1407 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 54 | PSU | 2y | 55 | 54 | - | 2/7/25/26 | 0/2/2/2 |
| 32 | M2G | 2a | 966 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | 5MC | 1A | 1942 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 54 | 4SU | 2y | 8 | 54 | - | 2/5/25/26 | 0/2/2/2 |
| 1 | OMU | 1A | 2552 | 1,56 | - | 0/7/27/28 | 0/2/2/2 |
| 32 | 5MC | 1a | 1400 | 32 | - | 2/5/25/26 | 0/2/2/2 |
| 54 | CM0 | 1w | 34 | 54 | - | 3/8/30/31 | 0/2/2/2 |
| 1 | 2MA | 1A | 2503 | 1,56 | - | 2/3/25/26 | 0/3/3/3 |
| 32 | PSU | 1a | 516 | 32,56 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | M2G | 1a | 966 | 32 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | OMC | 1A | 1920 | 1 | - | 1/7/27/28 | 0/2/2/2 |
| 54 | PSU | 2w | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1915 | 1 | - | 3/5/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|-----------|---------|
| 54 | CM0 | 1y | 34 | 54 | - | 2/8/30/31 | 0/2/2/2 |
| 54 | PSU | 1w | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | PSU | 2a | 516 | 32 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 4OC | 2a | 1402 | 32 | - | 6/9/29/30 | 0/2/2/2 |
| 55 | PSU | 1x | 55 | 55,56 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | PSU | 1y | 55 | 54 | - | 0/7/25/26 | 0/2/2/2 |
| 43 | 0TD | 2l | 92 | 43 | - | 1/3/12/14 | - |
| 1 | PSU | 2A | 2605 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1962 | 1,56 | - | 2/5/25/26 | 0/2/2/2 |
| 1 | PSU | 2A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 5MC | 1a | 1404 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 54 | CM0 | 2w | 34 | 54 | - | 5/8/30/31 | 0/2/2/2 |
| 55 | 5MC | 2x | 32 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 55 | 4SU | 1x | 8 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MU | 1A | 1939 | 1,56 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 2MG | 2a | 1207 | 32 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | OMC | 2A | 1920 | 1 | - | 1/7/27/28 | 0/2/2/2 |
| 1 | OMG | 2A | 2251 | 1,55,56 | - | 0/5/27/28 | 0/3/3/3 |
| 32 | 5MC | 2a | 1400 | 32 | - | 2/5/25/26 | 0/2/2/2 |
| 32 | 4OC | 1a | 1402 | 32 | - | 3/9/29/30 | 0/2/2/2 |
| 54 | 5MU | 2y | 54 | 54 | - | 3/5/25/26 | 0/2/2/2 |
| 1 | PSU | 1A | 1911 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MC | 1x | 32 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 55 | 5MU | 1x | 54 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 54 | 5MU | 1y | 54 | 54 | - | 4/5/25/26 | 0/2/2/2 |
| 32 | 2MG | 1a | 1207 | 32 | - | 0/5/27/28 | 0/3/3/3 |
| 54 | 7MG | 1y | 46 | 54 | - | 6/7/37/38 | 0/3/3/3 |
| 54 | 6MZ | 1y | 37 | 54 | - | 1/5/27/28 | 0/3/3/3 |
| 55 | PSU | 2x | 55 | 55 | - | 0/7/25/26 | 0/2/2/2 |
| 32 | 7MG | 2a | 527 | 32,56 | - | 3/7/37/38 | 0/3/3/3 |
| 54 | CM0 | 2y | 34 | 54 | - | 4/8/30/31 | 0/2/2/2 |
| 32 | MA6 | 2a | 1519 | 32 | - | 6/7/29/30 | 0/3/3/3 |
| 54 | 4SU | 1y | 8 | 54 | - | 2/5/25/26 | 0/2/2/2 |
| 54 | 6MZ | 1w | 37 | 54 | - | 0/5/27/28 | 0/3/3/3 |
| 32 | 7MG | 1a | 527 | 32,56 | - | 3/7/37/38 | 0/3/3/3 |
| 32 | MA6 | 1a | 1519 | 32 | - | 4/7/29/30 | 0/3/3/3 |
| 1 | PSU | 1A | 1917 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | OMU | 2A | 2552 | 1,56 | - | 0/7/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|---------|---------|-----------|---------|
| 32 | MA6 | 2a | 1518 | 32 | - | 3/7/29/30 | 0/3/3/3 |
| 54 | 5MU | 1w | 54 | 54 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | MA6 | 1a | 1518 | 32 | - | 1/7/29/30 | 0/3/3/3 |
| 54 | 7MG | 1w | 46 | 54 | - | 2/7/37/38 | 0/3/3/3 |
| 1 | OMG | 1A | 2251 | 1,55,56 | - | 0/5/27/28 | 0/3/3/3 |
| 54 | 7MG | 2w | 46 | 54 | - | 0/7/37/38 | 0/3/3/3 |
| 1 | 5MC | 1A | 1962 | 1 | - | 2/5/25/26 | 0/2/2/2 |
| 54 | 4SU | 2w | 8 | 54 | - | 1/5/25/26 | 0/2/2/2 |
| 54 | 6MZ | 2y | 37 | 54 | - | 1/5/27/28 | 0/3/3/3 |
| 32 | 5MC | 2a | 1407 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | UR3 | 2a | 1498 | 32 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 2MA | 2A | 2503 | 1 | - | 1/3/25/26 | 0/3/3/3 |
| 32 | 5MC | 1a | 967 | 32 | - | 2/5/25/26 | 0/2/2/2 |
| 54 | 6MZ | 2w | 37 | 54 | - | 2/5/27/28 | 0/3/3/3 |
| 1 | PSU | 1A | 2605 | 1,56 | - | 0/7/25/26 | 0/2/2/2 |
| 55 | 5MU | 2x | 54 | 55 | - | 0/5/25/26 | 0/2/2/2 |
| 1 | 5MC | 2A | 1942 | 1 | - | 0/5/25/26 | 0/2/2/2 |
| 32 | 5MC | 2a | 1404 | 32 | - | 2/5/25/26 | 0/2/2/2 |
| 54 | 7MG | 2y | 46 | 54 | - | 6/7/37/38 | 0/3/3/3 |
| 54 | 5MU | 2w | 54 | 54 | - | 0/5/25/26 | 0/2/2/2 |

All (126) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 43 | 1l | 92 | 0TD | CB-SB | -6.13 | 1.69 | 1.84 |
| 43 | 2l | 92 | 0TD | CB-SB | -6.04 | 1.69 | 1.84 |
| 54 | 2w | 46 | 7MG | C6-C5 | 5.20 | 1.48 | 1.41 |
| 32 | 1a | 527 | 7MG | C6-C5 | 5.16 | 1.48 | 1.41 |
| 32 | 2a | 527 | 7MG | C6-C5 | 5.02 | 1.48 | 1.41 |
| 54 | 1w | 46 | 7MG | C6-C5 | 4.97 | 1.48 | 1.41 |
| 54 | 1y | 46 | 7MG | C5-C4 | 4.93 | 1.48 | 1.39 |
| 32 | 2a | 967 | 5MC | C5-C4 | 4.89 | 1.48 | 1.41 |
| 32 | 2a | 1400 | 5MC | C5-C4 | 4.89 | 1.48 | 1.41 |
| 1 | 1A | 2503 | 2MA | C6-C5 | 4.88 | 1.48 | 1.41 |
| 55 | 2x | 32 | 5MC | C5-C4 | 4.88 | 1.48 | 1.41 |
| 32 | 2a | 1404 | 5MC | C5-C4 | 4.81 | 1.48 | 1.41 |
| 54 | 2y | 46 | 7MG | C5-C4 | 4.79 | 1.48 | 1.39 |
| 1 | 1A | 1962 | 5MC | C5-C4 | 4.77 | 1.48 | 1.41 |
| 1 | 2A | 1942 | 5MC | C5-C4 | 4.76 | 1.48 | 1.41 |
| 32 | 2a | 1407 | 5MC | C5-C4 | 4.72 | 1.48 | 1.41 |
| 55 | 1x | 32 | 5MC | C5-C4 | 4.71 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 32 | 1a | 1404 | 5MC | C5-C4 | 4.69 | 1.48 | 1.41 |
| 32 | 1a | 967 | 5MC | C5-C4 | 4.66 | 1.48 | 1.41 |
| 1 | 1A | 1942 | 5MC | C5-C4 | 4.64 | 1.48 | 1.41 |
| 32 | 1a | 1407 | 5MC | C5-C4 | 4.64 | 1.48 | 1.41 |
| 1 | 2A | 1917 | PSU | C5-C1' | -4.61 | 1.48 | 1.52 |
| 1 | 2A | 1962 | 5MC | C5-C4 | 4.60 | 1.48 | 1.41 |
| 1 | 2A | 2503 | 2MA | C6-C5 | 4.58 | 1.48 | 1.41 |
| 32 | 1a | 1400 | 5MC | C5-C4 | 4.54 | 1.48 | 1.41 |
| 32 | 1a | 527 | 7MG | C5-C4 | 4.50 | 1.48 | 1.39 |
| 32 | 2a | 1207 | 2MG | C6-C5 | 4.50 | 1.49 | 1.41 |
| 54 | 2w | 46 | 7MG | C5-C4 | 4.46 | 1.47 | 1.39 |
| 1 | 1A | 1917 | PSU | C5-C1' | -4.45 | 1.48 | 1.52 |
| 1 | 1A | 2605 | PSU | C5-C1' | -4.43 | 1.48 | 1.52 |
| 32 | 2a | 527 | 7MG | C5-C4 | 4.38 | 1.47 | 1.39 |
| 54 | 1y | 46 | 7MG | C6-C5 | 4.38 | 1.47 | 1.41 |
| 54 | 2y | 46 | 7MG | C6-C5 | 4.31 | 1.47 | 1.41 |
| 55 | 2x | 55 | PSU | C5-C1' | -4.22 | 1.48 | 1.52 |
| 54 | 1w | 46 | 7MG | C5-C4 | 4.22 | 1.47 | 1.39 |
| 1 | 1A | 2251 | OMG | C6-C5 | 4.21 | 1.48 | 1.41 |
| 32 | 1a | 966 | M2G | C6-C5 | 4.20 | 1.48 | 1.41 |
| 32 | 2a | 966 | M2G | C6-C5 | 4.20 | 1.48 | 1.41 |
| 32 | 1a | 1207 | 2MG | C6-C5 | 4.18 | 1.48 | 1.41 |
| 54 | 1w | 8 | 4SU | C4-S4 | -4.17 | 1.59 | 1.67 |
| 55 | 2x | 8 | 4SU | C4-S4 | -4.13 | 1.60 | 1.67 |
| 1 | 2A | 1911 | PSU | C5-C1' | -4.11 | 1.48 | 1.52 |
| 54 | 1y | 8 | 4SU | C4-S4 | -4.06 | 1.60 | 1.67 |
| 55 | 1x | 8 | 4SU | C4-S4 | -4.06 | 1.60 | 1.67 |
| 55 | 1x | 55 | PSU | C5-C1' | -4.03 | 1.48 | 1.52 |
| 54 | 1y | 55 | PSU | C5-C1' | -4.03 | 1.48 | 1.52 |
| 54 | 2y | 8 | 4SU | C4-S4 | -3.97 | 1.60 | 1.67 |
| 1 | 1A | 1911 | PSU | C5-C1' | -3.94 | 1.48 | 1.52 |
| 1 | 2A | 2605 | PSU | C5-C1' | -3.92 | 1.48 | 1.52 |
| 1 | 2A | 2251 | OMG | C6-C5 | 3.88 | 1.48 | 1.41 |
| 54 | 2w | 8 | 4SU | C4-S4 | -3.86 | 1.60 | 1.67 |
| 32 | 1a | 516 | PSU | C5-C1' | -3.72 | 1.49 | 1.52 |
| 54 | 1y | 46 | 7MG | C5-N7 | -3.67 | 1.33 | 1.39 |
| 32 | 2a | 516 | PSU | C5-C1' | -3.66 | 1.49 | 1.52 |
| 54 | 2y | 46 | 7MG | C5-N7 | -3.64 | 1.33 | 1.39 |
| 54 | 2y | 55 | PSU | C5-C1' | -3.61 | 1.49 | 1.52 |
| 54 | 2y | 34 | CM0 | C4-C5 | 3.61 | 1.49 | 1.40 |
| 1 | 2A | 1915 | 5MU | C4-C5 | 3.56 | 1.49 | 1.41 |
| 55 | 2x | 55 | PSU | C4-C5 | 3.51 | 1.49 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 32 | 1a | 527 | 7MG | C5-N7 | -3.51 | 1.33 | 1.39 |
| 54 | 1y | 54 | 5MU | C4-C5 | 3.50 | 1.49 | 1.41 |
| 54 | 1w | 54 | 5MU | C4-C5 | 3.50 | 1.49 | 1.41 |
| 54 | 1y | 34 | CM0 | C4-C5 | 3.49 | 1.48 | 1.40 |
| 32 | 1a | 966 | M2G | C2-N2 | 3.47 | 1.40 | 1.34 |
| 32 | 2a | 966 | M2G | C2-N2 | 3.47 | 1.40 | 1.34 |
| 55 | 2x | 54 | 5MU | C4-C5 | 3.46 | 1.48 | 1.41 |
| 54 | 2y | 55 | PSU | C4-C5 | 3.46 | 1.48 | 1.41 |
| 54 | 1w | 34 | CM0 | C4-C5 | 3.44 | 1.48 | 1.40 |
| 32 | 2a | 516 | PSU | C4-C5 | 3.42 | 1.48 | 1.41 |
| 1 | 2A | 1911 | PSU | C4-C5 | 3.40 | 1.48 | 1.41 |
| 1 | 1A | 1911 | PSU | C4-C5 | 3.39 | 1.48 | 1.41 |
| 54 | 2y | 54 | 5MU | C4-C5 | 3.36 | 1.48 | 1.41 |
| 32 | 1a | 516 | PSU | C4-C5 | 3.36 | 1.48 | 1.41 |
| 54 | 2w | 34 | CM0 | C4-C5 | 3.35 | 1.48 | 1.40 |
| 32 | 2a | 527 | 7MG | C5-N7 | -3.33 | 1.34 | 1.39 |
| 55 | 1x | 55 | PSU | C4-C5 | 3.33 | 1.48 | 1.41 |
| 54 | 2w | 46 | 7MG | C5-N7 | -3.33 | 1.34 | 1.39 |
| 54 | 1w | 55 | PSU | C4-C5 | 3.33 | 1.48 | 1.41 |
| 1 | 2A | 1917 | PSU | C4-C5 | 3.33 | 1.48 | 1.41 |
| 1 | 2A | 2605 | PSU | C4-C5 | 3.32 | 1.48 | 1.41 |
| 1 | 1A | 1915 | 5MU | C4-C5 | 3.29 | 1.48 | 1.41 |
| 55 | 1x | 54 | 5MU | C4-C5 | 3.29 | 1.48 | 1.41 |
| 54 | 1y | 55 | PSU | C4-C5 | 3.28 | 1.48 | 1.41 |
| 1 | 1A | 1939 | 5MU | C4-C5 | 3.28 | 1.48 | 1.41 |
| 54 | 2w | 55 | PSU | C4-C5 | 3.27 | 1.48 | 1.41 |
| 1 | 2A | 1939 | 5MU | C4-C5 | 3.23 | 1.48 | 1.41 |
| 1 | 1A | 1917 | PSU | C4-C5 | 3.23 | 1.48 | 1.41 |
| 54 | 1w | 46 | 7MG | C5-N7 | -3.21 | 1.34 | 1.39 |
| 1 | 1A | 2605 | PSU | C4-C5 | 3.19 | 1.48 | 1.41 |
| 55 | 1x | 8 | 4SU | C2-N3 | -3.18 | 1.31 | 1.38 |
| 54 | 2w | 54 | 5MU | C4-C5 | 3.15 | 1.48 | 1.41 |
| 54 | 2w | 55 | PSU | C5-C1' | -3.03 | 1.49 | 1.52 |
| 54 | 1w | 46 | 7MG | C4-N9 | -2.91 | 1.32 | 1.38 |
| 32 | 2a | 1518 | MA6 | C5-C4 | 2.68 | 1.48 | 1.40 |
| 32 | 2a | 966 | M2G | C5-C4 | 2.63 | 1.47 | 1.40 |
| 54 | 1w | 55 | PSU | C5-C1' | -2.62 | 1.50 | 1.52 |
| 32 | 2a | 1519 | MA6 | C5-C4 | 2.62 | 1.47 | 1.40 |
| 54 | 1y | 46 | 7MG | C4-N3 | 2.62 | 1.37 | 1.34 |
| 54 | 2y | 37 | 6MZ | C5-C4 | 2.58 | 1.47 | 1.40 |
| 32 | 2a | 1207 | 2MG | C5-C4 | 2.58 | 1.47 | 1.40 |
| 54 | 1y | 37 | 6MZ | C5-C4 | 2.55 | 1.47 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 54 | 2w | 37 | 6MZ | C5-C4 | 2.54 | 1.47 | 1.40 |
| 54 | 1w | 37 | 6MZ | C5-C4 | 2.53 | 1.47 | 1.40 |
| 32 | 1a | 966 | M2G | C5-C4 | 2.50 | 1.47 | 1.40 |
| 32 | 1a | 1518 | MA6 | C5-C4 | 2.49 | 1.47 | 1.40 |
| 1 | 1A | 2251 | OMG | C5-C4 | 2.48 | 1.47 | 1.40 |
| 32 | 1a | 1519 | MA6 | C5-C4 | 2.46 | 1.47 | 1.40 |
| 55 | 2x | 8 | 4SU | C2-N3 | -2.39 | 1.33 | 1.38 |
| 1 | 2A | 2251 | OMG | C5-C4 | 2.39 | 1.47 | 1.40 |
| 32 | 1a | 1207 | 2MG | C5-C4 | 2.36 | 1.47 | 1.40 |
| 32 | 2a | 527 | 7MG | C4-N9 | -2.34 | 1.34 | 1.38 |
| 32 | 1a | 516 | PSU | O4'-C1' | -2.28 | 1.41 | 1.44 |
| 1 | 1A | 2503 | 2MA | C5-C4 | 2.28 | 1.46 | 1.40 |
| 1 | 2A | 2503 | 2MA | C5-C4 | 2.26 | 1.46 | 1.40 |
| 32 | 1a | 527 | 7MG | C4-N9 | -2.25 | 1.34 | 1.38 |
| 54 | 2y | 46 | 7MG | C4-N3 | 2.20 | 1.37 | 1.34 |
| 1 | 1A | 2552 | OMU | C2-N3 | -2.20 | 1.33 | 1.38 |
| 1 | 1A | 2605 | PSU | C2-N3 | -2.10 | 1.34 | 1.38 |
| 1 | 2A | 2605 | PSU | C2-N3 | -2.10 | 1.34 | 1.38 |
| 1 | 1A | 1911 | PSU | C2-N3 | -2.10 | 1.34 | 1.38 |
| 55 | 1x | 54 | 5MU | C2-N3 | -2.07 | 1.34 | 1.38 |
| 1 | 1A | 1939 | 5MU | C2-N3 | -2.06 | 1.34 | 1.38 |
| 54 | 1y | 46 | 7MG | C2-N2 | 2.04 | 1.38 | 1.33 |
| 1 | 1A | 1917 | PSU | O4'-C1' | -2.01 | 1.41 | 1.44 |
| 1 | 1A | 2605 | PSU | O4'-C1' | -2.01 | 1.41 | 1.44 |
| 32 | 2a | 1498 | UR3 | C4-N3 | 2.00 | 1.41 | 1.38 |

All (311) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 43 | 1l | 92 | 0TD | CSB-SB-CB | -15.40 | 71.55 | 101.85 |
| 54 | 1y | 46 | 7MG | N3-C4-N9 | 10.44 | 140.32 | 126.91 |
| 54 | 2y | 46 | 7MG | N3-C4-N9 | 10.09 | 139.87 | 126.91 |
| 43 | 2l | 92 | 0TD | CSB-SB-CB | -9.76 | 82.66 | 101.85 |
| 32 | 1a | 527 | 7MG | N3-C4-N9 | 9.09 | 138.59 | 126.91 |
| 54 | 2w | 55 | PSU | N1-C2-N3 | -9.09 | 121.21 | 128.43 |
| 54 | 2w | 46 | 7MG | N3-C4-N9 | 9.02 | 138.49 | 126.91 |
| 54 | 1w | 55 | PSU | N1-C2-N3 | -8.98 | 121.30 | 128.43 |
| 32 | 2a | 516 | PSU | N1-C2-N3 | -8.86 | 121.39 | 128.43 |
| 32 | 2a | 527 | 7MG | N3-C4-N9 | 8.85 | 138.28 | 126.91 |
| 1 | 1A | 2605 | PSU | N1-C2-N3 | -8.80 | 121.44 | 128.43 |
| 1 | 2A | 1911 | PSU | N1-C2-N3 | -8.72 | 121.50 | 128.43 |
| 1 | 2A | 2605 | PSU | N1-C2-N3 | -8.52 | 121.65 | 128.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 1A | 1917 | PSU | N1-C2-N3 | -8.45 | 121.72 | 128.43 |
| 54 | 2y | 55 | PSU | N1-C2-N3 | -8.41 | 121.75 | 128.43 |
| 55 | 1x | 55 | PSU | N1-C2-N3 | -8.38 | 121.77 | 128.43 |
| 32 | 1a | 516 | PSU | N1-C2-N3 | -8.31 | 121.82 | 128.43 |
| 55 | 2x | 55 | PSU | N1-C2-N3 | -8.29 | 121.84 | 128.43 |
| 1 | 1A | 1911 | PSU | N1-C2-N3 | -8.23 | 121.88 | 128.43 |
| 54 | 1y | 55 | PSU | N1-C2-N3 | -8.18 | 121.93 | 128.43 |
| 1 | 2A | 1917 | PSU | N1-C2-N3 | -8.06 | 122.02 | 128.43 |
| 55 | 1x | 54 | 5MU | C4-N3-C2 | 8.06 | 121.95 | 115.14 |
| 54 | 1w | 46 | 7MG | N3-C4-N9 | 7.67 | 136.76 | 126.91 |
| 54 | 2w | 54 | 5MU | C4-N3-C2 | 7.51 | 121.49 | 115.14 |
| 54 | 2y | 54 | 5MU | C4-N3-C2 | 7.40 | 121.39 | 115.14 |
| 54 | 1w | 55 | PSU | C4-N3-C2 | 7.29 | 121.30 | 115.14 |
| 54 | 1y | 55 | PSU | C4-N3-C2 | 7.12 | 121.15 | 115.14 |
| 54 | 2w | 55 | PSU | C4-N3-C2 | 7.07 | 121.11 | 115.14 |
| 55 | 1x | 8 | 4SU | C2-N3-C4 | 7.01 | 125.31 | 115.15 |
| 1 | 1A | 1915 | 5MU | C4-N3-C2 | 6.93 | 121.00 | 115.14 |
| 55 | 2x | 54 | 5MU | C4-N3-C2 | 6.93 | 120.99 | 115.14 |
| 32 | 1a | 516 | PSU | C4-N3-C2 | 6.90 | 120.97 | 115.14 |
| 1 | 2A | 1911 | PSU | C4-N3-C2 | 6.90 | 120.97 | 115.14 |
| 55 | 1x | 55 | PSU | C4-N3-C2 | 6.84 | 120.92 | 115.14 |
| 54 | 2y | 55 | PSU | C4-N3-C2 | 6.79 | 120.87 | 115.14 |
| 32 | 2a | 516 | PSU | C4-N3-C2 | 6.77 | 120.86 | 115.14 |
| 1 | 2A | 2503 | 2MA | C2-N3-C4 | 6.76 | 121.01 | 115.52 |
| 1 | 1A | 2503 | 2MA | C2-N3-C4 | 6.75 | 121.01 | 115.52 |
| 1 | 1A | 1917 | PSU | C4-N3-C2 | 6.74 | 120.83 | 115.14 |
| 1 | 1A | 2605 | PSU | C4-N3-C2 | 6.70 | 120.80 | 115.14 |
| 1 | 2A | 1917 | PSU | C4-N3-C2 | 6.65 | 120.75 | 115.14 |
| 54 | 1y | 54 | 5MU | C4-N3-C2 | 6.60 | 120.72 | 115.14 |
| 54 | 1y | 46 | 7MG | C6-N1-C2 | 6.60 | 126.42 | 115.93 |
| 54 | 1w | 34 | CM0 | C4-N3-C2 | 6.59 | 120.71 | 115.14 |
| 55 | 2x | 8 | 4SU | C2-N3-C4 | 6.56 | 124.66 | 115.15 |
| 1 | 2A | 2605 | PSU | C4-N3-C2 | 6.50 | 120.63 | 115.14 |
| 1 | 1A | 1911 | PSU | C4-N3-C2 | 6.41 | 120.56 | 115.14 |
| 54 | 2y | 34 | CM0 | C4-N3-C2 | 6.41 | 120.55 | 115.14 |
| 55 | 2x | 55 | PSU | C4-N3-C2 | 6.38 | 120.53 | 115.14 |
| 1 | 2A | 1915 | 5MU | C4-N3-C2 | 6.37 | 120.52 | 115.14 |
| 54 | 1y | 34 | CM0 | C4-N3-C2 | 6.28 | 120.45 | 115.14 |
| 1 | 2A | 1939 | 5MU | C4-N3-C2 | 6.27 | 120.44 | 115.14 |
| 54 | 1w | 54 | 5MU | C4-N3-C2 | 6.20 | 120.38 | 115.14 |
| 54 | 2y | 46 | 7MG | C6-N1-C2 | 6.20 | 125.77 | 115.93 |
| 54 | 1y | 37 | 6MZ | C2-N1-C6 | 6.10 | 121.82 | 116.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 54 | 2w | 34 | CM0 | C4-N3-C2 | 6.10 | 120.29 | 115.14 |
| 54 | 1w | 37 | 6MZ | C2-N1-C6 | 6.01 | 121.75 | 116.59 |
| 54 | 2w | 37 | 6MZ | C2-N1-C6 | 6.00 | 121.73 | 116.59 |
| 54 | 2y | 37 | 6MZ | C2-N1-C6 | 5.96 | 121.70 | 116.59 |
| 1 | 1A | 1939 | 5MU | C4-N3-C2 | 5.88 | 120.10 | 115.14 |
| 54 | 1y | 55 | PSU | C5-C4-N3 | -5.75 | 117.95 | 125.36 |
| 54 | 1w | 46 | 7MG | N7-C8-N9 | -5.60 | 95.37 | 103.38 |
| 1 | 2A | 1917 | PSU | C5-C4-N3 | -5.57 | 118.18 | 125.36 |
| 32 | 2a | 527 | 7MG | N7-C8-N9 | -5.53 | 95.48 | 103.38 |
| 55 | 1x | 55 | PSU | C5-C4-N3 | -5.43 | 118.36 | 125.36 |
| 32 | 1a | 527 | 7MG | C5-C4-N3 | -5.43 | 117.63 | 126.49 |
| 54 | 1y | 46 | 7MG | C5-C4-N3 | -5.41 | 117.66 | 126.49 |
| 32 | 1a | 516 | PSU | C5-C4-N3 | -5.40 | 118.41 | 125.36 |
| 1 | 1A | 2251 | OMG | C2-N3-C4 | 5.38 | 121.50 | 115.36 |
| 55 | 2x | 55 | PSU | C5-C4-N3 | -5.37 | 118.44 | 125.36 |
| 54 | 2w | 46 | 7MG | C5-C4-N3 | -5.37 | 117.73 | 126.49 |
| 32 | 1a | 966 | M2G | C6-N1-C2 | 5.36 | 122.56 | 116.18 |
| 1 | 2A | 1911 | PSU | C5-C4-N3 | -5.32 | 118.50 | 125.36 |
| 1 | 1A | 1917 | PSU | C5-C4-N3 | -5.32 | 118.51 | 125.36 |
| 54 | 1w | 55 | PSU | C5-C4-N3 | -5.32 | 118.51 | 125.36 |
| 32 | 2a | 966 | M2G | C6-N1-C2 | 5.26 | 122.45 | 116.18 |
| 54 | 2y | 55 | PSU | C5-C4-N3 | -5.25 | 118.60 | 125.36 |
| 54 | 2y | 46 | 7MG | C5-C4-N3 | -5.21 | 117.99 | 126.49 |
| 54 | 2w | 46 | 7MG | N7-C8-N9 | -5.17 | 95.99 | 103.38 |
| 32 | 2a | 516 | PSU | C5-C4-N3 | -5.15 | 118.72 | 125.36 |
| 54 | 2w | 55 | PSU | C5-C4-N3 | -5.08 | 118.81 | 125.36 |
| 32 | 1a | 527 | 7MG | N7-C8-N9 | -5.08 | 96.11 | 103.38 |
| 32 | 2a | 527 | 7MG | C5-C4-N3 | -5.06 | 118.22 | 126.49 |
| 54 | 2y | 8 | 4SU | C2-N3-C4 | 5.06 | 122.49 | 115.15 |
| 1 | 1A | 2605 | PSU | C5-C4-N3 | -5.03 | 118.88 | 125.36 |
| 1 | 1A | 1911 | PSU | C5-C4-N3 | -5.03 | 118.88 | 125.36 |
| 32 | 1a | 966 | M2G | C2-N3-C4 | 5.02 | 120.98 | 115.28 |
| 32 | 2a | 1207 | 2MG | C2-N3-C4 | 4.96 | 120.91 | 115.28 |
| 54 | 2y | 46 | 7MG | N7-C8-N9 | -4.93 | 96.32 | 103.38 |
| 1 | 2A | 2605 | PSU | C5-C4-N3 | -4.93 | 119.01 | 125.36 |
| 32 | 2a | 966 | M2G | C2-N3-C4 | 4.90 | 120.84 | 115.28 |
| 32 | 2a | 1402 | 4OC | CM4-N4-C4 | -4.86 | 118.80 | 122.97 |
| 1 | 2A | 2503 | 2MA | C5-C6-N1 | -4.84 | 117.98 | 123.06 |
| 54 | 1w | 8 | 4SU | C2-N3-C4 | 4.78 | 122.08 | 115.15 |
| 54 | 2w | 8 | 4SU | C2-N3-C4 | 4.75 | 122.04 | 115.15 |
| 54 | 1y | 46 | 7MG | N7-C8-N9 | -4.74 | 96.60 | 103.38 |
| 1 | 1A | 2503 | 2MA | C5-C6-N1 | -4.71 | 118.12 | 123.06 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 1A | 1920 | OMC | C2-N3-C4 | 4.69 | 121.09 | 116.34 |
| 1 | 2A | 2251 | OMG | C2-N3-C4 | 4.68 | 120.71 | 115.36 |
| 55 | 2x | 55 | PSU | C5-C6-N1 | -4.62 | 118.76 | 124.44 |
| 54 | 1w | 46 | 7MG | C6-N1-C2 | 4.62 | 123.27 | 115.93 |
| 32 | 1a | 1207 | 2MG | C2-N3-C4 | 4.60 | 120.50 | 115.28 |
| 54 | 1y | 8 | 4SU | C2-N3-C4 | 4.54 | 121.74 | 115.15 |
| 54 | 1y | 46 | 7MG | C6-C5-C4 | 4.52 | 120.05 | 115.20 |
| 32 | 1a | 1207 | 2MG | C6-N1-C2 | 4.48 | 123.21 | 115.18 |
| 32 | 1a | 1207 | 2MG | C5-C6-N1 | -4.44 | 117.36 | 123.43 |
| 32 | 1a | 527 | 7MG | C6-C5-C4 | 4.44 | 119.97 | 115.20 |
| 32 | 2a | 527 | 7MG | C6-N1-C2 | 4.40 | 122.91 | 115.93 |
| 54 | 2y | 46 | 7MG | C6-C5-C4 | 4.39 | 119.92 | 115.20 |
| 32 | 2a | 1207 | 2MG | C5-C6-N1 | -4.36 | 117.47 | 123.43 |
| 32 | 1a | 966 | M2G | C6-C5-C4 | -4.33 | 116.66 | 120.80 |
| 54 | 1y | 55 | PSU | C5-C1'-C2' | -4.32 | 107.60 | 115.32 |
| 1 | 2A | 1917 | PSU | C5-C1'-C2' | -4.31 | 107.63 | 115.32 |
| 1 | 1A | 2605 | PSU | C5-C6-N1 | -4.31 | 119.14 | 124.44 |
| 1 | 1A | 2605 | PSU | C6-N1-C2 | 4.31 | 122.47 | 115.36 |
| 55 | 2x | 55 | PSU | C6-N1-C2 | 4.29 | 122.44 | 115.36 |
| 54 | 1w | 46 | 7MG | C5-C4-N3 | -4.27 | 119.51 | 126.49 |
| 1 | 2A | 2605 | PSU | C5-C6-N1 | -4.27 | 119.19 | 124.44 |
| 1 | 2A | 2605 | PSU | C6-N1-C2 | 4.26 | 122.39 | 115.36 |
| 1 | 2A | 1917 | PSU | C5-C6-N1 | -4.26 | 119.21 | 124.44 |
| 32 | 2a | 516 | PSU | C6-N1-C2 | 4.25 | 122.36 | 115.36 |
| 54 | 1y | 46 | 7MG | C5-C6-N1 | -4.24 | 114.43 | 123.14 |
| 32 | 1a | 527 | 7MG | C6-N1-C2 | 4.21 | 122.61 | 115.93 |
| 1 | 1A | 1911 | PSU | C5-C6-N1 | -4.20 | 119.28 | 124.44 |
| 1 | 2A | 2251 | OMG | C5-C6-N1 | -4.19 | 117.69 | 123.43 |
| 1 | 2A | 1911 | PSU | C6-N1-C2 | 4.19 | 122.28 | 115.36 |
| 1 | 1A | 1917 | PSU | C5-C6-N1 | -4.19 | 119.29 | 124.44 |
| 54 | 2y | 46 | 7MG | C5-C6-N1 | -4.17 | 114.57 | 123.14 |
| 1 | 2A | 1920 | OMC | C2-N3-C4 | 4.16 | 120.55 | 116.34 |
| 1 | 1A | 1911 | PSU | C6-N1-C2 | 4.15 | 122.20 | 115.36 |
| 1 | 2A | 2251 | OMG | C6-N1-C2 | 4.12 | 122.47 | 115.93 |
| 32 | 1a | 1207 | 2MG | C6-C5-C4 | -4.11 | 116.87 | 120.80 |
| 1 | 1A | 1917 | PSU | C6-N1-C2 | 4.11 | 122.14 | 115.36 |
| 32 | 2a | 966 | M2G | C5-C6-N1 | -4.10 | 117.82 | 123.43 |
| 54 | 2w | 46 | 7MG | C6-C5-C4 | 4.10 | 119.60 | 115.20 |
| 32 | 2a | 1207 | 2MG | C6-N1-C2 | 4.10 | 122.51 | 115.18 |
| 54 | 2w | 55 | PSU | C6-N1-C2 | 4.09 | 122.10 | 115.36 |
| 55 | 1x | 55 | PSU | C5-C6-N1 | -4.07 | 119.43 | 124.44 |
| 1 | 2A | 1911 | PSU | C5-C6-N1 | -4.05 | 119.46 | 124.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 54 | 2y | 55 | PSU | C6-N1-C2 | 4.05 | 122.04 | 115.36 |
| 32 | 2a | 516 | PSU | C5-C6-N1 | -4.03 | 119.49 | 124.44 |
| 1 | 2A | 1917 | PSU | C6-N1-C2 | 4.02 | 121.98 | 115.36 |
| 32 | 2a | 527 | 7MG | C6-C5-C4 | 4.01 | 119.51 | 115.20 |
| 55 | 1x | 55 | PSU | C6-N1-C2 | 4.01 | 121.97 | 115.36 |
| 54 | 2y | 55 | PSU | C5-C6-N1 | -3.97 | 119.56 | 124.44 |
| 1 | 1A | 2251 | OMG | C5-C6-N1 | -3.96 | 118.01 | 123.43 |
| 1 | 1A | 2251 | OMG | C6-N1-C2 | 3.94 | 122.19 | 115.93 |
| 32 | 1a | 516 | PSU | C6-N1-C2 | 3.92 | 121.83 | 115.36 |
| 32 | 1a | 1207 | 2MG | CM2-N2-C2 | -3.91 | 118.87 | 123.59 |
| 32 | 1a | 516 | PSU | C5-C6-N1 | -3.90 | 119.64 | 124.44 |
| 32 | 1a | 1402 | 4OC | CM4-N4-C4 | -3.89 | 119.63 | 122.97 |
| 32 | 1a | 1404 | 5MC | C2-N3-C4 | 3.89 | 120.71 | 116.02 |
| 54 | 1w | 55 | PSU | C6-N1-C2 | 3.88 | 121.77 | 115.36 |
| 54 | 2w | 46 | 7MG | C6-N1-C2 | 3.87 | 122.07 | 115.93 |
| 32 | 1a | 966 | M2G | C5-C6-N1 | -3.84 | 118.18 | 123.43 |
| 32 | 2a | 1407 | 5MC | C2-N3-C4 | 3.79 | 120.59 | 116.02 |
| 32 | 2a | 1207 | 2MG | C6-C5-C4 | -3.76 | 117.21 | 120.80 |
| 32 | 1a | 1407 | 5MC | C2-N3-C4 | 3.76 | 120.55 | 116.02 |
| 32 | 1a | 1400 | 5MC | C2-N3-C4 | 3.76 | 120.55 | 116.02 |
| 1 | 2A | 2605 | PSU | C5-C1'-C2' | -3.75 | 108.64 | 115.32 |
| 54 | 1w | 46 | 7MG | C5-C6-N1 | -3.74 | 115.46 | 123.14 |
| 55 | 1x | 8 | 4SU | C5-C4-N3 | -3.68 | 118.90 | 123.83 |
| 32 | 2a | 967 | 5MC | C2-N3-C4 | 3.68 | 120.46 | 116.02 |
| 54 | 1y | 55 | PSU | C6-N1-C2 | 3.68 | 121.42 | 115.36 |
| 32 | 1a | 527 | 7MG | C5-C6-N1 | -3.67 | 115.60 | 123.14 |
| 55 | 2x | 32 | 5MC | C2-N3-C4 | 3.67 | 120.44 | 116.02 |
| 32 | 2a | 1519 | MA6 | C4-C5-N7 | -3.66 | 105.59 | 109.40 |
| 1 | 2A | 1942 | 5MC | C2-N3-C4 | 3.65 | 120.43 | 116.02 |
| 32 | 1a | 967 | 5MC | C2-N3-C4 | 3.64 | 120.41 | 116.02 |
| 32 | 2a | 527 | 7MG | C5-C6-N1 | -3.63 | 115.68 | 123.14 |
| 1 | 1A | 1942 | 5MC | C2-N3-C4 | 3.63 | 120.39 | 116.02 |
| 32 | 2a | 1518 | MA6 | C4-C5-N7 | -3.62 | 105.62 | 109.40 |
| 55 | 1x | 32 | 5MC | C2-N3-C4 | 3.59 | 120.36 | 116.02 |
| 55 | 2x | 8 | 4SU | C5-C4-N3 | -3.58 | 119.03 | 123.83 |
| 54 | 1y | 37 | 6MZ | C9-N6-C6 | -3.58 | 119.79 | 122.87 |
| 1 | 2A | 1962 | 5MC | C2-N3-C4 | 3.57 | 120.33 | 116.02 |
| 54 | 1y | 55 | PSU | C5-C6-N1 | -3.57 | 120.06 | 124.44 |
| 54 | 2w | 55 | PSU | C5-C6-N1 | -3.56 | 120.06 | 124.44 |
| 32 | 1a | 1519 | MA6 | C4-C5-N7 | -3.51 | 105.74 | 109.40 |
| 1 | 1A | 2605 | PSU | C5-C1'-C2' | -3.49 | 109.08 | 115.32 |
| 32 | 2a | 1400 | 5MC | C2-N3-C4 | 3.47 | 120.20 | 116.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | 2A | 1911 | PSU | C5-C1'-C2' | -3.40 | 109.25 | 115.32 |
| 54 | 1w | 46 | 7MG | C6-C5-C4 | 3.39 | 118.84 | 115.20 |
| 32 | 2a | 1207 | 2MG | C4-C5-N7 | -3.38 | 105.87 | 109.40 |
| 32 | 2a | 966 | M2G | C6-C5-C4 | -3.37 | 117.58 | 120.80 |
| 54 | 2w | 46 | 7MG | C5-C6-N1 | -3.37 | 116.22 | 123.14 |
| 1 | 1A | 1917 | PSU | C5-C1'-C2' | -3.36 | 109.32 | 115.32 |
| 1 | 1A | 2251 | OMG | N3-C2-N1 | -3.36 | 122.74 | 127.22 |
| 32 | 1a | 1518 | MA6 | N3-C2-N1 | -3.35 | 123.44 | 128.68 |
| 54 | 2y | 37 | 6MZ | C9-N6-C6 | -3.35 | 119.99 | 122.87 |
| 32 | 1a | 1518 | MA6 | C4-C5-N7 | -3.33 | 105.92 | 109.40 |
| 1 | 1A | 2251 | OMG | C6-C5-C4 | -3.33 | 117.61 | 120.80 |
| 32 | 2a | 1404 | 5MC | C2-N3-C4 | 3.33 | 120.04 | 116.02 |
| 32 | 2a | 1518 | MA6 | N3-C2-N1 | -3.33 | 123.47 | 128.68 |
| 32 | 2a | 1519 | MA6 | C9-N6-C6 | -3.32 | 109.46 | 119.51 |
| 54 | 1y | 37 | 6MZ | N3-C2-N1 | -3.30 | 123.52 | 128.68 |
| 1 | 1A | 1962 | 5MC | C2-N3-C4 | 3.29 | 119.98 | 116.02 |
| 54 | 1w | 37 | 6MZ | C9-N6-C6 | -3.28 | 120.05 | 122.87 |
| 1 | 1A | 1939 | 5MU | C5-C6-N1 | -3.28 | 118.66 | 122.19 |
| 32 | 1a | 1519 | MA6 | N3-C2-N1 | -3.28 | 123.56 | 128.68 |
| 32 | 2a | 1518 | MA6 | C9-N6-C6 | -3.27 | 109.61 | 119.51 |
| 54 | 1y | 46 | 7MG | N2-C2-N3 | 3.27 | 122.33 | 117.25 |
| 54 | 2y | 37 | 6MZ | N3-C2-N1 | -3.19 | 123.69 | 128.68 |
| 1 | 2A | 2251 | OMG | C6-C5-C4 | -3.19 | 117.75 | 120.80 |
| 54 | 1y | 46 | 7MG | C5-C4-N9 | -3.16 | 102.01 | 106.44 |
| 1 | 2A | 2251 | OMG | N3-C2-N1 | -3.15 | 123.02 | 127.22 |
| 54 | 1y | 8 | 4SU | C5-C4-N3 | -3.13 | 119.64 | 123.83 |
| 32 | 1a | 1207 | 2MG | C4-C5-N7 | -3.12 | 106.14 | 109.40 |
| 54 | 2w | 37 | 6MZ | N3-C2-N1 | -3.12 | 123.80 | 128.68 |
| 32 | 2a | 1519 | MA6 | N3-C2-N1 | -3.11 | 123.82 | 128.68 |
| 54 | 2y | 34 | CM0 | O5-C5-C4 | 3.10 | 118.99 | 115.19 |
| 54 | 2y | 8 | 4SU | C5-C4-N3 | -3.09 | 119.69 | 123.83 |
| 54 | 1w | 55 | PSU | C5-C6-N1 | -3.09 | 120.64 | 124.44 |
| 54 | 2w | 8 | 4SU | C5-C4-N3 | -3.08 | 119.71 | 123.83 |
| 32 | 1a | 1519 | MA6 | C9-N6-C6 | -3.08 | 110.19 | 119.51 |
| 54 | 2y | 46 | 7MG | C5-C4-N9 | -3.07 | 102.14 | 106.44 |
| 32 | 1a | 1518 | MA6 | C9-N6-C6 | -3.07 | 110.21 | 119.51 |
| 32 | 2a | 1207 | 2MG | CM2-N2-C2 | -3.06 | 119.90 | 123.59 |
| 54 | 1w | 37 | 6MZ | N3-C2-N1 | -3.01 | 123.97 | 128.68 |
| 1 | 2A | 1939 | 5MU | C5-C6-N1 | -3.00 | 118.97 | 122.19 |
| 54 | 2y | 46 | 7MG | N2-C2-N3 | 2.98 | 121.89 | 117.25 |
| 54 | 2y | 37 | 6MZ | C4-C5-N7 | -2.97 | 106.30 | 109.40 |
| 55 | 1x | 55 | PSU | C5-C1'-C2' | -2.96 | 110.04 | 115.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 55 | 2x | 55 | PSU | C5-C1'-C2' | -2.95 | 110.05 | 115.32 |
| 1 | 1A | 2503 | 2MA | C4-C5-N7 | -2.93 | 106.35 | 109.40 |
| 1 | 1A | 1911 | PSU | C5-C1'-C2' | -2.93 | 110.10 | 115.32 |
| 54 | 1w | 37 | 6MZ | C4-C5-N7 | -2.91 | 106.37 | 109.40 |
| 1 | 2A | 2503 | 2MA | C4-C5-N7 | -2.90 | 106.38 | 109.40 |
| 54 | 1w | 8 | 4SU | C5-C4-N3 | -2.89 | 119.96 | 123.83 |
| 54 | 1y | 37 | 6MZ | C4-C5-N7 | -2.87 | 106.41 | 109.40 |
| 1 | 2A | 1962 | 5MC | N4-C4-N3 | 2.85 | 121.06 | 117.03 |
| 1 | 2A | 1915 | 5MU | C5-C6-N1 | -2.84 | 119.14 | 122.19 |
| 54 | 2y | 55 | PSU | C5-C1'-C2' | -2.83 | 110.26 | 115.32 |
| 54 | 2w | 55 | PSU | C5-C1'-C2' | -2.83 | 110.27 | 115.32 |
| 32 | 2a | 527 | 7MG | C8-N7-C5 | 2.82 | 116.29 | 108.94 |
| 54 | 1y | 34 | CM0 | O5-C5-C4 | 2.81 | 118.63 | 115.19 |
| 54 | 2y | 34 | CM0 | C7-O5-C5 | 2.81 | 123.29 | 117.76 |
| 54 | 1w | 34 | CM0 | O5-C5-C4 | 2.78 | 118.60 | 115.19 |
| 32 | 2a | 1407 | 5MC | N4-C4-N3 | 2.75 | 120.92 | 117.03 |
| 54 | 2w | 34 | CM0 | O5-C5-C4 | 2.75 | 118.56 | 115.19 |
| 54 | 2w | 46 | 7MG | C8-N7-C5 | 2.75 | 116.08 | 108.94 |
| 55 | 2x | 55 | PSU | O4'-C1'-C5 | 2.72 | 114.14 | 109.93 |
| 32 | 1a | 527 | 7MG | C8-N7-C5 | 2.72 | 116.00 | 108.94 |
| 32 | 1a | 1400 | 5MC | N4-C4-N3 | 2.71 | 120.86 | 117.03 |
| 54 | 2w | 37 | 6MZ | C4-C5-N7 | -2.71 | 106.58 | 109.40 |
| 1 | 1A | 2251 | OMG | C4-C5-N7 | -2.70 | 106.59 | 109.40 |
| 32 | 2a | 1207 | 2MG | N2-C2-N1 | 2.69 | 119.55 | 116.96 |
| 1 | 1A | 1962 | 5MC | C5-C6-N1 | -2.66 | 119.33 | 122.19 |
| 54 | 1w | 46 | 7MG | C8-N7-C5 | 2.66 | 115.84 | 108.94 |
| 32 | 2a | 1404 | 5MC | C5-C6-N1 | -2.63 | 119.36 | 122.19 |
| 32 | 1a | 1404 | 5MC | N4-C4-N3 | 2.62 | 120.73 | 117.03 |
| 54 | 1y | 34 | CM0 | C7-O5-C5 | 2.60 | 122.88 | 117.76 |
| 32 | 1a | 1407 | 5MC | N4-C4-N3 | 2.60 | 120.70 | 117.03 |
| 32 | 1a | 967 | 5MC | N4-C4-N3 | 2.58 | 120.68 | 117.03 |
| 54 | 1w | 54 | 5MU | C5-C6-N1 | -2.57 | 119.42 | 122.19 |
| 54 | 1y | 46 | 7MG | N1-C2-N3 | -2.55 | 121.42 | 125.42 |
| 55 | 1x | 32 | 5MC | N4-C4-N3 | 2.54 | 120.63 | 117.03 |
| 32 | 1a | 1207 | 2MG | N2-C2-N1 | 2.53 | 119.39 | 116.96 |
| 1 | 2A | 1942 | 5MC | N4-C4-N3 | 2.53 | 120.61 | 117.03 |
| 32 | 1a | 966 | M2G | C4-C5-N7 | -2.52 | 106.77 | 109.40 |
| 1 | 1A | 1920 | OMC | N4-C4-N3 | 2.52 | 120.47 | 116.49 |
| 54 | 1y | 46 | 7MG | C8-N7-C5 | 2.50 | 115.44 | 108.94 |
| 54 | 2y | 46 | 7MG | C8-N7-C5 | 2.50 | 115.43 | 108.94 |
| 1 | 2A | 2251 | OMG | C4-C5-N7 | -2.48 | 106.81 | 109.40 |
| 32 | 2a | 1400 | 5MC | C5-C6-N1 | -2.47 | 119.53 | 122.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54 | 1y | 34 | CM0 | C5-C4-N3 | -2.46 | 119.28 | 122.66 |
| 55 | 1x | 32 | 5MC | C5-C6-N1 | -2.46 | 119.54 | 122.19 |
| 1 | 1A | 1942 | 5MC | N4-C4-N3 | 2.43 | 120.47 | 117.03 |
| 54 | 2y | 34 | CM0 | C5-C4-N3 | -2.42 | 119.34 | 122.66 |
| 1 | 1A | 1962 | 5MC | N4-C4-N3 | 2.41 | 120.44 | 117.03 |
| 55 | 2x | 32 | 5MC | N4-C4-N3 | 2.39 | 120.41 | 117.03 |
| 54 | 2w | 34 | CM0 | C5-C4-N3 | -2.37 | 119.41 | 122.66 |
| 32 | 2a | 1518 | MA6 | C10-N6-C9 | -2.35 | 108.56 | 116.12 |
| 54 | 1w | 34 | CM0 | C5-C4-N3 | -2.34 | 119.45 | 122.66 |
| 1 | 1A | 1942 | 5MC | C5-C6-N1 | -2.34 | 119.68 | 122.19 |
| 32 | 2a | 1400 | 5MC | N4-C4-N3 | 2.34 | 120.34 | 117.03 |
| 54 | 1w | 55 | PSU | C5-C1'-C2' | -2.33 | 111.16 | 115.32 |
| 54 | 2w | 46 | 7MG | C2-N3-C4 | 2.31 | 120.29 | 113.89 |
| 32 | 2a | 966 | M2G | C4-C5-N7 | -2.31 | 106.99 | 109.40 |
| 32 | 1a | 1400 | 5MC | C5-C6-N1 | -2.29 | 119.73 | 122.19 |
| 32 | 1a | 1207 | 2MG | N3-C2-N1 | -2.26 | 122.66 | 126.23 |
| 32 | 2a | 1404 | 5MC | N4-C4-N3 | 2.26 | 120.22 | 117.03 |
| 32 | 2a | 967 | 5MC | N4-C4-N3 | 2.25 | 120.21 | 117.03 |
| 32 | 1a | 1518 | MA6 | C10-N6-C6 | -2.24 | 112.73 | 119.51 |
| 32 | 1a | 516 | PSU | O4'-C1'-C2' | 2.22 | 108.26 | 104.66 |
| 1 | 2A | 1962 | 5MC | C5-C6-N1 | -2.22 | 119.81 | 122.19 |
| 32 | 1a | 967 | 5MC | C5-C6-N1 | -2.22 | 119.81 | 122.19 |
| 32 | 2a | 966 | M2G | N3-C2-N2 | 2.21 | 119.43 | 117.18 |
| 54 | 1y | 46 | 7MG | C2-N3-C4 | 2.21 | 120.01 | 113.89 |
| 32 | 1a | 1407 | 5MC | C5-C6-N1 | -2.21 | 119.81 | 122.19 |
| 54 | 1w | 34 | CM0 | O3'-C3'-C2' | 2.20 | 118.94 | 111.82 |
| 32 | 1a | 1518 | MA6 | C10-N6-C9 | -2.20 | 109.04 | 116.12 |
| 1 | 2A | 1920 | OMC | N4-C4-N3 | 2.20 | 119.96 | 116.49 |
| 54 | 2w | 54 | 5MU | C5-C6-N1 | -2.19 | 119.83 | 122.19 |
| 32 | 1a | 527 | 7MG | C2-N3-C4 | 2.19 | 119.94 | 113.89 |
| 32 | 2a | 967 | 5MC | C5-C6-N1 | -2.19 | 119.84 | 122.19 |
| 55 | 2x | 54 | 5MU | C5-C6-N1 | -2.18 | 119.85 | 122.19 |
| 55 | 2x | 32 | 5MC | C5-C6-N1 | -2.14 | 119.89 | 122.19 |
| 32 | 2a | 527 | 7MG | C2-N3-C4 | 2.12 | 119.76 | 113.89 |
| 32 | 1a | 1519 | MA6 | N1-C6-N6 | 2.12 | 119.29 | 117.06 |
| 54 | 1y | 46 | 7MG | C4-N9-C1' | 2.12 | 131.63 | 126.60 |
| 54 | 2y | 46 | 7MG | N1-C2-N3 | -2.11 | 122.11 | 125.42 |
| 32 | 2a | 527 | 7MG | C5-C4-N9 | -2.11 | 103.49 | 106.44 |
| 54 | 1w | 46 | 7MG | N2-C2-N1 | 2.09 | 120.50 | 117.25 |
| 54 | 2y | 46 | 7MG | C2-N3-C4 | 2.08 | 119.64 | 113.89 |
| 55 | 1x | 54 | 5MU | C5-C6-N1 | -2.08 | 119.95 | 122.19 |
| 1 | 2A | 1942 | 5MC | C5-C6-N1 | -2.06 | 119.98 | 122.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1 | 2A | 2552 | OMU | C5-C4-N3 | -2.05 | 118.79 | 123.31 |
| 54 | 1w | 46 | 7MG | C2-N3-C4 | 2.05 | 119.56 | 113.89 |
| 32 | 1a | 1518 | MA6 | N1-C6-N6 | 2.04 | 119.20 | 117.06 |
| 54 | 1y | 54 | 5MU | C5-C6-N1 | -2.02 | 120.02 | 122.19 |

There are no chirality outliers.

All (103) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 1 | 1A | 1962 | 5MC | O4'-C1'-N1-C6 |
| 1 | 1A | 1962 | 5MC | C2'-C1'-N1-C6 |
| 43 | 1l | 92 | 0TD | O-C-CA-CB |
| 55 | 2x | 8 | 4SU | C2'-C1'-N1-C6 |
| 1 | 2A | 1939 | 5MU | C2'-C1'-N1-C6 |
| 1 | 2A | 1939 | 5MU | O4'-C1'-N1-C6 |
| 32 | 1a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 32 | 1a | 1519 | MA6 | C5-C6-N6-C10 |
| 32 | 1a | 1400 | 5MC | O4'-C4'-C5'-O5' |
| 32 | 1a | 1400 | 5MC | C3'-C4'-C5'-O5' |
| 54 | 1w | 34 | CM0 | C4-C5-O5-C7 |
| 1 | 1A | 1915 | 5MU | O4'-C1'-N1-C6 |
| 1 | 1A | 1915 | 5MU | C3'-C4'-C5'-O5' |
| 54 | 1y | 46 | 7MG | C4'-C5'-O5'-P |
| 54 | 1y | 46 | 7MG | C3'-C4'-C5'-O5' |
| 43 | 2l | 92 | 0TD | CG-CB-SB-CSB |
| 54 | 2w | 34 | CM0 | C4-C5-O5-C7 |
| 32 | 2a | 1207 | 2MG | C3'-C4'-C5'-O5' |
| 1 | 2A | 1920 | OMC | O4'-C1'-N1-C6 |
| 32 | 2a | 1400 | 5MC | O4'-C1'-N1-C6 |
| 32 | 2a | 1400 | 5MC | C2'-C1'-N1-C6 |
| 32 | 1a | 1402 | 4OC | C5-C4-N4-CM4 |
| 54 | 1y | 37 | 6MZ | N1-C6-N6-C9 |
| 54 | 2y | 54 | 5MU | C2'-C1'-N1-C6 |
| 54 | 2y | 54 | 5MU | C3'-C4'-C5'-O5' |
| 54 | 2y | 54 | 5MU | O4'-C4'-C5'-O5' |
| 54 | 1y | 54 | 5MU | C2'-C1'-N1-C6 |
| 54 | 1y | 54 | 5MU | O4'-C1'-N1-C6 |
| 54 | 1y | 54 | 5MU | C3'-C4'-C5'-O5' |
| 54 | 1y | 54 | 5MU | O4'-C4'-C5'-O5' |
| 54 | 2w | 8 | 4SU | C2'-C1'-N1-C6 |
| 1 | 1A | 1920 | OMC | C2'-C1'-N1-C6 |
| 32 | 2a | 527 | 7MG | C3'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 32 | 2a | 1519 | MA6 | O4'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | C5-C6-N6-C10 |
| 54 | 1y | 8 | 4SU | C2'-C1'-N1-C6 |
| 32 | 2a | 1518 | MA6 | C5-C6-N6-C10 |
| 32 | 2a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 32 | 2a | 1402 | 4OC | O4'-C1'-N1-C6 |
| 32 | 2a | 1402 | 4OC | C2'-C1'-N1-C6 |
| 54 | 1w | 46 | 7MG | O4'-C4'-C5'-O5' |
| 54 | 1w | 46 | 7MG | C3'-C4'-C5'-O5' |
| 54 | 2y | 37 | 6MZ | N1-C6-N6-C9 |
| 54 | 2w | 37 | 6MZ | C5-C6-N6-C9 |
| 54 | 2w | 37 | 6MZ | N1-C6-N6-C9 |
| 54 | 2y | 46 | 7MG | C4'-C5'-O5'-P |
| 54 | 2y | 46 | 7MG | C3'-C4'-C5'-O5' |
| 32 | 1a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 54 | 2y | 55 | PSU | O4'-C4'-C5'-O5' |
| 54 | 2y | 8 | 4SU | O4'-C4'-C5'-O5' |
| 1 | 1A | 1915 | 5MU | O4'-C4'-C5'-O5' |
| 32 | 2a | 1207 | 2MG | O4'-C4'-C5'-O5' |
| 32 | 1a | 1402 | 4OC | O4'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | C3'-C4'-C5'-O5' |
| 32 | 2a | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 54 | 2y | 55 | PSU | C3'-C4'-C5'-O5' |
| 54 | 2y | 8 | 4SU | C3'-C4'-C5'-O5' |
| 32 | 1a | 1402 | 4OC | C3'-C4'-C5'-O5' |
| 32 | 2a | 527 | 7MG | O4'-C4'-C5'-O5' |
| 32 | 1a | 967 | 5MC | O4'-C4'-C5'-O5' |
| 54 | 1w | 34 | CM0 | C8-C7-O5-C5 |
| 54 | 1y | 34 | CM0 | O4'-C4'-C5'-O5' |
| 54 | 1y | 46 | 7MG | O4'-C4'-C5'-O5' |
| 54 | 2y | 46 | 7MG | O4'-C4'-C5'-O5' |
| 54 | 2w | 34 | CM0 | C6-C5-O5-C7 |
| 32 | 2a | 1519 | MA6 | C5-C6-N6-C9 |
| 32 | 2a | 1518 | MA6 | C5-C6-N6-C9 |
| 32 | 1a | 1518 | MA6 | C5-C6-N6-C10 |
| 54 | 2w | 34 | CM0 | O4'-C4'-C5'-O5' |
| 54 | 2w | 34 | CM0 | C8-C7-O5-C5 |
| 54 | 2y | 34 | CM0 | C4-C5-O5-C7 |
| 32 | 1a | 527 | 7MG | C3'-C4'-C5'-O5' |
| 32 | 1a | 967 | 5MC | C3'-C4'-C5'-O5' |
| 54 | 1w | 34 | CM0 | C6-C5-O5-C7 |
| 54 | 1y | 46 | 7MG | C2'-C1'-N9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 54 | 1y | 34 | CM0 | C3'-C4'-C5'-O5' |
| 54 | 2w | 34 | CM0 | C3'-C4'-C5'-O5' |
| 32 | 2a | 1404 | 5MC | O4'-C4'-C5'-O5' |
| 54 | 2y | 34 | CM0 | C6-C5-O5-C7 |
| 32 | 2a | 1404 | 5MC | C3'-C4'-C5'-O5' |
| 54 | 2y | 46 | 7MG | C2'-C1'-N9-C8 |
| 1 | 1A | 2503 | 2MA | C4'-C5'-O5'-P |
| 32 | 2a | 527 | 7MG | C4'-C5'-O5'-P |
| 32 | 2a | 1519 | MA6 | C4'-C5'-O5'-P |
| 54 | 2y | 34 | CM0 | C8-C7-O5-C5 |
| 32 | 1a | 1519 | MA6 | C4'-C5'-O5'-P |
| 1 | 2A | 1962 | 5MC | O4'-C4'-C5'-O5' |
| 32 | 2a | 1519 | MA6 | N1-C6-N6-C9 |
| 32 | 2a | 1402 | 4OC | C3'-C2'-O2'-CM2 |
| 54 | 1y | 46 | 7MG | C2'-C1'-N9-C4 |
| 54 | 2y | 46 | 7MG | O4'-C1'-N9-C8 |
| 32 | 1a | 527 | 7MG | C4'-C5'-O5'-P |
| 54 | 1y | 8 | 4SU | O4'-C4'-C5'-O5' |
| 32 | 1a | 527 | 7MG | O4'-C4'-C5'-O5' |
| 1 | 2A | 2503 | 2MA | O4'-C4'-C5'-O5' |
| 32 | 2a | 1402 | 4OC | C1'-C2'-O2'-CM2 |
| 54 | 1y | 46 | 7MG | O4'-C1'-N9-C8 |
| 1 | 2A | 1962 | 5MC | C3'-C4'-C5'-O5' |
| 43 | 1l | 92 | 0TD | CG-CB-SB-CSB |
| 32 | 2a | 1518 | MA6 | N1-C6-N6-C9 |
| 1 | 1A | 2503 | 2MA | O4'-C4'-C5'-O5' |
| 54 | 2y | 34 | CM0 | O4'-C4'-C5'-O5' |
| 54 | 2y | 46 | 7MG | C2'-C1'-N9-C4 |

There are no ring outliers.

10 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | 2A | 1939 | 5MU | 1 | 0 |
| 1 | 1A | 2552 | OMU | 1 | 0 |
| 1 | 2A | 1962 | 5MC | 1 | 0 |
| 1 | 2A | 1917 | PSU | 1 | 0 |
| 1 | 1A | 1939 | 5MU | 1 | 0 |
| 1 | 2A | 1920 | OMC | 2 | 0 |
| 1 | 2A | 2251 | OMG | 1 | 0 |
| 1 | 2A | 2552 | OMU | 1 | 0 |
| 1 | 2A | 2503 | 2MA | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | 2A | 1942 | 5MC | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 | 4100 | - | 45,45,47 | 0.75 | 1 (2%) | 61,67,69 | 1.11 | 3 (4%) |
| 57 | LUJ | 2A | 3851 | - | 45,45,47 | 0.83 | 2 (4%) | 61,67,69 | 1.54 | 8 (13%) |
| 57 | LUJ | 2A | 3852 | - | 45,45,47 | 0.75 | 1 (2%) | 61,67,69 | 1.18 | 4 (6%) |
| 60 | SF4 | 1d | 501 | 35 | 0,12,12 | 0.00 | - | - | | |
| 60 | SF4 | 2d | 303 | 35 | 0,12,12 | 0.00 | - | - | | |
| 57 | LUJ | 1A | 4099 | - | 45,45,47 | 0.79 | 1 (2%) | 61,67,69 | 1.48 | 8 (13%) |
| 57 | LUJ | 2a | 3232 | - | 47,47,47 | 0.83 | 3 (6%) | 61,69,69 | 1.32 | 5 (8%) |
| 57 | LUJ | 1a | 1832 | 56 | 47,47,47 | 0.76 | 1 (2%) | 61,69,69 | 1.18 | 3 (4%) |

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 | 4100 | - | - | 5/18/94/97 | 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 |
| 60 | SF4 | 1d | 501 | 35 | - | - | 0/6/5/5 |
| 60 | SF4 | 2d | 303 | 35 | - | - | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 57 | LUJ | 1A | 4099 | - | - | 7/18/94/97 | 0/4/4/4 |
| 57 | LUJ | 2a | 3232 | - | - | 6/21/97/97 | 0/4/4/4 |
| 57 | LUJ | 1a | 1832 | 56 | - | 5/21/97/97 | 0/4/4/4 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 57 | 2A | 3851 | LUJ | O4'-C1' | 2.73 | 1.46 | 1.41 |
| 57 | 1A | 4100 | LUJ | O4'-C1' | 2.68 | 1.46 | 1.41 |
| 57 | 2A | 3851 | LUJ | CBE-CBD | -2.34 | 1.50 | 1.53 |
| 57 | 1a | 1832 | LUJ | CBG-CBE | -2.27 | 1.50 | 1.53 |
| 57 | 1A | 4099 | LUJ | OAB-CBC | 2.12 | 1.47 | 1.41 |
| 57 | 2a | 3232 | LUJ | O4'-C1' | 2.09 | 1.45 | 1.41 |
| 57 | 2a | 3232 | LUJ | C1'-C2' | -2.07 | 1.50 | 1.52 |
| 57 | 2A | 3852 | LUJ | C1'-C2' | -2.05 | 1.50 | 1.52 |
| 57 | 2a | 3232 | LUJ | CBE-CBD | -2.02 | 1.51 | 1.53 |

All (31) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57 | 2a | 3232 | LUJ | CBF-O3'-C3' | -6.22 | 102.56 | 117.96 |
| 57 | 1A | 4099 | LUJ | O1'-C1'-O4' | -5.36 | 105.63 | 111.43 |
| 57 | 1a | 1832 | LUJ | CBF-O3'-C3' | -5.23 | 105.01 | 117.96 |
| 57 | 2A | 3851 | LUJ | O1'-C1'-O4' | -5.10 | 105.91 | 111.43 |
| 57 | 2A | 3852 | LUJ | CBF-O3'-C3' | -4.69 | 106.35 | 117.96 |
| 57 | 1A | 4099 | LUJ | C1'-C2'-C3' | -4.21 | 97.04 | 102.10 |
| 57 | 2a | 3232 | LUJ | C1'-C2'-C3' | -4.14 | 97.13 | 102.10 |
| 57 | 2A | 3851 | LUJ | C1'-O1'-CAS | -4.12 | 107.78 | 117.96 |
| 57 | 1A | 4100 | LUJ | C2'-C3'-C4' | -4.09 | 95.98 | 103.22 |
| 57 | 2A | 3851 | LUJ | C2'-C3'-C4' | -4.01 | 96.12 | 103.22 |
| 57 | 1A | 4100 | LUJ | CBF-O3'-C3' | -3.91 | 108.30 | 117.96 |
| 57 | 1a | 1832 | LUJ | C2'-C3'-C4' | -3.76 | 96.55 | 103.22 |
| 57 | 1A | 4099 | LUJ | C1'-O1'-CAS | -3.73 | 108.73 | 117.96 |
| 57 | 2A | 3852 | LUJ | C1'-C2'-C3' | -3.64 | 97.73 | 102.10 |
| 57 | 2A | 3851 | LUJ | CBP-CBG-CBE | -3.58 | 107.35 | 112.15 |
| 57 | 2A | 3852 | LUJ | O4'-C1'-C2' | -3.39 | 100.61 | 104.98 |
| 57 | 1A | 4100 | LUJ | O1'-C1'-O4' | 3.33 | 115.04 | 111.43 |
| 57 | 2a | 3232 | LUJ | C2'-C3'-C4' | -3.13 | 97.68 | 103.22 |
| 57 | 1A | 4099 | LUJ | C2'-C3'-C4' | -2.81 | 98.24 | 103.22 |
| 57 | 2A | 3851 | LUJ | OAB-CBC-OAF | 2.80 | 118.50 | 110.67 |
| 57 | 1A | 4099 | LUJ | OAB-CBC-OAF | 2.74 | 118.32 | 110.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 57 | 1A | 4099 | LUJ | CBP-CBG-CBE | -2.73 | 108.49 | 112.15 |
| 57 | 1a | 1832 | LUJ | C1'-C2'-C3' | -2.73 | 98.82 | 102.10 |
| 57 | 2A | 3851 | LUJ | C1'-C2'-C3' | -2.64 | 98.93 | 102.10 |
| 57 | 2A | 3852 | LUJ | C2'-C3'-C4' | -2.51 | 98.77 | 103.22 |
| 57 | 2A | 3851 | LUJ | CBC-OAB-CAT | 2.34 | 123.77 | 117.96 |
| 57 | 1A | 4099 | LUJ | OAB-CAT-CAS | 2.29 | 113.30 | 107.48 |
| 57 | 1A | 4099 | LUJ | OAG-CBM-CBO | 2.20 | 110.10 | 106.01 |
| 57 | 2a | 3232 | LUJ | O4'-C1'-C2' | -2.15 | 102.21 | 104.98 |
| 57 | 2A | 3851 | LUJ | CBF-O3'-C3' | -2.02 | 112.97 | 117.96 |
| 57 | 2a | 3232 | LUJ | O3'-CBF-CBH | 2.00 | 111.66 | 108.22 |

There are no chirality outliers.

All (31) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 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' |
| 57 | 2A | 3852 | LUJ | O4'-C4'-C5'-O5' |
| 57 | 2a | 3232 | LUJ | C3'-C4'-C5'-O5' |
| 57 | 2A | 3852 | LUJ | C3'-C4'-C5'-O5' |
| 57 | 1A | 4099 | LUJ | OAF-CBC-OAB-CAT |
| 57 | 2A | 3851 | LUJ | OAF-CBC-OAB-CAT |
| 57 | 1A | 4100 | LUJ | O4'-C4'-C5'-O5' |
| 57 | 1a | 1832 | LUJ | OAF-CBI-CBN-OAM |
| 57 | 1A | 4100 | LUJ | C3'-C4'-C5'-O5' |
| 57 | 1a | 1832 | LUJ | CBG-CBI-CBN-OAM |
| 57 | 2a | 3232 | LUJ | CBG-CBP-CBQ-CBR |
| 57 | 1A | 4100 | LUJ | OAF-CBI-CBN-OAM |
| 57 | 2A | 3851 | LUJ | OAG-CBF-O3'-C3' |
| 57 | 1a | 1832 | LUJ | CBI-CBG-CBP-CBQ |
| 57 | 1A | 4099 | LUJ | C2'-C3'-O3'-CBF |
| 57 | 1A | 4100 | LUJ | CBG-CBI-CBN-OAM |
| 57 | 2A | 3852 | LUJ | CAS-CAT-OAB-CBC |
| 57 | 1A | 4100 | LUJ | OAF-CBC-OAB-CAT |
| 57 | 2a | 3232 | LUJ | CAS-CAT-OAB-CBC |
| 57 | 1a | 1832 | LUJ | CAS-CAT-OAB-CBC |
| 57 | 1A | 4099 | LUJ | OAG-CBM-CBO-NAR |
| 57 | 2A | 3851 | LUJ | OAG-CBM-CBO-NAR |
| 57 | 1A | 4099 | LUJ | CAS-CAT-OAB-CBC |
| 57 | 1A | 4099 | LUJ | OAG-CBF-O3'-C3' |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 57 | 2A | 3852 | LUJ | OAF-CBC-OAB-CAT |
| 57 | 2A | 3851 | LUJ | CAS-CAT-OAB-CBC |
| 57 | 1A | 4099 | LUJ | C2'-C1'-O1'-CAS |
| 57 | 1A | 4099 | LUJ | CBL-CBM-CBO-NAR |

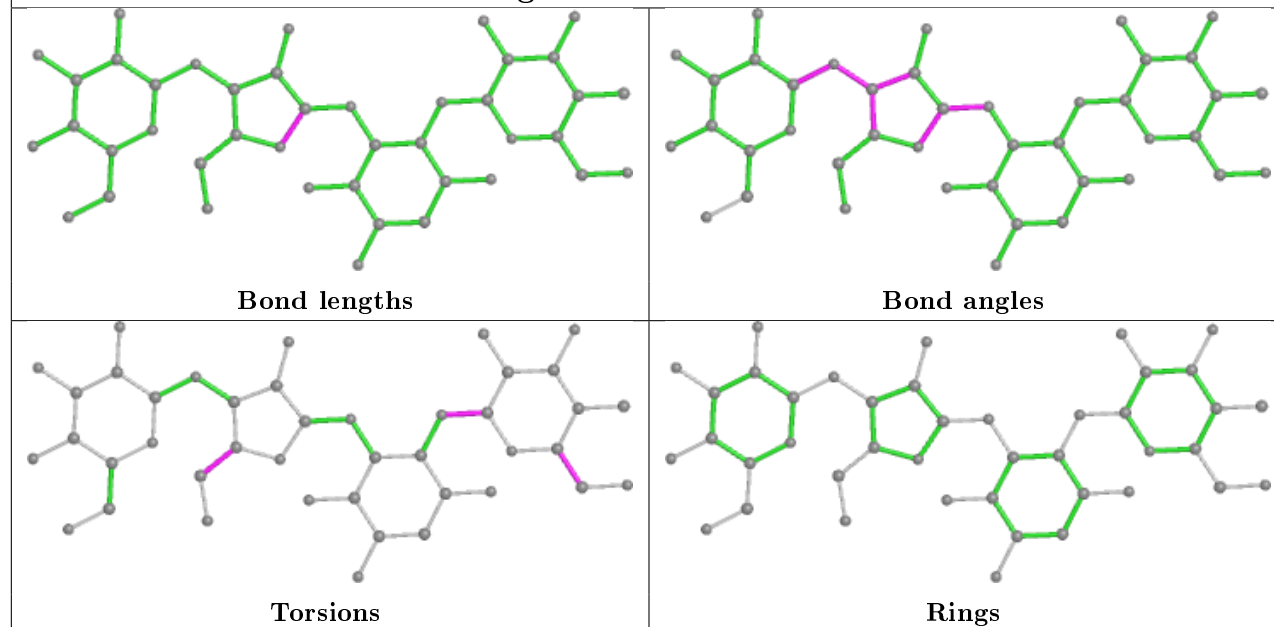
There are no ring outliers.

4 monomers are involved in 6 short contacts:

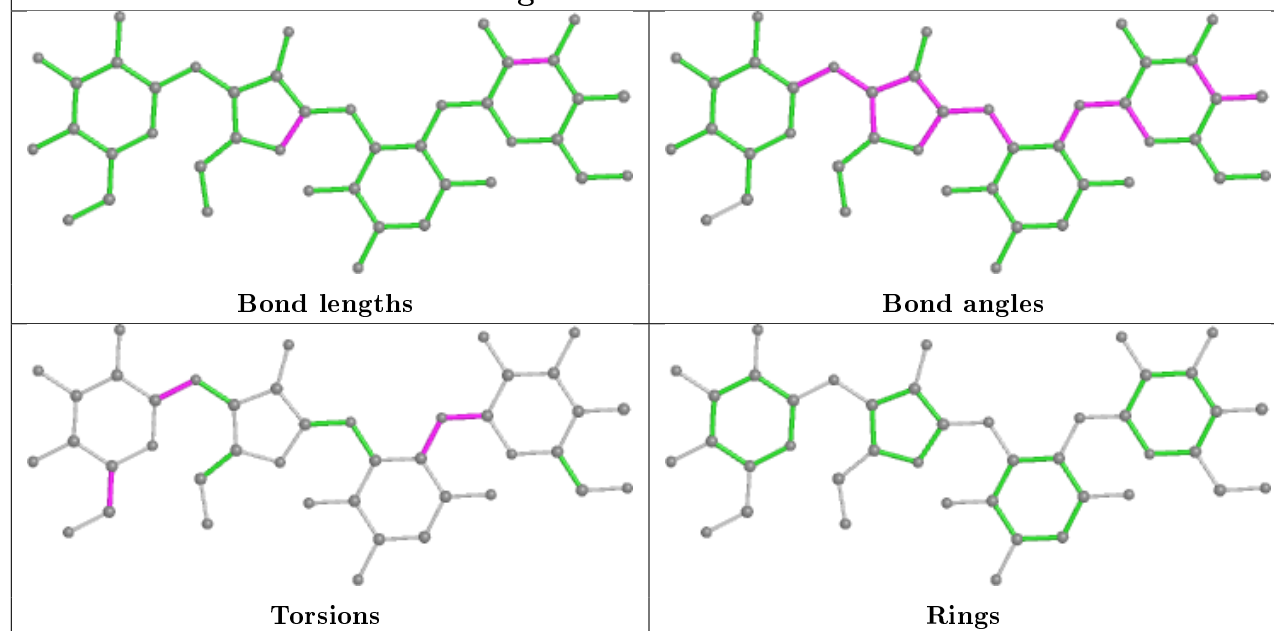
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57 | 1A | 4100 | LUJ | 1 | 0 |
| 57 | 2A | 3851 | LUJ | 2 | 0 |
| 57 | 2A | 3852 | LUJ | 1 | 0 |
| 57 | 1A | 4099 | LUJ | 2 | 0 |

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

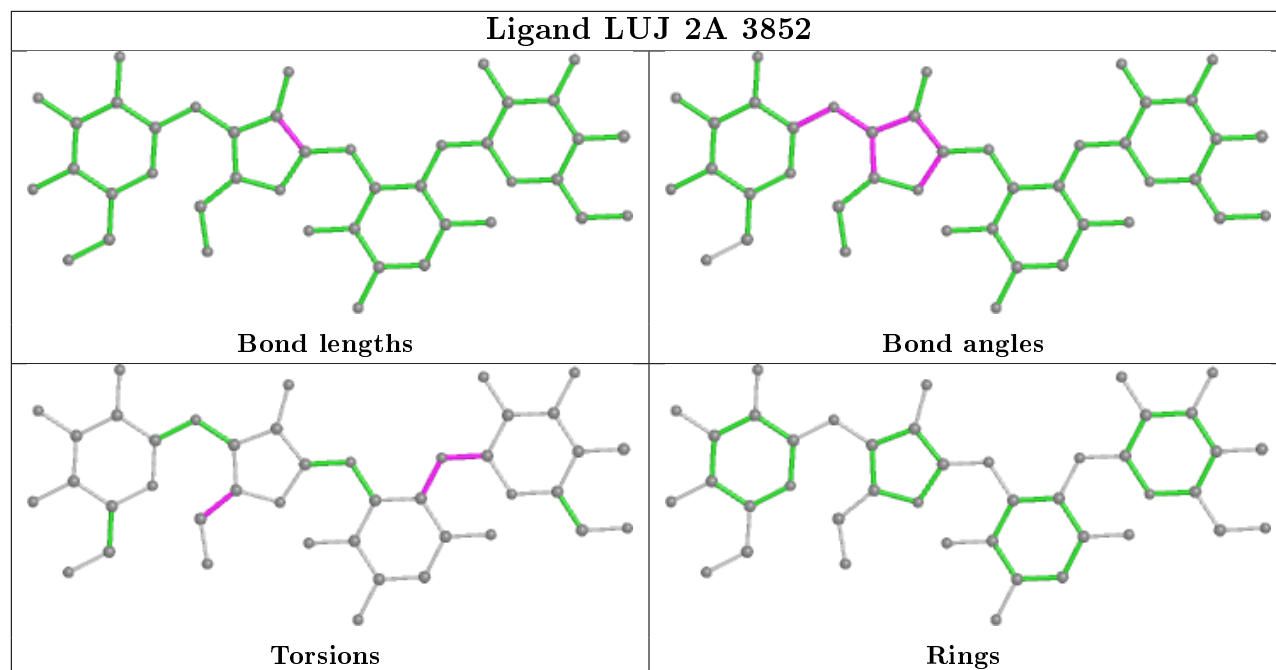
Ligand LUJ 1A 4100



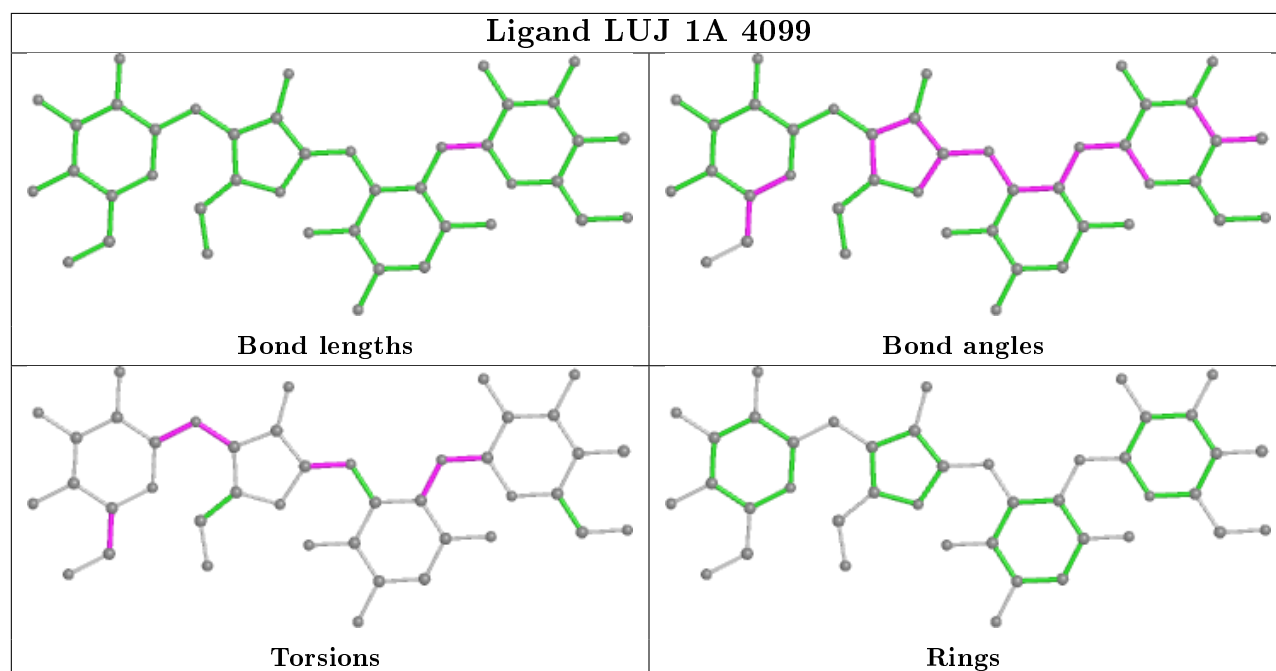
Ligand LUJ 2A 3851

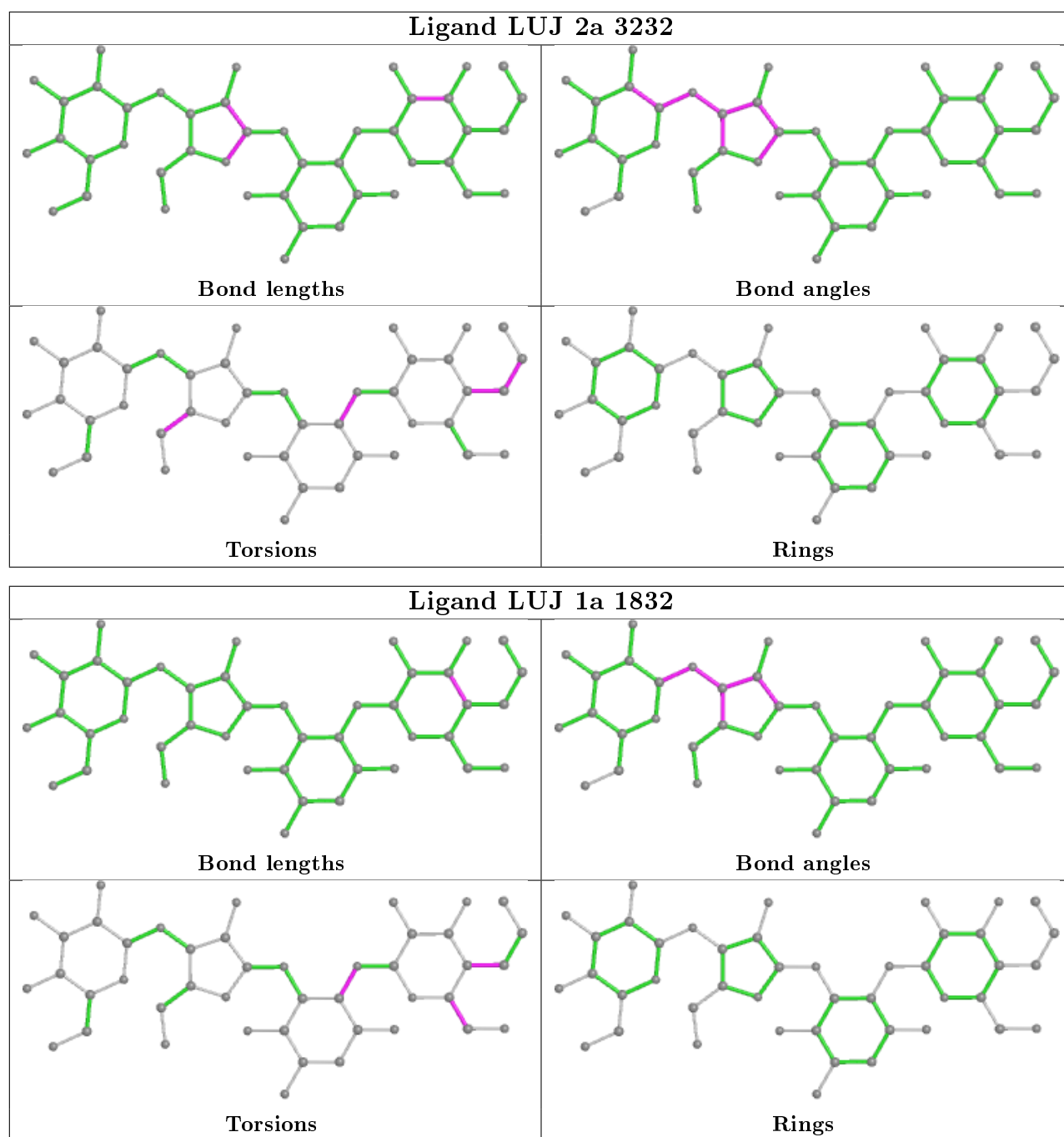


Ligand LUJ 2A 3852



Ligand LUJ 1A 4099





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | 1A | 2860/2915 (98%) | 0.32 | 22 (0%) 86 90 | 11, 28, 86, 98 | 0 |
| 1 | 2A | 2789/2915 (95%) | 0.23 | 57 (2%) 65 73 | 26, 53, 86, 100 | 0 |
| 2 | 1B | 120/121 (99%) | -0.03 | 0 100 100 | 21, 40, 53, 74 | 0 |
| 2 | 2B | 120/121 (99%) | -0.06 | 1 (0%) 86 90 | 55, 70, 79, 87 | 0 |
| 3 | 1D | 275/276 (99%) | 0.79 | 14 (5%) 28 34 | 13, 31, 45, 74 | 0 |
| 3 | 2D | 275/276 (99%) | 0.82 | 19 (6%) 16 20 | 24, 45, 58, 69 | 0 |
| 4 | 1E | 204/206 (99%) | 0.59 | 4 (1%) 65 73 | 12, 33, 52, 69 | 0 |
| 4 | 2E | 204/206 (99%) | 0.73 | 15 (7%) 14 17 | 29, 55, 68, 76 | 0 |
| 5 | 1F | 203/210 (96%) | 0.45 | 3 (1%) 73 81 | 13, 35, 60, 77 | 0 |
| 5 | 2F | 203/210 (96%) | 0.69 | 13 (6%) 19 23 | 31, 61, 75, 79 | 0 |
| 6 | 1G | 181/182 (99%) | 0.60 | 8 (4%) 34 41 | 35, 53, 66, 76 | 0 |
| 6 | 2G | 181/182 (99%) | 0.92 | 25 (13%) 2 3 | 57, 70, 78, 92 | 0 |
| 7 | 1H | 174/180 (96%) | 0.25 | 1 (0%) 89 92 | 31, 45, 57, 63 | 0 |
| 7 | 2H | 174/180 (96%) | 1.40 | 48 (27%) 0 0 | 63, 76, 84, 89 | 0 |
| 8 | 1I | 146/148 (98%) | 0.43 | 8 (5%) 25 30 | 38, 64, 75, 80 | 0 |
| 8 | 2I | 146/148 (98%) | 0.51 | 9 (6%) 20 25 | 53, 65, 74, 78 | 0 |
| 9 | 1N | 140/140 (100%) | 0.52 | 2 (1%) 75 82 | 18, 31, 51, 68 | 0 |
| 9 | 2N | 140/140 (100%) | 1.07 | 27 (19%) 1 1 | 43, 59, 70, 82 | 0 |
| 10 | 1O | 122/122 (100%) | 0.68 | 2 (1%) 72 79 | 20, 34, 51, 57 | 0 |
| 10 | 2O | 122/122 (100%) | 0.87 | 14 (11%) 4 5 | 43, 55, 65, 67 | 0 |
| 11 | 1P | 149/150 (99%) | 0.55 | 0 100 100 | 13, 39, 62, 68 | 0 |
| 11 | 2P | 149/150 (99%) | 0.99 | 26 (17%) 1 1 | 34, 61, 73, 80 | 0 |
| 12 | 1Q | 141/141 (100%) | 0.49 | 1 (0%) 87 91 | 20, 33, 49, 65 | 0 |
| 12 | 2Q | 141/141 (100%) | 1.49 | 39 (27%) 0 0 | 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%) | 0.52 | 0 100 100 | 16, 27, 43, 55 | 0 |
| 13 | 2R | 118/118 (100%) | 0.58 | 3 (2%) 57 66 | 36, 49, 58, 62 | 0 |
| 14 | 1S | 110/112 (98%) | 0.28 | 1 (0%) 84 89 | 29, 40, 52, 58 | 0 |
| 14 | 2S | 110/112 (98%) | 0.96 | 20 (18%) 1 1 | 52, 63, 75, 79 | 0 |
| 15 | 1T | 131/146 (89%) | 0.49 | 4 (3%) 49 58 | 26, 38, 61, 66 | 0 |
| 15 | 2T | 131/146 (89%) | 0.68 | 7 (5%) 26 31 | 45, 57, 72, 74 | 0 |
| 16 | 1U | 116/118 (98%) | 0.74 | 4 (3%) 45 53 | 14, 23, 36, 60 | 0 |
| 16 | 2U | 116/118 (98%) | 1.04 | 19 (16%) 1 1 | 38, 57, 70, 78 | 0 |
| 17 | 1V | 101/101 (100%) | 0.36 | 1 (0%) 82 87 | 13, 31, 48, 62 | 0 |
| 17 | 2V | 101/101 (100%) | 0.89 | 17 (16%) 1 1 | 43, 64, 72, 77 | 0 |
| 18 | 1W | 112/113 (99%) | 0.51 | 1 (0%) 84 89 | 16, 24, 43, 70 | 0 |
| 18 | 2W | 112/113 (99%) | 0.94 | 13 (11%) 4 5 | 37, 46, 60, 75 | 0 |
| 19 | 1X | 95/96 (98%) | 0.50 | 1 (1%) 80 86 | 17, 29, 48, 68 | 0 |
| 19 | 2X | 95/96 (98%) | 0.58 | 5 (5%) 26 31 | 41, 53, 65, 70 | 0 |
| 20 | 1Y | 107/110 (97%) | 0.54 | 2 (1%) 66 75 | 28, 43, 65, 70 | 0 |
| 20 | 2Y | 107/110 (97%) | 1.35 | 23 (21%) 0 0 | 56, 65, 77, 79 | 0 |
| 21 | 1Z | 154/206 (74%) | 0.47 | 5 (3%) 47 56 | 29, 56, 81, 89 | 0 |
| 21 | 2Z | 160/206 (77%) | 1.18 | 36 (22%) 0 0 | 55, 73, 87, 91 | 0 |
| 22 | 10 | 83/85 (97%) | 1.04 | 7 (8%) 11 13 | 20, 28, 53, 69 | 0 |
| 22 | 20 | 83/85 (97%) | 1.52 | 24 (28%) 0 0 | 39, 57, 71, 80 | 0 |
| 23 | 11 | 97/98 (98%) | 0.83 | 5 (5%) 27 33 | 18, 36, 62, 69 | 0 |
| 23 | 21 | 97/98 (98%) | 1.03 | 10 (10%) 6 7 | 30, 52, 69, 74 | 0 |
| 24 | 12 | 70/72 (97%) | 0.54 | 1 (1%) 75 82 | 26, 40, 54, 68 | 0 |
| 24 | 22 | 70/72 (97%) | 0.62 | 5 (7%) 16 19 | 50, 62, 71, 79 | 0 |
| 25 | 13 | 59/60 (98%) | 0.30 | 0 100 100 | 17, 28, 48, 62 | 0 |
| 25 | 23 | 59/60 (98%) | 1.61 | 17 (28%) 0 0 | 50, 61, 75, 82 | 0 |
| 26 | 14 | 69/71 (97%) | 0.61 | 8 (11%) 4 5 | 41, 68, 81, 85 | 0 |
| 26 | 24 | 69/71 (97%) | 0.81 | 12 (17%) 1 1 | 71, 77, 85, 87 | 0 |
| 27 | 15 | 59/60 (98%) | 0.55 | 2 (3%) 45 53 | 12, 24, 44, 55 | 0 |
| 27 | 25 | 59/60 (98%) | 0.63 | 5 (8%) 10 13 | 34, 47, 62, 67 | 0 |
| 28 | 16 | 53/54 (98%) | 0.45 | 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%) | 1.20 | 10 (18%) 1 1 | 42, 53, 63, 70 | 0 |
| 29 | 17 | 48/49 (97%) | 0.84 | 5 (10%) 6 7 | 14, 19, 50, 59 | 0 |
| 29 | 27 | 48/49 (97%) | 1.46 | 8 (16%) 1 1 | 29, 38, 57, 71 | 0 |
| 30 | 18 | 64/65 (98%) | 0.69 | 3 (4%) 31 37 | 18, 26, 35, 52 | 0 |
| 30 | 28 | 64/65 (98%) | 1.80 | 26 (40%) 0 0 | 39, 49, 56, 66 | 0 |
| 31 | 19 | 37/37 (100%) | 0.86 | 0 100 100 | 22, 32, 46, 47 | 0 |
| 31 | 29 | 37/37 (100%) | 1.39 | 11 (29%) 0 0 | 54, 66, 75, 77 | 0 |
| 32 | 1a | 1488/1521 (97%) | 0.10 | 9 (0%) 89 92 | 29, 57, 83, 98 | 0 |
| 32 | 2a | 1491/1521 (98%) | 0.24 | 52 (3%) 44 52 | 43, 69, 87, 100 | 0 |
| 33 | 1b | 231/256 (90%) | 0.62 | 23 (9%) 7 7 | 54, 70, 78, 84 | 0 |
| 33 | 2b | 231/256 (90%) | 1.61 | 75 (32%) 0 0 | 65, 78, 85, 92 | 0 |
| 34 | 1c | 206/239 (86%) | 0.74 | 18 (8%) 10 12 | 47, 63, 73, 78 | 0 |
| 34 | 2c | 206/239 (86%) | 1.29 | 56 (27%) 0 0 | 64, 75, 81, 88 | 0 |
| 35 | 1d | 208/209 (99%) | 0.90 | 28 (13%) 3 3 | 50, 60, 70, 76 | 0 |
| 35 | 2d | 208/209 (99%) | 1.03 | 36 (17%) 1 1 | 50, 64, 73, 82 | 0 |
| 36 | 1e | 148/162 (91%) | 0.72 | 18 (12%) 4 4 | 45, 56, 65, 71 | 0 |
| 36 | 2e | 148/162 (91%) | 1.48 | 47 (31%) 0 0 | 56, 70, 76, 82 | 0 |
| 37 | 1f | 100/101 (99%) | 0.43 | 2 (2%) 65 73 | 41, 55, 64, 73 | 0 |
| 37 | 2f | 100/101 (99%) | 0.27 | 2 (2%) 65 73 | 50, 61, 69, 76 | 0 |
| 38 | 1g | 155/156 (99%) | 0.74 | 22 (14%) 2 3 | 52, 63, 75, 83 | 0 |
| 38 | 2g | 155/156 (99%) | 0.79 | 28 (18%) 1 1 | 61, 70, 79, 82 | 0 |
| 39 | 1h | 137/138 (99%) | 0.94 | 22 (16%) 1 1 | 48, 58, 64, 74 | 0 |
| 39 | 2h | 137/138 (99%) | 1.44 | 36 (26%) 0 0 | 61, 69, 75, 79 | 0 |
| 40 | 1i | 127/128 (99%) | 1.07 | 29 (22%) 0 0 | 44, 66, 75, 80 | 0 |
| 40 | 2i | 127/128 (99%) | 2.23 | 66 (51%) 0 0 | 66, 75, 82, 85 | 0 |
| 41 | 1j | 97/105 (92%) | 0.73 | 15 (15%) 2 2 | 49, 70, 80, 90 | 0 |
| 41 | 2j | 96/105 (91%) | 2.02 | 38 (39%) 0 0 | 64, 76, 83, 88 | 0 |
| 42 | 1k | 114/129 (88%) | 0.61 | 5 (4%) 34 41 | 37, 57, 66, 75 | 0 |
| 42 | 2k | 114/129 (88%) | 0.85 | 13 (11%) 5 5 | 51, 65, 74, 76 | 0 |
| 43 | 1l | 121/132 (91%) | 0.55 | 7 (5%) 23 28 | 36, 45, 56, 62 | 0 |
| 43 | 2l | 121/132 (91%) | 1.20 | 25 (20%) 1 1 | 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%) | 0.94 | 14 (11%) 5 5 | 47, 62, 72, 85 | 0 |
| 44 | 2m | 122/126 (96%) | 1.84 | 36 (29%) 0 0 | 64, 73, 81, 90 | 0 |
| 45 | 1n | 60/61 (98%) | 0.93 | 5 (8%) 11 13 | 48, 57, 65, 69 | 0 |
| 45 | 2n | 60/61 (98%) | 3.70 | 49 (81%) 0 0 | 66, 76, 80, 81 | 0 |
| 46 | 1o | 88/89 (98%) | 0.95 | 15 (17%) 1 1 | 41, 54, 66, 70 | 0 |
| 46 | 2o | 88/89 (98%) | 1.32 | 22 (25%) 0 0 | 56, 66, 73, 78 | 0 |
| 47 | 1p | 82/88 (93%) | 1.61 | 30 (36%) 0 0 | 48, 59, 70, 79 | 0 |
| 47 | 2p | 82/88 (93%) | 1.11 | 12 (14%) 2 2 | 53, 62, 69, 75 | 0 |
| 48 | 1q | 99/105 (94%) | 0.93 | 11 (11%) 5 6 | 42, 57, 65, 71 | 0 |
| 48 | 2q | 99/105 (94%) | 1.71 | 44 (44%) 0 0 | 55, 66, 74, 76 | 0 |
| 49 | 1r | 68/88 (77%) | 0.67 | 4 (5%) 22 27 | 48, 57, 67, 73 | 0 |
| 49 | 2r | 68/88 (77%) | 0.70 | 8 (11%) 4 5 | 55, 65, 75, 83 | 0 |
| 50 | 1s | 83/93 (89%) | 0.45 | 4 (4%) 30 36 | 50, 61, 72, 78 | 0 |
| 50 | 2s | 83/93 (89%) | 1.85 | 37 (44%) 0 0 | 67, 77, 82, 86 | 0 |
| 51 | 1t | 96/106 (90%) | 1.07 | 19 (19%) 1 1 | 46, 60, 72, 74 | 0 |
| 51 | 2t | 96/106 (90%) | 1.19 | 19 (19%) 1 1 | 53, 64, 75, 77 | 0 |
| 52 | 1u | 23/27 (85%) | 2.22 | 13 (56%) 0 0 | 55, 59, 64, 65 | 0 |
| 52 | 2u | 23/27 (85%) | 3.35 | 15 (65%) 0 0 | 67, 74, 78, 80 | 0 |
| 53 | 1v | 13/27 (48%) | 1.87 | 4 (30%) 0 0 | 40, 50, 82, 92 | 0 |
| 53 | 2v | 13/27 (48%) | 2.52 | 6 (46%) 0 0 | 56, 72, 92, 94 | 0 |
| 54 | 1w | 67/76 (88%) | 0.90 | 15 (22%) 0 0 | 44, 81, 92, 95 | 0 |
| 54 | 1y | 67/76 (88%) | 1.09 | 12 (17%) 1 1 | 31, 89, 96, 96 | 0 |
| 54 | 2w | 67/76 (88%) | 2.00 | 28 (41%) 0 0 | 65, 89, 95, 101 | 0 |
| 54 | 2y | 67/76 (88%) | 1.28 | 14 (20%) 1 0 | 49, 92, 97, 99 | 0 |
| 55 | 1x | 72/77 (93%) | 0.15 | 0 100 100 | 30, 60, 74, 80 | 0 |
| 55 | 2x | 72/77 (93%) | 0.32 | 6 (8%) 11 13 | 50, 74, 82, 88 | 0 |
| All | All | 20878/21754 (95%) | 0.62 | 1793 (8%) 10 13 | 11, 57, 82, 101 | 0 |

All (1793) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 44 | 1m | 124 | PRO | 21.0 |
| 44 | 2m | 124 | PRO | 20.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 44 | 2m | 123 | ALA | 19.8 |
| 44 | 2m | 122 | LYS | 15.9 |
| 44 | 1m | 123 | ALA | 15.0 |
| 33 | 2b | 165 | VAL | 13.1 |
| 45 | 2n | 39 | LEU | 10.9 |
| 22 | 20 | 2 | ALA | 10.5 |
| 45 | 2n | 25 | VAL | 9.9 |
| 45 | 2n | 34 | TYR | 9.6 |
| 41 | 2j | 47 | PHE | 9.5 |
| 23 | 21 | 2 | SER | 9.0 |
| 52 | 2u | 14 | TRP | 9.0 |
| 22 | 20 | 7 | LEU | 8.7 |
| 21 | 2Z | 149 | SER | 8.5 |
| 44 | 2m | 102 | ARG | 8.1 |
| 34 | 2c | 198 | VAL | 8.1 |
| 54 | 2w | 56 | C | 8.0 |
| 44 | 2m | 121 | LYS | 7.8 |
| 40 | 2i | 115 | GLY | 7.7 |
| 33 | 2b | 187 | LEU | 7.7 |
| 41 | 2j | 65 | LEU | 7.5 |
| 54 | 2w | 71 | C | 7.4 |
| 38 | 1g | 79 | ARG | 7.2 |
| 38 | 1g | 80 | VAL | 7.1 |
| 40 | 2i | 66 | ARG | 7.0 |
| 40 | 2i | 125 | TYR | 7.0 |
| 44 | 2m | 6 | GLY | 7.0 |
| 46 | 2o | 87 | ILE | 7.0 |
| 21 | 2Z | 170 | THR | 6.8 |
| 45 | 2n | 42 | ILE | 6.8 |
| 54 | 2y | 36 | C | 6.7 |
| 22 | 10 | 7 | LEU | 6.6 |
| 22 | 20 | 4 | LYS | 6.5 |
| 33 | 2b | 133 | LYS | 6.5 |
| 7 | 2H | 113 | VAL | 6.5 |
| 29 | 17 | 48 | LYS | 6.5 |
| 29 | 27 | 47 | ARG | 6.4 |
| 3 | 1D | 276 | LYS | 6.4 |
| 50 | 2s | 84 | GLY | 6.4 |
| 52 | 2u | 17 | THR | 6.4 |
| 53 | 2v | 24 | C | 6.3 |
| 50 | 2s | 83 | HIS | 6.3 |
| 39 | 2h | 83 | ILE | 6.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 44 | 2m | 120 | LYS | 6.2 |
| 54 | 2w | 1 | G | 6.2 |
| 53 | 2v | 12 | A | 6.2 |
| 33 | 1b | 133 | LYS | 6.2 |
| 40 | 2i | 9 | ARG | 6.2 |
| 34 | 2c | 4 | LYS | 6.1 |
| 39 | 2h | 2 | LEU | 6.1 |
| 35 | 1d | 5 | ILE | 6.1 |
| 41 | 2j | 50 | ILE | 6.1 |
| 54 | 2w | 70 | C | 6.0 |
| 7 | 2H | 105 | LEU | 6.0 |
| 17 | 2V | 73 | SER | 6.0 |
| 3 | 2D | 2 | ALA | 6.0 |
| 52 | 2u | 11 | GLY | 6.0 |
| 40 | 2i | 7 | THR | 6.0 |
| 54 | 1w | 70 | C | 5.9 |
| 52 | 2u | 13 | ILE | 5.9 |
| 41 | 2j | 59 | SER | 5.9 |
| 52 | 2u | 22 | ARG | 5.9 |
| 29 | 27 | 1 | MET | 5.8 |
| 34 | 2c | 159 | GLY | 5.8 |
| 54 | 2w | 31 | C | 5.8 |
| 45 | 2n | 24 | CYS | 5.8 |
| 1 | 1A | 2141 | G | 5.8 |
| 22 | 10 | 5 | LYS | 5.8 |
| 40 | 2i | 36 | TYR | 5.8 |
| 34 | 2c | 157 | ILE | 5.7 |
| 45 | 2n | 36 | PHE | 5.7 |
| 55 | 2x | 70 | G | 5.7 |
| 53 | 1v | 13 | A | 5.7 |
| 38 | 1g | 156 | TRP | 5.7 |
| 45 | 2n | 35 | ARG | 5.7 |
| 36 | 2e | 12 | LEU | 5.6 |
| 39 | 2h | 99 | GLU | 5.6 |
| 12 | 2Q | 104 | PHE | 5.6 |
| 54 | 2w | 76 | A | 5.6 |
| 38 | 1g | 84 | ASN | 5.6 |
| 36 | 2e | 13 | ILE | 5.6 |
| 41 | 2j | 40 | LEU | 5.5 |
| 45 | 2n | 23 | ARG | 5.5 |
| 45 | 2n | 11 | LYS | 5.5 |
| 11 | 2P | 45 | LEU | 5.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | 2A | 2802 | G | 5.5 |
| 39 | 2h | 112 | LEU | 5.5 |
| 52 | 1u | 2 | GLY | 5.4 |
| 23 | 1l | 98 | LEU | 5.4 |
| 44 | 2m | 90 | LEU | 5.4 |
| 41 | 2j | 55 | LYS | 5.4 |
| 44 | 1m | 122 | LYS | 5.4 |
| 54 | 1y | 36 | C | 5.3 |
| 50 | 2s | 71 | LEU | 5.3 |
| 44 | 2m | 119 | GLY | 5.3 |
| 46 | 2o | 60 | VAL | 5.3 |
| 34 | 2c | 200 | ALA | 5.3 |
| 39 | 2h | 111 | ILE | 5.3 |
| 7 | 2H | 103 | LEU | 5.3 |
| 40 | 1i | 106 | ALA | 5.2 |
| 41 | 2j | 85 | LEU | 5.2 |
| 45 | 2n | 2 | ALA | 5.2 |
| 44 | 2m | 101 | GLN | 5.2 |
| 12 | 2Q | 37 | LEU | 5.2 |
| 34 | 2c | 193 | TYR | 5.2 |
| 22 | 10 | 6 | GLY | 5.1 |
| 41 | 2j | 48 | THR | 5.1 |
| 41 | 2j | 56 | HIS | 5.1 |
| 33 | 2b | 70 | PHE | 5.1 |
| 50 | 2s | 80 | TYR | 5.1 |
| 54 | 2w | 73 | A | 5.1 |
| 38 | 2g | 82 | GLY | 5.1 |
| 34 | 2c | 124 | ILE | 5.0 |
| 54 | 2w | 3 | G | 5.0 |
| 1 | 2A | 2146 | C | 5.0 |
| 33 | 2b | 197 | VAL | 5.0 |
| 43 | 2l | 8 | ASN | 5.0 |
| 1 | 2A | 2112 | G | 5.0 |
| 34 | 2c | 197 | GLY | 5.0 |
| 20 | 2Y | 106 | LEU | 5.0 |
| 45 | 2n | 53 | LEU | 5.0 |
| 45 | 2n | 29 | ARG | 5.0 |
| 33 | 2b | 185 | ILE | 4.9 |
| 26 | 24 | 49 | PHE | 4.9 |
| 21 | 2Z | 144 | LEU | 4.9 |
| 26 | 14 | 54 | GLY | 4.9 |
| 33 | 2b | 139 | LYS | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 42 | 2k | 126 | ARG | 4.9 |
| 22 | 10 | 3 | HIS | 4.9 |
| 33 | 2b | 188 | ALA | 4.9 |
| 27 | 15 | 60 | VAL | 4.9 |
| 29 | 27 | 48 | LYS | 4.9 |
| 44 | 2m | 87 | TYR | 4.8 |
| 17 | 2V | 72 | VAL | 4.8 |
| 38 | 2g | 16 | LEU | 4.8 |
| 34 | 2c | 149 | ALA | 4.8 |
| 24 | 22 | 1 | MET | 4.8 |
| 45 | 2n | 37 | PHE | 4.8 |
| 52 | 2u | 18 | TYR | 4.8 |
| 26 | 24 | 56 | VAL | 4.8 |
| 51 | 2t | 24 | LEU | 4.8 |
| 22 | 20 | 3 | HIS | 4.8 |
| 40 | 2i | 77 | ILE | 4.8 |
| 52 | 2u | 15 | ARG | 4.7 |
| 36 | 2e | 110 | LEU | 4.7 |
| 40 | 2i | 14 | VAL | 4.7 |
| 46 | 1o | 57 | LEU | 4.7 |
| 36 | 2e | 133 | TYR | 4.7 |
| 39 | 1h | 92 | ARG | 4.7 |
| 43 | 2l | 15 | ARG | 4.7 |
| 33 | 2b | 48 | MET | 4.7 |
| 1 | 2A | 2111 | C | 4.7 |
| 33 | 2b | 129 | GLU | 4.7 |
| 41 | 2j | 51 | ARG | 4.7 |
| 35 | 2d | 164 | ALA | 4.7 |
| 17 | 2V | 71 | LEU | 4.7 |
| 1 | 2A | 888 | C | 4.7 |
| 40 | 2i | 114 | TYR | 4.7 |
| 42 | 2k | 25 | TYR | 4.7 |
| 7 | 2H | 107 | VAL | 4.7 |
| 21 | 2Z | 140 | ASP | 4.7 |
| 34 | 2c | 188 | LEU | 4.6 |
| 40 | 2i | 65 | VAL | 4.6 |
| 53 | 2v | 14 | A | 4.6 |
| 26 | 24 | 50 | VAL | 4.6 |
| 33 | 2b | 93 | VAL | 4.6 |
| 48 | 2q | 37 | LYS | 4.6 |
| 21 | 2Z | 150 | LEU | 4.6 |
| 32 | 2a | 1257 | U | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 36 | 2e | 90 | VAL | 4.6 |
| 21 | 1Z | 168 | GLU | 4.6 |
| 32 | 2a | 1532 | U | 4.6 |
| 35 | 1d | 8 | VAL | 4.6 |
| 38 | 2g | 80 | VAL | 4.6 |
| 33 | 2b | 97 | TRP | 4.6 |
| 1 | 2A | 1026 | U | 4.6 |
| 7 | 2H | 55 | PRO | 4.5 |
| 3 | 1D | 2 | ALA | 4.5 |
| 36 | 2e | 86 | ALA | 4.5 |
| 45 | 2n | 41 | ARG | 4.5 |
| 45 | 2n | 6 | LEU | 4.5 |
| 54 | 2y | 1 | G | 4.5 |
| 1 | 2A | 2896 | C | 4.5 |
| 54 | 1w | 71 | C | 4.5 |
| 33 | 2b | 120 | ALA | 4.5 |
| 41 | 2j | 58 | ASP | 4.5 |
| 36 | 2e | 31 | LEU | 4.5 |
| 50 | 2s | 69 | HIS | 4.4 |
| 22 | 20 | 8 | GLY | 4.4 |
| 6 | 2G | 146 | TYR | 4.4 |
| 30 | 28 | 29 | LYS | 4.4 |
| 32 | 2a | 1030(A) | G | 4.4 |
| 43 | 2l | 32 | PHE | 4.4 |
| 33 | 2b | 95 | GLN | 4.4 |
| 36 | 2e | 82 | VAL | 4.4 |
| 39 | 2h | 129 | VAL | 4.4 |
| 34 | 2c | 6 | HIS | 4.4 |
| 12 | 2Q | 66 | ILE | 4.4 |
| 7 | 2H | 169 | VAL | 4.3 |
| 17 | 2V | 75 | PHE | 4.3 |
| 36 | 2e | 89 | ILE | 4.3 |
| 52 | 1u | 14 | TRP | 4.3 |
| 29 | 17 | 46 | VAL | 4.3 |
| 45 | 2n | 55 | GLY | 4.3 |
| 8 | 2l | 1 | MET | 4.3 |
| 36 | 2e | 123 | LEU | 4.3 |
| 6 | 2G | 49 | ASP | 4.3 |
| 45 | 2n | 44 | LEU | 4.3 |
| 54 | 2w | 13 | C | 4.3 |
| 45 | 2n | 38 | GLY | 4.3 |
| 1 | 2A | 2117 | A | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 32 | 2a | 80 | G | 4.2 |
| 29 | 27 | 46 | VAL | 4.2 |
| 52 | 2u | 16 | GLY | 4.2 |
| 16 | 2U | 17 | ILE | 4.2 |
| 12 | 2Q | 103 | MET | 4.2 |
| 33 | 2b | 81 | VAL | 4.2 |
| 45 | 2n | 26 | ARG | 4.2 |
| 19 | 2X | 69 | TYR | 4.2 |
| 53 | 2v | 13 | A | 4.2 |
| 39 | 2h | 128 | GLY | 4.2 |
| 50 | 2s | 59 | PRO | 4.2 |
| 32 | 2a | 1202 | G | 4.2 |
| 33 | 2b | 164 | VAL | 4.2 |
| 7 | 2H | 56 | SER | 4.2 |
| 54 | 2w | 4 | U | 4.2 |
| 33 | 2b | 114 | ARG | 4.2 |
| 41 | 2j | 46 | ARG | 4.2 |
| 46 | 2o | 64 | ARG | 4.2 |
| 41 | 2j | 63 | PHE | 4.2 |
| 39 | 1h | 3 | THR | 4.2 |
| 35 | 1d | 70 | ILE | 4.2 |
| 47 | 2p | 19 | ILE | 4.2 |
| 47 | 1p | 19 | ILE | 4.1 |
| 54 | 2w | 72 | C | 4.1 |
| 21 | 2Z | 148 | ASP | 4.1 |
| 50 | 2s | 40 | ILE | 4.1 |
| 8 | 2I | 12 | LEU | 4.1 |
| 25 | 23 | 26 | LEU | 4.1 |
| 6 | 1G | 139 | LEU | 4.1 |
| 45 | 2n | 7 | ILE | 4.1 |
| 32 | 1a | 1531 | A | 4.1 |
| 45 | 2n | 50 | LYS | 4.1 |
| 21 | 2Z | 139 | VAL | 4.1 |
| 41 | 2j | 66 | ARG | 4.1 |
| 41 | 2j | 11 | PHE | 4.1 |
| 33 | 2b | 118 | LEU | 4.1 |
| 44 | 1m | 96 | LEU | 4.1 |
| 10 | 2O | 1 | MET | 4.1 |
| 36 | 2e | 84 | PHE | 4.1 |
| 7 | 2H | 148 | ILE | 4.1 |
| 51 | 2t | 80 | ARG | 4.1 |
| 43 | 2l | 18 | VAL | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | 2n | 56 | VAL | 4.1 |
| 16 | 1U | 117 | GLN | 4.1 |
| 30 | 28 | 41 | ILE | 4.0 |
| 48 | 1q | 35 | VAL | 4.0 |
| 7 | 2H | 159 | GLU | 4.0 |
| 34 | 2c | 152 | ILE | 4.0 |
| 38 | 1g | 154 | TYR | 4.0 |
| 33 | 2b | 135 | GLN | 4.0 |
| 33 | 2b | 215 | LEU | 4.0 |
| 28 | 26 | 54 | ILE | 4.0 |
| 54 | 2y | 2 | G | 4.0 |
| 6 | 2G | 34 | LEU | 4.0 |
| 33 | 2b | 221 | LEU | 4.0 |
| 48 | 2q | 9 | VAL | 4.0 |
| 20 | 2Y | 105 | ALA | 4.0 |
| 25 | 23 | 60 | GLU | 4.0 |
| 35 | 1d | 157 | LEU | 4.0 |
| 36 | 2e | 120 | THR | 4.0 |
| 23 | 1l | 2 | SER | 4.0 |
| 48 | 2q | 90 | ILE | 4.0 |
| 38 | 1g | 83 | ALA | 4.0 |
| 34 | 2c | 2 | GLY | 4.0 |
| 52 | 2u | 6 | ARG | 4.0 |
| 35 | 1d | 104 | VAL | 4.0 |
| 40 | 2i | 128 | ARG | 3.9 |
| 1 | 2A | 2113 | U | 3.9 |
| 43 | 1l | 7 | ILE | 3.9 |
| 1 | 2A | 2155 | G | 3.9 |
| 40 | 1i | 113 | LYS | 3.9 |
| 40 | 2i | 33 | PHE | 3.9 |
| 38 | 2g | 4 | ARG | 3.9 |
| 45 | 2n | 31 | ARG | 3.9 |
| 20 | 2Y | 5 | MET | 3.9 |
| 39 | 2h | 3 | THR | 3.9 |
| 46 | 2o | 31 | LEU | 3.9 |
| 47 | 1p | 6 | LEU | 3.9 |
| 6 | 2G | 133 | LEU | 3.9 |
| 40 | 2i | 4 | TYR | 3.9 |
| 40 | 2i | 71 | SER | 3.9 |
| 9 | 2N | 8 | GLN | 3.9 |
| 21 | 2Z | 137 | ILE | 3.9 |
| 36 | 2e | 131 | ILE | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 48 | 1q | 36 | ILE | 3.9 |
| 54 | 1y | 33 | U | 3.9 |
| 7 | 2H | 96 | ALA | 3.9 |
| 43 | 2l | 55 | VAL | 3.9 |
| 45 | 2n | 22 | THR | 3.9 |
| 39 | 1h | 133 | LEU | 3.9 |
| 31 | 29 | 37 | GLY | 3.9 |
| 1 | 1A | 2132 | U | 3.9 |
| 32 | 2a | 1030(B) | C | 3.9 |
| 1 | 2A | 2154 | G | 3.9 |
| 6 | 2G | 136 | ARG | 3.9 |
| 51 | 2t | 62 | LEU | 3.9 |
| 40 | 2i | 64 | THR | 3.9 |
| 26 | 24 | 67 | TYR | 3.9 |
| 54 | 2w | 75 | C | 3.9 |
| 34 | 2c | 160 | ALA | 3.8 |
| 44 | 2m | 104 | ARG | 3.8 |
| 46 | 2o | 68 | ARG | 3.8 |
| 39 | 2h | 9 | MET | 3.8 |
| 40 | 2i | 72 | GLY | 3.8 |
| 38 | 1g | 85 | TYR | 3.8 |
| 3 | 2D | 276 | LYS | 3.8 |
| 30 | 28 | 16 | ILE | 3.8 |
| 34 | 1c | 14 | ILE | 3.8 |
| 41 | 1j | 98 | ILE | 3.8 |
| 44 | 2m | 5 | ALA | 3.8 |
| 44 | 2m | 7 | VAL | 3.8 |
| 20 | 1Y | 1 | MET | 3.8 |
| 33 | 2b | 163 | PHE | 3.8 |
| 43 | 2l | 7 | ILE | 3.8 |
| 33 | 2b | 149 | LEU | 3.8 |
| 40 | 2i | 17 | VAL | 3.8 |
| 40 | 2i | 79 | LEU | 3.8 |
| 1 | 2A | 2147 | G | 3.8 |
| 10 | 2O | 65 | THR | 3.8 |
| 50 | 2s | 79 | THR | 3.8 |
| 20 | 2Y | 1 | MET | 3.8 |
| 54 | 2w | 74 | C | 3.8 |
| 1 | 1A | 1026 | U | 3.8 |
| 34 | 2c | 186 | PHE | 3.8 |
| 40 | 1i | 77 | ILE | 3.8 |
| 40 | 2i | 28 | VAL | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | 2A | 2118 | U | 3.8 |
| 33 | 2b | 201 | ILE | 3.8 |
| 34 | 2c | 154 | SER | 3.8 |
| 1 | 1A | 2142 | C | 3.8 |
| 20 | 2Y | 24 | VAL | 3.8 |
| 38 | 1g | 78 | ARG | 3.8 |
| 22 | 10 | 4 | LYS | 3.8 |
| 29 | 17 | 47 | ARG | 3.7 |
| 38 | 1g | 34 | GLY | 3.8 |
| 22 | 10 | 2 | ALA | 3.7 |
| 7 | 2H | 35 | VAL | 3.7 |
| 52 | 2u | 5 | ASP | 3.7 |
| 47 | 2p | 1 | MET | 3.7 |
| 45 | 2n | 51 | GLY | 3.7 |
| 35 | 1d | 4 | TYR | 3.7 |
| 44 | 2m | 23 | TYR | 3.7 |
| 41 | 2j | 87 | THR | 3.7 |
| 45 | 2n | 27 | CYS | 3.7 |
| 12 | 2Q | 1 | MET | 3.7 |
| 25 | 23 | 17 | LYS | 3.7 |
| 35 | 1d | 3 | ARG | 3.7 |
| 45 | 2n | 45 | ARG | 3.7 |
| 46 | 2o | 61 | GLY | 3.7 |
| 50 | 2s | 30 | LEU | 3.7 |
| 34 | 2c | 184 | TYR | 3.7 |
| 55 | 2x | 72 | A | 3.7 |
| 41 | 2j | 49 | VAL | 3.7 |
| 16 | 2U | 43 | GLY | 3.7 |
| 54 | 2w | 2 | G | 3.7 |
| 39 | 2h | 13 | ILE | 3.7 |
| 44 | 2m | 65 | LYS | 3.7 |
| 14 | 2S | 3 | ARG | 3.7 |
| 45 | 2n | 12 | ARG | 3.7 |
| 50 | 2s | 78 | ARG | 3.7 |
| 40 | 2i | 10 | ARG | 3.7 |
| 52 | 1u | 21 | TYR | 3.7 |
| 34 | 2c | 199 | LYS | 3.7 |
| 36 | 2e | 20 | GLN | 3.7 |
| 48 | 2q | 100 | LYS | 3.7 |
| 40 | 1i | 19 | LEU | 3.7 |
| 34 | 2c | 201 | TYR | 3.7 |
| 43 | 2l | 39 | VAL | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 40 | 1i | 70 | LYS | 3.7 |
| 36 | 2e | 125 | SER | 3.7 |
| 11 | 2P | 51 | PHE | 3.6 |
| 41 | 2j | 54 | PHE | 3.6 |
| 41 | 2j | 62 | HIS | 3.6 |
| 40 | 2i | 52 | ALA | 3.6 |
| 32 | 1a | 1257 | U | 3.6 |
| 39 | 2h | 93 | VAL | 3.6 |
| 7 | 2H | 6 | ARG | 3.6 |
| 6 | 2G | 139 | LEU | 3.6 |
| 5 | 2F | 49 | ALA | 3.6 |
| 54 | 2w | 32 | C | 3.6 |
| 7 | 2H | 165 | ALA | 3.6 |
| 44 | 2m | 76 | ALA | 3.6 |
| 50 | 2s | 82 | GLY | 3.6 |
| 34 | 2c | 182 | ILE | 3.6 |
| 45 | 2n | 58 | LYS | 3.6 |
| 46 | 2o | 32 | LEU | 3.6 |
| 22 | 20 | 6 | GLY | 3.6 |
| 34 | 2c | 155 | GLY | 3.6 |
| 38 | 1g | 81 | GLY | 3.6 |
| 35 | 1d | 122 | ARG | 3.6 |
| 35 | 2d | 49 | ARG | 3.6 |
| 12 | 2Q | 38 | GLU | 3.6 |
| 34 | 2c | 10 | PHE | 3.6 |
| 26 | 14 | 45 | GLY | 3.6 |
| 12 | 2Q | 6 | ARG | 3.6 |
| 41 | 2j | 44 | VAL | 3.6 |
| 48 | 2q | 36 | ILE | 3.6 |
| 46 | 2o | 72 | ARG | 3.6 |
| 21 | 2Z | 171 | ILE | 3.6 |
| 33 | 2b | 210 | SER | 3.6 |
| 1 | 2A | 2174 | C | 3.6 |
| 48 | 2q | 88 | TYR | 3.6 |
| 35 | 1d | 21 | LEU | 3.6 |
| 40 | 2i | 127 | LYS | 3.6 |
| 38 | 2g | 27 | ILE | 3.6 |
| 50 | 2s | 70 | LYS | 3.6 |
| 1 | 2A | 2145 | C | 3.6 |
| 53 | 1v | 24 | C | 3.6 |
| 1 | 2A | 2132 | U | 3.5 |
| 33 | 2b | 34 | ALA | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | 2H | 114 | VAL | 3.5 |
| 36 | 1e | 82 | VAL | 3.5 |
| 11 | 2P | 30 | THR | 3.5 |
| 32 | 2a | 965 | A | 3.5 |
| 54 | 2w | 57 | G | 3.5 |
| 26 | 14 | 59 | PHE | 3.5 |
| 9 | 2N | 44 | PRO | 3.5 |
| 23 | 21 | 26 | ARG | 3.5 |
| 33 | 2b | 222 | ILE | 3.5 |
| 45 | 2n | 13 | THR | 3.5 |
| 52 | 2u | 10 | ARG | 3.5 |
| 9 | 2N | 116 | LEU | 3.5 |
| 22 | 20 | 5 | LYS | 3.5 |
| 14 | 2S | 20 | ARG | 3.5 |
| 33 | 2b | 137 | ARG | 3.5 |
| 50 | 2s | 38 | SER | 3.5 |
| 54 | 2y | 73 | A | 3.5 |
| 23 | 11 | 70 | VAL | 3.5 |
| 35 | 1d | 2 | GLY | 3.5 |
| 51 | 2t | 41 | ILE | 3.5 |
| 1 | 2A | 2897 | U | 3.5 |
| 16 | 2U | 20 | LEU | 3.5 |
| 40 | 2i | 62 | TYR | 3.5 |
| 39 | 2h | 35 | ILE | 3.5 |
| 50 | 1s | 71 | LEU | 3.5 |
| 33 | 2b | 152 | PHE | 3.5 |
| 33 | 2b | 92 | TYR | 3.5 |
| 21 | 2Z | 169 | GLU | 3.5 |
| 41 | 2j | 98 | ILE | 3.5 |
| 52 | 1u | 17 | THR | 3.5 |
| 23 | 11 | 97 | LEU | 3.5 |
| 12 | 2Q | 65 | PHE | 3.5 |
| 21 | 2Z | 121 | HIS | 3.5 |
| 32 | 2a | 974 | A | 3.5 |
| 33 | 1b | 130 | ARG | 3.5 |
| 40 | 1i | 121 | ARG | 3.5 |
| 42 | 1k | 126 | ARG | 3.5 |
| 54 | 1w | 56 | C | 3.5 |
| 10 | 2O | 7 | TYR | 3.5 |
| 25 | 23 | 51 | ALA | 3.5 |
| 40 | 1i | 8 | GLY | 3.5 |
| 40 | 1i | 30 | GLY | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | 2n | 30 | ALA | 3.5 |
| 6 | 2G | 29 | TRP | 3.4 |
| 47 | 1p | 28 | ARG | 3.5 |
| 33 | 2b | 140 | HIS | 3.4 |
| 8 | 1l | 1 | MET | 3.4 |
| 32 | 2a | 1116 | C | 3.4 |
| 32 | 2a | 1286 | A | 3.4 |
| 52 | 2u | 21 | TYR | 3.4 |
| 55 | 2x | 71 | C | 3.4 |
| 30 | 28 | 35 | GLN | 3.4 |
| 13 | 2R | 68 | ARG | 3.4 |
| 28 | 26 | 10 | LEU | 3.4 |
| 28 | 26 | 11 | LEU | 3.4 |
| 35 | 2d | 78 | LEU | 3.4 |
| 41 | 2j | 41 | PRO | 3.4 |
| 6 | 2G | 159 | VAL | 3.4 |
| 33 | 1b | 214 | ILE | 3.4 |
| 39 | 1h | 134 | ILE | 3.4 |
| 7 | 2H | 2 | SER | 3.4 |
| 45 | 2n | 17 | LYS | 3.4 |
| 51 | 2t | 59 | ALA | 3.4 |
| 35 | 2d | 160 | GLN | 3.4 |
| 33 | 1b | 131 | PRO | 3.4 |
| 44 | 2m | 97 | PRO | 3.4 |
| 33 | 2b | 71 | VAL | 3.4 |
| 44 | 2m | 103 | THR | 3.4 |
| 46 | 1o | 66 | LEU | 3.4 |
| 36 | 1e | 89 | ILE | 3.4 |
| 34 | 2c | 13 | GLY | 3.4 |
| 38 | 2g | 81 | GLY | 3.4 |
| 45 | 2n | 15 | LYS | 3.4 |
| 21 | 2Z | 96 | VAL | 3.4 |
| 21 | 2Z | 151 | HIS | 3.4 |
| 45 | 2n | 49 | HIS | 3.4 |
| 32 | 2a | 873 | A | 3.4 |
| 8 | 2l | 19 | VAL | 3.4 |
| 21 | 2Z | 126 | VAL | 3.4 |
| 41 | 1j | 72 | VAL | 3.4 |
| 34 | 2c | 202 | ILE | 3.4 |
| 5 | 2F | 62 | ARG | 3.4 |
| 36 | 2e | 81 | GLU | 3.4 |
| 51 | 2t | 73 | HIS | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | 2n | 61 | TRP | 3.4 |
| 1 | 2A | 2119 | A | 3.4 |
| 51 | 1t | 38 | LYS | 3.4 |
| 41 | 2j | 53 | PRO | 3.4 |
| 21 | 2Z | 145 | GLU | 3.4 |
| 35 | 2d | 70 | ILE | 3.4 |
| 41 | 2j | 38 | ILE | 3.4 |
| 51 | 1t | 80 | ARG | 3.4 |
| 16 | 2U | 39 | LEU | 3.4 |
| 35 | 1d | 120 | LEU | 3.4 |
| 7 | 2H | 49 | VAL | 3.4 |
| 7 | 2H | 97 | ARG | 3.4 |
| 33 | 2b | 101 | MET | 3.3 |
| 11 | 2P | 23 | PRO | 3.3 |
| 18 | 2W | 92 | ARG | 3.3 |
| 47 | 2p | 39 | TYR | 3.3 |
| 8 | 1I | 3 | VAL | 3.3 |
| 50 | 2s | 41 | VAL | 3.3 |
| 51 | 2t | 63 | ILE | 3.3 |
| 33 | 2b | 94 | ASN | 3.3 |
| 51 | 1t | 9 | ASN | 3.3 |
| 54 | 2w | 19 | G | 3.3 |
| 7 | 2H | 41 | MET | 3.3 |
| 50 | 2s | 81 | ARG | 3.3 |
| 33 | 2b | 200 | ILE | 3.3 |
| 39 | 2h | 6 | ILE | 3.3 |
| 32 | 2a | 1285 | A | 3.3 |
| 40 | 2i | 82 | ALA | 3.3 |
| 4 | 2E | 115 | GLY | 3.3 |
| 9 | 2N | 83 | LYS | 3.3 |
| 43 | 2l | 13 | LYS | 3.3 |
| 9 | 2N | 9 | VAL | 3.3 |
| 36 | 2e | 100 | VAL | 3.3 |
| 7 | 2H | 123 | PHE | 3.3 |
| 51 | 1t | 74 | LYS | 3.3 |
| 21 | 2Z | 160 | GLY | 3.3 |
| 32 | 2a | 1224 | G | 3.3 |
| 40 | 2i | 76 | ALA | 3.3 |
| 44 | 2m | 66 | LEU | 3.3 |
| 33 | 2b | 147 | LYS | 3.3 |
| 51 | 1t | 83 | ARG | 3.3 |
| 12 | 2Q | 47 | ILE | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | 2b | 214 | ILE | 3.3 |
| 54 | 2w | 39 | G | 3.3 |
| 40 | 1i | 65 | VAL | 3.3 |
| 40 | 2i | 63 | ILE | 3.3 |
| 18 | 2W | 86 | LEU | 3.3 |
| 32 | 2a | 1033 | G | 3.3 |
| 47 | 1p | 1 | MET | 3.3 |
| 40 | 1i | 128 | ARG | 3.3 |
| 25 | 23 | 25 | ALA | 3.2 |
| 33 | 1b | 187 | LEU | 3.2 |
| 33 | 2b | 232 | PRO | 3.2 |
| 54 | 1y | 21 | A | 3.2 |
| 45 | 2n | 47 | LEU | 3.2 |
| 12 | 2Q | 33 | GLY | 3.2 |
| 14 | 2S | 33 | LYS | 3.2 |
| 31 | 29 | 15 | LYS | 3.2 |
| 35 | 2d | 93 | PHE | 3.2 |
| 6 | 1G | 73 | ALA | 3.2 |
| 41 | 2j | 18 | ALA | 3.2 |
| 8 | 1I | 35 | LEU | 3.2 |
| 12 | 2Q | 39 | PRO | 3.2 |
| 14 | 2S | 32 | LEU | 3.2 |
| 40 | 2i | 123 | PRO | 3.2 |
| 49 | 1r | 31 | LEU | 3.2 |
| 40 | 1i | 14 | VAL | 3.2 |
| 44 | 2m | 98 | VAL | 3.2 |
| 16 | 2U | 47 | TYR | 3.2 |
| 45 | 2n | 21 | TYR | 3.2 |
| 54 | 1y | 24 | G | 3.2 |
| 33 | 2b | 77 | ALA | 3.2 |
| 48 | 2q | 53 | LEU | 3.2 |
| 51 | 2t | 72 | LEU | 3.2 |
| 25 | 23 | 54 | VAL | 3.2 |
| 50 | 2s | 52 | TYR | 3.2 |
| 33 | 2b | 123 | ALA | 3.2 |
| 1 | 2A | 2140 | C | 3.2 |
| 38 | 1g | 99 | LEU | 3.2 |
| 39 | 1h | 2 | LEU | 3.2 |
| 44 | 2m | 92 | HIS | 3.2 |
| 39 | 2h | 97 | VAL | 3.2 |
| 41 | 2j | 60 | ARG | 3.2 |
| 15 | 2T | 110 | ILE | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | 1c | 193 | TYR | 3.2 |
| 45 | 1n | 2 | ALA | 3.2 |
| 15 | 2T | 99 | LEU | 3.2 |
| 6 | 2G | 28 | VAL | 3.2 |
| 9 | 2N | 122 | VAL | 3.2 |
| 33 | 2b | 28 | PHE | 3.2 |
| 9 | 2N | 75 | TYR | 3.2 |
| 31 | 29 | 19 | ARG | 3.2 |
| 17 | 2V | 79 | VAL | 3.2 |
| 25 | 23 | 47 | VAL | 3.2 |
| 47 | 1p | 2 | VAL | 3.2 |
| 48 | 2q | 23 | VAL | 3.2 |
| 32 | 2a | 1032 | G | 3.2 |
| 38 | 2g | 154 | TYR | 3.2 |
| 40 | 2i | 106 | ALA | 3.2 |
| 39 | 2h | 131 | GLY | 3.2 |
| 40 | 2i | 30 | GLY | 3.2 |
| 44 | 1m | 106 | ASN | 3.2 |
| 40 | 1i | 120 | ARG | 3.2 |
| 41 | 2j | 9 | ARG | 3.2 |
| 7 | 2H | 133 | VAL | 3.1 |
| 48 | 2q | 21 | VAL | 3.1 |
| 32 | 2a | 1223 | C | 3.1 |
| 48 | 2q | 32 | TYR | 3.1 |
| 50 | 2s | 56 | GLN | 3.1 |
| 36 | 2e | 10 | MET | 3.1 |
| 3 | 2D | 205 | VAL | 3.1 |
| 12 | 2Q | 22 | LYS | 3.1 |
| 40 | 1i | 112 | LYS | 3.1 |
| 53 | 1v | 12 | A | 3.1 |
| 5 | 2F | 181 | LEU | 3.1 |
| 32 | 1a | 1027 | C | 3.1 |
| 36 | 2e | 107 | ARG | 3.1 |
| 36 | 2e | 126 | ARG | 3.1 |
| 40 | 2i | 67 | GLY | 3.1 |
| 33 | 2b | 31 | TYR | 3.1 |
| 41 | 1j | 65 | LEU | 3.1 |
| 45 | 2n | 46 | GLU | 3.1 |
| 14 | 2S | 5 | THR | 3.1 |
| 48 | 2q | 5 | VAL | 3.1 |
| 29 | 27 | 31 | LEU | 3.1 |
| 34 | 2c | 196 | LEU | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 39 | 2h | 132 | GLU | 3.1 |
| 45 | 2n | 10 | ALA | 3.1 |
| 43 | 2l | 5 | PRO | 3.1 |
| 54 | 1y | 38 | A | 3.1 |
| 44 | 2m | 109 | THR | 3.1 |
| 1 | 1A | 1176 | G | 3.1 |
| 9 | 2N | 84 | LYS | 3.1 |
| 34 | 1c | 182 | ILE | 3.1 |
| 35 | 2d | 162 | LEU | 3.1 |
| 38 | 2g | 7 | ALA | 3.1 |
| 17 | 2V | 81 | TYR | 3.1 |
| 35 | 2d | 122 | ARG | 3.1 |
| 44 | 1m | 102 | ARG | 3.1 |
| 12 | 2Q | 35 | VAL | 3.1 |
| 48 | 2q | 11 | VAL | 3.1 |
| 9 | 2N | 91 | LEU | 3.1 |
| 30 | 28 | 61 | LEU | 3.1 |
| 34 | 2c | 148 | GLY | 3.1 |
| 8 | 2l | 92 | VAL | 3.1 |
| 33 | 1b | 81 | VAL | 3.1 |
| 33 | 1b | 136 | VAL | 3.1 |
| 4 | 2E | 157 | ALA | 3.1 |
| 16 | 2U | 35 | ALA | 3.1 |
| 33 | 2b | 138 | LEU | 3.1 |
| 25 | 23 | 29 | ARG | 3.1 |
| 1 | 2A | 2125 | G | 3.1 |
| 30 | 28 | 21 | LYS | 3.1 |
| 16 | 2U | 40 | PHE | 3.1 |
| 1 | 2A | 884 | C | 3.1 |
| 46 | 1o | 67 | LEU | 3.1 |
| 3 | 2D | 271 | ILE | 3.1 |
| 12 | 2Q | 99 | PRO | 3.1 |
| 33 | 2b | 131 | PRO | 3.1 |
| 47 | 1p | 17 | TYR | 3.0 |
| 26 | 24 | 54 | GLY | 3.0 |
| 6 | 2G | 109 | VAL | 3.0 |
| 7 | 2H | 141 | VAL | 3.0 |
| 54 | 2w | 18 | G | 3.0 |
| 21 | 2Z | 51 | ALA | 3.0 |
| 39 | 2h | 84 | ARG | 3.0 |
| 40 | 2i | 12 | GLU | 3.0 |
| 40 | 2i | 15 | ALA | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 51 | 1t | 86 | ARG | 3.0 |
| 26 | 14 | 55 | ARG | 3.0 |
| 12 | 2Q | 20 | ALA | 3.0 |
| 17 | 1V | 77 | ALA | 3.0 |
| 1 | 1A | 2151 | G | 3.0 |
| 54 | 1w | 61 | C | 3.0 |
| 5 | 2F | 90 | PHE | 3.0 |
| 54 | 1w | 76 | A | 3.0 |
| 47 | 1p | 48 | TRP | 3.0 |
| 47 | 1p | 7 | ALA | 3.0 |
| 34 | 2c | 185 | GLY | 3.0 |
| 35 | 2d | 98 | GLU | 3.0 |
| 36 | 1e | 81 | GLU | 3.0 |
| 47 | 1p | 32 | TYR | 3.0 |
| 42 | 2k | 87 | THR | 3.0 |
| 1 | 2A | 1847 | A | 3.0 |
| 32 | 2a | 1196 | U | 3.0 |
| 49 | 1r | 78 | LEU | 3.0 |
| 20 | 2Y | 77 | PRO | 3.0 |
| 3 | 1D | 275 | LYS | 3.0 |
| 4 | 2E | 77 | ILE | 3.0 |
| 39 | 1h | 86 | ILE | 3.0 |
| 41 | 2j | 74 | ILE | 3.0 |
| 48 | 2q | 59 | ILE | 3.0 |
| 9 | 2N | 45 | ASN | 3.0 |
| 39 | 2h | 31 | PHE | 3.0 |
| 41 | 1j | 47 | PHE | 3.0 |
| 52 | 1u | 18 | TYR | 3.0 |
| 1 | 2A | 2115 | G | 3.0 |
| 5 | 2F | 89 | VAL | 3.0 |
| 7 | 2H | 144 | VAL | 3.0 |
| 40 | 2i | 109 | VAL | 3.0 |
| 54 | 2w | 40 | G | 3.0 |
| 14 | 2S | 58 | LEU | 3.0 |
| 30 | 28 | 34 | TRP | 3.0 |
| 34 | 2c | 33 | LEU | 3.0 |
| 34 | 2c | 178 | LEU | 3.0 |
| 40 | 2i | 80 | GLY | 3.0 |
| 54 | 1y | 47 | U | 3.0 |
| 39 | 1h | 6 | ILE | 3.0 |
| 26 | 24 | 63 | TYR | 3.0 |
| 48 | 2q | 27 | PHE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 39 | 1h | 103 | VAL | 3.0 |
| 43 | 1l | 11 | VAL | 3.0 |
| 49 | 1r | 79 | LEU | 3.0 |
| 50 | 2s | 37 | ARG | 3.0 |
| 11 | 2P | 39 | LYS | 3.0 |
| 14 | 2S | 11 | LYS | 3.0 |
| 48 | 2q | 71 | PHE | 3.0 |
| 40 | 2i | 110 | GLU | 3.0 |
| 54 | 2w | 61 | C | 2.9 |
| 23 | 2l | 60 | PHE | 2.9 |
| 9 | 2N | 72 | TYR | 2.9 |
| 14 | 2S | 17 | ARG | 2.9 |
| 48 | 2q | 35 | VAL | 2.9 |
| 17 | 2V | 74 | LYS | 2.9 |
| 28 | 26 | 20 | ASN | 2.9 |
| 50 | 1s | 40 | ILE | 2.9 |
| 20 | 2Y | 90 | LEU | 2.9 |
| 38 | 2g | 79 | ARG | 2.9 |
| 51 | 2t | 13 | LEU | 2.9 |
| 52 | 1u | 6 | ARG | 2.9 |
| 7 | 2H | 125 | VAL | 2.9 |
| 18 | 2W | 85 | VAL | 2.9 |
| 32 | 2a | 1531 | A | 2.9 |
| 40 | 2i | 119 | ALA | 2.9 |
| 35 | 2d | 158 | ILE | 2.9 |
| 1 | 2A | 2144 | U | 2.9 |
| 33 | 2b | 144 | ARG | 2.9 |
| 54 | 1w | 72 | C | 2.9 |
| 7 | 2H | 98 | LEU | 2.9 |
| 38 | 1g | 38 | LEU | 2.9 |
| 46 | 2o | 67 | LEU | 2.9 |
| 40 | 2i | 41 | VAL | 2.9 |
| 47 | 1p | 41 | PRO | 2.9 |
| 21 | 2Z | 154 | ASP | 2.9 |
| 40 | 2i | 42 | ARG | 2.9 |
| 43 | 1l | 91 | LYS | 2.9 |
| 40 | 1i | 115 | GLY | 2.9 |
| 41 | 2j | 10 | GLY | 2.9 |
| 54 | 2w | 47 | U | 2.9 |
| 6 | 2G | 149 | VAL | 2.9 |
| 33 | 1b | 165 | VAL | 2.9 |
| 43 | 1l | 90 | VAL | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 39 | 2h | 136 | GLU | 2.9 |
| 1 | 1A | 2152 | G | 2.9 |
| 10 | 2O | 2 | ILE | 2.9 |
| 35 | 2d | 47 | ARG | 2.9 |
| 38 | 1g | 153 | HIS | 2.9 |
| 51 | 1t | 22 | ARG | 2.9 |
| 40 | 2i | 126 | SER | 2.9 |
| 19 | 2X | 66 | LEU | 2.9 |
| 46 | 2o | 56 | LEU | 2.9 |
| 48 | 2q | 22 | LEU | 2.9 |
| 7 | 2H | 24 | VAL | 2.9 |
| 33 | 1b | 126 | GLU | 2.9 |
| 48 | 2q | 42 | TYR | 2.9 |
| 35 | 2d | 134 | ASP | 2.9 |
| 51 | 2t | 9 | ASN | 2.9 |
| 40 | 2i | 117 | HIS | 2.9 |
| 36 | 2e | 129 | ILE | 2.9 |
| 39 | 2h | 134 | ILE | 2.9 |
| 50 | 2s | 49 | ILE | 2.9 |
| 33 | 2b | 17 | PHE | 2.9 |
| 22 | 20 | 75 | LEU | 2.9 |
| 32 | 2a | 570 | G | 2.9 |
| 1 | 2A | 229 | A | 2.9 |
| 43 | 2l | 47 | LYS | 2.9 |
| 52 | 1u | 12 | LYS | 2.9 |
| 20 | 2Y | 7 | VAL | 2.9 |
| 20 | 2Y | 78 | ALA | 2.9 |
| 26 | 24 | 68 | ARG | 2.9 |
| 38 | 2g | 32 | ARG | 2.9 |
| 39 | 2h | 82 | HIS | 2.9 |
| 40 | 2i | 124 | GLN | 2.9 |
| 11 | 2P | 73 | GLY | 2.9 |
| 32 | 2a | 879 | C | 2.9 |
| 39 | 2h | 86 | ILE | 2.9 |
| 47 | 2p | 9 | PHE | 2.9 |
| 51 | 1t | 29 | LYS | 2.9 |
| 50 | 2s | 5 | LEU | 2.9 |
| 1 | 1A | 2190 | G | 2.9 |
| 14 | 2S | 13 | ARG | 2.9 |
| 40 | 1i | 119 | ALA | 2.9 |
| 38 | 1g | 82 | GLY | 2.8 |
| 43 | 2l | 27 | LEU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | 2Z | 82 | ARG | 2.8 |
| 47 | 1p | 8 | ARG | 2.8 |
| 12 | 2Q | 102 | VAL | 2.8 |
| 48 | 2q | 87 | LYS | 2.8 |
| 54 | 1y | 39 | G | 2.8 |
| 30 | 28 | 58 | ILE | 2.8 |
| 36 | 2e | 109 | ILE | 2.8 |
| 42 | 2k | 29 | ILE | 2.8 |
| 47 | 1p | 36 | ILE | 2.8 |
| 11 | 2P | 79 | ARG | 2.8 |
| 12 | 2Q | 17 | LEU | 2.8 |
| 32 | 2a | 89 | C | 2.8 |
| 34 | 1c | 15 | THR | 2.8 |
| 20 | 2Y | 29 | GLU | 2.8 |
| 30 | 28 | 10 | ALA | 2.8 |
| 40 | 2i | 61 | ALA | 2.8 |
| 43 | 1l | 43 | VAL | 2.8 |
| 48 | 2q | 28 | PRO | 2.8 |
| 10 | 2O | 25 | LEU | 2.8 |
| 48 | 2q | 6 | LEU | 2.8 |
| 51 | 1t | 20 | LEU | 2.8 |
| 51 | 1t | 84 | LEU | 2.8 |
| 47 | 1p | 29 | ASP | 2.8 |
| 1 | 2A | 2143 | C | 2.8 |
| 4 | 2E | 116 | VAL | 2.8 |
| 23 | 21 | 28 | GLY | 2.8 |
| 36 | 2e | 134 | ALA | 2.8 |
| 28 | 26 | 21 | TYR | 2.8 |
| 36 | 2e | 11 | ILE | 2.8 |
| 39 | 1h | 83 | ILE | 2.8 |
| 40 | 2i | 105 | ASP | 2.8 |
| 11 | 2P | 32 | THR | 2.8 |
| 22 | 20 | 52 | GLY | 2.8 |
| 12 | 2Q | 36 | ALA | 2.8 |
| 28 | 26 | 52 | VAL | 2.8 |
| 1 | 1A | 2145 | C | 2.8 |
| 1 | 2A | 2803 | C | 2.8 |
| 7 | 2H | 3 | ARG | 2.8 |
| 38 | 1g | 32 | ARG | 2.8 |
| 44 | 2m | 94 | ARG | 2.8 |
| 54 | 1y | 32 | C | 2.8 |
| 54 | 2y | 61 | C | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 17 | 2V | 80 | GLN | 2.8 |
| 33 | 1b | 222 | ILE | 2.8 |
| 33 | 2b | 80 | ILE | 2.8 |
| 35 | 2d | 206 | PHE | 2.8 |
| 1 | 1A | 2189 | U | 2.8 |
| 20 | 2Y | 12 | THR | 2.8 |
| 8 | 2I | 3 | VAL | 2.8 |
| 24 | 12 | 69 | ARG | 2.8 |
| 31 | 29 | 1 | MET | 2.8 |
| 36 | 2e | 21 | ALA | 2.8 |
| 43 | 2l | 48 | PRO | 2.8 |
| 44 | 1m | 117 | VAL | 2.8 |
| 38 | 1g | 3 | ARG | 2.8 |
| 46 | 2o | 65 | ARG | 2.8 |
| 8 | 2I | 29 | TYR | 2.8 |
| 54 | 2y | 39 | G | 2.8 |
| 26 | 24 | 51 | ASP | 2.8 |
| 8 | 2I | 35 | LEU | 2.8 |
| 33 | 1b | 61 | LEU | 2.8 |
| 39 | 2h | 135 | CYS | 2.8 |
| 46 | 1o | 34 | LEU | 2.8 |
| 48 | 1q | 90 | ILE | 2.8 |
| 34 | 2c | 158 | GLY | 2.8 |
| 39 | 1h | 90 | GLY | 2.8 |
| 44 | 1m | 105 | THR | 2.8 |
| 4 | 2E | 131 | ALA | 2.8 |
| 16 | 2U | 42 | ALA | 2.8 |
| 25 | 23 | 21 | ALA | 2.8 |
| 34 | 2c | 7 | PRO | 2.8 |
| 38 | 2g | 156 | TRP | 2.8 |
| 32 | 2a | 1117 | G | 2.8 |
| 34 | 2c | 39 | ILE | 2.8 |
| 39 | 1h | 112 | LEU | 2.8 |
| 3 | 2D | 217 | ARG | 2.8 |
| 6 | 2G | 115 | ARG | 2.8 |
| 15 | 2T | 60 | THR | 2.8 |
| 50 | 2s | 36 | ARG | 2.8 |
| 34 | 2c | 37 | GLN | 2.7 |
| 12 | 2Q | 32 | TYR | 2.7 |
| 3 | 2D | 5 | LYS | 2.7 |
| 33 | 2b | 55 | PHE | 2.7 |
| 33 | 2b | 98 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | 2b | 145 | LEU | 2.7 |
| 36 | 2e | 121 | LYS | 2.7 |
| 39 | 1h | 119 | LEU | 2.7 |
| 41 | 2j | 57 | LYS | 2.7 |
| 47 | 2p | 80 | PHE | 2.7 |
| 7 | 2H | 95 | ARG | 2.7 |
| 39 | 2h | 92 | ARG | 2.7 |
| 48 | 2q | 38 | ARG | 2.7 |
| 54 | 2y | 57 | G | 2.7 |
| 29 | 17 | 45 | ALA | 2.7 |
| 47 | 1p | 16 | HIS | 2.7 |
| 14 | 2S | 57 | LYS | 2.7 |
| 33 | 1b | 132 | LYS | 2.7 |
| 52 | 1u | 3 | LYS | 2.7 |
| 26 | 24 | 45 | GLY | 2.7 |
| 31 | 29 | 24 | TYR | 2.7 |
| 44 | 1m | 87 | TYR | 2.7 |
| 34 | 2c | 30 | ARG | 2.7 |
| 51 | 2t | 83 | ARG | 2.7 |
| 35 | 2d | 146 | ILE | 2.7 |
| 17 | 2V | 77 | ALA | 2.7 |
| 30 | 28 | 2 | PRO | 2.7 |
| 33 | 1b | 232 | PRO | 2.7 |
| 1 | 2A | 2585 | U | 2.7 |
| 14 | 2S | 29 | PHE | 2.7 |
| 14 | 2S | 92 | TYR | 2.7 |
| 21 | 2Z | 155 | LEU | 2.7 |
| 32 | 2a | 1150 | U | 2.7 |
| 34 | 2c | 167 | TRP | 2.7 |
| 30 | 28 | 63 | PRO | 2.7 |
| 45 | 2n | 14 | PRO | 2.7 |
| 18 | 2W | 47 | VAL | 2.7 |
| 6 | 2G | 48 | GLU | 2.7 |
| 46 | 1o | 81 | LEU | 2.7 |
| 47 | 2p | 6 | LEU | 2.7 |
| 54 | 1w | 47 | U | 2.7 |
| 18 | 2W | 96 | ILE | 2.7 |
| 44 | 2m | 105 | THR | 2.7 |
| 16 | 2U | 2 | PRO | 2.7 |
| 31 | 29 | 12 | ASP | 2.7 |
| 45 | 2n | 60 | SER | 2.7 |
| 52 | 2u | 23 | PRO | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 45 | 2n | 18 | VAL | 2.7 |
| 34 | 2c | 190 | ARG | 2.7 |
| 41 | 1j | 46 | ARG | 2.7 |
| 44 | 2m | 88 | ARG | 2.7 |
| 4 | 1E | 195 | LEU | 2.7 |
| 12 | 2Q | 18 | LYS | 2.7 |
| 12 | 2Q | 63 | LYS | 2.7 |
| 40 | 2i | 78 | LYS | 2.7 |
| 47 | 1p | 73 | LEU | 2.7 |
| 51 | 1t | 14 | LYS | 2.7 |
| 32 | 2a | 1321 | C | 2.7 |
| 17 | 2V | 70 | ILE | 2.7 |
| 16 | 2U | 50 | ARG | 2.7 |
| 23 | 21 | 68 | PRO | 2.7 |
| 33 | 1b | 13 | ALA | 2.7 |
| 36 | 2e | 24 | ARG | 2.7 |
| 40 | 2i | 93 | ARG | 2.7 |
| 45 | 1n | 57 | ARG | 2.7 |
| 50 | 2s | 50 | ALA | 2.7 |
| 40 | 2i | 108 | VAL | 2.7 |
| 19 | 2X | 33 | LYS | 2.7 |
| 36 | 2e | 88 | LYS | 2.7 |
| 40 | 2i | 8 | GLY | 2.7 |
| 4 | 2E | 151 | TYR | 2.7 |
| 35 | 2d | 54 | TYR | 2.7 |
| 6 | 2G | 39 | ILE | 2.7 |
| 34 | 1c | 39 | ILE | 2.7 |
| 39 | 2h | 4 | ASP | 2.7 |
| 45 | 2n | 57 | ARG | 2.7 |
| 1 | 2A | 2173 | A | 2.7 |
| 38 | 2g | 152 | ALA | 2.7 |
| 45 | 2n | 4 | LYS | 2.7 |
| 4 | 2E | 125 | GLY | 2.7 |
| 1 | 2A | 2149 | G | 2.7 |
| 25 | 23 | 6 | VAL | 2.7 |
| 25 | 23 | 50 | VAL | 2.7 |
| 32 | 2a | 1001(A) | G | 2.7 |
| 54 | 2w | 5 | G | 2.7 |
| 54 | 2w | 22 | G | 2.7 |
| 4 | 2E | 195 | LEU | 2.7 |
| 24 | 22 | 60 | LEU | 2.7 |
| 33 | 2b | 69 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | 2e | 119 | LEU | 2.7 |
| 39 | 2h | 127 | LEU | 2.7 |
| 43 | 2l | 10 | LEU | 2.7 |
| 10 | 2O | 19 | ILE | 2.7 |
| 46 | 1o | 87 | ILE | 2.7 |
| 12 | 2Q | 129 | THR | 2.7 |
| 22 | 20 | 9 | SER | 2.7 |
| 30 | 28 | 37 | SER | 2.7 |
| 1 | 2A | 2128 | C | 2.6 |
| 21 | 2Z | 172 | ALA | 2.6 |
| 30 | 18 | 2 | PRO | 2.6 |
| 54 | 1w | 4 | U | 2.6 |
| 39 | 1h | 93 | VAL | 2.6 |
| 1 | 2A | 896 | A | 2.6 |
| 12 | 2Q | 79 | LEU | 2.6 |
| 35 | 1d | 19 | LEU | 2.6 |
| 36 | 1e | 139 | LEU | 2.6 |
| 40 | 2i | 85 | LEU | 2.6 |
| 50 | 2s | 16 | LEU | 2.6 |
| 32 | 2a | 1516 | G | 2.6 |
| 20 | 2Y | 55 | TYR | 2.6 |
| 39 | 2h | 94 | TYR | 2.6 |
| 46 | 1o | 36 | ILE | 2.6 |
| 51 | 2t | 55 | ILE | 2.6 |
| 34 | 1c | 78 | GLY | 2.6 |
| 34 | 2c | 81 | GLY | 2.6 |
| 40 | 1i | 117 | HIS | 2.6 |
| 50 | 2s | 45 | VAL | 2.6 |
| 54 | 2y | 64 | U | 2.6 |
| 32 | 2a | 795 | C | 2.6 |
| 39 | 2h | 133 | LEU | 2.6 |
| 41 | 2j | 61 | GLU | 2.6 |
| 1 | 1A | 1077 | A | 2.6 |
| 33 | 1b | 137 | ARG | 2.6 |
| 29 | 27 | 27 | GLY | 2.6 |
| 54 | 1w | 1 | G | 2.6 |
| 10 | 2O | 41 | ALA | 2.6 |
| 48 | 2q | 29 | HIS | 2.6 |
| 4 | 2E | 52 | LEU | 2.6 |
| 44 | 2m | 99 | ARG | 2.6 |
| 50 | 1s | 78 | ARG | 2.6 |
| 49 | 2r | 43 | PHE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6 | 1G | 88 | ILE | 2.6 |
| 31 | 29 | 17 | ILE | 2.6 |
| 34 | 2c | 23 | TYR | 2.6 |
| 35 | 1d | 158 | ILE | 2.6 |
| 40 | 1i | 125 | TYR | 2.6 |
| 43 | 2l | 64 | TYR | 2.6 |
| 30 | 28 | 15 | LYS | 2.6 |
| 41 | 1j | 20 | ALA | 2.6 |
| 7 | 2H | 115 | VAL | 2.6 |
| 30 | 28 | 23 | VAL | 2.6 |
| 32 | 2a | 973 | G | 2.6 |
| 40 | 2i | 121 | ARG | 2.6 |
| 47 | 1p | 25 | ARG | 2.6 |
| 48 | 2q | 10 | VAL | 2.6 |
| 7 | 2H | 88 | LEU | 2.6 |
| 12 | 2Q | 125 | LEU | 2.6 |
| 19 | 2X | 92 | LEU | 2.6 |
| 51 | 1t | 72 | LEU | 2.6 |
| 36 | 2e | 45 | PHE | 2.6 |
| 44 | 2m | 69 | GLU | 2.6 |
| 45 | 1n | 50 | LYS | 2.6 |
| 48 | 2q | 40 | LYS | 2.6 |
| 54 | 2w | 38 | A | 2.6 |
| 5 | 1F | 89 | VAL | 2.6 |
| 40 | 1i | 109 | VAL | 2.6 |
| 9 | 2N | 112 | LEU | 2.6 |
| 12 | 2Q | 2 | LEU | 2.6 |
| 29 | 17 | 1 | MET | 2.6 |
| 35 | 2d | 19 | LEU | 2.6 |
| 44 | 2m | 82 | MET | 2.6 |
| 39 | 2h | 87 | SER | 2.6 |
| 21 | 2Z | 57 | ILE | 2.6 |
| 46 | 1o | 68 | ARG | 2.6 |
| 51 | 1t | 71 | THR | 2.6 |
| 54 | 1y | 56 | C | 2.6 |
| 21 | 2Z | 141 | VAL | 2.6 |
| 46 | 2o | 27 | VAL | 2.6 |
| 47 | 1p | 76 | GLN | 2.6 |
| 40 | 2i | 102 | LEU | 2.6 |
| 50 | 2s | 12 | ASP | 2.6 |
| 23 | 21 | 29 | GLY | 2.6 |
| 34 | 2c | 194 | GLY | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 38 | 1g | 26 | PHE | 2.6 |
| 52 | 1u | 16 | GLY | 2.6 |
| 1 | 1A | 2125 | G | 2.6 |
| 33 | 2b | 111 | ARG | 2.6 |
| 38 | 1g | 155 | ARG | 2.6 |
| 34 | 1c | 202 | ILE | 2.6 |
| 34 | 2c | 14 | ILE | 2.6 |
| 47 | 1p | 13 | HIS | 2.6 |
| 1 | 1A | 884 | C | 2.6 |
| 3 | 2D | 155 | LEU | 2.6 |
| 35 | 1d | 78 | LEU | 2.6 |
| 43 | 2l | 16 | GLU | 2.6 |
| 40 | 2i | 37 | PHE | 2.6 |
| 50 | 2s | 66 | MET | 2.6 |
| 29 | 27 | 23 | ARG | 2.6 |
| 45 | 1n | 23 | ARG | 2.6 |
| 46 | 1o | 65 | ARG | 2.6 |
| 3 | 1D | 203 | ASN | 2.5 |
| 7 | 2H | 89 | ILE | 2.5 |
| 16 | 1U | 17 | ILE | 2.5 |
| 41 | 2j | 42 | THR | 2.5 |
| 33 | 2b | 186 | ALA | 2.5 |
| 36 | 1e | 17 | ALA | 2.5 |
| 6 | 1G | 146 | TYR | 2.5 |
| 32 | 2a | 1021 | G | 2.5 |
| 13 | 2R | 69 | ASP | 2.5 |
| 15 | 2T | 114 | LEU | 2.5 |
| 22 | 20 | 67 | VAL | 2.5 |
| 31 | 29 | 16 | VAL | 2.5 |
| 35 | 2d | 64 | LEU | 2.5 |
| 11 | 2P | 1 | MET | 2.5 |
| 22 | 20 | 44 | ARG | 2.5 |
| 48 | 2q | 91 | ARG | 2.5 |
| 43 | 2l | 91 | LYS | 2.5 |
| 34 | 2c | 174 | PRO | 2.5 |
| 41 | 2j | 15 | THR | 2.5 |
| 42 | 2k | 117 | ASN | 2.5 |
| 6 | 2G | 169 | ALA | 2.5 |
| 54 | 1y | 35 | A | 2.5 |
| 7 | 2H | 52 | VAL | 2.5 |
| 12 | 2Q | 34 | LEU | 2.5 |
| 27 | 25 | 58 | LEU | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 22 | 20 | 55 | ARG | 2.5 |
| 12 | 2Q | 69 | PHE | 2.5 |
| 32 | 1a | 1030(C) | G | 2.5 |
| 41 | 1j | 60 | ARG | 2.5 |
| 32 | 2a | 1320 | C | 2.5 |
| 7 | 2H | 145 | ALA | 2.5 |
| 30 | 28 | 59 | LYS | 2.5 |
| 32 | 2a | 1358 | U | 2.5 |
| 33 | 1b | 221 | LEU | 2.5 |
| 44 | 1m | 60 | VAL | 2.5 |
| 49 | 2r | 66 | LEU | 2.5 |
| 51 | 2t | 84 | LEU | 2.5 |
| 52 | 2u | 12 | LYS | 2.5 |
| 55 | 2x | 76 | A | 2.5 |
| 5 | 2F | 56 | GLU | 2.5 |
| 32 | 2a | 823 | G | 2.5 |
| 1 | 1A | 1064 | C | 2.5 |
| 38 | 2g | 24 | THR | 2.5 |
| 45 | 2n | 54 | PRO | 2.5 |
| 52 | 2u | 24 | ARG | 2.5 |
| 10 | 2O | 8 | LEU | 2.5 |
| 16 | 2U | 24 | TYR | 2.5 |
| 33 | 2b | 184 | VAL | 2.5 |
| 35 | 2d | 157 | LEU | 2.5 |
| 51 | 1t | 18 | GLN | 2.5 |
| 48 | 2q | 58 | GLU | 2.5 |
| 34 | 2c | 164 | ARG | 2.5 |
| 1 | 2A | 2100 | G | 2.5 |
| 16 | 2U | 41 | ALA | 2.5 |
| 35 | 2d | 209 | ARG | 2.5 |
| 38 | 2g | 83 | ALA | 2.5 |
| 40 | 1i | 82 | ALA | 2.5 |
| 52 | 1u | 15 | ARG | 2.5 |
| 18 | 2W | 103 | ILE | 2.5 |
| 40 | 2i | 68 | GLY | 2.5 |
| 35 | 1d | 11 | LEU | 2.5 |
| 35 | 1d | 135 | LEU | 2.5 |
| 30 | 28 | 65 | GLU | 2.5 |
| 36 | 2e | 115 | VAL | 2.5 |
| 47 | 1p | 39 | TYR | 2.5 |
| 3 | 2D | 6 | PHE | 2.5 |
| 33 | 2b | 122 | PHE | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 48 | 2q | 82 | MET | 2.5 |
| 3 | 2D | 38 | LYS | 2.5 |
| 47 | 1p | 5 | ARG | 2.5 |
| 51 | 1t | 79 | ARG | 2.5 |
| 9 | 2N | 43 | THR | 2.5 |
| 27 | 15 | 2 | ALA | 2.5 |
| 40 | 2i | 81 | ILE | 2.5 |
| 1 | 1A | 1509 | C | 2.5 |
| 7 | 2H | 43 | VAL | 2.5 |
| 42 | 2k | 109 | VAL | 2.5 |
| 47 | 2p | 2 | VAL | 2.5 |
| 1 | 1A | 2112 | G | 2.5 |
| 26 | 24 | 43 | TYR | 2.5 |
| 32 | 2a | 112 | G | 2.5 |
| 47 | 2p | 17 | TYR | 2.5 |
| 14 | 2S | 9 | ARG | 2.5 |
| 34 | 2c | 179 | ARG | 2.5 |
| 41 | 1j | 45 | ARG | 2.5 |
| 47 | 1p | 66 | PRO | 2.5 |
| 48 | 1q | 28 | PRO | 2.5 |
| 1 | 2A | 2170 | A | 2.5 |
| 21 | 2Z | 124 | ILE | 2.5 |
| 32 | 2a | 969 | A | 2.5 |
| 41 | 2j | 71 | LEU | 2.5 |
| 48 | 2q | 84 | LEU | 2.5 |
| 54 | 2y | 66 | A | 2.5 |
| 3 | 1D | 113 | VAL | 2.5 |
| 36 | 2e | 105 | VAL | 2.5 |
| 21 | 2Z | 99 | TYR | 2.5 |
| 37 | 2f | 59 | TYR | 2.5 |
| 42 | 1k | 125 | PHE | 2.5 |
| 45 | 1n | 16 | PHE | 2.5 |
| 41 | 1j | 66 | ARG | 2.5 |
| 32 | 2a | 1222 | G | 2.5 |
| 1 | 1A | 271(K) | U | 2.4 |
| 10 | 2O | 27 | GLY | 2.4 |
| 14 | 2S | 8 | GLU | 2.4 |
| 35 | 1d | 7 | PRO | 2.4 |
| 3 | 2D | 59 | LYS | 2.4 |
| 36 | 1e | 134 | ALA | 2.4 |
| 5 | 2F | 78 | ILE | 2.4 |
| 28 | 26 | 7 | ILE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 38 | 1g | 120 | ILE | 2.4 |
| 47 | 1p | 33 | ILE | 2.4 |
| 6 | 1G | 149 | VAL | 2.4 |
| 26 | 14 | 56 | VAL | 2.4 |
| 35 | 2d | 198 | VAL | 2.4 |
| 40 | 1i | 108 | VAL | 2.4 |
| 9 | 2N | 1 | MET | 2.4 |
| 33 | 2b | 227 | GLY | 2.4 |
| 34 | 2c | 80 | GLY | 2.4 |
| 35 | 1d | 62 | GLN | 2.4 |
| 55 | 2x | 3 | C | 2.4 |
| 12 | 2Q | 114 | ALA | 2.4 |
| 32 | 1a | 204 | U | 2.4 |
| 34 | 2c | 176 | HIS | 2.4 |
| 42 | 2k | 31 | THR | 2.4 |
| 54 | 2y | 19 | G | 2.4 |
| 11 | 2P | 6 | LEU | 2.4 |
| 14 | 1S | 4 | LEU | 2.4 |
| 23 | 2l | 94 | LEU | 2.4 |
| 44 | 2m | 78 | ILE | 2.4 |
| 48 | 2q | 31 | LEU | 2.4 |
| 49 | 2r | 85 | LEU | 2.4 |
| 35 | 1d | 139 | ARG | 2.4 |
| 43 | 2l | 96 | VAL | 2.4 |
| 48 | 1q | 11 | VAL | 2.4 |
| 38 | 2g | 26 | PHE | 2.4 |
| 17 | 2V | 78 | LYS | 2.4 |
| 53 | 2v | 15 | A | 2.4 |
| 33 | 2b | 202 | PRO | 2.4 |
| 42 | 2k | 115 | PRO | 2.4 |
| 46 | 2o | 46 | HIS | 2.4 |
| 1 | 2A | 2150 | U | 2.4 |
| 10 | 1O | 47 | ILE | 2.4 |
| 15 | 2T | 102 | ILE | 2.4 |
| 16 | 1U | 18 | LEU | 2.4 |
| 26 | 14 | 62 | ARG | 2.4 |
| 38 | 2g | 22 | LEU | 2.4 |
| 15 | 1T | 109 | GLU | 2.4 |
| 33 | 1b | 75 | LYS | 2.4 |
| 54 | 1w | 3 | G | 2.4 |
| 7 | 2H | 164 | TYR | 2.4 |
| 35 | 2d | 165 | MET | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | 1D | 263 | ARG | 2.4 |
| 16 | 2U | 33 | ARG | 2.4 |
| 21 | 2Z | 122 | ARG | 2.4 |
| 54 | 1w | 69 | A | 2.4 |
| 39 | 1h | 39 | LEU | 2.4 |
| 1 | 1A | 885 | C | 2.4 |
| 8 | 1I | 4 | ILE | 2.4 |
| 11 | 2P | 29 | LYS | 2.4 |
| 33 | 1b | 127 | ILE | 2.4 |
| 33 | 2b | 8 | LYS | 2.4 |
| 36 | 1e | 88 | LYS | 2.4 |
| 48 | 2q | 24 | GLU | 2.4 |
| 22 | 20 | 71 | ASP | 2.4 |
| 33 | 1b | 93 | VAL | 2.4 |
| 20 | 2Y | 89 | PHE | 2.4 |
| 1 | 2A | 2116 | G | 2.4 |
| 3 | 2D | 4 | LYS | 2.4 |
| 9 | 2N | 10 | GLU | 2.4 |
| 14 | 2S | 34 | HIS | 2.4 |
| 41 | 1j | 57 | LYS | 2.4 |
| 3 | 2D | 37 | LEU | 2.4 |
| 9 | 2N | 23 | LEU | 2.4 |
| 38 | 1g | 22 | LEU | 2.4 |
| 9 | 2N | 71 | ILE | 2.4 |
| 11 | 2P | 40 | SER | 2.4 |
| 41 | 1j | 58 | ASP | 2.4 |
| 54 | 1y | 23 | A | 2.4 |
| 54 | 2y | 35 | A | 2.4 |
| 6 | 2G | 89 | GLY | 2.4 |
| 20 | 2Y | 80 | GLY | 2.4 |
| 32 | 1a | 1532 | U | 2.4 |
| 48 | 1q | 71 | PHE | 2.4 |
| 48 | 2q | 80 | GLY | 2.4 |
| 55 | 2x | 69 | C | 2.4 |
| 17 | 2V | 84 | LYS | 2.4 |
| 44 | 1m | 121 | LYS | 2.4 |
| 48 | 2q | 92 | ARG | 2.4 |
| 1 | 2A | 2319 | G | 2.4 |
| 11 | 2P | 35 | HIS | 2.4 |
| 42 | 2k | 35 | PRO | 2.4 |
| 3 | 2D | 240 | ALA | 2.4 |
| 46 | 2o | 57 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 10 | 2O | 81 | ASP | 2.4 |
| 30 | 28 | 20 | GLY | 2.4 |
| 35 | 2d | 2 | GLY | 2.4 |
| 31 | 29 | 25 | VAL | 2.4 |
| 39 | 1h | 31 | PHE | 2.4 |
| 1 | 2A | 2114 | A | 2.4 |
| 38 | 2g | 78 | ARG | 2.4 |
| 47 | 1p | 27 | LYS | 2.4 |
| 7 | 2H | 58 | GLU | 2.4 |
| 44 | 1m | 23 | TYR | 2.4 |
| 21 | 2Z | 167 | PRO | 2.4 |
| 48 | 1q | 45 | HIS | 2.4 |
| 16 | 2U | 31 | SER | 2.4 |
| 22 | 10 | 75 | LEU | 2.4 |
| 23 | 21 | 98 | LEU | 2.4 |
| 36 | 1e | 91 | LEU | 2.4 |
| 44 | 2m | 96 | LEU | 2.4 |
| 46 | 2o | 81 | LEU | 2.4 |
| 20 | 2Y | 61 | ILE | 2.4 |
| 33 | 2b | 18 | GLY | 2.4 |
| 35 | 2d | 161 | ASN | 2.4 |
| 40 | 2i | 6 | GLY | 2.4 |
| 40 | 2i | 112 | LYS | 2.4 |
| 41 | 1j | 50 | ILE | 2.4 |
| 54 | 1y | 1 | G | 2.4 |
| 54 | 2w | 15 | G | 2.4 |
| 11 | 2P | 50 | ARG | 2.4 |
| 12 | 2Q | 41 | TRP | 2.4 |
| 18 | 2W | 14 | PRO | 2.3 |
| 35 | 2d | 106 | TYR | 2.3 |
| 39 | 1h | 5 | PRO | 2.3 |
| 42 | 2k | 121 | PRO | 2.3 |
| 4 | 1E | 28 | ALA | 2.3 |
| 16 | 2U | 48 | ALA | 2.3 |
| 18 | 2W | 13 | SER | 2.3 |
| 39 | 2h | 124 | ALA | 2.3 |
| 40 | 1i | 7 | THR | 2.3 |
| 40 | 1i | 116 | LYS | 2.3 |
| 40 | 1i | 126 | SER | 2.3 |
| 41 | 1j | 32 | ALA | 2.3 |
| 51 | 1t | 24 | LEU | 2.3 |
| 52 | 1u | 11 | GLY | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | 1D | 204 | ILE | 2.3 |
| 15 | 1T | 108 | ARG | 2.3 |
| 33 | 2b | 68 | ILE | 2.3 |
| 43 | 2l | 100 | ILE | 2.3 |
| 46 | 1o | 12 | ILE | 2.3 |
| 48 | 2q | 78 | GLU | 2.3 |
| 20 | 2Y | 13 | VAL | 2.3 |
| 34 | 2c | 138 | VAL | 2.3 |
| 32 | 2a | 1220 | G | 2.3 |
| 47 | 1p | 59 | TRP | 2.3 |
| 15 | 2T | 113 | LYS | 2.3 |
| 32 | 2a | 90 | U | 2.3 |
| 41 | 2j | 68 | HIS | 2.3 |
| 48 | 1q | 34 | LYS | 2.3 |
| 50 | 2s | 42 | PRO | 2.3 |
| 6 | 2G | 173 | LEU | 2.3 |
| 9 | 2N | 26 | LEU | 2.3 |
| 9 | 2N | 120 | LEU | 2.3 |
| 1 | 2A | 885 | C | 2.3 |
| 11 | 2P | 22 | GLY | 2.3 |
| 33 | 1b | 124 | SER | 2.3 |
| 22 | 20 | 12 | ASN | 2.3 |
| 32 | 1a | 1030 | C | 2.3 |
| 40 | 1i | 61 | ALA | 2.3 |
| 51 | 2t | 79 | ARG | 2.3 |
| 24 | 22 | 57 | ILE | 2.3 |
| 33 | 2b | 41 | ILE | 2.3 |
| 33 | 2b | 162 | ILE | 2.3 |
| 21 | 2Z | 88 | PHE | 2.3 |
| 38 | 2g | 23 | VAL | 2.3 |
| 42 | 1k | 14 | VAL | 2.3 |
| 26 | 14 | 46 | GLN | 2.3 |
| 38 | 2g | 151 | TYR | 2.3 |
| 43 | 2l | 94 | PRO | 2.3 |
| 4 | 2E | 20 | ALA | 2.3 |
| 7 | 2H | 102 | ALA | 2.3 |
| 21 | 2Z | 76 | LEU | 2.3 |
| 34 | 1c | 19 | GLU | 2.3 |
| 26 | 14 | 58 | ARG | 2.3 |
| 30 | 28 | 32 | LEU | 2.3 |
| 46 | 1o | 56 | LEU | 2.3 |
| 54 | 2y | 5 | G | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | 28 | 17 | THR | 2.3 |
| 38 | 2g | 2 | ALA | 2.3 |
| 32 | 2a | 924 | C | 2.3 |
| 1 | 2A | 735 | A | 2.3 |
| 33 | 2b | 211 | ILE | 2.3 |
| 34 | 2c | 134 | ILE | 2.3 |
| 12 | 2Q | 109 | VAL | 2.3 |
| 21 | 1Z | 141 | VAL | 2.3 |
| 22 | 20 | 69 | PHE | 2.3 |
| 35 | 1d | 198 | VAL | 2.3 |
| 36 | 1e | 55 | VAL | 2.3 |
| 38 | 2g | 33 | ASP | 2.3 |
| 50 | 2s | 14 | HIS | 2.3 |
| 33 | 1b | 118 | LEU | 2.3 |
| 51 | 2t | 10 | LEU | 2.3 |
| 52 | 1u | 22 | ARG | 2.3 |
| 39 | 2h | 58 | TYR | 2.3 |
| 5 | 1F | 48 | THR | 2.3 |
| 18 | 2W | 60 | ASN | 2.3 |
| 53 | 1v | 23 | U | 2.3 |
| 1 | 2A | 2148 | G | 2.3 |
| 32 | 2a | 1061 | G | 2.3 |
| 40 | 2i | 38 | GLN | 2.3 |
| 10 | 2O | 43 | VAL | 2.3 |
| 12 | 1Q | 81 | VAL | 2.3 |
| 33 | 2b | 15 | VAL | 2.3 |
| 33 | 2b | 105 | PHE | 2.3 |
| 46 | 2o | 82 | ILE | 2.3 |
| 39 | 2h | 95 | VAL | 2.3 |
| 20 | 2Y | 62 | GLU | 2.3 |
| 28 | 26 | 42 | TRP | 2.3 |
| 35 | 2d | 73 | ARG | 2.3 |
| 40 | 2i | 39 | GLY | 2.3 |
| 8 | 2I | 30 | LEU | 2.3 |
| 25 | 23 | 23 | LEU | 2.3 |
| 34 | 2c | 12 | LEU | 2.3 |
| 9 | 2N | 117 | PHE | 2.3 |
| 12 | 2Q | 29 | PHE | 2.3 |
| 48 | 2q | 65 | ILE | 2.3 |
| 44 | 2m | 67 | GLU | 2.3 |
| 1 | 2A | 2110 | G | 2.3 |
| 16 | 2U | 36 | ARG | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | 24 | 55 | ARG | 2.3 |
| 35 | 2d | 57 | ARG | 2.3 |
| 39 | 2h | 122 | ARG | 2.3 |
| 40 | 2i | 75 | ASP | 2.3 |
| 6 | 2G | 177 | GLY | 2.3 |
| 3 | 2D | 275 | LYS | 2.3 |
| 20 | 2Y | 26 | LYS | 2.3 |
| 32 | 2a | 794 | A | 2.3 |
| 33 | 1b | 95 | GLN | 2.3 |
| 7 | 2H | 106 | THR | 2.3 |
| 40 | 1i | 114 | TYR | 2.3 |
| 45 | 2n | 40 | CYS | 2.3 |
| 34 | 2c | 206 | GLU | 2.3 |
| 1 | 2A | 2172 | U | 2.3 |
| 21 | 2Z | 44 | PHE | 2.3 |
| 26 | 24 | 14 | ILE | 2.3 |
| 43 | 2l | 101 | VAL | 2.3 |
| 50 | 2s | 9 | VAL | 2.3 |
| 11 | 2P | 76 | LYS | 2.3 |
| 7 | 2H | 65 | HIS | 2.3 |
| 7 | 2H | 84 | SER | 2.3 |
| 16 | 1U | 27 | LEU | 2.3 |
| 33 | 1b | 233 | SER | 2.3 |
| 32 | 2a | 1030 | C | 2.3 |
| 32 | 2a | 1149 | C | 2.3 |
| 44 | 1m | 107 | ALA | 2.3 |
| 21 | 1Z | 170 | THR | 2.3 |
| 5 | 2F | 64 | ILE | 2.3 |
| 5 | 2F | 82 | ILE | 2.3 |
| 9 | 2N | 118 | LYS | 2.3 |
| 12 | 2Q | 64 | ILE | 2.3 |
| 45 | 2n | 16 | PHE | 2.3 |
| 30 | 28 | 38 | GLY | 2.2 |
| 54 | 2w | 33 | U | 2.2 |
| 33 | 2b | 78 | GLN | 2.2 |
| 43 | 2l | 9 | GLN | 2.2 |
| 15 | 1T | 114 | LEU | 2.2 |
| 36 | 2e | 138 | ALA | 2.2 |
| 38 | 2g | 25 | ALA | 2.2 |
| 40 | 2i | 122 | ALA | 2.2 |
| 6 | 1G | 75 | LYS | 2.2 |
| 19 | 1X | 65 | ARG | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | 28 | 52 | LYS | 2.2 |
| 33 | 2b | 130 | ARG | 2.2 |
| 35 | 2d | 68 | TYR | 2.2 |
| 46 | 2o | 88 | ARG | 2.2 |
| 6 | 2G | 134 | GLY | 2.2 |
| 33 | 2b | 203 | GLY | 2.2 |
| 34 | 2c | 153 | VAL | 2.2 |
| 41 | 2j | 34 | VAL | 2.2 |
| 46 | 2o | 3 | ILE | 2.2 |
| 36 | 2e | 130 | ASN | 2.2 |
| 40 | 1i | 110 | GLU | 2.2 |
| 51 | 2t | 70 | SER | 2.2 |
| 21 | 2Z | 125 | LEU | 2.2 |
| 40 | 2i | 19 | LEU | 2.2 |
| 44 | 2m | 64 | TRP | 2.2 |
| 3 | 1D | 50 | THR | 2.2 |
| 7 | 2H | 132 | ARG | 2.2 |
| 22 | 20 | 77 | ARG | 2.2 |
| 27 | 25 | 11 | THR | 2.2 |
| 40 | 2i | 111 | ARG | 2.2 |
| 34 | 2c | 17 | ASP | 2.2 |
| 1 | 2A | 2175 | C | 2.2 |
| 36 | 2e | 124 | GLY | 2.2 |
| 6 | 2G | 160 | VAL | 2.2 |
| 25 | 23 | 9 | VAL | 2.2 |
| 40 | 2i | 53 | VAL | 2.2 |
| 47 | 1p | 4 | ILE | 2.2 |
| 48 | 2q | 56 | VAL | 2.2 |
| 54 | 2y | 18 | G | 2.2 |
| 11 | 2P | 74 | GLU | 2.2 |
| 30 | 28 | 19 | SER | 2.2 |
| 2 | 2B | 90 | A | 2.2 |
| 17 | 2V | 76 | LYS | 2.2 |
| 31 | 29 | 33 | LYS | 2.2 |
| 32 | 1a | 389 | A | 2.2 |
| 43 | 2l | 52 | LEU | 2.2 |
| 47 | 1p | 35 | LYS | 2.2 |
| 34 | 2c | 22 | TRP | 2.2 |
| 50 | 2s | 76 | PRO | 2.2 |
| 50 | 2s | 44 | MET | 2.2 |
| 52 | 1u | 10 | ARG | 2.2 |
| 18 | 2W | 93 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | 2b | 79 | ASP | 2.2 |
| 38 | 2g | 140 | ASP | 2.2 |
| 22 | 20 | 45 | PHE | 2.2 |
| 35 | 2d | 167 | GLY | 2.2 |
| 41 | 1j | 11 | PHE | 2.2 |
| 42 | 2k | 86 | GLY | 2.2 |
| 48 | 1q | 26 | GLN | 2.2 |
| 21 | 2Z | 161 | VAL | 2.2 |
| 36 | 1e | 80 | ILE | 2.2 |
| 43 | 2l | 43 | VAL | 2.2 |
| 8 | 1I | 9 | LEU | 2.2 |
| 35 | 1d | 101 | LEU | 2.2 |
| 47 | 2p | 73 | LEU | 2.2 |
| 33 | 2b | 90 | MET | 2.2 |
| 1 | 1A | 1095 | A | 2.2 |
| 8 | 1I | 20 | ASP | 2.2 |
| 49 | 2r | 47 | THR | 2.2 |
| 38 | 2g | 85 | TYR | 2.2 |
| 42 | 1k | 25 | TYR | 2.2 |
| 3 | 1D | 51 | VAL | 2.2 |
| 3 | 2D | 106 | ILE | 2.2 |
| 5 | 2F | 57 | VAL | 2.2 |
| 12 | 2Q | 97 | VAL | 2.2 |
| 36 | 2e | 101 | ILE | 2.2 |
| 39 | 1h | 61 | VAL | 2.2 |
| 49 | 2r | 50 | ILE | 2.2 |
| 35 | 1d | 209 | ARG | 2.2 |
| 47 | 2p | 8 | ARG | 2.2 |
| 7 | 2H | 71 | LEU | 2.2 |
| 14 | 2S | 54 | LEU | 2.2 |
| 17 | 2V | 87 | HIS | 2.2 |
| 23 | 21 | 46 | LEU | 2.2 |
| 35 | 1d | 40 | PRO | 2.2 |
| 36 | 2e | 139 | LEU | 2.2 |
| 46 | 2o | 66 | LEU | 2.2 |
| 48 | 2q | 43 | LEU | 2.2 |
| 1 | 2A | 2142 | C | 2.2 |
| 34 | 2c | 162 | GLN | 2.2 |
| 35 | 1d | 102 | ASP | 2.2 |
| 47 | 1p | 44 | THR | 2.2 |
| 32 | 2a | 977 | A | 2.2 |
| 38 | 2g | 43 | PHE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | 2D | 54 | ARG | 2.2 |
| 14 | 2S | 31 | SER | 2.2 |
| 18 | 2W | 24 | ILE | 2.2 |
| 34 | 2c | 8 | ILE | 2.2 |
| 3 | 2D | 206 | LEU | 2.2 |
| 22 | 20 | 59 | LEU | 2.2 |
| 25 | 23 | 12 | PRO | 2.2 |
| 25 | 23 | 16 | PRO | 2.2 |
| 34 | 1c | 196 | LEU | 2.2 |
| 37 | 1f | 61 | LEU | 2.2 |
| 49 | 1r | 44 | LEU | 2.2 |
| 7 | 2H | 90 | LYS | 2.2 |
| 11 | 2P | 36 | LYS | 2.2 |
| 39 | 2h | 116 | LYS | 2.2 |
| 43 | 2l | 14 | GLY | 2.2 |
| 51 | 1t | 59 | ALA | 2.2 |
| 27 | 25 | 29 | THR | 2.2 |
| 5 | 2F | 83 | PHE | 2.2 |
| 32 | 2a | 1062 | U | 2.2 |
| 35 | 1d | 118 | ARG | 2.2 |
| 46 | 2o | 15 | PHE | 2.2 |
| 1 | 2A | 2583 | G | 2.2 |
| 40 | 2i | 5 | TYR | 2.2 |
| 28 | 26 | 5 | VAL | 2.2 |
| 30 | 18 | 22 | VAL | 2.2 |
| 36 | 2e | 33 | VAL | 2.2 |
| 39 | 1h | 109 | ILE | 2.2 |
| 39 | 2h | 109 | ILE | 2.2 |
| 48 | 2q | 73 | VAL | 2.2 |
| 49 | 2r | 22 | VAL | 2.2 |
| 1 | 2A | 2169 | A | 2.2 |
| 32 | 2a | 1357 | A | 2.2 |
| 16 | 2U | 18 | LEU | 2.2 |
| 20 | 2Y | 82 | PRO | 2.2 |
| 34 | 2c | 47 | LEU | 2.2 |
| 43 | 1l | 27 | LEU | 2.2 |
| 46 | 1o | 31 | LEU | 2.2 |
| 5 | 2F | 76 | GLY | 2.2 |
| 19 | 2X | 1 | MET | 2.2 |
| 10 | 2O | 6 | THR | 2.2 |
| 48 | 2q | 7 | THR | 2.2 |
| 17 | 2V | 82 | ARG | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 38 | 2g | 76 | ARG | 2.2 |
| 51 | 2t | 17 | ARG | 2.2 |
| 40 | 1i | 59 | PHE | 2.2 |
| 10 | 2O | 29 | ASN | 2.1 |
| 22 | 20 | 19 | LYS | 2.1 |
| 35 | 1d | 138 | TYR | 2.1 |
| 43 | 1l | 98 | TYR | 2.1 |
| 42 | 2k | 108 | ILE | 2.1 |
| 47 | 1p | 62 | VAL | 2.1 |
| 4 | 2E | 132 | HIS | 2.1 |
| 11 | 2P | 27 | HIS | 2.1 |
| 45 | 2n | 52 | GLN | 2.1 |
| 35 | 2d | 29 | PRO | 2.1 |
| 47 | 1p | 49 | LEU | 2.1 |
| 34 | 1c | 205 | GLY | 2.1 |
| 36 | 2e | 22 | GLY | 2.1 |
| 36 | 2e | 114 | GLY | 2.1 |
| 8 | 1I | 27 | ARG | 2.1 |
| 29 | 27 | 45 | ALA | 2.1 |
| 39 | 2h | 91 | ARG | 2.1 |
| 44 | 2m | 72 | ALA | 2.1 |
| 15 | 2T | 1 | MET | 2.1 |
| 42 | 1k | 87 | THR | 2.1 |
| 47 | 2p | 22 | THR | 2.1 |
| 50 | 2s | 33 | THR | 2.1 |
| 11 | 2P | 46 | LYS | 2.1 |
| 17 | 2V | 85 | LYS | 2.1 |
| 48 | 1q | 78 | GLU | 2.1 |
| 36 | 2e | 60 | TYR | 2.1 |
| 54 | 1w | 13 | C | 2.1 |
| 7 | 2H | 151 | ILE | 2.1 |
| 14 | 2S | 40 | ILE | 2.1 |
| 41 | 2j | 72 | VAL | 2.1 |
| 51 | 2t | 33 | ILE | 2.1 |
| 7 | 2H | 111 | HIS | 2.1 |
| 47 | 2p | 74 | LEU | 2.1 |
| 48 | 2q | 33 | GLY | 2.1 |
| 10 | 1O | 17 | ARG | 2.1 |
| 25 | 23 | 30 | ARG | 2.1 |
| 35 | 2d | 3 | ARG | 2.1 |
| 1 | 2A | 2894 | G | 2.1 |
| 24 | 22 | 8 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 30 | 28 | 12 | LYS | 2.1 |
| 32 | 2a | 1034 | G | 2.1 |
| 34 | 1c | 72 | LYS | 2.1 |
| 35 | 1d | 166 | LYS | 2.1 |
| 36 | 1e | 95 | ALA | 2.1 |
| 40 | 1i | 118 | LYS | 2.1 |
| 40 | 1i | 127 | LYS | 2.1 |
| 1 | 2A | 2801(A) | A | 2.1 |
| 45 | 2n | 43 | CYS | 2.1 |
| 6 | 1G | 26 | GLN | 2.1 |
| 4 | 2E | 26 | ILE | 2.1 |
| 18 | 2W | 9 | TYR | 2.1 |
| 18 | 2W | 10 | VAL | 2.1 |
| 48 | 2q | 19 | VAL | 2.1 |
| 1 | 2A | 2138 | C | 2.1 |
| 12 | 2Q | 23 | GLY | 2.1 |
| 32 | 2a | 1354 | C | 2.1 |
| 35 | 2d | 108 | LEU | 2.1 |
| 35 | 2d | 168 | ARG | 2.1 |
| 44 | 1m | 119 | GLY | 2.1 |
| 54 | 1w | 31 | C | 2.1 |
| 34 | 1c | 206 | GLU | 2.1 |
| 36 | 1e | 86 | ALA | 2.1 |
| 38 | 1g | 150 | ALA | 2.1 |
| 23 | 2l | 34 | THR | 2.1 |
| 3 | 1D | 15 | PHE | 2.1 |
| 35 | 2d | 75 | PHE | 2.1 |
| 1 | 1A | 1093 | G | 2.1 |
| 1 | 2A | 910 | A | 2.1 |
| 32 | 2a | 1225 | A | 2.1 |
| 32 | 2a | 1363(A) | A | 2.1 |
| 9 | 1N | 140 | VAL | 2.1 |
| 9 | 2N | 52 | VAL | 2.1 |
| 9 | 2N | 87 | LEU | 2.1 |
| 11 | 2P | 59 | LEU | 2.1 |
| 20 | 2Y | 67 | LEU | 2.1 |
| 25 | 23 | 53 | LEU | 2.1 |
| 34 | 1c | 201 | TYR | 2.1 |
| 34 | 2c | 204 | LEU | 2.1 |
| 36 | 1e | 121 | LYS | 2.1 |
| 44 | 2m | 108 | ARG | 2.1 |
| 6 | 2G | 142 | PRO | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | 2N | 90 | MET | 2.1 |
| 11 | 2P | 58 | THR | 2.1 |
| 7 | 1H | 2 | SER | 2.1 |
| 14 | 2S | 12 | PHE | 2.1 |
| 21 | 1Z | 149 | SER | 2.1 |
| 51 | 2t | 21 | LYS | 2.1 |
| 15 | 1T | 87 | ASP | 2.1 |
| 6 | 2G | 140 | ILE | 2.1 |
| 30 | 18 | 14 | VAL | 2.1 |
| 1 | 1A | 2131 | G | 2.1 |
| 20 | 2Y | 35 | TYR | 2.1 |
| 33 | 2b | 58 | ILE | 2.1 |
| 34 | 1c | 152 | ILE | 2.1 |
| 36 | 1e | 13 | ILE | 2.1 |
| 46 | 2o | 43 | LEU | 2.1 |
| 50 | 1s | 67 | VAL | 2.1 |
| 50 | 2s | 15 | LEU | 2.1 |
| 32 | 2a | 978 | A | 2.1 |
| 36 | 2e | 83 | GLU | 2.1 |
| 54 | 1w | 10 | G | 2.1 |
| 54 | 1w | 14 | A | 2.1 |
| 53 | 2v | 23 | U | 2.1 |
| 3 | 1D | 214 | TRP | 2.1 |
| 36 | 1e | 18 | ARG | 2.1 |
| 36 | 1e | 24 | ARG | 2.1 |
| 51 | 1t | 8 | ARG | 2.1 |
| 4 | 2E | 158 | GLY | 2.1 |
| 8 | 2I | 20 | ASP | 2.1 |
| 20 | 2Y | 58 | GLY | 2.1 |
| 12 | 2Q | 105 | GLU | 2.1 |
| 20 | 1Y | 31 | LEU | 2.1 |
| 21 | 2Z | 91 | LEU | 2.1 |
| 22 | 20 | 37 | LEU | 2.1 |
| 24 | 22 | 61 | LEU | 2.1 |
| 4 | 1E | 77 | ILE | 2.1 |
| 7 | 2H | 37 | VAL | 2.1 |
| 36 | 1e | 123 | LEU | 2.1 |
| 38 | 1g | 91 | VAL | 2.1 |
| 49 | 2r | 44 | LEU | 2.1 |
| 33 | 2b | 148 | TYR | 2.1 |
| 11 | 2P | 38 | GLN | 2.1 |
| 1 | 2A | 2141 | G | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 34 | 1c | 160 | ALA | 2.1 |
| 35 | 1d | 111 | ALA | 2.1 |
| 36 | 2e | 47 | LYS | 2.1 |
| 42 | 2k | 123 | LYS | 2.1 |
| 1 | 2A | 1963 | U | 2.1 |
| 40 | 2i | 27 | THR | 2.1 |
| 27 | 25 | 12 | SER | 2.1 |
| 39 | 1h | 136 | GLU | 2.1 |
| 46 | 1o | 61 | GLY | 2.1 |
| 54 | 2w | 30 | C | 2.1 |
| 13 | 2R | 18 | LEU | 2.1 |
| 3 | 1D | 49 | ILE | 2.1 |
| 7 | 2H | 162 | ILE | 2.1 |
| 9 | 2N | 85 | ILE | 2.1 |
| 20 | 2Y | 51 | VAL | 2.1 |
| 21 | 2Z | 174 | VAL | 2.1 |
| 31 | 29 | 3 | VAL | 2.1 |
| 34 | 1c | 115 | LEU | 2.1 |
| 35 | 2d | 148 | VAL | 2.1 |
| 48 | 2q | 89 | LEU | 2.1 |
| 50 | 2s | 11 | VAL | 2.1 |
| 50 | 2s | 62 | ILE | 2.1 |
| 28 | 26 | 53 | LYS | 2.1 |
| 12 | 2Q | 121 | ALA | 2.1 |
| 11 | 2P | 33 | ARG | 2.1 |
| 35 | 2d | 115 | ARG | 2.1 |
| 44 | 2m | 93 | ARG | 2.1 |
| 46 | 2o | 38 | ARG | 2.1 |
| 51 | 1t | 15 | ARG | 2.1 |
| 41 | 2j | 64 | GLU | 2.1 |
| 1 | 2A | 2506 | U | 2.0 |
| 6 | 2G | 141 | PHE | 2.1 |
| 12 | 2Q | 100 | GLY | 2.1 |
| 32 | 2a | 1287 | A | 2.1 |
| 39 | 1h | 4 | ASP | 2.1 |
| 1 | 1A | 1092 | C | 2.0 |
| 14 | 2S | 4 | LEU | 2.0 |
| 16 | 2U | 16 | LYS | 2.0 |
| 16 | 2U | 19 | LYS | 2.0 |
| 21 | 1Z | 102 | LEU | 2.0 |
| 34 | 1c | 12 | LEU | 2.0 |
| 35 | 2d | 135 | LEU | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 38 | 2g | 38 | LEU | 2.0 |
| 48 | 2q | 4 | LYS | 2.0 |
| 12 | 2Q | 132 | VAL | 2.0 |
| 36 | 1e | 49 | PRO | 2.0 |
| 36 | 2e | 118 | ILE | 2.0 |
| 8 | 1I | 36 | ALA | 2.0 |
| 36 | 2e | 140 | ARG | 2.0 |
| 39 | 1h | 85 | ARG | 2.0 |
| 39 | 1h | 91 | ARG | 2.0 |
| 7 | 2H | 109 | PHE | 2.0 |
| 37 | 1f | 92 | LYS | 2.0 |
| 40 | 2i | 70 | LYS | 2.0 |
| 43 | 2l | 46 | LYS | 2.0 |
| 33 | 2b | 196 | LEU | 2.0 |
| 38 | 2g | 99 | LEU | 2.0 |
| 48 | 2q | 98 | LEU | 2.0 |
| 1 | 2A | 734 | A | 2.0 |
| 1 | 2A | 2151 | G | 2.0 |
| 4 | 1E | 196 | VAL | 2.0 |
| 9 | 2N | 140 | VAL | 2.0 |
| 12 | 2Q | 96 | VAL | 2.0 |
| 21 | 2Z | 86 | VAL | 2.0 |
| 32 | 1a | 1503 | A | 2.0 |
| 33 | 2b | 112 | VAL | 2.0 |
| 34 | 1c | 106 | VAL | 2.0 |
| 6 | 2G | 157 | ILE | 2.0 |
| 36 | 2e | 106 | PRO | 2.0 |
| 49 | 2r | 80 | PRO | 2.0 |
| 46 | 1o | 64 | ARG | 2.0 |
| 3 | 1D | 62 | TYR | 2.0 |
| 6 | 2G | 164 | GLU | 2.0 |
| 22 | 20 | 68 | GLU | 2.0 |
| 30 | 28 | 64 | TYR | 2.0 |
| 5 | 2F | 166 | ALA | 2.0 |
| 36 | 2e | 108 | ALA | 2.0 |
| 9 | 2N | 104 | LYS | 2.0 |
| 41 | 1j | 93 | GLY | 2.0 |
| 48 | 1q | 87 | LYS | 2.0 |
| 50 | 2s | 32 | LYS | 2.0 |
| 10 | 2O | 79 | PHE | 2.0 |
| 3 | 2D | 182 | LEU | 2.0 |
| 5 | 1F | 41 | LEU | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | 1D | 3 | VAL | 2.0 |
| 4 | 2E | 189 | PRO | 2.0 |
| 7 | 2H | 76 | VAL | 2.0 |
| 11 | 2P | 72 | PRO | 2.0 |
| 11 | 2P | 125 | VAL | 2.0 |
| 18 | 1W | 92 | ARG | 2.0 |
| 22 | 20 | 79 | VAL | 2.0 |
| 23 | 11 | 51 | VAL | 2.0 |
| 30 | 28 | 14 | VAL | 2.0 |
| 30 | 28 | 22 | VAL | 2.0 |
| 33 | 2b | 136 | VAL | 2.0 |
| 40 | 2i | 86 | VAL | 2.0 |
| 50 | 2s | 51 | VAL | 2.0 |
| 9 | 1N | 71 | ILE | 2.0 |
| 46 | 1o | 3 | ILE | 2.0 |
| 1 | 2A | 968 | G | 2.0 |
| 3 | 2D | 144 | ALA | 2.0 |
| 21 | 2Z | 9 | TYR | 2.0 |
| 32 | 2a | 1035 | A | 2.0 |
| 27 | 25 | 14 | ALA | 2.0 |
| 37 | 2f | 55 | ASP | 2.0 |
| 54 | 2y | 56 | C | 2.0 |
| 47 | 1p | 67 | THR | 2.0 |
| 4 | 2E | 51 | PHE | 2.0 |
| 6 | 1G | 82 | LEU | 2.0 |
| 22 | 20 | 11 | ARG | 2.0 |
| 17 | 2V | 5 | VAL | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 54 | PSU | 2w | 55 | 20/21 | 0.59 | 0.37 | 74,91,97,99 | 0 |
| 54 | 4SU | 2y | 8 | 20/21 | 0.68 | 0.19 | 92,97,104,113 | 0 |
| 54 | 7MG | 2y | 46 | 24/25 | 0.71 | 0.22 | 87,98,104,119 | 0 |
| 54 | PSU | 1w | 55 | 20/21 | 0.72 | 0.28 | 63,85,89,91 | 0 |
| 54 | CM0 | 2y | 34 | 25/26 | 0.73 | 0.49 | 82,94,105,114 | 0 |
| 54 | 7MG | 2w | 46 | 24/25 | 0.75 | 0.18 | 80,90,102,117 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54 | 6MZ | 2y | 37 | 23/24 | 0.76 | 0.31 | 82,87,100,116 | 0 |
| 54 | 4SU | 2w | 8 | 20/21 | 0.77 | 0.22 | 84,94,99,102 | 0 |
| 54 | PSU | 2y | 55 | 20/21 | 0.79 | 0.34 | 85,91,95,96 | 0 |
| 54 | 7MG | 1y | 46 | 24/25 | 0.79 | 0.23 | 82,91,96,99 | 0 |
| 54 | 4SU | 1y | 8 | 20/21 | 0.79 | 0.20 | 82,91,101,109 | 0 |
| 54 | 7MG | 1w | 46 | 24/25 | 0.80 | 0.18 | 74,82,92,94 | 0 |
| 54 | PSU | 1y | 55 | 20/21 | 0.81 | 0.25 | 79,88,95,98 | 0 |
| 54 | CM0 | 1y | 34 | 25/26 | 0.82 | 0.51 | 79,86,99,109 | 0 |
| 54 | 5MU | 2w | 54 | 21/22 | 0.84 | 0.23 | 74,81,87,90 | 0 |
| 54 | 5MU | 1y | 54 | 21/22 | 0.85 | 0.21 | 70,80,88,93 | 0 |
| 54 | 5MU | 2y | 54 | 21/22 | 0.86 | 0.28 | 82,90,102,115 | 0 |
| 55 | PSU | 2x | 55 | 20/21 | 0.86 | 0.16 | 67,73,86,93 | 0 |
| 54 | 6MZ | 1y | 37 | 23/24 | 0.86 | 0.32 | 77,82,92,107 | 0 |
| 54 | 4SU | 1w | 8 | 20/21 | 0.89 | 0.19 | 72,81,90,90 | 0 |
| 32 | PSU | 2a | 516 | 20/21 | 0.91 | 0.18 | 63,68,72,80 | 0 |
| 55 | 4SU | 2x | 8 | 20/21 | 0.91 | 0.13 | 71,76,79,87 | 0 |
| 32 | 2MG | 2a | 1207 | 24/25 | 0.91 | 0.17 | 54,77,82,86 | 0 |
| 32 | 5MC | 2a | 967 | 21/22 | 0.92 | 0.27 | 58,65,74,77 | 0 |
| 1 | 5MU | 2A | 1915 | 21/22 | 0.92 | 0.17 | 62,68,77,81 | 0 |
| 54 | 6MZ | 2w | 37 | 23/24 | 0.92 | 0.31 | 62,69,76,77 | 0 |
| 54 | CM0 | 2w | 34 | 25/26 | 0.92 | 0.23 | 60,71,78,90 | 0 |
| 32 | M2G | 2a | 966 | 25/26 | 0.92 | 0.26 | 53,63,72,76 | 0 |
| 43 | 0TD | 2l | 92 | 10/11 | 0.93 | 0.30 | 56,61,66,79 | 0 |
| 43 | 0TD | 1l | 92 | 10/11 | 0.93 | 0.21 | 35,41,44,49 | 0 |
| 55 | 4SU | 1x | 8 | 20/21 | 0.93 | 0.18 | 47,62,75,77 | 0 |
| 54 | CM0 | 1w | 34 | 25/26 | 0.94 | 0.20 | 53,60,68,73 | 0 |
| 32 | 7MG | 2a | 527 | 24/25 | 0.94 | 0.19 | 54,62,69,71 | 0 |
| 1 | 5MU | 1A | 1915 | 21/22 | 0.94 | 0.21 | 46,52,58,60 | 0 |
| 32 | 5MC | 2a | 1407 | 21/22 | 0.94 | 0.26 | 46,54,61,74 | 0 |
| 1 | PSU | 2A | 1917 | 20/21 | 0.94 | 0.18 | 48,58,66,68 | 0 |
| 55 | 5MU | 2x | 54 | 21/22 | 0.94 | 0.17 | 72,76,83,85 | 0 |
| 54 | 5MU | 1w | 54 | 21/22 | 0.94 | 0.18 | 52,67,79,83 | 0 |
| 32 | 5MC | 2a | 1400 | 21/22 | 0.94 | 0.29 | 56,62,67,67 | 0 |
| 55 | 5MC | 2x | 32 | 21/22 | 0.95 | 0.26 | 60,67,74,75 | 0 |
| 32 | MA6 | 2a | 1519 | 24/25 | 0.95 | 0.35 | 43,57,63,65 | 0 |
| 1 | PSU | 2A | 1911 | 20/21 | 0.95 | 0.19 | 53,58,60,63 | 0 |
| 54 | 6MZ | 1w | 37 | 23/24 | 0.95 | 0.23 | 40,46,53,54 | 0 |
| 32 | MA6 | 2a | 1518 | 24/25 | 0.95 | 0.32 | 43,54,61,63 | 0 |
| 55 | PSU | 1x | 55 | 20/21 | 0.95 | 0.16 | 50,62,65,72 | 0 |
| 32 | 4OC | 2a | 1402 | 22/23 | 0.95 | 0.22 | 45,58,61,62 | 0 |
| 55 | 5MU | 1x | 54 | 21/22 | 0.95 | 0.15 | 54,62,70,75 | 0 |
| 32 | 7MG | 1a | 527 | 24/25 | 0.96 | 0.21 | 28,38,44,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 1 | PSU | 2A | 2605 | 20/21 | 0.96 | 0.20 | 29,38,42,46 | 0 |
| 32 | 5MC | 1a | 1400 | 21/22 | 0.96 | 0.21 | 30,40,46,48 | 0 |
| 1 | OMC | 2A | 1920 | 21/22 | 0.96 | 0.23 | 49,58,60,62 | 0 |
| 1 | 5MC | 2A | 1962 | 21/22 | 0.96 | 0.17 | 39,50,54,56 | 0 |
| 1 | 5MC | 2A | 1942 | 21/22 | 0.96 | 0.19 | 47,56,62,68 | 0 |
| 32 | 5MC | 2a | 1404 | 21/22 | 0.96 | 0.22 | 46,51,57,58 | 0 |
| 32 | 4OC | 1a | 1402 | 22/23 | 0.96 | 0.22 | 27,41,47,53 | 0 |
| 32 | PSU | 1a | 516 | 20/21 | 0.96 | 0.17 | 40,49,51,54 | 0 |
| 1 | 5MC | 1A | 1962 | 21/22 | 0.97 | 0.19 | 26,32,35,45 | 0 |
| 1 | PSU | 1A | 1911 | 20/21 | 0.97 | 0.20 | 37,44,51,53 | 0 |
| 55 | 5MC | 1x | 32 | 21/22 | 0.97 | 0.21 | 36,49,52,56 | 0 |
| 32 | 5MC | 1a | 1404 | 21/22 | 0.97 | 0.21 | 28,31,36,37 | 0 |
| 1 | OMG | 2A | 2251 | 24/25 | 0.97 | 0.22 | 33,39,43,46 | 0 |
| 32 | UR3 | 2a | 1498 | 21/22 | 0.97 | 0.26 | 39,53,60,64 | 0 |
| 32 | 5MC | 1a | 967 | 21/22 | 0.97 | 0.23 | 40,46,50,53 | 0 |
| 32 | 2MG | 1a | 1207 | 24/25 | 0.97 | 0.17 | 51,59,62,69 | 0 |
| 1 | PSU | 1A | 1917 | 20/21 | 0.97 | 0.18 | 37,47,51,52 | 0 |
| 32 | M2G | 1a | 966 | 25/26 | 0.97 | 0.22 | 37,45,51,55 | 0 |
| 32 | MA6 | 1a | 1519 | 24/25 | 0.97 | 0.23 | 28,33,42,44 | 0 |
| 32 | MA6 | 1a | 1518 | 24/25 | 0.97 | 0.23 | 26,33,37,43 | 0 |
| 1 | 5MC | 1A | 1942 | 21/22 | 0.97 | 0.19 | 32,38,44,52 | 0 |
| 1 | 5MU | 2A | 1939 | 21/22 | 0.98 | 0.20 | 38,40,42,50 | 0 |
| 1 | OMU | 1A | 2552 | 21/22 | 0.98 | 0.20 | 18,26,30,31 | 0 |
| 1 | 2MA | 2A | 2503 | 23/24 | 0.98 | 0.23 | 25,29,36,40 | 0 |
| 1 | 5MU | 1A | 1939 | 21/22 | 0.98 | 0.21 | 15,23,26,36 | 0 |
| 32 | 5MC | 1a | 1407 | 21/22 | 0.98 | 0.23 | 31,35,39,44 | 0 |
| 1 | PSU | 1A | 2605 | 20/21 | 0.98 | 0.20 | 16,22,30,30 | 0 |
| 1 | OMC | 1A | 1920 | 21/22 | 0.98 | 0.21 | 30,40,46,51 | 0 |
| 1 | OMG | 1A | 2251 | 24/25 | 0.98 | 0.19 | 14,19,20,21 | 0 |
| 32 | UR3 | 1a | 1498 | 21/22 | 0.98 | 0.23 | 26,33,37,41 | 0 |
| 1 | 2MA | 1A | 2503 | 23/24 | 0.98 | 0.21 | 11,14,17,18 | 0 |
| 1 | OMU | 2A | 2552 | 21/22 | 0.98 | 0.21 | 27,37,43,48 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 56 | MG | 1a | 1786 | 1/1 | -0.11 | 0.28 | 84,84,84,84 | 0 |
| 56 | MG | 1A | 3993 | 1/1 | 0.18 | 0.60 | 86,86,86,86 | 0 |
| 56 | MG | 1l | 202 | 1/1 | 0.24 | 0.41 | 82,82,82,82 | 0 |
| 56 | MG | 2a | 3173 | 1/1 | 0.24 | 0.21 | 86,86,86,86 | 0 |
| 56 | MG | 2a | 3106 | 1/1 | 0.30 | 0.19 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3975 | 1/1 | 0.34 | 0.31 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3973 | 1/1 | 0.35 | 0.21 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 4036 | 1/1 | 0.42 | 0.28 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4075 | 1/1 | 0.42 | 0.21 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 4027 | 1/1 | 0.44 | 0.22 | 80,80,80,80 | 0 |
| 56 | MG | 2B | 209 | 1/1 | 0.44 | 0.19 | 72,72,72,72 | 0 |
| 56 | MG | 2a | 3077 | 1/1 | 0.47 | 0.18 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3824 | 1/1 | 0.48 | 0.20 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3912 | 1/1 | 0.48 | 0.24 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4045 | 1/1 | 0.48 | 0.22 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4028 | 1/1 | 0.50 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3097 | 1/1 | 0.52 | 0.28 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 4044 | 1/1 | 0.52 | 0.25 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3990 | 1/1 | 0.52 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1760 | 1/1 | 0.53 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1x | 114 | 1/1 | 0.53 | 0.35 | 74,74,74,74 | 0 |
| 56 | MG | 2Q | 202 | 1/1 | 0.54 | 0.33 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3141 | 1/1 | 0.55 | 0.21 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3881 | 1/1 | 0.56 | 0.17 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3318 | 1/1 | 0.56 | 0.21 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4014 | 1/1 | 0.56 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3781 | 1/1 | 0.56 | 0.14 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3888 | 1/1 | 0.57 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3135 | 1/1 | 0.58 | 0.10 | 78,78,78,78 | 0 |
| 56 | MG | 1A | 3591 | 1/1 | 0.59 | 0.18 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1793 | 1/1 | 0.60 | 0.15 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3784 | 1/1 | 0.60 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3947 | 1/1 | 0.61 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1B | 218 | 1/1 | 0.61 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3095 | 1/1 | 0.62 | 0.20 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 3100 | 1/1 | 0.62 | 0.38 | 61,61,61,61 | 0 |
| 56 | MG | 2B | 212 | 1/1 | 0.62 | 0.19 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3177 | 1/1 | 0.62 | 0.70 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1612 | 1/1 | 0.62 | 0.18 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4061 | 1/1 | 0.62 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3161 | 1/1 | 0.63 | 0.12 | 65,65,65,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3416 | 1/1 | 0.63 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3046 | 1/1 | 0.63 | 0.20 | 72,72,72,72 | 0 |
| 56 | MG | 1a | 1790 | 1/1 | 0.63 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3613 | 1/1 | 0.63 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3164 | 1/1 | 0.63 | 0.16 | 83,83,83,83 | 0 |
| 56 | MG | 2a | 3219 | 1/1 | 0.63 | 0.31 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3148 | 1/1 | 0.63 | 0.15 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3948 | 1/1 | 0.63 | 0.41 | 69,69,69,69 | 0 |
| 56 | MG | 2a | 3043 | 1/1 | 0.63 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3538 | 1/1 | 0.64 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 4040 | 1/1 | 0.64 | 0.35 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 4060 | 1/1 | 0.64 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4083 | 1/1 | 0.64 | 0.15 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3835 | 1/1 | 0.64 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3624 | 1/1 | 0.64 | 0.25 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 4017 | 1/1 | 0.64 | 0.41 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 4098 | 1/1 | 0.65 | 0.45 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1784 | 1/1 | 0.65 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3769 | 1/1 | 0.65 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3368 | 1/1 | 0.65 | 0.36 | 58,58,58,58 | 0 |
| 56 | MG | 2a | 3020 | 1/1 | 0.65 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3424 | 1/1 | 0.66 | 0.23 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3356 | 1/1 | 0.66 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1627 | 1/1 | 0.66 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3720 | 1/1 | 0.66 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4048 | 1/1 | 0.66 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3314 | 1/1 | 0.66 | 0.13 | 60,60,60,60 | 0 |
| 56 | MG | 1Q | 205 | 1/1 | 0.66 | 0.30 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3657 | 1/1 | 0.66 | 0.18 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3949 | 1/1 | 0.66 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 1E | 302 | 1/1 | 0.66 | 0.74 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1825 | 1/1 | 0.67 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1781 | 1/1 | 0.67 | 0.08 | 64,64,64,64 | 0 |
| 56 | MG | 1a | 1792 | 1/1 | 0.67 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3571 | 1/1 | 0.67 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3411 | 1/1 | 0.67 | 0.23 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3503 | 1/1 | 0.67 | 0.43 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3241 | 1/1 | 0.68 | 0.23 | 55,55,55,55 | 0 |
| 56 | MG | 1v | 101 | 1/1 | 0.68 | 0.49 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3072 | 1/1 | 0.68 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4054 | 1/1 | 0.68 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1815 | 1/1 | 0.68 | 0.19 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3943 | 1/1 | 0.68 | 0.21 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 4024 | 1/1 | 0.68 | 0.16 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3251 | 1/1 | 0.69 | 0.58 | 53,53,53,53 | 0 |
| 56 | MG | 2y | 103 | 1/1 | 0.69 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3750 | 1/1 | 0.69 | 0.20 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3062 | 1/1 | 0.69 | 0.25 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3821 | 1/1 | 0.70 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3091 | 1/1 | 0.70 | 0.82 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1675 | 1/1 | 0.70 | 0.21 | 68,68,68,68 | 0 |
| 56 | MG | 1x | 108 | 1/1 | 0.70 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | 2y | 102 | 1/1 | 0.70 | 0.11 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3355 | 1/1 | 0.70 | 0.27 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3065 | 1/1 | 0.71 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3775 | 1/1 | 0.71 | 0.36 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4021 | 1/1 | 0.71 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3015 | 1/1 | 0.71 | 0.56 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3373 | 1/1 | 0.71 | 0.19 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3133 | 1/1 | 0.71 | 0.09 | 76,76,76,76 | 0 |
| 56 | MG | 2y | 105 | 1/1 | 0.71 | 0.12 | 85,85,85,85 | 0 |
| 56 | MG | 1A | 3970 | 1/1 | 0.71 | 0.30 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3271 | 1/1 | 0.71 | 0.15 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3292 | 1/1 | 0.71 | 0.26 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3940 | 1/1 | 0.71 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3669 | 1/1 | 0.71 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3801 | 1/1 | 0.71 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3165 | 1/1 | 0.71 | 0.28 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1712 | 1/1 | 0.71 | 0.32 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3620 | 1/1 | 0.71 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3489 | 1/1 | 0.72 | 0.36 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1606 | 1/1 | 0.72 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3849 | 1/1 | 0.72 | 0.19 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 3218 | 1/1 | 0.72 | 0.14 | 69,69,69,69 | 0 |
| 56 | MG | 1x | 112 | 1/1 | 0.73 | 0.19 | 67,67,67,67 | 0 |
| 56 | MG | 1B | 227 | 1/1 | 0.73 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3433 | 1/1 | 0.73 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3162 | 1/1 | 0.73 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3392 | 1/1 | 0.73 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3500 | 1/1 | 0.73 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3789 | 1/1 | 0.73 | 0.17 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3216 | 1/1 | 0.73 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3567 | 1/1 | 0.73 | 0.15 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3627 | 1/1 | 0.73 | 0.13 | 15,15,15,15 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3419 | 1/1 | 0.73 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3625 | 1/1 | 0.73 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3104 | 1/1 | 0.73 | 0.35 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3945 | 1/1 | 0.73 | 0.22 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3232 | 1/1 | 0.73 | 0.40 | 65,65,65,65 | 0 |
| 56 | MG | 1y | 105 | 1/1 | 0.73 | 0.44 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 3478 | 1/1 | 0.73 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3360 | 1/1 | 0.73 | 0.78 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3649 | 1/1 | 0.73 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3253 | 1/1 | 0.74 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3911 | 1/1 | 0.74 | 0.18 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3224 | 1/1 | 0.74 | 0.09 | 69,69,69,69 | 0 |
| 56 | MG | 1a | 1718 | 1/1 | 0.74 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3942 | 1/1 | 0.74 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3370 | 1/1 | 0.74 | 0.15 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3641 | 1/1 | 0.74 | 0.10 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 4032 | 1/1 | 0.74 | 0.14 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3346 | 1/1 | 0.74 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3992 | 1/1 | 0.74 | 0.35 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3238 | 1/1 | 0.74 | 0.35 | 42,42,42,42 | 0 |
| 56 | MG | 2e | 201 | 1/1 | 0.74 | 0.13 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3080 | 1/1 | 0.74 | 0.15 | 63,63,63,63 | 0 |
| 56 | MG | 1a | 1639 | 1/1 | 0.75 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3647 | 1/1 | 0.75 | 0.58 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3266 | 1/1 | 0.75 | 0.27 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3759 | 1/1 | 0.75 | 0.34 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3280 | 1/1 | 0.75 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3878 | 1/1 | 0.75 | 0.15 | 13,13,13,13 | 0 |
| 56 | MG | 1a | 1801 | 1/1 | 0.75 | 0.23 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3857 | 1/1 | 0.75 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1808 | 1/1 | 0.75 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3652 | 1/1 | 0.75 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3722 | 1/1 | 0.75 | 0.29 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3797 | 1/1 | 0.75 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3288 | 1/1 | 0.75 | 0.82 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4006 | 1/1 | 0.75 | 0.08 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3565 | 1/1 | 0.75 | 0.33 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3149 | 1/1 | 0.76 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3982 | 1/1 | 0.76 | 0.14 | 10,10,10,10 | 0 |
| 56 | MG | 2A | 3319 | 1/1 | 0.76 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3629 | 1/1 | 0.76 | 0.15 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 4101 | 1/1 | 0.76 | 0.21 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3834 | 1/1 | 0.76 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3121 | 1/1 | 0.76 | 0.16 | 63,63,63,63 | 0 |
| 56 | MG | 2B | 210 | 1/1 | 0.76 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3749 | 1/1 | 0.76 | 0.12 | 68,68,68,68 | 0 |
| 56 | MG | 2a | 3027 | 1/1 | 0.76 | 0.63 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 3003 | 1/1 | 0.76 | 0.15 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3278 | 1/1 | 0.76 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3354 | 1/1 | 0.76 | 0.57 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1622 | 1/1 | 0.77 | 0.42 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1689 | 1/1 | 0.77 | 0.21 | 35,35,35,35 | 0 |
| 56 | MG | 1B | 209 | 1/1 | 0.77 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3996 | 1/1 | 0.77 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 2F | 303 | 1/1 | 0.77 | 0.82 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3268 | 1/1 | 0.77 | 0.11 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3106 | 1/1 | 0.77 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 2G | 201 | 1/1 | 0.77 | 0.13 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1706 | 1/1 | 0.77 | 0.25 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3978 | 1/1 | 0.77 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3512 | 1/1 | 0.77 | 0.11 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3869 | 1/1 | 0.77 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3674 | 1/1 | 0.77 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3962 | 1/1 | 0.77 | 0.23 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3049 | 1/1 | 0.77 | 0.52 | 73,73,73,73 | 0 |
| 56 | MG | 1a | 1807 | 1/1 | 0.77 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1812 | 1/1 | 0.77 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3321 | 1/1 | 0.77 | 0.36 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3359 | 1/1 | 0.77 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3780 | 1/1 | 0.78 | 0.07 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3048 | 1/1 | 0.78 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1823 | 1/1 | 0.78 | 0.16 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3519 | 1/1 | 0.78 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3837 | 1/1 | 0.78 | 0.22 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3001 | 1/1 | 0.78 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3995 | 1/1 | 0.78 | 0.08 | 36,36,36,36 | 0 |
| 56 | MG | 1I | 201 | 1/1 | 0.78 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3007 | 1/1 | 0.78 | 0.20 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3016 | 1/1 | 0.78 | 0.47 | 73,73,73,73 | 0 |
| 56 | MG | 2A | 3218 | 1/1 | 0.78 | 0.32 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3618 | 1/1 | 0.78 | 0.19 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3507 | 1/1 | 0.78 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3690 | 1/1 | 0.78 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3936 | 1/1 | 0.78 | 0.37 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1B | 231 | 1/1 | 0.78 | 0.22 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4111 | 1/1 | 0.78 | 0.31 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1759 | 1/1 | 0.78 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1810 | 1/1 | 0.78 | 0.28 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3721 | 1/1 | 0.78 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1751 | 1/1 | 0.78 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3756 | 1/1 | 0.78 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3845 | 1/1 | 0.78 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3449 | 1/1 | 0.78 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3941 | 1/1 | 0.78 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3812 | 1/1 | 0.78 | 0.18 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3854 | 1/1 | 0.79 | 0.58 | 39,39,39,39 | 0 |
| 56 | MG | 2F | 301 | 1/1 | 0.79 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1605 | 1/1 | 0.79 | 0.67 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1699 | 1/1 | 0.79 | 0.24 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3071 | 1/1 | 0.79 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3426 | 1/1 | 0.79 | 0.38 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1603 | 1/1 | 0.79 | 0.48 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1628 | 1/1 | 0.79 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3534 | 1/1 | 0.79 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3053 | 1/1 | 0.79 | 0.23 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1822 | 1/1 | 0.79 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4103 | 1/1 | 0.79 | 0.15 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3453 | 1/1 | 0.79 | 0.41 | 37,37,37,37 | 0 |
| 56 | MG | 1x | 101 | 1/1 | 0.79 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3011 | 1/1 | 0.79 | 0.20 | 58,58,58,58 | 0 |
| 56 | MG | 1G | 202 | 1/1 | 0.79 | 0.22 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3331 | 1/1 | 0.79 | 0.33 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3151 | 1/1 | 0.79 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3177 | 1/1 | 0.79 | 0.21 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3386 | 1/1 | 0.79 | 0.19 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3917 | 1/1 | 0.79 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3886 | 1/1 | 0.79 | 0.39 | 50,50,50,50 | 0 |
| 56 | MG | 1E | 305 | 1/1 | 0.79 | 0.14 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3951 | 1/1 | 0.79 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3466 | 1/1 | 0.79 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3028 | 1/1 | 0.79 | 0.13 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3525 | 1/1 | 0.79 | 0.83 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4030 | 1/1 | 0.79 | 0.07 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3414 | 1/1 | 0.79 | 0.30 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1796 | 1/1 | 0.79 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1662 | 1/1 | 0.79 | 0.16 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3750 | 1/1 | 0.79 | 0.29 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3178 | 1/1 | 0.80 | 0.42 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3103 | 1/1 | 0.80 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3539 | 1/1 | 0.80 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3522 | 1/1 | 0.80 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3259 | 1/1 | 0.80 | 0.36 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3204 | 1/1 | 0.80 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3148 | 1/1 | 0.80 | 0.27 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3761 | 1/1 | 0.80 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3335 | 1/1 | 0.80 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1818 | 1/1 | 0.80 | 0.12 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3969 | 1/1 | 0.80 | 0.17 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3326 | 1/1 | 0.80 | 0.33 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3225 | 1/1 | 0.80 | 0.27 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3154 | 1/1 | 0.80 | 0.12 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 3788 | 1/1 | 0.80 | 0.18 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3700 | 1/1 | 0.80 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3853 | 1/1 | 0.80 | 0.20 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1601 | 1/1 | 0.80 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3086 | 1/1 | 0.80 | 0.25 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3809 | 1/1 | 0.80 | 0.30 | 50,50,50,50 | 0 |
| 56 | MG | 1w | 106 | 1/1 | 0.80 | 0.19 | 75,75,75,75 | 0 |
| 56 | MG | 2A | 3413 | 1/1 | 0.80 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1761 | 1/1 | 0.80 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3457 | 1/1 | 0.80 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3844 | 1/1 | 0.80 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3070 | 1/1 | 0.80 | 0.21 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3737 | 1/1 | 0.80 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 1x | 109 | 1/1 | 0.80 | 0.21 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3702 | 1/1 | 0.80 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1817 | 1/1 | 0.80 | 0.16 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3680 | 1/1 | 0.80 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3173 | 1/1 | 0.80 | 0.28 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3725 | 1/1 | 0.80 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3425 | 1/1 | 0.80 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1615 | 1/1 | 0.80 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3747 | 1/1 | 0.80 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3604 | 1/1 | 0.80 | 0.11 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3807 | 1/1 | 0.80 | 0.37 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3070 | 1/1 | 0.80 | 0.48 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3776 | 1/1 | 0.80 | 0.16 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3246 | 1/1 | 0.80 | 0.32 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2a | 3229 | 1/1 | 0.80 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3670 | 1/1 | 0.80 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4053 | 1/1 | 0.80 | 1.07 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3184 | 1/1 | 0.81 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3191 | 1/1 | 0.81 | 0.38 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3047 | 1/1 | 0.81 | 0.13 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3098 | 1/1 | 0.81 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3298 | 1/1 | 0.81 | 0.24 | 60,60,60,60 | 0 |
| 56 | MG | 1B | 201 | 1/1 | 0.81 | 0.43 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3202 | 1/1 | 0.81 | 0.41 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3665 | 1/1 | 0.81 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3711 | 1/1 | 0.81 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3850 | 1/1 | 0.81 | 0.63 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 3197 | 1/1 | 0.81 | 0.08 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3646 | 1/1 | 0.81 | 0.22 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3469 | 1/1 | 0.81 | 0.28 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3621 | 1/1 | 0.81 | 0.19 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3407 | 1/1 | 0.81 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1672 | 1/1 | 0.81 | 0.34 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3684 | 1/1 | 0.81 | 0.14 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3420 | 1/1 | 0.81 | 0.56 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4095 | 1/1 | 0.81 | 0.31 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3320 | 1/1 | 0.81 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3271 | 1/1 | 0.81 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3085 | 1/1 | 0.81 | 0.16 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3777 | 1/1 | 0.81 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3640 | 1/1 | 0.81 | 0.29 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3240 | 1/1 | 0.81 | 0.30 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3306 | 1/1 | 0.81 | 0.57 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3477 | 1/1 | 0.81 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3069 | 1/1 | 0.81 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3988 | 1/1 | 0.81 | 0.09 | 75,75,75,75 | 0 |
| 56 | MG | 1A | 3316 | 1/1 | 0.82 | 0.19 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3913 | 1/1 | 0.82 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3075 | 1/1 | 0.82 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3821 | 1/1 | 0.82 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3470 | 1/1 | 0.82 | 0.30 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1782 | 1/1 | 0.82 | 0.08 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3325 | 1/1 | 0.82 | 0.34 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3269 | 1/1 | 0.82 | 0.19 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3842 | 1/1 | 0.82 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3159 | 1/1 | 0.82 | 0.10 | 66,66,66,66 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1a | 1641 | 1/1 | 0.82 | 0.21 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3281 | 1/1 | 0.82 | 0.17 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3594 | 1/1 | 0.82 | 0.16 | 71,71,71,71 | 0 |
| 56 | MG | 2a | 3167 | 1/1 | 0.82 | 0.07 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3830 | 1/1 | 0.82 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3488 | 1/1 | 0.82 | 0.82 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3110 | 1/1 | 0.82 | 0.32 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3755 | 1/1 | 0.82 | 0.22 | 16,16,16,16 | 0 |
| 56 | MG | 1a | 1633 | 1/1 | 0.82 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3916 | 1/1 | 0.82 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3910 | 1/1 | 0.82 | 0.06 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1619 | 1/1 | 0.82 | 0.11 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3405 | 1/1 | 0.82 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3256 | 1/1 | 0.82 | 0.18 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3699 | 1/1 | 0.82 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3144 | 1/1 | 0.82 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4064 | 1/1 | 0.82 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3178 | 1/1 | 0.82 | 0.11 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3199 | 1/1 | 0.82 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4057 | 1/1 | 0.82 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3919 | 1/1 | 0.82 | 0.13 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3741 | 1/1 | 0.82 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3425 | 1/1 | 0.82 | 0.11 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3213 | 1/1 | 0.82 | 0.24 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3357 | 1/1 | 0.82 | 0.24 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4029 | 1/1 | 0.82 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 1a | 1776 | 1/1 | 0.82 | 0.19 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3534 | 1/1 | 0.82 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 2y | 104 | 1/1 | 0.82 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3156 | 1/1 | 0.82 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1827 | 1/1 | 0.82 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3445 | 1/1 | 0.82 | 0.36 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3591 | 1/1 | 0.83 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3165 | 1/1 | 0.83 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3760 | 1/1 | 0.83 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3168 | 1/1 | 0.83 | 0.34 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3361 | 1/1 | 0.83 | 0.57 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1636 | 1/1 | 0.83 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1637 | 1/1 | 0.83 | 0.22 | 49,49,49,49 | 0 |
| 59 | ZN | 24 | 501 | 1/1 | 0.83 | 0.05 | 113,113,113,113 | 0 |
| 56 | MG | 2V | 202 | 1/1 | 0.83 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3766 | 1/1 | 0.83 | 0.08 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 25 | 101 | 1/1 | 0.83 | 0.29 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3983 | 1/1 | 0.83 | 0.15 | 21,21,21,21 | 0 |
| 56 | MG | 2a | 3037 | 1/1 | 0.83 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3155 | 1/1 | 0.83 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3809 | 1/1 | 0.83 | 0.18 | 12,12,12,12 | 0 |
| 56 | MG | 2A | 3252 | 1/1 | 0.83 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3166 | 1/1 | 0.83 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3735 | 1/1 | 0.83 | 0.17 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3539 | 1/1 | 0.83 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3545 | 1/1 | 0.83 | 0.18 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3313 | 1/1 | 0.83 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4023 | 1/1 | 0.83 | 0.24 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3798 | 1/1 | 0.83 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | 2B | 204 | 1/1 | 0.83 | 0.13 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3411 | 1/1 | 0.83 | 0.50 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3024 | 1/1 | 0.83 | 0.14 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3934 | 1/1 | 0.83 | 0.23 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3632 | 1/1 | 0.83 | 0.15 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3827 | 1/1 | 0.83 | 0.21 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3092 | 1/1 | 0.83 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3398 | 1/1 | 0.83 | 0.31 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3994 | 1/1 | 0.83 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3779 | 1/1 | 0.83 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3501 | 1/1 | 0.83 | 0.39 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3710 | 1/1 | 0.83 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3136 | 1/1 | 0.83 | 0.23 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3521 | 1/1 | 0.83 | 0.15 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3819 | 1/1 | 0.83 | 0.18 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3582 | 1/1 | 0.83 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1645 | 1/1 | 0.83 | 0.34 | 54,54,54,54 | 0 |
| 56 | MG | 1f | 202 | 1/1 | 0.83 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3395 | 1/1 | 0.83 | 0.39 | 29,29,29,29 | 0 |
| 56 | MG | 20 | 102 | 1/1 | 0.83 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3731 | 1/1 | 0.83 | 0.19 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3448 | 1/1 | 0.83 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3112 | 1/1 | 0.83 | 0.23 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4079 | 1/1 | 0.83 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1a | 1809 | 1/1 | 0.83 | 0.44 | 69,69,69,69 | 0 |
| 56 | MG | 10 | 105 | 1/1 | 0.83 | 0.24 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3597 | 1/1 | 0.83 | 0.06 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3140 | 1/1 | 0.84 | 0.23 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3651 | 1/1 | 0.84 | 0.12 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 4011 | 1/1 | 0.84 | 0.14 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3628 | 1/1 | 0.84 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3176 | 1/1 | 0.84 | 0.37 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4012 | 1/1 | 0.84 | 0.17 | 17,17,17,17 | 0 |
| 56 | MG | 2a | 3055 | 1/1 | 0.84 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3861 | 1/1 | 0.84 | 0.33 | 46,46,46,46 | 0 |
| 56 | MG | 2I | 101 | 1/1 | 0.84 | 0.78 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3514 | 1/1 | 0.84 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3596 | 1/1 | 0.84 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3549 | 1/1 | 0.84 | 0.08 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3146 | 1/1 | 0.84 | 0.19 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3370 | 1/1 | 0.84 | 0.36 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3459 | 1/1 | 0.84 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 1B | 236 | 1/1 | 0.84 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3490 | 1/1 | 0.84 | 0.30 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3230 | 1/1 | 0.84 | 0.37 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3220 | 1/1 | 0.84 | 0.23 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1709 | 1/1 | 0.84 | 0.55 | 56,56,56,56 | 0 |
| 56 | MG | 1x | 103 | 1/1 | 0.84 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3175 | 1/1 | 0.84 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3827 | 1/1 | 0.84 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3334 | 1/1 | 0.84 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1683 | 1/1 | 0.84 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3432 | 1/1 | 0.84 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3311 | 1/1 | 0.84 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3142 | 1/1 | 0.84 | 0.36 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3367 | 1/1 | 0.84 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3349 | 1/1 | 0.84 | 0.87 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3310 | 1/1 | 0.84 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3722 | 1/1 | 0.84 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3243 | 1/1 | 0.84 | 0.40 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3739 | 1/1 | 0.84 | 0.26 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3504 | 1/1 | 0.84 | 0.25 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3439 | 1/1 | 0.84 | 0.36 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3261 | 1/1 | 0.84 | 0.25 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3585 | 1/1 | 0.84 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3405 | 1/1 | 0.84 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3541 | 1/1 | 0.84 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3847 | 1/1 | 0.84 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3006 | 1/1 | 0.84 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1640 | 1/1 | 0.84 | 0.29 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3344 | 1/1 | 0.84 | 0.18 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3020 | 1/1 | 0.84 | 0.19 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3536 | 1/1 | 0.84 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3119 | 1/1 | 0.84 | 0.28 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3276 | 1/1 | 0.84 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3782 | 1/1 | 0.84 | 0.26 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3322 | 1/1 | 0.84 | 0.34 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3026 | 1/1 | 0.84 | 0.42 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3390 | 1/1 | 0.84 | 0.24 | 45,45,45,45 | 0 |
| 56 | MG | 2r | 101 | 1/1 | 0.84 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1693 | 1/1 | 0.85 | 0.40 | 66,66,66,66 | 0 |
| 56 | MG | 1a | 1730 | 1/1 | 0.85 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | 1N | 206 | 1/1 | 0.85 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3872 | 1/1 | 0.85 | 0.14 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3792 | 1/1 | 0.85 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3556 | 1/1 | 0.85 | 0.37 | 40,40,40,40 | 0 |
| 56 | MG | 1P | 202 | 1/1 | 0.85 | 0.11 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3124 | 1/1 | 0.85 | 0.20 | 68,68,68,68 | 0 |
| 56 | MG | 2A | 3448 | 1/1 | 0.85 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3024 | 1/1 | 0.85 | 1.25 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1797 | 1/1 | 0.85 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1614 | 1/1 | 0.85 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3403 | 1/1 | 0.85 | 0.18 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3267 | 1/1 | 0.85 | 0.38 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3744 | 1/1 | 0.85 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3586 | 1/1 | 0.85 | 0.25 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1795 | 1/1 | 0.85 | 0.13 | 58,58,58,58 | 0 |
| 56 | MG | 1Z | 304 | 1/1 | 0.85 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3752 | 1/1 | 0.85 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 1w | 102 | 1/1 | 0.85 | 0.31 | 60,60,60,60 | 0 |
| 56 | MG | 1B | 206 | 1/1 | 0.85 | 0.19 | 46,46,46,46 | 0 |
| 56 | MG | 1y | 103 | 1/1 | 0.85 | 0.12 | 72,72,72,72 | 0 |
| 56 | MG | 1A | 3007 | 1/1 | 0.85 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3359 | 1/1 | 0.85 | 0.30 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1767 | 1/1 | 0.85 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3421 | 1/1 | 0.85 | 0.17 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1834 | 1/1 | 0.85 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3082 | 1/1 | 0.85 | 0.22 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3876 | 1/1 | 0.85 | 0.40 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1727 | 1/1 | 0.85 | 0.43 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3861 | 1/1 | 0.85 | 0.31 | 30,30,30,30 | 0 |
| 56 | MG | 1F | 308 | 1/1 | 0.85 | 0.23 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3615 | 1/1 | 0.85 | 0.16 | 29,29,29,29 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 4071 | 1/1 | 0.85 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3367 | 1/1 | 0.85 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3956 | 1/1 | 0.85 | 0.41 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3754 | 1/1 | 0.85 | 0.14 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3665 | 1/1 | 0.85 | 0.15 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3016 | 1/1 | 0.85 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3025 | 1/1 | 0.85 | 0.95 | 57,57,57,57 | 0 |
| 56 | MG | 1w | 105 | 1/1 | 0.85 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 2B | 202 | 1/1 | 0.85 | 0.27 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3840 | 1/1 | 0.85 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3205 | 1/1 | 0.85 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3052 | 1/1 | 0.85 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3770 | 1/1 | 0.85 | 0.20 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3260 | 1/1 | 0.85 | 0.60 | 59,59,59,59 | 0 |
| 56 | MG | 1a | 1604 | 1/1 | 0.85 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3064 | 1/1 | 0.85 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3518 | 1/1 | 0.85 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3307 | 1/1 | 0.85 | 0.27 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1777 | 1/1 | 0.85 | 0.31 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3273 | 1/1 | 0.85 | 0.21 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3442 | 1/1 | 0.85 | 0.30 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3694 | 1/1 | 0.85 | 0.18 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1749 | 1/1 | 0.85 | 0.32 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3793 | 1/1 | 0.85 | 0.18 | 31,31,31,31 | 0 |
| 56 | MG | 2T | 204 | 1/1 | 0.85 | 0.29 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3781 | 1/1 | 0.85 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3786 | 1/1 | 0.85 | 0.13 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3914 | 1/1 | 0.85 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3600 | 1/1 | 0.85 | 0.23 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3667 | 1/1 | 0.85 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3155 | 1/1 | 0.85 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3329 | 1/1 | 0.85 | 0.58 | 58,58,58,58 | 0 |
| 56 | MG | 1B | 225 | 1/1 | 0.85 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3752 | 1/1 | 0.85 | 0.15 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3472 | 1/1 | 0.85 | 0.39 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3078 | 1/1 | 0.85 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3921 | 1/1 | 0.85 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3018 | 1/1 | 0.85 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | 2d | 301 | 1/1 | 0.85 | 0.16 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3343 | 1/1 | 0.85 | 0.11 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3788 | 1/1 | 0.85 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3139 | 1/1 | 0.85 | 0.49 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3108 | 1/1 | 0.85 | 0.35 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3187 | 1/1 | 0.85 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3779 | 1/1 | 0.85 | 0.49 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3598 | 1/1 | 0.85 | 0.18 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3233 | 1/1 | 0.85 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3207 | 1/1 | 0.85 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3615 | 1/1 | 0.85 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1771 | 1/1 | 0.85 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | 2T | 202 | 1/1 | 0.85 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3400 | 1/1 | 0.86 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3150 | 1/1 | 0.86 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3307 | 1/1 | 0.86 | 0.33 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3149 | 1/1 | 0.86 | 0.05 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3216 | 1/1 | 0.86 | 0.73 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3380 | 1/1 | 0.86 | 0.23 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3296 | 1/1 | 0.86 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3803 | 1/1 | 0.86 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3053 | 1/1 | 0.86 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3476 | 1/1 | 0.86 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1N | 204 | 1/1 | 0.86 | 0.72 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3354 | 1/1 | 0.86 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3447 | 1/1 | 0.86 | 0.37 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3442 | 1/1 | 0.86 | 0.35 | 44,44,44,44 | 0 |
| 56 | MG | 1Y | 203 | 1/1 | 0.86 | 0.19 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1780 | 1/1 | 0.86 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1799 | 1/1 | 0.86 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3137 | 1/1 | 0.86 | 0.05 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 4042 | 1/1 | 0.86 | 0.45 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 4066 | 1/1 | 0.86 | 0.33 | 62,62,62,62 | 0 |
| 56 | MG | 2a | 3065 | 1/1 | 0.86 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3712 | 1/1 | 0.86 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3475 | 1/1 | 0.86 | 0.26 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3965 | 1/1 | 0.86 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3483 | 1/1 | 0.86 | 0.15 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3107 | 1/1 | 0.86 | 0.29 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3332 | 1/1 | 0.86 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3286 | 1/1 | 0.86 | 0.42 | 56,56,56,56 | 0 |
| 56 | MG | 1y | 104 | 1/1 | 0.86 | 0.12 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3430 | 1/1 | 0.86 | 0.44 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3009 | 1/1 | 0.86 | 0.38 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3865 | 1/1 | 0.86 | 0.69 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3250 | 1/1 | 0.86 | 0.17 | 31,31,31,31 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1a | 1722 | 1/1 | 0.86 | 0.21 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3081 | 1/1 | 0.86 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3059 | 1/1 | 0.86 | 0.13 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3688 | 1/1 | 0.86 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | 1x | 113 | 1/1 | 0.86 | 0.20 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3603 | 1/1 | 0.86 | 0.18 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1788 | 1/1 | 0.86 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3528 | 1/1 | 0.86 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 2E | 307 | 1/1 | 0.86 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3180 | 1/1 | 0.86 | 0.89 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3829 | 1/1 | 0.86 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 2a | 3033 | 1/1 | 0.86 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3734 | 1/1 | 0.86 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3353 | 1/1 | 0.86 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3623 | 1/1 | 0.86 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3376 | 1/1 | 0.86 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3358 | 1/1 | 0.86 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | 1O | 201 | 1/1 | 0.86 | 0.16 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1720 | 1/1 | 0.86 | 0.26 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3129 | 1/1 | 0.86 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3445 | 1/1 | 0.86 | 1.56 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3431 | 1/1 | 0.86 | 0.18 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4052 | 1/1 | 0.86 | 0.20 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3523 | 1/1 | 0.86 | 0.07 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3364 | 1/1 | 0.86 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1714 | 1/1 | 0.86 | 0.24 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3577 | 1/1 | 0.86 | 0.23 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1667 | 1/1 | 0.86 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3626 | 1/1 | 0.86 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3998 | 1/1 | 0.86 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3161 | 1/1 | 0.86 | 0.25 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3058 | 1/1 | 0.86 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3333 | 1/1 | 0.86 | 0.34 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3727 | 1/1 | 0.86 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3532 | 1/1 | 0.86 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3795 | 1/1 | 0.86 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3971 | 1/1 | 0.86 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3257 | 1/1 | 0.86 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3944 | 1/1 | 0.86 | 0.07 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3953 | 1/1 | 0.86 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3251 | 1/1 | 0.86 | 0.19 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 4020 | 1/1 | 0.86 | 0.22 | 59,59,59,59 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2a | 3002 | 1/1 | 0.86 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3761 | 1/1 | 0.86 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | 1w | 101 | 1/1 | 0.86 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3524 | 1/1 | 0.86 | 0.18 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3244 | 1/1 | 0.86 | 0.26 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4007 | 1/1 | 0.86 | 0.14 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3219 | 1/1 | 0.86 | 0.28 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3263 | 1/1 | 0.86 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3681 | 1/1 | 0.86 | 0.07 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3172 | 1/1 | 0.86 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3787 | 1/1 | 0.86 | 0.15 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3679 | 1/1 | 0.86 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1739 | 1/1 | 0.86 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3771 | 1/1 | 0.86 | 0.15 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3308 | 1/1 | 0.86 | 0.33 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3572 | 1/1 | 0.86 | 0.19 | 75,75,75,75 | 0 |
| 56 | MG | 2a | 3171 | 1/1 | 0.86 | 0.15 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3384 | 1/1 | 0.86 | 0.18 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3541 | 1/1 | 0.86 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 4097 | 1/1 | 0.87 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1779 | 1/1 | 0.87 | 0.12 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3198 | 1/1 | 0.87 | 0.11 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3238 | 1/1 | 0.87 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3832 | 1/1 | 0.87 | 0.36 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3810 | 1/1 | 0.87 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3162 | 1/1 | 0.87 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3433 | 1/1 | 0.87 | 0.61 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3601 | 1/1 | 0.87 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | 1e | 201 | 1/1 | 0.87 | 0.66 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3285 | 1/1 | 0.87 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3010 | 1/1 | 0.87 | 0.30 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3810 | 1/1 | 0.87 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 1Q | 204 | 1/1 | 0.87 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3894 | 1/1 | 0.87 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3856 | 1/1 | 0.87 | 0.77 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3516 | 1/1 | 0.87 | 0.16 | 38,38,38,38 | 0 |
| 56 | MG | 14 | 101 | 1/1 | 0.87 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3342 | 1/1 | 0.87 | 0.98 | 30,30,30,30 | 0 |
| 56 | MG | 1N | 205 | 1/1 | 0.87 | 0.36 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3041 | 1/1 | 0.87 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3563 | 1/1 | 0.87 | 0.27 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3017 | 1/1 | 0.87 | 0.50 | 49,49,49,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3954 | 1/1 | 0.87 | 0.08 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3841 | 1/1 | 0.87 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3193 | 1/1 | 0.87 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3196 | 1/1 | 0.87 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3454 | 1/1 | 0.87 | 0.68 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3403 | 1/1 | 0.87 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3338 | 1/1 | 0.87 | 0.18 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3794 | 1/1 | 0.87 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3468 | 1/1 | 0.87 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3424 | 1/1 | 0.87 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3465 | 1/1 | 0.87 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1695 | 1/1 | 0.87 | 0.21 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1703 | 1/1 | 0.87 | 0.22 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3751 | 1/1 | 0.87 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3364 | 1/1 | 0.87 | 0.39 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3130 | 1/1 | 0.87 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3097 | 1/1 | 0.87 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3035 | 1/1 | 0.87 | 0.17 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 4037 | 1/1 | 0.87 | 0.09 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3968 | 1/1 | 0.87 | 0.10 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3467 | 1/1 | 0.87 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3609 | 1/1 | 0.87 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 2j | 202 | 1/1 | 0.87 | 0.12 | 70,70,70,70 | 0 |
| 56 | MG | 2a | 3054 | 1/1 | 0.87 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3044 | 1/1 | 0.87 | 0.17 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3259 | 1/1 | 0.87 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3481 | 1/1 | 0.87 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3474 | 1/1 | 0.87 | 0.20 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3396 | 1/1 | 0.87 | 0.13 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3500 | 1/1 | 0.87 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3088 | 1/1 | 0.87 | 0.17 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3759 | 1/1 | 0.87 | 0.10 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3071 | 1/1 | 0.87 | 0.85 | 47,47,47,47 | 0 |
| 56 | MG | 2F | 305 | 1/1 | 0.87 | 0.19 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3553 | 1/1 | 0.87 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4035 | 1/1 | 0.87 | 0.34 | 44,44,44,44 | 0 |
| 56 | MG | 2U | 203 | 1/1 | 0.87 | 0.44 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3535 | 1/1 | 0.87 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3034 | 1/1 | 0.87 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3499 | 1/1 | 0.87 | 0.23 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3004 | 1/1 | 0.87 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3602 | 1/1 | 0.87 | 0.14 | 26,26,26,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1a | 1743 | 1/1 | 0.87 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 2B | 206 | 1/1 | 0.87 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3592 | 1/1 | 0.88 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4031 | 1/1 | 0.88 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3522 | 1/1 | 0.88 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1625 | 1/1 | 0.88 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3482 | 1/1 | 0.88 | 0.20 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3214 | 1/1 | 0.88 | 0.13 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3101 | 1/1 | 0.88 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3922 | 1/1 | 0.88 | 0.21 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3323 | 1/1 | 0.88 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3702 | 1/1 | 0.88 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3116 | 1/1 | 0.88 | 0.14 | 65,65,65,65 | 0 |
| 56 | MG | 1a | 1728 | 1/1 | 0.88 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 1N | 202 | 1/1 | 0.88 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1a | 1794 | 1/1 | 0.88 | 0.21 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3099 | 1/1 | 0.88 | 0.16 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1690 | 1/1 | 0.88 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3668 | 1/1 | 0.88 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3188 | 1/1 | 0.88 | 0.14 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3930 | 1/1 | 0.88 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3495 | 1/1 | 0.88 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1x | 115 | 1/1 | 0.88 | 0.26 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3528 | 1/1 | 0.88 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 1Y | 202 | 1/1 | 0.88 | 0.23 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3462 | 1/1 | 0.88 | 0.41 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3379 | 1/1 | 0.88 | 0.21 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3560 | 1/1 | 0.88 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1a | 1711 | 1/1 | 0.88 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3718 | 1/1 | 0.88 | 0.22 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3807 | 1/1 | 0.88 | 0.08 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3616 | 1/1 | 0.88 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3365 | 1/1 | 0.88 | 0.41 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3006 | 1/1 | 0.88 | 0.09 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3923 | 1/1 | 0.88 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3111 | 1/1 | 0.88 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1657 | 1/1 | 0.88 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3504 | 1/1 | 0.88 | 0.32 | 37,37,37,37 | 0 |
| 56 | MG | 10 | 103 | 1/1 | 0.88 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3964 | 1/1 | 0.88 | 0.30 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3817 | 1/1 | 0.88 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 2E | 308 | 1/1 | 0.88 | 0.10 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3049 | 1/1 | 0.88 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1664 | 1/1 | 0.88 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | 2q | 201 | 1/1 | 0.88 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 1F | 304 | 1/1 | 0.88 | 0.34 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3716 | 1/1 | 0.88 | 0.14 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3770 | 1/1 | 0.88 | 0.14 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3245 | 1/1 | 0.88 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1658 | 1/1 | 0.88 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3634 | 1/1 | 0.88 | 0.16 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 4116 | 1/1 | 0.88 | 0.52 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3774 | 1/1 | 0.88 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3543 | 1/1 | 0.88 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3189 | 1/1 | 0.88 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3408 | 1/1 | 0.88 | 0.32 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3199 | 1/1 | 0.88 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4010 | 1/1 | 0.88 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | 2F | 302 | 1/1 | 0.88 | 0.21 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1666 | 1/1 | 0.88 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | 1a | 1735 | 1/1 | 0.88 | 0.16 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3675 | 1/1 | 0.88 | 0.14 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3277 | 1/1 | 0.88 | 0.48 | 61,61,61,61 | 0 |
| 56 | MG | 1B | 234 | 1/1 | 0.88 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3831 | 1/1 | 0.88 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3104 | 1/1 | 0.88 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3733 | 1/1 | 0.88 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3061 | 1/1 | 0.88 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3718 | 1/1 | 0.88 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3719 | 1/1 | 0.88 | 0.09 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3126 | 1/1 | 0.88 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3103 | 1/1 | 0.88 | 0.07 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3662 | 1/1 | 0.88 | 0.10 | 10,10,10,10 | 0 |
| 56 | MG | 2A | 3210 | 1/1 | 0.88 | 0.27 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3860 | 1/1 | 0.88 | 0.36 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3609 | 1/1 | 0.88 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | 1a | 1747 | 1/1 | 0.88 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3382 | 1/1 | 0.88 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3686 | 1/1 | 0.88 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1756 | 1/1 | 0.88 | 0.16 | 67,67,67,67 | 0 |
| 56 | MG | 2a | 3068 | 1/1 | 0.88 | 0.19 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3632 | 1/1 | 0.88 | 0.10 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3152 | 1/1 | 0.88 | 0.52 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 4056 | 1/1 | 0.88 | 0.11 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2a | 3158 | 1/1 | 0.88 | 0.10 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3346 | 1/1 | 0.88 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 4050 | 1/1 | 0.88 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 4086 | 1/1 | 0.88 | 0.23 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3239 | 1/1 | 0.88 | 0.28 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3157 | 1/1 | 0.88 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3907 | 1/1 | 0.88 | 0.55 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1652 | 1/1 | 0.88 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3160 | 1/1 | 0.88 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3554 | 1/1 | 0.88 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3153 | 1/1 | 0.88 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3633 | 1/1 | 0.88 | 0.19 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3309 | 1/1 | 0.88 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3401 | 1/1 | 0.88 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3224 | 1/1 | 0.88 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3190 | 1/1 | 0.88 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3352 | 1/1 | 0.88 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3374 | 1/1 | 0.88 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3090 | 1/1 | 0.88 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3017 | 1/1 | 0.88 | 0.13 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3014 | 1/1 | 0.88 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3062 | 1/1 | 0.88 | 0.19 | 30,30,30,30 | 0 |
| 56 | MG | 2a | 3081 | 1/1 | 0.88 | 0.20 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3790 | 1/1 | 0.88 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3094 | 1/1 | 0.88 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3324 | 1/1 | 0.88 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3205 | 1/1 | 0.88 | 0.22 | 26,26,26,26 | 0 |
| 56 | MG | 2B | 208 | 1/1 | 0.88 | 0.24 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3683 | 1/1 | 0.88 | 0.14 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3379 | 1/1 | 0.89 | 0.63 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3730 | 1/1 | 0.89 | 0.18 | 25,25,25,25 | 0 |
| 56 | MG | 1a | 1678 | 1/1 | 0.89 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3510 | 1/1 | 0.89 | 0.16 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3183 | 1/1 | 0.89 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 13 | 101 | 1/1 | 0.89 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3146 | 1/1 | 0.89 | 0.45 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3290 | 1/1 | 0.89 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3377 | 1/1 | 0.89 | 0.18 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3330 | 1/1 | 0.89 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3165 | 1/1 | 0.89 | 0.20 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4004 | 1/1 | 0.89 | 0.31 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 3349 | 1/1 | 0.89 | 0.18 | 41,41,41,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3255 | 1/1 | 0.89 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3391 | 1/1 | 0.89 | 0.23 | 58,58,58,58 | 0 |
| 56 | MG | 1w | 108 | 1/1 | 0.89 | 0.61 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3622 | 1/1 | 0.89 | 0.08 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3447 | 1/1 | 0.89 | 0.25 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3735 | 1/1 | 0.89 | 0.09 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3090 | 1/1 | 0.89 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1648 | 1/1 | 0.89 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3981 | 1/1 | 0.89 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 1F | 305 | 1/1 | 0.89 | 0.24 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3906 | 1/1 | 0.89 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | 2a | 3111 | 1/1 | 0.89 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3018 | 1/1 | 0.89 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3105 | 1/1 | 0.89 | 0.61 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3785 | 1/1 | 0.89 | 0.14 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3040 | 1/1 | 0.89 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3553 | 1/1 | 0.89 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1674 | 1/1 | 0.89 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3568 | 1/1 | 0.89 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3045 | 1/1 | 0.89 | 0.28 | 67,67,67,67 | 0 |
| 57 | LUJ | 2A | 3851 | 42/44 | 0.89 | 0.32 | 50,62,75,82 | 0 |
| 56 | MG | 2A | 3229 | 1/1 | 0.89 | 0.74 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3201 | 1/1 | 0.89 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3328 | 1/1 | 0.89 | 0.18 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3805 | 1/1 | 0.89 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4118 | 1/1 | 0.89 | 1.01 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3860 | 1/1 | 0.89 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3991 | 1/1 | 0.89 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3214 | 1/1 | 0.89 | 0.31 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3801 | 1/1 | 0.89 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3348 | 1/1 | 0.89 | 0.33 | 63,63,63,63 | 0 |
| 57 | LUJ | 2A | 3852 | 42/44 | 0.89 | 0.56 | 38,59,68,75 | 0 |
| 56 | MG | 2A | 3153 | 1/1 | 0.89 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3204 | 1/1 | 0.89 | 0.51 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3066 | 1/1 | 0.89 | 0.65 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3050 | 1/1 | 0.89 | 0.26 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3143 | 1/1 | 0.89 | 0.26 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3076 | 1/1 | 0.89 | 0.22 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3355 | 1/1 | 0.89 | 0.23 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3636 | 1/1 | 0.89 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 1B | 232 | 1/1 | 0.89 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 1F | 306 | 1/1 | 0.89 | 0.36 | 17,17,17,17 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1a | 1702 | 1/1 | 0.89 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1b | 301 | 1/1 | 0.89 | 0.16 | 76,76,76,76 | 0 |
| 56 | MG | 2A | 3815 | 1/1 | 0.89 | 0.08 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3451 | 1/1 | 0.89 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3136 | 1/1 | 0.89 | 0.15 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3265 | 1/1 | 0.89 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3548 | 1/1 | 0.89 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3427 | 1/1 | 0.89 | 0.55 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1682 | 1/1 | 0.89 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3999 | 1/1 | 0.89 | 0.16 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3843 | 1/1 | 0.89 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3144 | 1/1 | 0.89 | 0.09 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 4049 | 1/1 | 0.89 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | 1B | 230 | 1/1 | 0.89 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3754 | 1/1 | 0.89 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3569 | 1/1 | 0.89 | 0.80 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3663 | 1/1 | 0.89 | 0.14 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3904 | 1/1 | 0.89 | 0.20 | 11,11,11,11 | 0 |
| 56 | MG | 2A | 3785 | 1/1 | 0.89 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3341 | 1/1 | 0.89 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3140 | 1/1 | 0.89 | 0.18 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3171 | 1/1 | 0.89 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3234 | 1/1 | 0.89 | 0.29 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3317 | 1/1 | 0.89 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3270 | 1/1 | 0.89 | 0.56 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3380 | 1/1 | 0.89 | 0.14 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3082 | 1/1 | 0.89 | 0.42 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3728 | 1/1 | 0.89 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1654 | 1/1 | 0.89 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 10 | 102 | 1/1 | 0.89 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3440 | 1/1 | 0.89 | 0.49 | 33,33,33,33 | 0 |
| 56 | MG | 2l | 202 | 1/1 | 0.89 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3134 | 1/1 | 0.89 | 0.58 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3291 | 1/1 | 0.89 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3382 | 1/1 | 0.89 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3352 | 1/1 | 0.89 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | 2B | 201 | 1/1 | 0.89 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3207 | 1/1 | 0.89 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 2x | 103 | 1/1 | 0.89 | 0.10 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1729 | 1/1 | 0.89 | 0.26 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3474 | 1/1 | 0.89 | 0.57 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3599 | 1/1 | 0.89 | 0.14 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2a | 3078 | 1/1 | 0.89 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3618 | 1/1 | 0.89 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3515 | 1/1 | 0.89 | 0.18 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3021 | 1/1 | 0.89 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3619 | 1/1 | 0.89 | 0.14 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3791 | 1/1 | 0.89 | 0.19 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 4005 | 1/1 | 0.89 | 0.21 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3117 | 1/1 | 0.89 | 0.26 | 33,33,33,33 | 0 |
| 56 | MG | 2a | 3079 | 1/1 | 0.89 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3147 | 1/1 | 0.89 | 0.09 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3212 | 1/1 | 0.89 | 0.28 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3267 | 1/1 | 0.89 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3406 | 1/1 | 0.89 | 0.20 | 53,53,53,53 | 0 |
| 56 | MG | 2y | 106 | 1/1 | 0.89 | 0.14 | 72,72,72,72 | 0 |
| 56 | MG | 1B | 204 | 1/1 | 0.89 | 0.19 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3977 | 1/1 | 0.89 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3946 | 1/1 | 0.89 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3310 | 1/1 | 0.90 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3064 | 1/1 | 0.90 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1692 | 1/1 | 0.90 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3422 | 1/1 | 0.90 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3404 | 1/1 | 0.90 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3653 | 1/1 | 0.90 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3363 | 1/1 | 0.90 | 0.68 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3932 | 1/1 | 0.90 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3052 | 1/1 | 0.90 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2v | 103 | 1/1 | 0.90 | 0.39 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3187 | 1/1 | 0.90 | 0.21 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3480 | 1/1 | 0.90 | 0.28 | 67,67,67,67 | 0 |
| 56 | MG | 1a | 1691 | 1/1 | 0.90 | 0.30 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3608 | 1/1 | 0.90 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3765 | 1/1 | 0.90 | 0.30 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3057 | 1/1 | 0.90 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3200 | 1/1 | 0.90 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3177 | 1/1 | 0.90 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4026 | 1/1 | 0.90 | 0.44 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3197 | 1/1 | 0.90 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3705 | 1/1 | 0.90 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3874 | 1/1 | 0.90 | 0.17 | 22,22,22,22 | 0 |
| 56 | MG | 1a | 1687 | 1/1 | 0.90 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 1U | 206 | 1/1 | 0.90 | 0.44 | 36,36,36,36 | 0 |
| 56 | MG | 1B | 208 | 1/1 | 0.90 | 0.17 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 10 | 101 | 1/1 | 0.90 | 0.18 | 24,24,24,24 | 0 |
| 56 | MG | 2a | 3069 | 1/1 | 0.90 | 0.18 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3691 | 1/1 | 0.90 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3030 | 1/1 | 0.90 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1697 | 1/1 | 0.90 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3588 | 1/1 | 0.90 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3389 | 1/1 | 0.90 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3736 | 1/1 | 0.90 | 0.09 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3638 | 1/1 | 0.90 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3265 | 1/1 | 0.90 | 0.76 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3044 | 1/1 | 0.90 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3747 | 1/1 | 0.90 | 0.16 | 9,9,9,9 | 0 |
| 56 | MG | 2a | 3138 | 1/1 | 0.90 | 0.12 | 77,77,77,77 | 0 |
| 56 | MG | 1w | 103 | 1/1 | 0.90 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1631 | 1/1 | 0.90 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3275 | 1/1 | 0.90 | 0.30 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3121 | 1/1 | 0.90 | 0.77 | 29,29,29,29 | 0 |
| 56 | MG | 1a | 1766 | 1/1 | 0.90 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1789 | 1/1 | 0.90 | 0.28 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3362 | 1/1 | 0.90 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 1S | 201 | 1/1 | 0.90 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3446 | 1/1 | 0.90 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3726 | 1/1 | 0.90 | 0.21 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3148 | 1/1 | 0.90 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3716 | 1/1 | 0.90 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1813 | 1/1 | 0.90 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3120 | 1/1 | 0.90 | 0.19 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3927 | 1/1 | 0.90 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3067 | 1/1 | 0.90 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3143 | 1/1 | 0.90 | 0.10 | 73,73,73,73 | 0 |
| 56 | MG | 2a | 3112 | 1/1 | 0.90 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3939 | 1/1 | 0.90 | 0.38 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1713 | 1/1 | 0.90 | 0.33 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3215 | 1/1 | 0.90 | 0.40 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3336 | 1/1 | 0.90 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | 1E | 306 | 1/1 | 0.90 | 0.62 | 41,41,41,41 | 0 |
| 56 | MG | 2T | 203 | 1/1 | 0.90 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3303 | 1/1 | 0.90 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 4068 | 1/1 | 0.90 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3252 | 1/1 | 0.90 | 0.21 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3338 | 1/1 | 0.90 | 0.32 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3205 | 1/1 | 0.90 | 0.10 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1a | 1626 | 1/1 | 0.90 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3168 | 1/1 | 0.90 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3627 | 1/1 | 0.90 | 0.26 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3351 | 1/1 | 0.90 | 0.09 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3756 | 1/1 | 0.90 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3778 | 1/1 | 0.90 | 0.14 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3521 | 1/1 | 0.90 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3035 | 1/1 | 0.90 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3589 | 1/1 | 0.90 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3937 | 1/1 | 0.90 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 2a | 3060 | 1/1 | 0.90 | 0.24 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3679 | 1/1 | 0.90 | 0.14 | 7,7,7,7 | 0 |
| 56 | MG | 2A | 3200 | 1/1 | 0.90 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3823 | 1/1 | 0.90 | 0.13 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3650 | 1/1 | 0.90 | 0.19 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3114 | 1/1 | 0.90 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3105 | 1/1 | 0.90 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3670 | 1/1 | 0.90 | 0.13 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3010 | 1/1 | 0.90 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3808 | 1/1 | 0.90 | 0.18 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3489 | 1/1 | 0.90 | 0.21 | 64,64,64,64 | 0 |
| 56 | MG | 1x | 104 | 1/1 | 0.90 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3544 | 1/1 | 0.90 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4067 | 1/1 | 0.90 | 0.21 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3568 | 1/1 | 0.90 | 0.85 | 30,30,30,30 | 0 |
| 56 | MG | 1U | 201 | 1/1 | 0.90 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3260 | 1/1 | 0.90 | 0.45 | 35,35,35,35 | 0 |
| 56 | MG | 1x | 102 | 1/1 | 0.90 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3176 | 1/1 | 0.90 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3416 | 1/1 | 0.90 | 0.33 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3704 | 1/1 | 0.90 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3109 | 1/1 | 0.90 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2a | 3220 | 1/1 | 0.90 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3203 | 1/1 | 0.90 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3542 | 1/1 | 0.90 | 0.19 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3980 | 1/1 | 0.90 | 0.39 | 72,72,72,72 | 0 |
| 56 | MG | 2a | 3064 | 1/1 | 0.90 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3091 | 1/1 | 0.90 | 0.23 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3625 | 1/1 | 0.90 | 0.27 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1670 | 1/1 | 0.90 | 0.60 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3208 | 1/1 | 0.90 | 0.46 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3578 | 1/1 | 0.90 | 0.14 | 51,51,51,51 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3848 | 1/1 | 0.90 | 0.69 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3122 | 1/1 | 0.90 | 0.29 | 52,52,52,52 | 0 |
| 56 | MG | 2i | 201 | 1/1 | 0.90 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3415 | 1/1 | 0.90 | 0.39 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3437 | 1/1 | 0.90 | 0.36 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3083 | 1/1 | 0.90 | 0.14 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3304 | 1/1 | 0.90 | 0.15 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3179 | 1/1 | 0.90 | 0.25 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3036 | 1/1 | 0.90 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3611 | 1/1 | 0.90 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 1B | 233 | 1/1 | 0.90 | 0.32 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3197 | 1/1 | 0.90 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3308 | 1/1 | 0.90 | 0.15 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3240 | 1/1 | 0.90 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1802 | 1/1 | 0.90 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3582 | 1/1 | 0.90 | 0.64 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3614 | 1/1 | 0.90 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1774 | 1/1 | 0.90 | 0.11 | 42,42,42,42 | 0 |
| 56 | MG | 2d | 302 | 1/1 | 0.90 | 0.16 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3029 | 1/1 | 0.90 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3180 | 1/1 | 0.90 | 0.11 | 83,83,83,83 | 0 |
| 56 | MG | 2A | 3043 | 1/1 | 0.90 | 0.63 | 37,37,37,37 | 0 |
| 56 | MG | 1O | 204 | 1/1 | 0.90 | 0.31 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1750 | 1/1 | 0.90 | 0.13 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3223 | 1/1 | 0.90 | 0.62 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3678 | 1/1 | 0.90 | 0.13 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3184 | 1/1 | 0.90 | 0.23 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3329 | 1/1 | 0.90 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3566 | 1/1 | 0.90 | 0.22 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3531 | 1/1 | 0.90 | 0.14 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3215 | 1/1 | 0.90 | 0.38 | 71,71,71,71 | 0 |
| 56 | MG | 2A | 3031 | 1/1 | 0.91 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3305 | 1/1 | 0.91 | 0.26 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3662 | 1/1 | 0.91 | 0.06 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3496 | 1/1 | 0.91 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3699 | 1/1 | 0.91 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3116 | 1/1 | 0.91 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3768 | 1/1 | 0.91 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3013 | 1/1 | 0.91 | 0.16 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3755 | 1/1 | 0.91 | 0.09 | 76,76,76,76 | 0 |
| 56 | MG | 1A | 3057 | 1/1 | 0.91 | 0.15 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3147 | 1/1 | 0.91 | 0.39 | 32,32,32,32 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1a | 1804 | 1/1 | 0.91 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3107 | 1/1 | 0.91 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3890 | 1/1 | 0.91 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3124 | 1/1 | 0.91 | 0.42 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3406 | 1/1 | 0.91 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3049 | 1/1 | 0.91 | 0.14 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3390 | 1/1 | 0.91 | 0.22 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4074 | 1/1 | 0.91 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3015 | 1/1 | 0.91 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3661 | 1/1 | 0.91 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3287 | 1/1 | 0.91 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3208 | 1/1 | 0.91 | 0.16 | 66,66,66,66 | 0 |
| 56 | MG | 2a | 3132 | 1/1 | 0.91 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1N | 201 | 1/1 | 0.91 | 0.78 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3844 | 1/1 | 0.91 | 0.15 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3697 | 1/1 | 0.91 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3427 | 1/1 | 0.91 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3742 | 1/1 | 0.91 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3372 | 1/1 | 0.91 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3160 | 1/1 | 0.91 | 0.06 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3926 | 1/1 | 0.91 | 0.08 | 33,33,33,33 | 0 |
| 56 | MG | 1B | 220 | 1/1 | 0.91 | 0.22 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3842 | 1/1 | 0.91 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3045 | 1/1 | 0.91 | 0.25 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3092 | 1/1 | 0.91 | 0.22 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3870 | 1/1 | 0.91 | 0.09 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3673 | 1/1 | 0.91 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2B | 217 | 1/1 | 0.91 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3278 | 1/1 | 0.91 | 0.64 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3938 | 1/1 | 0.91 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3281 | 1/1 | 0.91 | 0.25 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1607 | 1/1 | 0.91 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3517 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3727 | 1/1 | 0.91 | 0.17 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3501 | 1/1 | 0.91 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3429 | 1/1 | 0.91 | 0.26 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3481 | 1/1 | 0.91 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3090 | 1/1 | 0.91 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3408 | 1/1 | 0.91 | 0.61 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3301 | 1/1 | 0.91 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3479 | 1/1 | 0.91 | 0.27 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3422 | 1/1 | 0.91 | 0.44 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1S | 203 | 1/1 | 0.91 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3583 | 1/1 | 0.91 | 0.52 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3099 | 1/1 | 0.91 | 0.38 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3593 | 1/1 | 0.91 | 0.15 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3136 | 1/1 | 0.91 | 0.24 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3125 | 1/1 | 0.91 | 0.15 | 42,42,42,42 | 0 |
| 56 | MG | 1b | 302 | 1/1 | 0.91 | 0.09 | 64,64,64,64 | 0 |
| 56 | MG | 1B | 221 | 1/1 | 0.91 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3118 | 1/1 | 0.91 | 0.37 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1748 | 1/1 | 0.91 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3782 | 1/1 | 0.91 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3813 | 1/1 | 0.91 | 0.12 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3284 | 1/1 | 0.91 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3733 | 1/1 | 0.91 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3095 | 1/1 | 0.91 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3575 | 1/1 | 0.91 | 0.26 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3764 | 1/1 | 0.91 | 0.12 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3080 | 1/1 | 0.91 | 0.34 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3334 | 1/1 | 0.91 | 0.30 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3219 | 1/1 | 0.91 | 0.42 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3312 | 1/1 | 0.91 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3129 | 1/1 | 0.91 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 28 | 101 | 1/1 | 0.91 | 0.23 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3666 | 1/1 | 0.91 | 0.10 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3437 | 1/1 | 0.91 | 0.18 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3051 | 1/1 | 0.91 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3081 | 1/1 | 0.91 | 0.46 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3298 | 1/1 | 0.91 | 0.21 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3643 | 1/1 | 0.91 | 0.08 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3316 | 1/1 | 0.91 | 0.30 | 45,45,45,45 | 0 |
| 56 | MG | 2a | 3088 | 1/1 | 0.91 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3897 | 1/1 | 0.91 | 0.12 | 40,40,40,40 | 0 |
| 56 | MG | 1a | 1816 | 1/1 | 0.91 | 0.08 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3073 | 1/1 | 0.91 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3885 | 1/1 | 0.91 | 0.45 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3312 | 1/1 | 0.91 | 0.46 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3692 | 1/1 | 0.91 | 0.26 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3241 | 1/1 | 0.91 | 0.36 | 27,27,27,27 | 0 |
| 59 | ZN | 29 | 102 | 1/1 | 0.91 | 0.10 | 69,69,69,69 | 0 |
| 56 | MG | 1A | 3144 | 1/1 | 0.91 | 0.55 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3063 | 1/1 | 0.91 | 0.15 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3836 | 1/1 | 0.91 | 0.08 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3091 | 1/1 | 0.91 | 0.14 | 14,14,14,14 | 0 |
| 56 | MG | 1w | 104 | 1/1 | 0.91 | 0.39 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3019 | 1/1 | 0.91 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3239 | 1/1 | 0.91 | 0.44 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3226 | 1/1 | 0.91 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3048 | 1/1 | 0.91 | 0.16 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3659 | 1/1 | 0.91 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3634 | 1/1 | 0.91 | 0.15 | 61,61,61,61 | 0 |
| 59 | ZN | 14 | 102 | 1/1 | 0.91 | 0.10 | 94,94,94,94 | 0 |
| 56 | MG | 1A | 3648 | 1/1 | 0.91 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3340 | 1/1 | 0.91 | 0.27 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3157 | 1/1 | 0.91 | 0.24 | 21,21,21,21 | 0 |
| 56 | MG | 2a | 3093 | 1/1 | 0.91 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1688 | 1/1 | 0.91 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1671 | 1/1 | 0.91 | 0.25 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4008 | 1/1 | 0.91 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3741 | 1/1 | 0.91 | 0.16 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 4039 | 1/1 | 0.91 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 18 | 101 | 1/1 | 0.91 | 0.58 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3235 | 1/1 | 0.91 | 0.29 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3198 | 1/1 | 0.91 | 0.29 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3284 | 1/1 | 0.91 | 0.19 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3428 | 1/1 | 0.91 | 0.80 | 50,50,50,50 | 0 |
| 57 | LUJ | 1A | 4100 | 42/44 | 0.91 | 0.35 | 23,39,54,62 | 0 |
| 56 | MG | 1A | 4009 | 1/1 | 0.91 | 0.17 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3856 | 1/1 | 0.91 | 0.14 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3062 | 1/1 | 0.91 | 0.17 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3811 | 1/1 | 0.91 | 0.18 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1708 | 1/1 | 0.91 | 0.13 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3060 | 1/1 | 0.91 | 0.11 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3515 | 1/1 | 0.91 | 0.12 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 4129 | 1/1 | 0.91 | 0.18 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3167 | 1/1 | 0.91 | 0.15 | 39,39,39,39 | 0 |
| 56 | MG | 1a | 1757 | 1/1 | 0.91 | 0.18 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3277 | 1/1 | 0.91 | 0.96 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3465 | 1/1 | 0.91 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3723 | 1/1 | 0.91 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3258 | 1/1 | 0.91 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3692 | 1/1 | 0.91 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3487 | 1/1 | 0.91 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2D | 301 | 1/1 | 0.91 | 0.13 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3302 | 1/1 | 0.91 | 0.21 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3409 | 1/1 | 0.91 | 0.42 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3179 | 1/1 | 0.91 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3511 | 1/1 | 0.91 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1758 | 1/1 | 0.91 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3696 | 1/1 | 0.91 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3368 | 1/1 | 0.91 | 0.46 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3004 | 1/1 | 0.91 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3630 | 1/1 | 0.91 | 0.89 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3266 | 1/1 | 0.91 | 0.33 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3146 | 1/1 | 0.91 | 0.37 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3186 | 1/1 | 0.91 | 0.07 | 77,77,77,77 | 0 |
| 56 | MG | 2A | 3009 | 1/1 | 0.91 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3587 | 1/1 | 0.91 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3011 | 1/1 | 0.91 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3701 | 1/1 | 0.91 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3336 | 1/1 | 0.91 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1B | 202 | 1/1 | 0.91 | 0.20 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 4096 | 1/1 | 0.91 | 0.17 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3158 | 1/1 | 0.91 | 0.52 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3542 | 1/1 | 0.91 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3194 | 1/1 | 0.91 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1752 | 1/1 | 0.91 | 0.15 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3261 | 1/1 | 0.91 | 0.27 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3478 | 1/1 | 0.91 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1V | 202 | 1/1 | 0.91 | 0.09 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3236 | 1/1 | 0.92 | 0.16 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3707 | 1/1 | 0.92 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3235 | 1/1 | 0.92 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3862 | 1/1 | 0.92 | 0.29 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3305 | 1/1 | 0.92 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 1W | 206 | 1/1 | 0.92 | 0.23 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 4046 | 1/1 | 0.92 | 0.09 | 24,24,24,24 | 0 |
| 56 | MG | 2a | 3172 | 1/1 | 0.92 | 0.05 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3960 | 1/1 | 0.92 | 0.12 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3483 | 1/1 | 0.92 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3769 | 1/1 | 0.92 | 0.22 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3804 | 1/1 | 0.92 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3818 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3181 | 1/1 | 0.92 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3805 | 1/1 | 0.92 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3556 | 1/1 | 0.92 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3828 | 1/1 | 0.92 | 0.12 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3245 | 1/1 | 0.92 | 0.58 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3547 | 1/1 | 0.92 | 0.37 | 43,43,43,43 | 0 |
| 56 | MG | 2P | 202 | 1/1 | 0.92 | 0.15 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3263 | 1/1 | 0.92 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3486 | 1/1 | 0.92 | 0.21 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3833 | 1/1 | 0.92 | 0.11 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3972 | 1/1 | 0.92 | 0.13 | 62,62,62,62 | 0 |
| 56 | MG | 1a | 1624 | 1/1 | 0.92 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3381 | 1/1 | 0.92 | 0.19 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3066 | 1/1 | 0.92 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3839 | 1/1 | 0.92 | 0.09 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3413 | 1/1 | 0.92 | 0.13 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3569 | 1/1 | 0.92 | 0.09 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3519 | 1/1 | 0.92 | 0.19 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3455 | 1/1 | 0.92 | 0.22 | 42,42,42,42 | 0 |
| 56 | MG | 1D | 311 | 1/1 | 0.92 | 0.56 | 17,17,17,17 | 0 |
| 56 | MG | 1a | 1754 | 1/1 | 0.92 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3152 | 1/1 | 0.92 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3895 | 1/1 | 0.92 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3358 | 1/1 | 0.92 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3477 | 1/1 | 0.92 | 0.16 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3790 | 1/1 | 0.92 | 0.06 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3837 | 1/1 | 0.92 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3288 | 1/1 | 0.92 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3022 | 1/1 | 0.92 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3456 | 1/1 | 0.92 | 0.19 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3170 | 1/1 | 0.92 | 0.26 | 84,84,84,84 | 0 |
| 56 | MG | 2A | 3765 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3233 | 1/1 | 0.92 | 0.64 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3319 | 1/1 | 0.92 | 0.23 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1742 | 1/1 | 0.92 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3708 | 1/1 | 0.92 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3100 | 1/1 | 0.92 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3612 | 1/1 | 0.92 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3473 | 1/1 | 0.92 | 0.27 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3006 | 1/1 | 0.92 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3283 | 1/1 | 0.92 | 0.24 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3121 | 1/1 | 0.92 | 0.20 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3671 | 1/1 | 0.92 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3551 | 1/1 | 0.92 | 0.74 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3464 | 1/1 | 0.92 | 0.11 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3209 | 1/1 | 0.92 | 0.18 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3054 | 1/1 | 0.92 | 0.20 | 28,28,28,28 | 0 |
| 56 | MG | 2y | 101 | 1/1 | 0.92 | 0.12 | 67,67,67,67 | 0 |
| 56 | MG | 2A | 3677 | 1/1 | 0.92 | 0.06 | 72,72,72,72 | 0 |
| 56 | MG | 1a | 1617 | 1/1 | 0.92 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3731 | 1/1 | 0.92 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3846 | 1/1 | 0.92 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 4047 | 1/1 | 0.92 | 0.15 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3211 | 1/1 | 0.92 | 0.46 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3123 | 1/1 | 0.92 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3557 | 1/1 | 0.92 | 0.09 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3143 | 1/1 | 0.92 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3201 | 1/1 | 0.92 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3376 | 1/1 | 0.92 | 0.48 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1820 | 1/1 | 0.92 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3682 | 1/1 | 0.92 | 0.19 | 15,15,15,15 | 0 |
| 56 | MG | 1a | 1685 | 1/1 | 0.92 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3073 | 1/1 | 0.92 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3100 | 1/1 | 0.92 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3758 | 1/1 | 0.92 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | 1a | 1705 | 1/1 | 0.92 | 0.15 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3724 | 1/1 | 0.92 | 0.11 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3402 | 1/1 | 0.92 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3337 | 1/1 | 0.92 | 0.26 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3047 | 1/1 | 0.92 | 0.32 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3309 | 1/1 | 0.92 | 0.17 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3155 | 1/1 | 0.92 | 0.29 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3451 | 1/1 | 0.92 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3180 | 1/1 | 0.92 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3345 | 1/1 | 0.92 | 0.72 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3094 | 1/1 | 0.92 | 0.13 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3013 | 1/1 | 0.92 | 0.42 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3192 | 1/1 | 0.92 | 0.23 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3065 | 1/1 | 0.92 | 0.19 | 22,22,22,22 | 0 |
| 56 | MG | 25 | 102 | 1/1 | 0.92 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 2k | 201 | 1/1 | 0.92 | 0.13 | 56,56,56,56 | 0 |
| 56 | MG | 1F | 310 | 1/1 | 0.92 | 0.23 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3086 | 1/1 | 0.92 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3231 | 1/1 | 0.92 | 0.08 | 73,73,73,73 | 0 |
| 56 | MG | 1A | 3089 | 1/1 | 0.92 | 0.19 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3535 | 1/1 | 0.92 | 0.16 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3726 | 1/1 | 0.92 | 0.26 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1653 | 1/1 | 0.92 | 0.25 | 58,58,58,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3725 | 1/1 | 0.92 | 0.38 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3248 | 1/1 | 0.92 | 0.12 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3078 | 1/1 | 0.92 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3689 | 1/1 | 0.92 | 0.11 | 25,25,25,25 | 0 |
| 56 | MG | 2a | 3098 | 1/1 | 0.92 | 0.70 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3497 | 1/1 | 0.92 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 2l | 201 | 1/1 | 0.92 | 0.14 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1677 | 1/1 | 0.92 | 0.37 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3056 | 1/1 | 0.92 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1B | 205 | 1/1 | 0.92 | 0.17 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3418 | 1/1 | 0.92 | 0.30 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3480 | 1/1 | 0.92 | 0.11 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3766 | 1/1 | 0.92 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3610 | 1/1 | 0.92 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3767 | 1/1 | 0.92 | 0.20 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3723 | 1/1 | 0.92 | 0.18 | 31,31,31,31 | 0 |
| 56 | MG | 2Q | 201 | 1/1 | 0.92 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1723 | 1/1 | 0.92 | 0.17 | 29,29,29,29 | 0 |
| 56 | MG | 1Y | 204 | 1/1 | 0.92 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1661 | 1/1 | 0.92 | 0.25 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3595 | 1/1 | 0.92 | 0.18 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3871 | 1/1 | 0.92 | 0.12 | 14,14,14,14 | 0 |
| 56 | MG | 2B | 216 | 1/1 | 0.92 | 0.23 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3485 | 1/1 | 0.92 | 0.38 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3022 | 1/1 | 0.92 | 0.95 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3217 | 1/1 | 0.92 | 0.39 | 47,47,47,47 | 0 |
| 56 | MG | 19 | 101 | 1/1 | 0.92 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1F | 302 | 1/1 | 0.92 | 0.38 | 28,28,28,28 | 0 |
| 56 | MG | 2a | 3193 | 1/1 | 0.92 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3046 | 1/1 | 0.92 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3347 | 1/1 | 0.92 | 0.38 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3857 | 1/1 | 0.92 | 0.18 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3575 | 1/1 | 0.92 | 0.51 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3034 | 1/1 | 0.92 | 0.25 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3648 | 1/1 | 0.92 | 0.21 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3664 | 1/1 | 0.92 | 0.15 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3986 | 1/1 | 0.92 | 0.16 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3745 | 1/1 | 0.92 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3400 | 1/1 | 0.92 | 0.25 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3598 | 1/1 | 0.92 | 0.10 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3436 | 1/1 | 0.92 | 0.16 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3561 | 1/1 | 0.92 | 0.21 | 35,35,35,35 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2f | 201 | 1/1 | 0.92 | 0.07 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 4062 | 1/1 | 0.92 | 0.15 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3763 | 1/1 | 0.92 | 0.14 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3032 | 1/1 | 0.92 | 0.77 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3513 | 1/1 | 0.92 | 0.08 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1763 | 1/1 | 0.92 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3620 | 1/1 | 0.92 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3835 | 1/1 | 0.92 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 4070 | 1/1 | 0.92 | 0.09 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3724 | 1/1 | 0.92 | 0.32 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3826 | 1/1 | 0.92 | 0.16 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3757 | 1/1 | 0.92 | 0.23 | 30,30,30,30 | 0 |
| 56 | MG | 2a | 3061 | 1/1 | 0.92 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3979 | 1/1 | 0.92 | 0.30 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3527 | 1/1 | 0.92 | 0.33 | 57,57,57,57 | 0 |
| 56 | MG | 2B | 213 | 1/1 | 0.92 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3513 | 1/1 | 0.92 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3967 | 1/1 | 0.92 | 0.27 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3279 | 1/1 | 0.92 | 0.18 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3924 | 1/1 | 0.92 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3976 | 1/1 | 0.92 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3559 | 1/1 | 0.92 | 0.14 | 33,33,33,33 | 0 |
| 56 | MG | 17 | 104 | 1/1 | 0.92 | 0.10 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3449 | 1/1 | 0.92 | 0.32 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3494 | 1/1 | 0.92 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3275 | 1/1 | 0.92 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3101 | 1/1 | 0.92 | 0.09 | 65,65,65,65 | 0 |
| 56 | MG | 1y | 106 | 1/1 | 0.92 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3985 | 1/1 | 0.92 | 0.14 | 16,16,16,16 | 0 |
| 56 | MG | 1a | 1629 | 1/1 | 0.92 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3139 | 1/1 | 0.92 | 0.33 | 68,68,68,68 | 0 |
| 56 | MG | 1A | 3738 | 1/1 | 0.92 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3496 | 1/1 | 0.92 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3762 | 1/1 | 0.92 | 0.08 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3135 | 1/1 | 0.92 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3340 | 1/1 | 0.92 | 0.18 | 65,65,65,65 | 0 |
| 56 | MG | 1U | 207 | 1/1 | 0.92 | 1.38 | 71,71,71,71 | 0 |
| 56 | MG | 1A | 3506 | 1/1 | 0.92 | 0.25 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3166 | 1/1 | 0.92 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3054 | 1/1 | 0.92 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3799 | 1/1 | 0.92 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3394 | 1/1 | 0.92 | 0.27 | 34,34,34,34 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 4022 | 1/1 | 0.92 | 0.13 | 60,60,60,60 | 0 |
| 56 | MG | 2U | 202 | 1/1 | 0.93 | 0.55 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3850 | 1/1 | 0.93 | 0.09 | 33,33,33,33 | 0 |
| 56 | MG | 1a | 1630 | 1/1 | 0.93 | 0.16 | 39,39,39,39 | 0 |
| 57 | LUJ | 2a | 3232 | 44/44 | 0.93 | 0.28 | 40,55,62,65 | 0 |
| 56 | MG | 2A | 3432 | 1/1 | 0.93 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3682 | 1/1 | 0.93 | 0.24 | 48,48,48,48 | 0 |
| 57 | LUJ | 1A | 4099 | 42/44 | 0.93 | 0.24 | 32,44,54,57 | 0 |
| 56 | MG | 2A | 3410 | 1/1 | 0.93 | 0.16 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3651 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 2Q | 204 | 1/1 | 0.93 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3129 | 1/1 | 0.93 | 0.32 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1602 | 1/1 | 0.93 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1f | 201 | 1/1 | 0.93 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3654 | 1/1 | 0.93 | 0.15 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3488 | 1/1 | 0.93 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3738 | 1/1 | 0.93 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3736 | 1/1 | 0.93 | 0.11 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3984 | 1/1 | 0.93 | 0.15 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3531 | 1/1 | 0.93 | 0.09 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3407 | 1/1 | 0.93 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3745 | 1/1 | 0.93 | 0.22 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3393 | 1/1 | 0.93 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3485 | 1/1 | 0.93 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3506 | 1/1 | 0.93 | 0.12 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3297 | 1/1 | 0.93 | 0.39 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3343 | 1/1 | 0.93 | 0.39 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3101 | 1/1 | 0.93 | 0.38 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3249 | 1/1 | 0.93 | 0.21 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3464 | 1/1 | 0.93 | 0.34 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3014 | 1/1 | 0.93 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1701 | 1/1 | 0.93 | 0.16 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3594 | 1/1 | 0.93 | 0.16 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3737 | 1/1 | 0.93 | 0.25 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3482 | 1/1 | 0.93 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3463 | 1/1 | 0.93 | 0.19 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3444 | 1/1 | 0.93 | 0.09 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3109 | 1/1 | 0.93 | 0.20 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3455 | 1/1 | 0.93 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3060 | 1/1 | 0.93 | 0.11 | 27,27,27,27 | 0 |
| 56 | MG | 2a | 3019 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1724 | 1/1 | 0.93 | 0.20 | 56,56,56,56 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3058 | 1/1 | 0.93 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3160 | 1/1 | 0.93 | 0.23 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3753 | 1/1 | 0.93 | 0.24 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3255 | 1/1 | 0.93 | 0.14 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3508 | 1/1 | 0.93 | 0.24 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 4077 | 1/1 | 0.93 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3703 | 1/1 | 0.93 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3211 | 1/1 | 0.93 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4059 | 1/1 | 0.93 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3188 | 1/1 | 0.93 | 0.09 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3032 | 1/1 | 0.93 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | 1Z | 302 | 1/1 | 0.93 | 0.17 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3327 | 1/1 | 0.93 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4115 | 1/1 | 0.93 | 0.37 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3739 | 1/1 | 0.93 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3730 | 1/1 | 0.93 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3009 | 1/1 | 0.93 | 0.10 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3061 | 1/1 | 0.93 | 0.36 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3169 | 1/1 | 0.93 | 0.20 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3814 | 1/1 | 0.93 | 0.17 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 4110 | 1/1 | 0.93 | 0.34 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3113 | 1/1 | 0.93 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3777 | 1/1 | 0.93 | 0.17 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3057 | 1/1 | 0.93 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 20 | 101 | 1/1 | 0.93 | 0.10 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3130 | 1/1 | 0.93 | 0.21 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3671 | 1/1 | 0.93 | 0.15 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3412 | 1/1 | 0.93 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3712 | 1/1 | 0.93 | 0.13 | 28,28,28,28 | 0 |
| 56 | MG | 2T | 201 | 1/1 | 0.93 | 0.17 | 57,57,57,57 | 0 |
| 56 | MG | 12 | 3701 | 1/1 | 0.93 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3183 | 1/1 | 0.93 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4058 | 1/1 | 0.93 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3820 | 1/1 | 0.93 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3848 | 1/1 | 0.93 | 0.15 | 55,55,55,55 | 0 |
| 56 | MG | 2O | 202 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3289 | 1/1 | 0.93 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 4073 | 1/1 | 0.93 | 0.27 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3112 | 1/1 | 0.93 | 0.23 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 4085 | 1/1 | 0.93 | 0.20 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3397 | 1/1 | 0.93 | 0.37 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3211 | 1/1 | 0.93 | 0.15 | 60,60,60,60 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3562 | 1/1 | 0.93 | 0.12 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3552 | 1/1 | 0.93 | 0.20 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3028 | 1/1 | 0.93 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | 1P | 203 | 1/1 | 0.93 | 0.48 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3509 | 1/1 | 0.93 | 0.37 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3484 | 1/1 | 0.93 | 0.14 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3410 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3824 | 1/1 | 0.93 | 0.15 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3222 | 1/1 | 0.93 | 0.42 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3414 | 1/1 | 0.93 | 0.13 | 55,55,55,55 | 0 |
| 56 | MG | 1R | 202 | 1/1 | 0.93 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3028 | 1/1 | 0.93 | 0.12 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1732 | 1/1 | 0.93 | 0.26 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3436 | 1/1 | 0.93 | 0.83 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3150 | 1/1 | 0.93 | 0.21 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3570 | 1/1 | 0.93 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1734 | 1/1 | 0.93 | 0.24 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3409 | 1/1 | 0.93 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3080 | 1/1 | 0.93 | 0.13 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3118 | 1/1 | 0.93 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3299 | 1/1 | 0.93 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1659 | 1/1 | 0.93 | 0.18 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3417 | 1/1 | 0.93 | 0.12 | 22,22,22,22 | 0 |
| 56 | MG | 2P | 201 | 1/1 | 0.93 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3145 | 1/1 | 0.93 | 0.38 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3232 | 1/1 | 0.93 | 0.31 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3689 | 1/1 | 0.93 | 0.14 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3475 | 1/1 | 0.93 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3021 | 1/1 | 0.93 | 0.32 | 45,45,45,45 | 0 |
| 56 | MG | 1W | 201 | 1/1 | 0.93 | 0.22 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3083 | 1/1 | 0.93 | 1.15 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3674 | 1/1 | 0.93 | 0.21 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3272 | 1/1 | 0.93 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1726 | 1/1 | 0.93 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3068 | 1/1 | 0.93 | 0.14 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3672 | 1/1 | 0.93 | 0.08 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3215 | 1/1 | 0.93 | 0.42 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3194 | 1/1 | 0.93 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1764 | 1/1 | 0.93 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3097 | 1/1 | 0.93 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3584 | 1/1 | 0.93 | 0.15 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3458 | 1/1 | 0.93 | 0.23 | 20,20,20,20 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3347 | 1/1 | 0.93 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1651 | 1/1 | 0.93 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3264 | 1/1 | 0.93 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3203 | 1/1 | 0.93 | 0.20 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3705 | 1/1 | 0.93 | 0.21 | 35,35,35,35 | 0 |
| 56 | MG | 2a | 3142 | 1/1 | 0.93 | 0.06 | 61,61,61,61 | 0 |
| 56 | MG | 2x | 102 | 1/1 | 0.93 | 0.07 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3138 | 1/1 | 0.93 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3863 | 1/1 | 0.93 | 0.38 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3043 | 1/1 | 0.93 | 0.25 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3218 | 1/1 | 0.93 | 0.22 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3697 | 1/1 | 0.93 | 0.07 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3168 | 1/1 | 0.93 | 0.29 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4087 | 1/1 | 0.93 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 1a | 1665 | 1/1 | 0.93 | 0.50 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3817 | 1/1 | 0.93 | 0.11 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3050 | 1/1 | 0.93 | 0.12 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3653 | 1/1 | 0.93 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | 2U | 201 | 1/1 | 0.93 | 0.13 | 29,29,29,29 | 0 |
| 56 | MG | 1a | 1673 | 1/1 | 0.93 | 0.42 | 43,43,43,43 | 0 |
| 56 | MG | 18 | 104 | 1/1 | 0.93 | 0.30 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3113 | 1/1 | 0.93 | 0.46 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3696 | 1/1 | 0.93 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3242 | 1/1 | 0.93 | 0.26 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3085 | 1/1 | 0.93 | 0.42 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3931 | 1/1 | 0.93 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3099 | 1/1 | 0.93 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3686 | 1/1 | 0.93 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3366 | 1/1 | 0.93 | 0.41 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3220 | 1/1 | 0.93 | 0.47 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3103 | 1/1 | 0.93 | 0.24 | 19,19,19,19 | 0 |
| 56 | MG | 2E | 305 | 1/1 | 0.93 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3385 | 1/1 | 0.93 | 0.27 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3164 | 1/1 | 0.93 | 0.06 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3115 | 1/1 | 0.93 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3685 | 1/1 | 0.93 | 0.11 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3678 | 1/1 | 0.93 | 0.15 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3067 | 1/1 | 0.93 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3026 | 1/1 | 0.93 | 0.19 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1800 | 1/1 | 0.93 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3599 | 1/1 | 0.93 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1783 | 1/1 | 0.93 | 0.07 | 38,38,38,38 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3339 | 1/1 | 0.93 | 0.12 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3264 | 1/1 | 0.93 | 0.61 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3063 | 1/1 | 0.93 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3879 | 1/1 | 0.93 | 0.08 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3039 | 1/1 | 0.93 | 0.15 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3157 | 1/1 | 0.93 | 0.12 | 67,67,67,67 | 0 |
| 56 | MG | 1I | 101 | 1/1 | 0.93 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | 2N | 201 | 1/1 | 0.93 | 0.58 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1635 | 1/1 | 0.93 | 0.23 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3050 | 1/1 | 0.93 | 0.22 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3237 | 1/1 | 0.93 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1773 | 1/1 | 0.93 | 0.09 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3543 | 1/1 | 0.93 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3285 | 1/1 | 0.93 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1a | 1826 | 1/1 | 0.93 | 0.07 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3721 | 1/1 | 0.93 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3905 | 1/1 | 0.93 | 0.20 | 17,17,17,17 | 0 |
| 56 | MG | 1E | 304 | 1/1 | 0.93 | 0.17 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3375 | 1/1 | 0.93 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3394 | 1/1 | 0.93 | 0.31 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3128 | 1/1 | 0.93 | 0.32 | 26,26,26,26 | 0 |
| 56 | MG | 1B | 212 | 1/1 | 0.93 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3548 | 1/1 | 0.93 | 0.20 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3402 | 1/1 | 0.93 | 0.30 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3849 | 1/1 | 0.93 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3254 | 1/1 | 0.93 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1746 | 1/1 | 0.93 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3282 | 1/1 | 0.93 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3127 | 1/1 | 0.93 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3952 | 1/1 | 0.93 | 0.08 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3714 | 1/1 | 0.93 | 0.23 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3056 | 1/1 | 0.93 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3587 | 1/1 | 0.93 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 2E | 301 | 1/1 | 0.93 | 0.55 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3549 | 1/1 | 0.93 | 0.28 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3421 | 1/1 | 0.93 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3227 | 1/1 | 0.93 | 0.52 | 31,31,31,31 | 0 |
| 56 | MG | 1a | 1681 | 1/1 | 0.93 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3315 | 1/1 | 0.93 | 0.19 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3655 | 1/1 | 0.93 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3507 | 1/1 | 0.93 | 0.16 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3987 | 1/1 | 0.93 | 0.11 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3109 | 1/1 | 0.93 | 0.23 | 25,25,25,25 | 0 |
| 56 | MG | 1a | 1668 | 1/1 | 0.93 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3249 | 1/1 | 0.93 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1686 | 1/1 | 0.93 | 0.22 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4033 | 1/1 | 0.93 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3714 | 1/1 | 0.93 | 0.22 | 51,51,51,51 | 0 |
| 56 | MG | 2X | 101 | 1/1 | 0.93 | 0.15 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3901 | 1/1 | 0.93 | 0.60 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3461 | 1/1 | 0.93 | 0.13 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3847 | 1/1 | 0.93 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3661 | 1/1 | 0.93 | 0.12 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3002 | 1/1 | 0.93 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3147 | 1/1 | 0.93 | 0.35 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3646 | 1/1 | 0.93 | 0.16 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3438 | 1/1 | 0.93 | 0.71 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3955 | 1/1 | 0.93 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3863 | 1/1 | 0.93 | 0.06 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3040 | 1/1 | 0.93 | 0.24 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3896 | 1/1 | 0.93 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3783 | 1/1 | 0.93 | 0.16 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3900 | 1/1 | 0.93 | 0.29 | 31,31,31,31 | 0 |
| 56 | MG | 1x | 105 | 1/1 | 0.93 | 0.20 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 4089 | 1/1 | 0.93 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3117 | 1/1 | 0.93 | 0.07 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3672 | 1/1 | 0.93 | 0.12 | 34,34,34,34 | 0 |
| 58 | K | 1A | 4137 | 1/1 | 0.93 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3254 | 1/1 | 0.93 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3623 | 1/1 | 0.94 | 0.27 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3486 | 1/1 | 0.94 | 0.56 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3693 | 1/1 | 0.94 | 0.12 | 9,9,9,9 | 0 |
| 56 | MG | 2A | 3456 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1B | 223 | 1/1 | 0.94 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1716 | 1/1 | 0.94 | 0.15 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3586 | 1/1 | 0.94 | 0.55 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3502 | 1/1 | 0.94 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3868 | 1/1 | 0.94 | 0.08 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3853 | 1/1 | 0.94 | 0.26 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1660 | 1/1 | 0.94 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1830 | 1/1 | 0.94 | 0.34 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3369 | 1/1 | 0.94 | 0.36 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3958 | 1/1 | 0.94 | 0.14 | 30,30,30,30 | 0 |
| 56 | MG | 2a | 3005 | 1/1 | 0.94 | 0.08 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3561 | 1/1 | 0.94 | 0.24 | 54,54,54,54 | 0 |
| 56 | MG | 2a | 3107 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3145 | 1/1 | 0.94 | 0.43 | 33,33,33,33 | 0 |
| 56 | MG | 2a | 3225 | 1/1 | 0.94 | 0.10 | 60,60,60,60 | 0 |
| 56 | MG | 1y | 101 | 1/1 | 0.94 | 0.19 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3058 | 1/1 | 0.94 | 0.12 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3669 | 1/1 | 0.94 | 0.12 | 20,20,20,20 | 0 |
| 56 | MG | 2a | 3134 | 1/1 | 0.94 | 0.22 | 60,60,60,60 | 0 |
| 56 | MG | 1a | 1738 | 1/1 | 0.94 | 0.20 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4041 | 1/1 | 0.94 | 0.08 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3510 | 1/1 | 0.94 | 0.62 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3508 | 1/1 | 0.94 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 4113 | 1/1 | 0.94 | 0.54 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1762 | 1/1 | 0.94 | 0.15 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3229 | 1/1 | 0.94 | 0.25 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3154 | 1/1 | 0.94 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3362 | 1/1 | 0.94 | 0.13 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3036 | 1/1 | 0.94 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3001 | 1/1 | 0.94 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3270 | 1/1 | 0.94 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3487 | 1/1 | 0.94 | 0.50 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3680 | 1/1 | 0.94 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3401 | 1/1 | 0.94 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | 1Q | 203 | 1/1 | 0.94 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4126 | 1/1 | 0.94 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 4134 | 1/1 | 0.94 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3073 | 1/1 | 0.94 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3892 | 1/1 | 0.94 | 0.45 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3175 | 1/1 | 0.94 | 0.07 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3640 | 1/1 | 0.94 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3660 | 1/1 | 0.94 | 0.17 | 9,9,9,9 | 0 |
| 56 | MG | 2A | 3074 | 1/1 | 0.94 | 0.44 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3055 | 1/1 | 0.94 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3463 | 1/1 | 0.94 | 0.46 | 42,42,42,42 | 0 |
| 56 | MG | 1X | 105 | 1/1 | 0.94 | 0.24 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3153 | 1/1 | 0.94 | 0.17 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3540 | 1/1 | 0.94 | 0.23 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3560 | 1/1 | 0.94 | 0.13 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3201 | 1/1 | 0.94 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3729 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3642 | 1/1 | 0.94 | 0.21 | 66,66,66,66 | 0 |
| 56 | MG | 2A | 3037 | 1/1 | 0.94 | 0.25 | 47,47,47,47 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3458 | 1/1 | 0.94 | 0.23 | 48,48,48,48 | 0 |
| 56 | MG | 1a | 1737 | 1/1 | 0.94 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3313 | 1/1 | 0.94 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 1X | 104 | 1/1 | 0.94 | 0.50 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3492 | 1/1 | 0.94 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3862 | 1/1 | 0.94 | 0.19 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3657 | 1/1 | 0.94 | 0.20 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 4093 | 1/1 | 0.94 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3607 | 1/1 | 0.94 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 2x | 101 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3156 | 1/1 | 0.94 | 0.14 | 74,74,74,74 | 0 |
| 56 | MG | 1a | 1719 | 1/1 | 0.94 | 0.11 | 33,33,33,33 | 0 |
| 56 | MG | 1R | 204 | 1/1 | 0.94 | 0.25 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 4055 | 1/1 | 0.94 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 1E | 301 | 1/1 | 0.94 | 0.27 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3025 | 1/1 | 0.94 | 0.26 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3174 | 1/1 | 0.94 | 0.12 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3262 | 1/1 | 0.94 | 0.15 | 27,27,27,27 | 0 |
| 56 | MG | 2a | 3008 | 1/1 | 0.94 | 0.15 | 58,58,58,58 | 0 |
| 56 | MG | 1B | 210 | 1/1 | 0.94 | 0.32 | 43,43,43,43 | 0 |
| 56 | MG | 1w | 107 | 1/1 | 0.94 | 0.06 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3749 | 1/1 | 0.94 | 0.19 | 29,29,29,29 | 0 |
| 59 | ZN | 2n | 501 | 1/1 | 0.94 | 0.07 | 84,84,84,84 | 0 |
| 56 | MG | 1G | 201 | 1/1 | 0.94 | 0.17 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3656 | 1/1 | 0.94 | 0.07 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3210 | 1/1 | 0.94 | 0.22 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3743 | 1/1 | 0.94 | 0.08 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3613 | 1/1 | 0.94 | 0.18 | 16,16,16,16 | 0 |
| 58 | K | 2A | 3434 | 1/1 | 0.94 | 0.17 | 67,67,67,67 | 0 |
| 56 | MG | 1A | 3024 | 1/1 | 0.94 | 0.14 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3460 | 1/1 | 0.94 | 0.25 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3114 | 1/1 | 0.94 | 0.14 | 60,60,60,60 | 0 |
| 56 | MG | 2A | 3096 | 1/1 | 0.94 | 0.20 | 65,65,65,65 | 0 |
| 56 | MG | 2A | 3154 | 1/1 | 0.94 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3257 | 1/1 | 0.94 | 0.17 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3811 | 1/1 | 0.94 | 0.10 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3855 | 1/1 | 0.94 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3079 | 1/1 | 0.94 | 0.22 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3748 | 1/1 | 0.94 | 0.17 | 44,44,44,44 | 0 |
| 56 | MG | 1a | 1621 | 1/1 | 0.94 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3079 | 1/1 | 0.94 | 0.45 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3443 | 1/1 | 0.94 | 0.17 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3133 | 1/1 | 0.94 | 0.17 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3182 | 1/1 | 0.94 | 0.27 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3096 | 1/1 | 0.94 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3417 | 1/1 | 0.94 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3843 | 1/1 | 0.94 | 0.12 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3772 | 1/1 | 0.94 | 0.24 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3076 | 1/1 | 0.94 | 0.10 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3126 | 1/1 | 0.94 | 0.15 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3698 | 1/1 | 0.94 | 0.12 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3658 | 1/1 | 0.94 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | 1T | 202 | 1/1 | 0.94 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3195 | 1/1 | 0.94 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3526 | 1/1 | 0.94 | 0.10 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3434 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3503 | 1/1 | 0.94 | 0.29 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3859 | 1/1 | 0.94 | 0.22 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3585 | 1/1 | 0.94 | 0.10 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3471 | 1/1 | 0.94 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3151 | 1/1 | 0.94 | 0.27 | 63,63,63,63 | 0 |
| 56 | MG | 1A | 3852 | 1/1 | 0.94 | 0.21 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 4043 | 1/1 | 0.94 | 0.07 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3186 | 1/1 | 0.94 | 0.39 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3825 | 1/1 | 0.94 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3595 | 1/1 | 0.94 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3550 | 1/1 | 0.94 | 0.22 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3700 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3573 | 1/1 | 0.94 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3051 | 1/1 | 0.94 | 0.34 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3039 | 1/1 | 0.94 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3377 | 1/1 | 0.94 | 0.17 | 12,12,12,12 | 0 |
| 56 | MG | 2A | 3660 | 1/1 | 0.94 | 0.11 | 47,47,47,47 | 0 |
| 56 | MG | 1a | 1787 | 1/1 | 0.94 | 0.23 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3635 | 1/1 | 0.94 | 0.15 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3339 | 1/1 | 0.94 | 0.13 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3227 | 1/1 | 0.94 | 0.51 | 39,39,39,39 | 0 |
| 56 | MG | 2a | 3012 | 1/1 | 0.94 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4003 | 1/1 | 0.94 | 0.09 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 4088 | 1/1 | 0.94 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3141 | 1/1 | 0.94 | 0.20 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3537 | 1/1 | 0.94 | 0.07 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3715 | 1/1 | 0.94 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3457 | 1/1 | 0.94 | 0.13 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3429 | 1/1 | 0.94 | 0.42 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3293 | 1/1 | 0.94 | 0.22 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 4091 | 1/1 | 0.94 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3593 | 1/1 | 0.94 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 3042 | 1/1 | 0.94 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | 1a | 1806 | 1/1 | 0.94 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3206 | 1/1 | 0.94 | 0.60 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3787 | 1/1 | 0.94 | 0.11 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3123 | 1/1 | 0.94 | 0.16 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1721 | 1/1 | 0.94 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3231 | 1/1 | 0.94 | 0.31 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 4125 | 1/1 | 0.94 | 0.55 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3467 | 1/1 | 0.94 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3295 | 1/1 | 0.94 | 0.18 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3398 | 1/1 | 0.94 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3269 | 1/1 | 0.94 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3573 | 1/1 | 0.94 | 0.56 | 18,18,18,18 | 0 |
| 56 | MG | 2a | 3140 | 1/1 | 0.94 | 0.35 | 77,77,77,77 | 0 |
| 56 | MG | 1A | 3523 | 1/1 | 0.94 | 0.15 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3795 | 1/1 | 0.94 | 0.08 | 17,17,17,17 | 0 |
| 56 | MG | 2a | 3195 | 1/1 | 0.94 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3247 | 1/1 | 0.94 | 0.37 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3174 | 1/1 | 0.94 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 2a | 3030 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3838 | 1/1 | 0.94 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3490 | 1/1 | 0.94 | 0.25 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3302 | 1/1 | 0.94 | 0.19 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3137 | 1/1 | 0.94 | 0.21 | 38,38,38,38 | 0 |
| 56 | MG | 1E | 303 | 1/1 | 0.94 | 0.15 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3667 | 1/1 | 0.94 | 0.19 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3518 | 1/1 | 0.94 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3439 | 1/1 | 0.94 | 0.49 | 30,30,30,30 | 0 |
| 56 | MG | 1F | 301 | 1/1 | 0.94 | 0.22 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3170 | 1/1 | 0.94 | 0.52 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3069 | 1/1 | 0.94 | 0.16 | 14,14,14,14 | 0 |
| 56 | MG | 2x | 104 | 1/1 | 0.94 | 0.14 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3337 | 1/1 | 0.94 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3778 | 1/1 | 0.94 | 0.24 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3324 | 1/1 | 0.94 | 0.23 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3461 | 1/1 | 0.94 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3645 | 1/1 | 0.94 | 0.11 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3412 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2B | 214 | 1/1 | 0.94 | 0.52 | 69,69,69,69 | 0 |
| 56 | MG | 2A | 3859 | 1/1 | 0.94 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | 1V | 201 | 1/1 | 0.94 | 0.22 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3516 | 1/1 | 0.94 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3636 | 1/1 | 0.94 | 0.24 | 57,57,57,57 | 0 |
| 56 | MG | 1B | 224 | 1/1 | 0.94 | 0.19 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4120 | 1/1 | 0.94 | 0.62 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3612 | 1/1 | 0.94 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1831 | 1/1 | 0.94 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3072 | 1/1 | 0.94 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3713 | 1/1 | 0.94 | 0.10 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3014 | 1/1 | 0.94 | 0.33 | 25,25,25,25 | 0 |
| 56 | MG | 2a | 3110 | 1/1 | 0.94 | 0.17 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3748 | 1/1 | 0.94 | 0.09 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3366 | 1/1 | 0.94 | 0.26 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3820 | 1/1 | 0.94 | 0.06 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3083 | 1/1 | 0.94 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3095 | 1/1 | 0.94 | 0.15 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3469 | 1/1 | 0.94 | 0.26 | 52,52,52,52 | 0 |
| 56 | MG | 1D | 301 | 1/1 | 0.94 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3950 | 1/1 | 0.94 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | 17 | 102 | 1/1 | 0.94 | 0.28 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3734 | 1/1 | 0.94 | 0.19 | 8,8,8,8 | 0 |
| 56 | MG | 2A | 3520 | 1/1 | 0.94 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3228 | 1/1 | 0.94 | 0.11 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3187 | 1/1 | 0.94 | 0.17 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3005 | 1/1 | 0.94 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 4034 | 1/1 | 0.94 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3145 | 1/1 | 0.94 | 0.06 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3800 | 1/1 | 0.94 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3579 | 1/1 | 0.94 | 0.26 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3441 | 1/1 | 0.94 | 1.14 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3397 | 1/1 | 0.94 | 0.43 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1731 | 1/1 | 0.94 | 0.19 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1609 | 1/1 | 0.94 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3645 | 1/1 | 0.94 | 0.06 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3350 | 1/1 | 0.94 | 0.34 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3185 | 1/1 | 0.94 | 0.12 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3378 | 1/1 | 0.94 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3120 | 1/1 | 0.94 | 0.13 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1634 | 1/1 | 0.94 | 0.25 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3322 | 1/1 | 0.94 | 0.10 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2v | 102 | 1/1 | 0.94 | 0.70 | 52,52,52,52 | 0 |
| 56 | MG | 11 | 102 | 1/1 | 0.94 | 0.42 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 4107 | 1/1 | 0.94 | 0.41 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3806 | 1/1 | 0.94 | 0.58 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3045 | 1/1 | 0.94 | 0.10 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3929 | 1/1 | 0.94 | 0.07 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3256 | 1/1 | 0.94 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3546 | 1/1 | 0.94 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 2D | 303 | 1/1 | 0.94 | 0.26 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 4069 | 1/1 | 0.94 | 0.28 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3169 | 1/1 | 0.94 | 0.11 | 37,37,37,37 | 0 |
| 56 | MG | 2E | 304 | 1/1 | 0.94 | 0.30 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3558 | 1/1 | 0.94 | 0.14 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3327 | 1/1 | 0.94 | 0.24 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1608 | 1/1 | 0.94 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3170 | 1/1 | 0.94 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3915 | 1/1 | 0.94 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3836 | 1/1 | 0.94 | 0.16 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3399 | 1/1 | 0.94 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3564 | 1/1 | 0.94 | 0.23 | 49,49,49,49 | 0 |
| 56 | MG | 1a | 1821 | 1/1 | 0.94 | 0.09 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3209 | 1/1 | 0.94 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3435 | 1/1 | 0.95 | 0.43 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3798 | 1/1 | 0.95 | 0.32 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3698 | 1/1 | 0.95 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3867 | 1/1 | 0.95 | 0.36 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3732 | 1/1 | 0.95 | 0.17 | 15,15,15,15 | 0 |
| 56 | MG | 16 | 102 | 1/1 | 0.95 | 0.47 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3076 | 1/1 | 0.95 | 0.26 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3641 | 1/1 | 0.95 | 0.06 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3268 | 1/1 | 0.95 | 0.33 | 15,15,15,15 | 0 |
| 56 | MG | 2a | 3200 | 1/1 | 0.95 | 0.14 | 56,56,56,56 | 0 |
| 56 | MG | 2a | 3227 | 1/1 | 0.95 | 0.12 | 65,65,65,65 | 0 |
| 56 | MG | 1D | 306 | 1/1 | 0.95 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3880 | 1/1 | 0.95 | 0.15 | 14,14,14,14 | 0 |
| 56 | MG | 2Q | 203 | 1/1 | 0.95 | 0.25 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3085 | 1/1 | 0.95 | 0.11 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3015 | 1/1 | 0.95 | 0.18 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3391 | 1/1 | 0.95 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3602 | 1/1 | 0.95 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3019 | 1/1 | 0.95 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3033 | 1/1 | 0.95 | 0.13 | 19,19,19,19 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3562 | 1/1 | 0.95 | 0.49 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3743 | 1/1 | 0.95 | 0.15 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3273 | 1/1 | 0.95 | 0.28 | 16,16,16,16 | 0 |
| 56 | MG | 1a | 1710 | 1/1 | 0.95 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3695 | 1/1 | 0.95 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3001 | 1/1 | 0.95 | 0.23 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 4018 | 1/1 | 0.95 | 0.11 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3566 | 1/1 | 0.95 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 1R | 203 | 1/1 | 0.95 | 0.12 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3369 | 1/1 | 0.95 | 0.16 | 36,36,36,36 | 0 |
| 56 | MG | 2F | 304 | 1/1 | 0.95 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3592 | 1/1 | 0.95 | 0.13 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3873 | 1/1 | 0.95 | 0.13 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3192 | 1/1 | 0.95 | 0.14 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1620 | 1/1 | 0.95 | 0.19 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 4001 | 1/1 | 0.95 | 0.23 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3183 | 1/1 | 0.95 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 1a | 1824 | 1/1 | 0.95 | 0.06 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3250 | 1/1 | 0.95 | 0.17 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3133 | 1/1 | 0.95 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1N | 207 | 1/1 | 0.95 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | 1a | 1828 | 1/1 | 0.95 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3525 | 1/1 | 0.95 | 0.28 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1643 | 1/1 | 0.95 | 0.16 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3729 | 1/1 | 0.95 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3213 | 1/1 | 0.95 | 0.35 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3234 | 1/1 | 0.95 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 3989 | 1/1 | 0.95 | 0.07 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3420 | 1/1 | 0.95 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3027 | 1/1 | 0.95 | 0.26 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3291 | 1/1 | 0.95 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3545 | 1/1 | 0.95 | 0.13 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3175 | 1/1 | 0.95 | 0.30 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3392 | 1/1 | 0.95 | 0.25 | 35,35,35,35 | 0 |
| 56 | MG | 1O | 202 | 1/1 | 0.95 | 0.27 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3399 | 1/1 | 0.95 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3440 | 1/1 | 0.95 | 0.35 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3034 | 1/1 | 0.95 | 0.36 | 25,25,25,25 | 0 |
| 56 | MG | 2a | 3119 | 1/1 | 0.95 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 12 | 3702 | 1/1 | 0.95 | 0.22 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 4076 | 1/1 | 0.95 | 0.18 | 8,8,8,8 | 0 |
| 56 | MG | 1A | 3567 | 1/1 | 0.95 | 0.13 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1D | 312 | 1/1 | 0.95 | 0.20 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3247 | 1/1 | 0.95 | 0.31 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3684 | 1/1 | 0.95 | 0.14 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3935 | 1/1 | 0.95 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3328 | 1/1 | 0.95 | 0.28 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3619 | 1/1 | 0.95 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3106 | 1/1 | 0.95 | 0.26 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3053 | 1/1 | 0.95 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 1E | 307 | 1/1 | 0.95 | 0.22 | 35,35,35,35 | 0 |
| 56 | MG | 1X | 101 | 1/1 | 0.95 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | 1U | 202 | 1/1 | 0.95 | 0.59 | 29,29,29,29 | 0 |
| 56 | MG | 1W | 202 | 1/1 | 0.95 | 0.23 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3404 | 1/1 | 0.95 | 0.40 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3565 | 1/1 | 0.95 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3335 | 1/1 | 0.95 | 0.27 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3258 | 1/1 | 0.95 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3554 | 1/1 | 0.95 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 1N | 203 | 1/1 | 0.95 | 0.21 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3149 | 1/1 | 0.95 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3728 | 1/1 | 0.95 | 0.09 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 4117 | 1/1 | 0.95 | 0.55 | 21,21,21,21 | 0 |
| 56 | MG | 2a | 3221 | 1/1 | 0.95 | 0.12 | 61,61,61,61 | 0 |
| 56 | MG | 1A | 3818 | 1/1 | 0.95 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1638 | 1/1 | 0.95 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 1a | 1819 | 1/1 | 0.95 | 0.08 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4094 | 1/1 | 0.95 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3512 | 1/1 | 0.95 | 0.39 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3179 | 1/1 | 0.95 | 0.14 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3185 | 1/1 | 0.95 | 0.07 | 55,55,55,55 | 0 |
| 56 | MG | 2a | 3102 | 1/1 | 0.95 | 0.06 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3476 | 1/1 | 0.95 | 0.16 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3966 | 1/1 | 0.95 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3772 | 1/1 | 0.95 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3466 | 1/1 | 0.95 | 0.22 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3610 | 1/1 | 0.95 | 0.14 | 25,25,25,25 | 0 |
| 56 | MG | 1a | 1613 | 1/1 | 0.95 | 0.17 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3883 | 1/1 | 0.95 | 0.20 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3450 | 1/1 | 0.95 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3115 | 1/1 | 0.95 | 0.33 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3753 | 1/1 | 0.95 | 0.15 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3290 | 1/1 | 0.95 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 1a | 1616 | 1/1 | 0.95 | 0.11 | 46,46,46,46 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2q | 203 | 1/1 | 0.95 | 0.07 | 70,70,70,70 | 0 |
| 56 | MG | 2A | 3126 | 1/1 | 0.95 | 0.18 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3887 | 1/1 | 0.95 | 0.21 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3189 | 1/1 | 0.95 | 0.48 | 61,61,61,61 | 0 |
| 59 | ZN | 2Y | 202 | 1/1 | 0.95 | 0.11 | 88,88,88,88 | 0 |
| 56 | MG | 15 | 101 | 1/1 | 0.95 | 0.53 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3248 | 1/1 | 0.95 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3828 | 1/1 | 0.95 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3717 | 1/1 | 0.95 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3428 | 1/1 | 0.95 | 0.09 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3520 | 1/1 | 0.95 | 0.47 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3375 | 1/1 | 0.95 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3450 | 1/1 | 0.95 | 0.11 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3540 | 1/1 | 0.95 | 0.15 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3974 | 1/1 | 0.95 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3446 | 1/1 | 0.95 | 0.40 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3997 | 1/1 | 0.95 | 0.10 | 31,31,31,31 | 0 |
| 56 | MG | 1Z | 303 | 1/1 | 0.95 | 0.20 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3294 | 1/1 | 0.95 | 0.25 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3695 | 1/1 | 0.95 | 0.13 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3119 | 1/1 | 0.95 | 0.20 | 21,21,21,21 | 0 |
| 56 | MG | 1U | 204 | 1/1 | 0.95 | 0.52 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3108 | 1/1 | 0.95 | 0.37 | 29,29,29,29 | 0 |
| 56 | MG | 1a | 1680 | 1/1 | 0.95 | 0.16 | 38,38,38,38 | 0 |
| 56 | MG | 1G | 204 | 1/1 | 0.95 | 0.14 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3701 | 1/1 | 0.95 | 0.28 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3858 | 1/1 | 0.95 | 0.43 | 60,60,60,60 | 0 |
| 56 | MG | 1A | 3114 | 1/1 | 0.95 | 0.39 | 22,22,22,22 | 0 |
| 56 | MG | 1R | 201 | 1/1 | 0.95 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3604 | 1/1 | 0.95 | 0.17 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3295 | 1/1 | 0.95 | 0.29 | 47,47,47,47 | 0 |
| 56 | MG | 1F | 303 | 1/1 | 0.95 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3771 | 1/1 | 0.95 | 0.20 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3237 | 1/1 | 0.95 | 0.29 | 41,41,41,41 | 0 |
| 56 | MG | 1W | 204 | 1/1 | 0.95 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | 2a | 3184 | 1/1 | 0.95 | 0.13 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 4132 | 1/1 | 0.95 | 0.42 | 24,24,24,24 | 0 |
| 56 | MG | 2t | 201 | 1/1 | 0.95 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 15 | 103 | 1/1 | 0.95 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3161 | 1/1 | 0.95 | 0.67 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3196 | 1/1 | 0.95 | 0.12 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1717 | 1/1 | 0.95 | 0.16 | 53,53,53,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2a | 3223 | 1/1 | 0.95 | 0.08 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3713 | 1/1 | 0.95 | 0.18 | 69,69,69,69 | 0 |
| 56 | MG | 1x | 106 | 1/1 | 0.95 | 0.05 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3243 | 1/1 | 0.95 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3928 | 1/1 | 0.95 | 0.12 | 15,15,15,15 | 0 |
| 56 | MG | 1a | 1755 | 1/1 | 0.95 | 0.08 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3190 | 1/1 | 0.95 | 0.11 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3505 | 1/1 | 0.95 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1a | 1644 | 1/1 | 0.95 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 2q | 202 | 1/1 | 0.95 | 0.09 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3242 | 1/1 | 0.95 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3419 | 1/1 | 0.95 | 0.16 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3690 | 1/1 | 0.95 | 0.13 | 7,7,7,7 | 0 |
| 56 | MG | 1A | 4105 | 1/1 | 0.95 | 0.11 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3786 | 1/1 | 0.95 | 0.15 | 13,13,13,13 | 0 |
| 56 | MG | 1x | 110 | 1/1 | 0.95 | 0.09 | 59,59,59,59 | 0 |
| 56 | MG | 1B | 228 | 1/1 | 0.95 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3590 | 1/1 | 0.95 | 0.13 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3323 | 1/1 | 0.95 | 0.11 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3066 | 1/1 | 0.95 | 0.24 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3608 | 1/1 | 0.95 | 0.14 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3658 | 1/1 | 0.95 | 0.26 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3563 | 1/1 | 0.95 | 0.15 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3224 | 1/1 | 0.95 | 0.22 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3230 | 1/1 | 0.95 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3570 | 1/1 | 0.95 | 0.65 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3452 | 1/1 | 0.95 | 0.18 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3423 | 1/1 | 0.95 | 0.12 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3675 | 1/1 | 0.95 | 0.11 | 23,23,23,23 | 0 |
| 56 | MG | 29 | 101 | 1/1 | 0.95 | 0.18 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3845 | 1/1 | 0.95 | 0.17 | 16,16,16,16 | 0 |
| 56 | MG | 1a | 1618 | 1/1 | 0.95 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3152 | 1/1 | 0.95 | 0.14 | 61,61,61,61 | 0 |
| 56 | MG | 2a | 3113 | 1/1 | 0.95 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 4072 | 1/1 | 0.95 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1814 | 1/1 | 0.95 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3262 | 1/1 | 0.95 | 0.82 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3186 | 1/1 | 0.95 | 0.30 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3363 | 1/1 | 0.95 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3704 | 1/1 | 0.95 | 0.07 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3276 | 1/1 | 0.95 | 0.46 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3188 | 1/1 | 0.95 | 0.39 | 30,30,30,30 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3051 | 1/1 | 0.95 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3550 | 1/1 | 0.95 | 0.64 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3933 | 1/1 | 0.95 | 0.12 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3294 | 1/1 | 0.95 | 0.16 | 55,55,55,55 | 0 |
| 56 | MG | 2A | 3629 | 1/1 | 0.95 | 0.12 | 53,53,53,53 | 0 |
| 56 | MG | 2a | 3213 | 1/1 | 0.95 | 0.23 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3444 | 1/1 | 0.95 | 0.22 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3505 | 1/1 | 0.95 | 0.24 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3495 | 1/1 | 0.95 | 0.11 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1803 | 1/1 | 0.95 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 1B | 219 | 1/1 | 0.95 | 0.21 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3514 | 1/1 | 0.95 | 0.18 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3614 | 1/1 | 0.95 | 0.07 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3536 | 1/1 | 0.95 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | 2a | 3125 | 1/1 | 0.95 | 0.04 | 58,58,58,58 | 0 |
| 56 | MG | 2A | 3059 | 1/1 | 0.95 | 0.16 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3021 | 1/1 | 0.95 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3767 | 1/1 | 0.95 | 0.35 | 70,70,70,70 | 0 |
| 56 | MG | 1A | 3789 | 1/1 | 0.95 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 2a | 3210 | 1/1 | 0.95 | 0.09 | 64,64,64,64 | 0 |
| 56 | MG | 2A | 3791 | 1/1 | 0.95 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3246 | 1/1 | 0.95 | 0.17 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3816 | 1/1 | 0.95 | 0.08 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3557 | 1/1 | 0.95 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 1X | 103 | 1/1 | 0.95 | 0.22 | 19,19,19,19 | 0 |
| 56 | MG | 2a | 3222 | 1/1 | 0.95 | 0.13 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3832 | 1/1 | 0.95 | 0.09 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3808 | 1/1 | 0.95 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3093 | 1/1 | 0.95 | 0.17 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4092 | 1/1 | 0.95 | 0.31 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3814 | 1/1 | 0.95 | 0.12 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3851 | 1/1 | 0.95 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3055 | 1/1 | 0.95 | 0.07 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4130 | 1/1 | 0.95 | 0.60 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3068 | 1/1 | 0.95 | 0.17 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 4090 | 1/1 | 0.95 | 0.13 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3202 | 1/1 | 0.95 | 0.17 | 64,64,64,64 | 0 |
| 56 | MG | 1A | 3214 | 1/1 | 0.95 | 0.39 | 32,32,32,32 | 0 |
| 56 | MG | 2O | 201 | 1/1 | 0.95 | 0.06 | 50,50,50,50 | 0 |
| 56 | MG | 2A | 3203 | 1/1 | 0.96 | 0.26 | 55,55,55,55 | 0 |
| 56 | MG | 1a | 1778 | 1/1 | 0.96 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3104 | 1/1 | 0.96 | 0.17 | 25,25,25,25 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3740 | 1/1 | 0.96 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3033 | 1/1 | 0.96 | 0.55 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1753 | 1/1 | 0.96 | 0.24 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3963 | 1/1 | 0.96 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3762 | 1/1 | 0.96 | 0.17 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3706 | 1/1 | 0.96 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3042 | 1/1 | 0.96 | 0.13 | 24,24,24,24 | 0 |
| 56 | MG | 1t | 201 | 1/1 | 0.96 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3925 | 1/1 | 0.96 | 0.13 | 12,12,12,12 | 0 |
| 56 | MG | 2A | 3694 | 1/1 | 0.96 | 0.20 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3493 | 1/1 | 0.96 | 0.29 | 22,22,22,22 | 0 |
| 56 | MG | 1a | 1663 | 1/1 | 0.96 | 0.11 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3511 | 1/1 | 0.96 | 0.14 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3231 | 1/1 | 0.96 | 0.27 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3077 | 1/1 | 0.96 | 0.17 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3687 | 1/1 | 0.96 | 0.21 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 4065 | 1/1 | 0.96 | 0.07 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 4119 | 1/1 | 0.96 | 0.21 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3374 | 1/1 | 0.96 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3222 | 1/1 | 0.96 | 0.10 | 20,20,20,20 | 0 |
| 56 | MG | 1a | 1745 | 1/1 | 0.96 | 0.08 | 32,32,32,32 | 0 |
| 56 | MG | 2a | 3230 | 1/1 | 0.96 | 0.08 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3829 | 1/1 | 0.96 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 1B | 213 | 1/1 | 0.96 | 0.13 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3325 | 1/1 | 0.96 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3020 | 1/1 | 0.96 | 0.15 | 26,26,26,26 | 0 |
| 56 | MG | 2a | 3026 | 1/1 | 0.96 | 0.09 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3509 | 1/1 | 0.96 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3666 | 1/1 | 0.96 | 0.15 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3776 | 1/1 | 0.96 | 0.07 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3839 | 1/1 | 0.96 | 0.22 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3797 | 1/1 | 0.96 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 4000 | 1/1 | 0.96 | 0.12 | 15,15,15,15 | 0 |
| 56 | MG | 2a | 3131 | 1/1 | 0.96 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3236 | 1/1 | 0.96 | 0.21 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3840 | 1/1 | 0.96 | 0.14 | 12,12,12,12 | 0 |
| 56 | MG | 2A | 3683 | 1/1 | 0.96 | 0.13 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3443 | 1/1 | 0.96 | 0.23 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 4082 | 1/1 | 0.96 | 0.20 | 31,31,31,31 | 0 |
| 56 | MG | 1Z | 301 | 1/1 | 0.96 | 0.36 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3472 | 1/1 | 0.96 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | 1W | 203 | 1/1 | 0.96 | 0.22 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1a | 1684 | 1/1 | 0.96 | 0.19 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3606 | 1/1 | 0.96 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | 1F | 307 | 1/1 | 0.96 | 0.25 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3652 | 1/1 | 0.96 | 0.21 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3226 | 1/1 | 0.96 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4104 | 1/1 | 0.96 | 0.43 | 24,24,24,24 | 0 |
| 56 | MG | 2a | 3150 | 1/1 | 0.96 | 0.18 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 4078 | 1/1 | 0.96 | 0.17 | 6,6,6,6 | 0 |
| 56 | MG | 1A | 4127 | 1/1 | 0.96 | 0.74 | 27,27,27,27 | 0 |
| 56 | MG | 1a | 1676 | 1/1 | 0.96 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 27 | 101 | 1/1 | 0.96 | 0.80 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3169 | 1/1 | 0.96 | 0.28 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3804 | 1/1 | 0.96 | 0.13 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3172 | 1/1 | 0.96 | 0.10 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3244 | 1/1 | 0.96 | 0.12 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3884 | 1/1 | 0.96 | 0.25 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3572 | 1/1 | 0.96 | 0.48 | 33,33,33,33 | 0 |
| 56 | MG | 2a | 3044 | 1/1 | 0.96 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1a | 1669 | 1/1 | 0.96 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3431 | 1/1 | 0.96 | 0.14 | 37,37,37,37 | 0 |
| 56 | MG | 1D | 308 | 1/1 | 0.96 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3122 | 1/1 | 0.96 | 0.13 | 31,31,31,31 | 0 |
| 56 | MG | 1D | 304 | 1/1 | 0.96 | 0.60 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3624 | 1/1 | 0.96 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3077 | 1/1 | 0.96 | 0.28 | 41,41,41,41 | 0 |
| 56 | MG | 2a | 3115 | 1/1 | 0.96 | 0.20 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3063 | 1/1 | 0.96 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3029 | 1/1 | 0.96 | 0.20 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1740 | 1/1 | 0.96 | 0.13 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3626 | 1/1 | 0.96 | 0.22 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3596 | 1/1 | 0.96 | 0.14 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3357 | 1/1 | 0.96 | 0.24 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3017 | 1/1 | 0.96 | 0.14 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3792 | 1/1 | 0.96 | 0.13 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3784 | 1/1 | 0.96 | 0.18 | 11,11,11,11 | 0 |
| 56 | MG | 1a | 1811 | 1/1 | 0.96 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3796 | 1/1 | 0.96 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3182 | 1/1 | 0.96 | 0.06 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3013 | 1/1 | 0.96 | 0.23 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3764 | 1/1 | 0.96 | 0.05 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3395 | 1/1 | 0.96 | 0.13 | 24,24,24,24 | 0 |
| 56 | MG | 1e | 202 | 1/1 | 0.96 | 0.06 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2a | 3084 | 1/1 | 0.96 | 0.12 | 57,57,57,57 | 0 |
| 56 | MG | 1A | 3668 | 1/1 | 0.96 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3578 | 1/1 | 0.96 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3746 | 1/1 | 0.96 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3656 | 1/1 | 0.96 | 0.12 | 9,9,9,9 | 0 |
| 56 | MG | 1a | 1770 | 1/1 | 0.96 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3361 | 1/1 | 0.96 | 0.06 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1744 | 1/1 | 0.96 | 0.20 | 50,50,50,50 | 0 |
| 56 | MG | 2a | 3191 | 1/1 | 0.96 | 0.30 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3056 | 1/1 | 0.96 | 0.17 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1733 | 1/1 | 0.96 | 0.20 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1646 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3093 | 1/1 | 0.96 | 0.08 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3693 | 1/1 | 0.96 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3484 | 1/1 | 0.96 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3156 | 1/1 | 0.96 | 0.32 | 18,18,18,18 | 0 |
| 56 | MG | 2j | 201 | 1/1 | 0.96 | 0.09 | 74,74,74,74 | 0 |
| 56 | MG | 2A | 3460 | 1/1 | 0.96 | 0.21 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3673 | 1/1 | 0.96 | 0.12 | 12,12,12,12 | 0 |
| 56 | MG | 1A | 3796 | 1/1 | 0.96 | 0.57 | 20,20,20,20 | 0 |
| 56 | MG | 1a | 1715 | 1/1 | 0.96 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3221 | 1/1 | 0.96 | 0.20 | 12,12,12,12 | 0 |
| 56 | MG | 2E | 303 | 1/1 | 0.96 | 0.25 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3178 | 1/1 | 0.96 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3580 | 1/1 | 0.96 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3555 | 1/1 | 0.96 | 0.23 | 38,38,38,38 | 0 |
| 56 | MG | 15 | 102 | 1/1 | 0.96 | 0.32 | 28,28,28,28 | 0 |
| 56 | MG | 2a | 3087 | 1/1 | 0.96 | 0.11 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3195 | 1/1 | 0.96 | 0.12 | 17,17,17,17 | 0 |
| 56 | MG | 1a | 1785 | 1/1 | 0.96 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3468 | 1/1 | 0.96 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3959 | 1/1 | 0.96 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3067 | 1/1 | 0.96 | 0.15 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3493 | 1/1 | 0.96 | 0.21 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3574 | 1/1 | 0.96 | 0.15 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3189 | 1/1 | 0.96 | 0.29 | 23,23,23,23 | 0 |
| 56 | MG | 1W | 207 | 1/1 | 0.96 | 0.24 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3882 | 1/1 | 0.96 | 0.10 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3292 | 1/1 | 0.96 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 10 | 104 | 1/1 | 0.96 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3717 | 1/1 | 0.96 | 0.13 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3831 | 1/1 | 0.96 | 0.12 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2R | 3003 | 1/1 | 0.96 | 0.10 | 40,40,40,40 | 0 |
| 56 | MG | 2a | 3031 | 1/1 | 0.96 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3530 | 1/1 | 0.96 | 0.25 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3611 | 1/1 | 0.96 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3644 | 1/1 | 0.96 | 0.19 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3032 | 1/1 | 0.96 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 2Q | 205 | 1/1 | 0.96 | 0.12 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 4019 | 1/1 | 0.96 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 1D | 309 | 1/1 | 0.96 | 0.28 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3538 | 1/1 | 0.96 | 0.16 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3529 | 1/1 | 0.96 | 0.20 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3108 | 1/1 | 0.96 | 0.24 | 40,40,40,40 | 0 |
| 56 | MG | 1O | 203 | 1/1 | 0.96 | 0.42 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3118 | 1/1 | 0.96 | 0.69 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3159 | 1/1 | 0.96 | 0.19 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3120 | 1/1 | 0.96 | 0.17 | 59,59,59,59 | 0 |
| 56 | MG | 2A | 3430 | 1/1 | 0.96 | 0.11 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3813 | 1/1 | 0.96 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3280 | 1/1 | 0.96 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3758 | 1/1 | 0.96 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | 2A | 3216 | 1/1 | 0.96 | 0.12 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3293 | 1/1 | 0.96 | 0.13 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3317 | 1/1 | 0.96 | 0.31 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3793 | 1/1 | 0.96 | 0.19 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3228 | 1/1 | 0.96 | 0.54 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3127 | 1/1 | 0.96 | 0.17 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3010 | 1/1 | 0.96 | 0.14 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3909 | 1/1 | 0.96 | 0.14 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3306 | 1/1 | 0.96 | 0.15 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3022 | 1/1 | 0.96 | 0.13 | 11,11,11,11 | 0 |
| 56 | MG | 1A | 3279 | 1/1 | 0.96 | 0.35 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3303 | 1/1 | 0.96 | 0.15 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3706 | 1/1 | 0.96 | 0.07 | 62,62,62,62 | 0 |
| 56 | MG | 1Y | 205 | 1/1 | 0.96 | 0.50 | 48,48,48,48 | 0 |
| 56 | MG | 2a | 3206 | 1/1 | 0.96 | 0.09 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 4080 | 1/1 | 0.96 | 0.10 | 11,11,11,11 | 0 |
| 56 | MG | 1A | 3812 | 1/1 | 0.96 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | 2v | 101 | 1/1 | 0.96 | 0.11 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3192 | 1/1 | 0.96 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3576 | 1/1 | 0.96 | 0.10 | 33,33,33,33 | 0 |
| 56 | MG | 1B | 226 | 1/1 | 0.96 | 0.12 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3780 | 1/1 | 0.96 | 0.21 | 36,36,36,36 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3877 | 1/1 | 0.96 | 0.09 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3492 | 1/1 | 0.96 | 0.11 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3957 | 1/1 | 0.96 | 0.09 | 37,37,37,37 | 0 |
| 56 | MG | 2a | 3023 | 1/1 | 0.96 | 0.14 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3132 | 1/1 | 0.96 | 0.13 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3396 | 1/1 | 0.96 | 0.38 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3365 | 1/1 | 0.96 | 0.25 | 57,57,57,57 | 0 |
| 56 | MG | 2a | 3105 | 1/1 | 0.96 | 0.06 | 66,66,66,66 | 0 |
| 56 | MG | 1A | 3854 | 1/1 | 0.96 | 0.43 | 54,54,54,54 | 0 |
| 56 | MG | 1D | 302 | 1/1 | 0.96 | 0.36 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3287 | 1/1 | 0.96 | 0.19 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3351 | 1/1 | 0.96 | 0.18 | 36,36,36,36 | 0 |
| 56 | MG | 2A | 3072 | 1/1 | 0.96 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 2A | 3621 | 1/1 | 0.96 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3826 | 1/1 | 0.96 | 0.07 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3822 | 1/1 | 0.96 | 0.26 | 62,62,62,62 | 0 |
| 56 | MG | 2A | 3605 | 1/1 | 0.96 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3125 | 1/1 | 0.96 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 1a | 1768 | 1/1 | 0.96 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3655 | 1/1 | 0.96 | 0.12 | 31,31,31,31 | 0 |
| 56 | MG | 1a | 1698 | 1/1 | 0.96 | 0.18 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3274 | 1/1 | 0.96 | 0.27 | 19,19,19,19 | 0 |
| 56 | MG | 1a | 1611 | 1/1 | 0.96 | 0.09 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3875 | 1/1 | 0.96 | 0.16 | 34,34,34,34 | 0 |
| 57 | LUJ | 1a | 1832 | 44/44 | 0.96 | 0.26 | 29,39,44,48 | 0 |
| 56 | MG | 1A | 3605 | 1/1 | 0.96 | 0.20 | 29,29,29,29 | 0 |
| 56 | MG | 1a | 1736 | 1/1 | 0.96 | 0.15 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3331 | 1/1 | 0.96 | 0.15 | 36,36,36,36 | 0 |
| 56 | MG | 1a | 1707 | 1/1 | 0.96 | 0.19 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3773 | 1/1 | 0.96 | 0.34 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3589 | 1/1 | 0.96 | 0.14 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3283 | 1/1 | 0.96 | 0.15 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3023 | 1/1 | 0.96 | 0.58 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3846 | 1/1 | 0.96 | 0.10 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3088 | 1/1 | 0.96 | 0.12 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3102 | 1/1 | 0.96 | 0.17 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3527 | 1/1 | 0.96 | 0.21 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3607 | 1/1 | 0.96 | 0.18 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1610 | 1/1 | 0.96 | 0.12 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 4121 | 1/1 | 0.96 | 0.66 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3075 | 1/1 | 0.96 | 0.47 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 4112 | 1/1 | 0.96 | 0.09 | 43,43,43,43 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3590 | 1/1 | 0.96 | 0.13 | 15,15,15,15 | 0 |
| 56 | MG | 2A | 3664 | 1/1 | 0.96 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3775 | 1/1 | 0.96 | 0.06 | 28,28,28,28 | 0 |
| 56 | MG | 17 | 101 | 1/1 | 0.96 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 2B | 203 | 1/1 | 0.96 | 0.18 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3304 | 1/1 | 0.96 | 0.14 | 42,42,42,42 | 0 |
| 56 | MG | 2a | 3212 | 1/1 | 0.96 | 0.21 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1694 | 1/1 | 0.96 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3223 | 1/1 | 0.96 | 0.81 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3371 | 1/1 | 0.96 | 0.61 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3371 | 1/1 | 0.96 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 2a | 3082 | 1/1 | 0.96 | 0.11 | 72,72,72,72 | 0 |
| 56 | MG | 2A | 3135 | 1/1 | 0.96 | 0.23 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1704 | 1/1 | 0.96 | 0.14 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3920 | 1/1 | 0.96 | 0.15 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3372 | 1/1 | 0.96 | 0.21 | 24,24,24,24 | 0 |
| 56 | MG | 1Q | 202 | 1/1 | 0.96 | 0.21 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3622 | 1/1 | 0.96 | 0.16 | 9,9,9,9 | 0 |
| 56 | MG | 2A | 3344 | 1/1 | 0.96 | 0.16 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3185 | 1/1 | 0.97 | 0.38 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3898 | 1/1 | 0.97 | 0.11 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1623 | 1/1 | 0.97 | 0.19 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3098 | 1/1 | 0.97 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 1a | 1805 | 1/1 | 0.97 | 0.24 | 49,49,49,49 | 0 |
| 56 | MG | 1B | 211 | 1/1 | 0.97 | 0.34 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3564 | 1/1 | 0.97 | 0.35 | 21,21,21,21 | 0 |
| 56 | MG | 1F | 309 | 1/1 | 0.97 | 0.09 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3030 | 1/1 | 0.97 | 0.20 | 9,9,9,9 | 0 |
| 56 | MG | 1A | 3855 | 1/1 | 0.97 | 0.09 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3388 | 1/1 | 0.97 | 0.30 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1655 | 1/1 | 0.97 | 0.14 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3087 | 1/1 | 0.97 | 0.18 | 59,59,59,59 | 0 |
| 56 | MG | 2a | 3196 | 1/1 | 0.97 | 0.14 | 63,63,63,63 | 0 |
| 56 | MG | 2A | 3800 | 1/1 | 0.97 | 0.10 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3004 | 1/1 | 0.97 | 0.19 | 17,17,17,17 | 0 |
| 56 | MG | 1a | 1798 | 1/1 | 0.97 | 0.08 | 48,48,48,48 | 0 |
| 56 | MG | 2A | 3517 | 1/1 | 0.97 | 0.20 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3075 | 1/1 | 0.97 | 0.27 | 22,22,22,22 | 0 |
| 56 | MG | 2a | 3092 | 1/1 | 0.97 | 0.22 | 45,45,45,45 | 0 |
| 56 | MG | 2A | 3529 | 1/1 | 0.97 | 0.13 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3122 | 1/1 | 0.97 | 0.41 | 23,23,23,23 | 0 |
| 56 | MG | 2B | 218 | 1/1 | 0.97 | 0.21 | 40,40,40,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1y | 102 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3040 | 1/1 | 0.97 | 0.44 | 21,21,21,21 | 0 |
| 56 | MG | 1B | 214 | 1/1 | 0.97 | 0.20 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3899 | 1/1 | 0.97 | 0.08 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3318 | 1/1 | 0.97 | 0.10 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3162 | 1/1 | 0.97 | 0.44 | 25,25,25,25 | 0 |
| 56 | MG | 1A | 3217 | 1/1 | 0.97 | 0.17 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 4108 | 1/1 | 0.97 | 0.21 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3182 | 1/1 | 0.97 | 0.28 | 36,36,36,36 | 0 |
| 56 | MG | 1D | 310 | 1/1 | 0.97 | 0.20 | 29,29,29,29 | 0 |
| 56 | MG | 2a | 3128 | 1/1 | 0.97 | 0.15 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3181 | 1/1 | 0.97 | 0.17 | 24,24,24,24 | 0 |
| 56 | MG | 1a | 1725 | 1/1 | 0.97 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | 1D | 307 | 1/1 | 0.97 | 0.74 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3638 | 1/1 | 0.97 | 0.17 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3498 | 1/1 | 0.97 | 0.26 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3007 | 1/1 | 0.97 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3070 | 1/1 | 0.97 | 0.32 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3441 | 1/1 | 0.97 | 0.20 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1791 | 1/1 | 0.97 | 0.12 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3029 | 1/1 | 0.97 | 0.42 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 4038 | 1/1 | 0.97 | 0.12 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3637 | 1/1 | 0.97 | 0.15 | 54,54,54,54 | 0 |
| 56 | MG | 1A | 3300 | 1/1 | 0.97 | 0.10 | 17,17,17,17 | 0 |
| 56 | MG | 2a | 3163 | 1/1 | 0.97 | 0.09 | 62,62,62,62 | 0 |
| 56 | MG | 1A | 3491 | 1/1 | 0.97 | 0.37 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 4106 | 1/1 | 0.97 | 0.29 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3132 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3202 | 1/1 | 0.97 | 0.14 | 41,41,41,41 | 0 |
| 56 | MG | 2A | 3537 | 1/1 | 0.97 | 0.08 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3583 | 1/1 | 0.97 | 0.20 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3908 | 1/1 | 0.97 | 0.09 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3387 | 1/1 | 0.97 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 1D | 313 | 1/1 | 0.97 | 0.30 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3473 | 1/1 | 0.97 | 0.23 | 38,38,38,38 | 0 |
| 56 | MG | 1B | 217 | 1/1 | 0.97 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3326 | 1/1 | 0.97 | 0.10 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3454 | 1/1 | 0.97 | 0.19 | 52,52,52,52 | 0 |
| 56 | MG | 2a | 3181 | 1/1 | 0.97 | 0.14 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3025 | 1/1 | 0.97 | 0.12 | 33,33,33,33 | 0 |
| 59 | ZN | 26 | 501 | 1/1 | 0.97 | 0.16 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3289 | 1/1 | 0.97 | 0.10 | 57,57,57,57 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3773 | 1/1 | 0.97 | 0.13 | 37,37,37,37 | 0 |
| 59 | ZN | 1Y | 206 | 1/1 | 0.97 | 0.18 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3494 | 1/1 | 0.97 | 0.21 | 31,31,31,31 | 0 |
| 56 | MG | 2a | 3207 | 1/1 | 0.97 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 2A | 3633 | 1/1 | 0.97 | 0.10 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3128 | 1/1 | 0.97 | 0.10 | 39,39,39,39 | 0 |
| 56 | MG | 16 | 101 | 1/1 | 0.97 | 0.16 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3600 | 1/1 | 0.97 | 0.16 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 4063 | 1/1 | 0.97 | 0.12 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3715 | 1/1 | 0.97 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3110 | 1/1 | 0.97 | 0.15 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3533 | 1/1 | 0.97 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3087 | 1/1 | 0.97 | 0.19 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3644 | 1/1 | 0.97 | 0.15 | 24,24,24,24 | 0 |
| 56 | MG | 2a | 3190 | 1/1 | 0.97 | 0.15 | 56,56,56,56 | 0 |
| 56 | MG | 2A | 3163 | 1/1 | 0.97 | 0.19 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3581 | 1/1 | 0.97 | 0.11 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3617 | 1/1 | 0.97 | 0.30 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3173 | 1/1 | 0.97 | 0.16 | 10,10,10,10 | 0 |
| 56 | MG | 2A | 3654 | 1/1 | 0.97 | 0.27 | 57,57,57,57 | 0 |
| 56 | MG | 1a | 1700 | 1/1 | 0.97 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3650 | 1/1 | 0.97 | 0.13 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3116 | 1/1 | 0.97 | 0.15 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3041 | 1/1 | 0.97 | 0.19 | 41,41,41,41 | 0 |
| 56 | MG | 1A | 3603 | 1/1 | 0.97 | 0.12 | 8,8,8,8 | 0 |
| 56 | MG | 1B | 203 | 1/1 | 0.97 | 0.25 | 33,33,33,33 | 0 |
| 56 | MG | 1l | 201 | 1/1 | 0.97 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3864 | 1/1 | 0.97 | 0.50 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3710 | 1/1 | 0.97 | 0.14 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3732 | 1/1 | 0.97 | 0.11 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3751 | 1/1 | 0.97 | 0.10 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3649 | 1/1 | 0.97 | 0.16 | 11,11,11,11 | 0 |
| 56 | MG | 2A | 3498 | 1/1 | 0.97 | 0.13 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3141 | 1/1 | 0.97 | 0.45 | 25,25,25,25 | 0 |
| 56 | MG | 1T | 201 | 1/1 | 0.97 | 0.10 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1772 | 1/1 | 0.97 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3601 | 1/1 | 0.97 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 2A | 3532 | 1/1 | 0.97 | 0.10 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4122 | 1/1 | 0.97 | 0.24 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3228 | 1/1 | 0.97 | 0.20 | 55,55,55,55 | 0 |
| 56 | MG | 1A | 4002 | 1/1 | 0.97 | 0.15 | 11,11,11,11 | 0 |
| 56 | MG | 2a | 3059 | 1/1 | 0.97 | 0.13 | 48,48,48,48 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3588 | 1/1 | 0.97 | 0.24 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3037 | 1/1 | 0.97 | 0.26 | 24,24,24,24 | 0 |
| 56 | MG | 2A | 3111 | 1/1 | 0.97 | 0.16 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3002 | 1/1 | 0.97 | 0.28 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3131 | 1/1 | 0.97 | 0.13 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3470 | 1/1 | 0.97 | 0.21 | 21,21,21,21 | 0 |
| 56 | MG | 1a | 1632 | 1/1 | 0.97 | 0.11 | 25,25,25,25 | 0 |
| 56 | MG | 2W | 201 | 1/1 | 0.97 | 0.09 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3206 | 1/1 | 0.97 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1W | 205 | 1/1 | 0.97 | 0.28 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3134 | 1/1 | 0.97 | 0.13 | 38,38,38,38 | 0 |
| 56 | MG | 1a | 1656 | 1/1 | 0.97 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3086 | 1/1 | 0.97 | 0.16 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3384 | 1/1 | 0.97 | 0.45 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3031 | 1/1 | 0.97 | 0.37 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3096 | 1/1 | 0.97 | 0.17 | 17,17,17,17 | 0 |
| 56 | MG | 2A | 3127 | 1/1 | 0.97 | 0.33 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3802 | 1/1 | 0.97 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 2A | 3551 | 1/1 | 0.97 | 0.08 | 58,58,58,58 | 0 |
| 56 | MG | 1a | 1769 | 1/1 | 0.97 | 0.10 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3571 | 1/1 | 0.97 | 0.28 | 25,25,25,25 | 0 |
| 56 | MG | 2a | 3209 | 1/1 | 0.97 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3117 | 1/1 | 0.97 | 0.40 | 54,54,54,54 | 0 |
| 56 | MG | 2A | 3350 | 1/1 | 0.97 | 0.28 | 42,42,42,42 | 0 |
| 56 | MG | 1A | 3581 | 1/1 | 0.97 | 0.15 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3889 | 1/1 | 0.97 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 1a | 1649 | 1/1 | 0.97 | 0.21 | 53,53,53,53 | 0 |
| 56 | MG | 2A | 3003 | 1/1 | 0.97 | 0.24 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 4133 | 1/1 | 0.97 | 0.75 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3164 | 1/1 | 0.97 | 0.26 | 26,26,26,26 | 0 |
| 56 | MG | 17 | 103 | 1/1 | 0.97 | 0.23 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3373 | 1/1 | 0.97 | 0.17 | 20,20,20,20 | 0 |
| 56 | MG | 2E | 306 | 1/1 | 0.97 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3130 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3426 | 1/1 | 0.97 | 0.23 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3151 | 1/1 | 0.97 | 0.15 | 45,45,45,45 | 0 |
| 56 | MG | 1a | 1679 | 1/1 | 0.97 | 0.09 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3794 | 1/1 | 0.97 | 0.08 | 18,18,18,18 | 0 |
| 56 | MG | 2R | 3002 | 1/1 | 0.97 | 0.13 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3891 | 1/1 | 0.97 | 0.28 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3094 | 1/1 | 0.97 | 0.23 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3274 | 1/1 | 0.97 | 0.09 | 39,39,39,39 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3311 | 1/1 | 0.97 | 0.08 | 34,34,34,34 | 0 |
| 56 | MG | 1a | 1833 | 1/1 | 0.97 | 0.16 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3036 | 1/1 | 0.97 | 0.67 | 26,26,26,26 | 0 |
| 56 | MG | 1D | 305 | 1/1 | 0.97 | 0.09 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3580 | 1/1 | 0.97 | 0.22 | 15,15,15,15 | 0 |
| 56 | MG | 18 | 103 | 1/1 | 0.97 | 0.18 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3574 | 1/1 | 0.97 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3253 | 1/1 | 0.97 | 0.17 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3016 | 1/1 | 0.97 | 0.16 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3768 | 1/1 | 0.97 | 0.09 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3139 | 1/1 | 0.97 | 0.16 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3176 | 1/1 | 0.97 | 0.21 | 31,31,31,31 | 0 |
| 56 | MG | 1Y | 201 | 1/1 | 0.97 | 0.40 | 47,47,47,47 | 0 |
| 56 | MG | 2A | 3038 | 1/1 | 0.97 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | 1G | 203 | 1/1 | 0.97 | 0.06 | 61,61,61,61 | 0 |
| 56 | MG | 2A | 3552 | 1/1 | 0.97 | 0.12 | 23,23,23,23 | 0 |
| 56 | MG | 2A | 3606 | 1/1 | 0.97 | 0.08 | 31,31,31,31 | 0 |
| 56 | MG | 18 | 102 | 1/1 | 0.97 | 0.11 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3332 | 1/1 | 0.97 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3171 | 1/1 | 0.97 | 0.18 | 17,17,17,17 | 0 |
| 56 | MG | 1A | 3816 | 1/1 | 0.97 | 0.13 | 28,28,28,28 | 0 |
| 56 | MG | 1P | 201 | 1/1 | 0.97 | 0.32 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3774 | 1/1 | 0.97 | 0.06 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3300 | 1/1 | 0.97 | 0.18 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3617 | 1/1 | 0.97 | 0.10 | 14,14,14,14 | 0 |
| 56 | MG | 2A | 3631 | 1/1 | 0.97 | 0.43 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3841 | 1/1 | 0.97 | 0.19 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3163 | 1/1 | 0.97 | 0.15 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3711 | 1/1 | 0.97 | 0.07 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3742 | 1/1 | 0.97 | 0.10 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3676 | 1/1 | 0.97 | 0.26 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3802 | 1/1 | 0.97 | 0.18 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3647 | 1/1 | 0.97 | 0.16 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3360 | 1/1 | 0.97 | 0.11 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4114 | 1/1 | 0.97 | 0.37 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3005 | 1/1 | 0.97 | 0.17 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3707 | 1/1 | 0.97 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3039 | 1/1 | 0.97 | 0.12 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3035 | 1/1 | 0.97 | 0.11 | 13,13,13,13 | 0 |
| 56 | MG | 2A | 3089 | 1/1 | 0.97 | 0.12 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3961 | 1/1 | 0.97 | 0.19 | 26,26,26,26 | 0 |
| 56 | MG | 1B | 222 | 1/1 | 0.97 | 0.12 | 44,44,44,44 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3381 | 1/1 | 0.97 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3659 | 1/1 | 0.97 | 0.09 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3530 | 1/1 | 0.97 | 0.16 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3579 | 1/1 | 0.97 | 0.12 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3011 | 1/1 | 0.97 | 0.14 | 28,28,28,28 | 0 |
| 56 | MG | 1a | 1741 | 1/1 | 0.97 | 0.19 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 3799 | 1/1 | 0.97 | 0.12 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3555 | 1/1 | 0.97 | 0.18 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3052 | 1/1 | 0.97 | 0.17 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3635 | 1/1 | 0.97 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3630 | 1/1 | 0.97 | 0.09 | 60,60,60,60 | 0 |
| 56 | MG | 2a | 3159 | 1/1 | 0.97 | 0.08 | 64,64,64,64 | 0 |
| 56 | MG | 2a | 3048 | 1/1 | 0.97 | 0.09 | 51,51,51,51 | 0 |
| 56 | MG | 1A | 3212 | 1/1 | 0.97 | 0.11 | 36,36,36,36 | 0 |
| 56 | MG | 2B | 205 | 1/1 | 0.97 | 0.11 | 52,52,52,52 | 0 |
| 56 | MG | 1A | 3558 | 1/1 | 0.97 | 0.23 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3225 | 1/1 | 0.97 | 0.11 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3639 | 1/1 | 0.97 | 0.15 | 32,32,32,32 | 0 |
| 56 | MG | 1G | 205 | 1/1 | 0.97 | 0.14 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3435 | 1/1 | 0.97 | 0.13 | 19,19,19,19 | 0 |
| 56 | MG | 1A | 3282 | 1/1 | 0.97 | 0.36 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 4102 | 1/1 | 0.97 | 0.41 | 26,26,26,26 | 0 |
| 56 | MG | 2A | 3438 | 1/1 | 0.97 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 2B | 207 | 1/1 | 0.97 | 0.17 | 60,60,60,60 | 0 |
| 56 | MG | 1x | 111 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3320 | 1/1 | 0.97 | 0.14 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3744 | 1/1 | 0.97 | 0.10 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3709 | 1/1 | 0.97 | 0.17 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3008 | 1/1 | 0.97 | 0.12 | 12,12,12,12 | 0 |
| 56 | MG | 1A | 4013 | 1/1 | 0.97 | 0.07 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3003 | 1/1 | 0.97 | 0.12 | 17,17,17,17 | 0 |
| 56 | MG | 2A | 3459 | 1/1 | 0.97 | 0.10 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3166 | 1/1 | 0.97 | 0.23 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3783 | 1/1 | 0.97 | 0.09 | 59,59,59,59 | 0 |
| 56 | MG | 1A | 3825 | 1/1 | 0.97 | 0.24 | 58,58,58,58 | 0 |
| 56 | MG | 2B | 215 | 1/1 | 0.98 | 0.17 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3479 | 1/1 | 0.98 | 0.13 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3204 | 1/1 | 0.98 | 0.16 | 24,24,24,24 | 0 |
| 60 | SF4 | 2d | 303 | 8/8 | 0.98 | 0.17 | 55,66,68,68 | 0 |
| 56 | MG | 2A | 3577 | 1/1 | 0.98 | 0.13 | 43,43,43,43 | 0 |
| 60 | SF4 | 1d | 501 | 8/8 | 0.98 | 0.17 | 38,50,55,61 | 0 |
| 56 | MG | 1A | 3174 | 1/1 | 0.98 | 0.09 | 13,13,13,13 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2l | 204 | 1/1 | 0.98 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 2a | 3074 | 1/1 | 0.98 | 0.11 | 58,58,58,58 | 0 |
| 56 | MG | 1A | 3102 | 1/1 | 0.98 | 0.32 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3760 | 1/1 | 0.98 | 0.11 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3208 | 1/1 | 0.98 | 0.14 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3418 | 1/1 | 0.98 | 0.17 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3193 | 1/1 | 0.98 | 0.19 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 4109 | 1/1 | 0.98 | 0.43 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3452 | 1/1 | 0.98 | 0.07 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 4051 | 1/1 | 0.98 | 0.23 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3642 | 1/1 | 0.98 | 0.15 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3296 | 1/1 | 0.98 | 0.33 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3046 | 1/1 | 0.98 | 0.16 | 16,16,16,16 | 0 |
| 56 | MG | 2A | 3383 | 1/1 | 0.98 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 4135 | 1/1 | 0.98 | 0.14 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 4016 | 1/1 | 0.98 | 0.18 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3822 | 1/1 | 0.98 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 4131 | 1/1 | 0.98 | 0.27 | 20,20,20,20 | 0 |
| 56 | MG | 2A | 3834 | 1/1 | 0.98 | 0.09 | 53,53,53,53 | 0 |
| 56 | MG | 1a | 1829 | 1/1 | 0.98 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3301 | 1/1 | 0.98 | 0.07 | 49,49,49,49 | 0 |
| 56 | MG | 1A | 3559 | 1/1 | 0.98 | 0.47 | 22,22,22,22 | 0 |
| 56 | MG | 1A | 3194 | 1/1 | 0.98 | 0.15 | 11,11,11,11 | 0 |
| 56 | MG | 1A | 3286 | 1/1 | 0.98 | 0.13 | 33,33,33,33 | 0 |
| 56 | MG | 2A | 3389 | 1/1 | 0.98 | 0.25 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3643 | 1/1 | 0.98 | 0.08 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3893 | 1/1 | 0.98 | 0.32 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3315 | 1/1 | 0.98 | 0.30 | 14,14,14,14 | 0 |
| 56 | MG | 1A | 3314 | 1/1 | 0.98 | 0.29 | 20,20,20,20 | 0 |
| 56 | MG | 1Z | 305 | 1/1 | 0.98 | 0.11 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3676 | 1/1 | 0.98 | 0.15 | 14,14,14,14 | 0 |
| 56 | MG | 1a | 1642 | 1/1 | 0.98 | 0.08 | 49,49,49,49 | 0 |
| 56 | MG | 2a | 3089 | 1/1 | 0.98 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3546 | 1/1 | 0.98 | 0.46 | 27,27,27,27 | 0 |
| 56 | MG | 2A | 3709 | 1/1 | 0.98 | 0.08 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3757 | 1/1 | 0.98 | 0.09 | 32,32,32,32 | 0 |
| 56 | MG | 1A | 3631 | 1/1 | 0.98 | 0.20 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3330 | 1/1 | 0.98 | 0.09 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3663 | 1/1 | 0.98 | 0.06 | 39,39,39,39 | 0 |
| 56 | MG | 1B | 207 | 1/1 | 0.98 | 0.13 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3740 | 1/1 | 0.98 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 1a | 1765 | 1/1 | 0.98 | 0.18 | 52,52,52,52 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1A | 3047 | 1/1 | 0.98 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3199 | 1/1 | 0.98 | 0.10 | 12,12,12,12 | 0 |
| 56 | MG | 2U | 204 | 1/1 | 0.98 | 0.06 | 37,37,37,37 | 0 |
| 56 | MG | 2x | 105 | 1/1 | 0.98 | 0.09 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 4081 | 1/1 | 0.98 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3462 | 1/1 | 0.98 | 0.10 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3137 | 1/1 | 0.98 | 0.19 | 16,16,16,16 | 0 |
| 56 | MG | 2E | 302 | 1/1 | 0.98 | 0.18 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3393 | 1/1 | 0.98 | 0.47 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 4124 | 1/1 | 0.98 | 0.13 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3902 | 1/1 | 0.98 | 0.13 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3838 | 1/1 | 0.98 | 0.06 | 51,51,51,51 | 0 |
| 56 | MG | 2A | 3415 | 1/1 | 0.98 | 0.12 | 36,36,36,36 | 0 |
| 56 | MG | 1A | 4015 | 1/1 | 0.98 | 0.08 | 23,23,23,23 | 0 |
| 56 | MG | 1a | 1647 | 1/1 | 0.98 | 0.17 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3823 | 1/1 | 0.98 | 0.17 | 18,18,18,18 | 0 |
| 56 | MG | 2A | 3491 | 1/1 | 0.98 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3345 | 1/1 | 0.98 | 0.59 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 4084 | 1/1 | 0.98 | 0.20 | 32,32,32,32 | 0 |
| 56 | MG | 2l | 203 | 1/1 | 0.98 | 0.25 | 50,50,50,50 | 0 |
| 56 | MG | 1A | 3815 | 1/1 | 0.98 | 0.10 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3124 | 1/1 | 0.98 | 0.36 | 28,28,28,28 | 0 |
| 56 | MG | 2A | 3833 | 1/1 | 0.98 | 0.13 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3341 | 1/1 | 0.98 | 0.30 | 38,38,38,38 | 0 |
| 56 | MG | 2A | 3356 | 1/1 | 0.98 | 0.20 | 39,39,39,39 | 0 |
| 56 | MG | 1B | 229 | 1/1 | 0.98 | 0.17 | 42,42,42,42 | 0 |
| 56 | MG | 2A | 3012 | 1/1 | 0.98 | 0.26 | 38,38,38,38 | 0 |
| 56 | MG | 1Q | 201 | 1/1 | 0.98 | 0.14 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3806 | 1/1 | 0.98 | 0.09 | 40,40,40,40 | 0 |
| 56 | MG | 2A | 3803 | 1/1 | 0.98 | 0.10 | 65,65,65,65 | 0 |
| 56 | MG | 1A | 3708 | 1/1 | 0.98 | 0.15 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3830 | 1/1 | 0.98 | 0.13 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 4025 | 1/1 | 0.98 | 0.17 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3191 | 1/1 | 0.98 | 0.12 | 29,29,29,29 | 0 |
| 56 | MG | 1A | 3333 | 1/1 | 0.98 | 0.10 | 28,28,28,28 | 0 |
| 56 | MG | 2a | 3217 | 1/1 | 0.98 | 0.10 | 57,57,57,57 | 0 |
| 56 | MG | 2B | 211 | 1/1 | 0.98 | 0.21 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 4136 | 1/1 | 0.98 | 0.24 | 29,29,29,29 | 0 |
| 56 | MG | 2A | 3685 | 1/1 | 0.98 | 0.13 | 28,28,28,28 | 0 |
| 56 | MG | 1A | 3866 | 1/1 | 0.98 | 0.31 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3084 | 1/1 | 0.98 | 0.07 | 46,46,46,46 | 0 |
| 56 | MG | 1a | 1775 | 1/1 | 0.98 | 0.12 | 26,26,26,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1a | 1696 | 1/1 | 0.98 | 0.24 | 37,37,37,37 | 0 |
| 56 | MG | 1A | 3858 | 1/1 | 0.98 | 0.09 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 4123 | 1/1 | 0.98 | 0.26 | 32,32,32,32 | 0 |
| 56 | MG | 2A | 3584 | 1/1 | 0.98 | 0.16 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3387 | 1/1 | 0.98 | 0.24 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3544 | 1/1 | 0.98 | 0.08 | 50,50,50,50 | 0 |
| 56 | MG | 2D | 302 | 1/1 | 0.98 | 0.59 | 39,39,39,39 | 0 |
| 56 | MG | 1A | 3903 | 1/1 | 0.98 | 0.11 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3038 | 1/1 | 0.98 | 0.07 | 47,47,47,47 | 0 |
| 56 | MG | 2a | 3038 | 1/1 | 0.98 | 0.18 | 57,57,57,57 | 0 |
| 56 | MG | 2A | 3027 | 1/1 | 0.98 | 0.10 | 38,38,38,38 | 0 |
| 56 | MG | 2a | 3042 | 1/1 | 0.98 | 0.29 | 63,63,63,63 | 0 |
| 56 | MG | 1U | 203 | 1/1 | 0.98 | 0.40 | 22,22,22,22 | 0 |
| 56 | MG | 2V | 201 | 1/1 | 0.98 | 0.70 | 56,56,56,56 | 0 |
| 56 | MG | 1A | 3131 | 1/1 | 0.98 | 0.14 | 11,11,11,11 | 0 |
| 56 | MG | 1A | 3158 | 1/1 | 0.98 | 0.96 | 24,24,24,24 | 0 |
| 56 | MG | 1A | 3388 | 1/1 | 0.98 | 0.19 | 18,18,18,18 | 0 |
| 56 | MG | 1A | 3321 | 1/1 | 0.98 | 0.22 | 39,39,39,39 | 0 |
| 56 | MG | 2A | 3687 | 1/1 | 0.98 | 0.10 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3526 | 1/1 | 0.98 | 0.13 | 30,30,30,30 | 0 |
| 56 | MG | 2A | 3639 | 1/1 | 0.98 | 0.16 | 44,44,44,44 | 0 |
| 56 | MG | 1U | 205 | 1/1 | 0.98 | 0.20 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3597 | 1/1 | 0.98 | 0.14 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3628 | 1/1 | 0.98 | 0.08 | 8,8,8,8 | 0 |
| 56 | MG | 1A | 3576 | 1/1 | 0.98 | 0.05 | 31,31,31,31 | 0 |
| 56 | MG | 1A | 3297 | 1/1 | 0.98 | 0.26 | 27,27,27,27 | 0 |
| 56 | MG | 1A | 3677 | 1/1 | 0.98 | 0.13 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3023 | 1/1 | 0.98 | 0.24 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3703 | 1/1 | 0.98 | 0.12 | 10,10,10,10 | 0 |
| 56 | MG | 1A | 3691 | 1/1 | 0.98 | 0.09 | 9,9,9,9 | 0 |
| 56 | MG | 1A | 3142 | 1/1 | 0.98 | 0.20 | 17,17,17,17 | 0 |
| 56 | MG | 2A | 3547 | 1/1 | 0.98 | 0.17 | 31,31,31,31 | 0 |
| 56 | MG | 2A | 3688 | 1/1 | 0.98 | 0.39 | 45,45,45,45 | 0 |
| 56 | MG | 1A | 3502 | 1/1 | 0.98 | 0.12 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3084 | 1/1 | 0.98 | 0.19 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3763 | 1/1 | 0.98 | 0.09 | 21,21,21,21 | 0 |
| 56 | MG | 2A | 3681 | 1/1 | 0.98 | 0.07 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3272 | 1/1 | 0.98 | 0.17 | 13,13,13,13 | 0 |
| 56 | MG | 2a | 3198 | 1/1 | 0.98 | 0.10 | 52,52,52,52 | 0 |
| 56 | MG | 2R | 3001 | 1/1 | 0.98 | 0.26 | 46,46,46,46 | 0 |
| 56 | MG | 2A | 3353 | 1/1 | 0.98 | 0.17 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3342 | 1/1 | 0.98 | 0.13 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 2A | 3008 | 1/1 | 0.98 | 0.11 | 30,30,30,30 | 0 |
| 56 | MG | 2Y | 201 | 1/1 | 0.98 | 0.16 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3386 | 1/1 | 0.98 | 0.16 | 40,40,40,40 | 0 |
| 56 | MG | 1A | 3719 | 1/1 | 0.98 | 0.14 | 13,13,13,13 | 0 |
| 56 | MG | 1A | 3348 | 1/1 | 0.98 | 0.17 | 30,30,30,30 | 0 |
| 56 | MG | 1A | 3524 | 1/1 | 0.99 | 0.22 | 32,32,32,32 | 0 |
| 59 | ZN | 1n | 102 | 1/1 | 0.99 | 0.15 | 47,47,47,47 | 0 |
| 56 | MG | 1A | 3071 | 1/1 | 0.99 | 0.16 | 20,20,20,20 | 0 |
| 56 | MG | 1B | 215 | 1/1 | 0.99 | 0.07 | 37,37,37,37 | 0 |
| 56 | MG | 1l | 203 | 1/1 | 0.99 | 0.21 | 48,48,48,48 | 0 |
| 56 | MG | 1A | 3746 | 1/1 | 0.99 | 0.14 | 23,23,23,23 | 0 |
| 56 | MG | 1A | 3138 | 1/1 | 0.99 | 0.18 | 9,9,9,9 | 0 |
| 56 | MG | 2A | 3819 | 1/1 | 0.99 | 0.10 | 47,47,47,47 | 0 |
| 56 | MG | 1S | 202 | 1/1 | 0.99 | 0.14 | 35,35,35,35 | 0 |
| 56 | MG | 1n | 101 | 1/1 | 0.99 | 0.11 | 26,26,26,26 | 0 |
| 56 | MG | 1A | 3123 | 1/1 | 0.99 | 0.16 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3074 | 1/1 | 0.99 | 0.14 | 15,15,15,15 | 0 |
| 56 | MG | 1A | 3497 | 1/1 | 0.99 | 0.10 | 44,44,44,44 | 0 |
| 56 | MG | 1D | 303 | 1/1 | 0.99 | 0.49 | 34,34,34,34 | 0 |
| 56 | MG | 1A | 3299 | 1/1 | 0.99 | 0.15 | 15,15,15,15 | 0 |
| 56 | MG | 2a | 3226 | 1/1 | 0.99 | 0.12 | 44,44,44,44 | 0 |
| 56 | MG | 1A | 3167 | 1/1 | 0.99 | 0.25 | 29,29,29,29 | 0 |
| 56 | MG | 1x | 107 | 1/1 | 0.99 | 0.19 | 74,74,74,74 | 0 |
| 56 | MG | 1A | 3637 | 1/1 | 0.99 | 0.15 | 21,21,21,21 | 0 |
| 56 | MG | 1A | 3533 | 1/1 | 0.99 | 0.19 | 12,12,12,12 | 0 |
| 56 | MG | 2A | 3378 | 1/1 | 0.99 | 0.08 | 43,43,43,43 | 0 |
| 56 | MG | 2A | 3385 | 1/1 | 0.99 | 0.15 | 36,36,36,36 | 0 |
| 59 | ZN | 16 | 103 | 1/1 | 0.99 | 0.22 | 35,35,35,35 | 0 |
| 56 | MG | 1A | 3918 | 1/1 | 0.99 | 0.12 | 46,46,46,46 | 0 |
| 56 | MG | 1A | 3041 | 1/1 | 0.99 | 0.20 | 20,20,20,20 | 0 |
| 56 | MG | 1a | 1650 | 1/1 | 0.99 | 0.09 | 42,42,42,42 | 0 |
| 59 | ZN | 15 | 104 | 1/1 | 0.99 | 0.23 | 38,38,38,38 | 0 |
| 56 | MG | 1A | 3720 | 1/1 | 0.99 | 0.14 | 9,9,9,9 | 0 |
| 56 | MG | 2A | 3616 | 1/1 | 0.99 | 0.19 | 50,50,50,50 | 0 |
| 59 | ZN | 19 | 102 | 1/1 | 0.99 | 0.18 | 33,33,33,33 | 0 |
| 56 | MG | 1A | 3383 | 1/1 | 0.99 | 0.23 | 20,20,20,20 | 0 |
| 56 | MG | 1A | 3012 | 1/1 | 0.99 | 0.08 | 16,16,16,16 | 0 |
| 56 | MG | 1A | 3499 | 1/1 | 0.99 | 0.16 | 35,35,35,35 | 0 |
| 56 | MG | 2A | 3018 | 1/1 | 0.99 | 0.13 | 53,53,53,53 | 0 |
| 56 | MG | 1A | 4128 | 1/1 | 0.99 | 0.11 | 18,18,18,18 | 0 |
| 59 | ZN | 25 | 103 | 1/1 | 0.99 | 0.20 | 51,51,51,51 | 0 |
| 56 | MG | 1q | 201 | 1/1 | 0.99 | 0.06 | 39,39,39,39 | 0 |

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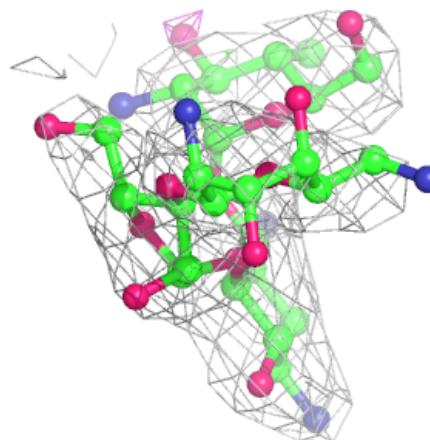
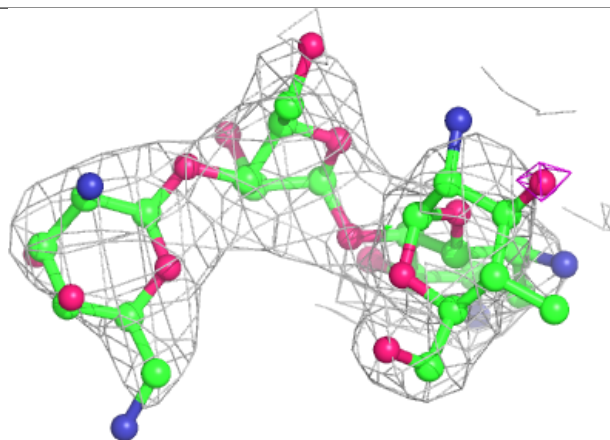
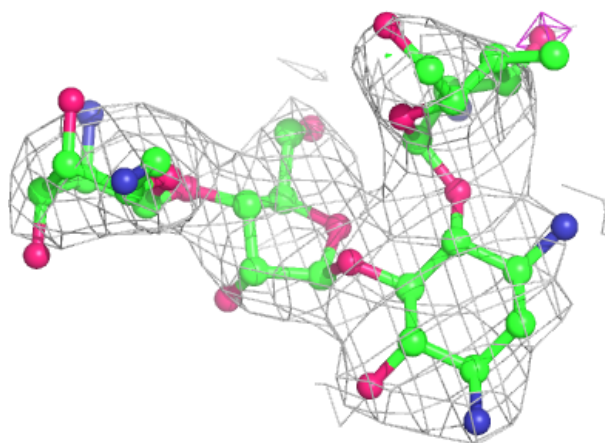
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 56 | MG | 1B | 216 | 1/1 | 0.99 | 0.20 | 22,22,22,22 | 0 |
| 56 | MG | 2A | 3453 | 1/1 | 0.99 | 0.28 | 33,33,33,33 | 0 |
| 56 | MG | 1X | 102 | 1/1 | 0.99 | 0.21 | 17,17,17,17 | 0 |
| 56 | MG | 1B | 235 | 1/1 | 0.99 | 0.04 | 37,37,37,37 | 0 |
| 56 | MG | 2A | 3471 | 1/1 | 0.99 | 0.12 | 25,25,25,25 | 0 |
| 56 | MG | 2A | 3221 | 1/1 | 1.00 | 0.21 | 43,43,43,43 | 0 |
| 56 | MG | 1A | 3423 | 1/1 | 1.00 | 0.20 | 45,45,45,45 | 0 |

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

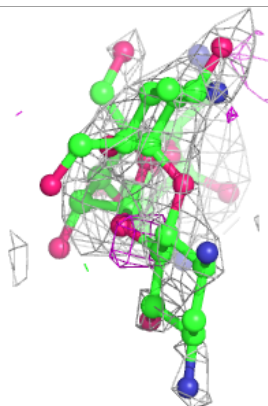
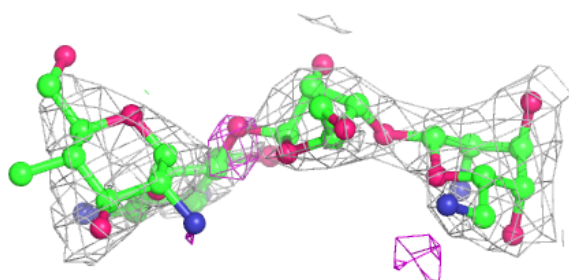
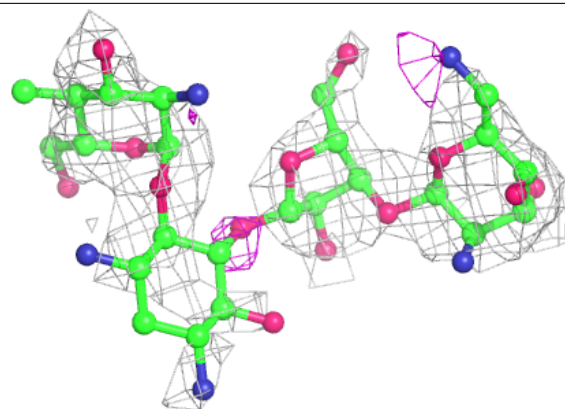
Electron density around LUJ 2A 3851:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

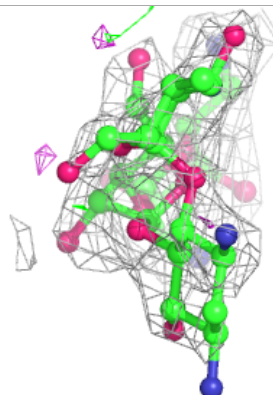
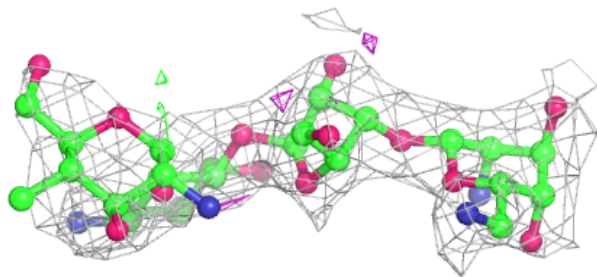
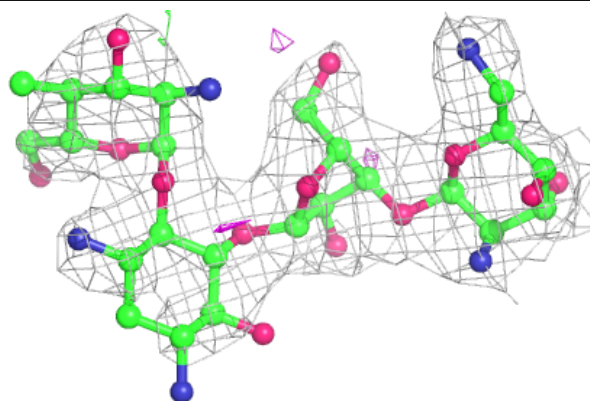


Electron density around LUJ 2A 3852:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

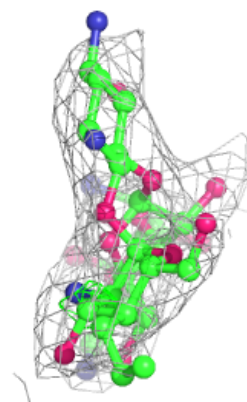
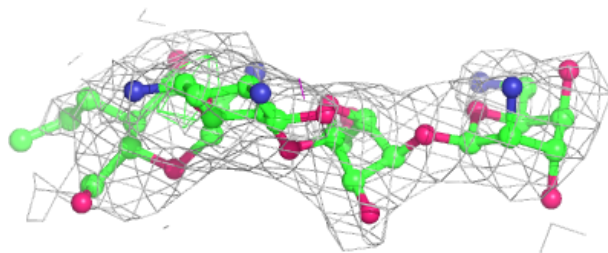
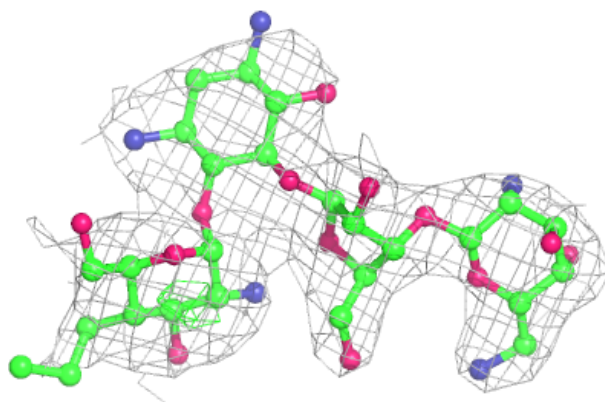
**Electron density around LUJ 1A 4100:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



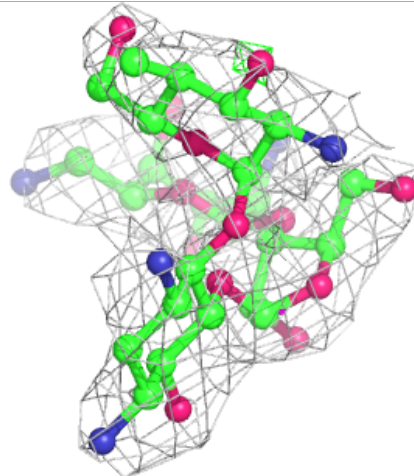
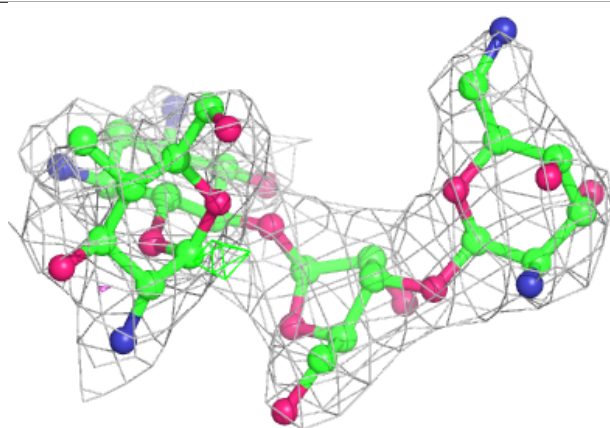
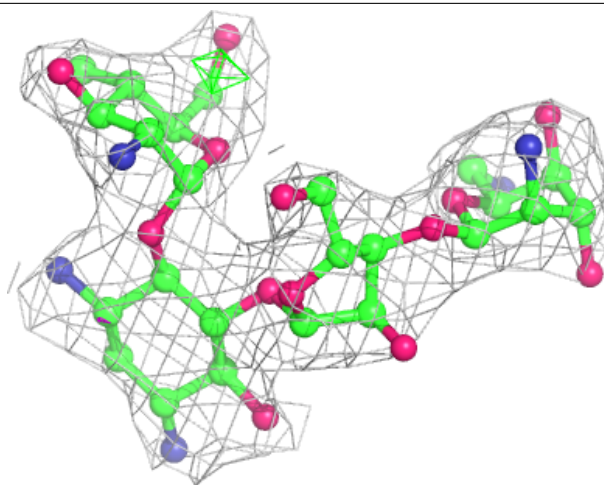
Electron density around LUJ 2a 3232:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



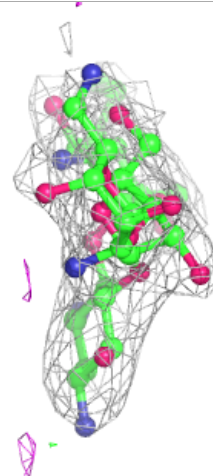
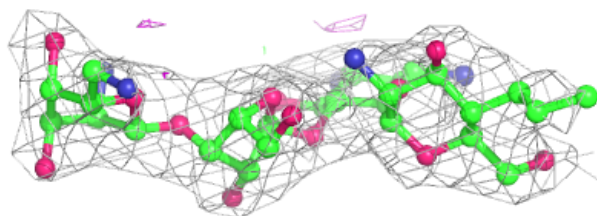
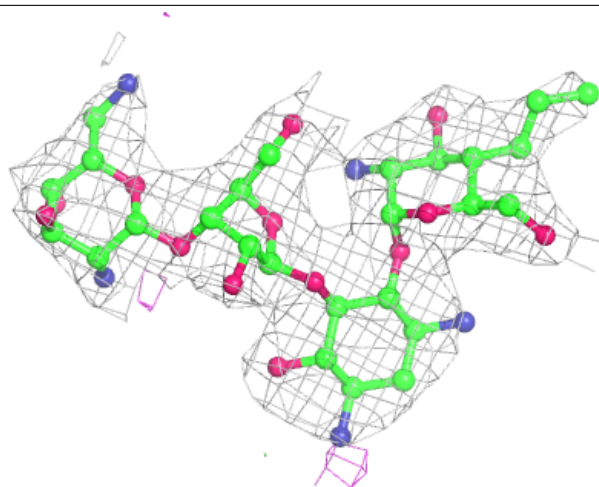
Electron density around LUJ 1A 4099:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LUJ 1a 1832:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.